STUDIES ON POLYMORPHISM AND MOLECULAR RECOGNITION IN CHOLIC ACID INCLUSION CRYSTALS

（コール酸包接結晶における多形現象と分子認識に関する研究）

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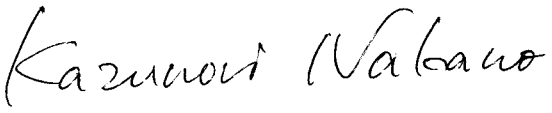
Preface

The work in this thesis has been performed under the direction of Professor Mikiji Miyata at Material and Life Science, Graduate School of Engineering, Osaka University and at Nagoya Municipal Industrial Research Institute.



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General Introduction

Molecular recognition and self-assembly plays a fundamental role in numerous biological processes in living cells. The processes are, for example, the highly specific substrate recognition by enzymes, the formation of the double helix structure of DNA by pairing of complementary nucleoside, and the formation of membranes and ribosomes. Supramolecular chemistry[1] generally encompasses the chemistry of molecular recognition and self-assembly. Molecular recognition relies on complementary of shape, size, and chemical functionalities, and resulting assemblies consist of smaller molecules through the noncovalent bonds, such as hydrogen bonds, π–π stacking, and van der Waals interactions. The structural features involving chemical properties of the resulting molecular assemblies are distinct from the original molecules. The molecular assemblies studied in supramolecular chemistry are not only biological compounds but also artificial compounds involving membranes, liquid crystals, gels, and crystals. In particular, crystals have advantages to study arrays and interactions of a molecular unit in detail because of recent advances of rapid X-ray structural analyses and computer graphic softwares for visualization of crystal structures.

Host-guest chemistry, wherein a host compound spatially accommodates a guest molecule or ion, is one of the important fields in supramolecular chemistry. This is because that inclusion compounds have received a great deal of attention from scientific interest and practical appreciation. For example, a selective formation of inclusion complex from mixtures can be considered as a simple model of a process of molecular recognition in living cells; selective enclathration is one of the most useful processes for the separation. Crown ethers are a classical example of hosts that are capable of incorporating guest molecules or ions within their confines.[2] More recent efforts in this area have focused on creating macromolecular capsules, such as cavitands,[3] cyclodextrins,[4] and calixarenes.[3d,5] These macrocyclic compounds are constructed readily by covalent bonds to yield expected cavities with guest recognitions in solution.

In solid state, porous molecular frameworks have also been developed in cooperation of development of crystal engineering, which has been defined as the understanding of intermolecular interactions in the context of crystal packing.[6] The origins of crystal engineering lie in the work of Gerhard Schmidt who realized, more than twenty-five years ago, that the systematic development of organic solid state chemistry required a proper theory of crystal packing. Although since then many efforts to understand intermolecular interactions have devoted, until now no one has achieved the design of new solids with desired physical and chemical properties due to complexity of the intermolecular forces. This is particularly true of crystalline lattice compounds. There are several reports for design and synthesis of host frameworks using multiple and divergent hydrogen bond functional groups as the connectivities.[7] These studies attempt to reveal the effect of func-

tional groups of a host molecule on the resulting host frameworks. However, it is difficult to find the general rule of the effect because of an inability to predict and control molecular organization mentioned above. Even in the designed hosts, the host frameworks often isomerize in response to guest components and collapse to the close packed guest-free forms without suitable guest components. The flexibility of the host frameworks is a substantial characteristic for organic host compounds constructed by noncovalent bonds. The discovery dates back to 1950's soon after the structural confirmation of the organic clathrate compounds. Powell and co-worker first reported that two types of host frameworks in a series of tri-*o*-thymotide inclusion compounds and that the length of the guest components affected the host frameworks.[8] Since then many hosts have been reported to form several host framework types dependent on the guest sizes, shapes, and functional groups.[9,10] The host framework flexibility necessarily effect not only on the formation of inclusion compounds but also on their molecular recognition and other properties. This prevents a progress of a potential application of lattice inclusion compounds, such as catalysis and chemical separations. Therefore, it is expected to reveal a question as to what is a factor for the formation of diverse host frameworks by a host.

With these backgrounds, the author studied a host of cholic acid (3α, 7α, 12α,-trihydroxy-5β-cholan-24-oic acid, **CA**), which is a commercially available steroidal bile acid and has an unusual facially amphiphilic molecular structure.[9] All three hydroxy groups are directed to steroidal α-face to form a hydrophilic face and two methyl groups are to the other β-face to form a lipophilic face. The face differentiating molecular structure has been utilized as a molecular scaffold for artificial receptors or combinatorial chemistry.[11] The molecular complexes with small alcohols in crystalline states have been known since last century, and the crystallographic study revealed that guest alcohols are included in a cage-type host cavity.[12] More recently, it has been reported that **CA** includes a wide range of organic compounds and that **CA** can also form bilayer-type structures constructed by hydrogen bonds between hydrophilic faces and by van der Waals associations between lipophilic faces.[13,14] The guest compounds are entrapped by van der Waals force and steric complementary in a one-dimensional host cavity, a molecular channel, running in the lipophilic layer. These facts indicate that **CA** is one of the appropriate hosts to investigate the flexibility of the host frameworks systematically. The advantages are summarized as follows:

(1) **CA** is a commercially available and not expensive.

(2) **CA** forms inclusion compounds with many organic substances and gives a good single crystal for many guests.

(3) It is possible that **CA** forms many types of host frameworks due to the characteristic molecular structure: asymmetric structure involving eleven chiral carbons; multi-functional structure involving three hydroxy groups and a carboxy group; amphiphilic structure consisting of rigid steroidal unit and flexible methylene unit.

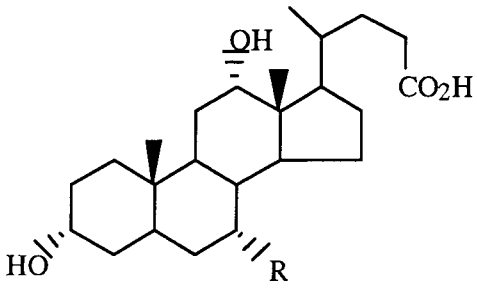
(4) The resulting **CA** host frameworks can be comparable to old host of deoxycholic acid (**DCA**) and many derivatives synthesized from the host.

The author systematically studied a host of **CA**: inclusion phenomena, molecular assembly, polymorphism, molecular recognition, intercalation phenomena, and inclusion polymerization. This thesis consists of following six chapters. Chapter 1 describes that **CA** forms inclusion compounds with various guest using appropriate solvents. The formation of inclusion compounds involving hydrocarbons and related compounds enables us to compare the molecular assemblies with old host of deoxycholic acid. Chapter 2 describes dependence of host frameworks in response to guest size. **CA** can form four host frameworks with mono-substituted benzenes owing to conformational isomerizations of the side-chain and stacking modes in lipophilic layers and stacking modes in hydrophilic layers. Packing coefficient of host cavity (PC_{cavity}), volume ratio of the guest compound to the host cavity, permits to clarify the relation between the guest volume and isomerizations of the host frameworks. Chapter 3 describes guest shape dependence of **CA** host frameworks and molecular recognition for xylenes. Selective enclathration of xylene isomers can be understood by PC_{cavity}. X-ray crystallography proved existence of "clathrate" solid solution crystals, leading to non-selective enclathration. Chapter 4 describes the drastic isomerization of host frameworks depending mainly on the guest volumes. Systematic investigation enables us to find polymorphism of inclusion compounds composed of the same host-guest complex with the same stoichiometry. Chapter 5 describes intercalation phenomena of **CA** inclusion crystal with the same guest. The reversible change of layers in host frameworks can be caused by absorption-release of guest molecules. Chapter 6 describes reaction in a one-dimensional cavity of **CA** can be achieved by controlling the formation of host framework types. The systematic research of steroidal hosts having various channels reveal space effect of molecular-level spaces on polymerization.

Chapter 1. Inclusion Phenomenon of Cholic Acid

1. Introduction

Cholic acid (**CA**) is a new host, while deoxycholic acid (**DCA**)[1] is an old one. They serve as a fascinating pair of hosts for multimolecular inclusion compounds. The reason is that the hosts enable us to prove that only a slight difference in their molecular structures brings about great differences in their molecular assemblies with hydrogen bonding networks,[2] molecular arrangements,[3] dynamics,[4,5] and molecular recognition.[6,7] However, their inclusion phenomena and the resulting molecular assemblies could not be compared precisely, since the inclusion compounds of **CA** with various hydrocarbons and related compounds, which are common guests for **DCA**, were obtained due to their low solubilities.[8] This problem has been resolved by using appropriate solvents at recrystallization. In this chapter, the author report the first preparation of inclusion compounds of **CA** with hydrocarbons and related compounds as well as crystallographic evidence for the simplest inclusion compound of **CA** with benzene (**1**).



R=OH: Cholic Acid (**CA**)
R=H: Deoxycholic Acid (**DCA**)

2. Experimental

General Methods

All chemicals and solvents were commercially available and used without any purification. Infrared spectra were recorded on a JASCO IR-Report-100 spectrometer. Differential scanning calorimetry (DSC), and thermal gravimetry (TG), were performed on a Rigaku TAS100 system; ca.10 mg from 40 to 230°C at a heating rate of 5°C min^{-1}.

Crystal Structure Determinations

X-ray diffraction data were collected on a Rigaku AFC-7R four-circle diffractometer with graphite-monochromatized Mo-Kα radiation. Lattice parameters were obtained by least-squares analysis of 25 reflections measured in the range $20< 2\theta < 25$ in the four-circle diffractometer. Direct methods (SHELEX86) were used for the structure solution. The structure was refined by the full matrix least-squares procedure with the program TEXSAN[9] using observed reflections ($|Fo|>3\sigma(|Fo|)$). All non-hydrogen atoms were refined with anisotropic displacement parameters and hydrogen atoms of the host molecule were placed in idealized positions and refined as riding atoms with the relative isotropic displacement parameters. Hydrogen atoms of the guest molecule were placed in idealized positions and not refined. All calculations were performed using the TEXSAN[9] crystallographic software package.

3. Results and Discussion

Commonly, solvents for preparing inclusion compounds are determined by trial and error. For example, in the case of **DCA**, methanol and ethanol have been empirically used as solvents.[1] However, these alcohols can not be applied to **CA**, since they form stable crystals with **CA**.[10] Therefore, the inclusion compounds of **CA** have been obtained by direct recrystallization from liquid guests.[8] Recently, a plausible mechanism for selective inclusion of **CA** derivative against alcoholic guests via hydrogen bonding double hooks has been reported.[11] This suggests that the other alcohols should serve as appropriate solvents, and that solvents for preparing the inclusion compounds can be reasonably found.

First, preparation of the inclusion compound of **CA** with benzene using various alcohols as solvents was systematically investigated. Excess amounts of **1** were added to saturated alcoholic solutions of **CA**. The resulting crystals had completely different components for guests, as shown in Table 1-1. In the case of methanol, ethanol and 1-propanol, **CA** exclusively yielded the stable inclusion compounds with the corresponding alcohols, but not with **1**. The reverse was observed in the case of other alcohols, such as various butanols and pentanols. Among the alcohols checked, 1-butanol, 2-butanol and 2-methyl-1-propanol were easy to treat owing to moderate solubilities and viscosity against **CA** and various guests.

Next, inclusion compounds with various hydrocarbons were prepared in the same way by using 2-butanol. Molar ratios and release temperatures of the resulting crystals were determined by TG-DSC, as shown in Table 1-2. Most of aromatic hydrocarbons employed gave thermally stable inclusion compounds. For example, molecules of **1** were released from the crystals at 123°C, which is 43°C higher than the boiling point itself. Introduction of a methyl or ethyl group leads to a decrease of the release temperatures. In the case of ethylbenzene and tetralin, a two-step-release was observed. Although naphthalene gave no complex, 1-methylnaphthalene gave a 2:1 complex.

Table 1-1. Formation of inclusion compounds of **CA** in the presence of alcoholic solvents

Solvent	Volume of solvent [a] [mL]	Included guest [b]	Inclusion crystal [mg]	Solvent	Volume of solvent [a] [mL]	Included guest [b]	Inclusion crystal [mg]
methanol	0.6	methanol	60	1-pentanol	0.4	**1**	83
ethanol	1.6	ethanol	69	2-pentanol	0.6	**1**	85
1-propanol	1.4	1-propanol	77	2-methyl-1-butanol	0.4	**1**	81
2-propanol	1.0	**1**	15	2-methyl-2-butanol	0.7	**1**	88
1-butanol	0.4	**1**	86	1-hexanol	0.4	**1**	80
2-butanol	0.5	**1**	80	2-hexanol	0.6	**1**	77
2-methyl-1-propanol	0.4	**1**	81	1-octanol	0.4	**1**	86
2-methyl-2-propanol	1.0	**1**	82	2-octanol	0.6	**1**	80

[a] **CA** (100mg) was dissolved in alcoholic solvents.
[b] **1** (1.0mL) was added to saturated alcoholic solutions.

Table 1-2. Guest release temperatures and molar ratios of inclusion compounds of **CA** with hydrocarbons and related compounds

Guest	Guest release temperature [a] [°C]	Host-guest molar ratio [a,b]	Guest	Guest release temperature [a] [°C]	Host-guest molar ratio [a,b]
benzene	123	1 : 1	cyclohexane	Not clear	3 : 2
toluene	89	1 : 1	ethylcyclohexane	110	2 : 1
ethylbenzene	70, 116	1 : 1	2,5-norbornadiene	142	1 : 1
tetralin	89, 113	3 : 2	chlorobenzene	122	1 : 1
1-methylnaphthalene	126	2 : 1	di-*n*-butyl ether	109	2 : 1
1,5-hexadiene	Not clear	1 : 1	*β*-ionone	142	2 : 1
myrcene	117	2 : 1	methyl *n*-decanoate	118	2 : 1

[a] Determined by TG-DSC.
[b] Determined by ^{1}H-NMR.

Aliphatic hydrocarbons also yielded inclusion compounds. For example, cyclohexane gave an unstable compound, while methyl or ethylcyclohexane did stable ones. Saturated hydrocarbons such as hexane, 2,3-dimethylbutane and decalin gave crystals without any guests. Unsaturated hydrocarbons such as cyclohexene, 1,5-hexadiene and 2,3-dimethyl-1,3-butadiene gave the thermally unstable compounds, while 2,5-norbornadiene did stable ones. Terpenes, such as myrcene and (+)-limonene, were also included. It is noteworthy that aromatic or long-chain compounds involving functional groups, such as chlorobenzene, dibutyl ether, β-ionone, and methyl decanoate, yielded stable inclusion compounds.

In order to confirm the incorporation of hydrocarbons without solvents, the inclusion compound of **CA** with **1** was analyzed by X-ray crystallography. Needle-like crystals were obtained by

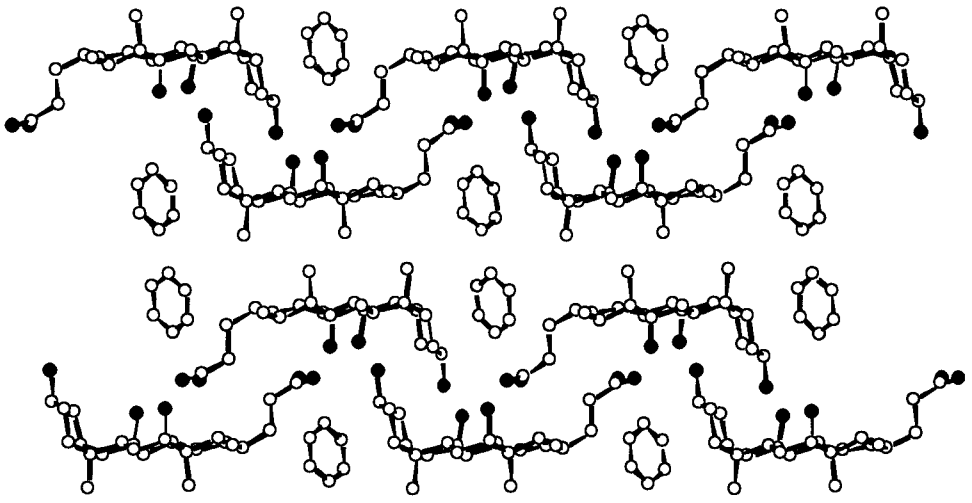


Figure 1-1 The crystal structure of the inclusion compound of **CA** with benzene (1:1) viewed down along the crystallographic *b*-axis. Hydrogen atoms are omitted for clarity. Carbon and oxygen atoms are represented by empty and filled circles, respectively.

recrystallization from a solution of **CA** in **1** and 2-butanol. X-ray crystallographic study revealed that the resulting single crystal consists of a 1:1 bilayer structure with channel cavity. The structure are shown in Figure 1-1. The structure is basically identical to those with γ-valerolactone,[6] acetophenone,[7] nitrobenzene and aniline.[12] The side-chain of **CA** molecules adopt *gauche* conformation as in the case of acetophenone. Facial amphiphilicity forces the molecules to yield bilayers composed of hydrophilic and lipophilic sides. On the hydrophilic side four hydrogen bonding groups form cyclic networks, leading to a molecular arrangement in a *head-to-head* and *tail-to-tail* fashion. On the lipophilic side the steroidal skeletons stack together so as to leave channels between them. The channels have large side-pockets where benzene molecules fit closely, explaining the thermal stability of the inclusion compound mentioned above. Other structural details are described in next chapter.

4. Conclusion

This study demonstrates that **CA** can include not only polar but also nonopolar guest components. The incorporation of hydrocarbons and related compounds in **CA** cavity enable us to compare inclusion behaviors of **CA** and **DCA**. The crystal structure of inclusion compound of **CA** with **1** shows the accommodation of the guest molecules in channel cavity without incorporation of alcoholic solvents. The important difference in channels between **CA** and **DCA** lead us to the idea that the two hosts provide significantly different molecular-level space for inclusion polymerization[13] described in Chapter 6.

Chapter 2. Guest Size Dependence of Host Framework Isomerization in Cholic Acid Inclusion Crystals

1. Introduction

It is well known that steric complementary between host cavities and guest components is required to form host-guest compounds due to key-and-lock mechanism in molecular recognitions. In particular, the sizes of the included components play a primary role for guest inclusions in the open host frameworks.[1] Qualitatively, the guest compounds just fitted to the steric dimensions of the host cavities are included, while larger or smaller compounds are not included. However, there have been few reports concerned with quantitative analyses and estimations of size of the host cavities and the guest compounds. Recently, Rebek J. Jr. and Mecozzi[2] estimated the volumes and introduced packing coefficients of the host cavities (PC_{cavity}), which is defined as the ratio between the molecular volume of the guest component included in the host cavity and the void in the host cavity, as the parameter to estimate the steric fit between the host and the guest. According to molecular mechanic calculations, a value for PC_{cavity} of 0.55±0.1 give the best binding constants for the resulting host-guest complexes. However, in the crystalline state, there have been no reports that have attempted to understand the guest inclusions by PC_{cavity}. Only, molecular volumes have been used for discussion on the specific reactions or guest recognitions in solid state.[3,4] For example, Ohashi and co-workers revealed that photoisomerization of ligands in a series of cobaloxime complexes is controlled by the molecular volumes of the reaction cavities.[3] Gerdil used molecular volumes to rationalize optical resolutions and isomerizations of *trans*-stilbene in the host frameworks of tri-*o*-thymotide.[4]

Because importance of the guest size for the formation of the lattice inclusion crystals are empirically known as well, systematic investigations of PC_{cavity} of inclusion crystals can reveal guest-dependent isomerization of the open host frameworks. Recently, the isomerizations have been widely accepted as substantial property of organic host compounds because of the discovery in many hosts.[5-15] In Chapter 1, the author proved that **CA** could form inclusion compounds with a variety of organic substances. Therefore, **CA** would be a suitable host compound for investigating the role of steric fitting between the guest components and the host cavities. In this chapter, crystal structures of **CA** with mono-substituted benzenes (Chart 1) are systematically revealed to clarify the steric factors of guest incorporations and guest-dependent isomerizations of the host frameworks.

2. Experimental

General Methods

All chemicals and solvents were commercially available and used without any purification.

Infrared spectra were recorded on a JASCO IR-Report-100 or JASCO IR-810 spectrometer. Differential scanning calorimetry (DSC), and thermal gravimetry (TG), were performed on a Rigaku TAS100 system; ca.10 mg from 40 to 230°C at a heating rate of 5°Cmin^{-1}. X-ray powder diffraction (XRD) patterns were measured by using Rigaku RINT-1100 at room temperature.

Preparation of Inclusion Crystals

Method A. **CA** (100 mg) was dissolved with warming in the liquid guest (usually 2-3 mL), and the resulting solution allowed to stand to room temperature. The needle-like crystals were collected and dried on the filter papers.

Method B. If **CA** was insufficiently soluble in the liquid guest, 1-butanol is used as solvent: **CA** (100 mg) was dissolved with warming in the 1-butanol (0.4 ml), and the liquid guest (usually 1-2 ml) was poured into the resulting solution. The crystals were isolated in the same manner as in Method A.

Crystal Structure Determinations

X-ray diffraction data were collected on a Rigaku AFC-7R four-circle diffractometer or a RAXIS-IV diffractometer with a two-dimensional area detector with graphite-monochromatized Mo-Kα radiation. Lattice parameters were obtained by least-squares analysis of 25 reflections measured in the range $20 < 2\theta < 25$ in the four-circle diffractometer and reflections for 3 oscillation images in the area detector. Direct methods (SHELEX86 or SIR92) were used for the structure solution. The structure was refined by the full matrix least-squares procedure with the program TEXSAN.[20] In the case of **CA•3, CA•15, CA•17, CA•45, CA•50, CA•51, CA•54** and **CA•57**, non-hydrogen atoms of the host compound were refined with anisotropic displacement parameters. The guest molecules were located unambiguously in difference electron density maps and refined anisotropically with bond length restraints. Hydrogen atoms were placed in idealized positions and were not subjected to further refinement. In the case of **CA•56**, only the host molecule was refined with anisotropic displacement parameters because the guest molecule was completely disordered. In all the other crystals, all non-hydrogen atoms were refined with anisotropic displacement parameters and hydrogen atoms of the host molecule were placed in idealized positions and refined as riding atoms with the relative isotropic displacement parameters. Hydrogen atoms of the guest molecule were placed in idealized positions and not refined. All calculations were performed using the TEXSAN crystallographic software package.[20] The condition of measurement and structural details are listed Table II-1 (Appendix).

Molecular Graphics

Molecular graphics study was carried out by with the computer software based on MODRASTE.[21] The atomic radii of hydrogen, carbon, and oxygen in the cross-sectional views are fixed at 1.20Å, 1.60Å, and 1.45Å, respectively.

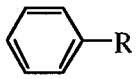
Calculations

The volumes of the host cavities were calculated from the atomic coordinations with the program Free Volume[22] in the software package Cerius^2 (version 4.0).[23] The following values were used for the atomic radii: hydrogen=1.20Å, carbon=1.70Å, nitrogen=1.65Å, oxygen=1.60Å, fluorine=1.47Å, chlorine=1.75Å, bromine=1.85Å, iodine=1.98Å. The calculation involves rolling of a spherical probe along the interior surface, but there is no universally accepted radius of the probe. Rebek J., Jr. et al. reported that the packing coefficient of 55±9% gives the best binding of host-guest complex in solution when a 0.7Å radius probe is used.[2] Rebek also stated that the size of the probe give rise to a tolerance error range for a larger cavity calculation. The same size probe was used to calculate the **CA** cavities because all of the cavities have enough volume. The employment of the same size probe would permit to compare cavity volumes and the packing coefficients between in solutions and in solid state. The cavity volumes or packing coefficients are not used as absolute value but as relative value for each crystal.

3. Results and Discussion

Formation of Inclusion Crystals and Bilayer Structures of CA

Chart 1 shows monosubstituted benzenes included by **CA**. The host-guest ratios and the crystallographic parameters are summarized in Tables 2-1 and 2-2, respectively. Figures 2-1, 2-2,



1: R=H
2: R=CH_3
3: R=CH_2CH_3
4: R=$CH=CH_2$
5: R=C≡CH
6: R=$(CH_2)_2CH_3$
7: R=$CH_2CH=CH_2$
8: R=$C(CH_3)=CH_2$
9: R=$(CH_2)_3CH_3$
10: R=$CH_2CH(CH_3)_2$
11: R=$(CH_2)_4CH_3$
12: R=$(CH_2)_5CH_3$
13: R=C_6H_{11}
14: R=$CH_2C_6H_5$
15: R=F
16: R=Cl
17: R=Br
18: R=I
19: R=CH_2Cl
20: R=CH_2Br
21: R=C(=O)H
22: R=$C(=O)CH_3$
23: R=$C(=O)CH_2CH_3$
24: R=$C(=O)(CH_2)_2CH_3$
25: R=$C(=O)CH(CH_3)_2$
26: R=$C(=O)(CH_2)_3CH_3$
27: R=$C(=O)(CH_2)_4CH_3$
28: R=$C(=O)C_6H_5$
29: R=$(CH_2)_2C(=O)CH_3$
30: R=CO_2CH_3
31: R=$CO_2CH_2CH_3$
32: R=$CO_2(CH_2)_2CH_3$
33: R=$CO_2CH(CH_3)_2$
34: R=$CO_2(CH_2)_3CH_3$
35: R=$CO_2CH_2CH(CH_3)_2$
36: R=$CO_2C(CH_3)_3$
37: R=$CO_2(CH_2)_4CH_3$
38: R=$CO_2(CH_2)_2CH(CH_3)_2$
39: R=$CO_2(CH_2)_5CH_3$
40: R=$CO_2C_6H_5$
41: R=$CH_2CO_2CH_3$
42: R=$CH_2CO_2CH_2CH_3$
43: R=$OCOCH_3$
44: R=$OCOCH_2CH_3$
45: R=CH_2OCOH
46: R=CH_2OCOCH_3
47: R=$CH_2OCOCH_2CH_3$
48: R=$CH_2OCOC(CH_3)=CH_2$
49: R=$CH_2OCO(CH_2)_2CH_3$
50: R=OCH_3
51: R=OCH_2CH_3
52: R=OC_6H_5
53: R=$OCH_2C_6H_5$
54: R=CH_2OCH_3
55: R=C≡N
56: R=OH
57: R=CH_2OH
58: R=NH_2
59: R=$NHCH_3$
60: R=$NHCH_2CH_3$
61: R=NO_2

Chart 1

Table 2-1. Host-guest ratios, molecular volumes and host frameworks of inclusion compounds of **CA**.

Guest R	Host-guest ratio	Molecular volume [Å^3]	Host framework	Guest R	Host-guest ratio	Molecular volume [Å^3]	Host framework
H(**1**)	1:1	83	α-*gauche*	$CO_2CH_2CH_3$(**31**)	2:1	149	α-*trans*
F(**15**)	1:1	88	α-*gauche*	$CH_2CO_2CH_3$(**41**)	2:1	149	α-*trans*
OH(**56**)	1:1	93	β-*trans*	CH_2OCOCH_3(**46**)	2:1	150	α-*trans*
NH_2(**58**)	1:1	96	α-*gauche*	$OCOCH_2CH_3$(**44**)	2:1	150	α-*trans*
Cl(**16**)	1:1	98	α-*gauche*	$CH_2CH(CH_3)_2$(**10**)	2:1	153	α-*trans*
CH_3(**2**)	1:1	101	α-*gauche*	$(CH_2)_3CH_3$(**9**)	2:1	153	α-*trans*
Br(**17**)	1:1	102	α-*gauche*	$C(=O)(CH_2)_2CH_3$(**24**)	2:1	156	α-*trans*
C≡N(**55**)	1:1	102	α-*gauche*	$(CH_2)_2C(=O)CH_3$(**29**)	2:1	156	α-*gauche*
C(=O)H(**21**)	1:1	104	α-*gauche*	$C(=O)CH(CH_3)_2$(**25**)	2:1	156	α-*trans*
C≡CH(**5**)	1:1	105	β-*gauche*	$CO_2CH(CH_3)_2$(**33**)	2:1	166	α-*gauche*
I(**18**)	1:1	108	α-*gauche*	OC_6H_5(**52**)	2:1	166	α-*gauche*
NO_2(**61**)	1:1	110	α-*gauche*	$CH_2CO_2CH_2CH_3$(**42**)	2:1	167	α-*gauche*
OCH_3(**50**)	1:1	110	α-*gauche*	$CO_2(CH_2)_2CH_3$(**32**)	2:1	167	α-*trans*
CH_2OH(**57**)	1:1	111	α-*trans*	$CH_2OCOCH_2CH_3$(**47**)	2:1	167	α-*trans*
$CH=CH_2$(**4**)	1:1	111	α-*gauche*	$(CH_2)_4CH_3$(**11**)	2:1	171	α-*gauche*
$NHCH_3$(**59**)	1:1	113	β-*trans*	$C(=O)(CH_2)_3CH_3$(**26**)	2:1	174	α-*trans*
CH_2Cl(**19**)	1:1	115	β-*trans*	$CH_2C_6H_5$(**14**)	2:1	174	α-*trans*
CH_2CH_3(**3**)	1:1	118	β-*trans*	$C(=O)C_6H_5$(**28**)	2:1	176	α-*trans*
CH_2Br(**20**)	1:1	119	β-*trans*	C_6H_{11}(**13**)	2:1	176	α-*trans*
$C(=O)CH_3$(**22**)	1:1	121	α-*gauche*	$CH_2OCOC(CH_3)=CH_2$(**48**)	2:1	177	α-*trans*
CH_2OCH_3(**54**)	1:1	128	β-*trans*	$CO_2C(CH_3)_3$(**36**)	2:1	183	α-*trans*
$C(CH_3)=CH_2$(**8**)	1:1	128	α-*gauche*	$OCH_2C_6H_5$(**53**)	2:1	183	α-*gauche*
$CH_2CH=CH_2$(**7**)	1:1	128	β-*trans*	$CO_2(CH_2)_3CH_3$(**34**)	2:1	184	α-*trans*
OCH_2CH_3(**51**)	1:1	128	β-*trans*	$CO_2CH_2CH(CH_3)_2$(**35**)	2:1	184	α-*gauche*
$NHCH_2CH_3$(**60**)	1:1	130	β-*trans*	$CH_2OCO(CH_2)_2CH_3$(**49**)	2:1	185	α-*gauche*
$OCOCH_3$(**43**)	1:1	131	β-*trans*	$CO_2C_6H_5$(**40**)	2:1	186	α-*gauche*
CO_2CH_3(**30**)	1:1	132	β-*trans*	$(CH_2)_5CH_3$(**12**)	2:1	189	α-*gauche*
CH_2OCOH(**45**)	1:1	132	β-*trans*	$C(=O)(CH_2)_4CH_3$(**27**)	2:1	191	α-*trans*
$(CH_2)_2CH_3$(**6**)	1:1	136	β-*trans*	$CO_2(CH_2)_4CH_3$(**37**)	2:1	202	α-*trans*
$C(=O)CH_2CH_3$(**23**)	1:1	139	β-*trans*	$CO_2(CH_2)_2CH(CH_3)_2$(**38**)	2:1	202	α-*trans*
				$CO_2(CH_2)_5CH_3$(**39**)	2:1	220	α-*trans*

2-3, and 2-4 illustrate the crystal structures viewed down along crystallographic *b*-axis. A common feature found in the crystal structures is a bilayer structure with alternate stacking of lipophilic layers and hydrophilic layers. Facially amphiphilic molecular structure of **CA** give rise to the bilayer structure by means of van der Waals association of the hydrophilic faces and hydrogen bonding between the hydrophilic faces.[15a] The rigid molecular shape makes the layer corrugated, and the offset stacking of the lipophilic faces yields one-dimensional host channels in the lipophilic

Table 2-2. Lattice parameters and dihedral angles for 1:1 inclusion compounds of **CA**.

Guest	Space group	*a* [Å]	*b* [Å]	*c* [Å]	*a* [°]	*b* [°]	*c* [°]	*V* [Å^3]	Ψ [°]	Reference
α-gauche										
benzene(**1**)	$P2_1$	13.63	8.04	14.08		114.3		1406	63	[16d]
fluorobenzene(**15**)	$P2_1$	13.57	8.06	14.10		114.4		1405	62	this work
aniline(**58**)	$P2_1$	13.80	8.07	14.09		116.0		1410	61	[17a,18a]
chlorobenzene(**16**)	$P2_1$	13.66	8.10	14.03		114.6		1411	60	this work
toluene(**2**)	$P2_1$	13.74	8.04	14.01		114.1		1421	61	this work
bromobenzene(**17**)	$P2_1$	13.69	8.10	14.01		114.6		1413	65	this work
benzonitrile(**55**)	$P2_1$	13.64	8.16	14.03		113.9		1428	58	this work
benzaldehyde(**21**)	$P2_1$	13.57	8.11	14.06		113.7		1417	58	this work
iodobenzene(**18**)	$P2_1$	13.68	8.10	14.09		114.2		1423	61	this work
nitrobenzene(**61**)	$P2_1$	13.58	8.11	14.05		113.5		1418	60	[18a]
anisole(**50**)	$P2_1$	13.57	8.08	14.23		114.7		1417	59	this work
styrene(**4**)	$P2_1$	13.57	8.15	14.24		114.6		1431	60	this work
acetophenone(**22**)	$P2_1$	13.72	8.09	14.23		113.7		1447	58	[16b]
ethyl acetate	$P2_1$	13.67	7.82	14.10		113.5		1382		[18b]
ethyl propionate	$P2_1$	13.57	7.97	14.24		113.5		1411		[18b]
2-fluoroaniline	$P2_1$	13.61	8.15	14.03		113.7		1425		[17d]
4-fluoroaniline	$P2_1$	13.83	8.11	13.99		115.5		1416		[17d]
3,4-difluoroaniline	$P2_1$	13.93	8.14	14.03		115.9		1430		[17d]
4-fluoroacetophenone	$P2_1$	13.54	8.15	14.35		113.3		1456		[17c]
2-fluorobenzylalchohol	$P2_1$	13.42	8.51	13.98		113.2		1467		[17e]
β-trans										
phenol(**56**)	$P2_1$	12.07	7.92	16.39		111.9		1455	-163	this work
N-methylaniline(**59**)	$P2_1$	12.00	7.96	16.22		111.6		1441	-167	this work
benzyl chloride(**19**)	$P2_1$	12.34	7.82	16.24		111.7		1456	-174	this work
ethylbenzene(**3**)	$P2_1$	12.41	7.83	16.28		111.8		1469	-174	this work
benzyl bromide(**20**)	$P2_1$	12.29	7.83	16.30		111.5		1459	-169	this work
benzylmethyl ether(**54**)	$P2_1$	12.11	7.94	16.24		109.9		1468	-169	this work
allylbenzene(**7**)	$P2_1$	12.43	7.88	16.33		112.1		1483	-173	this work
phenetol(**51**)	$P2_1$	12.11	7.97	16.12		108.5		1475	-171	this work
N-ethylaniline(**60**)	$P2_1$	12.14	7.95	16.14		108.2		1481	-171	this work
phenyl acetate(**43**)	$P2_1$	12.26	7.90	16.67		109.7		1478	-180	this work
benzyl formate(**45**)	$P2_1$	12.09	7.96	16.21		109.7		1468	-169	this work
n-propylbenzene(**6**)	$P2_1$	12.07	7.84	16.25		109.8		1447	-172	this work
n-propiophenone(**23**)	$P2_1$	12.30	7.94	16.24		109.2		1499	-170	this work, [18a]
3-fluoroacetophenone	$P2_1$	12.79	7.81	16.17		113.1		1486		[17c]
2-chloroacetophenone	$P2_1$	12.58	7.98	16.05		112.2		1492		[17c]
3-methyl, *N*-nitrosopiperidine	$P2_1$	12.35	7.68	16.36		111.1		1447		[18b]
1,5-dimethyl, *N*-nitrosopiperidine	$P2_1$	12.75	7.88	16.36		112.0		1525		[18b]
4-fluoro-*n*-propiophenone	$P2_1$	16.67	8.15	12.06		113.2		1506		[18a]

Table 2-2. Lattice parameters and dihedral angles for 1:1 inclusion compounds of **CA**. (Continued)

Guest	Space group	*a* [Å]	*b* [Å]	*c* [Å]	*a* [°]	*b* [°]	*c* [°]	*V* [Å^3]	Ψ [°]	Reference
β-*gauche*										
ethynylbenzene(**5**)	$P2_1$	12.26	7.80	15.47		106.8		1417	70	this work
n-propyl acetate	$P2_1$	16.80	7.88	12.11		118.1		1415		[18b]
isopropyl acetate	$P2_1$	16.60	7.98	12.14		117.8		1423		[18b]
α-*trans*										
benzylalcohol(**57**)	$P2_1$	12.64	8.61	13.90		105.2		1459	-160	this work
acryronitrile	$P2_1$	12.18	7.88	14.30		104.2		1331		[15c]
methacryronitrile	$P1$	12.53	14.16	8.28	90.9	94.9	107.2	1396		[15d]
γ-valerolactone	$P2_1$	13.01	8.00	14.05		104.8		1414		[16c]
4-fluorobenzylalcohol	$P2_1$	12.63	8.61	13.81		105.2		1449		[17e]
methyl acetate	$P1$	12.22	8.19	14.20	90.2	105.7	94.0	1364		[18b]
methyl acetate+isopropyl acetate	$P1$	12.29	8.24	14.25	90.4	105.8	95.0	1382		[18e]
acetone+*o*-dichlorobenzene	$P1$	12.47	8.25	14.21	91.1	106.3	94.4	1399		[18e]
N-nitrosopiperidine	$P2_1$	13.27	7.91	13.82		106.0		1394		[19b]

layers.

All the crystal structures, except that with **57**, contain identical host-host hydrogen bond networks irrespective of the chemical properties of the guest compounds. Figure 2-5(a) shows the hydrogen bond network of **CA** with **1** as a typical example. The cyclic hydrogen bond network enables the arrangement of the host molecules into a two-dimensional array. The hydroxy group of **57** is inserted into the cyclic host-host hydrogen bond network, while the amino group of **58**[17a,18a] forms weak hydrogen bonds with the hydroxy groups of the host molecules, as shown in Figure 2-5(b) and (c). Unfortunately, disorder of the guest **56** in the host cavity is so severe that the orientations of the guest component cannot be accurately investigated. However, the hydroxyl group of **56** probably forms a guest-to-host hydrogen bond in the similar manner to **58**.

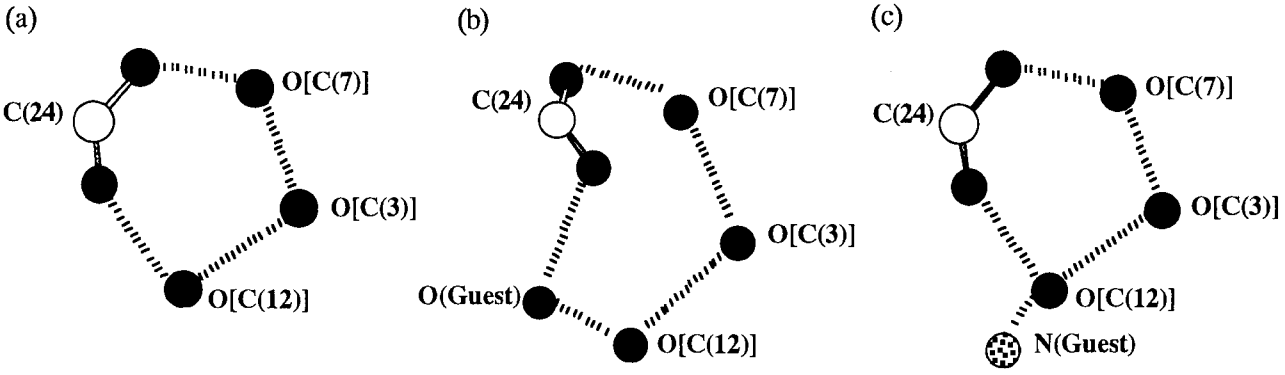


Figure 2-5. Hydrogen bond networks of **CA** with (a) **1**, (b) **57**, and (c) **58**. The carbon, nitrogen, and oxygen atoms are represented by open, dotted, and filled circle, respectively.

Classification of Host Frameworks

The bilayer structures are robust, common structural motifs of the **CA** inclusion crystals. These crystals are classified into four sub-types based on two conformations (*gauche* and *trans*) of the steroidal side chain, and two types of interdigitation of methyl groups (α and β) in the lipophilic faces. [15a] A combination of the two factors gives the four types; α–*gauche*, β–*gauche*, α–*trans*, and β–*trans*, which are illustrated in Figures 2-1, 2-2, 2-3, and 2-4, respectively.

(a) α–*Gauche* Type This host framework (Figure 2-1) was found as the first example of channel-type crystal structure of **CA** with **22** in 1988.[16b] Since this discovery, some monosubstituted benzenes, such as **1**,[16d] **58**[17a,17a] and **61**[18a], and other compounds[17b-e,18b] have been reported to give this type. The dihedral angles of the side chain at C17-C20-C22-C23 (ψ) are between 58° and 65°. This conformation refers to the *gauche* type. In the lipophilic layers, the methyl carbon C(19) in the upper layer is located between the methyl carbons C(18) and C(19) of the opposite layer. The stacking is of the α–type. Therefore, this host arrangement is classified as α–*gauche*. In addition nine compounds with the aromatic guest compounds (**2, 4, 15, 16, 17, 18, 21, 50**, and **55**) are included in this type. The crystallographic parameters of all of these host-guest compounds are in a narrow range: 13.565 < *a* < 13.801Å, 8.038 < *b* < 8.164Å, 14.011 < *c* < 14.235Å, 113.52 < *β* < 116.01°, 1405.4 < *V* < 1446.7 Å^3.

(b) β–*Trans* Type The torsion angles ψ are in the range from -167° to -180°. This conformation refers to the *trans* type (Figure 2-2). In the lipophilic layers, the methyl carbon C(18) in the upper layer is located between the methyl carbons C(18) and C(19) of the opposite layer. This is β–type stacking. Sliding of the upper layer of the α–type stacking by approximately 4.5Å gives the β–type stacking. This host framework already has been reported in the crystal structures of **CA** with other aliphatic compounds.[17c,19a,19b] Thirteen aromatic compounds (**3, 6, 7, 19, 20, 23, 43, 45, 51, 54, 56, 59**, and **60**) are included in this host framework. Regardless of the guest species, the lattice parameters of the β–*trans* type are also within a narrow range; 12.001 < *a* < 12.434Å, 7.821 < *b* < 7.965Å, 16.118 < *c* < 16.671Å, 108.194 < *β* < 112.060°, 1441.3 < *V* < 1498.8 Å^3.

(c) β–*Gauche* Type From this current study of aromatic guests, only guest **5** affords the β–*gauche* type structure in the **CA** host-guest compound (Figure 2-3). The torsion angle of the side-chain is 70°, which corresponds to the α–*gauche* type. The interdigitation of the methyl groups in the lipophilic layer is same as the β–*trans* type. This type of structure, however, is known in the crystal structures of **CA** with aliphatic esters. [18b]

(d) α–*Trans* Type From this current study of aromatic guests, the only guest **57** affords a 1:1 α–*trans* type (Figure 2-4). The torsion angle is -160°, which corresponds to the *trans* type. The interdigitation of the methyl groups in the lipophilic side is the α–stacking. Since the X-ray crystallographic study of the inclusion compounds of **CA** with γ-valerolactone,[16c] there have been reports that some aliphatic compounds also afforded this host framework, which is further classified

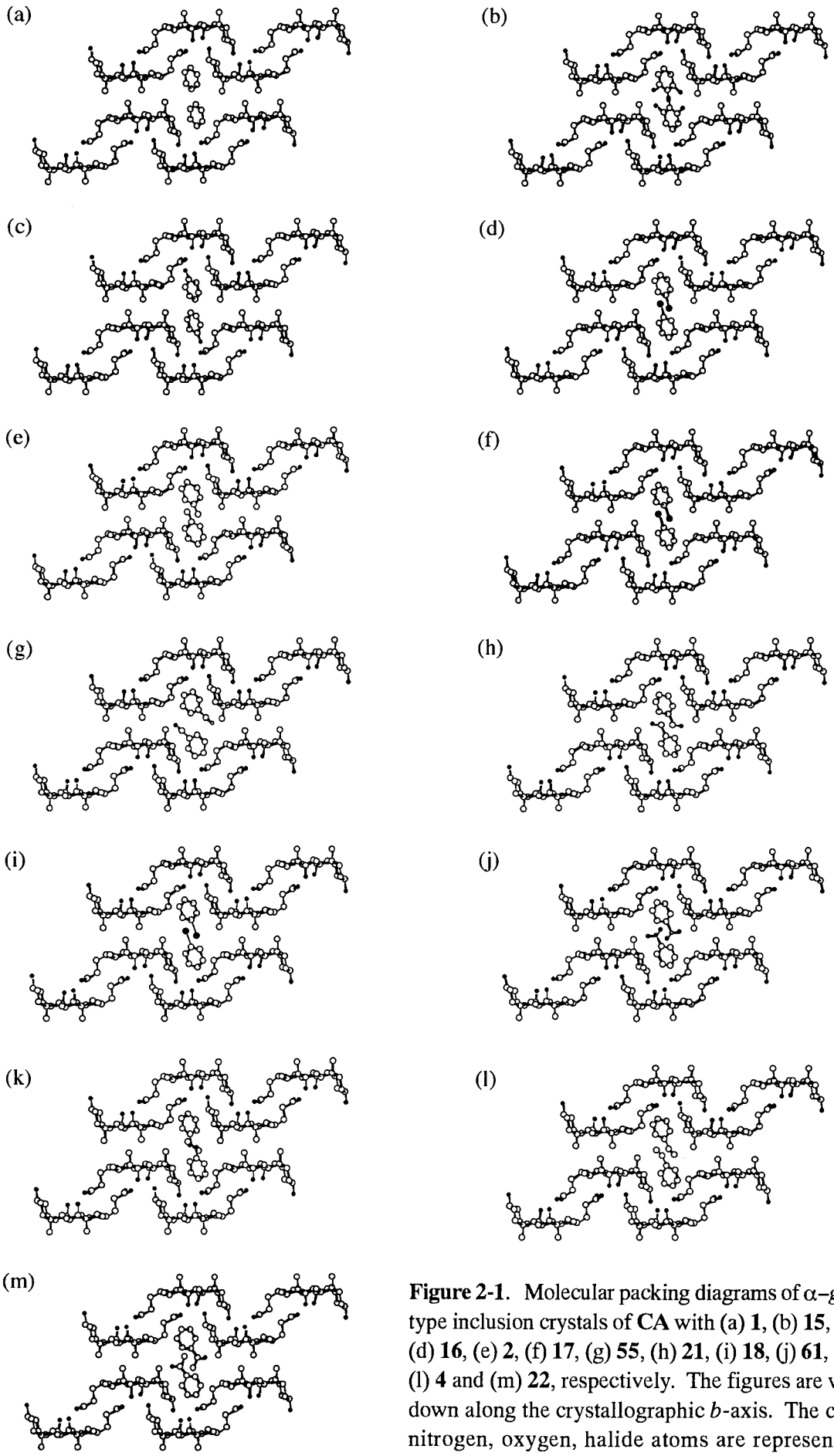


Figure 2-1. Molecular packing diagrams of α-*gauche* type inclusion crystals of **CA** with (a) **1**, (b) **15**, (c) **58**, (d) **16**, (e) **2**, (f) **17**, (g) **55**, (h) **21**, (i) **18**, (j) **61**, (k) **50**, (l) **4** and (m) **22**, respectively. The figures are viewed down along the crystallographic *b*-axis. The carbon, nitrogen, oxygen, halide atoms are represented by open, dotted, filled, and shadowed circle, respectively.

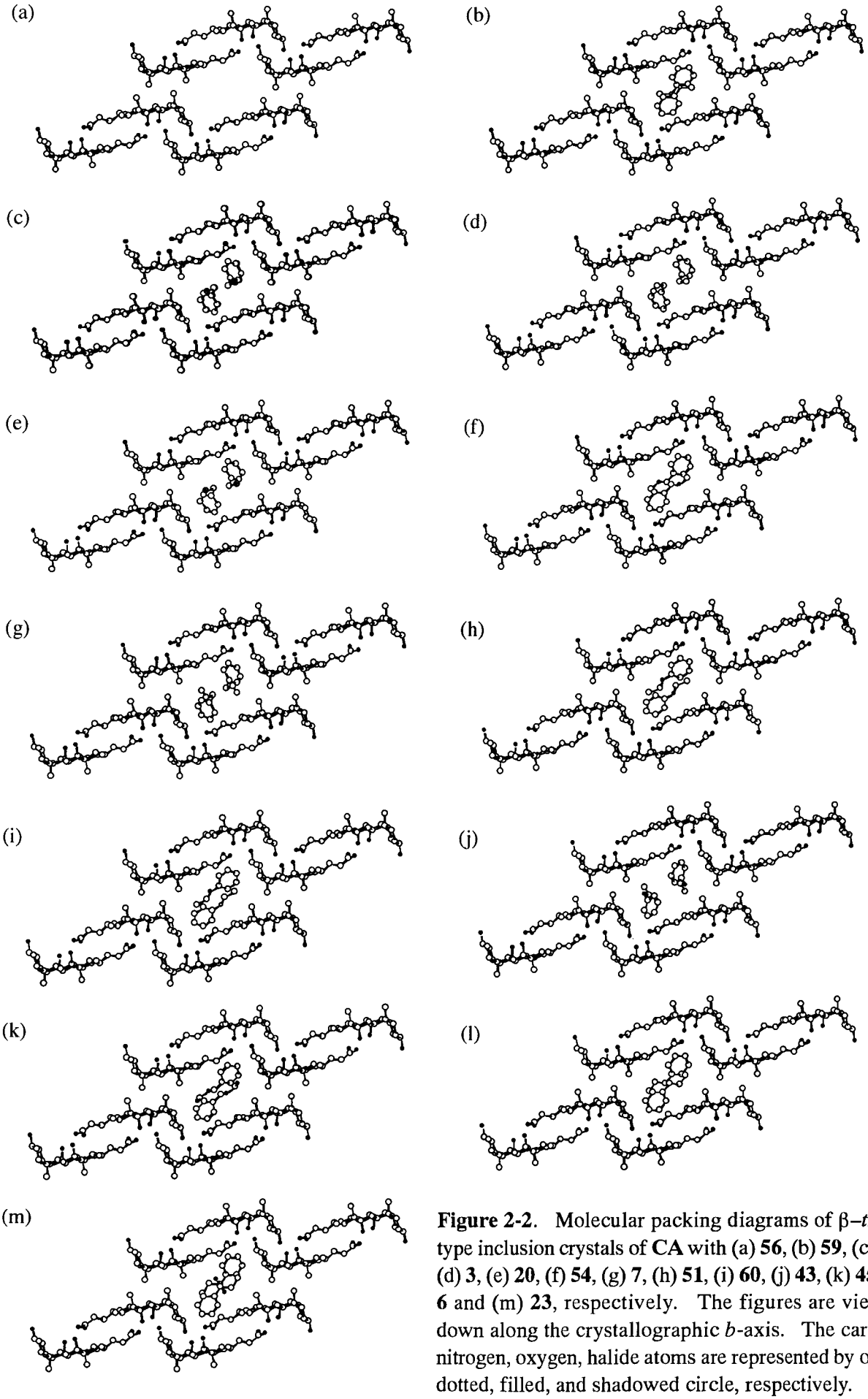


Figure 2-2. Molecular packing diagrams of β–*trans* type inclusion crystals of **CA** with (a) **56**, (b) **59**, (c) **19**, (d) **3**, (e) **20**, (f) **54**, (g) **7**, (h) **51**, (i) **60**, (j) **43**, (k) **45**, (l) **6** and (m) **23**, respectively. The figures are viewed down along the crystallographic *b*-axis. The carbon, nitrogen, oxygen, halide atoms are represented by open, dotted, filled, and shadowed circle, respectively.

into two crystal systems; monoclinic[15c,16e,17e,19b] and triclinic.[15d,18b,18e]

Sizes and Shapes of Host Cavities

The crystal structures of the host frameworks are affected by the guest compounds. However, differences of the lattice parameters of the α–*gauche* type or the β–*trans* type are within only 3%. This indicates that the size and the shape of the host cavities are essentially identical within the same host framework, regardless of the functional groups or the steric dimensions of the guest components. Variations of the host channels only originate from four types of the host architectures. Namely, **CA** can provide at least four different host cavities to include the monosubstituted benzenes by isomerization of the host frameworks. Table 2-3 summarizes free volumes of the host cavities in a unit cell, calculated by Cerius2.[23] The mean values of the host cavities in unit cell of the α–*gauche* type and the β–*trans* type are 330±14 Å^3 and 392±11 Å^3, respectively, when the volumes of the host cavities were calculated using a 0.7Å radius probe. The difference in volume is 62 Å^3, which is similar to the volume difference calculated using a 1.0Å radius probe.[24] The free volumes of **CA** with **5** in the β–*gauche* host framework and with **57** in the α–*trans* are 351 Å^3 and 354 Å^3, respectively. Therefore, the order of the volumes is as follows; α–*gauche* < α–*trans*, β–*gauche* < β–*trans*. The β–*trans* type host frameworks have the largest host cavities of the **CA** host.

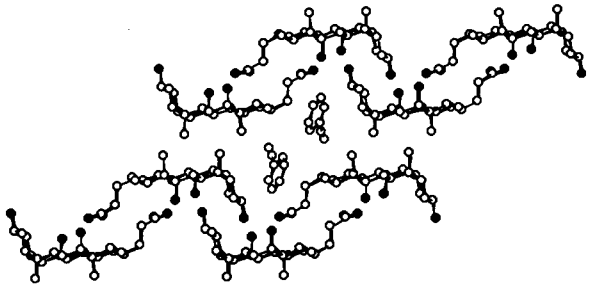


Figure 2-3. Molecular packing diagram of a β–*gauche* type inclusion crystal of **CA** with **5**. The figure is viewed down along the crystallographic *b*-axis. The carbon and oxygen atoms are represented by open and filled circle, respectively.

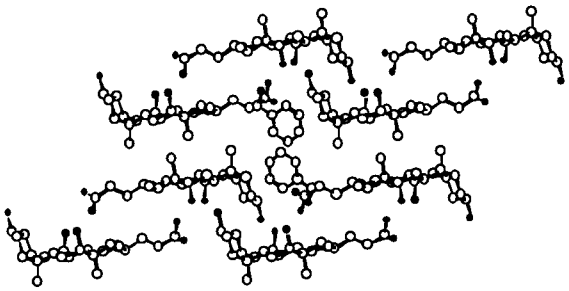


Figure 2-4. Molecular packing diagram of a α–*trans* type inclusion crystal of **CA** with **57**. The figure is viewed down along the crystallographic *b*-axis. The carbon and oxygen atoms are represented by open and filled circle, respectively.

Figures 2-6 and 2-7 illustrate the cross-sectional views sliced perpendicular or parallel to the axis of the channel at the same positions. The perpendicular cross sections of α–*gauche*, β–*trans*, β–*gauche*, and α–*trans*, are nearly ellipse, larger ellipse, distorted round, and round, respectively. The parallel cross-sections permit us to clarify the difference of the shapes between the *gauche* and the *trans* type. The host cavities in the α– and the β–*gauche* types have square grooves, while those in the α– and the β–*trans* types have the triangular grooves.

Size-Dependent Isomerization of Host Frameworks

Most of the monosubstituted benzenes are incorporated in two common types, α–*gauche* and β–*trans*. The sizes of the guest compounds contribute to isomerization of the host framework. The

Table 2-3. Molecular volume, cavity volume, packing coefficient, and length and thickness of guest molecules.

Guest R	Molecular volume [Å^3]	V_{cavity} [a] [Å^3]	PC_{cavity} [b] [%]	$PC_{crystal}$ [c] [%]	L [Å]	Th [Å]
α-gauche						
H(**1**)	83	298	56	72	7.4	3.4
F(**15**)	88	319	55	71	7.9	3.4
NH_2(**58**)	96	336	57	71	8.1	3.4
Cl(**16**)	98	328	58	72	8.5	3.5
CH_3(**2**)	101	335	60	71	8.2	4.3
Br(**17**)	102	319	64	72	8.9	3.7
C≡N(**55**)	102	328	62	73	9.2	3.4
C(=O)H(**21**)	104	331	63	73	8.7	3.4
I(**18**)	108	352	61	72	9.1	4.0
NO_2(**61**)	110	326	67	74	8.7	3.4
OCH_3(**50**)	110	332	67	73	9.5	4.3
$CH{=}CH_2$(**4**)	111	346	64	72	9.7	3.4
$C(=O)CH_3$(**22**)	121	345	70	74	9.6	4.3
β-trans						
OH(**56**)	93	390	48	-d	8.0	3.4
$NHCH_3$(**59**)	113	374	61	72	9.6	4.3
CH_2Cl(**19**)	115	370	62	71	9.0	5.1
CH_2CH_3(**3**)	118	386	61	71	9.5	4.9
CH_2Br(**20**)	119	400	60	72	9.2	5.3
CH_2OCH_3(**54**)	128	399	64	72	10.0	5.2
$CH_2CH{=}CH_2$(**7**)	128	394	65	72	9.5	5.8
OCH_2CH_3(**51**)	128	389	66	72	11.0	4.3
$NHCH_2CH_3$(**60**)	130	407	64	71	11.0	4.3
$OCOCH_3$(**43**)	131	399	66	72	10.0	5.5
CH_2OCOH(**45**)	132	388	68	73	11.0	5.4
$(CH_2)_2CH_3$(**6**)	136	387	70	74	10.0	5.1
$C(=O)CH_2CH_3$(**23**)	139	408	68	74	11.0	4.3
β-gauche						
C≡CH(**5**)	105	351	60	72	10.0	3.4
α-trans						
CH_2OH(**57**)	111	354	63	71	8.7	5.2

[a] V_{cavity} is the volume of the cavity in unit cell calculated using a 0.7Å radius probe.

[b] PC_{cavity} means packing coefficient of the guest components in the host cavity:

PC_{cavity}=(molecular volume)×2/V_{cavity}×100.

[c] $PC_{crystal}$ means packing coefficient of the whole crystal.

[d] $PC_{crystal}$ cannot be calculated because of the disorder.

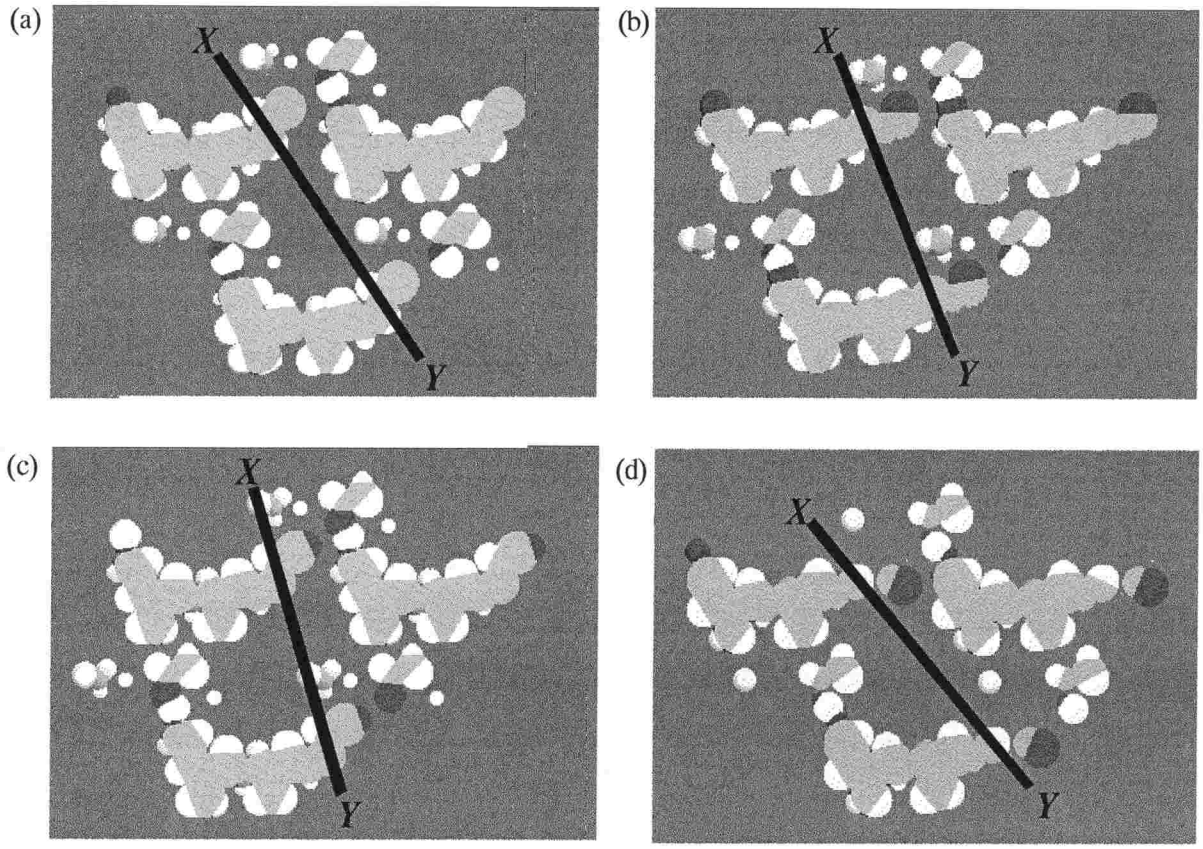


Figure 2-6. Cross sections of the host channels sliced perpendicular to the direction of the channel; (a) **CA** with **1** as a typical example for α–*gauche* type, (b) **CA** with **3** as β-*trans* type, (c) **CA** with **5** as β-*gauche* type, and (d) **CA** with **57** as α–*trans* type, respectively. The guest molecules are omitted. Carbon, hydrogen, and oxygen atoms are represented in gray, white, and black, respectively. The bold line of ***X-Y*** indicates the position sliced parallel to the direction of the channel which is shown in Figure 2-7.

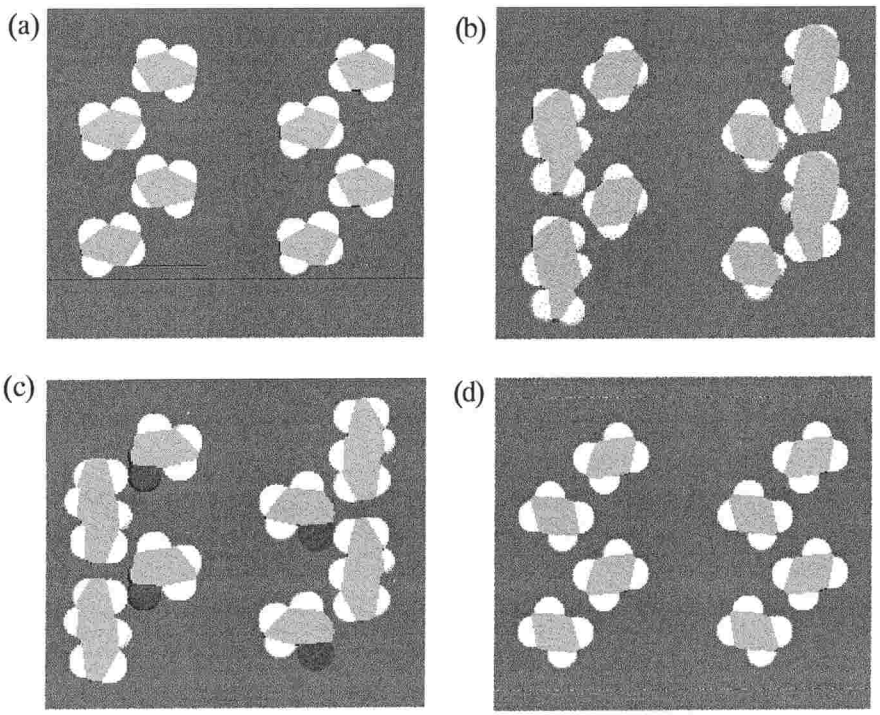


Figure 2-7. Cross sections of the host channels sliced parallel to the direction of the channel; (a) **CA** with **1** as a typical example for α–*gauche* type, (b) **CA** with **3** as β-*trans* type, (c) **CA** with **5** as β-*gauche* type, and (d) **CA** with **57** as α–*trans* type, respectively. The guest molecules are omitted. Carbon, hydrogen, and oxygen atoms are represented in gray, white, and black, respectively.

smaller guests in the range of 83.4-127.7Å^3 prefer the α–*gauche* type and the larger guests in the range of 93.0-138.9Å^3 tend to form the β–*trans* type, as shown in Table 2-1. This is a good agreement to the fact that the β–*trans* host framework has a 119% larger cavity than the α–*gauche* framework. When the molecular volumes of the guest compounds exceed the upper limit of the β–*trans* type, 140 Å^3, the host-guest ratios change from 1:1 to 2:1 and simultaneously the host frameworks isomerize from the β–*trans* type to the α–types. As the α–types have smaller cavities than β–*trans*, the number of the guest components in the unit cell is reduced. Both of the host frameworks and the host-guest ratios change with increase in guest volume in the order, α–*gauche* lattice at 1:1 stoichiometry < β–*trans* lattice at 1:1 stoichiometry < α–*gauche* or α–*trans* lattice at 2:1 stoichiometry. This indicates that the guest-dependent isomerization of the host frameworks as well as the change of the host-guest stoichiometries enable **CA** to include a variety of the monofunctional benzenes.

Shape-Dependent Isomerization of Host Frameworks

The volumes of the guest compounds play a primary role for the isomerization of the host frameworks. Small and large guest compounds are included in the α–*gauche* or the β–*trans* type, respectively. However, it is possible to incorporate the medium-size guests (93.0-127.7 Å^3) in both of the host lattices. In these cases, the shape of the guest compounds determines the host frameworks. To specify the shapes, two parameters are introduced; length of the molecular longitudinal molecular axis *L*, and thickness of the guest molecules *Th* (Figure 2-8). They are estimated based on geometrical calculation from the molecular models.

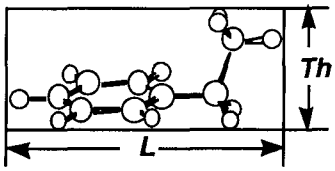


Figure 2-8. Length (*L*) and thickness (*Th*) of guest molecules were defined from molecular modeling.

The guest compounds included in the α–*gauche* type have *L*<9.7 Å and *Th* <4.3 Å, while those in the β–*trans* type have *L*>9.0 Å and *Th* >4.3 Å, respectively, except for **56**. This means that the shorter and thinner molecules prefer to form the α–*gauche* lattice and that longer and thicker molecules prefer the β–*trans* lattice. For example, **50** and **3** have similar volumes and *L* on account of the similar sizes of the substitutent groups. However, *Th* of the former is smaller than that of the latter, because the torsion angle between the terminal methyl group and the phenyl ring in the former guests is 0°, but in the latter it is 90°. The difference between the thicknesses gives the different host frameworks. When the molecular volumes are in the boundary between the two host frameworks, the shape determines the host frameworks. Furthermore, the characteristic shapes of **5** and **57** give an explanation of the two less common types. The length (*L*=10.0) of **5** is too large to be incorporated in the α–*gauche* lattice but the volume is too small for it to be incorporated in the β–*trans* lattice. It prefers the unique cavity of the β–*gauche* lattice. The center of the cavity is narrowed because of the *gauche* conformation of the side chain. The acetylene moiety just fits into the narrow corridor, as shown in Figure 2-6(c). For guest **57**, the thickness (*Th*=5.2 Å) is beyond the

range in the α–*gauche* framework (3.4Å < *Th* < 4.3 Å), and the volume is too small for the β–*gauche* lattice. Therefore, the molecular shape and the hydroxy group of **57** contribute to the formation of the α–*trans* type. Molecule **56** is an exceptional guest. In spite of the small volume (93.1 Å^3) and the short thin molecular shape (*L*=8.0 Å, *Th*=3.4 Å), it has a β–*trans* type host. Unfortunately, even at low temperature, the orientation of the guest compounds in the host cavity could not be confirmed because of the disorder of the phenyl ring, while the host framework is found to be the β–*trans* type. The disorder can be understood by the fact that the size of the guest molecule is too small for the host cavity. The host-guest hydrogen bonding between **56** and the host compound may force the phenyl ring of guest molecule to arrange in the specific direction to yield the β–*trans* lattice.

Packing Coefficients of Host Cavities

In order to understand the size-dependent isomerizations and the guest recogintions of **CA**, the estimations of the steric fit between the host cavities and guest components are required. The packing coefficients of the host cavities (PC_{cavity}) as a parameter for the steric fit of the guest component in the host cavity were used. This parameter is calculated from the free volume of the host cavities and the molecular volume of the guest compounds in the unit cell. Table 2-3 summarizes the PC_{cavity} of all the examined inclusion crystals, together with $PC_{crystal}$, the ratios between the volumes of the unit cell and the molecular volumes of all components in the unit cell. PC_{cavity} of the α–*gauche* and the β–*trans* host cavities, except for the complex with **56** is statistically distributed in the range of 62±5% and 65±3%, respectively. The similar values found for each host framework indicate that the PC_{cavity} is independent of the shape and size of the host frameworks.

In a series of the guest compounds included in the same host frameworks, PC_{cavity} tends to increase with increasing guest volumes, because the volumes of the host cavities are less sensitive than those of the guest molecules. Guests with packing coefficients of >70% do not form the stable inclusion crystals; they induces isomerization to another host framework that have larger host cavities or/and reduce the host-to-guest ratios. This is because close packing gives rise to steric repulsion between the host molecules and the guest components and restrictions in the freedom of motion of the guest components in the host cavities. On the other hand, guests with packing coefficients of <55% also do not form the inclusion crystals and induce isomerization to another host framework that have smaller host cavities. Therefore, the optimal values PC_{cavity} (55-70%) should be required to form the stable inclusion compounds, particularly when the guest components are entrapped in the host cavities by the steric dimensions and van der Waals forces. These results indicate that PC_{cavity} is a good parameter for the estimation of the steric fit and plays an important role for the formation of the host-guest compounds, the host-guest ratios, and the isomerizations of the host frameworks. On the other hand, guest **56**, which has a hydrogen-bonding functional group, has the lowest PC_{cavity} (48%). The size of the guest components is small, but the host framework

is the biggest. This steric misfit decreases the packing coefficient of **56**. The host-guest hydrogen bonding would hold the guest molecule within the relatively large host cavity. Therefore, additional strong intermolecular interactions, such as π-π interaction and hydrogen bonds, between a host cavity and a guest compound expand the range of PC_{cavity}.

Since there have been many examples of the host-guest compounds in crystalline state, PC_{cavity} of the selected host-guest compounds that have one dimensional host channels without any host-guest hydrogen bonds was calculated, as shown in Table 2-4. The packing coefficients of the host cavities are in the range of those observed in the host frameworks of **CA**. Larger packing coefficients are reached if the compounds are stabilized by π-π interactions. Unfortunately, the upper and lower limits of the PC_{cavity} are not clear because of a lack of systematic structural investigation of each host framework. However, these results indicate that the appropriate PC_{cavity} (55-70%) should be required to form the stable inclusion compounds. These facts suggest that the optimal PC_{cavity} is independent on both the host compounds and the host frameworks. Upper and lower limits of the PC_{cavity} are affected by the interactions between host cavities and guest components.

Behavior of the packing coefficients with respect to the formation of the inclusion crystals is quite similar to those of the tennis-ball type host compounds in solution.[2] Suitable packing coefficients of the host cavities are required to form stable complexes. Comparison of the absolute value of PC_{cavity} between them may have no sense because an accurate estimation of host cavities has been never achieved even in solid state nor in solution. However, the range of packing coefficient in the inclusion cavities is smaller than those of the organic crystals (66-77%)[25] or protein core[26], and a slightly larger than those of the calculated results of the encapsulated complexes in the solution (46-64%) or the liquid state (44-56%) (Figure 2-9).[2] This indicates that guest molecules in the host cavities of lattice inclusion compounds have an intermediate mobility and anisot-

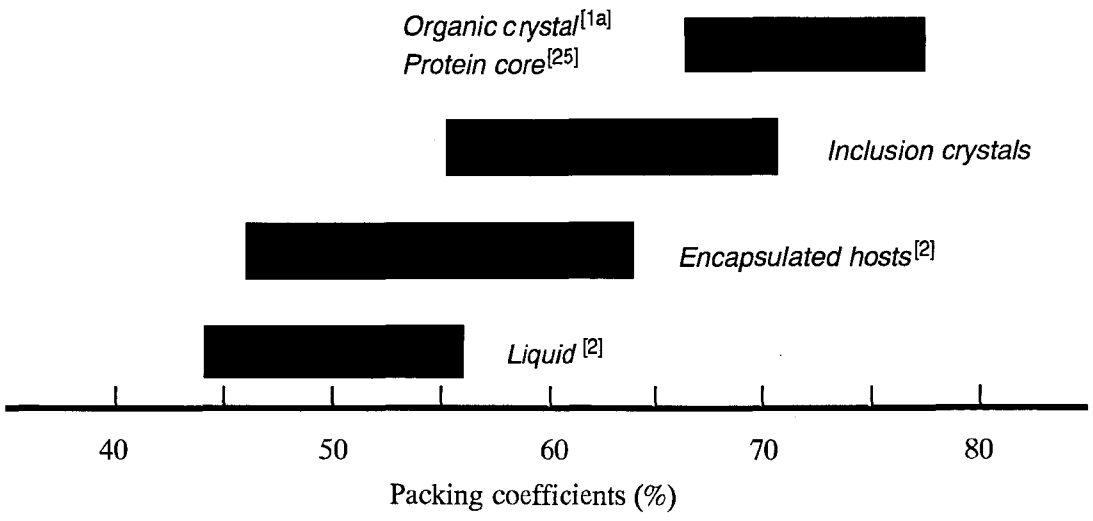


Figure 2-9. Packing coefficients in various states; organic crystals, protein cores, inclusion crystals, encapsulated hosts, and liquid state.

Table 2-4. Packing coefficents of the selected crystalline inclusion compounds.

No.	Host	Guest	Number of guest molecule in unit cell	Molecular volume	V_{cavity}[a] [Å^3]	PC_{cavity}[b] [%]	Reference
1	9-(3,5-dihydroxyphenyl)anthracene	methyl acetate	4	77	487	63	[10]
2	9-(3,5-dihydroxyphenyl)anthracene	ethyl acetate	4	94	551	68	[10]
3	9-(3,5-dihydroxyphenyl)anthracene	acetone	4	66	440	60	[10]
4	9-(3,5-dihydroxyphenyl)anthracene	2-butanone	4	84	506	66	[10]
5	9-(3,5-dihydroxyphenyl)anthracene	3-pentanone	4	101	613	66	[10]
6	9-(3,5-dihydroxyphenyl)anthracene	3-hexanone	4	119	684	70	[10]
7	9-(3,5-dihydroxyphenyl)anthracene	4-heptanone	4	136	743	73	[10]
8	9-(3,5-dihydroxyphenyl)anthracene	cyclohexanone	4	106	606	70	[10]
9	9-(3,5-dihydroxyphenyl)anthracene	methyl benzoate	4	132	669	79	[10]
10	9-(3,5-dihydroxyphenyl)anthracene	isoprpyl benzoate	4	166	867	77	[10]
11	9-(3,5-dihydroxyphenyl)anthracene	isoprpylbenzoate	4	166	898	74	[10]
12	9-(3,5-dihydroxyphenyl)anthracene	acetophenone	4	121	669	72	[10]
13	9-(3,5-dihydroxyphenyl)anthracene	benzoquinone	4	98	547	71	[10]
14	9-(3,5-dihydroxyphenyl)anthracene	tetramethylbenzoquinone	4	165	805	82	[10]
15	9-(3,5-dihydroxyphenyl)anthracene	nitrobenzene	12	110	1819	72	[10]
16	(guanidinium)$_2$ azobenzene-4,4'-disulfonate	1,4-dibromobenzene	1	120	176	68	[14b]
17	(guanidinium)$_2$ azobenzene-4,4'-disulfonate	1,4-divinylbenzene	1	139	190	74	[14b]
18	(guanidinium)$_2$ 4,4'-biphenyldisulfonate	1,4-dibromobenzene	4	120	712	67	[14c]
19	(guanidinium)$_2$ 4,4'-biphenyldisulfonate	1,4-divinylbenzene	6	139	1249	67	[14c]
20	(guanidinium)$_2$ 4,4'-biphenyldisulfonate	nitorobenzene	8	110	1203	73	[14c]
21	(guanidinium)$_2$ 4,4'-biphenyldisulfonate	1-nitoronaphtalene	4	153	717	85	[14c]
22	(guanidinium)$_2$ 4,4'-biphenyldisulfonate	naphtalene	1	127	150	85	[14c]
23	1,1',6,6',7,7'-hexahydroxy-3,3'-dimethyl-5,5'-di-isopropyl-(2,2'-binaphthalene)-8,8'-dicarboxaldehyde	acetone	2	66	226	59	[12]
24	1,1',6,6',7,7'-hexahydroxy-3,3'-dimethyl-5,5'-di-isopropyl-(2,2'-binaphthalene)-8,8'-dicarboxaldehyde	1-butanal	2	84	225	75	[12]
25	1,1'-binaphthyl-2,2'-dicarboxylic acid	bromobenzene	2	102	314	65	[13b]
26	1,1'-binaphthyl-2,2'-dicarboxylic acid	*o*-xylene	4	118	704	67	[13a]
27	1,1'-binaphthyl-2,2'-dicarboxylic acid	*m*-xylene	2	118	354	67	[13a]
28	1,1'-binaphthyl-2,2'-dicarboxylic acid	*p*-xylene	2	118	340	69	[13a]

[a] V_{cavity} is the volume of the cavity in unit cell calculated using a 0.7 radius probe.

[b] PC_{cavity}=(molecular volume)×(number of guest molecule in unit cell)/V_{cavity}×100.

ropy, which corresponds to dynamic properties and selective reactions of guest components in the host cavities.

4. Conclusion

The systematic structural investigations of inclusion compounds of **CA** with a series of mono-substituted benzenes were described. The four host frameworks are acquired by change in the conformation of the side chain and the type of interdigitation between methyl groups. Each host framework can include a limited range of the guest compounds. Moreover, formation of the host-guest compounds, host-guest ratios, and the structures of the host frameworks depend mainly on the volumes of the guest components. This indicates that the spatial fit between the guest components and the host cavities play a primary role for guest inclusion in crystalline state, and that the guest compounds act as templates for the host frameworks.

In order to clarify the role of the guest volume to enclathration in crystalline state more precisely, packing coefficients of the host cavities of inclusion crystals of **CA** as well as other known host compounds were calculated. This is the first application of PC_{cavity} for lattice inclusion compounds. The values of PC_{cavity} are statistically distributed in the range of 55-70%, when the guest components are included in the host cavities by van der Waals interaction and steric complementation. The optimal PC_{cavity} should be required to form the stable inclusion crystals, because compounds out of this range give rise to isomerization or collapse the host frameworks. Moreover, PC_{cavity} was not dependent on the host compounds and the host frameworks. Calculations of the PC_{cavity} of the guest candidates help to predict the boundary of isomerization of the host framework and the host-guest ratio. Guest candidates should be carefully designed to have the appropriate packing coefficients in order to construct expected host frameworks.

On the other hand, importance of the guest components to construct the designed host frameworks has been recently recognized.[5] This means that guest compounds acts as template for host frameworks. The results support this idea and give us insight for designing guest components and establishing the desired host frameworks. Computer-aided molecular modeling enables us to calculate void volumes of the host cavity on the basis of the host frameworks designed from molecular structure. The spatial requirement of the volume of the guest components can be estimated from PC_{cavity} and the volumes of the designed host cavity. Therefore, the packing coefficient will be useful for designing and predicting host frameworks. This should become the first step for designing the organic host compounds directed specific guest recognitions.

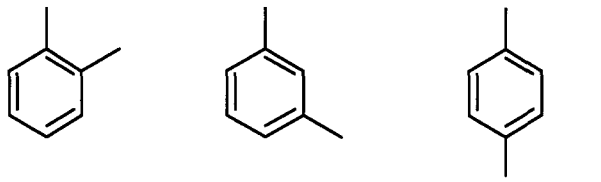
Finally, this work indicates that PC_{cavity} of the inclusion compound is intermediate between liquid state and solid state and that packing coefficients can be correlated with mobility and anisotropy of the included components. These results link molecular recognitions in solid state with that in solutions.

Chapter 3. Guest Shape Dependence of Cholic Acid Host Framework and Molecular Recognition

1. Introduction

Organic lattice inclusion compounds[1] are well known to exhibit high selectivity in guest recognitions.[2] Recently, constructing of open host frameworks by hydrogen bond networks have attracted much attention.[3] However, it is still hard to design host frameworks oriented specific guest molecules due to the following reasons. Firstly, there has been no general design of the reliable supramolecular building blocks in crystal engineering due to the complexity of non-covalent bonds. Secondly, most of host compounds have many open host frameworks whose cavities have different steric dimensions and chemical environments.[4] Thirdly, estimation and comparison of thermodynamic stability in crystalline state are still hard. This hinders us from designing the most suitable guest components for the host cavities. In order to overcome these difficulties, PC_{cavity} was introduced as a parameter for the stability of the lattice inclusion compounds.[5] As described in Chapter 2, PC_{cavity} of inclusion crystals of **CA** with aromatic compounds is in the range of 55% to 70%. In solution, Rebek Jr. and his coworker have already reported the correlation between stability constants and PC_{cavity} in the dimeric encapsulated host-guest compounds.[6] They concluded that stability constants largely decrease, when the *PC*cavity is lower or higher than the range of 55±9%. Therefore, it is of importance to clarify the correlation between PC_{cavity} and guest selectivity in lattice inclusion compounds.

In Chapter 2, the author described that volumes of the guest components played a crucial role for isomerizations of the host frameworks and host-guest ratios in **CA** inclusion crystals with monosubstituted benzenes.[5] The shapes of the guest molecules act as the secondary role for the host framework isomerizations, because the width of the host cavity is just suitable for a benzene ring. In order to clarify the role of the shapes of the guest components, the crystal structures of **CA** with xylenes (Chart 1) are investigated. In this chapter, crystal structures and PC_{cavity} of the inclusion crystals of **CA** with xylenes and the molecular recognitions by enclathration were described. Comparison of PC_{cavity} with guest selectivity indicates that PC_{cavity} is also useful for prediction and explanation of the guest recognitions in solid state host-guest compounds.



o-xylene (**62**) *m*-xylene (**63**) *p*-xylene (**64**)

Chart 1

2. Experimental

Preparation of inclusion crystals

The inclusion crystals of **CA** with **62** (Form I) were obtained by recrystallization using a solvent at room temperature. **CA** (100 mg) was dissolved with warming in 1-butanol (0.4 mL), and the xylene (2 mL) was added. The resulting solution was allowed to stand at room temperature. On the other hand, the recrystallization at 30 °C gave the inclusion crystals of **CA** with **62** (Form II). The inclusion crystals of **CA** with **63** or **64** were obtained by recrystallization in the presence of 1-butanol at room temperature. Competitive recrystallization from the mixture solution (host-guest ratio = 3:1, 2:1, 1:1, 1:2, 1:3, 1:4, 1:5) was also carried out in the similar way. **CA** (100 mg) was dissolved with warming in 1-butanol (0.4 mL), and the prescribed mixed solution (2 mL) of two guest compounds was added. The resulting feed solution was allowed to settle overnight at room temperature to attain crystallization equilibrium.

X-ray structural analysis

X-ray diffractions were collected by Rigaku RAXIS-CS imaging plate two-dimensional area detector using graphite-monochromatized Mo-*Kα* radiation (l=0.71070Å). All the crystallographic calculations were performed by using TEXSAN[7] software package of the Molecular Structure Corporation. Each crystal structure was solved by the direct methods (MULTAN, SHEXL97), and refined by the full-matrix least squares or SHEXL93.

All non-hydrogen atoms were refined anisotropically. Hydrogen atoms attached to carbon atoms were located in the calculated positions. The positions of hydrogen atoms attached to oxygen atoms were obtained from the difference Fourier syntheses. The crystal data of these crystals were shown in Tables 3-1 and 3-3.

Gas chromatography analysis

The obtained polycrystals of inclusion compounds **CA** with mixed xylenes (20 mg) were dissolved with methanol (0.4 mL) and the ratios of xylene isomers in the solution were analyzed by gas chromatography (GPC) using a Shimadzu GC-14A instrument equipped with a ULBON HR-20M capillary column.

Molecular graphics and calculations

Cross sections of host channels were depicted by using the MODRASTE.[8] The atomic radii of hydrogen, carbon, and oxygen in the cross-sectional views are 1.20Å, 1.60Å, and 1.45Å, respectively.

The volumes of the host cavities were calculated from the atomic coordinations by using Free Volume program[9] in Cerius^2 (version 4.0) software package.[10] The volumes of the **CA** cavities were calculated by a 0.7Å radius probe.[5,6] The atomic radii were adopted as following values: hydrogen=1.20Å, carbon=1.70Å, and oxygen=1.60Å.

3. Results and Discussion

Host-guest Complexes of CA with Xylenes

CA formed inclusion crystals with *m*-xylene (**63**) and *p*-xylene (**64**) at 1:1 host-guest ratios, while *o*-xylene (**62**) gave two polymorphs of the host-guest crystals at 2:1 host-guest stoichiometry. The crystal structures were characterized by X-ray structural analysis. The crystal data and packing diagrams are shown in Table 3-1 and Figure 3-1, respectively. The common structural feature is a bilayer structure, which consists of the alternative stacking of lipophilic layers and hydrophilic layers. In the hydrophilic layer, three hydroxy groups and one carboxylic acid group construct a 2D extended hydrogen bond network. In the lipophilic layer, two methyl groups on the steroidal β-face are interdigitated and a host cavity runs between the layers because of the anchored molecular structure of **CA**. Interestingly, the stacking mode of **CA•62** (Form I)[11a] is different from those of the others. The crystal of Form I has a parallel stacking in the lipophilic layer and an anti-parallel stacking in the hydrophilic layer, termed as *DCA* type, because this arrangement is identical to those of inclusion crystals of deoxycholic acid.[11b, 12] This result indicates that host arrangement is not inherent in a host molecular structure and can be changed by a guest compound. The other host frameworks have anti-parallel stacking both in the lipophilic layer and in the hydrophilic layer.

Table 3-1. Crystallographic Data of **CA** with xylenes.

Compound	**CA•62** (Form I)	**CA•62** (Form II)	**CA•63**	**CA•64**
Host:Guest	2:1	2:1	1:1	1:1
Formula	$C_{56}H_{90}O_{10}$	$C_{56}H_{90}O_{10}$	$C_{32}H_{50}O_5$	$C_{32}H_{50}O_5$
Formula weight	923.32	923.32	514.74	514.74
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P1$	$P2_1$	$P2_1$	$P2_1$
a [Å]	7.515(10)	12.331(3)	12.076(2)	13.584(2)
b [Å]	25.612(6)	7.9166(9)	8.165(1)	8.302(1)
c [Å]	13.827(9)	14.325(2)	15.973(5)	14.239(5)
β [deg]	90.99(8)	105.01(2)	109.25(2)	114.46(3)
V [Å^3]	2661(2)	1350.7(4)	1486.9(6)	1461.6(6)
Z	1	2	2	2
Dc [g/cm^3]	1.152	1.135	1.150	1.170
Number of unique reflections	5816	2762	2486	2568
Number of observed reflections	3796	2761	2485	2566
R_1,R_w	0.082/0.086	0.101/0.259[a]	0.090/0.243[a]	0.084/0.222[a]
GOF	4.53	2.01	1.21	1.20
2θmax [deg]	55	60.1	59.8	59.9
R/P	4.94	8.57	7.37	17.22
Temperature [°C]	25	-170	25	25
Host framework	*DCA*	α-*trans*	β-*trans*	α-*gauche*

[a] $wR_2 = [\Sigma w (F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$ (for all data)

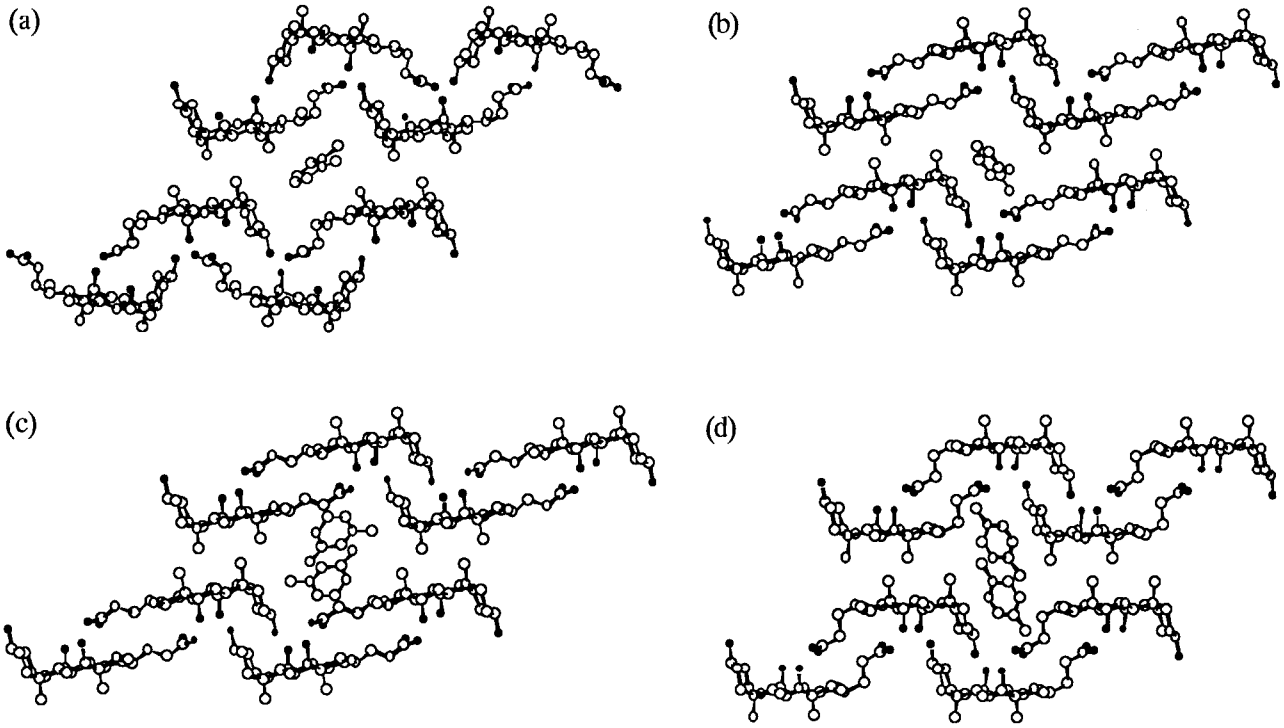


Figure 3-1. Molecular packing diagrams of **CA** with (a) **62** (Form I), (b) **62** (Form II), (c) **63**, and (d) **64**. The figures are viewed down along the crystallographic *b*-axis. In the case of **CA•62** (Form II), one of the two sites of the disordered guest molecules is omitted for clarity. The carbon and oxygen atoms are represented by open and filled circle, respectively. The hydrogen atoms are omitted for clarity.

The arrangments are characteristic for the host frameworks of **CA** inclusion crystals. They are finely classified into the four sub-groups described in Chapter 2.[11b] **CA•62** (Form II), **CA•63** and **CA•64** give α-*trans*, β-*trans*, and α-*gauche* type host frameworks, respectively.

Hydrogen bond networks are depicted in Figure 3-2. *DCA* type has the linear hydrogen bond networks involving two hydroxyl groups at OH (C3) and OH (C12), and the carboxylic acid along *c*-axis. This linear hydrogen bond connects one host molecule with four adjacent host molecules to yield a 2D sheet structure. The hydroxy group at 7 position weakly connects to the hydrogen bond network. The other host frameworks yield a cyclic hydrogen-bonding network involving in the sequence of OH (C3), OH (C7), OH (C12), OH (C24). This cyclic hydrogen bonding connects one host molecule with the surrounding twelve host molecules. All hydrogen bond donors and acceptors take part in the network to yield the robust structural motif.

Shape-Dependent Isomerizations of Host Framework

In order to estimate the size fit between host cavity and guest components, *PC*cavity of host-guest complex in **CA** crystals was calculated. Table 3-2 shows volumes of the host cavities for one guest molecule and PC_{cavity}. Among the four types of the host frameworks, the α-*gauche* type has the smallest volume and the highest PC_{cavity}. This indicates that the volume is the most suitable for xylenes. However, only **64** forms α-*gauche* type framework and the other isomers do other types. This indicates that the shape plays an important role for isomerization of the host frame-

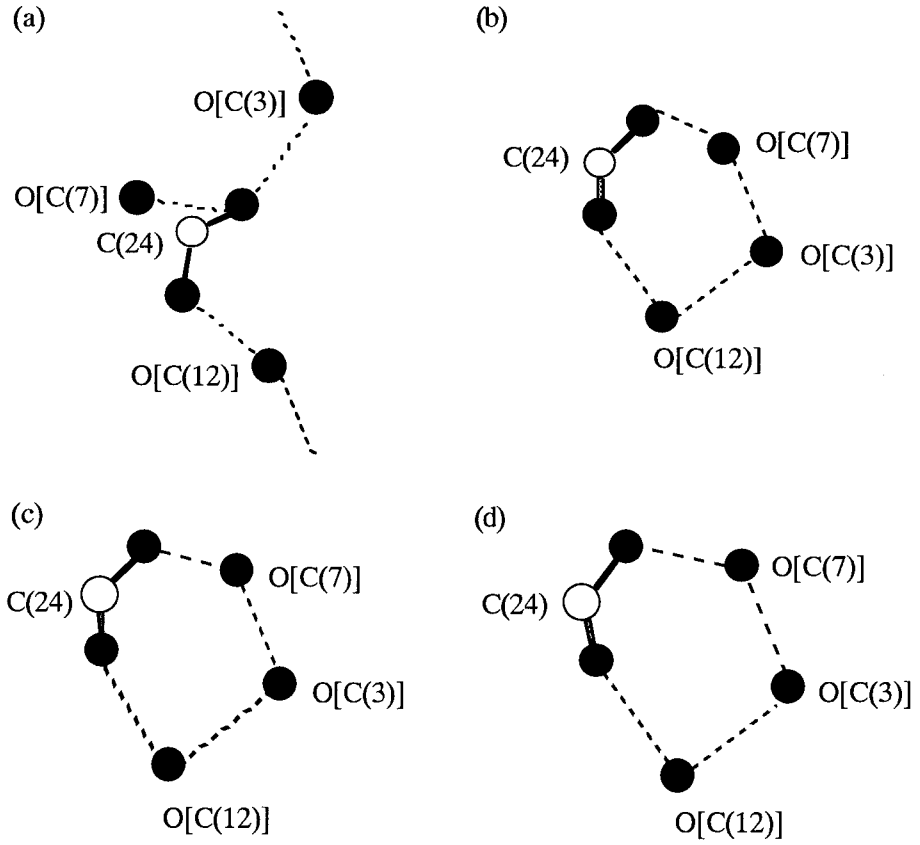


Figure 3-2. Hydrogen bond networks of **CA** with (a) **62** (Form I), (b) **62** (Form II), (c) **63**, and (d) **64**. The carbon and oxygen atoms are represented by open and filled circle, respectively.

Table 3-2. Molecular volumes, number of guest in a unit cell, cavity volumes of host cavity, PC_{cavity} and $PC_{crystal}$ for inclusion compounds of **CA** with xylenes.

Compound	Molecular volume [Å^3]	Number of guests in a unit cell	Volume of cavity[a] in a unit cell [Å^3]	Volume of cavity[a] per one guest molecule [Å^3]	PC_{cavity} [b] [%]	$PC_{crystal}$ [c] [%]
CA•62 (Form I)	118	2	497	248	47	70
CA•62 (Form II)	118	1	289	289	41	68
CA•63	118	2	408	204	58	71
CA•64	118	2	363	181	65	71

[a] Volumes of the cavity in unit cell calculated using a 0.7 radius probe.

[b] PC_{cavity} is a packing coefficient of the guest components in the host cavity, given as the following equation: PC_{cavity} [%]=(Molecular volume)×(Number of guests)/V_{cavity}×100.

[c] $PC_{crystal}$ is packing coefficient of the whole crystal.

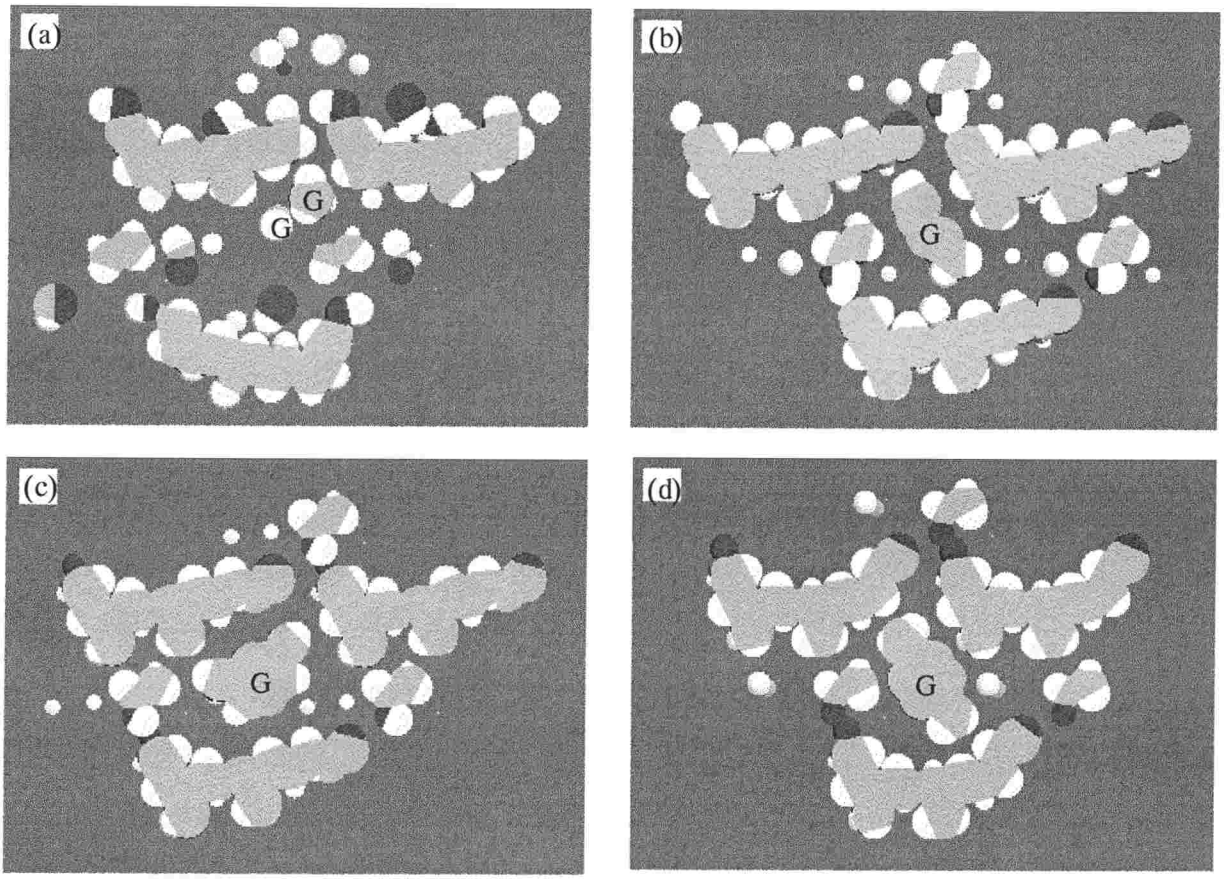


Figure 3-3. Cross sections of the host channels sliced perpendicular to the direction of the channel of **CA** with (a) **62** (Form I), (b) **62** (Form II), (c) **63**, and (d) **64**, respectively. The letter G stands for a guest molecule. In the case of **CA•62** (Form II), one of the two sites of the disordered guest molecules is shown for clarity. Carbon, hydrogen, and oxygen atoms are represented in gray, white, and black, respectively.

works. Figure 3-3 shows the cross-sectional views sliced perpendicular to the axis of the channel. The shapes of the isomers are longer and narrower in the order **64**, **63**, **62**. The ellipse cavity of α-*gauche* type just fit the shape of *p*-substituted benzenes, and the cavity would be too narrow for other isomers. The wider cavity of β-*trans* framework can incorporate **63** molecule, although the largest host cavity would be too narrow to accommodate **62**. Consequently, **62** cannot form the inclusion compounds with **CA** at a 1:1 host-guest ratio and gives *DCA* or α-*trans* type host framework having smaller host cavities at 2:1 host-guest ratios with reducing the number of the guest components in the unit cell in spite of the low packing coefficient. These results indicate that steric fitness of shape and volume between the guest molecule and host cavity play an important role for the selection of host framework types by guest molecules.

Polymorphism of CA•62 Clathrates

It is noteworthy that **CA•62** exhibits polymorphism dependent on the incubation temperatures. Polymorphism of organic crystals by changing recrystallization conditions has been well documented and has attracted attention, because chemical and physical properties depend on the crystal structures.[13] However, a few examples have been reported for inclusion compounds with identical host-guest combinations and identical host-guest ratios.[4d,11c,11d] Recrystallization at

25° C gave *DCA* type crystals, while α-*trans* type crystals were formed at higher temperature above 30° C. Both polymorphs have low *PC*cavity indicating no good steric fitness between the guest molecule and host cavity. On the other hand, *DCA* type crystal (PC_{cavity} = 47.4%) has better steric fitness than α-*trans* type (PC_{cavity} = 40.8%), though the host framework is uncommon due to the partially weak hydrogen bond. These facts suggest that the balance between steric fitness and the other factors involving hydrogen bonds lead free energy differences among the polymorphs to be quite small.

Competitive Recrystallization from Mixed Xylenes

Competitive recrystallization using equimolar mixtures of xylenes exhibits characteristic molecular recognition. Recrystallization from 1:1 mixtures of **62** and **63**, or **62** and **64** exclusively afforded **CA•63** or **CA•64**, respectively. On the other hand, recrystallization from 1:1 mixture of **63** and **64** yielded a crystal that included both guest components at the similar guest ratio to the bulk mixtures. A 1:1:1 mixture of all isomers also yielded 1:1 mixture of **63** and **64**. The selectivity seems to be dependent on the host frameworks and combinations of the guest components. The structures of inclusion crystals from mixed xylenes were systematically investigated.

Crystal Structures from Mixed Xylenes

Crystallographic data of the inclusion crystals from xylene mixtures are shown in Table 3-3. A 1:1 mixture of **62** and **63** yielded inclusion crystals with β-*trans* type host framework, and that of **62** and **64** did α-*gauche*. These frameworks are identical to those from the corresponding pure xylenes and are in a good agreement to the results of the competitive recrystallization. Namely, **62** acts as a solvent and is not included in **CA** at all.

In contrast to competitive recrystallization with **62**, inclusion crystals from a 1:1 mixture of **63** and **64**, and a 1:1:1 mixture of all isomers afforded only β-*trans* type frameworks that were formed from neat **63**. Both **63** and **64** were included in the β-*trans* type at the similar 1:1 guest ratio. These results indicate that the larger host cavity of β-*trans* type enables to incorporate both isomers. The structures of the single crystals from the mixtures of **63** and **64** at various ratios (= 3:1, 2:1, 1:1, 1:2, 1:3, 1:4, 1:5) were revealed. They all gave the β-*trans* type host frameworks irrespective of the starting isomer ratios. In order to confirm the disorder of guest molecules in the single crystals, the difference Fourier (F_o-F_c) map without guest components was calculated. Electron densities around methyl group of xylene isomers are broad so that both of **63** and **64** are included in the inclusion cavity at random. Models of **63** and **64** in difference Fourier map can be located, as shown in Figure 3-4. Further calculations including refinement of the population improve *R* factors in a great deal. This indicates that xylenes in the host cavity exhibit the location static disorder. The ratios between **63** and **64** in single crystals can be determined by refinement of the populations of both sites by X-ray structural analyses. Figure 3-5 illustrates the plots of the guest ratios in single crystals against the feed ratios as well as those in bulk crystals determined by

Table 3-3. Crystallographic data of **CA** with mixed xylenes.

Guest mixture	**62+63**	**62+64**	**63+64**	**63+64**	**63+64**
Mixed ratio	1:1	1:1	3:1	2:1	1:1
Formula	$C_{32}H_{50}O_5$	$C_{32}H_{50}O_5$	$C_{32}H_{50}O_5$	$C_{32}H_{50}O_5$	$C_{32}H_{50}O_5$
Formula weight	514.74	514.74	514.74	514.74	514.74
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1$	$P2_1$	$P2_1$	$P2_1$	$P2_1$
a [Å]	12.096(2)	13.581(3)	12.013(3)	11.987(3)	11.964(4)
b [Å]	8.170(3)	8.304(5)	8.173(6)	8.173(3)	8.178(5)
c [Å]	15.968(2)	14.184(3)	16.025(3)	16.076(3)	16.131(3)
β [deg]	109.51(1)	114.25(2)	109.47(2)	109.68(1)	109.86(2)
V [Å^3]	1487.4(6)	1458.5(9)	1483.4(10)	1483.0(7)	1484.4(9)
Z	2	2	2	2	2
Dc [g/cm^3]	1.149	1.172	1.152	1.153	1.152
Number of unique reflections	3664	3589	3660	3832	3658
Number of observed reflections	1647	990	1777	3665	2166
R_1,R_w	0.082/0.090[a]	0.106/0.375[a]	0.083/0.238[a]	0.064/0.196[a]	0.078/0.427[a]
GOF	1.57	1.386	1.05	1.04	0.93
2θmax [deg]	55.0	55.0	55.0	55.0	55.0
R/P	4.29	2.96	9.71	5.73	5.64
Temperature [°C]	23.0	23.0	23.0	23.0	23.0
Host framework	β-*trans*	α-*gauche*	β-*trans*	β-*trans*	β-*trans*

Guest mixture	**63+64**	**63+64**	**63+64**	**63+64**	**62+63+64**
Mixed ratio	1:2	1:3	1:4	1:5	1:1:1
Formula	$C_{32}H_{50}O_5$	$C_{32}H_{50}O_5$	$C_{32}H_{50}O_5$	$C_{32}H_{50}O_5$	$C_{32}H_{50}O_5$
Formula weight	514.74	514.74	514.74	514.74	514.74
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1$	$P2_1$	$P2_1$	$P2_1$	$P2_1$
a [Å]	11.928(10)	11.935(4)	11.932(4)	11.919(4)	11.92(1)
b [Å]	8.177(2)	8.282(5)	8.182(3)	8.186(5)	8.160(2)
c [Å]	16.127(4)	16.175(4)	16.178(3)	16.177(3)	16.082(4)
β [deg]	109.63(6)	109.95	109.97(2)	109.96(6)	109.56(6)
V [Å^3]	1481(1)	1484(1)	1484.3(7)	1483.6(9)	1474(1)
Z	2	2	2	2	2
Dc [g/cm^3]	1.154	1.152	1.152	1.152	1.152
Number of unique reflections	3623	3659	3660	3658	3755
Number of observed reflections	3614	1436	2428	2516	3754
R_1,R_w	0.051/0.141[a]	0.075/0.236[a]	0.072/0.236[a]	0.071/0.267[a]	0.047/0.139[a]
GOF	1.03	0.96	1.09	1.05	0.97
2θmax [deg]	59.9	55.0	55.0	55.0	60.1
R/P	8.86	3.50	5.95	6.17	9.20
Temperature [°C]	23.0	23.0	23.0	23.0	25.0
Host framework	β-*trans*	β-*trans*	β-*trans*	β-*trans*	β-*trans*

[a] $wR_2 = [\Sigma w (F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$ (for all data)

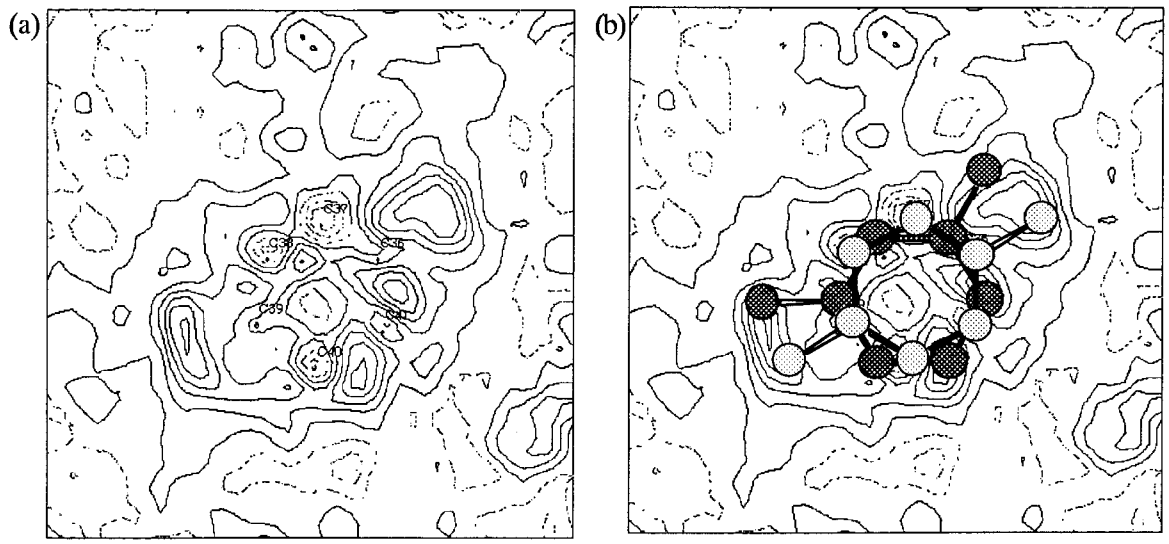


Figure 3-4. (a) Difference Fourier (F_O-F_C) map without guest components in the host cavity of **CA•63+64** (1:1), (b) Models of **63** and **64** applied in the difference Fourier map of the host cavity of **CA•63+64** (1:1). The filled and shadowed circles represent **63** and **64**, respectively.

chromatography. It is noteworthy that the guest ratios in the single crystals are in a good agreement to those in the bulk crystals and the mixed ratios. **CA** includes **64** a little bit superior to **63**, but both components are included in **CA** host lattice simultaneously. This indicates that **CA** cannot recognize **63** or **64** from their mixtures.

***PC*cavity and Guest Selectivity**

Competitive experiments are useful methods to estimate the relative stability of the host guest complexes in solution. However, there have been little attentions to estimate the order of the stability of inclusion crystals from competitive recrystallization.

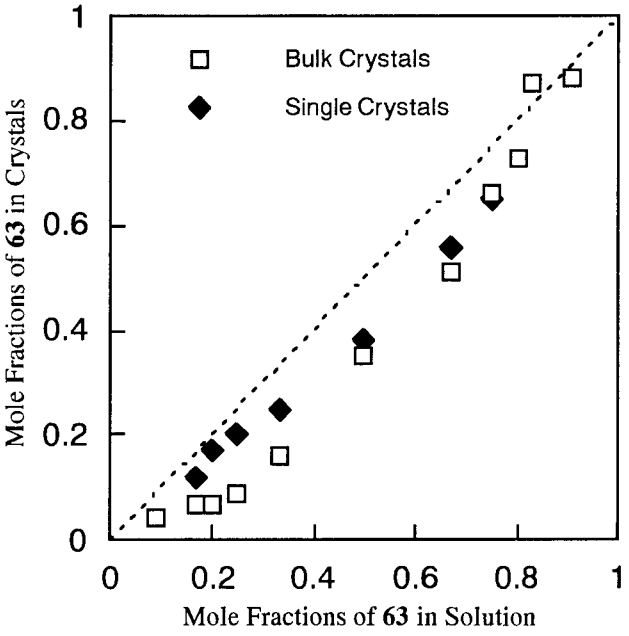


Figure 3-5. Mole fractions of **63** in the single crystals and in the bulk crystals are plotted against those of the starting mixed solvents of **63** and **64**.

Moreover, most of the structural studies have been devoted to the crystal structures of selective recognition from mixed guest components[3] or from pure guest compounds[1]. Less attention has been paid for the host compounds that exhibit non or less selective enclathrations. Our competitive experiments indicate that relative stability between **63** clathrate and **64** clathrate is small and that these two complexes are much more stable than **62**. The order of the stability of the inclusion crystals is in a good agreement to that expected from PC_{cavity} of the individual inclusion crystals. These results indicate that PC_{cavity} is a useful parameter to estimate stability of the host-guest crys-

tals and give explanations for guest recognitions in solid state.

Host Frameworks from Mixed Guests and Mechanism of Non-selective Inclusions.

The non-selective inclusion of **63-64** mixtures is explained by two presumable mechanisms. One is mixed inclusion crystals of **64** in the α-*gauche* type and **63** in the β-*trans* type, and the other is a formation of a unique host framework, α-*gauche*, β-*trans* or another host framework, including both guest components. Since the host frameworks of the **63-64** mixtures belong to all β-*trans* type, and the guest compounds are static disordered in the host cavities, this non-selective enclathration is attributed to the mechanism of solid solution. Consequently, recrystallization of **CA** from the mixtures of **63** and **64** affords the pseudo-diastereomeric solid solution, that is, "clathrate" solid solution crystals. This leads to low efficiency of the guest recognitions.

Difference of the size of the host cavities between these two host frameworks give an explanation for formation of the "clathrate" solid solution. The host cavity of the β-*trans* type has enough size and shape to accommodate both **63** and **64**, and α-*gauche* can only **64**. In addition, the stability difference between **63** in β-*trans* and **64** in α-*gauche* would be small, because their *PC*cavity are in appropriate range. Therefore, the formation of the clathrate solid solution in β-*trans* type is favorable to that of the selective formations of **64** or **63** complexes, because the former is expected to be more stable than the latter due to the term of mixing entropy.

4. Conclusion

The inclusion phenomena and crystal structures of **CA** with xylene isomers were demonstrated. The host frameworks and host-guest stoichiometries depend on shapes of the incorporated isomers. All xylenes are accommodated in the different host frameworks. Interestingly, **CA** forms two types of **CA•62** at the same host-guest stoichiometry by changing the incubation temperatures. The details of the polymorphism of the inclusion crystals are described in next chapter.

Competitive recrystallization from mixed xylenes revealed that **CA** exhibits selective and non-selective inclusion phenomena toward xylenes. The drastic change of the guest selectivities is consistent to difference of the stability estimated from PC_{cavity} of the individual host-guest crystals. Moreover, in the non-selective enclathrations, X-ray diffraction studies revealed that the ratios of the guest components of the recrystallization mixtures are quite similar to those both in the single crystals and in the bulk crystals. This indicates that non-selective inclusions are attributed to formation of "clathrate" solid solution crystals of the guest mixtures, not to that of mixtures of the individual inclusion crystals. This would be the first report that pointed out the similarity between the guest recognition by enclathration and chiral recognitions by the diastereomer salt formations. Molecular recognitions by using the crystalline state may have the same mechanisms and that PC_{cavity} must be one of the useful parameters to estimate stability of the host-guest crystals and give explanations for guest recognitions in solid state.

Chapter 4. Polymorphism of Cholic Acid Host Frameworks and Inclusion Crystals

1. Introduction

Isomerization of host frameworks is observed in many hosts and are substantial properties of organic host compounds because their host lattices are maintained by noncovalent bonds.[1] In many cases, the guest molecules induce subtle change in the structure and dimensions of a host framework with the retention of the general architecture.[2-4] On the other hand, some host compounds can form completely different host frameworks with dimensionally different cavities.[5] In every case, it is empirically known that host framework isomerizations are mainly attributed to the size fitting between a host cavity and guest molecule, as shown in Figure 4-1.

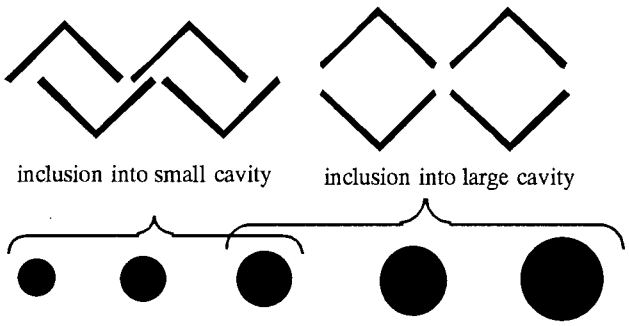


Figure 4-1. Schematic representation of incorporation of small and large molecules into small and large cavities.

In Chapter 2, the author clarified that the relationship between the **CA** host framework isomerizations of bilayer structures and included guest volumes using the parameter of PC_{cavity}. Moreover, the author also revealed that PC_{cavity} could explain the guest recognitions *via* selective enclathration in **CA** cavities of bilayer structures in Chapter 3. These facts lead to the idea that PC_{cavity} can be extensively applied not only to bilayer structure but also to another structures. **CA** can form not only a bilayer structure with a channel cavity but also a crossing structure with a cage-like cavity for smaller molecules.[6] Figure 4-2 shows the schematic representation of the two structures. The former framework is commonly maintained by cyclic hydrogen bond network, while the

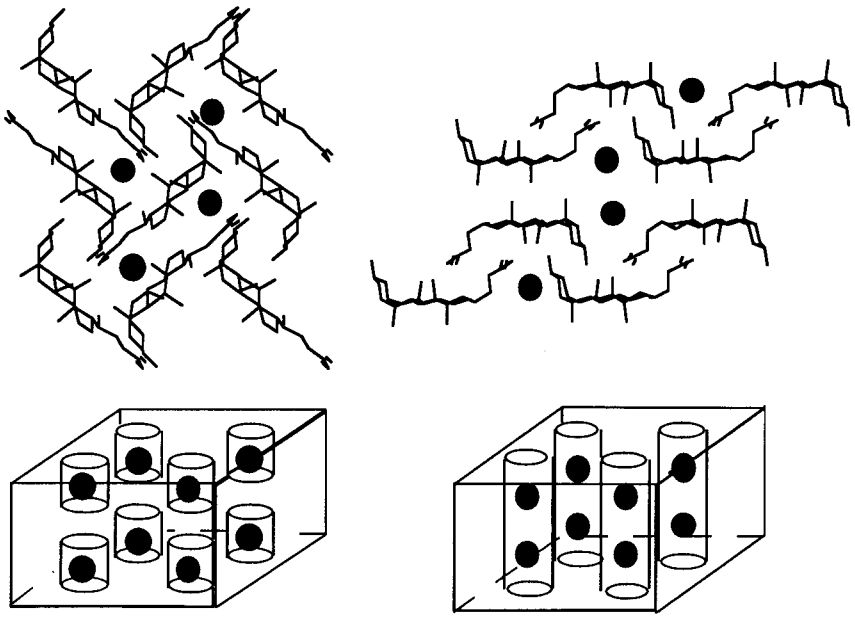


Figure 4-2. Schematic representation of (a) a crossing structure and (b) a bilayer structure.

R–CO_2H

65: R=H
66: R=CH_3
67: R=CH=CH_2
68: R=CH_2CH_3
69: R=C(CH_3)=CH_2
70: R=$(CH_2)_2CH_3$
71: R=$CH(CH_3)_2$
72: R=CH_3CH=$CHCH_2$
73: R=R=CH_3CH_2CH=CH
74: R=$(CH_2)_3CH_3$
75: R=$(CH_2)_4CH_3$

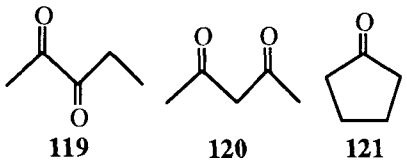
R–OH

76: R=CH_3
77: R=C≡CH
78: R=CH_2CH_3
79: R=$(CH_2)_2OH$
80: R=$CH(CH_3)_2$
81: R=$(CH_2)_2CH_3$
82: R=CH_2CHCH_2O

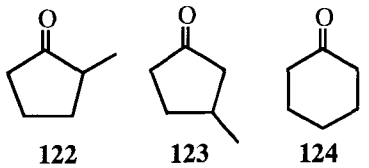
83: R=$(CH_2)_3CH_3$
84: R=$CH_2CH(CH_3)CH_3$
85: R=$CH(CH_3)CH_2CH_3$
86: R=$C(CH_3)_3$
87: R=$C(CH_3)_2CH_2CH_3$
88: R=$CH(CH_3)CH(CH_3)_2$
89: R=$CH_2C(CH_3)_3$
90: R=$(CH_2)_4CH_3$
91: R=$CH(CH_3)(CH_2)_3CH_3$
92: R=$(CH_2)_2CH(CH_3)_2$
93: R=$CH(CH_2CH_3)_2$
94: R=$CH_2CH(CH_3)CH_2CH_3$
95: R=C_6H_{11}
96: R=$C(CH_3)_2(CH_2)_2CH_3$
97: R=$CH(CH_3)CH(CH_3)CH_2CH_3$
98: R=$C(CH_3)(CH_2CH_3)_2$
99: R=$C(CH_3)_2CH(CH_3)_2$
100: R=$CH(CH_3)C(CH_3)_3$
101: R=$CH(CH_3)CH_2CH(CH_3)_2$
102: R=$CH(CH_3)(CH_2)_3CH_3$
103: R=$CH(CH_2CH_3)(CH_2CH_2CH_3)$
104: R=$CH_2CH(CH_2CH_3)_2$
105: R=$(CH_2)_3CH(CH_3)_2$
106: R=$(CH_2)_5CH_3$
107: R=$CH(CH_2CH_3)CH(CH_3)_2$
108: R=$(CH_2)_2CH(CH_3)CH_2CH_3$
109: R=$CH_2CH(CH_3)(CH_2)_2CH_3$

R–C(=O)–R'

110: R=CH_3 R'=CH_3
111: R=CH_3 R'=CH_2CH_3
112: R=H R'=$(CH_2)_3CH_3$
113: R=CH_2CH_3 R'=CH_2CH_3
114: R=CH_3 R'=$CH(CH_3)_2$
115: R=CH_3 R'=$(CH_2)_2CH_3$
116: R=CH_3 R'=$CH_2CH(CH_3)_2$
117: R=CH_2CH_3 R'=$(CH_2)_2CH_3$
118: R=CH_3 R'=$(CH_2)_3CH_3$



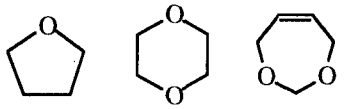
119 **120** **121**



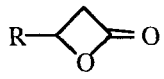
122 **123** **124**

R–O–R'

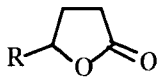
125: R=CH=CH_2 R'=CH_2CH_3
126: R=CH_2CH_3 R'=CH_2CH_3
127: R=CH_2CH=CH_2 R'=CH_2CH=CH_2
128: R=CH=CH_2 R'=$(CH_2)_3CH_3$
129: R=$(CH_2)_2CH_3$ R'=$(CH_2)_2CH_3$
130: R=$CH(CH_3)_2$ R'=$CH(CH_3)_2$



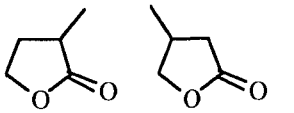
131 **132** **133**



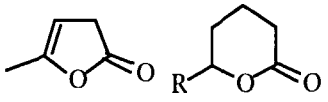
134: R=H
135: R=CH_3
136: R=CH_2CH_3
137: R=$(CH_2)_2CH_3$



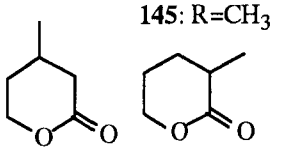
138: R=H
139: R=CH_3
140: R=CH_2CH_3



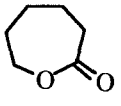
141 **142**



143 **144**: R=H **145**: R=CH_3



146 **147**



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R–C≡N

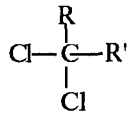
184: R=CH_3
185: R=CH=CH_2
186: R=CH_2CH_3
187: R=C(CH_3)=CH_2
188: R=CH_2CH=CH_2
189: R=CH=CH_2CH_3
190: R=$CH(CH_3)_2$
191: R=$(CH_2)_2CH_3$
192: R=$C(CH_3)_3$
193: R=$CH_2CH(CH_3)_2$
194: R=$(CH_2)_3CH_3$
195: R=$(CH_2)_4CH_3$

R–NO_2

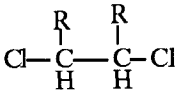
196: R=CH_3
197: R=CH_2CH_3
198: R=$(CH_2)_2CH_3$
199: R=$CH(CH_3)_2$

R–CO_2R'

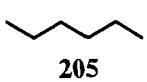
149: R=H R'=CH_3
150: R=CH_3 R'=CH_3
151: R=H R'=CH_2CH_3
152: R=CH_3 R'=CH=CH_2
153: R=CH_2=CH R'=CH_3
154: R=H R'=$CH(CH_3)_2$
155: R=CH_3 R'=CH_2CH_3
156: R=CH_2CH_3 R'=CH_3
157: R=H R'=$(CH_2)_2CH_3$
158: R=CH_2=CH R'=CH_2=CH
159: R=CH_3 R'=CH_2CH=CH_2
160: R=CH_3 R'=C(CH_3)=CH_2
161: R=CH=$CHCH_3$ R'=CH_3
162: R=CH_2=CH R'=CH_2CH_3
163: R=C(CH_3)=CH_2 R'=CH_3
164: R=CH_3 R'=$CH(CH_3)_2$
165: R=CH_2CH_3 R'=CH_2CH_3
166: R=CH_2CH_3 R'=CH_3
167: R=H R'=$(CH_2)_3CH_3$
168: R=H R'=$CH_2CH(CH_3)_2$
169: R=CH=$CHCH_3$ R'=CH=CH_2
170: R=CH_3 R'=$(CH_2)_2CH_3$
171: R=$(CH_2)_2CH_3$ R'=CH=CH_2
172: R=C(CH_3)=CH_2 R'=CH_2CH_3
173: R=CH=$CHCH_3$ R'=CH_2CH_3
174: R=CH_2CH_3 R'=$(CH_2)_2CH_3$
175: R=CH_2CH_3 R'=$CH(CH_3)_2$
176: R=$(CH_2)_2CH_3$ R'=CH_2CH_3
177: R=CH_3 R'=$(CH_2)_3CH_3$
178: R=CH_3 R'=$CH(CH_3)CH_2CH_3$
179: R=CH_3 R'=$C(CH_3)_3$
180: R=CH_3 R'=$CH_2CH(CH_3)_2$
181: R=$(CH_2)_3CH_3$ R'=CH_3
182: R=H R'=$(CH_2)_2CH(CH_3)_2$
183: R=H R'=$(CH_2)_4CH_3$



200: R=H R'=H
201: R=H R'=Cl
202: R=Cl R'=Cl



203: R=H
204: R=Cl



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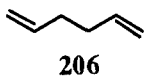

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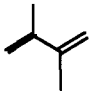

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208

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Chart 1

latter framework by spiral one. In order to clarify the guest-dependent isomerizations of the two host frameworks, we systematically investigated the host frameworks of **CA** in a series of the aliphatic molecules having C6 or less as guest (Chart 1).

Furthermore, the systematic investigation enables us to find a rare example of two-component polymorphism of inclusion crystals. Polymorphism is an important phenomenon to solid state chemistry because chemical and physical properties are dependent on polymorphs.[7] Commonly, polymorphism is divided into two types; (i) packing the same molecules into different arrangements or (ii) packing conformational isomers into similar or different arrangements, named as conformational polymorphism.[8-10] Most studies of polymorphism have been applied for one-component system. More recently, polymorphism of inclusion compounds has been reported only to an inclusion compound of urea.[11] Urea yielded two types of the inclusion crystals that have the same host-guest combinations and host-guest ratios. In the crystal structure, the host and guest have the same conformations but different molecular arrangements. This indicates that they are classified as the former type polymorphism of two-component system. Table 4-1 summaries classification of polymorphs in organic compounds. In this chapter, the formation of both types of two-component polymorphs in **CA** crystals are described. Furthermore, the selective preparation of a polymorph and the mechanism of the formation are revealed.

Table 1 Polymorphism on organic crystals.

	(i)	(ii)
one-component	known[7]	known[8-10]
two-component	ura[11], **CA**	**CA**

2. Experimental

General Methods

All chemicals and solvents were commercially available and used without any purification. Infrared spectra were recorded on a JASCO IR-Report-100 or JASCO IR-810 spectrometer. Differential scanning calorimetry (DSC), and thermal gravimetry (TG), were performed on a Rigaku TAS100 system; ca.10 mg from 40 to 230°C at a heating rate of 5°Cmin^{-1}. X-ray powder diffraction (XRD) patterns were measured by using Rigaku RINT-1100 at room temperature.

Preparation of Inclusion Crystals

Method A **CA** (100 mg) was dissolved with warming in the liquid guest (usually 2-3 mL), and the resulting solution allowed to stand to room temperature. The needle-like crystals were collected and dried on the filter papers.

Method B If **CA** was insufficiently soluble in the liquid guest, 1-butanol is used as solvent: **CA** (100 mg) was dissolved with warming in the 1-butanol (0.4 mL), and the liquid guest (usually 1-2 mL) was poured into the resulting solution. The crystals were isolated in the same manner as in Method A.

Method C In the case of the liquid guests, **65** and **79**, cyclohexane or isopentyl acetate was used as solvent due to high solubility of **CA** in the guests: **CA** (500 mg) was dissolved with warming in the guest (0.5 mL), and the solvent (usually 1-2 mL) was poured into the resulting solution. The crystals were isolated in the same manner as in Method A.

Method D In the case of the liquid guest **196**, 1-butanol and isopentyl acetate was used as solvent because the guest, if Method B was applied due to low solubility of **CA** in the guest, is immiscible with 1-butanol: **CA** (100 mg) was dissolved with warming in the 1-butanol (0.4 mL), and isopentyl acetate (0.1-0.2 mL) and the liquid guest (0.1-0.5 mL) were poured into the resulting solution. The crystals were isolated in the same manner as in Method A.

Crystal Structure Determinations

X-ray diffraction data were collected on a Rigaku AFC-7R four-circle diffractometer or a RAXIS-IV diffractometer with a two-dimensional area detector with graphite-monochromatized Mo-Kα radiation. Lattice parameters were obtained by least-squares analysis of 25 reflections measured in the range $20 < 2\theta < 25$ in the four-circle diffractometer and reflections for 3 oscillation images in the area detector. Direct methods (SHELEX86 or SIR92) were used for the structure solution. The structure was refined by the full matrix least-squares procedure with the program TEXSAN.[12] All non-hydrogen atoms were refined with anisotropic displacement parameters and hydrogen atoms of the host molecule were placed in idealized positions and refined as riding atoms with the relative isotropic displacement parameters. Hydrogen atoms of the guest molecule were placed in idealized positions and not refined. All calculations were performed using the TEXSAN crystallographic software package.[12] The condition of measurement and structural details are listed Table IV-1 (Appendix).

Molecular Graphics and Calculations

Molecular graphics study was carried out by with the computer software based on MODRASTE.[13] The atomic radii of hydrogen, carbon, and oxygen in the cross-sectional views are fixed at 1.20Å, 1.60Å, and 1.45Å, respectively. The volumes of the host cavities were calculated from the atomic coordinations with the program Free Volume[14] in the software package Cerius^2 (version 4.0).[15] The following values were used for the atomic radii: hydrogen=1.20Å, carbon=1.70Å, nitrogen=1.65Å, oxygen=1.60Å, chlorine=1.75Å.

3. Results and Discussion

Formation of Inclusion Compounds

CA forms inclusion compounds with approximately one hundred organic substances having C6 or less. Table 4-2 summarizes the incorporated guest compounds, corresponding host-guest ratios, molecular volumes, and types of host frameworks discussed later. The organic compounds that give guest-free crystals are listed in Table 4-3 with corresponding molecular volumes. Follow-

Table 4-2. Host-guest ratios,molecular volumes and host structures of inclusion compounds of **CA**.

Guest	Host-guest ratio	Molecular volume [Å^3]	Host framework
carboxylic acid			
formic acid(**65**)	1:1	43	crossing
acetic acid(**66**)	1:1, 1:2	60	crossing, bilayer
acryic acid(**67**)	1:1	70	crossing
propionic acid(**68**)	1:1	77	crossing
methacryic acid(**69**)	1:1	88	bilayer
isobutylic acid(**71**)	1:1	94	bilayer
3-pentenoic acid(**72**)	1:1	104	bilayer
alchohol			
methanol(**76**)	1:1	39	crossing
propargyl alcohol(**77**)	1:1	55	crossing
ethanol(**78**)	1:1	56	crossing
ethyleneglycol(**79**)	1:1	66	crossing
2-propanol(**80**)	1:1	73	monolayer
1-propanol(**81**)	1:1	73	crossing
glycidol(**82**)	1:1	76	crossing
1-pentanol(**90**)	1:1	108	bilayer
1-hexanol(**106**)	1:1	126	bilayer
ketone			
acetone(**110**)	1:1	66	bilayer
2-butanone(**111**)	1:1	84	bilayer
n-butylaldehyde(**112**)	1:1	84	bilayer
3-pentanone(**113**)	1:1	101	bilayer
3-methyl-2-butanone(**114**)	1:1	101	bilayer
2-pentanone(**115**)	1:1	101	bilayer
2,4-pentadione(**120**)	1:1	103	bilayer
3-methylcyclopentanone(**123**)	1:1	107	bilayer
cyclohexanone(**124**)	1:1	107	bilayer
4-methyl-2-pentanone(**116**)	1:1	118	bilayer
3-hexanone(**117**)	1:1	118	bilayer
2-hexanone(**118**)	1:1	119	bilayer
ether			
ethyl vinyl ether(**125**)	1:1	84	bilayer
diethyl ether(**126**)	1:1	91	bilayer
4,7-dihydro-1,3-dioxepin(**133**)	1:1	98	bilayer
diallyl ether(**127**)	1:1	110	bilayer
n-butyl vinyl ether(**128**)	1:1	119	bilayer
n-propylether(**129**)	1:1	126	bilayer
isopropylether(**130**)	1:1	126	bilayer

Table 4-2. Host-guest ratios,molecular volumes and host structures of inclusion compounds of CA. (Continued)

Guest	Host-guest ratio	Molecular volume [Å^3]	Host framework
lactone			
α-angelicalactone(**143**)	1:1	85	bilayer
β-butyrolactone(**135**)	1:1	85	bilayer
γ-valerolactone(**139**)	1:1	100	bilayer
δ-valerolactone(**144**)	1:1	101	bilayer
α-methyl-γ-butyrolactone(**141**)	1:1	101	bilayer
β-methyl-γ-butyrolactone(**142**)	1:1	101	bilayer
β-valerolactone(**136**)	1:1	102	bilayer
β-hexalactone(**137**)	1:1	110	bilayer
β-methyl-γ-valerolactone(**146**)	1:1	111	bilayer
ε-hexalactone(**148**)	1:1	118	bilayer
δ-hexalactone(**145**)	1:1	118	bilayer
γ-hexalactone(**140**)	1:1	119	bilayer
ester			
methyl formate(**149**)	1:1	60	bilayer
methyl acetate(**150**)	1:1	77	bilayer
ethy formate(**151**)	1:1	77	bilayer
vinly acetate(**152**)	1:1	88	bilayer
methy acrylate(**153**)	1:1	88	bilayer
isopropyl formate(**154**)	1:1	94	bilayer
ethyl acetate(**155**)	1:1	94	bilayer
methyl propionate(**156**)	1:1	95	bilayer
n-propyl formate(**157**)	1:1	95	bilayer
vinly acrylate(**158**)	1:1	99	bilayer
allyl acetate(**159**)	1:1	104	bilayer
isopropenyl acetate(**160**)	1:1	104	bilayer
methyl crotonate(**161**)	1:1	104	bilayer
ethyl acryrate(**162**)	1:1	105	bilayer
methyl methacryrate(**163**)	1:1	105	bilayer
isopropyl acetate(**164**)	1:1	111	bilayer
ethyl propionate(**165**)	1:1	112	bilayer
methyl butylate(**166**)	1:1	112	bilayer
n-butyl formate(**167**)	1:1	112	bilayer
isobutyl formate(**168**)	1:1	112	bilayer
vinylcrotonate(**169**)	1:1	116	bilayer
n-propyl acetate(**170**)	1:1	117	bilayer
vinyl butyrate(**171**)	1:1	122	bilayer
ethyl methacrylate(**172**)	1:1	122	bilayer
n-propyl propionate(**174**)	1:1	128	bilayer

Table 4-2. Host-guest ratios,molecular volumes and host structures of inclusion compounds of **CA**. (Continued)

Guest	Host-guest ratio	Molecular volume [Å^3]	Host framework
isopropyl propionate(**175**)	1:1	129	bilayer
ethyl butyrate(**176**)	1:1	129	bilayer
n-butyl acetate(**177**)	1:1	129	bilayer
isopentyl formate(**182**)	1:1	130	bilayer
n-pentyl formate(**183**)	1:1	130	bilayer
nitrile			
acetonitrile(**184**)	1:1	48	bilayer
acryronitrile(**185**)	1:1	57	crossing, bilayer
propionitrile(**186**)	1:1	65	crossing
methacrylonitrile(**187**)	1:1	74	crossing, bilayer
allyl cianide(**188**)	1:1	74	bilayer
crotononitrile(**189**)	1:1	74	bilayer
isobutyronitrile(**190**)	1:1	82	bilayer
n-butyronitrile(**191**)	1:1	83	bilayer
nitro			
nitromethane(**196**)	1:1	56	crossing, bilayer
nitroethane(**197**)	1:1	73	bilayer
1-nitropropane(**198**)	1:1	90	bilayer
2-nitropropane(**199**)	1:1	90	bilayer
halide			
dichloromethane(**200**)	1:1	57	bilayer
chloroform(**201**)	1:1	70	bilayer
1,2-dichloroethane(**202**)	1:1	74	bilayer
carbontetrachloride(**203**)	1:1	84	bilayer
1,1,2,2-tetrachloroethane(**204**)	1:1	102	bilayer
hydrocarbon			
cyclohexene(**208**)	1:1	96	bilayer
1,5-hexadiene(**206**)	1:1	100	bilayer
2,3-dimethyl-1,3-butadiene(**207**)	1:1	101	bilayer
cyclohexane(**209**)	1:1	104	bilayer

ing points are remarkable to the inclusion ability of **CA**. (1) **CA** forms inclusion compounds with a variety of organic compounds, such as carboxylic acids (**65-72**), alcohols (**76-82, 90, 106**), ketones (**110-118, 120, 123, 124**), ethers (**125-130, 133**), lactone (**135-137, 139-146, 148**), esters (**149-172, 174-177, 182, 183**), nitriles (**184-191**), nitro (**196-199**), halides (**200-204**), and hydrocarbons (**206-209**). (2) Organic compounds having 38-130Å^3 can give inclusion compounds, while compounds having more than 90Å^3, especially alcohols, often give guest-free crystals as well. (3)

Table 4-3. Molecular volumes of solvents for guest-free crystals of **CA**.

Guest	Molecular Volume [Å^3]	Guest	Molecular Volume [Å^3]
carboxylic acid		2-methyl-3-pentanol(**107**)	126
butanoic acid(**70**)	94	3-methyl-1-pentanol(**108**)	126
2-pentenoic acid(**73**)	105	2-methyl-1-pentanol(**109**)	126
pentanoic acid(**74**)	112	**ketone**	
hexanoic acid(**75**)	129	cyclopentanone(**121**)	90
alcohol		2,3-pentadione(**119**)	105
1-butanol(**83**)	90	2-methylcyclopentanone(**122**)	107
2-butanol(**84**)	90	**ether**	
2-methyl-1-propanol(**85**)	90	THF(**131**)	80
2-methyl-2-propanol(**86**)	90	1,4-dioxane(**132**)	89
2-methyl-2-butanol(**87**)	107	**lactone**	
3-methyl-2-butanol(**88**)	107	β-propiolactone(**134**)	60
2,2-dimethyl-1-propanol(**89**)	108	γ-butyrolactone(**138**)	83
2-pentanol(**91**)	108	α-methyl-γ-valerolactone(**147**)	111
3-methyl-1-butanol(**92**)	108	**ester**	
3-pentanol(**93**)	108	ethyl crotonate(**173**)	123
2-methyl-1-butanol(**94**)	109	*sec*-butyl acetate(**178**)	129
cyclohexanol(**95**)	113	*tert*-butyl acetate(**179**)	129
2-methyl-2-pentanol(**96**)	124	isobutyl acetate(**180**)	129
3-methyl-2-pentanol(**97**)	124	metyl pentanoate(**181**)	129
3-methyl-3-pentanol(**98**)	125	**nitrile**	
2,3-dimethyl-2-butanol(**99**)	125	2,2-dimethyl propionitrile(**192**)	99
3,3-dimethyl-2-butanol(**100**)	125	isovaleronitrile(**193**)	100
4-methyl-2-pentanol(**101**)	125	*n*-valeronitrile(**194**)	100
2-hexanol(**102**)	125	*n*-hexanitrile(**195**)	117
3-hexanol(**103**)	125	**hydrocarbon**	
2-ethyl-1-butanol(**104**)	125	*n*-hexane(**205**)	115
4-methyl-1-pentanol(**105**)	125		

Aliphatic amides do not give good crystalline materials at all due to high solubility. (4) All guest molecules except **66** are incorporated in **CA** inclusion compounds at a 1:1 host-guest ratio. These inclusion behaviors must be closely related with their crystal structures.

Crystal Structures of Inclusion Crystals

X-ray powder diffraction revealed that all the guest molecule except **80** give two types of crystal structures, a crossing and bilayer structure, dependent on incorporated guest molecules. The bilayer structure, except the case of **66** and **184**, can be further classified into four sub-types (α-*gauche*, α-*trans*, β-*gauche*, and β-*trans* types) that have been discussed previous chapters. Table

4-4 shows the lattice parameters of analyzed crystals by X-ray crystallography and important data discussed later. The hydrogen bond networks of the typical crossing and bilayer structures are shown in Figures 4-3 and 4-4, respectively. The crossing structures have basically spiral host-host hydrogen bond networks. In the inclusion crystals of **CA** with carboxylic acids and alcohols, carboxy or hydroxy group of guest molecule insert the spiral networks between OH[C(3)] and OH[C(7)]. In contrast to the crossing structure, the bilayer structure has host-host cyclic, and cyclic and spiral hydrogen bond networks in monoclinic and triclinic forms, respectively. In addition, the host-guest or guest-guest hydrogen bonds are observed in the crystals of **CA** with carboxylic acids and alcohols.

In the inclusion crystals of **CA** with aliphatic compounds, functional groups of guest mol-

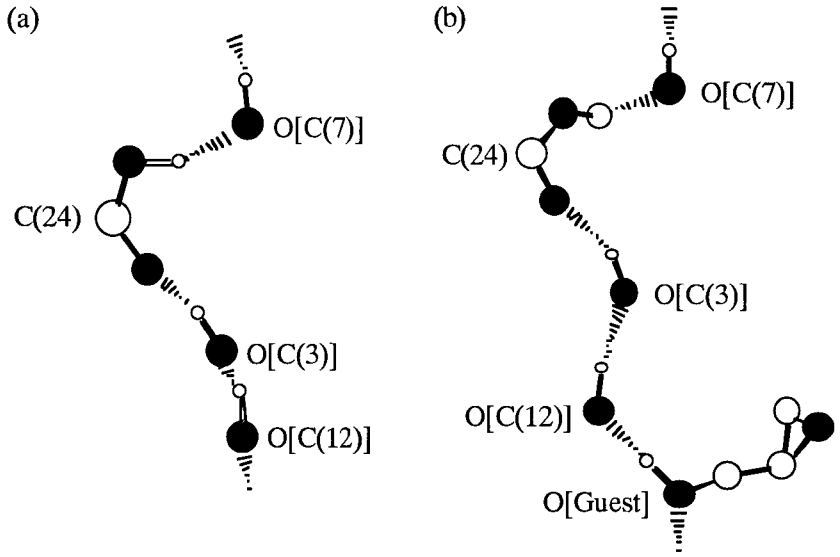


Figure 4-3. Hydrogen bond networks of typical crossing structures of **CA** with (a) **196**, (b) **82**. Hydrogen atoms of a guest molecule are omitted for clarity. The carbon and oxygen atoms are represented by open and filled circle, respectively.

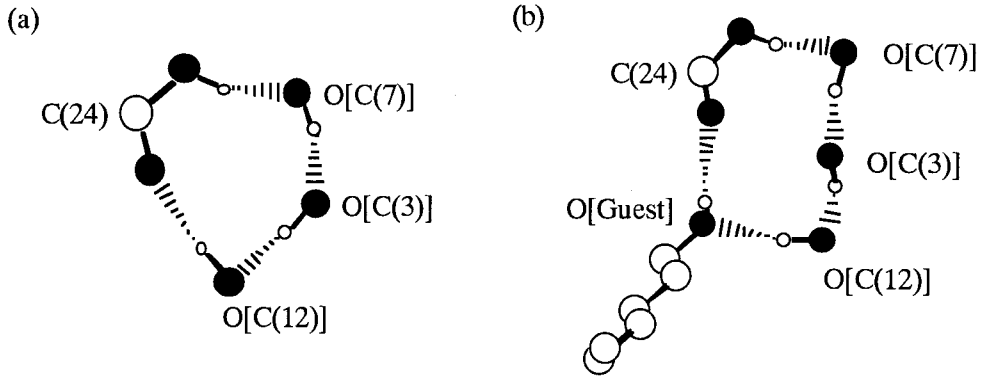


Figure 4-4. Hydrogen bond networks of typical bilayer structures of **CA** with (a) **113**, (b) **106**. Hydrogen atoms of a guest molecule are omitted for clarity. The carbon and oxygen atoms are represented by open and filled circle, respectively.

ecules effect on the host frameworks, though such tendency is not observed in the crystals of **CA** with aromatic compounds. Four compounds, acids, alcohols, nitriles, nitro, can form the two structures, while the other give only bilayer structure.

carboxylic acid Smaller (<78Å^3) and larger (>87Å^3) acids tend to give a crossing and bilayer structures, respectively. Only **66** can afford the two types of crystals, which are obtained by controlling the recrystallization condition. Direct recrystallization yielded 1:1 crossing structure (Figure 4-5(a)) with the helical hydrogen-bonded networks involving the carboxyl groups of the guest

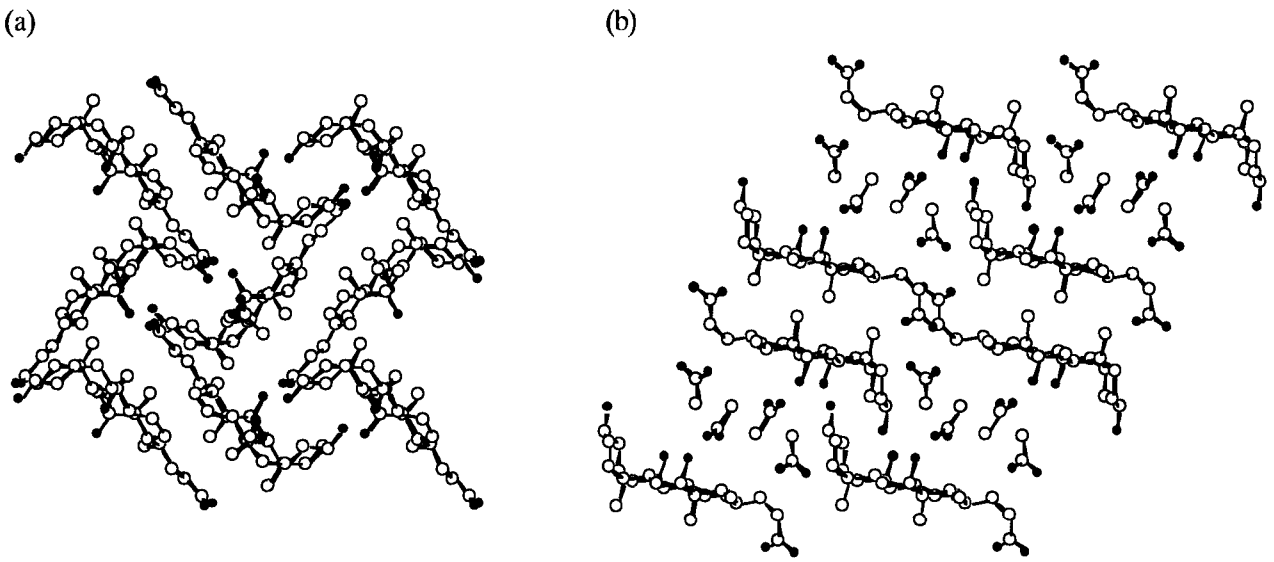


Figure 4-5. Molecular packing diagrams of **CA** with **66**: (a) 1:1 crossing structure, (b) 1:2 bilayer structure. Hydrogen atoms are omitted for clarity. The carbon and oxygen atoms are represented by open and filled circle, respectively.

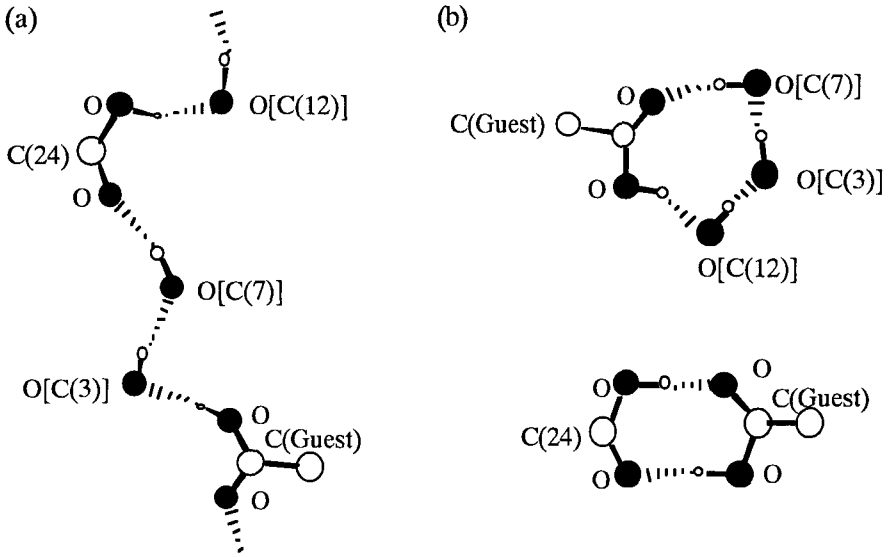


Figure 4-6. Hydrogen bond networks of **CA** with **66**: (a) 1:1 crossing structure, (b) 1:2 bilayer structure. Hydrogen atoms of guest molecules are omitted for clarity. The carbon and oxygen atoms are represented by open and filled circle, respectively.

molecule (Figure 4-6(a)). On the other hand, recrystallization involving cyclohexane as the third component yielded 1:2 bilayer structure (Figure 4-5(b)) with two kinds of cyclic hydrogen-bonded networks (Figure 4-6(b)). Although the former crystal has similar crossing structure to other crystals, the latter crystal has an uncommon bilayer structure that cannot be classified into the four sub-types. The side-chain conformation is different from the other bilayer structures due to host-guest cyclic hydrogen bonds of their carboxylic acids.

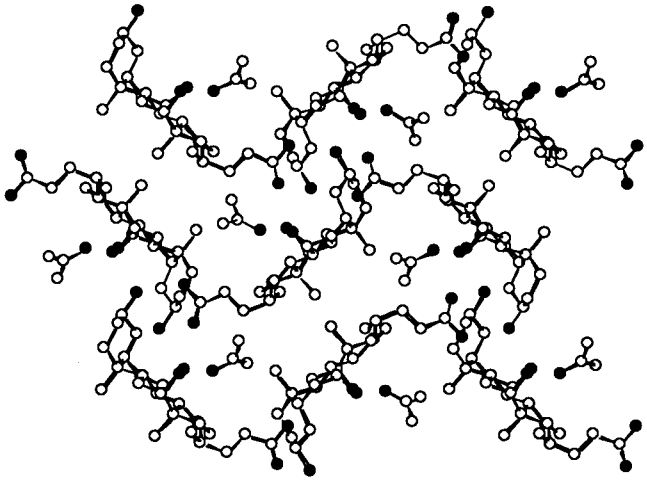


Figure 4-7. Molecular packing diagrams of **CA** with **80**. Hydrogen atoms are omitted for clarity. The carbon and oxygen atoms are represented by open and filled circle, respectively.

alcohol As the case of carboxylic acid, smaller (<76Å^3) and larger (>108Å^3) alcohols tend to give a crossing and bilayer structure, respectively. Only **80** affords new host framework that is monolayer structure comprised of wavy molecular sheet, as shown in Figure 4-7. The structure is maintained by host-host and host-guest spiral hydrogen networks of ···OH[C(7)]···O=C-OH[C(24)]···OH[C(3)]···OH[C(12)]···OH[guest]···, as shown in Figure 4-8. The guest molecules are incorporated among crests and troughs of the wavy sheets.

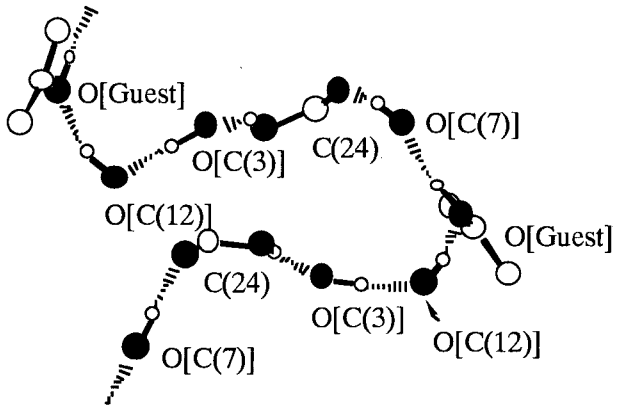


Figure 4-8. Hydrogen bond networks of **CA** with **80**. The carbon and oxygen atoms are represented by open and filled circle, respectively.

nitrile The crystal of **CA•184** have uncommon bilayer structure due to the different interdigitation manners of methyl groups in the lipophilic faces.[16a] Other nitriles give a common crossing and/or bilayer structures. Two nitriles, **185** and **187**, can form two structures with the same host-guest stoichiometry, indicating two-component polymorphism of inclusion compounds described latter.

nitro **196** can form the two structures with the same host-guest stoichiometry as the case of nitriles mentioned above. Larger nitros (>72Å^3) give only bilayer structure.

others Keton, ether, lactone,[17] ester,[16b] halide, and hydrocarbon give only bilayer structure irrespective of their molecular volumes (56-130Å^3).

Figure 4-9 shows the relationship between number of guest or solvent molecules and the

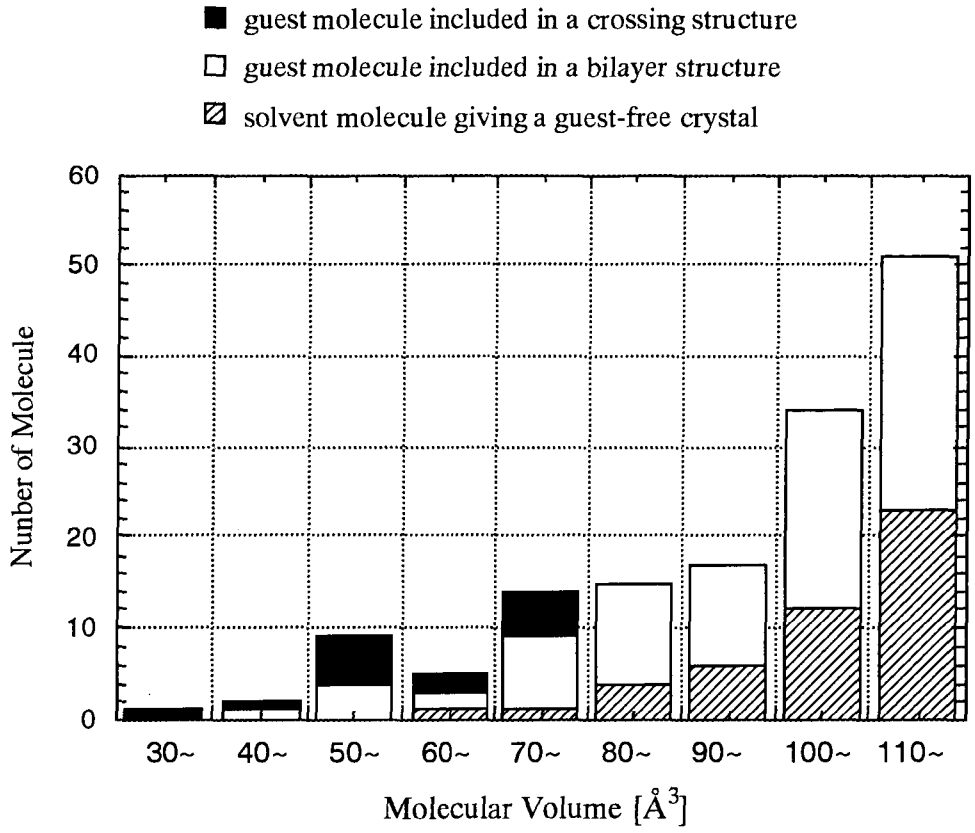


Figure 4-9. Relationship between number of guest or solvent molecule and the corresponding molecular volume.

corresponding molecular volume. The incorporated guests in crossing and bilayer structure have 39-77Å^3 and 48-130Å^3 molecular volume in this research. The high inclusion ability of bilayer structure is attributed to the fact that there are four sub-types and two specific types depending on the steric requirement of guest molecules.

Host Cavities

The crossing and monolayer structures have cage-like cavities, which are surrounded by host molecule three-dimensionally. In contrast, bilayer structures except **CA•184** have a one-dimensional cavity in the lipophilic layer, which run perpendicularly to the direction of the layer. The crystal of **CA•184** has cage-like cavity like that of crossing and monolayer structures. Table 4-4 summarizes free volumes of the host cavities of each host framework calculated by Cerius^2. The common host cavity volumes of crossing and bilayer structures are 89-131(106±14)Å^3/guest molecule and 137-203(161±15)Å^3/guest molecule, respectively. The bilayer structures have apparently larger cavities than crossing structures, though the cavity volumes are slightly different even in the same host framework depending on the incorporated guest molecules. The difference of the cavity size between two structures agrees with that of the incorporated guest size: 62±12 Å^3 in cage-like cavity and 99±19 Å^3 in channel.

In order to clarify the size dependence of the host frameworks, we calculate the packing

Table 4-4. Lattice parameters for inclusion compounds of **CA** with aliphatic compounds.

Guest	Space Group	a [Å]	b [Å]	c [Å]	α [°]	β [°]	γ [°]	V [Å^3]	Number of guest molecule in unit cell	V_{guest} [Å^3]	V_{cavity} [Å^3]	PC_{cavity} [%]	Reference
crossing type													
acetic acid(**66**)	$P2_12_12_1$	13.83	15.36	12.40				2634	4	60	423	56	this work
acrylic acid(**67**)	$P2_12_12_1$	14.43	15.34	12.44				2755	4	60	510	47	this work
propionic acid(**68**)	$P2_12_12_1$	12.77	12.94	16.66				2753	4	77	525	59	this work
methanol(**76**)	$P2_12_12_1$	15.20	11.63	14.56				2572	4	39	369	42	[6b]
propargyl alcohol(**77**)	$P2_12_12_1$	14.40	15.11	11.60				2523	4	55	362	61	this work
ethanol(**78**)	$P2_12_12_1$	14.65	11.74	15.05				2588	4	56	381	58	[6a,6b]
ethylene glycol(**79**)	$P2_12_12_1$	14.45	15.15	11.65				2550	4	66	432	61	this work
1-propanol(**81**)	$P2_12_12_1$	15.03	11.86	14.95				2655	4	73	461	64	[6b]
glycidol(**82**)	$P2_12_12_1$	14.86	15.03	11.90				2658	4	76	441	69	this work
acryronitrile(**185**)	$P2_12_12_1$	16.88	17.62	8.50				2528	4	57	393	58	this work
methacrylonitrile(**187**)	$P2_12_12_1$	16.71	17.85	8.65				2579	4	74	425	70	this work
nitromethane(**196**)	$P2_12_12_1$	16.62	17.76	8.42				2485	4	56	355	63	this work
bilayer type													
acetic acid(**66**)	$P2_1$	13.35	8.19	14.00		112.2		1417	4	60	303	79	this work
methacryic acid(**69**)	$P2_1$	13.14	8.00	14.23		113.5		1372	2	88	284	62	this work
3-pentenoic acid(**72**)	$P1$	12.37	14.14	8.26	90.2	92.9	106.1	1386	2	104	304	68	this work
1-pentanol(**90**)	$P2_1$	12.32	7.96	14.06		104.6		1336	2	108	290	75	this work
1-hexanol(**106**)	$P2_1$	13.38	8.66	14.12		113.0		1506	2	126	407	62	this work
3-pentanone(**113**)	$P2_1$	12.79	8.12	13.96		103.8		1408	2	101	319	63	this work
2,4-pentadione(**120**)	$P1$	12.26	14.15	8.18	90.5	92.9	105.2	1397	2	103	314	66	this work
ethyl vinyl ether(**125**)	$P2_1$	13.69	7.72	14.03		115.0		1343	2	84	278	61	this work
4,7-dihydro-1,3-dioxepin(**133**)	$P2_1$	13.54	8.01	14.06		113.4		1398	2	98	312	63	this work
α-angelicalactone(**143**)	$P2_1$	12.75	8.00	14.10		105.2		1388	2	85	316	54	[17b]

Table 4-4. Lattice parameters for inclusion compounds of **CA** with aliphatic compounds.

Guest	Space Group	a [Å]	b [Å]	c [Å]	α [°]	β [°]	γ [°]	V [Å^3]	Number of guest molecule in unit cell	V_{guest} [Å^3]	V_{cavity} [Å^3]	PC_{cavity} [%]	Reference
β-butyrolactone(**135**)	$P2_1$	12.63	7.93	14.30		103.8		1365	2	85	304	56	[17b]
β-valerolactone(**136**)	$P2_1$	12.70	8.04	14.05		103.9		1392	2	102	322	63	[17b]
γ-valerolactone(**139**)	$P2_1$	12.92	7.98	14.04		104.5		1402	2	100	328	61	[17b]
δ-valerolactone(**144**)	$P2_1$	13.16	7.92	13.97		105.9		1400	2	101	342	59	[17b]
α-methyl-γ-butyrolactone(**141**)	$P2_1$	13.00	7.95	14.00		104.2		1403	2	101	333	60	[17b]
ε-hexalactone(**148**)	$P2_1$	12.70	8.16	14.02		104.1		1419	2	118	354	67	[17b]
δ-hexalactone(**145**)	$P2_1$	13.05	8.08	13.87		104.2		1417	2	118	338	70	[17b]
γ-hexalactone(**140**)	$P2_1$	13.36	7.97	13.90		106.6		1417	2	119	343	70	[17b]
methyl acetate(**150**)	$P\bar{1}$	12.22	8.19	14.20	90.2	105.7	94.0	1364	2	77	285	54	[17b]
ethyl acetate(**155**)	$P2_1$	13.67	7.82	14.10		113.5		1382	2	94	385	49	[16b]
ethyl acetate(**155**)	$P\bar{1}$	12.28	14.16	8.24	90.4	94.2	105.7	1376	2	94	310	61	[16b]
allyl acetate(**159**)	$P2_1$	12.22	7.76	15.21		104.9		1394	2	104	298	70	this work
methyl crotonate(**161**)	$P\bar{1}$	12.29	14.37	8.36	90.5	95.3	107.2	1404	2	104	334	63	this work
ethyl acryrate(**162**)	$P2_1$	12.40	7.70	15.26		105.4		1404	2	105	332	63	this work
isopropyl acetate(**164**)	$P2_1$	16.60	7.98	12.14		117.8		1423	2	111	346	64	[16b]
ethyl propionate(**165**)	$P2_1$	13.57	7.97	14.24		113.5		1411	2	112	328	68	[16b]
vinyl crotonate(**169**)	$P2_1$	12.37	7.73	15.43		106.5		1415	2	116	333	70	this work
n-propyl acetate(**170**)	$P2_1$	16.80	7.88	12.11		118.1		1415	2	117	344	68	[16b]
acetonitrile(**184**)	$P2_1$	9.65	8.40	15.75		101.0		1253	2	48	167	57	[16a]
acryronitrile(**185**)	$P2_1$	12.18	7.88	14.30		104.2		1331	2	57	274	42	this work
methacrylonitrile(**187**)	$P2_1$	12.53	14.16	8.28	90.9	94.9	107.2	1396	2	74	313	47	this work
monolayer type													
2-propanol(**80**)	$P2_12_12_1$	15.50	18.90	9.01				2639	4	73	460	64	this work

coefficients of the host cavities (PC_{cavity}) as parameter for the steric fitness of the guest component in the host cavity.[1,18,19] Table 4-4 shows *PCcavity* calculated from the free volumes of the host cavities and the molecular volumes of the guest compounds in the unit cell. PC_{cavity} of the host cavities lies in the range of 42-75% in two common structures (59±8% in a crossing structure and 60±7% in a bilayer structure) to form the stable inclusion compounds. Furthermore, we noticed that the host framework isomerization of **CA** crystals could be understood through PC_{cavity}. Figure 4-10 shows the relationship between the molecular volume and PC_{cavity} of 1:1 inclusion crystals with (i) aliphatic compounds in a crossing structure, (ii) aliphatic compounds in a bilayer structure (α-*gauche*, β-*gauche* and α-*trans* type), (iii) aromatic compounds in a bilayer structure (α-*gauche*, β-*gauche* and α-*trans* type), and (iv) aromatic compounds in a bilayer structure (β-*trans* type). The data of (iii) and (iv) are described in Chapter 2. Irrespective of functional groups of guest molecules, *PCcavity* tends to increase with increase of the guest volumes within the same host frameworks, indicating that the volumes of the host cavities are less sensitive than that of the guest molecules. The host frameworks change with increase in guest volume in the order, crossing structure < bilayer structure (α-*gauche*, β-*gauche* and α-*trans* type) < bilayer structure (β-*trans* type). Further large molecules are included in bilayer structures at 2:1 host-guest stoichiometry. From the relationship in Figure 4-10, the monolayer structure involving **80** and bilayer structure involving **184** are found to have similar cavity with crossing structures, whereas the bilayer structure involving **66** has a specific cavity.

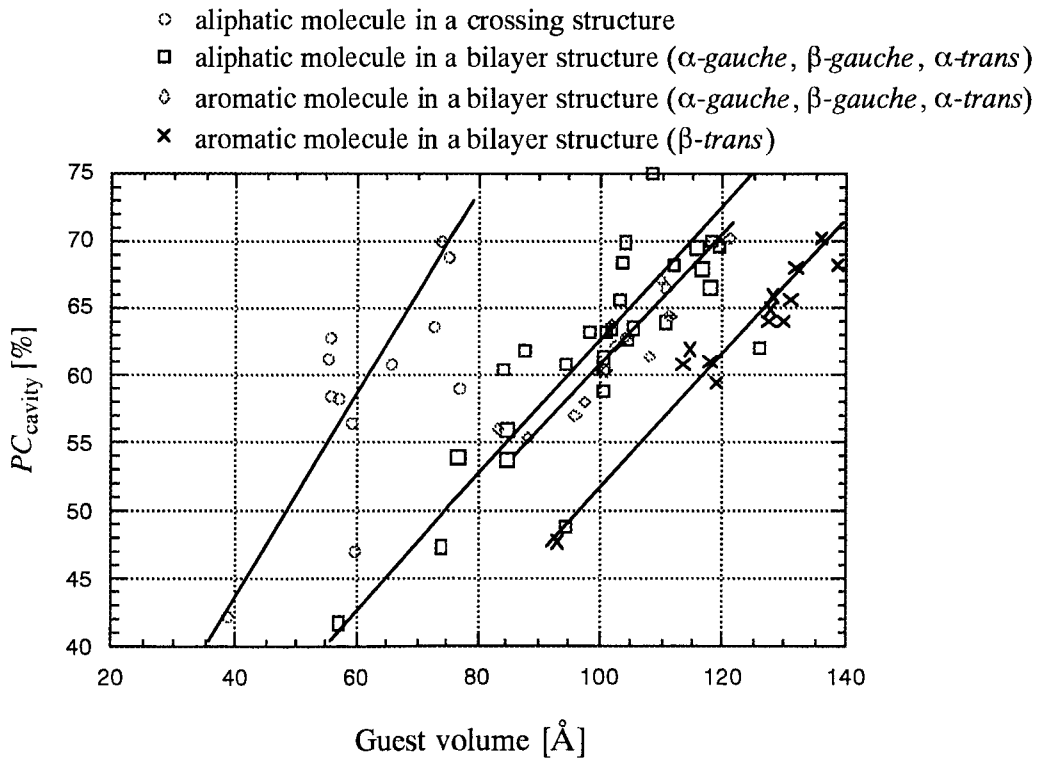


Figure 4-10. Relationship between molecular volumes and PC_{cavity} of crossing and bilayer structure.

It should be noted that PC_{cavity} can explain effect of hydrogen bonds on the formation of bilayer structure. **CA•90** crystal has high value of PC_{cavity} for the molecular volume, while **CA•106** has low value. Two crystals have similar cyclic hydrogen bond networks involving hydroxy group of the guest molecule, as shown in Figure 4-6(b). This suggests that the host-guest hydrogen bonding is not always useful for the incorporation in the host cavities. This assumption is supported by the results of the inclusion phenomena as follows: most of the alcohols having 90Å^3 or more volume gave guest-free crystals, while many esters having similar molecular volume afforded inclusion crystals; inclusion crystals of **CA•67** and **CA•68** have low value of PC_{cavity} for their molecular volume in comparison with the crystals involving nitriles. This indicates that the host-guest hydrogen bonding rather work to prevent the incorporation of guest molecules. The reason may be due to the fact that the host-guest hydrogen bond network restricts the orientation of the guest molecule and make difficult to achieve stable arrangement in the cavity. Consequently, the host-guest hydrogen bond may lead to steric misfit between host cavity and guest molecule to fail to form the inclusion crystals with alcohols and acids having C4 or more. The formation of guest-free crystals by other compounds involving ketones, ethers e.t.c., may be shape misfit between a host cavity and a guest molecule. In addition, compounds having <90Å^3 volume, if they form bilayer structures, may give low PC_{cavity} (<57%) to yield unstable inclusion compounds. In fact, guest molecules were released at room temperature in inclusion crystals of **CA** with **110** (66Å^3), **149** (60Å^3), or **200** (57Å^3).

Polymorphism of inclusion crystals

The systematic investigation led us to find two-component polymorphs of inclusion crystals that have the same host-guest combinations and host-guest ratios. **CA** forms two types of the crystal structures, crossing and bilayer structures, with nitriles, **185** and **187**. Moreover, **CA** forms two types of bilayer structure with *o*-xylene (**62**) described in Chapter 3 and **155**. The former polymorphs were consequence of different arrangements of the same molecules, while the latter are consequence of packing of conformational isomers.

Polymorphs of CA•185 and CA•187 Figure 4-11 shows crystal structures of **CA·185** and **CA·187**. They have 1:1 host-guest ratios and have similar host frameworks to other crossing and bilayer structures. The crossing structures of two crystals belong to the same space group (orthorhombic, $P2_12_12_1$), while bilayer structures belong to the different space groups (monoclinic $P2_1$ and triclinic $P1$). This affects the hydrogen bond networks, as shown in Figure 4-12. The crystal of **CA•185** has a cyclic network, but **CA•187** has cyclic and spiral networks. To clarify the source of the formation of polymorphs, **CA** was recrystallized on various conditions. First, solvent effects with a definite temperature were examined in the presence of an equimolar amount of a guest and a solvent. The inclusion crystals of **CA•185** and **CA•187** were prepared by using four butanol isomers as the solvents. **CA** was dissolved in the hot butanols and cooled to 25°C, and neat **185** and

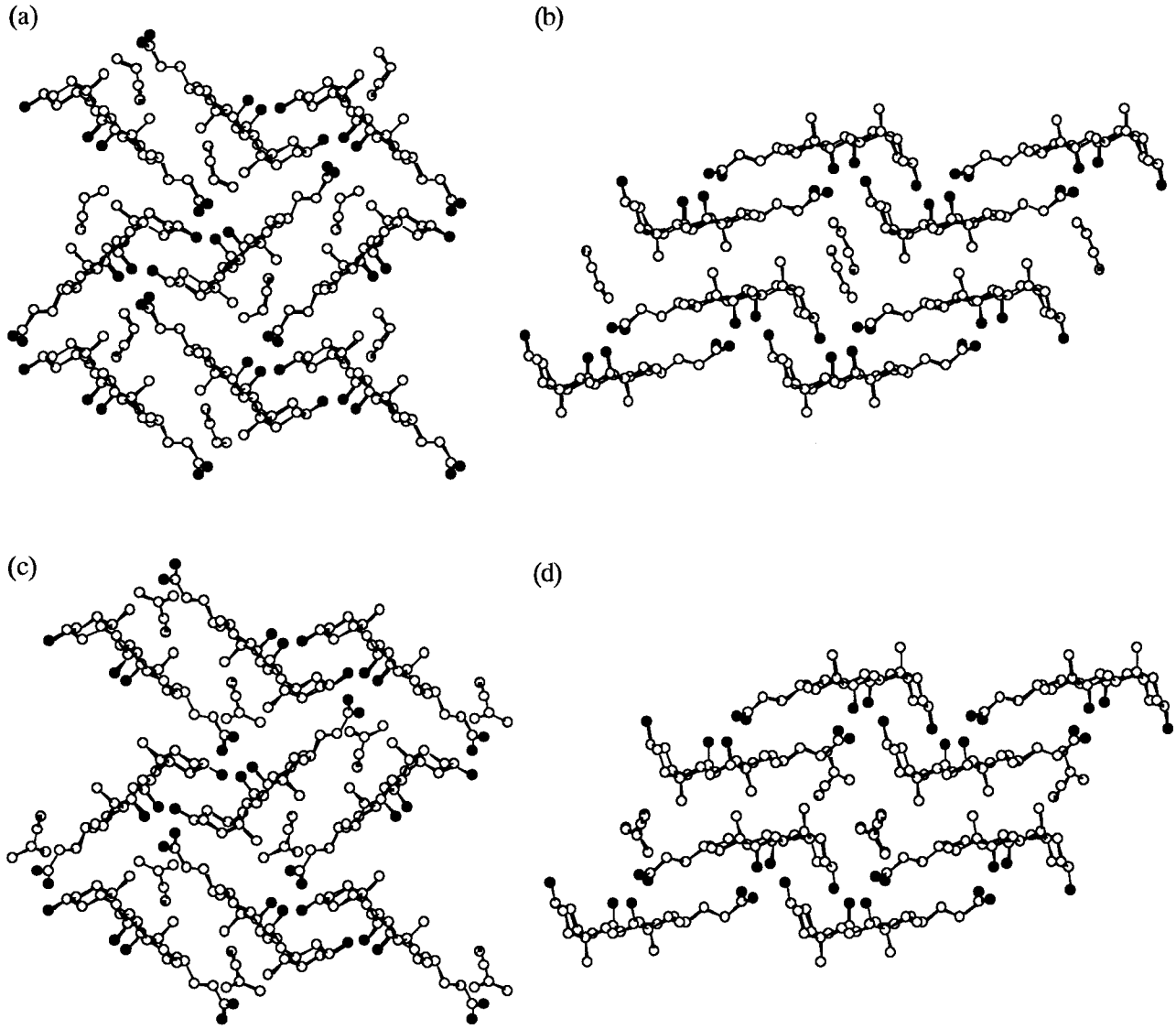


Figure 4-11. Molecular packing diagrams of (a) a crossing structure of **CA•185**, (b) a bilayer structure of **CA•185**, (c) a crossing structure of **CA•187**, and (d) a bilayer structure of **CA•187**. The carbon, nitrogen, and oxygen atoms are represented by open, dotted, and filled circle, respectively.

187, which were kept at 25°C, were added into the solution. The resulting solution was maintained at 25°C. As shown in Table 4-5, the polymorphs of **CA•185** and **CA•187** were obtained depending on the alcoholic solvents. Secondly, an effect of temperature was examined. In the case of **CA•185**, recrystallization using 1-butanol or 2-methyl-1-propanol at high and low temperature gave a crossing and bilayer structures. The borderline for separation of the two structures lies in about 30°C. On the other hand, only a bilayer structure was formed in the case of **187** irrespective of the solvents. As for concentration effects, the bilayer crystals tend to be obtained in the presence of an excess amount of the liquid guests compared to the amount of the solvents. In addition, seeding was also effective for the formation of a desirable polymorph.

Polymorph of CA•155 Figure 4-13 shows crystal structures of **CA•155**. Recrystallization of

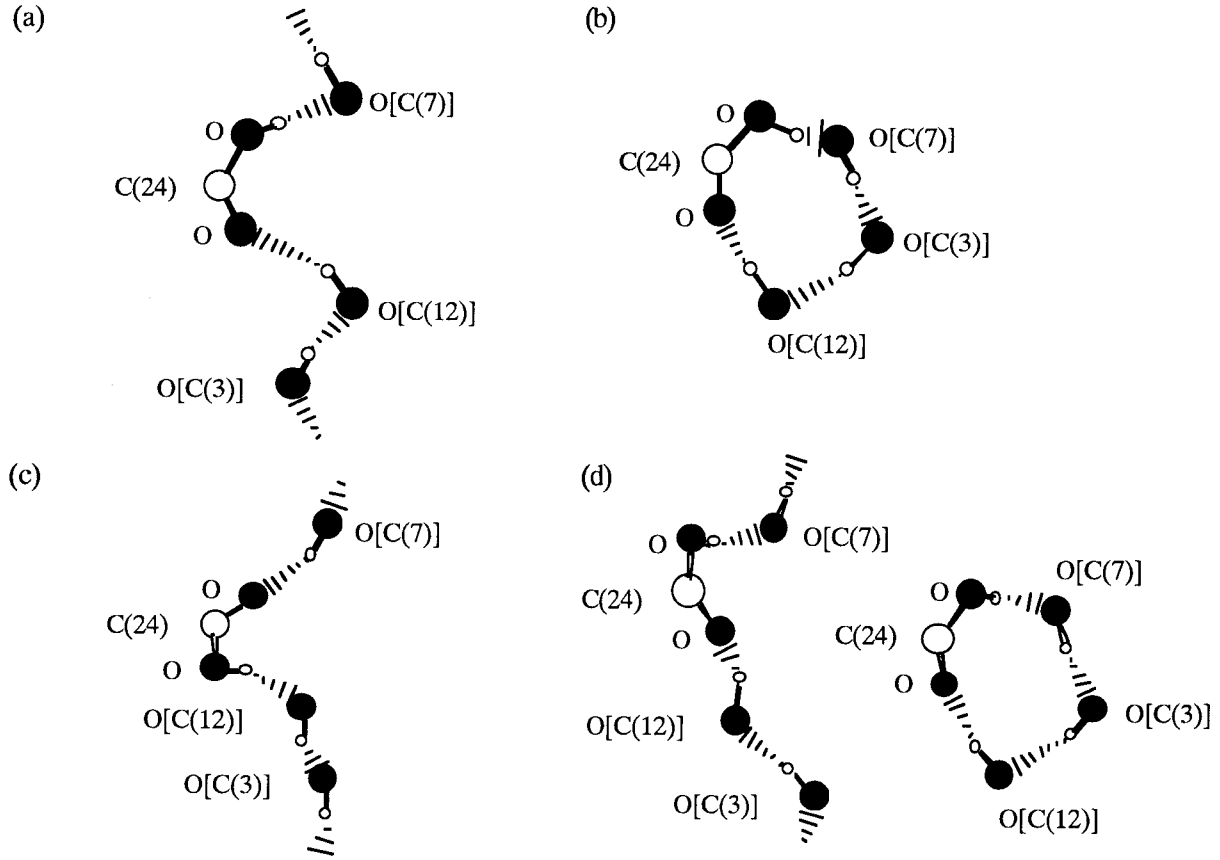


Figure 4-12. Hydrogen bond networks of (a) a crossing structure of **CA•185**, (b) a bilayer structure of **CA•185**, (c) a crossing structure of **CA•187**, and (d) a bilayer structure of **CA•187**. The carbon and oxygen atoms are represented by open and filled circle, respectively.

a salt of **CA** and 1-naphthylmethylamine from **155** gave a 1:1 inclusion crystal of **CA•155** that belongs to triclinic *P*1 (Form II) and does not involve 1-naphthylmethylamine. This crystal structure is different from the reported crystal structure of **CA•155** (Form I)[16b] that was obtained by direct recrystallization of **CA** from liquid **155**. In the latter, the dihedral angle at C17-C20-C22-C23 (ψ) is 65°, referred to as the *gauche* type, but in the former, they are -158° and -168°, referred to as the *trans* type.[20] This affects the hydrogen bond networks, as shown in Figure 4-14. Form I has a cyclic network, but Form II has cyclic and spiral networks. The difference of the side-chain conformation changes the shape of the host channels as well. Figure 4-15 illustrates typical cross-sections of the host cavities sliced parallel to the axis of the channel at the height that shows the cross-sections surrounded by the side chains. This shows that difference in the cavity shape affects the orientations of the guest molecules. In the Form I the guest molecules lie with their long molecular axis approximately perpendicular to the channel.[16b] On the other hand, in the Form II the guest molecules adopt with their long molecular axis in two directions: approximately at 45° and 70° to the channel. In spite of these differences, the two polymorphs have common features in most of the bilayer structures ever found. In addition, the interdigitation manners of methyl groups

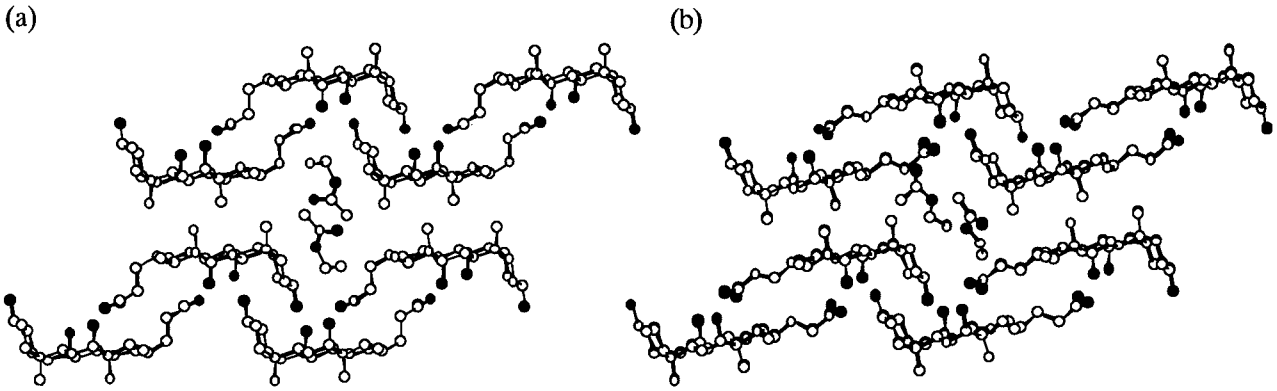


Figure 4-13. Molecular packing diagrams of **CA•155**; (a) Form I and (b) Form II. The carbon and oxygen atoms are represented by open and filled circle, respectively. The carbon and oxygen atoms are represented by open and filled circle, respectively.

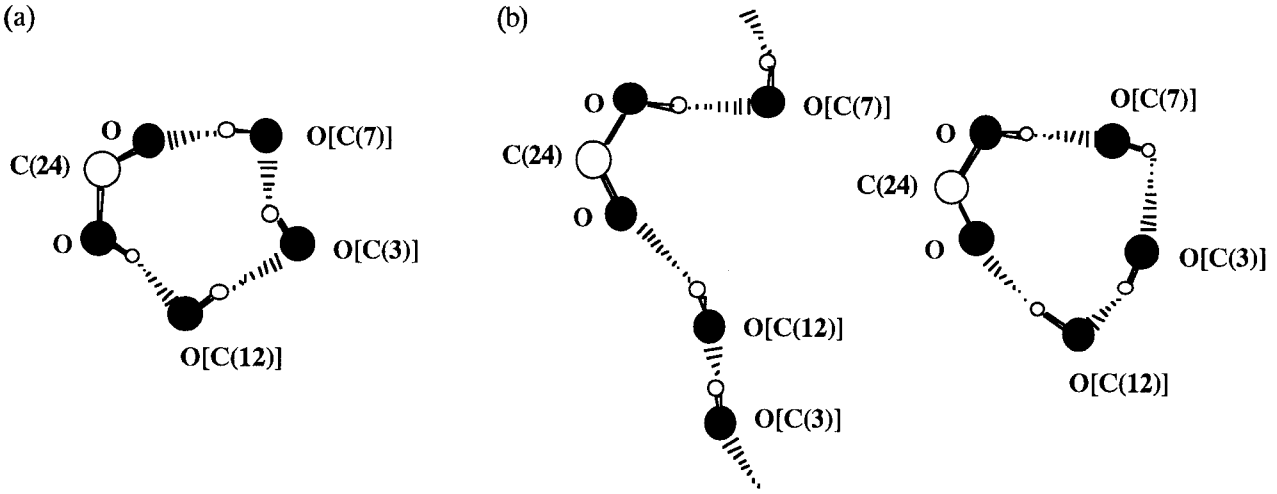


Figure 4-14. Hydrogen bond networks of **CA•155**; (a) Form I and (b) Form II. The carbon and oxygen atoms are represented by open and filled circle, respectively.

in the lipophilic faces are the same α-type.[20] This is a good contrast with polymorphism in inclusion crystals of **CA** with nitriles.

The polymorphism in inclusion crystals of **CA** with nitriles can be understood from limitation of guest volumes in crossing and bilayer structures. Because PC_{cavity} mostly lies in the range of 42-70% to retain the inclusion crystals, the volume of the guest molecules, if there is no specific interaction, should be in the range of 35-80Å^3 in a crossing structure and 55-140Å^3 in a bilayer structure, respectively. These facts indicate that the middle-size molecules having 55-80Å^3 molecular volume have possibility to incorporate in both host frameworks and that the molecules out of this range give only one host framework. This idea prompts us to investigate polymorphism of **CA** with the middle-size molecules systematically and enabled us to find polymorphs of **CA** with **196**. **196** molecule gave a crossing and bilayer structures as the case of nitriles. The former structure was confirmed by X-ray crystallography, while the latter was confirmed by X-ray powder

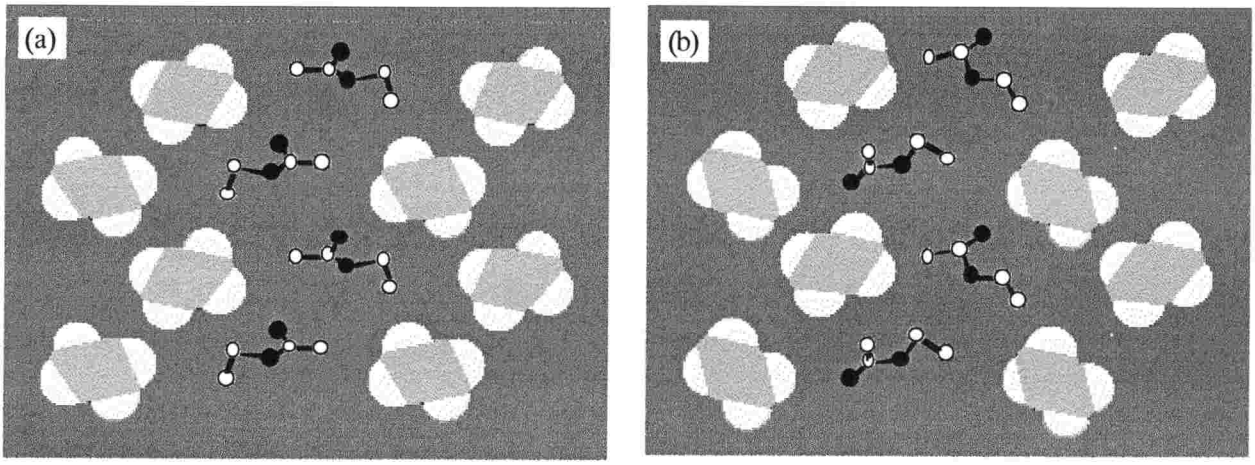


Figure 4-15. Cross sections of the host channels sliced parallel to the direction of the channel (carbon, hydrogen atoms are represented in gray and white, respectively) with arrays of included guest molecules (hydrogen atoms are omitted for clarity, and carbon and oxygen atoms are represented in white and black, respectively); (a) Form I and (b) Form II.

diffraction due to the low crystallinity. The other molecules having similar molecular volume, such as **78**, **200**, etc., gave only one host framework in spite of careful recrystallization. This may be due to the fact that the hydrogen bonds and/or steric interaction between host and guest molecules stabilize one-side crystal.

4. Conclusion

The formation of inclusion compounds of **CA** with a series of molecules having C6 or less was described. Systematic structural investigations illustrate that all the molecules, except **66**, **80**, and **184**, afford two common host frameworks of a crossing structure with a small cavity and a bilayer structure with a large cavity. The former includes small guest compounds (<78Å^3), the latter includes large ones (>56Å^3). Middle-size compounds (56-78Å^3) can be incorporated in both cavities, indicating that they can give two-component polymorphs of inclusion crystals. The host frameworks thus mainly depend on the volume fitness between the guest components and the host cavities. Because PC_{cavity} of the inclusion crystals lies in the range of 42-70% to retain the crystals, PC_{cavity} is a good parameter for the prediction of structural types. PC_{cavity} also gives a good explanation for the effect of host-guest hydrogen bonds, which often lead to the formation of the guest-free crystals. In addition, this work revealed that **CA** is a specific host having at least five polymorphs of inclusion crystals. This is due to the characteristic molecular structure of **CA**, which involves three hydroxy groups and a carboxy group, and consists of rigid steroidal unit and flexible methylene unit. The former feature may cause the polymorphs of different arrangements of the same molecules, and the latter may cause the polymorphs of packing of conformational isomers. Systematic research through PC_{cavity} would lead to the discovery of novel polymorphs in other hosts.

Chapter 5. Intercalation Phenomena in Cholic Acid Crystal with the Same Guest

1. Introduction

Porous inorganic materials, such as zeolite, graphite and clay, have much attention because of their practical and potential applications.[1] Absorption and/or desorption of the guest molecules are one of the most important features of these inorganic porous materials. During absorption and/or desorption, zeolites retain the frameworks due to their rigid covalent bonds, while graphite and clay having two-dimensional host frameworks vary their interlayer distance to the steric requirements and structures of guest components, which is known as intercalation phenomena. Recently, the intercalation phenomena have been reported in organic crystals.[2] Inclusion crystals of **CA** can absorb or exchange guest molecules with change the structural types but with retention of crystalline state. Since the discovery, the dynamic behavior of organic crystals have been reported in other host compounds.[3-6] In these reports, intercalation phenomena occur when the original crystals were soaked into the different liquid from incorporated guest liquid. Using the same guest, intercalation phenomena are expected to be observed in the **CA** crystals, because **CA** forms two types of host frameworks with identical guests,[7] as described in Chapter 4. Here, the author report the intercalation phenomena in **CA** crystals involving the same guests, where the lipophilic layers can reversibly slide without any transition to amorphous states.

2. Experimental

All chemicals and solvents were commercially available and used without any purification. **CA** (100 mg) was dissolved with warming in the 1-butanol (0.4 mL) solution, and the liquid guest (usually 2 mL) was poured into the resulting solution. The needle-like crystals were collected and dried on the filter papers. Infrared spectra were recorded on a JASCO IR-Report-100 spectrometer. Differential scanning calorimetry (DSC), and thermal gravimetry (TG), were performed on a Rigaku TAS100 system; ca.10 mg from 40 to 230° C at a heating rate of 5° C min^{-1}. X-ray powder diffraction (XRD) patterns were measured by using Rigaku RINT-1100 at room temperature.

3. Results and Discussion

As described in Chapter 2, the inclusion crystal of **CA** with *n*-propylbenzene (**6**) has the β-trans type bilayer structure.[8] Thermogravimetry (TG) and differential scanning calorimetry (DSC) revealed that the **CA•6** crystal have a characteristic thermal behavior. As shown in Figure 5-1, the crystals exhibited a two-step release of the guest with two peaks at 90 and 120° C, although most of the crystals employed so far have a one step release. At the first stage, just half an amount of the guest component released from the starting 1:1 inclusion crystals. At the second stage, the half

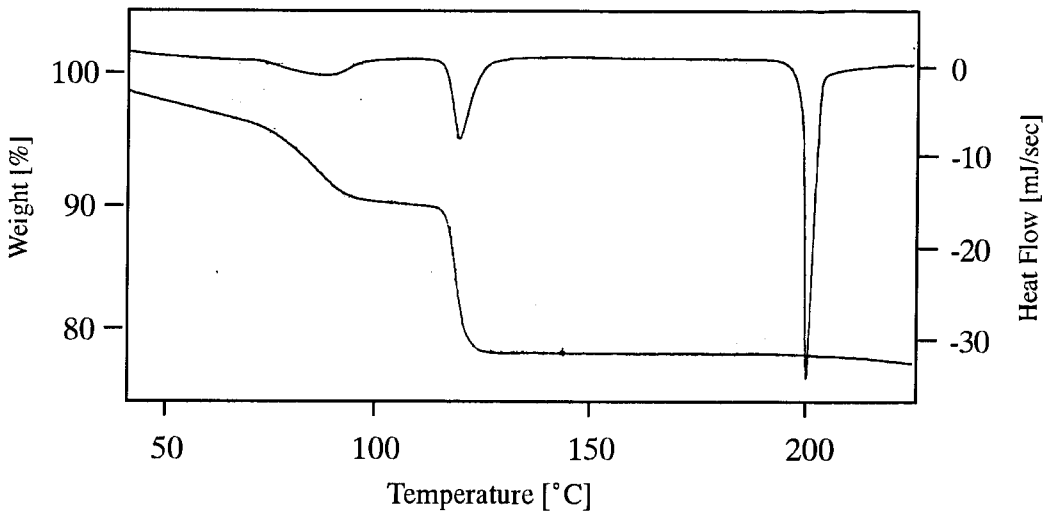


Figure 5-1. TG-DSC diagram of the inclusion crystals of **CA** with **6**.

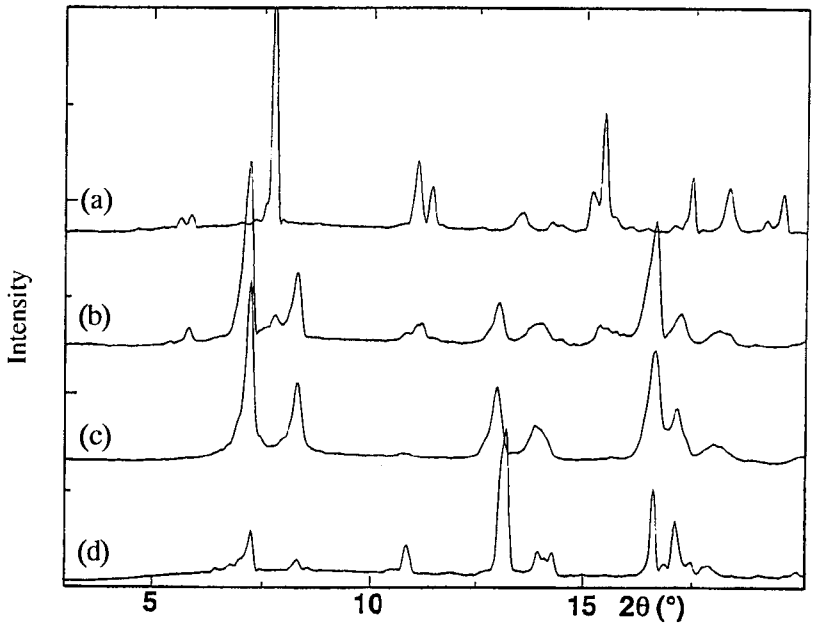


Figure 5-2. X-ray powder diffraction patterns of the inclusion crystals of (a) **CA** with **6**, (b) after heating at 70° C for 10 minutes, (c) after heating at 70° C for one hour, and (d) **CA** with **139**.

remainder released to yield guest-free crystals. This result indicates that an intermediate inclusion crystals at a 2:1 host-guest stoichiometry form between 90° C and 120° C, though the 2:1 crystals could not be obtained by recrystallization at any conditions.

X-ray powder diffraction revealed the crystal structures of the intermediate inclusion crystals. The 1:1 crystals were heated at 70° C, where the guest **6** began to release in the TG diagram. The original diffraction pattern changed a little after ten minutes and completely after one hour, as shown in Figure 5-2. The latter pattern was very similar to that of the inclusion crystal of **CA** with γ-valerolactone (**139**).[9] This indicates that the β-*trans* type framework changed to α-*trans* type.

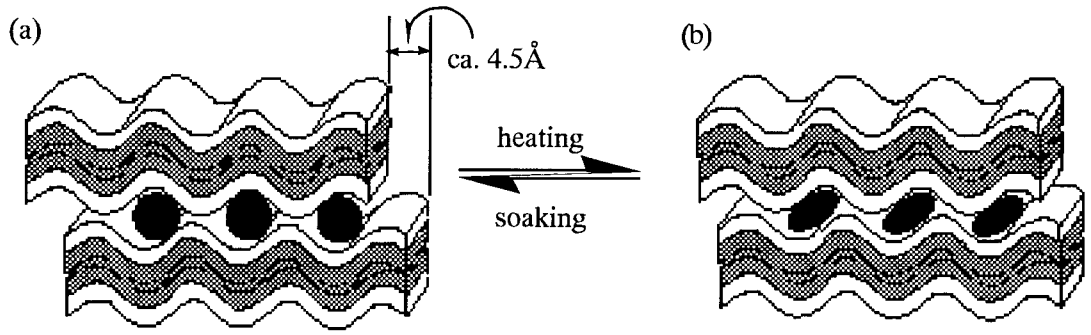


Figure 5-3. Schematic representation of the reversible sliding of bilayers on the lipophilic sides in the inclusion crystals of **CA**: (a) after heating of 1:1 β-*trans* type structures, (b) after soaking of 2:1 α-*trans* type structures.

Compared with the two host frameworks, the bilayers slide approximately 4.5Å in the horizontal direction, as schematically shown in Figure 5-3. The change of the host frameworks must be attributed to the formation of smaller cavities in order to compensate loss of the guest molecules. In addition, it should be noted that the crystals did not turn to amorphous state or guest-free crystals.

Interestingly, the opposite sliding of the bilayers was observed when the intermediate 2:1 crystals were soaked into a liquid **6** at room temperature for one hour. X-ray powder diffraction and TG-DSC analysis revealed that the resulting crystals were identical to the 1:1 original crystals. That is, the bilayers can slide back to the initial position without any deformation of the crystalline state (Figure 5-3). Such a reversible sliding of the bilayers was repeated more than two times through the heating and soaking cycles. In this way the host framework of **CA** has a reversible and dynamical property so as to bring about any cavities suitable for guests.

Further study made clear that such a bilayer sliding in crystals of **CA** was not specific for **6**. For example, the two-step release was observed in the compounds of **CA** with *m*-xylene (**63**) and methyl benzoate (**30**).[8,10] The 1:1 inclusion crystals of **CA** with these guests have the same 1:1 β-*trans* bilayer structures as those with **6**, described in Chapter 2 and 3. These crystals also can absorb and desorb the guest molecules with reversibly sliding of the lipophilic layers.

4. Conclusion

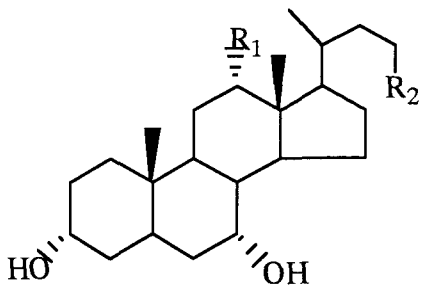
This study demonstrates the dynamic properties of guest-dependent polymorphic **CA** crystals. Heat treatment of 1:1 **CA·6** crystals gave the intermediate inclusion crystals with the same guests at 2:1 stoichiometry. The resulting crystals returned to the original crystals by soaking into the liquid **6**. During the absorption and desorption of the guests, the host framework reversibly changed to α-trans or β-trans type depending on the host-guest stoichiometries. The reversible change of the layers in **CA** crystal is very similar to intercalation phenomena in inorganic compounds having two-dimensional host frameworks, such as graphite and clay. The intercalation phenomena may be observed in other polymorphic inclusion crystals.

Chapter 6. Inclusion Polymerization in Polymorphic Crystals of Cholic Acid

1. Introduction

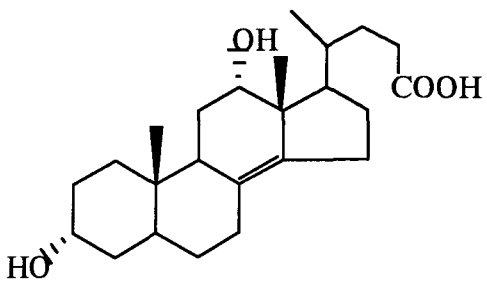
Many efforts have been devoted to the control of polymerizability on the basis of molecular assemblies, such as membranes,[1] liquid crystals,[2] gels,[3] or crystals.[4] In these assemblies, monomers are arrayed in a specific direction by noncovalent interactions, such as hydrogen-bonding and van der Waals interaction, to give characteristic polymers. In particular, some solid-state polymerizations provide clear relations between the orientation of monomers and stereoregularity of the resulting polymers.[4]

Inclusion compounds are useful assemblies for controlling the orientation of monomer molecules.[5] Nanometer-level spaces of the compounds force guest molecules to be arranged in a specific direction. If the arrangements of various monomers are retained during polymerization, polymers with highly controlled stereochemical structures may be obtained. So far, successful examples are known for only limited combinations of hosts and monomers. New hosts suitable for such polymerization using inclusion compounds should thus be found. Urea, thiourea, and perhydrotriphenylene are primary hosts for inclusion polymerization. These hosts yield highly stereoregular polymers from a limited range of diene monomers.[6-9] A pair of steroidal hosts, deoxycholic acid (**DCA**) and apocholic acid (**ACA**), were adopted to evaluate the polymerizability of comprehensive diene monomers on the basis of relative space effects at the nanometer level.[5,10-12] Methyl cholate (**MCA**) and chenodeoxycholic acid (**CDCA**), were confirmed to serve as hosts for inclusion polymerization.[13-15]



Chenodeoxycholic acid (CDCA) ; R_1=H R_2=CO_2H
Methyl cholate (MCA) ; R_1=OH R_2=CO_2CH_3

As described in the previous chapters, **CA** forms inclusion crystals with various organic substances and the crystals have bilayer structures with channels, as in the case of **DCA** and **ACA**.[16] However, polymerization in **CA** channels has not been proved. This was explained by the fact that **CA** crystals exhibit different polymorphism and dynamics from **DCA** and **ACA**.[16-19] Systematic studies made clear that such polymorphism is guest- and/or environment-dependent, leading to decisive evi-



Apocholic acid (ACA)

dence supporting that inclusion polymerization proceeds even in **CA** channels. This chapter describes inclusion polymerization of vinyl and diene monomers in **CA** crystals. The effects of the polymorphic crystals are discussed in detail.

2. Experimental

Formation of Inclusion Crystals

All compounds were commercially obtained and used without purification. Polymorphic crystals of **CA** were obtained by recrystallization and intercalation. In the case of acrylonitrile (**185**) and methacrylonitrile (**187**), crossing-type inclusion crystals of **CA** were prepared by direct recrystallization. **CA** (100 mg) was dissolved with warming in the liquid guest (12 mL), and the resulting solution was allowed to stand at room temperature. Channel-type inclusion crystals of **CA** with **185**, **187**, 2-chloroacrylonitrile (**210**), vinyl acetate (**152**), and 2,3-dimethyl-1,3-butadiene (**207**) were prepared by intercalation: starting inclusion crystals (100 mg) were obtained by direct recrystallization from acetophenone (**22**) and *n*-propylbenzene (**6**), and soaked in liquid guest (1 mL) and allowed to stand at room temperature for seven days.

Inclusion Polymerization

The inclusion crystals (*ca.* 500mg) were placed in a glass tube 10 mm in diameter and sealed under vacuum. The tube was exposed to γ-irradiation from a ^{60}Co source at 0° C for one hour at 1.0 Mrad. After irradiation, the tube was allowed to stand at room temperature for one day. The contents were poured into excess methanol to separate the polymer from **CA**. The methanol-insoluble fraction was filtered, dried under vacuum and weighed.

Measurements

Infrared spectra were recorded on a JASCO IR-Report-100 spectrometer. ^{1}H Nuclear magnetic resonance spectra were measured at 100° C with JEOL 270 MHz spectrometer. Differential scanning calorimetry (DSC) and thermal gravimetry (TG) were performed on a Rigaku TAS 100 system. About 10 mg crystals were heated from 40 to 230° C at 5° C min^{-1}. X-Ray powder diffraction was recorded using a Rigaku RINT-2000 with Cu-K_α radiation at room temperature. Diffraction patterns of 2θ(°) angle with relative intensity in parenthesis are as follows.

CA•187 (crossing type) : 7.21(21), 9.57(32), 11.18(23), 12.47(11).

CA•187 (bilayer type) : 7.44(100), 8.28(5), 11.26(2), 12.96(2).

CA•187 (bilayer type, after γ-irradiation) : 7.07(31), 7.49(100), 8.35(8), 11.33(2), 13.02(6).

CA•210 : 7.45(44), 8.35(30), 11.23(5), 13.00(22).

CA•152 : 7.57(100), 8.49(10), 11.19(3), 13.04(8).

CA•207 : 7.20(10), 8.36(58), 10.88(1), 13.04(21).

CA•207 (after γ-irradiation) : 7.20(24), 8.32(43), 10.84(3), 13.00(20).

Average molecular weight and molecular weight distribution of polymers were measured by

a modular system for gel permeation chromatography (GPC) consisting of a Shodex Degas, JASCO Model 880-PU solvent delivery system, Shodex Model AO-50 injector and column oven system, and Shodex RI SE-61 differential refractometer interfaced with a System Instruments Chromatocorder 12. AC-803 and AC-80M Columns and polystyrene standards were from Showa Denko K.K.

Molecular Graphics

A molecular graphics study was carried out using computer software based on MODRASTE.[22] Atomic radii of hydrogen, carbon, and oxygen in the cross-sectional views were 1.20Å, 1.60Å, and 1.45Å, respectively.

3. Results and Discussion

Polymorphic Inclusion Crystals of CA with Vinyl Monomers

CA forms many guest-dependent polymorphic crystals. As described in Chapter 4, a typical crystal has a crossing structure with cage-like cavities or bilayer structure with one-dimensional cavities, called channels, as shown in Figure 6-1. A guest component usually adopts only one structure, but the same guest component may induce multiple polymorphic crystals. Therefore, preparation of the crystals by direct recrystallization and intercalation or guest-exchange was carefully tested. In the case of the guest **185** and **187**, the same guest gave crossing and bilayer structures by recrystallization,[20,21] as described in Chapter 4. Recrystallization of **CA** from liquid **185** and **187** yielded only the former crystals with the same 1:1 molar ratio of host to guest, while recrystallization using an alcohol as solvent could give the latter crystals with nitriles. Intercalation easily afforded the latter bilayer crystals. At first, inclusion crystals of **CA** with **22**[23] were prepared by recrystallization, and the crystals were soaked in **187** for seven days. X-Ray diffraction revealed that α-*gauche* type **CA•22** crystals slightly changed to α-*trans* type **CA•187** crystals that is very similar to the crystals obtained from recrystallization, as shown in Figure 6-2. Instead of **CA•22** crystals, when inclusion crystals of **CA** with ethanol (**78**) were used as original crystals, guest-exchange did not occur. This would be due to host lattice types of the original crystals. Since **CA•78** crystals have a crossing

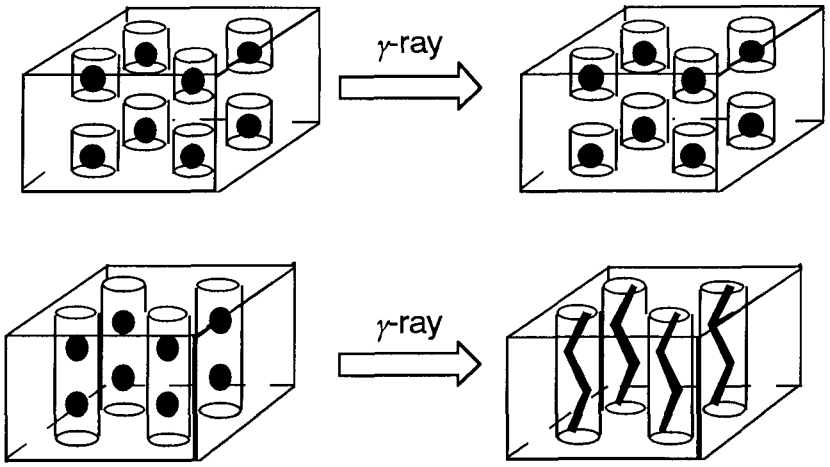


Figure 6-1. Inclusion polymerization in **CA** crystals of (a) crossing structure with cage-like cavities and (b) bilayer structure with channel cavities.

structure with cage-like cavities,[24] exchange to **CA•187** crystals requires dynamic change of the host framework with hydrogen bond networks. **CA•22** crystals have a bilayer structure, so that exchange occurs with retention of the hydrogen bond networks to yield **CA•187** crystals. The resulting crystals of **CA•187** were so stable that they did not transform to the crossing type for months. In contrast, the same α-*trans* type bilayer crystals of **CA•185** were unstable and transformed to the crossing type, meaning that the crystals were not suitable for inclusion polymerization.

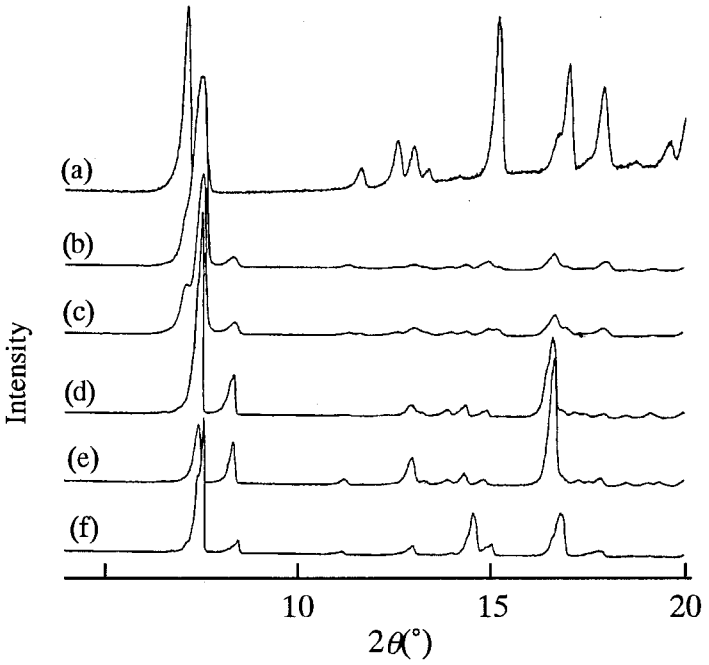


Figure 6-2. X-Ray diffraction patterns of inclusion compounds of (a) **CA•22** obtained by recrystallization, (b) guest-exchanged **CA•187**, (c) guest-exchanged **CA•187** after γ-irradiation, (d) channel-type **CA•187** obtained by recrystallization, (e) **CA•210**, and (f) **CA•152**.

Inclusion Polymerization of Vinyl Monomers

The incorporation of identical monomers in different inclusion spaces prompted us to examine cavities as reaction spaces for inclusion polymerization. The polymerization of the polymorphs of **CA•187** was carried out in a similar way to other steroidal hosts.[10-15] The results are summarized in Table 6-1. Polymers were obtained from crystals having channels but not cage-like cavities. As shown in Figure 6-1, monomers in cage-like cavities cannot react with adjacent monomers owing to hindrance of host molecules. The different results for the same host and the monomer prove that polymerization occurs in channels not outside crystals. The resulting polymers had no

Table 6-1. Inclusion polymerization of vinyl and diene monomers.

Monomer	Method [a]	Inclusion space	Yield [%] [b]	M_n / x10^4 [c]	M_w/M_n [c]
methacrylonitrile(**187**)	R	cage	0	-	-
methacrylonitrile(**187**)	E	channel	34	15	3.2
chloroacrylonitrile(**210**)	E	channel	26	0.48	2.3
vinyl acetate(**152**)	E	channel	0	-	-
2,3-dimethyl-1,3-butadiene(**207**)	E	channel	34	- [d]	- [d]

[a] R=Recrystallization, E=Guest-exchange.
[b] Methanol-insoluble fractions were weighted.
[c] M_w and M_n are based on the calibration of standard polystyrene.
[d] Not determined due to insoluble polymers.

significant differences in microstructures from polymers obtained by free-radical polymerization in solution. Polymerization in channels was confirmed by X-Ray powder diffraction. Comparison of diffraction of **CA•187** crystals before and after γ-irradiation showed they were very similar, as shown in Figure 6-2. The α-*trans* bilayer structure is thus maintained during the polymerization.

Inclusion polymerization of **210** and **152** was examined. The crystals had similar patterns to that of **CA•187** crystals, as shown in Figure 6-2, indicating that the two monomers are incorporated into channels of α-*trans* type frameworks like **187** molecules. γ-Irradiation generated the polymers from inclusion crystals of **CA•210**, but not of **CA•152**, due to different arrangements of monomers in the channels.

Figure 6-3 shows an arrangement of **187** molecules in a **CA** channel, where -C=C- double bond moieties of **187** molecules lie in the center of the channel. Similar arrangement may be achieved by **210** molecules because of the similar molecular structure with **187**, while **152** molecules may have no suitable arrangement for the reaction. Inclusion polymerization may thus require not only channel structures but also appropriate arrangements of included monomers in the channels.

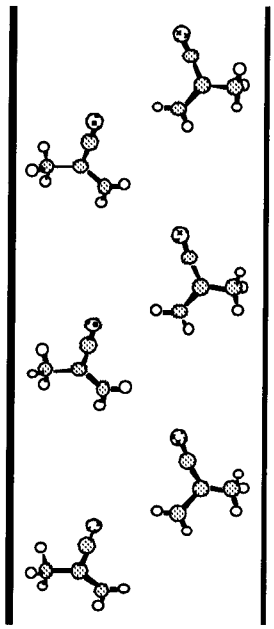


Figure 6-3. Arrangement of **187** molecules in a **CA** channel. Carbon, hydrogen, and nitrogen atoms are represented in gray, white, and dotted, respectively.

Inclusion Polymerization of Diene Monomer

As in the case of bilayer crystal of **CA•187**, inclusion compounds of **CA** with **207** were prepared by guest-exchange. When inclusion crystals of **CA•6**[15] were used as original crystals, **CA•207** crystals were easily obtained. TG-DSC measurement confirmed that inclusion crystals have 1:1 host-guest stoichiometry. When inclusion crystals of **CA•78** were used as original crystals, guest-exchange did not occur as in the case of **CA•187**. Even bilayer crystals, such as **CA•22** and **CA•139**,[25] did not give guest-exchanged **CA•207** crystals. Guest-exchange may be attributed to the channel size; the β-*trans* type crystal of **CA•6** have larger cavities than the α-type crystal of **CA•22** and **CA•139**, as described in Chapter 2. The larger cavities would lead to guest-exchange to give **CA•207** crystals easily. Appropriate original crystals should be thus selected to obtain inclusion crystals with monomers.

X-Ray powder diffraction revealed that the structures of the resulting **CA•207** crystals were different host frameworks from the original. As shown in Figure 6-4, the resulting crystals have α-*trans* type bilayer structures similar to **CA•187** crystals. Diffraction peaks of guest-exchanged

CA•207 crystals are similar to those after γ-irradiation, indicating that polymerization proceeds with retention of the same host framework with cahnnels.

γ-Irradiation of **CA•207** crystals led to solid polymer **207** as in the case of **DCA** and **ACA**, or rubber-like polymers as with **MCA** and **CDCA**. The infrared spectrum of the polymer had a strong absorption band at 1150 cm^{-1} characteristic of 1,4-addition, whereas tiny bands at 1630 cm^{-1} and 890 cm^{-1} characteristic of 1,2-addition. In the ^1H NMR spectrum, methylene resonance appeared at 2.24 ppm for the 1,4-*cis*-addition and 2.16 ppm for the 1,4-*trans*-addition, and tiny peaks for the 1,2-addition appear at 4.85 and 4.90 ppm corresponding to the double bond.[26] This shows that the polymer contained 52% of 1,4-*trans*-addition, 44% of 1,4-*cis*-addition, and 4% of 1,2-addition.

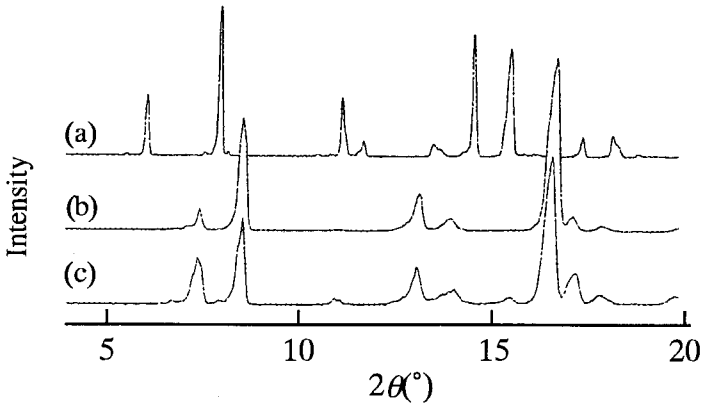


Figure 6-4. X-Ray diffraction patterns of inclusion compounds of (a) **CA•6**, (b) guest-exchanged **CA•207**, and (c) guest-exchanged **CA•207** after γ-irradiation.

Comparison with Other Steroidal Hosts

Space effects of **CA** channel may be found on the basis of the microstructure of polymer **207** obtained using steroidal hosts. As shown in Table 6-2, stereoregularity of the polymer in the case of **CA** is much lower than with **DCA**, **ACA** and **MCA**, but slightly higher than with **CDCA**. In spite of similar stereoregularity of the polymers from **CA** and **CDCA**, solubility for organic solvents differed; the polymer from **CDCA** was easily soluble in tetrahydrofuran, but not the polymer from **CA**.

Difference in the stereoregularity may be understood by comparison with channel size of each host. Host lattices of four steroidal hosts, **DCA**, **ACA**, **CA**, and **CDCA**, for **207** differ each other,[20,27-29] whereas the host lattice of **MCA•207** is unknown due to the guest-dependent structure.[14] Figure 6-5 shows cross sections of four host channels sliced perpendicular to the direction

Table 6-2. Microstructure of polymer **207** obtained using steroidal hosts.

Host	1,4-*trans* -addition [%]	1,4-*cis* -addition [%]	1,2-addition [%]	Reference
DCA	>99	0	0	[10]
ACA	>99	0	0	[12]
MCA	90	10	0	[13,14]
CA	54	42	4	this work
CDCA (None)	54	38	8	[15,(26)]

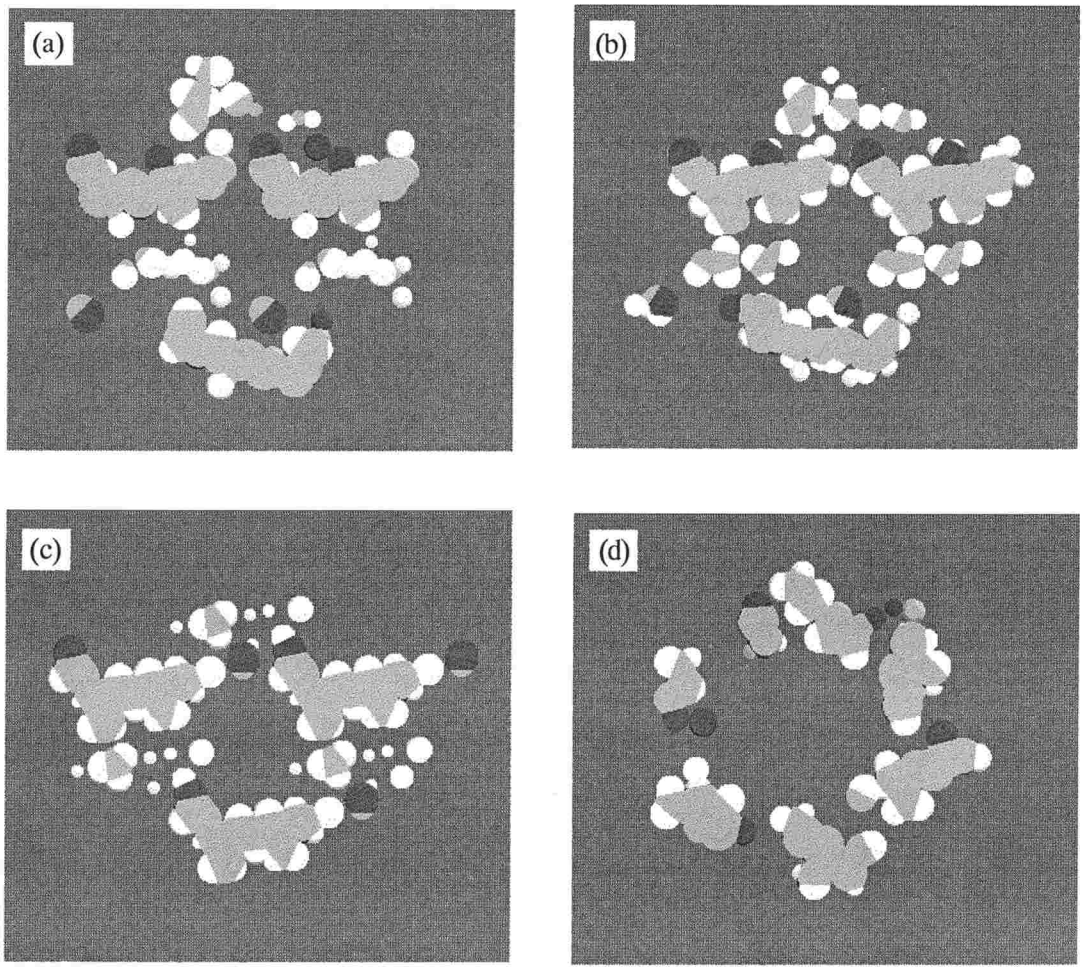


Figure 6-5. Cross sections of steroidal host channels sliced perpendicular to direction of the channel of (a) **DCA**, (b) **ACA**, (c) **CA**, and (d) **CDCA**. Guest molecules are omitted. Carbon, hydrogen, and oxygen atoms are represented in gray, white, and black, respectively.

of the channels. Cross sections of host cavities of **DCA**, **ACA**, **CA**, and **CDCA**, were nearly a 8×3.5Å square, 6.5Å in diameter, 8Å in diameter, and 12Å in diameter, respectively.

The shape of the **207** molecule is nearly a 7.4×6.5×4.2Å box, as estimated from geometrical calculation from molecular models, as shown in Figure 6-6. The microstructures of obtained polymers thus agree with channel size. The narrow channels of **DCA** and **ACA** would just fit **207** molecules and force them to be arranged in a specific direction. In contrast, the **207** molecules may move freely in **CDCA** channel as in solution. In a medium-size **CA** channel, **207** molecules move with restriction of direction. Although the host lattice of **MCA•207** is unknown as described above, the lattice may have one-dimensional

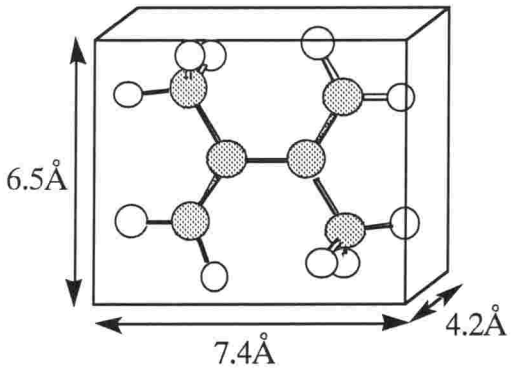


Figure 6-6. Shape of **207** molecule based on molecular modeling. Atom coding is identical to that in Figure 6-3.

cavities smaller than those of **CA** but larger than those of **ACA**.

4. Conclusion

The first inclusion polymerization using **CA** is described. As with other steroidal hosts, the monomers can be incorporated into **CA** channel of bilayer structure to give polymers. The stereoregularity of the resulting polymers was in good agreement with channel sizes of host lattices.

The control of host framework types of the monomer-included crystals was important for inclusion polymerization. The formation of desirable crystals could be achieved by the development of recrystalization method described in Chapter 1 and 4, and intercalation method described in Cahpter 5. This study should promote further research on inclusion polymerization using other hosts.

Summary

This thesis deals with systematic study of **CA** inclusion compounds: inclusion phenomena, assembly modes, polymorphism, molecular recognition, intercalation phenomena, and inclusion polymerization.

In Chapter 1, the author revealed that **CA** can form crystalline inclusion compounds with various hydrocarbons and related compounds by using alcoholic solvents. The crystal structure of inclusion compound of **CA** with benzene (**1**) shows the accommodation of the guest molecules in channel cavity without incorporation of solvents. This study enables us to compare the inclusion behaviors between **CA** and **DCA**.

In Chapter 2, the crystal structures of inclusion compounds of **CA** with 28 monosubstituted benzenes have been systematically investigated. All of the crystals belong to the monoclinic space group $P2_1$ and have bilayer structures with one-dimensional molecular channels that can include guest compounds. They are classified into four types of host frameworks that depend on the conformations of host molecules and stacking modes of the lipophilic layers. The host frameworks and the host-guest ratios depend primarily on the molecular volumes of the guest compounds. The packing coefficient of the host cavity (PC_{cavity}) is used to clarify the relationship between the guest volume and isomerization of the host frameworks. The value of PC_{cavity} for stable inclusion compounds lies in the range of 55±70 %. Compounds out of this range induce isomerization of the host frameworks or change their host-guest ratios. The packing coefficients of other host-guest compounds, in which the guest components are included in the host cavities through steric dimensions and van der Waals forces, are also in this range. These results indicate that PC_{cavity} is a useful parameter correlation for guest recognition and isomerization of the host frameworks.

In Chapter 3, molecular recognition of **CA** through enclathration of xylene isomers was described. All xylenes give lattice inclusion crystals with **CA**. Crystallographic studies revealed that they are included in the different open host frameworks. In particular, *o*-xylene (**62**) has two polymorphic forms dependent on the recrystallization temperatures. Competitive recrystallizations from mixed xylenes exhibit selective and non-selective enclathration. The selective enclathration of guest molecules was explained by the difference of the stability of **CA** inclusion crystals, judging from the *PC*cavity. The non-selective enclathration were explained by formation of "clathrate solid solutions." Recrystallization from mixture of *m*-xylene (**63**) and *p*-xylene (**64**) yielded inclusion crystals that accommodate both guest components. The host frameworks are same as that from pure **63**, and the guest components are statically disordered in the host cavity. The ratios of xylenes in single crystals are similar to those of the starting recrystallization mixtures as well as in the resulting bulk crystals. This study revealed the mechanism of the selectivity through enclathration and would develop the separation technology using lattice inclusion com-

pounds.

In Chapter 4, the formation of inclusion compounds of **CA** with a variety of organic substances having C6 or less was described. Most of the inclusion crystals have a crossing or bilayer structure depending mainly on the guest volumes. A cage-like cavity of a crossing structure is apparently smaller than a channel cavity of a bilayer structure and the difference of the cavity size agrees with that of the incorporated guest size. PC_{cavity} of two structures is in a range of 42-75% to retain the inclusion crystal. The parameter of PC_{cavity} gives a good explanation for the host framework isomerization as well as for the formation of the guest-free crystals by solvents that cannot be included. In addition, **CA** can form polymorphs of inclusion crystals for five guests. Three guests, acrylonitrile (**185**), methacrylonitrile (**187**), and nitromethane (**196**), give polymorphs consisting of 1:1 crossing and bilayer structures. They are consequence of packing in different arrangements of the same molecule. In contrast, two guests, ethyl acetate (**155**) and *o*-xylene (**62**), give two types of bilayer structures that are packing of conformation isomers. Moreover, PC_{cavity} can explain and predict the formation of the former type two-component polymorphs of inclusion compounds. This study would lead to the discovery of novel two-component polymorphs in other hosts.

In Chapter 5, dynamic property of **CA** crystals involving the same guest was described. Absorption and desorption of guests by heat treatment and soaking into the liquid guest induced the reversible change of the layers. The phenomena are very similar to intercalation phenomena in inorganic compounds having two-dimensional host frameworks, such as graphite and clay. The intercalation phenomena can be observed in **CA** crystals that have a two-step release of the guest components at heat treatment.

In Chapter 6, inclusion polymerization of vinyl and diene monomers was studied by using **CA** as a host. It was found that polymorphism of **CA** inclusion crystals played a decisive role in determining polymerizability of the monomers. The polymorphic crystals were obtained by two methods; recrystallization and guest-exchange on intercalation. In the case of methacrylonitrile (**187**), inclusion polymerization could be achieved in a bilayer structure with one-dimensional channels, but not in a crossing structure with cage-like cavities. In the case of 2,3-dimethyl-1,3-butadiene (**207**), the intercalation method yielded only the bilayer crystals. The microstructure of the resulting polymer was compared with those of the polymers obtained by using other steroidal hosts. The different stereoregularity can be explained on the basis of different channel sizes of these hosts. Study of inclusion polymerization in **CA** cavity should promote further research on inclusion polymerization using other hosts.

Through the systematic study of **CA** inclusion compounds, the parameter, PC_{cavity}, which is available universally in estimating size fitness between guest molecules and host cavities for all inclusion compounds, has been successfully introduced. In addition to the prediction of the host framework isomerization and the separation of organic compounds, as described in Chapters 2 and

3, the parameter would be useful in estimating the stability of inclusion compounds, designing host frameworks, and predicting guest molecules that can be incorporated. Such fundamental knowledge is indispensable to the further application of inclusion compounds to high functional materials including sensor, catalyst, and medicine. Finally, the author believes the novel concept of PC_{cavity} is promising in all the systems of molecular recognition and self-assembly, beyond the field of host-guest chemistry.

Appendix

Table II-1. Crystallographic data of **CA** with monosubstituted benzenes.

Compound	**CA•1**	**CA•2**	**CA•3**	**CA•4**	**CA•5**
Formula	$C_{30}H_{46}O_5$	$C_{31}H_{48}O_5$	$C_{32}H_{50}O_5$	$C_{32}H_{48}O_5$	$C_{32}H_{46}O_5$
Formula weight	486.69	500.72	514.74	512.73	510.71
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1$	$P2_1$	$P2_1$	$P2_1$	$P2_1$
a [Å]	13.627(4)	13.740(2)	12.408(7)	13.57(1)	12.264(2)
b [Å]	8.0379(9)	8.083(3)	7.828(1)	8.150(1)	7.8032(8)
c [Å]	14.076(4)	14.011(2)	16.281(6)	14.235(5)	15.465(3)
β [deg]	114.25(2)	114.05(1)	111.77(3)	114.63(4)	106.798(2)
V [Å^3]	1405.8(6)	1420.9(5)	1468.5(10)	1431.0(1)	1416.9(3)
Z	2	2	2	2	2
D_C [g/cm^3]	1.150	1.17	1.164	1.189	1.197
Number of unique reflections	3473	2677	2031	2404	2205
Number of observed reflections	1528	1898	1851	2337	2052
$R1,R_W$	0.049 ; 0.032	0.059 ; 0.146	0.058 ; 0.109	0.072 ; 0.198	0.056 ; 0.106
GOF	2.02	1.40	1.46	1.57	1.55
2θmax [deg]	55	50	50	50	50
R/P	3.51	5.82	5.54	7.00	6.14
Temperature [°C]	25	25	-70	-70	-70
Host framework	α-*gauche*	α-*gauche*	β-*trans*	α-*gauche*	β-*gauche*

Compound	**CA•6**	**CA•7**	**CA•15**	**CA•16**	**CA•17**
Formula	$C_{33}H_{52}O_5$	$C_{33}H_{50}O_5$	$C_{30}H_{45}O_5F$	$C_{30}H_{45}O_5Cl$	$C_{30}H_{45}O_5Br$
Formula weight	528.76	526.75	504.68	521.14	565.59
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1$	$P2_1$	$P2_1$	$P2_1$	$P2_1$
a [Å]	12.069(3)	12.434(4)	13.571(3)	13.663(5)	13.685(5)
b [Å]	7.843(3)	7.8811(7)	8.0647(9)	8.096(1)	8.0974(9)
c [Å]	16.245(4)	16.328(1)	14.100(4)	14.029(2)	14.013(3)
β [deg]	109.80(2)	112.060(2)	114.399(3)	114.62(3)	114.55(3)
V [Å^3]	1446.7(7)	1482.9(4)	1405.4(5)	1410.8(7)	1412.5(6)
Z	2	2	2	2	2
D_C [g/cm^3]	1.214	1.18	1.193	1.227	1.33
Number of unique reflections	3357	2446	2230	2078	2268
Number of observed reflections	2118	2303	2116	1895	2098
$R1,R_W$	0.108	0.057 ; 0.113	0.053 ; 0.121	0.068 ; 0.163	0.086 ; 0.228
GOF	3.51	1.47	1.39	1.17	1.94
2θmax [deg]	50	50	50	50	50
R/P	7.73	6.71	6.17	6.94	6.44
Temperature [°C]	-80	-70	-63	-63	-69
Host framework	β-*trans*	β-*trans*	α-*gauche*	α-*gauche*	α-*gauche*

Table II-1. Crystallographic data of **CA** with monosubstituted benzenes. (continued)

Compound	**CA•18**	**CA•19**	**CA•20**	**CA•21**	**CA•43**
Formula	$C_{30}H_{45}O_5I$	$C_{31}H_{47}O_5Cl$	$C_{31}H_{47}O_5Br$	$C_{31}H_{46}O_6$	$C_{32}H_{48}O_7$
Formula weight	612.59	535.16	579.61	514.7	544.73
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1$	$P2_1$	$P2_1$	$P2_1$	$P2_1$
a [Å]	13.681(5)	12.336(4)	12.289(8)	13.565(2)	12.256(2)
b [Å]	8.0954(9)	7.821(1)	7.829(1)	8.1110(9)	7.8972(8)
c [Å]	14.087(2)	16.238(7)	16.30(1)	14.055(6)	16.671(4)
β [deg]	114.206(2)	111.65(5)	111.50(6)	113.651(1)	109.671(4)
V [Å^3]	1423.0(4)	1456.1(9)	1459(1)	1416.5(5)	1477.6(5)
Z	2	2	2	2	2
D_C [g/cm^3]	1.43	1.22	1.319	1.207	1.224
Number of unique reflections	2468	2392	2303	2172	2574
Number of observed reflections	2397	2308	2168	2071	2490
$R1,R_W$	0.065 ; 0.178	0.050 ; 0.108	0.069 ; 0.168	0.070 ; 0.172	0.046 ; 0.106
GOF	1.85	1.83	1.34	1.41	1.40
2θmax [deg]	50	50	50	50	50
R/P	7.35	6.91	6.49	6.20	7.07
Temperature [°C]	-70	-70	-70	-70	-70
Host framework	α-*gauche*	β-*trans*	β-*trans*	α-*gauche*	β-*trans*

Compound	**CA•45**	**CA•50**	**CA•51**	**CA•54**	**CA•55**
Formula	$C_{32}H_{50}O_5$	$C_{31}H_{48}O_6$	$C_{32}H_{50}O_6$	$C_{32}H_{50}O_6$	$C_{31}H_{45}O_5N$
Formula weight	544.73	516.72	530.74	530.74	511.70
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1$	$P2_1$	$P2_1$	$P2_1$	$P2_1$
a [Å]	12.085(5)	13.566(4)	12.110(3)	12.108(3)	13.644(5)
b [Å]	7.961(2)	8.0846(9)	7.965(2)	7.9419(8)	8.164(1)
c [Å]	16.208(7)	14.225(2)	16.118(2)	16.236(3)	14.028(3)
β [deg]	109.697(1)	114.748(2)	108.47(1)	109.887(3)	113.93(4)
V [Å^3]	1468.1(7)	1416.8(2)	1474.5(5)	1468.1(4)	1428.1(7)
Z	2	2	2	2	2
D_C [g/cm^3]	1.232	1.211	1.195	1.201	1.19
Number of unique reflections	2098	2060	2024	1895	2374
Number of observed reflections	1905	1899	1897	1626	2300
$R1,R_W$	0.066 ; 0.113	0.071 ; 0.152	0.074 ; 0.199	0.085 ; 0.172	0.041 ; 0.102
GOF	1.45	1.73	1.80	1.50	1.13
2θmax [deg]	50	50	50	50	50
R/P	5.41	5.69	5.53	5.79	6.89
Temperature [°C]	-70	-70	23	-70	-70
Host framework	β-*trans*	α-*gauche*	β-*trans*	β-*trans*	α-*gauche*

Table II-1. Crystallographic data of **CA** with monosubstituted benzenes. (continued)

Compound	**CA•56**	**CA•57**	**CA•59**	**CA•60**
Formula	$C_{30}H_{46}O_6$	$C_{31}H_{48}O_6$	$C_{31}H_{49}NO_5$	$C_{32}H_{51}NO_5$
Formula weight	502.69	516.72	515.73	529.76
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1$	$P2_1$	$P2_1$	$P2_1$
a [Å]	12.068(2)	12.636(3)	12.001(4)	12.143(3)
b [Å]	7.924(2)	8.609(2)	7.9622(2)	7.953(2)
c [Å]	16.394(3)	13.90(1)	16.218(8)	16.14(1)
β [deg]	111.90(1)	105.18(5)	111.55(3)	108.194(3)
V [Å^3]	1454.5(5)	1459(1)	1441.3(9)	1480.9(10)
Z	2	2	2	2
D_C [g/cm^3]	1.148	1.176	1.188	1.188
Number of unique reflections	2371	2032	2591	2426
Number of observed reflections	2221	1852	2518	2324
$R1,R_W$	0.120;0.316	0.080 ; 0.193	0.046 ; 0.106	0.064 ; 0.153
GOF	1.88	1.98	1.62	1.51
2θmax [deg]	50.1	50.1	50	50
R/P	8.48	5.54	7.54	6.78
Temperature [°C]	-63	-70	-70	-70
Host framework	β-*trans*	α-*trans*	β-*trans*	β-*trans*

Table IV-1. Crystallographic data of **CA** with aliphatic compounds.

Compound	**CA•66**	**CA•66**	**CA•67**	**CA•68**	**CA•69**
Formula	$C_{26}H_{44}O_7$	$C_{28}H_{48}O_9$	$C_{27}H_{44}O_7$	$C_{27}H_{46}O_7$	$C_{29}H_{46}O_7$
Formula weight	468.63	528.68	480.64	482.66	506.68
Crystal system	orthorhombic	monoclinic	orthorhombic	orthorhombic	monoclinic
Space group	$P2_12_12_1$	$P2_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_1$
a [Å]	13.831(3)	13.353(2)	14.434(2)	12.7745(6)	13.144(3)
b [Å]	15.363(5)	8.189(2)	15.345(2)	12.939(1)	8.003(2)
c [Å]	12.400(3)	13.993(1)	12.4374(8)	16.658(2)	14.226(4)
α [deg]	90	90	90	90	90
β [deg]	90	112.175(8)	90	90	113.45(2)
γ [deg]	90	90	90	90	90
V [Å^3]	2634(1)	1416.9(4)	2754.8(6)	2753.3(5)	13728(6)
Z	4	2	4	4	2
D_C [g/cm^3]	1.181	1.239	1.159	1.164	1.226
Number of unique reflections	3407	3491	2711	2819	1551
Number of observed reflections	2161	2280	801	1156	1074
$R1$,R_W	0.051 ; 0.034	0.051 ; 0.034	0.068 ; 0.236	0.051 ; 0.162	0.203 ; 0.506
GOF	2.83	2.33	0.846	0.753	4.955
2θmax [deg]	55	55	50	50	50
R/P	7.25	6.85	2.61	3.75	4.08
Temperature [°C]	-65	-65	25	-70	-80
Host framework	crossing	bilayer	crossing	crossing	*α-gauche*

Compound	**CA•72**	**CA•77**	**CA•79**	**CA•80**	**CA•82**
Formula	$C_{29}H_{48}O_7$	$C_{27}H_{44}O_6$	$C_{26}H_{46}O_7$	$C_{27}H_{48}O_6$	$C_{27}H_{46}O_7$
Formula weight	508.69	464.64	470.65	468.67	482.66
Crystal system	triclinic	orthorhombic	orthorhombic	orthorhombic	orthorhombic
Space group	$P1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
a [Å]	12.367(4)	14.400(2)	14.454(3)	15.440(1)	14.8587(7)
b [Å]	14.136(6)	15.107(2)	15.149(3)	18.848(1)	15.0298(6)
c [Å]	8.255(3)	11.600(4)	11.654(2)	8.9747(5)	11.8956(5)
α [deg]	90.22(4)	90	90	90	90
β [deg]	92.93(3)	90	90	90	90
γ [deg]	106.07(3)	90	90	90	90
V [Å^3]	1384.7(9)	2523.5(9)	2551.7(8)	2611.8(3)	2656.6(2)
Z	1	4	4	4	4
D_C [g/cm^3]	1.220	1.223	1.224	1.192	1.207
Number of unique reflections	6372	1924	3279	2720	3422
Number of observed reflections	3377	1727	1445	2365	2133
$R1$,R_W	0.071 ; 0.171	0.123 ; 0.317	0.082 ; 0.229	0.054 : 0.143	0.080; 0.188
GOF	1.097	1.712	1.323	1.482	1.807
2θmax [deg]	50	50	50	50	50
R/P	5.22	5.78	4.83	7.91	6.93
Temperature [°C]	-50	-75	-80	-75	23
Host framework	*α-trans*	crossing	crossing	monolayer	crossing

Table IV-1. Crystallographic data of **CA** with aliphatic compounds. (continued)

Compound	**CA•90**	**CA•106**	**CA•113**	**CA•120**	**CA•125**
Formula	$C_{29}H_{52}O_6$	$C_{30}H_{54}O_6$	$C_{29}H_{50}O_6$	$C_{29}H_{48}O_7$	$C_{28}H_{48}O_6$
Formula weight	496.73	510.75	494.71	508.69	480.68
Crystal system	monoclinic	monoclinic	monoclinic	triclinic	monoclinic
Space group	$P2_1$	$P2_1$	$P2_1$	$P1$	$P2_1$
a [Å]	12.320(3)	13.3792(6)	12.621(2)	12.264(2)	13.6856(8)
b [Å]	7.967(1)	8.6640(3)	8.087(1)	14.452(7)	7.7174(4)
c [Å]	14.065(3)	14.1228(6)	13.921(2)	8.178(2)	14.0292(8)
α [deg]	90	90	90	90.48(3)	90
β [deg]	104.639(6)	112.9523(9)	103.122(4)	92.88(1)	114.978(3)
γ [deg]	90	90	90	105.19(2)	90
V [Å^3]	1335.8(5)	1507.5(1)	1383.8(4)	1396.8(1)	1343.1(1)
Z	2	2	2	1	2
D_C [g/cm^3]	1.235	1.125	1.187	1.209	1.188
Number of unique reflections	2512	3671	2497	4237	2616
Number of observed reflections	2110	1980	2085	3972	2340
$R1,R_W$	0.101 ; 0.280	0.059 ; 0.173	0.068 ; 0.181	0.052 ; 0.123	0.044 ; 0.110
GOF	1.923	0.948	1.833	1.766	1.322
2θmax [deg]	50	50	50	50	50
R/P	8.02	6.07	6.58	6.11	7.60
Temperature [°C]	-75	23	-75	15	-73
Host framework	α-*trans*	α-*gauche*	α-*trans*	α-*trans*	α-*trans*

Compound	**CA•133**	**CA•155**	**CA•159**	**CA•161**	**CA•162**
Formula	$C_{29}H_{48}O_7$	$C_{56}H_{96}O_{14}$	$C_{29}H_{48}O_7$	$C_{58}H_{96}O_{14}$	$C_{29}H_{48}O_7$
Formula weight	508.69	993.37	508.69	1017.39	508.69
Crystal system	monoclinic	triclinic	monoclinic	triclinic	monoclinic
Space group	$P2_1$	$P2_1$	$P2_1$	$P1$	$P2_1$
a [Å]	13.540(3)	12.279(1)	12.223(2)	12.2853(7)	12.40(2)
b [Å]	8.005(2)	14.157(1)	7.760(2)	14.3679(9)	7.696(2)
c [Å]	14.055(3)	8.2446(7)	15.214(3)	8.3632(5)	15.262(5)
α [deg]	90	90.408(3)	90	90.528(2)	90
β [deg]	113.43(1)	94.234(3)	104.91(1)	95.262(3)	105.42(6)
γ [deg]	90	105.690(5)	90	107.179(2)	90
V[Å^3]	1397.7	1375.5(2)	1394.4(5)	1403.4(1)	1404(1)
Z	2	2	2	1	2
D_C [g/cm^3]	1.209	1.199	1.211	1.204	1.203
Number of unique reflections	3451	4484	3436	4630	2538
Number of observed reflections	2474	4428	2218	4108	2312
$R1,R_W$	0.070 ; 0.1757	0.066 ; 0.166	0.059 ; 0.147	0.058 ; 0.147	0.062 ; 0.163
GOF	1.709	2.378	1.182	1.850	1.263
2θmax [deg]	50	50	50	50	50
R/P	7.61	7.01	6.82	6.32	7.09
Temperature [°C]	-70	-68	25	-75	15
Host framework	α-*gauche*	α-*trans*	β-*gauche*	α-*trans*	β-*gauche*

Table IV-1. Crystallographic data of **CA** with aliphatic compounds. (continued)

Compound	**CA•169**	**CA•185**	**CA•185**	**CA•187**	**CA•187**
Formula	$C_{30}H_{48}O_7$	$C_{27}H_{43}O_5N$	$C_{27}H_{43}O_5N$	$C_{28}H_{45}O_5N$	$C_{28}H_{45}O_5N$
Formula weight	520.71	461.64	461.64	475.67	475.67
Crystal system	monoclinic	orthorhombic	monoclinic	orthorhombic	triclinic
Space group	$P2_1$	$P2_12_12_1$	$P2_1$	$P2_12_12_1$	$P1$
a [Å]	12.367(2)	16.882(3)	12.183(2)	16.708(2)	12.533(6)
b [Å]	7.731(5)	17.619(2)	7.878(1)	17.848(1)	14.16(1)
c [Å]	15.429(5)	8.497(1)	14.300(3)	8.648(1)	8.277(2)
α [deg]	90	90	90	90	90.94(4)
β [deg]	106.53(2)	90	104.16(1)	90	94.86(3)
γ [deg]	90	90	90	90	107.23(4)
V [Å^3]	1414.1(10)	2527.5(5)	1330.8(4)	2578.77(4)	1396(1)
Z	2	4	2	4	1
D_C [g/cm^3]	1.223	1.213	1.152	1.205	1.092
Number of unique reflections	3476	3303	3284	3774	6633
Number of observed reflections	1917	1378	1566	2255	5014
$R1,R_W$	0.062 ; 0.153	0.089 ; 0.088	0.055 ; 0.036	0.057 ; 0.058	0.047 ; 0.049
GOF	1.109	2.74	1.93	1.98	2.02
2θmax [deg]	50	55	55	55	55
R/P	5.74	5.12	5.27	7.34	8.21
Temperature [°C]	-70	-70	-65	-65	-65
Host framework	β-*gauche*	crossing	α-*trans*	crossing	α-*trans*

Compound	**CA•196**
Formula	$C_{25}H_{43}O_7N$
Formula weight	469.62
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a [Å]	16.640(1)
b [Å]	17.910(1)
c [Å]	8.4482(5)
α [deg]	90
β [deg]	90
γ [deg]	90
V [Å^3]	2517.8(3)
Z	4
D_C [g/cm^3]	1.239
Number of unique reflections	2579
Number of observed reflections	1736
$R1,R_W$	0.053 ; 0.137
GOF	0.885
2θmax [deg]	50
R/P	5.81
Temperature [°C]	-68
Host framework	crossing

Atomic coordinates and thermal parameters

CA·1

atom	x	y	z	U	atom	x	y	z	U
O(25)	1.0912(6)	-0.2789	0.6202(4)	0.055(2)	H(4B)	1.033(5)	-0.383(9)	0.435(5)	0.0469
O(26)	0.8183(4)	0.034(1)	0.1937(4)	0.049(2)	H(5)	1.229(5)	-0.407(9)	0.419(4)	0.0456
O(27)	0.3468(6)	-0.227(1)	-0.1492(5)	0.099(3)	H(6A)	1.156(5)	-0.529(9)	0.274(5)	0.0507
O(28)	0.2999(5)	0.040(1)	-0.1952(5)	0.092(3)	H(6B)	1.126(5)	-0.648(8)	0.357(5)	0.0507
O(29)	0.9156(5)	-0.507(1)	0.2693(4)	0.049(2)	H(7)	0.973(5)	-0.576(8)	0.158(4)	0.0481
C(1)	1.1802(6)	-0.076(1)	0.4269(6)	0.043(2)	H(8)	1.024(4)	-0.311(8)	0.139(4)	0.0380
C(2)	1.1289(6)	-0.092(1)	0.5062(5)	0.041(2)	H(9)	0.980(5)	-0.179(9)	0.302(4)	0.0405
C(3)	1.1488(6)	-0.265(1)	0.5546(6)	0.046(3)	H(11A)	1.013(5)	0.074(9)	0.258(5)	0.0481
C(4)	1.1053(6)	-0.394(1)	0.4684(6)	0.040(2)	H(11B)	1.052(4)	0.032(8)	0.166(4)	0.0481
C(5)	1.1526(6)	-0.381(1)	0.3868(6)	0.040(2)	H(12)	0.874(5)	0.151(8)	0.099(5)	0.0481
C(6)	1.1073(6)	-0.520(1)	0.3051(5)	0.043(3)	H(14)	0.815(4)	-0.263(8)	0.158(4)	0.0418
C(7)	0.9924(5)	-0.488(1)	0.2244(5)	0.039(2)	H(15A)	0.805(5)	-0.499(9)	0.048(5)	0.0532
C(8)	0.9793(6)	-0.310(1)	0.1779(5)	0.033(2)	H(15B)	0.850(5)	-0.433(9)	-0.019(5)	0.0532
C(9)	1.0211(6)	-0.174(1)	0.2618(6)	0.033(2)	H(16A)	0.645(5)	-0.340(10)	-0.071(6)	0.0595
C(10)	1.1412(5)	-0.204(1)	0.3399(5)	0.038(2)	H(16B)	0.700(6)	-0.319(9)	-0.127(5)	0.0595
C(11)	1.0004(6)	-0.001(1)	0.2115(5)	0.039(2)	H(17)	0.681(4)	-0.110(8)	0.046(4)	0.0443
C(12)	0.8822(6)	0.032(1)	0.1339(5)	0.041(2)	H(18A)	0.873(5)	-0.180(9)	-0.089(5)	0.0507
C(13)	0.8442(5)	-0.104(1)	0.0508(5)	0.033(2)	H(18B)	0.988(5)	-0.100(8)	0.023(5)	0.0507
C(14)	0.8627(6)	-0.275(1)	0.1069(5)	0.033(2)	H(18C)	0.891(5)	0.047(9)	-0.060(5)	0.0507
C(15)	0.8040(7)	-0.399(1)	0.0184(6)	0.045(3)	H(19B)	1.185(5)	-0.230(10)	0.209(5)	0.0646
C(16)	0.7051(7)	-0.302(1)	-0.0543(7)	0.048(3)	H(19C)	1.220(6)	-0.079(9)	0.264(5)	0.0646
C(17)	0.7192(5)	-0.117(1)	-0.0175(5)	0.033(2)	H(19A)	1.309(5)	-0.23(1)	0.344(5)	0.0646
C(18)	0.9047(6)	-0.085(1)	-0.0210(6)	0.044(3)	H(20)	0.703(5)	-0.011(9)	-0.156(4)	0.0507
C(19)	1.2176(7)	-0.191(1)	0.2810(7)	0.055(3)	H(21B)	0.756(5)	0.23(1)	-0.058(5)	0.0633
C(20)	0.6643(6)	0.002(1)	-0.1102(5)	0.041(2)	H(21C)	0.644(5)	0.27(1)	-0.130(5)	0.0633
C(21)	0.6826(7)	0.185(1)	-0.0802(7)	0.054(3)	H(21A)	0.657(6)	0.21(1)	-0.026(5)	0.0633
C(22)	0.5439(6)	-0.038(1)	-0.1659(5)	0.044(3)	H(22B)	0.516(5)	0.042(9)	-0.214(5)	0.0507
C(23)	0.4811(7)	-0.015(2)	-0.0991(6)	0.060(3)	H(22A)	0.535(5)	-0.167(8)	-0.192(5)	0.0507
C(24)	0.3681(7)	-0.083(2)	-0.1499(6)	0.056(3)	H(23B)	0.513(6)	-0.07(1)	-0.034(5)	0.0760
C(30)	1.392(2)	0.317(3)	0.530(1)	0.163(10)	H(23A)	0.478(6)	0.13(1)	-0.089(5)	0.0760
C(31)	1.343(1)	0.285(2)	0.594(2)	0.160(8)	H(25)	1.106(8)	-0.33(1)	0.652(6)	0.0760
C(32)	1.362(1)	0.376(2)	0.680(1)	0.128(7)	H(26)	0.778(6)	0.06(1)	0.176(7)	0.0697
C(33)	1.437(1)	0.496(2)	0.701(1)	0.149(7)	H(28)	0.258(6)	0.01(1)	-0.221(6)	0.1077
C(34)	1.490(1)	0.531(3)	0.642(2)	0.18(1)	H(29)	0.911(7)	-0.57(1)	0.301(6)	0.0595
C(35)	1.468(1)	0.436(3)	0.557(2)	0.175(10)	H(30)	1.3742	0.2551	0.4680	0.1824
H(1A)	1.253(5)	-0.100(9)	0.465(5)	0.0507	H(31)	1.2938	0.1942	0.5769	0.1824
H(1B)	1.176(5)	0.051(9)	0.396(5)	0.0507	H(32)	1.3260	0.3533	0.7252	0.1520
H(2A)	1.037(5)	-0.068(8)	0.456(4)	0.0481	H(33)	1.4533	0.5607	0.7633	0.1672
H(2B)	1.159(4)	-0.002(9)	0.561(4)	0.0481	H(34)	1.5396	0.6191	0.6584	0.2153
H(3)	1.230(5)	-0.277(9)	0.605(4)	0.0545	H(35)	1.5083	0.4493	0.5157	0.1963
H(4A)	1.119(5)	-0.494(9)	0.510(5)	0.0469					

CA·2

atom	x	y	z	U	atom	x	y	z	U
O(1)	1.0926(3)	0.132(1)	1.1215(2)	0.058(1)	H(7)	1.0268	0.0292	0.9335	0.0596
O(2)	0.9158(2)	-0.095(1)	0.7694(2)	0.0544(10)	H(8)	1.2241	0.0147	0.9217	0.0602
O(3)	0.8143(2)	0.445(1)	0.6925(2)	0.0528(9)	H(9)	1.1512	-0.1045	0.7642	0.0688
O(4)	0.3496(4)	0.179(1)	0.3514(4)	0.121(2)	H(10)	1.1110	-0.2045	0.8355	0.0688
O(5)	0.2988(3)	0.442(1)	0.3075(3)	0.108(2)	H(11)	0.9735	-0.1511	0.6676	0.0552
C(1)	1.1760(4)	0.336(1)	0.9260(3)	0.050(1)	H(12)	1.0174	0.1096	0.6338	0.0518
C(2)	1.1257(4)	0.319(1)	1.0048(3)	0.047(1)	H(13)	0.9735	0.2310	0.8000	0.0495
C(3)	1.1451(4)	0.149(1)	1.0516(3)	0.050(1)	H(14)	1.0148	0.4912	0.7616	0.0555
C(4)	1.1036(4)	0.020(1)	0.9669(3)	0.044(1)	H(15)	1.0379	0.4200	0.6701	0.0555
C(5)	1.1482(3)	0.034(1)	0.8842(3)	0.049(1)	H(16)	0.8751	0.5458	0.6007	0.0547
C(6)	1.1041(4)	-0.100(1)	0.8018(3)	0.051(1)	H(17)	0.8228	0.1397	0.6487	0.0459
C(7)	0.9903(4)	-0.072(1)	0.7231(3)	0.046(1)	H(18)	0.8453	-0.0168	0.4805	0.0698
C(8)	0.9766(3)	0.103(1)	0.6755(3)	0.0394(10)	H(19)	0.7822	-0.0831	0.5424	0.0698
C(9)	1.0168(3)	0.239(1)	0.7596(3)	0.0370(10)	H(20)	0.6971	0.1054	0.3735	0.0691
C(10)	1.1361(3)	0.209(1)	0.8360(3)	0.046(1)	H(21)	0.6407	0.0646	0.4467	0.0691
C(11)	0.9949(4)	0.410(1)	0.7097(3)	0.045(1)	H(22)	0.6815	0.3066	0.5267	0.0532
C(12)	0.8782(3)	0.441(1)	0.6327(3)	0.043(1)	H(23)	0.9736	0.3171	0.5156	0.0698
C(13)	0.8395(3)	0.307(1)	0.5479(3)	0.039(1)	H(24)	0.8764	0.2464	0.4219	0.0698
C(14)	0.8605(3)	0.137(1)	0.6040(3)	0.037(1)	H(25)	0.8846	0.4350	0.4442	0.0698
C(15)	0.8033(4)	0.015(1)	0.5163(3)	0.050(1)	H(26)	1.2814	0.2024	0.8213	0.0805
C(16)	0.7039(4)	0.109(1)	0.4445(4)	0.054(1)	H(27)	1.1868	0.1464	0.7199	0.0805
C(17)	0.7183(3)	0.293(1)	0.4817(3)	0.042(1)	H(28)	1.2041	0.3329	0.7479	0.0805
C(18)	0.8999(4)	0.325(1)	0.4766(3)	0.053(1)	H(29)	0.6943	0.3895	0.3387	0.0647
C(19)	1.2108(4)	0.226(1)	0.7776(4)	0.066(2)	H(30)	0.7504	0.6215	0.4494	0.0772
C(20)	0.6614(3)	0.411(1)	0.3890(3)	0.047(1)	H(31)	0.6443	0.6598	0.3545	0.0772
C(21)	0.6779(4)	0.593(1)	0.4188(4)	0.060(1)	H(32)	0.6436	0.6185	0.4624	0.0772
C(22)	0.5418(4)	0.371(1)	0.3335(3)	0.053(1)	H(33)	0.5085	0.4405	0.2743	0.0724
C(23)	0.4798(4)	0.385(1)	0.4011(4)	0.063(2)	H(34)	0.5329	0.2569	0.3078	0.0724
C(24)	0.3689(4)	0.323(2)	0.3505(4)	0.069(1)	H(35)	0.5167	0.3214	0.4656	0.0843
C(25)	0.5709(8)	0.324(2)	0.961(1)	0.162(4)	H(36)	0.4823	0.4992	0.4236	0.0843
C(26)	0.6514(8)	0.226(2)	0.9675(9)	0.148(3)	H(37)	0.5931	0.4014	1.1056	0.0755
C(27)	0.676(1)	0.214(2)	0.883(1)	0.186(6)	H(38)	0.4738	0.4198	1.0306	0.0669
C(28)	0.630(1)	0.293(2)	0.794(1)	0.161(6)	H(39)	0.5202	0.2465	1.0723	0.0669
C(29)	0.549(1)	0.387(2)	0.792(1)	0.186(6)	H(40)	0.4516	0.4843	0.8524	0.1565
C(30)	0.5114(8)	0.409(2)	0.869(1)	0.179(5)	H(41)	0.6950	0.1718	1.0443	0.1604
C(31)	0.544(1)	0.341(3)	1.047(1)	0.27(1)	H(42)	0.7420	0.1390	0.9101	0.2101
H(1)	1.1618	0.4446	0.8962	0.0696	H(43)	0.6604	0.2760	0.7373	0.2159
H(2)	1.2519	0.3241	0.9626	0.0696	H(44)	0.5033	0.4368	0.7135	0.2140
H(3)	1.1554	0.3992	1.0583	0.0622	H(45)	1.1277	0.0435	1.1930	0.1880
H(4)	1.0510	0.3369	0.9694	0.0622	H(48)	0.9266	-0.1704	0.8325	0.2315
H(5)	1.2201	0.1332	1.0896	0.0654	H(49)	0.7766	0.5698	0.6733	0.2315
H(6)	1.1190	-0.0884	0.9992	0.0596	H(50)	0.2166	0.4135	0.2558	0.2315

CA·3

atom	x	y	z	U	atom	x	y	z	U
O(1)	-0.6080(3)	-0.132(1)	-0.6009(3)	0.039(1)	H(8)	-0.3058	-0.0202	-0.6348	0.0320
O(2)	-0.2533(3)	0.098(1)	-0.3837(2)	0.0258(9)	H(9)	-0.1510	0.1142	-0.5409	0.0364
O(3)	-0.1926(3)	-0.447(1)	-0.2868(2)	0.033(1)	H(10)	-0.2571	0.2095	-0.5342	0.0364
O(4)	0.1826(4)	-0.225(1)	0.1719(3)	0.044(1)	H(11)	-0.1070	0.1638	-0.3963	0.0311
O(5)	0.2728(3)	-0.467(1)	0.2291(2)	0.037(1)	H(12)	-0.0458	-0.1032	-0.4135	0.0268
C(1)	-0.3368(5)	-0.352(1)	-0.5988(3)	0.033(1)	H(13)	-0.2615	-0.2344	-0.4302	0.0284
C(2)	-0.4523(5)	-0.329(1)	-0.5864(3)	0.032(1)	H(14)	-0.0759	-0.4340	-0.4333	0.0345
C(3)	-0.5029(5)	-0.151(1)	-0.6183(3)	0.029(1)	H(15)	-0.1953	-0.5059	-0.4398	0.0345
C(4)	-0.4141(4)	-0.017(1)	-0.5663(4)	0.029(1)	H(16)	-0.0533	-0.5484	-0.2992	0.0359
C(5)	-0.2949(5)	-0.037(1)	-0.5749(4)	0.025(1)	H(17)	-0.1382	-0.1298	-0.2834	0.0269
C(6)	-0.2143(4)	0.106(1)	-0.5217(3)	0.030(1)	H(18)	0.0711	0.0361	-0.2555	0.0335
C(7)	-0.1658(4)	0.081(1)	-0.4218(3)	0.025(1)	H(19)	-0.0322	0.1073	-0.2340	0.0335
C(8)	-0.1123(4)	-0.098(1)	-0.3975(3)	0.021(1)	H(20)	0.1389	-0.0705	-0.1195	0.0394
C(9)	-0.1956(5)	-0.242(1)	-0.4467(3)	0.023(1)	H(21)	0.0225	-0.0355	-0.1074	0.0394
C(10)	-0.2419(5)	-0.220(1)	-0.5491(3)	0.027(1)	H(22)	-0.0467	-0.2952	-0.1534	0.0296
C(11)	-0.1395(4)	-0.419(1)	-0.4139(3)	0.027(1)	H(23)	0.1569	-0.2271	-0.2561	0.0390
C(12)	-0.0930(5)	-0.442(1)	-0.3136(3)	0.028(1)	H(24)	0.1410	-0.4239	-0.2606	0.0390
C(13)	-0.0075(4)	-0.298(1)	-0.2647(3)	0.024(1)	H(25)	0.0870	-0.3146	-0.3456	0.0390
C(14)	-0.0702(4)	-0.127(1)	-0.2971(3)	0.021(1)	H(26)	-0.0813	-0.1679	-0.5543	0.0441
C(15)	0.0095(4)	0.007(1)	-0.2364(3)	0.027(1)	H(27)	-0.1150	-0.3586	-0.5737	0.0441
C(16)	0.0571(5)	-0.083(1)	-0.1456(4)	0.032(1)	H(28)	-0.1715	-0.2215	-0.6456	0.0441
C(17)	0.0235(4)	-0.279(1)	-0.1634(3)	0.023(1)	H(29)	0.1896	-0.3625	-0.0973	0.0334
C(18)	0.1053(5)	-0.318(1)	-0.2837(4)	0.033(2)	H(30)	0.0242	-0.6191	-0.1124	0.0462
C(19)	-0.1419(5)	-0.244(1)	-0.5838(4)	0.036(2)	H(31)	0.1571	-0.6488	-0.0699	0.0462
C(20)	0.1162(4)	-0.392(1)	-0.0950(3)	0.026(1)	H(32)	0.0990	-0.6116	-0.1704	0.0462
C(21)	0.0971(5)	-0.586(1)	-0.1135(4)	0.038(2)	H(33)	0.1306	-0.2290	0.0056	0.0375
C(22)	0.1205(5)	-0.347(1)	-0.0024(3)	0.031(1)	H(34)	0.0476	-0.3805	0.0002	0.0375
C(23)	0.2145(5)	-0.434(1)	0.0752(3)	0.033(1)	H(35)	0.1981	-0.5533	0.0744	0.0418
C(24)	0.2220(4)	-0.362(1)	0.1630(4)	0.031(1)	H(36)	0.2872	-0.4188	0.0694	0.0418
C(25)	-0.5030(7)	-0.540(1)	-0.1081(5)	0.067(2)	H(37)	-0.6529	-0.0345	-0.6278	0.0488
C(26)	-0.3863(7)	-0.518(2)	-0.0992(7)	0.118(3)	H(38)	-0.3033	0.1949	-0.3985	0.0333
C(27)	-0.3567(9)	-0.384(2)	-0.147(1)	0.142(6)	H(39)	-0.1670	-0.5286	-0.2397	0.0416
C(28)	-0.445(1)	-0.281(2)	-0.1998(8)	0.125(5)	H(40)	0.2927	-0.4355	0.2894	0.0462
C(29)	-0.551(1)	-0.307(2)	-0.2053(6)	0.108(4)	H(41)	-0.3261	-0.5947	-0.0612	0.0892
C(30)	-0.5806(6)	-0.430(1)	-0.1630(5)	0.071(3)	H(42)	-0.2766	-0.3768	-0.1396	0.0892
C(31)	-0.5417(10)	-0.681(1)	-0.0626(6)	0.110(4)	H(43)	-0.4208	-0.1943	-0.2317	0.0892
C(32)	-0.5990(10)	-0.825(2)	-0.1224(6)	0.127(4)	H(44)	-0.6144	-0.2297	-0.2454	0.0892
H(1)	-0.3088	-0.4639	-0.5784	0.0418	H(45)	-0.6638	-0.4477	-0.1670	0.0892
H(2)	-0.3516	-0.3442	-0.6601	0.0418	H(46)	-0.4765	-0.7247	-0.0161	0.1292
H(3)	-0.4402	-0.3407	-0.5254	0.0406	H(47)	-0.5957	-0.6349	-0.0395	0.1292
H(4)	-0.5060	-0.4134	-0.6194	0.0406	H(48)	-0.6668	-0.7855	-0.1690	0.1552
H(5)	-0.5185	-0.1415	-0.6794	0.0369	H(49)	-0.5477	-0.8752	-0.1456	0.1552
H(6)	-0.4445	0.0912	-0.5886	0.0363	H(50)	-0.6225	-0.9099	-0.0893	0.1552
H(7)	-0.4040	-0.0264	-0.5061	0.0363					

CA·4

atom	x	y	z	U	atom	x	y	z	U
O(1)	-0.9124(2)	-0.085(1)	0.1199(2)	0.0478(8)	H(7)	-0.9760	-0.1864	-0.0661	0.0467
O(2)	-1.0898(2)	-0.315(1)	-0.2309(2)	0.0415(7)	H(8)	-0.7735	-0.2254	-0.0701	0.0498
O(3)	-1.1701(2)	0.225(1)	-0.3031(2)	0.0486(8)	H(9)	-0.8485	-0.3479	-0.2232	0.0512
O(4)	-1.6604(3)	-0.030(1)	-0.6437(3)	0.088(1)	H(10)	-0.8986	-0.4332	-0.1559	0.0512
O(5)	-1.6975(2)	0.232(1)	-0.6847(3)	0.0705(10)	H(11)	-1.0247	-0.3767	-0.3263	0.0447
C(1)	-0.8112(3)	0.099(1)	-0.0665(3)	0.046(1)	H(12)	-0.9744	-0.1254	-0.3565	0.0392
C(2)	-0.8665(3)	0.092(1)	0.0075(3)	0.0442(10)	H(13)	-1.0160	0.0051	-0.1959	0.0402
C(3)	-0.8550(3)	-0.080(1)	0.0539(3)	0.0419(9)	H(14)	-0.9688	0.2593	-0.2316	0.0489
C(4)	-0.9003(3)	-0.206(1)	-0.0297(3)	0.0389(9)	H(15)	-0.9442	0.1874	-0.3203	0.0489
C(5)	-0.8482(3)	-0.201(1)	-0.1077(3)	0.0416(9)	H(16)	-1.1095	0.3187	-0.3941	0.0489
C(6)	-0.8957(3)	-0.335(1)	-0.1898(3)	0.0428(10)	H(17)	-1.1729	-0.0812	-0.3513	0.0398
C(7)	-1.0086(3)	-0.300(1)	-0.2723(3)	0.0372(8)	H(18)	-1.2134	-0.3013	-0.4531	0.0473
C(8)	-1.0173(3)	-0.128(1)	-0.3182(3)	0.0326(8)	H(19)	-1.1482	-0.2381	-0.5131	0.0473
C(9)	-0.9730(3)	0.008(1)	-0.2343(3)	0.0335(8)	H(20)	-1.3562	-0.1485	-0.5485	0.0509
C(10)	-0.8544(3)	-0.026(1)	-0.1566(3)	0.0410(9)	H(21)	-1.2991	-0.1132	-0.6208	0.0509
C(11)	-0.9896(3)	0.178(1)	-0.2847(3)	0.0406(9)	H(22)	-1.3080	0.0872	-0.4681	0.0461
C(12)	-1.1076(3)	0.215(1)	-0.3625(3)	0.0406(9)	H(23)	-1.1170	0.0179	-0.5715	0.0583
C(13)	-1.1492(3)	0.082(1)	-0.4467(3)	0.0363(8)	H(24)	-1.0950	0.2025	-0.5443	0.0583
C(14)	-1.1327(3)	-0.086(1)	-0.3922(2)	0.0332(8)	H(25)	-1.0131	0.0715	-0.4771	0.0583
C(15)	-1.1920(3)	-0.207(1)	-0.4787(3)	0.0394(9)	H(26)	-0.7706	0.0887	-0.2308	0.0629
C(16)	-1.2924(3)	-0.107(1)	-0.5517(3)	0.0425(9)	H(27)	-0.8002	-0.0912	-0.2674	0.0629
C(17)	-1.2739(3)	0.074(1)	-0.5140(3)	0.0385(8)	H(28)	-0.7051	-0.0550	-0.1613	0.0629
C(18)	-1.0876(3)	0.094(1)	-0.5166(3)	0.049(1)	H(29)	-1.3003	0.1749	-0.6528	0.0593
C(19)	-0.7749(3)	-0.021(1)	-0.2091(3)	0.052(1)	H(30)	-1.3491	0.4403	-0.6344	0.0735
C(20)	-1.3301(3)	0.194(1)	-0.6041(3)	0.0493(10)	H(31)	-1.2348	0.3976	-0.5507	0.0735
C(21)	-1.3100(4)	0.374(1)	-0.5753(4)	0.061(1)	H(32)	-1.3337	0.3990	-0.5228	0.0735
C(22)	-1.4527(3)	0.157(1)	-0.6599(3)	0.052(1)	H(33)	-1.4844	0.2342	-0.7146	0.0626
C(23)	-1.5145(3)	0.166(1)	-0.5901(4)	0.064(1)	H(34)	-1.4610	0.0497	-0.6878	0.0626
C(24)	-1.6288(3)	0.115(1)	-0.6446(4)	0.058(1)	H(35)	-1.5126	0.2769	-0.5674	0.0767
C(25)	-1.432(1)	0.087(2)	-0.083(1)	0.174(4)	H(36)	-1.4796	0.0973	-0.5321	0.0767
C(26)	-1.347(1)	0.001(2)	-0.0656(7)	0.166(4)	H(37)	-0.8832	-0.1715	0.1681	0.0566
C(27)	-1.3092(7)	0.001(2)	-0.1490(9)	0.141(3)	H(38)	-1.0835	-0.3866	-0.1764	0.0494
C(28)	-1.3632(6)	0.084(1)	-0.2342(7)	0.103(2)	H(39)	-1.2158	0.3134	-0.3413	0.0567
C(29)	-1.4428(8)	0.165(1)	-0.2477(8)	0.130(3)	H(40)	-1.7853	0.1969	-0.7118	0.0822
C(30)	-1.4794(8)	0.174(2)	-0.1733(9)	0.147(4)	H(41)	-1.3090	-0.0576	-0.0034	0.1986
C(31)	-1.460(1)	0.097(2)	0.0021(8)	0.35(1)	H(42)	-1.2462	-0.0576	-0.1417	0.1688
C(32)	-1.433(1)	0.059(3)	0.0900(8)	0.28(1)	H(43)	-1.3393	0.0806	-0.2880	0.1232
H(1)	-0.8211	0.2069	-0.0954	0.0555	H(44)	-1.4789	0.2226	-0.3110	0.1565
H(2)	-0.7360	0.0798	-0.0278	0.0555	H(45)	-1.5402	0.2430	-0.1848	0.1778
H(3)	-0.8338	0.1701	0.0614	0.0531	H(46)	-1.5242	0.1616	-0.0177	0.4316
H(4)	-0.9413	0.1178	-0.0292	0.0531	H(47)	-1.3683	-0.0069	0.1229	0.3557
H(5)	-0.7804	-0.1015	0.0941	0.0504	H(48)	-1.4730	0.0894	0.1269	0.3557
H(6)	-0.8886	-0.3106	0.0015	0.0467					

CA·5

atom	x	y	z	U	atom	x	y	z	U
O(1)	0.5197(2)	-0.0548(9)	0.3958(2)	0.0375(7)	H(6)	0.3620	-0.2632	0.4092	0.0397
O(2)	0.3479(2)	-0.2833(9)	0.6173(2)	0.0364(7)	H(7)	0.3970	-0.1500	0.4953	0.0397
O(3)	0.3889(2)	0.2755(9)	0.7269(2)	0.0344(7)	H(8)	0.1866	-0.1214	0.3644	0.0385
O(4)	0.5135(3)	0.224(1)	1.2075(2)	0.107(2)	H(9)	0.2158	-0.3768	0.4679	0.0421
O(5)	0.4942(3)	-0.027(1)	1.1344(3)	0.094(1)	H(10)	0.1067	-0.2720	0.4631	0.0421
C(1)	0.2548(3)	0.1850(9)	0.4051(2)	0.0311(10)	H(11)	0.1907	-0.3199	0.6140	0.0385
C(2)	0.3815(3)	0.1562(9)	0.4155(3)	0.0313(9)	H(12)	0.1182	-0.0468	0.6009	0.0380
C(3)	0.4008(3)	-0.0208(9)	0.3830(2)	0.0305(9)	H(13)	0.3263	0.0626	0.5757	0.0319
C(4)	0.3539(3)	-0.1536(9)	0.4336(3)	0.032(1)	H(14)	0.2588	0.3363	0.5678	0.0369
C(5)	0.2273(3)	-0.1292(9)	0.4285(2)	0.0307(10)	H(15)	0.1425	0.2712	0.5756	0.0369
C(6)	0.1874(3)	-0.2695(9)	0.4818(3)	0.0337(10)	H(16)	0.2389	0.3853	0.7121	0.0366
C(7)	0.2277(3)	-0.2450(9)	0.5839(2)	0.0305(8)	H(17)	0.3283	-0.0316	0.7147	0.0380
C(8)	0.2012(3)	-0.0670(9)	0.6107(2)	0.0264(8)	H(18)	0.2608	-0.2718	0.7773	0.0435
C(9)	0.2458(3)	0.0760(9)	0.5600(3)	0.0254(8)	H(19)	0.1396	-0.1940	0.7567	0.0435
C(10)	0.2005(3)	0.0554(9)	0.4563(2)	0.0283(8)	H(20)	0.3199	-0.1303	0.9062	0.0465
C(11)	0.2228(3)	0.2536(9)	0.5948(2)	0.0301(9)	H(21)	0.1929	-0.0896	0.8955	0.0465
C(12)	0.2647(3)	0.2775(9)	0.6977(2)	0.0288(8)	H(22)	0.3541	0.1243	0.8530	0.0380
C(13)	0.2180(3)	0.1368(9)	0.7474(2)	0.0260(8)	H(23)	0.0530	0.1509	0.6642	0.0432
C(14)	0.2491(3)	-0.0370(9)	0.7128(2)	0.0269(9)	H(24)	0.0725	0.2679	0.7484	0.0432
C(15)	0.2188(3)	-0.1686(9)	0.7755(3)	0.035(1)	H(25)	0.0591	0.0716	0.7575	0.0432
C(16)	0.2523(3)	-0.0794(10)	0.8680(3)	0.038(1)	H(26)	0.0329	0.0109	0.4533	0.0456
C(17)	0.2748(3)	0.1143(9)	0.8514(2)	0.0289(9)	H(27)	0.0542	0.2011	0.4339	0.0456
C(18)	0.0882(3)	0.1590(9)	0.7272(3)	0.036(1)	H(28)	0.0435	0.0639	0.3594	0.0456
C(19)	0.0703(3)	0.0856(10)	0.4224(3)	0.037(1)	H(29)	0.1569	0.2405	0.9150	0.0407
C(20)	0.2366(3)	0.2288(10)	0.9176(2)	0.0333(9)	H(30)	0.3234	0.4464	0.9020	0.0547
C(21)	0.2482(4)	0.422(1)	0.9031(3)	0.045(1)	H(31)	0.2317	0.4832	0.9509	0.0547
C(22)	0.2977(3)	0.1783(9)	1.0168(3)	0.042(1)	H(32)	0.1957	0.4542	0.8472	0.0547
C(23)	0.4237(3)	0.220(1)	1.0480(3)	0.053(1)	H(33)	0.2617	0.2361	1.0550	0.0515
C(24)	0.4834(4)	0.140(1)	1.1394(3)	0.059(1)	H(34)	0.2899	0.0577	1.0227	0.0515
C(25)	-0.1453(4)	-0.057(1)	0.8487(3)	0.060(1)	H(35)	0.4320	0.3415	1.0538	0.0658
C(26)	-0.0930(5)	0.079(1)	0.9025(4)	0.083(2)	H(36)	0.4582	0.1804	1.0046	0.0658
C(27)	-0.1536(8)	0.226(1)	0.9033(5)	0.114(3)	H(37)	0.5708	0.0447	0.4009	0.0471
C(28)	-0.2634(8)	0.244(1)	0.8526(5)	0.122(3)	H(38)	0.3968	-0.2248	0.6853	0.0464
C(29)	-0.3162(6)	0.110(1)	0.7999(4)	0.106(2)	H(39)	0.4040	0.3378	0.6731	0.0435
C(30)	-0.2582(5)	-0.040(1)	0.7972(3)	0.070(2)	H(40)	0.5307	-0.0915	1.1882	0.1140
C(31)	-0.0841(4)	-0.215(1)	0.8493(3)	0.064(2)	H(41)	-0.0148	0.0697	0.9386	0.1003
C(32)	-0.0357(5)	-0.344(1)	0.8493(4)	0.090(2)	H(42)	-0.1190	0.3195	0.9408	0.1388
H(1)	0.2461	0.2966	0.4269	0.0385	H(43)	-0.3031	0.3487	0.8515	0.1474
H(2)	0.2146	0.1788	0.3426	0.0385	H(44)	-0.3940	0.1189	0.7657	0.1307
H(3)	0.4228	0.1674	0.4775	0.0386	H(45)	-0.2956	-0.1334	0.7599	0.0866
H(4)	0.4067	0.2391	0.3811	0.0386	H(46)	0.0042	-0.4489	0.8498	0.1079
H(5)	0.3639	-0.0358	0.3196	0.0381					

CA·6

atom	x	y	z	U	atom	x	y	z	U
O(1)	0.4830(5)	0.5357	0.5958(3)	0.030(2)	H(8)	0.8282	0.4354	0.6274	0.0203
O(2)	0.5960(5)	0.851(1)	0.2848(3)	0.028(2)	H(9)	0.8971	0.3079	0.5328	0.0291
O(3)	0.5253(8)	0.610(1)	-0.1728(5)	0.087(3)	H(10)	0.7878	0.2014	0.5305	0.0291
O(4)	0.5350(6)	0.866(1)	-0.2284(4)	0.057(2)	H(11)	0.7975	0.2407	0.3889	0.0215
O(5)	0.6401(5)	0.3021(10)	0.3818(3)	0.026(2)	H(12)	0.8769	0.5226	0.4001	0.0279
C(1)	0.7572(7)	0.760(1)	0.5911(5)	0.024(2)	H(13)	0.6738	0.6296	0.4356	0.0203
C(2)	0.6282(7)	0.733(1)	0.5814(5)	0.023(2)	H(14)	0.7487	0.9089	0.4352	0.0279
C(3)	0.6084(7)	0.559(1)	0.6123(5)	0.023(2)	H(15)	0.8609	0.8357	0.4220	0.0291
C(4)	0.6494(7)	0.426(1)	0.5615(5)	0.023(2)	H(16)	0.7441	0.9580	0.2850	0.0291
C(5)	0.7784(7)	0.445(1)	0.5675(4)	0.018(2)	H(17)	0.6515	0.5292	0.2859	0.0253
C(6)	0.8136(7)	0.308(1)	0.5158(5)	0.025(2)	H(18)	0.7144	0.2998	0.2305	0.0342
C(7)	0.7638(7)	0.327(1)	0.4164(4)	0.019(2)	H(19)	0.8390	0.3753	0.2475	0.0342
C(8)	0.7934(7)	0.509(1)	0.3912(5)	0.022(2)	H(20)	0.6423	0.4386	0.1050	0.0380
C(9)	0.7537(7)	0.650(1)	0.4395(4)	0.017(2)	H(21)	0.7710	0.4831	0.1137	0.0380
C(10)	0.8052(7)	0.629(1)	0.5412(5)	0.021(2)	H(22)	0.6112	0.6857	0.1557	0.0266
C(11)	0.7780(7)	0.823(1)	0.4066(4)	0.021(2)	H(23)	0.9182	0.6400	0.2415	0.0304
C(12)	0.7222(7)	0.851(1)	0.3072(5)	0.025(2)	H(24)	0.9060	0.8359	0.2482	0.0304
C(13)	0.7621(7)	0.707(1)	0.2574(5)	0.020(2)	H(25)	0.9376	0.7241	0.3317	0.0304
C(14)	0.7350(7)	0.534(1)	0.2932(5)	0.020(2)	H(26)	0.9730	0.6032	0.5335	0.0304
C(15)	0.7576(8)	0.401(1)	0.2312(5)	0.029(2)	H(27)	0.9589	0.7733	0.5777	0.0304
C(16)	0.7131(8)	0.491(1)	0.1413(5)	0.030(2)	H(28)	0.9755	0.6036	0.6296	0.0304
C(17)	0.6896(7)	0.684(1)	0.1580(5)	0.023(2)	H(29)	0.7926	0.7678	0.1005	0.0304
C(18)	0.8935(7)	0.729(1)	0.2710(5)	0.028(2)	H(30)	0.7296	1.0504	0.0654	0.0507
C(19)	0.9416(7)	0.655(1)	0.5736(5)	0.026(2)	H(31)	0.7437	1.0143	0.1624	0.0507
C(20)	0.7116(7)	0.797(1)	0.0881(5)	0.026(2)	H(32)	0.6194	1.0145	0.0914	0.0507
C(21)	0.7000(10)	0.987(1)	0.1033(6)	0.043(3)	H(33)	0.5469	0.7737	-0.0043	0.0443
C(22)	0.6240(8)	0.743(1)	-0.0020(5)	0.036(3)	H(34)	0.6288	0.6230	-0.0070	0.0443
C(23)	0.6445(8)	0.824(2)	-0.0799(5)	0.049(3)	H(35)	0.6366	0.9438	-0.0780	0.0608
C(24)	0.5595(9)	0.755(2)	-0.1645(6)	0.048(3)	H(36)	0.7239	0.7983	-0.0776	0.0608
C(25)	0.899(1)	0.197(2)	0.9358(8)	0.1942	H(37)	0.4816	0.4506	0.6384	0.0355
C(26)	0.900(1)	0.112(2)	0.861(1)	0.1942	H(38)	0.5588	0.9263	0.2389	0.0342
C(27)	0.799(2)	0.112(2)	0.7860(8)	0.1942	H(39)	0.4640	0.8452	-0.2816	0.0684
C(28)	0.698(1)	0.197(2)	0.7863(8)	0.1942	H(40)	0.6182	0.1841	0.3923	0.0304
C(29)	0.697(1)	0.283(2)	0.861(1)	0.1942	H(41)	0.969(2)	0.053(3)	0.862(2)	0.2048
C(30)	0.798(2)	0.283(2)	0.9361(8)	0.1942	H(42)	0.801(3)	0.051(3)	0.736(1)	0.2048
C(31)	1.0038	0.2189	1.0217	0.4759	H(43)	0.630(2)	0.194(4)	0.735(1)	0.2048
C(32)	0.984(2)	0.117(4)	1.087(1)	0.2602	H(44)	0.628(2)	0.340(3)	0.861(2)	0.2048
C(33)	1.094(2)	0.123(4)	1.168(1)	0.2239	H(45)	0.796(3)	0.341(3)	0.987(1)	0.2048
H(1)	0.969(2)	0.053(3)	0.861(2)	0.1942	H(46)	1.0105	0.3349	1.0394	0.6332
H(2)	0.800(3)	0.053(3)	0.735(1)	0.1942	H(47)	1.0744	0.1841	1.0129	0.6332
H(3)	0.630(2)	0.197(3)	0.735(1)	0.1942	H(48)	0.9702	0.0014	1.0672	0.3040
H(4)	0.629(2)	0.341(3)	0.862(2)	0.1942	H(49)	0.9177	0.1573	1.0999	0.3040
H(5)	0.797(3)	0.341(3)	0.987(1)	0.1942	H(50)	1.1070	0.2388	1.1885	0.2660
H(6)	0.6399	0.3165	0.5835	0.0291	H(51)	1.1593	0.0825	1.1559	0.2660
H(7)	0.6011	0.4335	0.5016	0.0291	H(52)	1.0813	0.0560	1.2137	0.2660

CA·7

atom	x	y	z	U	atom	x	y	z	U
O(1)	1.6089(2)	0.2363(9)	0.5994(2)	0.0452(8)	H(7)	1.4469	0.4575	0.5877	0.0415
O(2)	1.2517(2)	0.4692(8)	0.3839(1)	0.0328(7)	H(8)	1.3065	0.3534	0.6391	0.0391
O(3)	1.1924(2)	-0.0767(9)	0.2881(2)	0.0375(7)	H(9)	1.2670	0.6004	0.5415	0.0407
O(4)	0.8168(3)	0.1520(9)	-0.1724(2)	0.0524(9)	H(10)	1.1413	0.4666	0.5361	0.0407
O(5)	0.7296(2)	-0.0919(9)	-0.2286(2)	0.0425(7)	H(11)	1.1077	0.5220	0.3971	0.0416
C(1)	1.3385(3)	0.0194(9)	0.5978(2)	0.0364(9)	H(12)	1.0400	0.2731	0.4139	0.0380
C(2)	1.4534(3)	0.0406(9)	0.5857(2)	0.0377(10)	H(13)	1.2509	0.1330	0.4282	0.0380
C(3)	1.5021(3)	0.2167(9)	0.6168(2)	0.0375(9)	H(14)	1.1918	-0.1433	0.4332	0.0401
C(4)	1.4158(3)	0.3493(9)	0.5662(2)	0.0337(9)	H(15)	1.0646	-0.0580	0.4351	0.0401
C(5)	1.2960(3)	0.3311(9)	0.5745(2)	0.0312(9)	H(16)	1.0483	-0.1802	0.2913	0.0397
C(6)	1.2150(3)	0.4727(9)	0.5229(2)	0.0328(9)	H(17)	1.1459	0.2396	0.2815	0.0380
C(7)	1.1652(3)	0.4485(9)	0.4225(2)	0.0296(8)	H(18)	1.0367	0.4894	0.2376	0.0401
C(8)	1.1119(3)	0.2715(9)	0.3972(2)	0.0270(8)	H(19)	0.9229	0.4027	0.2512	0.0401
C(9)	1.1953(3)	0.1270(10)	0.4467(2)	0.0269(8)	H(20)	0.9804	0.3323	0.1089	0.0426
C(10)	1.2423(3)	0.1500(9)	0.5491(2)	0.0315(8)	H(21)	0.8640	0.2962	0.1200	0.0426
C(11)	1.1377(3)	-0.0458(9)	0.4143(2)	0.0329(9)	H(22)	1.0618	0.0779	0.1613	0.0380
C(12)	1.0935(3)	-0.0718(9)	0.3134(2)	0.0320(8)	H(23)	0.9121	0.0750	0.3438	0.0444
C(13)	1.0070(3)	0.0723(9)	0.2645(2)	0.0280(8)	H(24)	0.8649	-0.0566	0.2680	0.0444
C(14)	1.0718(3)	0.2415(9)	0.2978(2)	0.0285(8)	H(25)	0.8401	0.1351	0.2484	0.0444
C(15)	0.9914(3)	0.3748(9)	0.2365(2)	0.0327(9)	H(26)	1.1854	0.1456	0.6529	0.0495
C(16)	0.9456(3)	0.2853(9)	0.1466(2)	0.0347(9)	H(27)	1.0848	0.1923	0.5591	0.0495
C(17)	0.9794(3)	0.0930(9)	0.1634(2)	0.0285(8)	H(28)	1.1170	-0.0071	0.5696	0.0495
C(18)	0.8954(3)	0.0558(9)	0.2827(2)	0.036(1)	H(29)	0.8158	0.0038	0.0942	0.0381
C(19)	1.1450(3)	0.1274(9)	0.5851(2)	0.040(1)	H(30)	0.8971	-0.2383	0.1663	0.0565
C(20)	0.8860(3)	-0.0201(9)	0.0951(2)	0.0310(8)	H(31)	0.8495	-0.2717	0.0653	0.0565
C(21)	0.9059(4)	-0.2100(10)	0.1123(3)	0.046(1)	H(32)	0.9810	-0.2399	0.1161	0.0565
C(22)	0.8824(3)	0.0280(9)	0.0021(2)	0.0366(10)	H(33)	0.8729	0.1467	-0.0044	0.0453
C(23)	0.7865(4)	-0.0554(10)	-0.0744(2)	0.045(1)	H(34)	0.9549	-0.0038	-0.0010	0.0453
C(24)	0.7796(3)	0.0146(10)	-0.1627(2)	0.0370(9)	H(35)	0.7920	-0.1831	-0.0741	0.0533
C(25)	1.4895(5)	-0.149(1)	0.1099(4)	0.085(2)	H(36)	0.7174	-0.0284	-0.0749	0.0533
C(26)	1.5727(5)	-0.048(1)	0.1665(4)	0.077(2)	H(37)	1.6463	0.3242	0.6392	0.0561
C(27)	1.5513(8)	0.076(1)	0.2138(5)	0.113(3)	H(38)	1.3006	0.5638	0.4037	0.0404
C(28)	1.4498(10)	0.103(1)	0.2126(6)	0.138(4)	H(39)	1.1731	-0.1635	0.2373	0.0470
C(29)	1.3541(7)	0.014(2)	0.1594(9)	0.158(4)	H(40)	0.7576	-0.0506	-0.2713	0.0520
C(30)	1.3759(6)	-0.117(1)	0.1056(6)	0.147(3)	H(41)	1.6523	-0.0696	0.1734	0.0942
C(31)	1.5179(9)	-0.294(1)	0.0600(5)	0.168(4)	H(42)	1.6152	0.1468	0.2486	0.1346
C(32)	1.5614(7)	-0.449(1)	0.1215(5)	0.121(3)	H(43)	1.4440	0.1902	0.2522	0.1627
C(33)	1.6567(8)	-0.516(1)	0.1380(7)	0.159(4)	H(44)	1.2798	0.0381	0.1601	0.1805
H(1)	1.3085	-0.0950	0.5770	0.0444	H(45)	1.3141	-0.1848	0.0674	0.1708
H(2)	1.3468	0.0301	0.6541	0.0444	H(46)	1.4518	-0.3245	0.0110	0.2021
H(3)	1.4313	0.0248	0.5085	0.0473	H(47)	1.5786	-0.2597	0.0415	0.2021
H(4)	1.5093	-0.0496	0.6169	0.0473	H(48)	1.5104	-0.4943	0.1485	0.1444
H(5)	1.5193	0.2306	0.6833	0.0456	H(49)	1.6785	-0.6106	0.1763	0.1913
H(6)	1.4050	0.3402	0.5053	0.0415	H(50)	1.7067	-0.4712	0.1120	0.1913

CA·15

atom	x	y	z	U	atom	x	y	z	U
F(1)	-0.003(2)	0.576(4)	0.509(2)	0.16(1)	H(5)	0.7256	0.3422	0.5977	0.0498
F(2)	0.140(1)	0.391(2)	0.568(1)	0.195(6)	H(6)	0.6134	0.1186	0.4991	0.0536
F(3)	-0.067(1)	0.765(2)	0.338(1)	0.189(6)	H(7)	0.5253	0.2444	0.4330	0.0536
O(1)	0.5876(2)	0.3482(9)	0.6204(2)	0.0440(8)	H(8)	0.7308	0.2194	0.4277	0.0471
O(2)	0.4151(2)	0.1197(9)	0.2697(2)	0.0403(7)	H(9)	0.6126	0.0029	0.3395	0.0489
O(3)	0.3218(2)	0.6616(9)	0.1958(2)	0.0433(7)	H(10)	0.6564	0.0996	0.2698	0.0560
O(4)	-0.1590(3)	0.4089(10)	-0.1514(3)	0.077(1)	H(11)	0.4736	0.0575	0.1682	0.0477
O(5)	-0.2025(2)	0.6747(10)	-0.1979(3)	0.0640(9)	H(12)	0.5219	0.3220	0.1368	0.0432
C(1)	0.6849(3)	0.5458(9)	0.4318(3)	0.043(1)	H(13)	0.4777	0.4443	0.3037	0.0439
C(2)	0.6298(3)	0.5327(10)	0.5079(3)	0.0373(10)	H(14)	0.5238	0.7043	0.2622	0.0445
C(3)	0.6465(3)	0.3604(9)	0.5546(3)	0.0392(10)	H(15)	0.5455	0.6263	0.1721	0.0445
C(4)	0.6040(3)	0.2320(9)	0.4699(3)	0.0369(10)	H(16)	0.3812	0.7636	0.1017	0.0476
C(5)	0.6543(3)	0.243(1)	0.3896(3)	0.0380(10)	H(17)	0.3255	0.3524	0.1498	0.0383
C(6)	0.6081(3)	0.1071(9)	0.3061(3)	0.0401(9)	H(18)	0.3519	0.1983	-0.0149	0.0535
C(7)	0.4932(3)	0.1400(9)	0.2258(3)	0.0362(8)	H(19)	0.2893	0.1282	0.0467	0.0535
C(8)	0.4811(3)	0.3130(10)	0.1790(3)	0.0319(8)	H(20)	0.1921	0.3159	-0.1260	0.0486
C(9)	0.5243(3)	0.4502(9)	0.2648(3)	0.0310(8)	H(21)	0.1385	0.2802	-0.0500	0.0486
C(10)	0.6438(3)	0.4192(10)	0.3405(3)	0.0364(9)	H(22)	0.1866	0.5291	0.0292	0.0522
C(11)	0.5038(3)	0.6241(10)	0.2131(3)	0.0374(9)	H(23)	0.3836	0.4503	-0.0707	0.0552
C(12)	0.3860(3)	0.6568(9)	0.1362(3)	0.0360(9)	H(24)	0.3903	0.6408	-0.0542	0.0552
C(13)	0.3462(3)	0.5212(9)	0.0513(3)	0.0316(8)	H(25)	0.4823	0.5277	0.0200	0.0552
C(14)	0.3656(3)	0.3519(9)	0.1069(3)	0.0316(8)	H(26)	0.6973	0.3526	0.2250	0.0623
C(15)	0.3045(3)	0.2289(9)	0.0195(3)	0.0385(10)	H(27)	0.7174	0.5382	0.2560	0.0623
C(16)	0.2042(3)	0.3253(10)	-0.0538(3)	0.0398(9)	H(28)	0.7920	0.4031	0.3289	0.0623
C(17)	0.2211(3)	0.5115(10)	-0.0174(3)	0.0334(8)	H(29)	0.1996	0.6066	-0.1586	0.0489
C(18)	0.4071(3)	0.5372(10)	-0.0203(3)	0.041(1)	H(30)	0.1546	0.8856	-0.1382	0.0668
C(19)	0.7219(3)	0.432(1)	0.2853(3)	0.051(1)	H(31)	0.1504	0.8408	-0.0329	0.0668
C(20)	0.1668(3)	0.6315(9)	-0.1087(3)	0.0370(8)	H(32)	0.2601	0.8396	-0.0427	0.0668
C(21)	0.1838(3)	0.8141(10)	-0.0796(3)	0.046(1)	H(33)	0.0155	0.6627	-0.2259	0.0562
C(22)	0.0441(3)	0.5938(9)	-0.1657(3)	0.0418(10)	H(34)	0.0372	0.4783	-0.1923	0.0562
C(23)	-0.0191(3)	0.6125(9)	-0.0984(3)	0.051(1)	H(35)	-0.0146	0.7271	-0.0762	0.0664
C(24)	-0.1326(3)	0.552(1)	-0.1511(3)	0.0469(9)	H(36)	0.0188	0.5493	-0.0327	0.0664
C(25)	0.0374(5)	0.560(1)	0.4431(6)	0.108(2)	H(37)	0.6248	0.2570	0.6818	0.0538
C(26)	0.1175(5)	0.442(1)	0.4653(6)	0.114(2)	H(38)	0.4186	0.0386	0.3176	0.0680
C(27)	0.1662(6)	0.414(1)	0.3993(6)	0.114(3)	H(39)	0.2714	0.7176	0.1658	0.0520
C(28)	0.1401(5)	0.508(1)	0.3107(5)	0.097(2)	H(40)	-0.2840	0.6353	-0.2287	0.0764
C(29)	0.0615(5)	0.627(1)	0.2888(5)	0.099(2)	H(41)	0.0019	0.5759	0.4884	0.1307
C(30)	0.0122(6)	0.654(1)	0.3548(5)	0.116(3)	H(42)	0.1390	0.3757	0.5261	0.1337
H(1)	0.6787	0.6555	0.4027	0.0568	H(43)	0.2342	0.3432	0.4072	0.1337
H(2)	0.7642	0.5278	0.4705	0.0568	H(44)	0.1790	0.4971	0.2526	0.1155
H(3)	0.6538	0.6144	0.5608	0.0506	H(45)	0.0332	0.6913	0.2147	0.1201
H(4)	0.5519	0.5461	0.4693	0.0506	H(46)	-0.0409	0.7372	0.3374	0.1413

CA·16

atom	x	y	z	U	atom	x	y	z	U
Cl(1)	-0.9744(3)	-0.088(2)	-0.4502(2)	0.121(1)	H(6)	-0.3813	-0.5404	-0.4980	0.0348
O(1)	-0.4131(3)	-0.317(2)	-0.3782(3)	0.037(1)	H(7)	-0.4735	-0.4220	-0.5654	0.0348
O(2)	-0.5836(3)	-0.547(2)	-0.7323(3)	0.037(1)	H(8)	-0.2699	-0.4339	-0.5716	0.0392
O(3)	-0.6806(3)	-0.002(2)	-0.8071(3)	0.032(1)	H(9)	-0.3887	-0.6552	-0.6567	0.0395
O(4)	-1.1565(5)	-0.262(2)	-1.1484(5)	0.071(2)	H(10)	-0.3447	-0.5648	-0.7283	0.0395
O(5)	-1.2026(4)	0.003(2)	-1.1924(4)	0.058(2)	H(11)	-0.5175	-0.6044	-0.8273	0.0412
C(1)	-0.3199(5)	-0.116(2)	-0.5670(5)	0.035(2)	H(12)	-0.4771	-0.3382	-0.8628	0.0323
C(2)	-0.3732(5)	-0.131(2)	-0.4921(5)	0.031(2)	H(13)	-0.5174	-0.2229	-0.6910	0.0373
C(3)	-0.3554(5)	-0.303(2)	-0.4449(5)	0.031(2)	H(14)	-0.4545	-0.0282	-0.8241	0.0324
C(4)	-0.3955(5)	-0.431(2)	-0.5303(5)	0.029(2)	H(15)	-0.4809	0.0442	-0.7351	0.0324
C(5)	-0.3458(5)	-0.415(2)	-0.6090(5)	0.031(2)	H(16)	-0.6176	0.0972	-0.8988	0.0393
C(6)	-0.3909(5)	-0.552(2)	-0.6939(5)	0.033(2)	H(17)	-0.6767	-0.3118	-0.8530	0.0296
C(7)	-0.5044(5)	-0.521(2)	-0.7759(5)	0.030(1)	H(18)	-0.7126	-0.5375	-0.9596	0.0480
C(8)	-0.5192(5)	-0.349(2)	-0.8228(4)	0.026(1)	H(19)	-0.6498	-0.4663	-1.0204	0.0480
C(9)	-0.4773(4)	-0.213(2)	-0.7362(5)	0.026(1)	H(20)	-0.8581	-0.3856	-1.0529	0.0518
C(10)	-0.3579(5)	-0.239(2)	-0.6572(5)	0.032(1)	H(21)	-0.8046	-0.3477	-1.1286	0.0518
C(11)	-0.4992(5)	-0.039(2)	-0.7891(5)	0.031(1)	H(22)	-0.8172	-0.1432	-0.9770	0.0299
C(12)	-0.6169(5)	-0.009(2)	-0.8670(5)	0.030(1)	H(23)	-0.6178	-0.2217	-1.0769	0.0525
C(13)	-0.6565(5)	-0.145(2)	-0.9524(4)	0.027(1)	H(24)	-0.6255	-0.0309	-1.0723	0.0525
C(14)	-0.6360(5)	-0.311(2)	-0.8959(4)	0.026(1)	H(25)	-0.5245	-0.1221	-0.9932	0.0525
C(15)	-0.6963(5)	-0.435(2)	-0.9842(5)	0.035(2)	H(26)	-0.3013	-0.3046	-0.7705	0.0547
C(16)	-0.7965(5)	-0.339(2)	-1.0572(5)	0.036(2)	H(27)	-0.2845	-0.1187	-0.7414	0.0547
C(17)	-0.7805(5)	-0.155(2)	-1.0207(4)	0.026(1)	H(28)	-0.2087	-0.2497	-0.6658	0.0547
C(18)	-0.5977(5)	-0.126(2)	-1.0247(5)	0.036(2)	H(29)	-0.8058	-0.0617	-1.1639	0.0350
C(19)	-0.2803(5)	-0.224(2)	-0.7127(5)	0.046(2)	H(30)	-0.7466	0.1734	-1.0505	0.0471
C(20)	-0.8381(4)	-0.036(2)	-1.1138(4)	0.030(1)	H(31)	-0.8535	0.1697	-1.0368	0.0471
C(21)	-0.8198(5)	0.146(2)	-1.0842(5)	0.040(2)	H(32)	-0.8546	0.2128	-1.1450	0.0471
C(22)	-0.9601(5)	-0.075(2)	-1.1681(5)	0.033(2)	H(33)	-0.9710	-0.1843	-1.1971	0.0410
C(23)	-1.0200(5)	-0.059(2)	-1.0980(5)	0.042(2)	H(34)	-0.9914	0.0017	-1.2247	0.0410
C(24)	-1.1335(5)	-0.118(2)	-1.1495(5)	0.039(1)	H(35)	-0.9786	-0.1238	-1.0317	0.0552
C(25)	-0.9355(6)	-0.116(2)	-0.5502(5)	0.0811	H(36)	-1.0158	0.0534	-1.0730	0.0552
C(26)	-0.8577(5)	-0.235(2)	-0.5392(4)	0.0811	H(37)	-0.3840	-0.4093	-0.3141	0.0451
C(27)	-0.8214(5)	-0.255(2)	-0.6179(5)	0.0811	H(38)	-0.5782	-0.6220	-0.7021	0.0426
C(28)	-0.8630(5)	-0.157(2)	-0.7075(4)	0.0811	H(39)	-0.7475	0.0324	-0.8342	0.0388
C(29)	-0.9408(5)	-0.038(2)	-0.7185(4)	0.0811	H(40)	-1.2702	-0.0410	-1.2051	0.0693
C(30)	-0.9771(5)	-0.017(2)	-0.6398(5)	0.0811	H(41)	-0.8294(8)	-0.302(2)	-0.4782(6)	0.0811
H(1)	-0.2438	-0.1289	-0.5276	0.0457	H(42)	-0.7684(7)	-0.336(2)	-0.6104(8)	0.0811
H(2)	-0.3320	-0.0067	-0.5974	0.0457	H(43)	-0.8383(8)	-0.171(2)	-0.7611(6)	0.0811
H(3)	-0.3476	-0.0506	-0.4366	0.0365	H(44)	-0.9691(8)	0.029(2)	-0.7795(5)	0.0811
H(4)	-0.4515	-0.1118	-0.5289	0.0365	H(45)	-1.0301(7)	0.064(2)	-0.6473(8)	0.0811
H(5)	-0.2784	-0.3206	-0.4085	0.0359					

CA·17

atom	x	y	z	U	atom	x	y	z	U
Br(1)	0.5285(1)	0.462(2)	0.5558(1)	0.1026(6)	H(6)	0.0228	0.1554	0.4264	0.0374
O(1)	0.0882(5)	0.237(2)	0.6228(3)	0.036(2)	H(7)	0.1045	0.0219	0.4917	0.0374
O(2)	-0.0846(4)	0.010(2)	0.2660(4)	0.034(1)	H(8)	0.2284	0.1248	0.4320	0.0395
O(3)	-0.1809(4)	0.553(2)	0.1927(3)	0.033(1)	H(9)	0.1170	-0.0837	0.3434	0.0381
O(4)	-0.6553(7)	0.296(2)	-0.1481(6)	0.075(3)	H(10)	0.1592	0.0184	0.2747	0.0381
O(5)	-0.7019(5)	0.556(2)	-0.1890(5)	0.057(2)	H(11)	-0.0151	-0.0451	0.1697	0.0369
C(1)	0.1789(6)	0.444(2)	0.4305(5)	0.033(2)	H(12)	0.0178	0.2191	0.1324	0.0309
C(2)	0.1248(6)	0.426(2)	0.5069(5)	0.029(2)	H(13)	-0.0176	0.3409	0.3025	0.0274
C(3)	0.1445(6)	0.255(2)	0.5553(6)	0.027(2)	H(14)	0.0189	0.5990	0.2653	0.0335
C(4)	0.1031(6)	0.128(2)	0.4686(6)	0.028(2)	H(15)	0.0429	0.5325	0.1734	0.0335
C(5)	0.1519(6)	0.141(2)	0.3900(6)	0.031(2)	H(16)	-0.1162	0.6560	0.1055	0.0375
C(6)	0.1100(6)	0.004(2)	0.3070(6)	0.031(2)	H(17)	-0.1744	0.2485	0.1488	0.0245
C(7)	-0.0067(7)	0.034(2)	0.2229(6)	0.031(2)	H(18)	-0.2163	0.0285	0.0378	0.0413
C(8)	-0.0210(6)	0.209(2)	0.1765(5)	0.026(2)	H(19)	-0.1536	0.0999	-0.0231	0.0413
C(9)	0.0216(6)	0.348(2)	0.2608(5)	0.023(2)	H(20)	-0.3567	0.1741	-0.0526	0.0376
C(10)	0.1425(6)	0.317(2)	0.3420(6)	0.030(2)	H(21)	-0.3027	0.2133	-0.1278	0.0376
C(11)	-0.0007(6)	0.516(2)	0.2118(5)	0.029(2)	H(22)	-0.3159	0.4161	0.0248	0.0220
C(12)	-0.1177(6)	0.549(2)	0.1316(6)	0.029(2)	H(23)	-0.1096	0.5397	-0.0554	0.0327
C(13)	-0.1548(6)	0.415(2)	0.0474(5)	0.022(2)	H(24)	-0.1191	0.3505	-0.0746	0.0327
C(14)	-0.1356(6)	0.244(2)	0.1053(5)	0.021(2)	H(25)	-0.0211	0.4227	0.0193	0.0327
C(15)	-0.1960(7)	0.124(2)	0.0139(6)	0.031(2)	H(26)	0.2178	0.4463	0.2596	0.0591
C(16)	-0.2960(7)	0.217(2)	-0.0586(6)	0.031(2)	H(27)	0.2040	0.2603	0.2305	0.0591
C(17)	-0.2806(6)	0.402(2)	-0.0213(5)	0.023(2)	H(28)	0.2927	0.3167	0.3371	0.0591
C(18)	-0.0960(6)	0.431(2)	-0.0224(5)	0.029(2)	H(29)	-0.3018	0.5056	-0.1605	0.0364
C(19)	0.2199(7)	0.333(2)	0.2891(7)	0.044(3)	H(30)	-0.2467	0.7295	-0.0500	0.0438
C(20)	-0.3368(6)	0.520(2)	-0.1133(5)	0.029(2)	H(31)	-0.3566	0.7688	-0.1416	0.0438
C(21)	-0.3199(7)	0.700(2)	-0.0824(7)	0.036(2)	H(32)	-0.3513	0.7211	-0.0324	0.0438
C(22)	-0.4595(6)	0.481(2)	-0.1702(6)	0.034(2)	H(33)	-0.4678	0.3666	-0.1917	0.0472
C(23)	-0.5206(7)	0.499(2)	-0.0983(6)	0.040(2)	H(34)	-0.4896	0.5455	-0.2352	0.0472
C(24)	-0.6314(7)	0.439(2)	-0.1464(5)	0.037(2)	H(35)	-0.4863	0.4758	-0.0352	0.0478
C(25)	0.5696(8)	0.433(2)	0.4427(10)	0.068(3)	H(36)	-0.5348	0.6329	-0.1012	0.0478
C(26)	0.6493(9)	0.326(2)	0.4533(9)	0.067(3)	H(37)	0.0946	0.2397	0.6861	0.0541
C(27)	0.679(1)	0.309(3)	0.371(1)	0.088(5)	H(38)	-0.0833	-0.0839	0.2848	0.0507
C(28)	0.6364(10)	0.405(2)	0.281(1)	0.076(4)	H(39)	-0.2270	0.6310	0.1744	0.0502
C(29)	0.561(1)	0.512(2)	0.2808(9)	0.085(4)	H(40)	-0.7802	0.5361	-0.2571	0.0856
C(30)	0.5204(10)	0.530(2)	0.355(1)	0.079(4)	H(41)	0.6790	0.2648	0.5188	0.0847
H(1)	0.1691	0.5545	0.4023	0.0440	H(42)	0.7333	0.2314	0.3797	0.1184
H(2)	0.2551	0.4290	0.4713	0.0440	H(43)	0.6662	0.3992	0.2336	0.1004
H(3)	0.0456	0.4386	0.4637	0.0307	H(44)	0.5217	0.5781	0.2163	0.0965
H(4)	0.1444	0.5126	0.5560	0.0307	H(45)	0.4636	0.6052	0.3449	0.0943
H(5)	0.2225	0.2394	0.5951	0.0318					

CA·18

atom	x	y	z	U	atom	x	y	z	U
I(1)	1.03600(5)	0.233(2)	1.06275(4)	0.0824(2)	H(6)	0.6159	-0.1988	0.9987	0.0323
O(1)	0.5888(4)	0.028(2)	1.1207(3)	0.036(1)	H(7)	0.5265	-0.0763	0.9332	0.0323
O(2)	0.4155(3)	-0.202(2)	0.7682(3)	0.035(1)	H(8)	0.7263	-0.1002	0.9243	0.0332
O(3)	0.3198(3)	0.342(2)	0.6934(3)	0.034(1)	H(9)	0.6524	-0.2221	0.7689	0.0393
O(4)	-0.1573(6)	0.077(2)	0.3532(6)	0.077(2)	H(10)	0.6063	-0.3148	0.8379	0.0393
O(5)	-0.2000(4)	0.342(2)	0.3138(5)	0.060(2)	H(11)	0.4788	-0.2583	0.6688	0.0335
C(1)	0.6811(4)	0.226(2)	0.9305(4)	0.032(1)	H(12)	0.5221	-0.0031	0.6383	0.0263
C(2)	0.6273(5)	0.213(2)	1.0064(4)	0.031(1)	H(13)	0.4784	0.1215	0.8002	0.0253
C(3)	0.6452(5)	0.040(2)	1.0534(4)	0.030(1)	H(14)	0.5189	0.3785	0.7641	0.0335
C(4)	0.6015(5)	-0.086(2)	0.9684(4)	0.028(1)	H(15)	0.5450	0.3101	0.6743	0.0335
C(5)	0.6524(5)	-0.073(2)	0.8882(4)	0.029(1)	H(16)	0.3820	0.4347	0.6014	0.0320
C(6)	0.6068(5)	-0.208(2)	0.8045(5)	0.033(1)	H(17)	0.3260	0.0274	0.6476	0.0252
C(7)	0.4938(5)	-0.176(2)	0.7237(4)	0.029(1)	H(18)	0.3490	-0.1247	0.4823	0.0358
C(8)	0.4808(4)	-0.004(2)	0.6784(4)	0.022(1)	H(19)	0.2869	-0.1919	0.5448	0.0358
C(9)	0.5203(4)	0.134(2)	0.7610(4)	0.022(1)	H(20)	0.1954	-0.0085	0.3737	0.0352
C(10)	0.6407(4)	0.103(2)	0.8401(4)	0.030(1)	H(21)	0.1411	-0.0452	0.4488	0.0352
C(11)	0.5002(5)	0.304(2)	0.7104(4)	0.029(1)	H(22)	0.1872	0.1957	0.5282	0.0277
C(12)	0.3850(5)	0.336(2)	0.6335(4)	0.028(1)	H(23)	0.4787	0.2058	0.5181	0.0387
C(13)	0.3437(4)	0.201(2)	0.5490(4)	0.021(1)	H(24)	0.3810	0.1322	0.4259	0.0387
C(14)	0.3641(4)	0.031(2)	0.6049(4)	0.022(1)	H(25)	0.3884	0.3212	0.4457	0.0387
C(15)	0.3054(5)	-0.090(2)	0.5178(4)	0.031(1)	H(26)	0.7870	0.0882	0.8314	0.0465
C(16)	0.2034(5)	0.005(2)	0.4444(5)	0.030(1)	H(27)	0.6940	0.0369	0.7275	0.0465
C(17)	0.2210(4)	0.189(2)	0.4822(4)	0.024(1)	H(28)	0.7129	0.2219	0.7583	0.0465
C(18)	0.4042(4)	0.220(2)	0.4780(4)	0.033(1)	H(29)	0.1947	0.2845	0.3415	0.0323
C(19)	0.7167(5)	0.118(2)	0.7841(5)	0.041(2)	H(30)	0.2578	0.5044	0.4533	0.0480
C(20)	0.1650(4)	0.310(2)	0.3905(4)	0.027(1)	H(31)	0.1523	0.5490	0.3591	0.0480
C(21)	0.1837(6)	0.489(2)	0.4202(6)	0.041(2)	H(32)	0.1505	0.5093	0.4661	0.0480
C(22)	0.0417(4)	0.266(2)	0.3352(4)	0.032(1)	H(33)	0.0089	0.3328	0.2779	0.0379
C(23)	-0.0164(5)	0.281(2)	0.4060(5)	0.038(2)	H(34)	0.0349	0.1494	0.3104	0.0379
C(24)	-0.1316(4)	0.221(2)	0.3548(4)	0.039(1)	H(35)	0.0197	0.2097	0.4664	0.0435
C(25)	1.0757(6)	0.207(2)	0.9339(6)	0.054(2)	H(36)	-0.0162	0.3872	0.4254	0.0435
C(26)	1.1643(7)	0.116(2)	0.9439(7)	0.058(2)	H(37)	0.5951	-0.0407	1.1517	0.0434
C(27)	1.1911(7)	0.106(2)	0.8586(7)	0.063(2)	H(38)	0.4084	-0.3438	0.7943	0.0409
C(28)	1.1348(7)	0.192(2)	0.7691(7)	0.062(2)	H(39)	0.2860	0.4092	0.6889	0.0404
C(29)	1.0480(8)	0.280(2)	0.7615(7)	0.069(3)	H(40)	-0.2595	0.3143	0.2812	0.0723
C(30)	1.0178(7)	0.290(2)	0.8421(7)	0.065(2)	H(41)	1.2079	0.0584	1.0097	0.0697
H(1)	0.6685	0.3300	0.9025	0.0381	H(42)	1.2491	0.0320	0.8615	0.0768
H(2)	0.7556	0.2046	0.9685	0.0381	H(43)	1.1549	0.1822	0.7109	0.0744
H(3)	0.6580	0.2864	1.0608	0.0363	H(44)	1.0098	0.3361	0.6990	0.0810
H(4)	0.5529	0.2275	0.9709	0.0363	H(45)	0.9545	0.3453	0.8344	0.0756
H(5)	0.7195	0.0155	1.0931	0.0336					

CA·19

atom	x	y	z	U	atom	x	y	z	U
Cl(1)	0.5790(2)	-0.7130(7)	-0.37489(10)	0.1317(6)	H(6)	0.4455	0.2466	0.0913	0.0351
O(1)	0.6086(2)	0.0268(7)	0.1011(1)	0.0411(6)	H(7)	0.4052	0.1318	0.0075	0.0351
O(2)	0.2538(2)	0.2574(7)	-0.1161(1)	0.0281(5)	H(8)	0.3065	0.1360	0.1355	0.0336
O(3)	0.1924(2)	-0.2872(7)	-0.2134(1)	0.0331(5)	H(9)	0.1483	0.2668	0.0410	0.0340
O(4)	-0.1853(2)	-0.0635(7)	-0.6721(1)	0.0431(7)	H(10)	0.2540	0.3668	0.0355	0.0340
O(5)	-0.2730(2)	-0.3088(7)	-0.7296(1)	0.0360(6)	H(11)	0.1068	0.3202	-0.1038	0.0339
C(1)	0.3356(3)	-0.1922(8)	0.0987(2)	0.0306(7)	H(12)	0.0448	0.0537	-0.0866	0.0289
C(2)	0.4530(3)	-0.1708(8)	0.0879(2)	0.0341(8)	H(13)	0.2619	-0.0784	-0.0696	0.0293
C(3)	0.5024(3)	0.0054(8)	0.1184(2)	0.0315(7)	H(14)	0.1943	-0.3465	-0.0595	0.0365
C(4)	0.4152(2)	0.1404(7)	0.0682(2)	0.0279(7)	H(15)	0.0744	-0.2722	-0.0668	0.0365
C(5)	0.2952(2)	0.1210(8)	0.0749(2)	0.0264(7)	H(16)	0.0528	-0.3926	-0.2008	0.0339
C(6)	0.2126(2)	0.2643(7)	0.0224(2)	0.0268(7)	H(17)	0.1386	0.0261	-0.2162	0.0278
C(7)	0.1655(2)	0.2398(8)	-0.0778(2)	0.0263(7)	H(18)	-0.0712	0.1926	-0.2438	0.0354
C(8)	0.1115(2)	0.0620(8)	-0.1028(2)	0.0227(7)	H(19)	0.0325	0.2629	-0.2659	0.0354
C(9)	0.1955(2)	-0.0824(8)	-0.0530(2)	0.0230(7)	H(20)	-0.1398	0.0839	-0.3791	0.0410
C(10)	0.2409(3)	-0.0604(8)	0.0500(2)	0.0270(7)	H(21)	-0.0236	0.1200	-0.3922	0.0410
C(11)	0.1381(3)	-0.2573(8)	-0.0859(2)	0.0284(7)	H(22)	0.0465	-0.1370	-0.3473	0.0322
C(12)	0.0923(2)	-0.2830(7)	-0.1869(2)	0.0264(7)	H(23)	-0.1535	-0.0603	-0.2368	0.0380
C(13)	0.0055(2)	-0.1388(8)	-0.2353(2)	0.0227(7)	H(24)	-0.1482	-0.2574	-0.2451	0.0380
C(14)	0.0702(3)	0.0322(8)	-0.2023(2)	0.0218(7)	H(25)	-0.0871	-0.1700	-0.1539	0.0380
C(15)	-0.0098(3)	0.1655(8)	-0.2629(2)	0.0285(7)	H(26)	0.1704	-0.0659	0.1469	0.0406
C(16)	-0.0572(3)	0.0749(8)	-0.3535(2)	0.0322(8)	H(27)	0.0804	-0.0091	0.0558	0.0406
C(17)	-0.0241(2)	-0.1181(8)	-0.3372(2)	0.0251(7)	H(28)	0.1130	-0.2008	0.0737	0.0406
C(18)	-0.1061(3)	-0.1559(8)	-0.2157(2)	0.0311(8)	H(29)	-0.1910	-0.2063	-0.4020	0.0336
C(19)	0.1418(3)	-0.0840(7)	0.0850(2)	0.0330(8)	H(30)	-0.0976	-0.4522	-0.3289	0.0489
C(20)	-0.1174(2)	-0.2323(8)	-0.4044(2)	0.0262(7)	H(31)	-0.1580	-0.4893	-0.4294	0.0489
C(21)	-0.0976(3)	-0.4240(8)	-0.3864(2)	0.0387(9)	H(32)	-0.0244	-0.4587	-0.3887	0.0489
C(22)	-0.1201(3)	-0.1880(8)	-0.4976(2)	0.0298(7)	H(33)	-0.1286	-0.0707	-0.5051	0.0371
C(23)	-0.2159(3)	-0.2733(8)	-0.5748(2)	0.0335(8)	H(34)	-0.0469	-0.2243	-0.5002	0.0371
C(24)	-0.2221(3)	-0.2023(8)	-0.6629(2)	0.0301(7)	H(35)	-0.2017	-0.3954	-0.5735	0.0421
C(25)	0.5024(4)	-0.3839(9)	-0.3958(3)	0.060(1)	H(36)	-0.2889	-0.2563	-0.5689	0.0421
C(26)	0.5817(3)	-0.2784(9)	-0.3374(3)	0.060(1)	H(37)	0.6598	0.1186	0.1350	0.0544
C(27)	0.5485(6)	-0.1508(9)	-0.2946(3)	0.093(2)	H(38)	0.2875	0.3519	-0.0967	0.0362
C(28)	0.4346(8)	-0.131(1)	-0.3069(5)	0.120(2)	H(39)	0.1775	-0.3871	-0.2489	0.0421
C(29)	0.3522(6)	-0.234(1)	-0.3647(7)	0.137(3)	H(40)	-0.2637	-0.2812	-0.7840	0.0447
C(30)	0.3850(4)	-0.363(1)	-0.4092(4)	0.114(2)	H(41)	0.6622	-0.2967	-0.3263	0.0730
C(31)	0.5411(5)	-0.5247(10)	-0.4410(3)	0.093(2)	H(42)	0.6069	-0.0802	-0.2552	0.1140
H(1)	0.3070	-0.3056	0.0773	0.0391	H(43)	0.4147	-0.0446	-0.2747	0.1465
H(2)	0.3497	-0.1884	0.1602	0.0391	H(44)	0.2735	-0.2190	-0.3717	0.1641
H(3)	0.5060	-0.2572	0.1225	0.0428	H(45)	0.3275	-0.4375	-0.4491	0.1413
H(4)	0.4422	-0.1873	0.0274	0.0428	H(46)	0.6080	-0.4900	-0.4517	0.1115
H(5)	0.5191	0.0135	0.1801	0.0400	H(47)	0.4804	-0.5537	-0.4951	0.1115

CA·20

atom	x	y	z	U	atom	x	y	z	U
Br(1)	-1.0898(1)	-0.755(2)	-0.13198(7)	0.1127(5)	H(6)	-0.9462	0.2220	-0.5885	0.0426
O(1)	-1.1086(4)	0.003(2)	-0.6009(4)	0.050(1)	H(7)	-0.9061	0.1044	-0.5063	0.0426
O(2)	-0.7533(3)	0.233(2)	-0.3833(3)	0.040(1)	H(8)	-0.8031	0.1121	-0.6336	0.0410
O(3)	-0.6918(4)	-0.312(2)	-0.2855(3)	0.043(1)	H(9)	-0.7526	0.3397	-0.5337	0.0426
O(4)	-0.3154(4)	-0.088(2)	0.1720(3)	0.054(1)	H(10)	-0.6462	0.2402	-0.5390	0.0426
O(5)	-0.2259(4)	-0.332(2)	0.2293(3)	0.045(1)	H(11)	-0.6049	0.2954	-0.3951	0.0435
C(1)	-0.8329(5)	-0.215(2)	-0.5962(4)	0.039(2)	H(12)	-0.5425	0.0293	-0.4116	0.0398
C(2)	-0.9514(5)	-0.195(2)	-0.5866(5)	0.039(2)	H(13)	-0.7603	-0.1012	-0.4289	0.0383
C(3)	-1.0001(5)	-0.019(2)	-0.6173(5)	0.039(2)	H(14)	-0.6970	-0.3711	-0.4386	0.0486
C(4)	-0.9145(5)	0.115(2)	-0.5660(4)	0.035(2)	H(15)	-0.5759	-0.3026	-0.4329	0.0486
C(5)	-0.7928(5)	0.097(2)	-0.5731(4)	0.034(1)	H(16)	-0.5520	-0.4159	-0.2975	0.0426
C(6)	-0.7111(5)	0.237(2)	-0.5204(4)	0.035(1)	H(17)	-0.6388	0.0042	-0.2831	0.0391
C(7)	-0.6631(5)	0.215(2)	-0.4211(4)	0.036(1)	H(18)	-0.5295	0.2387	-0.2319	0.0456
C(8)	-0.6100(5)	0.037(2)	-0.3958(4)	0.033(1)	H(19)	-0.4257	0.1661	-0.2537	0.0456
C(9)	-0.6935(5)	-0.107(2)	-0.4451(4)	0.032(1)	H(20)	-0.4767	0.0944	-0.1070	0.0502
C(10)	-0.7398(5)	-0.086(2)	-0.5482(4)	0.034(1)	H(21)	-0.3593	0.0582	-0.1191	0.0502
C(11)	-0.6373(6)	-0.283(2)	-0.4129(4)	0.039(1)	H(22)	-0.5463	-0.1605	-0.1518	0.0392
C(12)	-0.5917(5)	-0.307(2)	-0.3114(4)	0.035(1)	H(23)	-0.3357	-0.1044	-0.2464	0.0532
C(13)	-0.5058(5)	-0.163(2)	-0.2638(4)	0.032(1)	H(24)	-0.3637	-0.2951	-0.2709	0.0532
C(14)	-0.5692(5)	0.008(2)	-0.2966(4)	0.034(1)	H(25)	-0.4082	-0.1555	-0.3431	0.0532
C(15)	-0.4885(5)	0.141(2)	-0.2352(4)	0.037(2)	H(26)	-0.5774	-0.0331	-0.5540	0.0517
C(16)	-0.4424(6)	0.048(2)	-0.1463(5)	0.041(2)	H(27)	-0.6100	-0.2244	-0.5729	0.0517
C(17)	-0.4753(5)	-0.142(2)	-0.1617(4)	0.032(1)	H(28)	-0.6676	-0.0882	-0.6449	0.0517
C(18)	-0.3924(5)	-0.180(2)	-0.2825(4)	0.044(2)	H(29)	-0.3082	-0.2320	-0.0971	0.0430
C(19)	-0.6380(6)	-0.107(2)	-0.5823(5)	0.043(2)	H(30)	-0.4815	-0.4780	-0.1213	0.0578
C(20)	-0.3833(5)	-0.257(2)	-0.0954(4)	0.035(1)	H(31)	-0.3881	-0.4800	-0.1644	0.0578
C(21)	-0.4035(6)	-0.448(2)	-0.1135(5)	0.048(2)	H(32)	-0.3515	-0.5136	-0.0641	0.0578
C(22)	-0.3801(5)	-0.213(2)	-0.0020(4)	0.040(2)	H(33)	-0.4532	-0.2476	0.0005	0.0502
C(23)	-0.2852(6)	-0.297(2)	0.0742(4)	0.045(2)	H(34)	-0.3715	-0.0941	0.0046	0.0502
C(24)	-0.2767(6)	-0.225(2)	0.1621(4)	0.042(1)	H(35)	-0.2992	-0.4167	0.0723	0.0547
C(25)	-1.0028(7)	-0.409(2)	-0.1042(6)	0.066(2)	H(36)	-0.2118	-0.2783	0.0668	0.0547
C(26)	-1.0790(7)	-0.302(2)	-0.1661(6)	0.070(3)	H(37)	-1.1400	0.1128	-0.6196	0.0608
C(27)	-1.045(1)	-0.179(2)	-0.2093(7)	0.103(4)	H(38)	-0.7871	0.3411	-0.3962	0.0486
C(28)	-0.924(2)	-0.167(2)	-0.191(1)	0.121(5)	H(39)	-0.6806	-0.3765	-0.2341	0.0742
C(29)	-0.845(1)	-0.272(3)	-0.130(1)	0.129(6)	H(40)	-0.2556	-0.3147	0.2754	0.0654
C(30)	-0.8854(8)	-0.389(2)	-0.0877(9)	0.108(4)	H(41)	-1.1592	-0.3191	-0.1791	0.0851
C(31)	-1.048(1)	-0.548(2)	-0.0605(7)	0.090(3)	H(42)	-1.0984	-0.1064	-0.2494	0.1231
H(1)	-0.8451	-0.2119	-0.6566	0.0456	H(43)	-0.8946	-0.0870	-0.2199	0.1444
H(2)	-0.8035	-0.3281	-0.5738	0.0456	H(44)	-0.7632	-0.2651	-0.1185	0.1565
H(3)	-0.9435	-0.2144	-0.5274	0.0473	H(45)	-0.8314	-0.4658	-0.0441	0.1307
H(4)	-1.0041	-0.2830	-0.6226	0.0473	H(46)	-0.9870	-0.5792	-0.0036	0.1079
H(5)	-1.0147	-0.0099	-0.6791	0.0471	H(47)	-1.1134	-0.5099	-0.0484	0.1079

CA·21

atom	x	y	z	U	atom	x	y	z	U
O(1)	1.0890(3)	0.210(1)	1.1206(2)	0.0477(9)	H(6)	1.1146	-0.0135	0.9986	0.0457
O(2)	0.9122(3)	-0.018(1)	0.7700(2)	0.0443(9)	H(7)	1.0257	0.1098	0.9334	0.0457
O(3)	0.8215(3)	0.522(1)	0.6949(2)	0.0460(9)	H(8)	1.2253	0.0789	0.9225	0.0461
O(4)	0.3404(4)	0.264(1)	0.3471(4)	0.081(1)	H(9)	1.1505	-0.0438	0.7679	0.0544
O(5)	0.3008(3)	0.529(1)	0.3077(3)	0.064(1)	H(10)	1.1052	-0.1345	0.8389	0.0544
O(6)	0.623(2)	0.311(3)	1.1272(10)	0.36(1)	H(11)	0.9728	-0.0780	0.6704	0.0501
C(1)	1.1841(4)	0.404(1)	0.9281(3)	0.043(1)	H(12)	1.0209	0.1769	0.6373	0.0407
C(2)	1.1311(4)	0.392(1)	1.0072(3)	0.039(1)	H(13)	0.9809	0.3026	0.8041	0.0413
C(3)	1.1456(4)	0.219(1)	1.0530(3)	0.041(1)	H(14)	1.0491	0.4920	0.6760	0.0468
C(4)	1.1015(4)	0.094(1)	0.9679(3)	0.038(1)	H(15)	1.0224	0.5617	0.7657	0.0468
C(5)	1.1506(4)	0.102(1)	0.8864(3)	0.038(1)	H(16)	0.8845	0.6180	0.6030	0.0498
C(6)	1.1051(4)	-0.033(1)	0.8043(3)	0.044(1)	H(17)	0.8248	0.2147	0.6488	0.0412
C(7)	0.9896(4)	0.000(1)	0.7251(3)	0.039(1)	H(18)	0.8489	0.0586	0.4824	0.0462
C(8)	0.9790(3)	0.174(1)	0.6774(3)	0.0341(10)	H(19)	0.7840	-0.0064	0.5439	0.0462
C(9)	1.0222(4)	0.309(1)	0.7629(3)	0.0338(10)	H(20)	0.6428	0.1451	0.4505	0.0502
C(10)	1.1424(4)	0.278(1)	0.8378(4)	0.040(1)	H(21)	0.6998	0.1821	0.3767	0.0502
C(11)	1.0033(4)	0.481(1)	0.7121(3)	0.039(1)	H(22)	0.6881	0.3835	0.5305	0.0445
C(12)	0.8872(4)	0.514(1)	0.6355(3)	0.039(1)	H(23)	0.8808	0.3156	0.4263	0.0536
C(13)	0.8458(4)	0.380(1)	0.5505(3)	0.035(1)	H(24)	0.8960	0.5029	0.4502	0.0536
C(14)	0.8643(3)	0.212(1)	0.6061(3)	0.0337(10)	H(25)	0.9814	0.3784	0.5197	0.0536
C(15)	0.8053(4)	0.090(1)	0.5182(3)	0.038(1)	H(26)	1.1963	0.2111	0.7267	0.0654
C(16)	0.7059(4)	0.188(1)	0.4463(3)	0.041(1)	H(27)	1.2163	0.3963	0.7556	0.0654
C(17)	0.7227(4)	0.371(1)	0.4840(3)	0.036(1)	H(28)	1.2895	0.2633	0.8298	0.0654
C(18)	0.9071(4)	0.396(1)	0.4799(3)	0.044(1)	H(29)	0.6985	0.4737	0.3441	0.0482
C(19)	1.2180(4)	0.288(1)	0.7820(4)	0.054(2)	H(30)	0.6555	0.7411	0.3633	0.0623
C(20)	0.6672(4)	0.491(1)	0.3927(3)	0.040(1)	H(31)	0.6493	0.6993	0.4685	0.0623
C(21)	0.6845(4)	0.674(1)	0.4239(4)	0.050(1)	H(32)	0.7593	0.6956	0.4589	0.0623
C(22)	0.5461(4)	0.453(1)	0.3362(3)	0.043(1)	H(33)	0.5396	0.3443	0.3088	0.0562
C(23)	0.4824(4)	0.462(1)	0.4043(4)	0.050(1)	H(34)	0.5162	0.5293	0.2810	0.0562
C(24)	0.3684(4)	0.407(1)	0.3508(4)	0.050(1)	H(35)	0.5172	0.3933	0.4629	0.0623
C(25)	0.5801(9)	0.383(2)	0.961(2)	0.215(6)	H(36)	0.4836	0.5727	0.4260	0.0623
C(26)	0.515(1)	0.471(3)	0.874(2)	0.223(8)	H(37)	1.1223	0.1324	1.1778	0.0578
C(27)	0.540(1)	0.477(2)	0.789(1)	0.231(6)	H(38)	0.9276	-0.1079	0.8204	0.0558
C(28)	0.617(1)	0.391(2)	0.7798(7)	0.149(4)	H(39)	0.8229	0.5213	0.7436	0.0739
C(29)	0.6784(7)	0.302(2)	0.8625(7)	0.104(3)	H(40)	0.2172	0.5037	0.2853	0.0769
C(30)	0.6576(7)	0.300(1)	0.9498(5)	0.093(2)	H(41)	0.4526	0.5340	0.8688	0.2675
C(31)	0.548(2)	0.412(3)	1.044(2)	0.30(1)	H(42)	0.5042	0.5453	0.7301	0.2629
H(1)	1.2593	0.3865	0.9650	0.0513	H(43)	0.6307	0.3863	0.7169	0.1722
H(2)	1.1720	0.5114	0.8992	0.0513	H(44)	0.7378	0.2399	0.8619	0.1238
H(3)	1.1634	0.4702	1.0613	0.0476	H(45)	0.7030	0.2347	1.0071	0.1089
H(4)	1.0561	0.4161	0.9728	0.0476	H(46)	0.4879	0.4740	1.0409	0.3617
H(5)	1.2198	0.1985	1.0920	0.0511					

CA·43

atom	x	y	z	U	atom	x	y	z	U
O(1)	-1.0166(2)	-0.5803(7)	-0.4049(1)	0.0352(5)	H(6)	-0.8976	-0.6839	-0.4965	0.0349
O(2)	-0.8585(2)	-0.8143(7)	-0.6172(1)	0.0299(5)	H(7)	-0.8598	-0.7975	-0.4137	0.0349
O(3)	-0.9035(2)	-0.2680(7)	-0.7127(1)	0.0307(5)	H(8)	-0.6778	-0.6853	-0.3703	0.0350
O(4)	-0.9781(2)	-0.4986(7)	-1.1761(1)	0.0459(6)	H(9)	-0.7169	-0.9137	-0.4685	0.0372
O(5)	-0.9732(2)	-0.2419(7)	-1.2322(1)	0.0386(6)	H(10)	-0.6064	-0.8125	-0.4635	0.0372
O(6)	-0.4492(2)	-0.6869(7)	-0.8255(2)	0.0555(7)	H(11)	-0.6974	-0.8669	-0.6061	0.0323
O(7)	-0.3778(3)	-0.8593(7)	-0.9038(2)	0.086(1)	H(12)	-0.6269	-0.5985	-0.5940	0.0309
C(1)	-0.7449(2)	-0.3611(7)	-0.4070(2)	0.0298(7)	H(13)	-0.8296	-0.4781	-0.5731	0.0299
C(2)	-0.8732(2)	-0.3832(7)	-0.4178(2)	0.0296(7)	H(14)	-0.6440	-0.2776	-0.5757	0.0340
C(3)	-0.8943(2)	-0.5586(8)	-0.3875(2)	0.0305(6)	H(15)	-0.7563	-0.2081	-0.5640	0.0340
C(4)	-0.8510(2)	-0.6914(7)	-0.4363(2)	0.0284(7)	H(16)	-0.7554	-0.1621	-0.7065	0.0323
C(5)	-0.7237(2)	-0.6712(7)	-0.4302(2)	0.0284(7)	H(17)	-0.8466	-0.5826	-0.7171	0.0305
C(6)	-0.6884(2)	-0.8106(7)	-0.4818(2)	0.0304(7)	H(18)	-0.7857	-0.8126	-0.7685	0.0398
C(7)	-0.7346(2)	-0.7881(7)	-0.5809(2)	0.0263(6)	H(19)	-0.6627	-0.7384	-0.7505	0.0398
C(8)	-0.7086(2)	-0.6098(7)	-0.6077(2)	0.0251(6)	H(20)	-0.8534	-0.6760	-0.8949	0.0413
C(9)	-0.7479(2)	-0.4689(7)	-0.5580(2)	0.0242(6)	H(21)	-0.7265	-0.6286	-0.8841	0.0413
C(10)	-0.6951(2)	-0.4908(7)	-0.4563(2)	0.0268(6)	H(22)	-0.8899	-0.4285	-0.8468	0.0331
C(11)	-0.7254(2)	-0.2944(7)	-0.5918(2)	0.0278(7)	H(23)	-0.5824	-0.4815	-0.7502	0.0399
C(12)	-0.7791(2)	-0.2707(7)	-0.6915(2)	0.0271(6)	H(24)	-0.5683	-0.3680	-0.6691	0.0399
C(13)	-0.7388(2)	-0.4104(7)	-0.7416(2)	0.0252(6)	H(25)	-0.6020	-0.2876	-0.7617	0.0399
C(14)	-0.7653(2)	-0.5826(7)	-0.7060(2)	0.0248(6)	H(26)	-0.5296	-0.5409	-0.4533	0.0432
C(15)	-0.7429(3)	-0.7137(7)	-0.7676(2)	0.0323(8)	H(27)	-0.5326	-0.4803	-0.3631	0.0432
C(16)	-0.7850(3)	-0.6245(8)	-0.8578(2)	0.0339(7)	H(28)	-0.5468	-0.3504	-0.4378	0.0432
C(17)	-0.8103(2)	-0.4363(8)	-0.8414(2)	0.0271(6)	H(29)	-0.7173	-0.3314	-0.9127	0.0346
C(18)	-0.6107(2)	-0.3858(7)	-0.7296(2)	0.0324(7)	H(30)	-0.8002	-0.0650	-0.9421	0.0445
C(19)	-0.5634(2)	-0.4641(8)	-0.4248(2)	0.0353(7)	H(31)	-0.7596	-0.0974	-0.8419	0.0445
C(20)	-0.7944(2)	-0.3194(8)	-0.9126(2)	0.0278(6)	H(32)	-0.8897	-0.1144	-0.8976	0.0445
C(21)	-0.8127(3)	-0.1329(8)	-0.8971(2)	0.0368(8)	H(33)	-0.9542	-0.3699	-0.9996	0.0430
C(22)	-0.8776(3)	-0.3778(7)	-1.0015(2)	0.0353(8)	H(34)	-0.8595	-0.4899	-1.0102	0.0430
C(23)	-0.8745(2)	-0.2746(8)	-1.0805(2)	0.0328(7)	H(35)	-0.7963	-0.2663	-1.0791	0.0403
C(24)	-0.9467(2)	-0.3513(8)	-1.1661(2)	0.0301(6)	H(36)	-0.9023	-0.1621	-1.0765	0.0403
C(25)	-0.3786(3)	-0.5543(8)	-0.8364(2)	0.0468(9)	H(37)	-1.0253	-0.6664	-0.3612	0.0433
C(26)	-0.2668(3)	-0.5417(8)	-0.7819(2)	0.0537(10)	H(38)	-0.8804	-0.9199	-0.5952	0.0371
C(27)	-0.1988(4)	-0.4084(9)	-0.7925(3)	0.063(1)	H(39)	-0.9320	-0.1948	-0.7567	0.0374
C(28)	-0.2458(4)	-0.2905(8)	-0.8572(3)	0.072(1)	H(40)	-1.0226	-0.2920	-1.2863	0.0470
C(29)	-0.3577(4)	-0.3047(9)	-0.9117(3)	0.078(1)	H(41)	-0.2360	-0.6211	-0.7366	0.0654
C(30)	-0.4278(4)	-0.4370(9)	-0.9018(3)	0.064(1)	H(42)	-0.1201	-0.3974	-0.7554	0.0775
C(31)	-0.4415(3)	-0.8373(8)	-0.8625(2)	0.056(1)	H(43)	-0.1999	-0.1964	-0.8636	0.0870
C(32)	-0.5212(4)	-0.9673(9)	-0.8472(3)	0.069(1)	H(44)	-0.3878	-0.2225	-0.9573	0.0927
H(1)	-0.7014	-0.3675	-0.3464	0.0367	H(45)	-0.5073	-0.4440	-0.9382	0.0780
H(2)	-0.7352	-0.2495	-0.4276	0.0367	H(46)	-0.5768	-0.9972	-0.9014	0.0837
H(3)	-0.9187	-0.3683	-0.4781	0.0362	H(47)	-0.5597	-0.9184	-0.8103	0.0837
H(4)	-0.8951	-0.2980	-0.3844	0.0362	H(48)	-0.4777	-1.0613	-0.8196	0.0837
H(5)	-0.8540	-0.5673	-0.3261	0.0367					

CA·45

atom	x	y	z	U	atom	x	y	z	U
O(1)	-0.4806(3)	-0.470(1)	-0.0952(2)	0.033(1)	O(1)	-0.4806(3)	-0.470(1)	-0.0952(2)	0.033(1)
O(2)	-0.6384(3)	-0.702(1)	0.1193(2)	0.027(1)	H(6)	-0.5984	-0.5676	-0.0012	0.0304
O(3)	-0.6006(3)	-0.157(1)	0.2134(2)	0.030(1)	H(7)	-0.6350	-0.6834	-0.0829	0.0304
O(4)	-0.5207(4)	-0.398(1)	0.6745(3)	0.060(1)	H(8)	-0.8209	-0.5744	-0.1284	0.0299
O(5)	-0.5329(4)	-0.144(1)	0.7287(2)	0.045(1)	H(9)	-0.8956	-0.6994	-0.0354	0.0297
O(6)	-0.9896(5)	-0.955(1)	0.4294(3)	0.078(2)	H(10)	-0.7844	-0.8015	-0.0310	0.0297
O(7)	-1.095(2)	-0.842(2)	0.3144(5)	0.424(9)	H(11)	-0.7971	-0.7618	0.1005	0.0274
C(1)	-0.7578(5)	-0.252(1)	-0.0923(3)	0.026(1)	H(12)	-0.8753	-0.4892	0.0946	0.0264
C(2)	-0.6278(5)	-0.275(1)	-0.0822(4)	0.029(1)	H(13)	-0.6715	-0.3652	0.0734	0.0239
C(3)	-0.6051(5)	-0.450(1)	-0.1112(3)	0.025(1)	H(14)	-0.7478	-0.1018	0.0640	0.0286
C(4)	-0.6452(5)	-0.579(1)	-0.0611(4)	0.025(1)	H(15)	-0.8624	-0.1728	0.0737	0.0286
C(5)	-0.7755(5)	-0.562(1)	-0.0683(3)	0.024(1)	H(16)	-0.7658	-0.0473	0.2043	0.0305
C(6)	-0.8121(5)	-0.700(1)	-0.0173(3)	0.024(1)	H(17)	-0.6544	-0.4698	0.2181	0.0258
C(7)	-0.7644(5)	-0.678(1)	0.0827(3)	0.023(1)	H(18)	-0.7120	-0.6992	0.2690	0.0398
C(8)	-0.7924(5)	-0.500(1)	0.1091(3)	0.021(1)	H(19)	-0.8373	-0.6287	0.2525	0.0398
C(9)	-0.7550(5)	-0.360(1)	0.0580(3)	0.019(1)	H(20)	-0.7704	-0.5208	0.3864	0.0441
C(10)	-0.8068(5)	-0.382(1)	-0.0429(3)	0.023(1)	H(21)	-0.6415	-0.5616	0.3948	0.0441
C(11)	-0.7795(5)	-0.189(1)	0.0910(3)	0.022(1)	H(22)	-0.6115	-0.3130	0.3474	0.0309
C(12)	-0.7280(5)	-0.164(1)	0.1916(3)	0.025(1)	H(23)	-0.9232	-0.3793	0.2502	0.0353
C(13)	-0.7649(5)	-0.302(1)	0.2415(3)	0.021(1)	H(24)	-0.9405	-0.2676	0.1683	0.0353
C(14)	-0.7370(5)	-0.474(1)	0.2066(3)	0.021(1)	H(25)	-0.9088	-0.1859	0.2603	0.0353
C(15)	-0.7566(6)	-0.604(1)	0.2683(4)	0.033(2)	H(26)	-0.9753	-0.4333	-0.0476	0.0334
C(16)	-0.7134(6)	-0.515(1)	0.3585(4)	0.036(2)	H(27)	-0.9707	-0.3734	-0.1375	0.0334
C(17)	-0.6922(5)	-0.327(1)	0.3417(3)	0.025(1)	H(28)	-0.9589	-0.2441	-0.0634	0.0334
C(18)	-0.8968(5)	-0.285(1)	0.2286(4)	0.030(2)	H(29)	-0.7908	-0.2313	0.4112	0.0322
C(19)	-0.9413(5)	-0.358(1)	-0.0758(3)	0.028(1)	H(30)	-0.7158	0.0384	0.4423	0.0486
C(20)	-0.7137(5)	-0.214(1)	0.4114(4)	0.027(1)	H(31)	-0.6296	0.0013	0.3920	0.0486
C(21)	-0.7037(6)	-0.027(1)	0.3960(4)	0.041(2)	H(32)	-0.7639	0.0073	0.3419	0.0486
C(22)	-0.6283(6)	-0.264(1)	0.5017(4)	0.039(2)	H(33)	-0.5515	-0.2284	0.5038	0.0486
C(23)	-0.6476(6)	-0.191(1)	0.5811(4)	0.046(2)	H(34)	-0.6317	-0.3793	0.5058	0.0486
C(24)	-0.5606(5)	-0.255(1)	0.6659(4)	0.036(2)	H(35)	-0.6398	-0.0697	0.5799	0.0562
C(25)	-0.8840(8)	-0.826(1)	0.5660(5)	0.071(2)	H(36)	-0.7242	-0.2166	0.5796	0.0562
C(26)	-0.8985(9)	-0.911(1)	0.6356(6)	0.079(3)	H(37)	-0.4780	-0.5817	-0.1389	0.0392
C(27)	-0.811(2)	-0.914(2)	0.7129(7)	0.156(5)	H(38)	-0.6062	-0.7949	0.0991	0.0328
C(28)	-0.715(2)	-0.843(3)	0.730(1)	0.250(8)	H(39)	-0.5673	-0.0528	0.2547	0.0375
C(29)	-0.693(1)	-0.756(2)	0.660(1)	0.189(7)	H(40)	-0.4646	-0.1735	0.7898	0.0529
C(30)	-0.775(1)	-0.747(1)	0.5817(9)	0.111(4)	H(41)	-0.9710	-0.9611	0.6294	0.0932
C(31)	-0.980(1)	-0.816(2)	0.4797(6)	0.210(6)	H(42)	-0.8222	-0.9743	0.7599	0.1750
C(32)	-1.055(1)	-0.949(2)	0.3468(6)	0.133(4)	H(43)	-0.6587	-0.8415	0.7860	0.2853
H(1)	-0.7669	-0.1404	-0.0707	0.0319	H(44)	-0.6189	-0.7009	0.6700	0.2234
H(2)	-0.8030	-0.2555	-0.1528	0.0319	H(45)	-0.7620	-0.6823	0.5351	0.1322
H(3)	-0.5814	-0.2561	-0.0226	0.0350	H(46)	-0.9666	-0.7167	0.4495	0.2489
H(4)	-0.6071	-0.1908	-0.1174	0.0350	H(47)	-1.0533	-0.7961	0.4905	0.2489
H(5)	-0.6381	-0.4394	-0.1750	0.0302	H(48)	-1.0690	-1.0486	0.3150	0.1564

CA·50

atom	x	y	z	U	atom	x	y	z	U
O(1)	-0.0886(3)	-0.033(1)	-0.1203(3)	0.040(1)	H(7)	-0.1203	0.1878	-0.0010	0.0365
O(2)	0.0846(3)	0.196(1)	0.2309(3)	0.0360(10)	H(8)	-0.2257	0.1077	0.0799	0.0410
O(3)	0.1754(3)	-0.346(1)	0.3050(3)	0.040(1)	H(9)	-0.1115	0.3072	0.1561	0.0458
O(4)	0.6562(4)	-0.089(1)	0.6425(4)	0.077(2)	H(10)	-0.1583	0.2152	0.2241	0.0458
O(5)	0.7020(3)	-0.350(1)	0.6911(4)	0.062(1)	H(11)	0.0341	0.2490	0.3237	0.0397
O(6)	0.5175(5)	-0.295(1)	0.0318(4)	0.101(2)	H(12)	-0.0271	-0.0032	0.3562	0.0332
C(1)	-0.1857(4)	-0.230(1)	0.0654(4)	0.035(1)	H(13)	0.0192	-0.1376	0.2080	0.0380
C(2)	-0.1300(4)	-0.216(1)	-0.0087(4)	0.035(1)	H(14)	-0.0518	-0.3173	0.3211	0.0400
C(3)	-0.1463(5)	-0.044(1)	-0.0555(4)	0.035(1)	H(15)	-0.0263	-0.3885	0.2325	0.0400
C(4)	-0.1054(4)	0.084(1)	0.0292(4)	0.030(1)	H(16)	0.1138	-0.4454	0.3947	0.0411
C(5)	-0.1559(4)	0.071(1)	0.1069(4)	0.035(1)	H(17)	0.1724	-0.0395	0.3511	0.0335
C(6)	-0.1108(4)	0.207(1)	0.1908(4)	0.037(1)	H(18)	0.1487	0.1148	0.5133	0.0418
C(7)	0.0031(4)	0.176(1)	0.2710(4)	0.032(1)	H(19)	0.2131	0.1793	0.4527	0.0418
C(8)	0.0159(4)	0.002(1)	0.3178(4)	0.027(1)	H(20)	0.3559	0.0292	0.5476	0.0450
C(9)	-0.0266(4)	-0.137(1)	0.2339(4)	0.028(1)	H(21)	0.2994	-0.0070	0.6203	0.0450
C(10)	-0.1454(4)	-0.104(1)	0.1555(4)	0.033(1)	H(22)	0.2982	-0.1978	0.4570	0.0392
C(11)	-0.0063(4)	-0.306(1)	0.2857(4)	0.034(1)	H(23)	0.0995	-0.3316	0.5455	0.0486
C(12)	0.1118(4)	-0.339(1)	0.3636(4)	0.034(1)	H(24)	0.0161	-0.2001	0.4792	0.0486
C(13)	0.1512(4)	-0.204(1)	0.4475(4)	0.032(1)	H(25)	0.1201	-0.1456	0.5739	0.0486
C(14)	0.1326(4)	-0.035(1)	0.3924(4)	0.027(1)	H(26)	-0.2261	-0.2297	0.2311	0.0586
C(15)	0.1917(4)	0.085(1)	0.4781(4)	0.035(1)	H(27)	-0.2964	-0.0891	0.1606	0.0586
C(16)	0.2923(4)	-0.011(1)	0.5508(4)	0.037(1)	H(28)	-0.2022	-0.0468	0.2665	0.0586
C(17)	0.2762(4)	-0.195(1)	0.5150(4)	0.032(1)	H(29)	0.3122	-0.2894	0.6709	0.0426
C(18)	0.0917(5)	-0.221(1)	0.5184(4)	0.040(2)	H(30)	0.3619	-0.5598	0.6358	0.0547
C(19)	-0.2257(4)	-0.117(1)	0.2083(5)	0.048(2)	H(31)	0.3269	-0.5173	0.5199	0.0547
C(20)	0.3332(4)	-0.312(1)	0.6067(4)	0.036(1)	H(32)	0.2410	-0.5234	0.5653	0.0547
C(21)	0.3135(5)	-0.495(1)	0.5780(5)	0.047(2)	H(33)	0.4861	-0.3502	0.7167	0.0467
C(22)	0.4550(4)	-0.275(1)	0.6611(4)	0.040(1)	H(34)	0.4628	-0.1647	0.6852	0.0467
C(23)	0.5158(4)	-0.290(1)	0.5918(5)	0.048(2)	H(35)	0.5161	-0.4051	0.5738	0.0560
C(24)	0.6315(5)	-0.234(1)	0.6453(5)	0.044(1)	H(36)	0.4800	-0.2280	0.5312	0.0560
C(25)	0.4591(6)	-0.246(1)	0.0888(6)	0.073(2)	H(37)	-0.0756	0.0686	-0.1465	0.0480
C(26)	0.4911(7)	-0.319(1)	0.1824(6)	0.081(2)	H(38)	0.0688	0.2682	0.1872	0.0436
C(27)	0.4376(7)	-0.290(2)	0.2433(6)	0.086(3)	H(39)	0.2386	-0.4139	0.3307	0.0465
C(28)	0.3522(7)	-0.183(2)	0.2111(8)	0.084(3)	H(40)	0.7881	-0.3322	0.7146	0.0720
C(29)	0.3238(8)	-0.106(1)	0.1173(8)	0.092(3)	H(41)	0.5531	-0.3999	0.2084	0.0775
C(30)	0.3778(6)	-0.139(1)	0.0537(6)	0.075(2)	H(42)	0.4587	-0.3437	0.3102	0.0775
C(31)	0.482(1)	-0.232(2)	-0.0715(7)	0.129(4)	H(43)	0.3123	-0.1583	0.2507	0.0775
H(1)	-0.1725	-0.3410	0.0949	0.0416	H(44)	0.2603	-0.0292	0.0894	0.0775
H(2)	-0.2616	-0.2178	0.0270	0.0416	H(45)	0.3548	-0.0854	-0.0125	0.0775
H(3)	-0.1613	-0.2977	-0.0626	0.0423	H(46)	0.4834	-0.1197	-0.0716	0.1336
H(4)	-0.0550	-0.2400	0.0283	0.0423	H(47)	0.5272	-0.2790	-0.1018	0.1336
H(5)	-0.2216	-0.0276	-0.0962	0.0426	H(48)	0.4088	-0.2732	-0.1118	0.1336
H(6)	-0.0289	0.0673	0.0662	0.0365					

CA·51

atom	x	y	z	U	atom	x	y	z	U
O(1)	-0.4810(3)	-0.428(1)	-1.0953(3)	0.050(1)	H(7)	-0.5969	-0.5263	-1.0043	0.0441
O(2)	-0.6416(3)	-0.664(1)	-0.8801(2)	0.0431(10)	H(8)	-0.8213	-0.5290	-1.1285	0.0289
O(3)	-0.6059(3)	-0.115(1)	-0.7878(2)	0.0447(10)	H(9)	-0.8910	-0.6576	-1.0316	0.0334
O(4)	-0.5223(6)	-0.358(1)	-0.3246(3)	0.089(2)	H(10)	-0.7790	-0.7557	-1.0284	0.0334
O(5)	-0.5296(4)	-0.100(1)	-0.2719(3)	0.064(1)	H(11)	-0.8067	-0.7128	-0.8960	0.0300
O(6)	-1.0764(5)	-0.271(1)	-0.4713(3)	0.074(1)	H(12)	-0.8738	-0.4471	-0.9075	0.0260
C(1)	-0.7568(5)	-0.216(1)	-1.0901(3)	0.038(1)	H(13)	-0.6725	-0.3320	-0.9238	0.0205
C(2)	-0.6283(5)	-0.235(1)	-1.0812(3)	0.039(1)	H(14)	-0.7494	-0.0632	-0.9348	0.0365
C(3)	-0.6034(5)	-0.409(1)	-1.1098(3)	0.039(1)	H(15)	-0.8625	-0.1334	-0.9220	0.0365
C(4)	-0.6447(4)	-0.538(1)	-1.0594(3)	0.038(1)	H(16)	-0.7556	-0.0117	-0.7939	0.0289
C(5)	-0.7731(4)	-0.522(1)	-1.0672(3)	0.035(1)	H(17)	-0.6583	-0.4289	-0.7787	0.0305
C(6)	-0.8097(5)	-0.660(1)	-1.0147(3)	0.037(1)	H(18)	-0.8395	-0.5945	-0.7494	0.0340
C(7)	-0.7658(5)	-0.638(1)	-0.9169(3)	0.034(1)	H(19)	-0.7133	-0.6586	-0.7322	0.0340
C(8)	-0.7939(4)	-0.462(1)	-0.8899(3)	0.031(1)	H(20)	-0.7782	-0.4662	-0.6115	0.0410
C(9)	-0.7561(4)	-0.322(1)	-0.9398(3)	0.031(1)	H(21)	-0.6496	-0.5119	-0.5997	0.0410
C(10)	-0.8042(5)	-0.344(1)	-1.0411(3)	0.035(1)	H(22)	-0.6154	-0.2732	-0.6539	0.0338
C(11)	-0.7812(5)	-0.150(1)	-0.9066(3)	0.037(1)	H(23)	-0.9076	-0.1394	-0.7329	0.0441
C(12)	-0.7293(5)	-0.123(1)	-0.8076(3)	0.034(1)	H(24)	-0.9388	-0.2227	-0.8245	0.0441
C(13)	-0.7688(4)	-0.266(1)	-0.7552(3)	0.033(1)	H(25)	-0.9266	-0.3320	-0.7424	0.0441
C(14)	-0.7396(5)	-0.433(1)	-0.7919(3)	0.034(1)	H(26)	-0.9569	-0.2137	-1.0580	0.0319
C(15)	-0.7620(6)	-0.566(1)	-0.7300(3)	0.045(2)	H(27)	-0.9645	-0.3331	-1.1357	0.0319
C(16)	-0.7205(6)	-0.474(1)	-0.6396(3)	0.051(1)	H(28)	-0.9687	-0.4058	-1.0474	0.0319
C(17)	-0.6960(5)	-0.289(1)	-0.6572(3)	0.037(1)	H(29)	-0.7937	-0.1965	-0.5860	0.0357
C(18)	-0.8972(5)	-0.244(1)	-0.7669(3)	0.044(1)	H(30)	-0.6276	0.0434	-0.5956	0.0639
C(19)	-0.9371(5)	-0.322(1)	-1.0742(3)	0.045(1)	H(31)	-0.7579	0.0557	-0.6513	0.0639
C(20)	-0.7154(5)	-0.175(1)	-0.5867(3)	0.042(1)	H(32)	-0.7215	0.0736	-0.5504	0.0639
C(21)	-0.7043(7)	0.013(1)	-0.6022(4)	0.064(2)	H(33)	-0.6177	-0.3394	-0.4933	0.0578
C(22)	-0.6277(6)	-0.227(1)	-0.4971(4)	0.056(2)	H(34)	-0.5511	-0.1742	-0.4959	0.0578
C(23)	-0.6437(6)	-0.153(1)	-0.4169(4)	0.059(2)	H(35)	-0.6530	-0.0423	-0.4207	0.0669
C(24)	-0.5593(5)	-0.217(1)	-0.3346(4)	0.051(1)	H(36)	-0.7214	-0.2062	-0.4191	0.0669
C(25)	-1.1365(6)	-0.288(1)	-0.5585(4)	0.061(2)	H(37)	-0.4659	-0.5373	-1.1145	0.0426
C(26)	-1.0975(7)	-0.377(2)	-0.6172(5)	0.074(2)	H(38)	-0.6241	-0.7758	-0.8931	0.0410
C(27)	-1.1654(9)	-0.387(2)	-0.7045(5)	0.091(3)	H(39)	-0.5720	-0.0873	-0.7260	0.0411
C(28)	-1.272(1)	-0.313(2)	-0.7306(6)	0.108(3)	H(40)	-0.4730	-0.1138	-0.2171	0.0709
C(29)	-1.3084(9)	-0.216(2)	-0.6727(8)	0.102(3)	H(41)	-1.0196	-0.4289	-0.5941	0.0944
C(30)	-1.2412(7)	-0.204(2)	-0.5895(6)	0.081(2)	H(42)	-1.1392	-0.4423	-0.7521	0.0942
C(31)	-0.9836(7)	-0.383(2)	-0.4340(5)	0.080(2)	H(43)	-1.3329	-0.3275	-0.7837	0.1001
C(32)	-0.9383(9)	-0.363(2)	-0.3383(5)	0.100(3)	H(44)	-1.3852	-0.1462	-0.6938	0.1038
H(1)	-0.7689	-0.1036	-1.0687	0.0334	H(45)	-1.2734	-0.1472	-0.5444	0.0900
H(2)	-0.7981	-0.2202	-1.1498	0.0334	H(46)	-1.0097	-0.4930	-0.4512	0.0977
H(3)	-0.6080	-0.1453	-1.1117	0.0445	H(47)	-0.9221	-0.3560	-0.4582	0.0977
H(4)	-0.5868	-0.2139	-1.0178	0.0445	H(48)	-1.0007	-0.3902	-0.3106	0.0995
H(5)	-0.6436	-0.4257	-1.1702	0.0380	H(49)	-0.8761	-0.4388	-0.3092	0.0995
H(6)	-0.6338	-0.6399	-1.0867	0.0441	H(50)	-0.9140	-0.2519	-0.3177	0.0995

CA·54

atom	x	y	z	U	atom	x	y	z	U
O(1)	-0.4812(5)	-0.464(2)	-0.5948(4)	0.030(2)	H(7)	-0.5998	-0.5637	-0.5009	0.0334
O(2)	-0.6361(5)	-0.694(2)	-0.3806(3)	0.031(2)	H(8)	-0.8239	-0.5692	-0.6282	0.0289
O(3)	-0.6015(5)	-0.149(2)	-0.2881(3)	0.028(2)	H(9)	-0.7833	-0.7970	-0.5297	0.0334
O(4)	-0.5219(7)	-0.388(2)	0.1738(4)	0.058(2)	H(10)	-0.8949	-0.6957	-0.5347	0.0334
O(5)	-0.5347(5)	-0.136(2)	0.2283(3)	0.041(2)	H(11)	-0.7930	-0.7567	-0.3880	0.0380
O(6)	-1.0211(10)	-0.411(2)	0.0769(7)	0.118(3)	H(12)	-0.8758	-0.4860	-0.4053	0.0261
C(1)	-0.7578(8)	-0.245(2)	-0.5933(5)	0.028(2)	H(13)	-0.6708	-0.3671	-0.4221	0.0243
C(2)	-0.6292(8)	-0.269(2)	-0.5836(5)	0.027(2)	H(14)	-0.7470	-0.0965	-0.4367	0.0283
C(3)	-0.6055(8)	-0.444(2)	-0.6110(5)	0.028(2)	H(15)	-0.8618	-0.1666	-0.4274	0.0283
C(4)	-0.6480(7)	-0.571(2)	-0.5614(6)	0.026(2)	H(16)	-0.7536	-0.0492	-0.2944	0.0294
C(5)	-0.7771(7)	-0.558(2)	-0.5698(5)	0.024(2)	H(17)	-0.6486	-0.4579	-0.2858	0.0258
C(6)	-0.8126(7)	-0.694(2)	-0.5170(5)	0.025(2)	H(18)	-0.7072	-0.6928	-0.2298	0.0409
C(7)	-0.7631(7)	-0.670(2)	-0.4178(5)	0.025(2)	H(19)	-0.8339	-0.6270	-0.2479	0.0409
C(8)	-0.7916(7)	-0.498(2)	-0.3915(5)	0.023(2)	H(20)	-0.6427	-0.5564	-0.1048	0.0410
C(9)	-0.7561(7)	-0.353(2)	-0.4418(5)	0.020(2)	H(21)	-0.7724	-0.5161	-0.1160	0.0410
C(10)	-0.8059(7)	-0.379(2)	-0.5428(5)	0.021(2)	H(22)	-0.6120	-0.3069	-0.1530	0.0319
C(11)	-0.7787(7)	-0.183(2)	-0.4087(5)	0.021(2)	H(23)	-0.9223	-0.3736	-0.2511	0.0365
C(12)	-0.7273(7)	-0.156(2)	-0.3086(5)	0.026(2)	H(24)	-0.9074	-0.1796	-0.2425	0.0365
C(13)	-0.7652(7)	-0.297(2)	-0.2590(5)	0.023(2)	H(25)	-0.9379	-0.2644	-0.3336	0.0365
C(14)	-0.7343(7)	-0.464(2)	-0.2930(5)	0.023(2)	H(26)	-0.9759	-0.4283	-0.5484	0.0345
C(15)	-0.7547(8)	-0.598(2)	-0.2312(5)	0.033(3)	H(27)	-0.9585	-0.2388	-0.5638	0.0345
C(16)	-0.7139(8)	-0.507(2)	-0.1424(6)	0.034(2)	H(28)	-0.9719	-0.3681	-0.6382	0.0345
C(17)	-0.6910(8)	-0.317(2)	-0.1588(5)	0.027(2)	H(29)	-0.7817	-0.2198	-0.0700	0.0334
C(18)	-0.8946(7)	-0.278(2)	-0.2729(5)	0.029(2)	H(30)	-0.7785	0.0199	-0.1493	0.0532
C(19)	-0.9421(7)	-0.352(2)	-0.5771(5)	0.030(2)	H(31)	-0.6438	0.0031	-0.1265	0.0532
C(20)	-0.7161(7)	-0.207(2)	-0.0897(5)	0.025(2)	H(32)	-0.6954	0.0422	-0.0533	0.0532
C(21)	-0.7074(9)	-0.018(2)	-0.1059(6)	0.044(3)	H(33)	-0.5503	-0.2184	0.0034	0.0471
C(22)	-0.6275(9)	-0.256(2)	0.0008(6)	0.037(3)	H(34)	-0.6271	-0.3733	0.0058	0.0471
C(23)	-0.6488(9)	-0.184(2)	0.0811(5)	0.044(3)	H(35)	-0.6419	-0.0621	0.0790	0.0578
C(24)	-0.5618(8)	-0.248(2)	0.1648(6)	0.036(2)	H(36)	-0.7255	-0.2109	0.0776	0.0578
C(25)	-1.1060(8)	-0.319(2)	-0.0666(5)	0.0836	H(37)	-0.4790	-0.5478	-0.6505	0.0383
C(26)	-1.0983(8)	-0.393(2)	-0.1424(7)	0.0836	H(38)	-0.6044	-0.7934	-0.4019	0.0356
C(27)	-1.1947(10)	-0.389(2)	-0.2199(5)	0.0836	H(39)	-0.5678	-0.0703	-0.2410	0.0354
C(28)	-1.2987(8)	-0.311(2)	-0.2216(5)	0.0836	H(40)	-0.4876	-0.1649	0.2934	0.0517
C(29)	-1.3064(8)	-0.237(2)	-0.1457(7)	0.0836	H(41)	-1.0275(9)	-0.445(3)	-0.1412(10)	0.0836
C(30)	-1.2101(10)	-0.241(2)	-0.0682(5)	0.0836	H(42)	-1.189(1)	-0.439(3)	-0.2715(7)	0.0836
C(31)	-1.003(2)	-0.313(3)	0.018(1)	0.146(7)	H(43)	-1.3643(10)	-0.308(3)	-0.2743(6)	0.0836
C(32)	-0.930(1)	-0.406(2)	0.1620(8)	0.089(4)	H(44)	-1.3773(9)	-0.184(3)	-0.1469(10)	0.0836
H(1)	-0.7668	-0.1350	-0.5715	0.0334	H(45)	-1.215(1)	-0.190(3)	-0.0166(6)	0.0836
H(2)	-0.8040	-0.2491	-0.6539	0.0334	H(46)	-0.9400	-0.3285	0.0104	0.2053
H(3)	-0.6097	-0.1865	-0.6191	0.0351	H(47)	-1.0093	-0.1944	0.0425	0.2053
H(4)	-0.5835	-0.2513	-0.5243	0.0351	H(48)	-0.8606	-0.4361	0.1579	0.1058
H(5)	-0.6545	-0.4256	-0.6756	0.0380	H(49)	-0.9265	-0.2877	0.1828	0.1058
H(6)	-0.6358	-0.6808	-0.5822	0.0334	H(50)	-0.9569	-0.4719	0.1987	0.1058

CA·55

atom	x	y	z	U	atom	x	y	z	U
O(1)	-0.0862(2)	0.4039(6)	-0.1205(1)	0.0399(5)	H(5)	-0.2239	0.3890	-0.0943	0.0363
O(2)	0.0912(1)	0.1751(6)	0.2315(1)	0.0350(4)	H(6)	-0.1042	0.1823	0.0035	0.0378
O(3)	0.1761(1)	0.7131(6)	0.3044(1)	0.0372(5)	H(7)	-0.0211	0.3051	0.0659	0.0380
O(4)	0.6616(2)	0.4575(6)	0.6538(2)	0.0598(7)	H(8)	-0.2289	0.2701	0.0739	0.0380
O(5)	0.6976(2)	0.7219(6)	0.6922(2)	0.0508(6)	H(9)	-0.1443	0.1418	0.2375	0.0419
N(1)	0.3371(4)	0.4248(8)	-0.1525(3)	0.097(1)	H(10)	-0.1004	0.0316	0.1599	0.0380
C(1)	-0.1831(2)	0.5907(7)	0.0715(2)	0.0360(7)	H(11)	0.0366	0.1145	0.3381	0.0380
C(2)	-0.1304(2)	0.5807(7)	-0.0062(2)	0.0347(6)	H(12)	-0.0197	0.3663	0.3617	0.0380
C(3)	-0.1434(2)	0.4106(7)	-0.0533(2)	0.0348(6)	H(13)	0.0221	0.4947	0.1960	0.0380
C(4)	-0.0979(2)	0.2846(6)	0.0325(2)	0.0320(6)	H(14)	-0.0425	0.6776	0.3286	0.0355
C(5)	-0.1476(2)	0.2916(7)	0.1130(2)	0.0336(6)	H(15)	-0.0268	0.7542	0.2363	0.0355
C(6)	-0.1009(2)	0.1565(7)	0.1962(2)	0.0349(6)	H(16)	0.1160	0.8155	0.3992	0.0380
C(7)	0.0131(2)	0.1916(7)	0.2766(2)	0.0317(6)	H(17)	0.1744	0.4072	0.3530	0.0380
C(8)	0.0232(2)	0.3637(7)	0.3229(2)	0.0282(5)	H(18)	0.2206	0.1782	0.4540	0.0380
C(9)	-0.0212(2)	0.4985(6)	0.2387(2)	0.0274(5)	H(19)	0.1488	0.2532	0.5210	0.0406
C(10)	-0.1404(2)	0.4647(7)	0.1621(2)	0.0310(6)	H(20)	0.3676	0.3342	0.5544	0.0392
C(11)	-0.0032(2)	0.6697(7)	0.2902(2)	0.0326(6)	H(21)	0.3013	0.3681	0.6332	0.0392
C(12)	0.1135(2)	0.7044(6)	0.3661(2)	0.0313(6)	H(22)	0.3100	0.5755	0.4663	0.0380
C(13)	0.1560(2)	0.5704(7)	0.4515(2)	0.0285(6)	H(23)	0.0964	0.6995	0.5501	0.0453
C(14)	0.1386(2)	0.4024(7)	0.3957(2)	0.0277(6)	H(24)	0.0137	0.5548	0.4936	0.0453
C(15)	0.1983(2)	0.2814(7)	0.4831(2)	0.0336(6)	H(25)	0.1211	0.5102	0.5834	0.0453
C(16)	0.2981(2)	0.3797(7)	0.5557(2)	0.0355(6)	H(26)	-0.1890	0.4172	0.2846	0.0506
C(17)	0.2798(2)	0.5613(7)	0.5176(2)	0.0303(6)	H(27)	-0.2909	0.4413	0.1738	0.0506
C(18)	0.0962(2)	0.5844(6)	0.5237(2)	0.0369(7)	H(28)	-0.2264	0.5903	0.2399	0.0506
C(19)	-0.2160(2)	0.4739(7)	0.2189(2)	0.0423(7)	H(29)	0.3024	0.6524	0.6629	0.0380
C(20)	0.3351(2)	0.6805(7)	0.6094(2)	0.0325(6)	H(30)	0.3605	0.9374	0.6367	0.0497
C(21)	0.3175(2)	0.8614(7)	0.5779(2)	0.0413(7)	H(31)	0.3430	0.8927	0.5174	0.0497
C(22)	0.4563(2)	0.6420(7)	0.6657(2)	0.0366(6)	H(32)	0.2399	0.8957	0.5541	0.0380
C(23)	0.5166(2)	0.6501(7)	0.5944(2)	0.0434(7)	H(33)	0.4901	0.7246	0.7237	0.0396
C(24)	0.6316(2)	0.5979(7)	0.6491(2)	0.0368(6)	H(34)	0.4623	0.5244	0.6954	0.0396
C(25)	0.3804(3)	0.5190(7)	0.0374(3)	0.0588(8)	H(35)	0.5161	0.7631	0.5724	0.0538
C(26)	0.3090(3)	0.4811(7)	0.0806(3)	0.0618(10)	H(36)	0.4854	0.5789	0.5353	0.0538
C(27)	0.3274(4)	0.5388(8)	0.1787(3)	0.077(1)	H(37)	-0.1149	0.3287	-0.1676	0.0667
C(28)	0.4177(4)	0.6339(8)	0.2329(3)	0.087(1)	H(38)	0.0819	0.0790	0.1909	0.1353
C(29)	0.4859(4)	0.6663(9)	0.1870(4)	0.096(1)	H(39)	0.2243	0.8027	0.3269	0.1305
C(30)	0.4679(3)	0.6119(8)	0.0903(3)	0.076(1)	H(40)	0.7634	0.6902	0.7164	0.1168
C(31)	0.3580(3)	0.4659(7)	-0.0677(3)	0.066(1)	H(41)	0.2491	0.4153	0.0420	0.0719
H(1)	-0.1704	0.7080	0.0991	0.0427	H(42)	0.2776	0.5118	0.2121	0.0935
H(2)	-0.2585	0.5650	0.0337	0.0427	H(43)	0.4322	0.6807	0.3036	0.1023
H(3)	-0.1612	0.6563	-0.0619	0.0402	H(44)	0.5505	0.7333	0.2258	0.1089
H(4)	-0.0447	0.6076	0.0319	0.0402	H(45)	0.5173	0.6400	0.0566	0.0934

CA·56

atom	x	y	z	U	atom	x	y	z	U
O(1)	-1.1109(3)	-0.234(2)	-0.5969(3)	0.046(1)	H(7)	-0.9036	-0.1321	-0.5020	0.0378
O(2)	-0.7479(3)	-0.003(2)	-0.3801(3)	0.040(1)	H(8)	-0.8016	-0.1247	-0.6279	0.0331
O(3)	-0.6905(4)	-0.548(2)	-0.2866(3)	0.045(1)	H(9)	-0.6412	0.0036	-0.5342	0.0392
O(4)	-0.2905(10)	-0.312(2)	0.1744(5)	0.140(3)	H(10)	-0.7494	0.1001	-0.5275	0.0392
O(5)	-0.2308(5)	-0.567(2)	0.2253(3)	0.074(2)	H(11)	-0.5947	0.0527	-0.3890	0.0361
C(1)	-0.8325(5)	-0.449(2)	-0.5952(4)	0.035(1)	H(12)	-0.5330	-0.2118	-0.4060	0.0356
C(2)	-0.9506(5)	-0.427(2)	-0.5832(4)	0.040(2)	H(13)	-0.7570	-0.3401	-0.4258	0.0319
C(3)	-1.0023(5)	-0.252(2)	-0.6118(4)	0.039(1)	H(14)	-0.6866	-0.6065	-0.4374	0.0358
C(4)	-0.9132(5)	-0.120(2)	-0.5619(4)	0.036(2)	H(15)	-0.5630	-0.5315	-0.4261	0.0358
C(5)	-0.7892(5)	-0.138(2)	-0.5683(4)	0.033(1)	H(16)	-0.5480	-0.6540	-0.2974	0.0411
C(6)	-0.7061(5)	0.000(2)	-0.5153(4)	0.037(1)	H(17)	-0.6332	-0.2383	-0.2806	0.0360
C(7)	-0.6568(5)	-0.025(2)	-0.4161(4)	0.034(1)	H(18)	-0.4154	-0.0785	-0.2485	0.0448
C(8)	-0.6020(5)	-0.200(2)	-0.3913(4)	0.032(1)	H(19)	-0.5219	-0.0074	-0.2280	0.0448
C(9)	-0.6891(5)	-0.341(2)	-0.4426(4)	0.031(1)	H(20)	-0.3492	-0.1893	-0.1155	0.0560
C(10)	-0.7348(5)	-0.318(2)	-0.5440(4)	0.034(1)	H(21)	-0.4686	-0.1505	-0.1040	0.0560
C(11)	-0.6308(5)	-0.515(2)	-0.4105(4)	0.035(1)	H(22)	-0.5442	-0.4022	-0.1517	0.0424
C(12)	-0.5880(5)	-0.545(2)	-0.3107(4)	0.039(2)	H(23)	-0.3498	-0.5340	-0.2592	0.0412
C(13)	-0.4983(5)	-0.404(2)	-0.2599(4)	0.036(1)	H(24)	-0.3997	-0.4108	-0.3381	0.0412
C(14)	-0.5618(5)	-0.232(2)	-0.2935(4)	0.034(1)	H(25)	-0.3277	-0.3415	-0.2447	0.0412
C(15)	-0.4800(5)	-0.102(2)	-0.2307(4)	0.043(2)	H(26)	-0.6042	-0.4579	-0.5696	0.0441
C(16)	-0.4345(7)	-0.193(2)	-0.1426(5)	0.051(2)	H(27)	-0.6606	-0.3188	-0.6394	0.0441
C(17)	-0.4719(5)	-0.384(2)	-0.1607(4)	0.039(1)	H(28)	-0.5683	-0.2706	-0.5474	0.0441
C(18)	-0.3834(5)	-0.422(2)	-0.2768(4)	0.038(2)	H(29)	-0.2999	-0.4806	-0.0942	0.0506
C(19)	-0.6311(5)	-0.340(2)	-0.5773(4)	0.044(2)	H(30)	-0.4774	-0.7167	-0.1069	0.0723
C(20)	-0.3763(6)	-0.499(2)	-0.0917(4)	0.046(2)	H(31)	-0.4028	-0.7185	-0.1662	0.0723
C(21)	-0.4016(8)	-0.687(2)	-0.1106(5)	0.063(2)	H(32)	-0.3416	-0.7550	-0.0664	0.0723
C(22)	-0.3722(6)	-0.454(2)	0.0004(4)	0.050(2)	H(33)	-0.3765	-0.3410	0.0046	0.0535
C(23)	-0.2671(8)	-0.514(2)	0.0749(5)	0.091(3)	H(34)	-0.4409	-0.5094	0.0068	0.0535
C(24)	-0.2644(7)	-0.449(2)	0.1624(5)	0.070(2)	H(35)	-0.2678	-0.6376	0.0758	0.1012
H(1)	-0.8038	-0.5642	-0.5768	0.0381	H(36)	-0.1980	-0.4792	0.0663	0.1012
H(2)	-0.8475	-0.4428	-0.6567	0.0381	H(37)	-1.1449	-0.1289	-0.6170	0.0501
H(3)	-1.0065	-0.5133	-0.6166	0.0409	H(38)	-0.7811	0.1039	-0.3939	0.0440
H(4)	-0.9380	-0.4440	-0.5227	0.0409	H(39)	-0.6653	-0.5750	-0.2253	0.0502
H(5)	-1.0182	-0.2453	-0.6737	0.0396	H(40)	-0.2258	-0.5462	0.2827	0.0823
H(6)	-0.9445	-0.0170	-0.5845	0.0378					

CA·57

atom	x	y	z	U	atom	x	y	z	U
O(1)	-0.0880(3)	0.549(1)	-0.1159(3)	0.041(1)	H(7)	-0.0173	0.4482	0.0642	0.0456
O(2)	0.1040(3)	0.324(1)	0.2178(3)	0.034(1)	H(8)	-0.2208	0.4063	0.1072	0.0456
O(3)	0.1663(3)	0.833(1)	0.2709(3)	0.040(1)	H(9)	-0.0878	0.2011	0.1683	0.0547
O(4)	0.6355(4)	0.707(1)	0.8118(4)	0.070(2)	H(10)	-0.1420	0.2752	0.2453	0.0547
O(5)	0.6801(3)	0.893(1)	0.7197(4)	0.054(2)	H(11)	0.0496	0.2644	0.3270	0.0471
O(6)	0.3828(4)	0.923(2)	0.2869(4)	0.065(2)	H(12)	-0.0216	0.4920	0.3631	0.0441
C(1)	-0.1948(5)	0.702(1)	0.0945(4)	0.041(2)	H(13)	0.0125	0.6171	0.1850	0.0410
C(2)	-0.1390(5)	0.705(2)	0.0102(4)	0.037(2)	H(14)	-0.0351	0.8589	0.2342	0.0502
C(3)	-0.1443(5)	0.544(1)	-0.0358(4)	0.037(2)	H(15)	-0.0593	0.7911	0.3296	0.0502
C(4)	-0.0929(5)	0.425(2)	0.0395(4)	0.036(2)	H(16)	0.1208	0.9238	0.3860	0.0471
C(5)	-0.1440(5)	0.419(2)	0.1304(4)	0.036(2)	H(17)	0.1785	0.5297	0.3238	0.0456
C(6)	-0.0952(5)	0.294(1)	0.2037(4)	0.042(2)	H(18)	0.2251	0.3413	0.4308	0.0471
C(7)	0.0202(5)	0.335(2)	0.2715(4)	0.035(1)	H(19)	0.1545	0.4004	0.4993	0.0471
C(8)	0.0231(5)	0.498(1)	0.3173(4)	0.034(1)	H(20)	0.3636	0.4875	0.5071	0.0517
C(9)	-0.0261(5)	0.621(2)	0.2374(4)	0.032(1)	H(21)	0.3006	0.5218	0.5867	0.0517
C(10)	-0.1464(5)	0.585(1)	0.1800(5)	0.036(2)	H(22)	0.3231	0.7231	0.4306	0.0471
C(11)	-0.0128(5)	0.787(2)	0.2857(4)	0.037(2)	H(23)	0.1121	0.6374	0.5544	0.0578
C(12)	0.1040(5)	0.824(1)	0.3442(4)	0.036(2)	H(24)	0.0958	0.8143	0.5347	0.0578
C(13)	0.1489(5)	0.707(1)	0.4260(4)	0.034(1)	H(25)	0.0102	0.6975	0.4746	0.0578
C(14)	0.1397(5)	0.541(1)	0.3763(4)	0.033(1)	H(26)	-0.2043	0.4983	0.2948	0.0597
C(15)	0.2000(5)	0.434(2)	0.4576(4)	0.038(2)	H(27)	-0.2199	0.6765	0.2815	0.0597
C(16)	0.2976(6)	0.529(2)	0.5184(5)	0.039(2)	H(28)	-0.2975	0.5640	0.2085	0.0597
C(17)	0.2754(5)	0.706(2)	0.4766(5)	0.037(2)	H(29)	0.2841	0.8020	0.6086	0.0502
C(18)	0.0850(5)	0.716(1)	0.5047(5)	0.044(2)	H(30)	0.2292	1.0122	0.5034	0.0608
C(19)	-0.2239(5)	0.582(2)	0.2469(5)	0.049(2)	H(31)	0.3366	1.0063	0.4692	0.0608
C(20)	0.3246(5)	0.823(2)	0.5613(4)	0.041(2)	H(32)	0.3396	1.0600	0.5765	0.0608
C(21)	0.3056(6)	0.993(2)	0.5240(5)	0.049(2)	H(33)	0.4574	0.6822	0.6093	0.0623
C(22)	0.4463(5)	0.793(1)	0.6051(5)	0.046(2)	H(34)	0.4852	0.8349	0.5620	0.0623
C(23)	0.4934(5)	0.861(2)	0.7099(5)	0.049(2)	H(35)	0.4497	0.8265	0.7523	0.0593
C(24)	0.6088(6)	0.810(2)	0.7529(5)	0.048(2)	H(36)	0.4912	0.9701	0.7055	0.0593
C(25)	0.4262(6)	0.754(2)	0.1599(6)	0.061(2)	H(37)	-0.1474	0.5256	-0.1758	0.0532
C(26)	0.3254(6)	0.675(2)	0.1239(6)	0.056(2)	H(38)	0.0921	0.2383	0.1631	0.0429
C(27)	0.2967(7)	0.613(2)	0.0291(6)	0.067(3)	H(39)	0.2510	0.8302	0.2840	0.0579
C(28)	0.3669(8)	0.629(2)	-0.0299(6)	0.090(3)	H(40)	0.7543	0.8444	0.7394	0.0654
C(29)	0.4660(8)	0.707(2)	0.0012(8)	0.098(4)	H(41)	0.2764	0.6612	0.1649	0.0719
C(30)	0.4925(7)	0.767(2)	0.0945(7)	0.075(3)	H(42)	0.2276	0.5630	0.0040	0.0844
C(31)	0.4607(7)	0.817(2)	0.2628(7)	0.074(3)	H(43)	0.3489	0.5824	-0.0946	0.1056
H(1)	-0.2697	0.6759	0.0664	0.0517	H(44)	0.5154	0.7184	-0.0392	0.1206
H(2)	-0.1884	0.8013	0.1222	0.0517	H(45)	0.5594	0.8202	0.1157	0.0967
H(3)	-0.1758	0.7744	-0.0393	0.0486	H(46)	0.5263	0.8716	0.2689	0.0941
H(4)	-0.0650	0.7318	0.0351	0.0486	H(47)	0.4705	0.7333	0.3078	0.0941
H(5)	-0.2193	0.5150	-0.0645	0.0486	H(48)	0.3549	0.9893	0.2349	0.0806
H(6)	-0.1004	0.3247	0.0084	0.0456					

CA·59

atom	x	y	z	U	atom	x	y	z	U
O(1)	0.5170(1)	0.0330(6)	0.4042(1)	0.0338(4)	H(7)	0.4091	-0.0721	0.4949	0.0331
O(2)	0.3675(1)	-0.1960(6)	0.61767(9)	0.0274(4)	H(8)	0.1642	-0.0798	0.3598	0.0331
O(3)	0.4053(1)	0.3438(6)	0.71179(9)	0.0318(4)	H(9)	0.2103	-0.2973	0.4674	0.0331
O(4)	0.4674(2)	0.1118(6)	1.1784(1)	0.0512(5)	H(10)	0.0987	-0.2150	0.4645	0.0331
O(5)	0.4549(1)	0.3686(6)	1.22725(9)	0.0404(5)	H(11)	0.2083	-0.2604	0.6061	0.0305
N(1)	0.0364(3)	0.1058(7)	1.0448(2)	0.095(1)	H(12)	0.1150	0.0094	0.5843	0.0283
C(1)	0.2366(2)	0.2465(6)	0.4025(1)	0.0272(5)	H(13)	0.3375	0.1315	0.5760	0.0274
C(2)	0.3686(2)	0.2265(6)	0.4145(1)	0.0279(5)	H(14)	0.1319	0.3339	0.5718	0.0307
C(3)	0.3906(2)	0.0523(6)	0.3849(1)	0.0274(5)	H(15)	0.2468	0.4034	0.5573	0.0307
C(4)	0.3498(2)	-0.0798(6)	0.4341(1)	0.0269(5)	H(16)	0.2480	0.4478	0.6997	0.0315
C(5)	0.2194(2)	-0.0623(6)	0.4272(1)	0.0248(5)	H(17)	0.3574	0.0289	0.7159	0.0290
C(6)	0.1878(2)	-0.2010(6)	0.4803(1)	0.0270(5)	H(18)	0.1616	-0.1359	0.7450	0.0381
C(7)	0.2392(2)	-0.1754(6)	0.5805(1)	0.0250(5)	H(19)	0.2929	-0.2114	0.7689	0.0381
C(8)	0.2082(2)	-0.0013(6)	0.6052(1)	0.0232(5)	H(20)	0.3607	-0.0672	0.8993	0.0429
C(9)	0.2460(2)	0.1397(6)	0.5554(1)	0.0222(5)	H(21)	0.2185	-0.0207	0.8820	0.0429
C(10)	0.1887(2)	0.1166(6)	0.4521(1)	0.0236(5)	H(22)	0.3889	0.1854	0.8472	0.0307
C(11)	0.2203(2)	0.3121(6)	0.5874(1)	0.0252(5)	H(23)	0.0870	0.3230	0.7341	0.0383
C(12)	0.2776(2)	0.3381(6)	0.6888(1)	0.0254(5)	H(24)	0.0789	0.1421	0.7617	0.0383
C(13)	0.2390(2)	0.1981(6)	0.7382(1)	0.0229(5)	H(25)	0.0519	0.1884	0.6639	0.0383
C(14)	0.2687(2)	0.0290(6)	0.7052(1)	0.0235(5)	H(26)	0.0312	0.2537	0.4233	0.0394
C(15)	0.2498(2)	-0.1023(6)	0.7673(1)	0.0313(6)	H(27)	0.0095	0.0647	0.4485	0.0394
C(16)	0.2911(2)	-0.0118(6)	0.8568(1)	0.0347(6)	H(28)	0.0192	0.1092	0.3543	0.0394
C(17)	0.3129(2)	0.1764(6)	0.8401(1)	0.0248(5)	H(29)	0.2061	0.2670	0.9089	0.0380
C(18)	0.1055(2)	0.2159(6)	0.7228(1)	0.0313(6)	H(30)	0.2488	0.5219	0.8325	0.0512
C(19)	0.0520(2)	0.1395(6)	0.4186(1)	0.0319(6)	H(31)	0.3056	0.5438	0.9419	0.0512
C(20)	0.2892(2)	0.2926(6)	0.9077(1)	0.0278(5)	H(32)	0.3915	0.4825	0.8966	0.0512
C(21)	0.3054(3)	0.4777(6)	0.8911(1)	0.0421(7)	H(33)	0.3749	0.1342	1.0101	0.0410
C(22)	0.3731(2)	0.2417(6)	1.0010(1)	0.0339(6)	H(34)	0.4458	0.2685	1.0100	0.0410
C(23)	0.3433(2)	0.3137(6)	1.0766(1)	0.0409(7)	H(35)	0.2633	0.2899	1.0677	0.0498
C(24)	0.4278(2)	0.2532(6)	1.1654(1)	0.0306(5)	H(36)	0.3473	0.4359	1.0755	0.0498
C(25)	-0.0670(3)	0.1479(7)	0.9726(3)	0.0705(9)	H(37)	0.5279	-0.0362	0.3716	0.0415
C(26)	-0.1569(3)	0.2352(7)	0.9844(3)	0.072(1)	H(38)	0.3851	-0.3059	0.6052	0.0336
C(27)	-0.2583(3)	0.2791(7)	0.9114(3)	0.078(1)	H(39)	0.4397	0.4144	0.7594	0.0397
C(28)	-0.2706(4)	0.2349(8)	0.8265(3)	0.091(1)	H(40)	0.5024	0.3241	1.2776	0.0632
C(29)	-0.1783(5)	0.1465(9)	0.8149(3)	0.100(1)	H(41)	-0.1509	0.2682	1.0428	0.0860
C(30)	-0.0779(4)	0.1055(8)	0.8869(3)	0.087(1)	H(42)	-0.3203	0.3455	0.9208	0.0939
C(31)	0.0381(4)	0.1082(9)	1.1331(3)	0.115(2)	H(43)	-0.3411	0.2640	0.7776	0.1109
H(1)	0.1837	0.2264	0.3385	0.0333	H(44)	-0.1847	0.1155	0.7568	0.1185
H(2)	0.2225	0.3603	0.4219	0.0333	H(45)	-0.0133	0.0501	0.8788	0.1033
H(3)	0.4230	0.2402	0.4822	0.0342	H(46)	-0.0312	0.0573	1.1352	0.1368
H(4)	0.3856	0.3168	0.3747	0.0342	H(47)	0.0393	0.2251	1.1517	0.1368
H(5)	0.3499	0.0334	0.3197	0.0380	H(48)	0.1078	0.0557	1.1722	0.1368
H(6)	0.3602	-0.1864	0.4123	0.0331	H(49)	0.0755	0.0105	1.0296	0.1126

CA·60

atom	x	y	z	U	atom	x	y	z	U
O(1)	-0.4796(2)	-0.4732(10)	-0.5943(2)	0.0441(8)	H(8)	-0.8165	-0.5792	-0.6258	0.0395
O(2)	-0.6431(2)	-0.7091(9)	-0.3802(2)	0.0368(7)	H(9)	-0.7847	-0.8075	-0.5298	0.0445
O(3)	-0.6031(2)	-0.1630(9)	-0.2866(2)	0.0388(7)	H(10)	-0.8942	-0.7039	-0.5330	0.0445
O(4)	-0.5200(3)	-0.403(1)	0.1768(2)	0.073(1)	H(11)	-0.8038	-0.7614	-0.3907	0.0380
O(5)	-0.5271(3)	-0.146(1)	0.2299(2)	0.0568(9)	H(12)	-0.8762	-0.4969	-0.4021	0.0388
N(1)	-1.0700(7)	-0.317(1)	0.0270(4)	0.144(2)	H(13)	-0.6725	-0.3728	-0.4239	0.0363
C(1)	-0.7546(3)	-0.2564(9)	-0.5897(2)	0.0345(9)	H(14)	-0.8614	-0.1786	-0.4202	0.0412
C(2)	-0.6260(3)	-0.2781(10)	-0.5810(2)	0.0354(9)	H(15)	-0.7489	-0.1067	-0.4328	0.0412
C(3)	-0.6033(3)	-0.453(1)	-0.6098(2)	0.0353(9)	H(16)	-0.7538	-0.0631	-0.2909	0.0418
C(4)	-0.6456(3)	-0.5834(10)	-0.5594(2)	0.0328(9)	H(17)	-0.6588	-0.4785	-0.2817	0.0392
C(5)	-0.7738(3)	-0.5655(10)	-0.5661(2)	0.0313(9)	H(18)	-0.7198	-0.7086	-0.2293	0.0511
C(6)	-0.8116(3)	-0.7050(10)	-0.5153(2)	0.0341(9)	H(19)	-0.8423	-0.6338	-0.2434	0.0511
C(7)	-0.7665(3)	-0.6830(10)	-0.4160(2)	0.0314(8)	H(20)	-0.7750	-0.5262	-0.1105	0.0562
C(8)	-0.7945(3)	-0.5062(10)	-0.3890(2)	0.0296(8)	H(21)	-0.6486	-0.5722	-0.1044	0.0562
C(9)	-0.7545(3)	-0.3654(10)	-0.4386(2)	0.0272(8)	H(22)	-0.6144	-0.3258	-0.1529	0.0409
C(10)	-0.8050(3)	-0.3872(10)	-0.5405(2)	0.0300(8)	H(23)	-0.9409	-0.2892	-0.3262	0.0493
C(11)	-0.7800(3)	-0.1937(10)	-0.4052(2)	0.0329(9)	H(24)	-0.9221	-0.3697	-0.2352	0.0493
C(12)	-0.7279(3)	-0.1703(9)	-0.3062(2)	0.0324(8)	H(25)	-0.9081	-0.1771	-0.2434	0.0493
C(13)	-0.7667(3)	-0.3101(10)	-0.2555(2)	0.0292(8)	H(26)	-0.9667	-0.3797	-0.6341	0.0515
C(14)	-0.7405(3)	-0.4798(10)	-0.2918(2)	0.0311(9)	H(27)	-0.9734	-0.4359	-0.5437	0.0515
C(15)	-0.7625(4)	-0.6097(10)	-0.2291(2)	0.041(1)	H(28)	-0.9558	-0.2476	-0.5612	0.0515
C(16)	-0.7182(4)	-0.522(1)	-0.1394(3)	0.045(1)	H(29)	-0.7869	-0.2342	-0.0817	0.0464
C(17)	-0.6940(3)	-0.335(1)	-0.1565(2)	0.0331(9)	H(30)	-0.6212	-0.0137	-0.1056	0.0669
C(18)	-0.8966(3)	-0.286(1)	-0.2659(2)	0.041(1)	H(31)	-0.7531	-0.0009	-0.1544	0.0669
C(19)	-0.9376(3)	-0.362(1)	-0.5730(2)	0.041(1)	H(32)	-0.7065	0.0321	-0.0548	0.0669
C(20)	-0.7106(4)	-0.220(1)	-0.0842(2)	0.0378(10)	H(33)	-0.5494	-0.2445	0.0029	0.0576
C(21)	-0.6964(4)	-0.034(1)	-0.1013(3)	0.053(1)	H(34)	-0.6318	-0.3902	0.0082	0.0576
C(22)	-0.6253(4)	-0.274(1)	0.0035(2)	0.046(1)	H(35)	-0.6310	-0.0754	0.0820	0.0699
C(23)	-0.6420(4)	-0.196(1)	0.0841(3)	0.056(1)	H(36)	-0.7183	-0.2162	0.0846	0.0699
C(24)	-0.5580(4)	-0.261(1)	0.1671(3)	0.045(1)	H(37)	-0.4571	-0.5423	-0.6306	0.0664
C(25)	-1.1354(6)	-0.332(1)	-0.0595(3)	0.076(2)	H(38)	-0.6112	-0.8069	-0.3961	0.0468
C(26)	-1.2447(7)	-0.254(1)	-0.0892(6)	0.096(2)	H(39)	-0.5558	-0.1184	-0.2325	0.0494
C(27)	-1.3116(8)	-0.266(1)	-0.1734(8)	0.133(3)	H(40)	-0.4770	-0.2073	0.2878	0.0684
C(28)	-1.271(1)	-0.350(2)	-0.2314(6)	0.137(3)	H(41)	-1.2721	-0.1883	-0.0492	0.1185
C(29)	-1.1729(9)	-0.422(1)	-0.2067(5)	0.109(3)	H(42)	-1.3875	-0.2161	-0.1937	0.1626
C(30)	-1.1011(5)	-0.416(1)	-0.1241(4)	0.079(2)	H(43)	-1.3146	-0.3557	-0.2922	0.1690
C(31)	-0.9895(8)	-0.418(2)	0.0709(6)	0.160(3)	H(44)	-1.1505	-0.4825	-0.2482	0.1383
C(32)	-0.9293(8)	-0.407(1)	0.1666(5)	0.123(3)	H(45)	-1.0270	-0.4682	-0.1096	0.0957
H(1)	-0.7979	-0.2619	-0.6500	0.0442	H(46)	-1.0273	-0.5223	0.0639	0.2052
H(2)	-0.7648	-0.1465	-0.5684	0.0442	H(47)	-0.9334	-0.4119	0.0438	0.2052
H(3)	-0.6045	-0.1950	-0.6160	0.0443	H(48)	-0.8693	-0.4896	0.1815	0.1474
H(4)	-0.5810	-0.2608	-0.5216	0.0443	H(49)	-0.8917	-0.2974	0.1796	0.1474
H(5)	-0.6426	-0.4635	-0.6704	0.0471	H(50)	-0.9795	-0.4208	0.1990	0.1474
H(6)	-0.6353	-0.6890	-0.5810	0.0410	H(51)	-1.0556	-0.1975	0.0461	0.1716
H(7)	-0.6014	-0.5726	-0.4998	0.0410					

CA·62 (Form II)

atom	x	y	z	Beq	atom	x	y	z	Beq
O(1)	-0.093(8)	0.4234(4)	-0.1077(6)	4.0(2)	H(7)	-0.1751	0.1400	-0.0374	4.0655
O(2)	0.080(8)	0.6476(4)	0.2090(6)	3.6(2)	H(8)	-0.2227	0.4200	-0.0670	4.0655
O(3)	0.178(8)	0.0998(4)	0.2784(6)	4.0(2)	H(9)	-0.1198	0.6200	0.0153	4.0655
O(4)	0.70(1)	0.0699(4)	0.7617(8)	4.9(2)	H(10)	-0.0404	0.5400	0.0698	4.0655
O(5)	0.66(1)	0.3228(4)	0.6929(8)	5.7(2)	H(11)	-0.2213	0.5600	0.0999	4.0655
C(1)	-0.20(1)	0.2204(5)	0.0920(9)	3.8(2)	H(12)	-0.1374	0.7600	0.1684	4.0655
C(2)	-0.14(1)	0.2348(5)	0.0096(9)	3.8(2)	H(13)	-0.1646	0.6600	0.2402	4.0655
C(3)	-0.16(1)	0.4067(5)	-0.0352(9)	3.6(2)	H(14)	0.0189	0.7200	0.3016	4.0655
C(4)	-0.11(1)	0.5373(5)	0.0426(9)	3.5(2)	H(15)	-0.0320	0.4600	0.3407	4.0655
C(5)	-0.17(1)	0.5292(5)	0.1270(9)	3.6(2)	H(16)	0.0125	0.3000	0.1949	4.0655
C(6)	-0.12(1)	0.6663(6)	0.2009(9)	4.2(2)	H(17)	-0.0538	0.1400	0.3294	4.0655
C(7)	0.00(1)	0.6352(5)	0.2619(9)	3.6(2)	H(18)	-0.0316	0.0600	0.2403	4.0655
C(8)	0.01(1)	0.4565(5)	0.3088(8)	3.0(2)	H(19)	0.1128	0.0000	0.3754	4.0655
C(9)	-0.03(1)	0.3160(4)	0.2338(8)	3.1(2)	H(20)	0.1649	0.4400	0.3240	4.0655
C(10)	-0.16(1)	0.3493(5)	0.1744(9)	3.4(2)	H(21)	0.1485	0.5800	0.4730	4.0655
C(11)	-0.01(1)	0.1468(5)	0.2826(9)	3.6(2)	H(22)	0.1948	0.6400	0.4067	4.0655
C(12)	0.11(1)	0.1106(5)	0.3439(8)	3.4(2)	H(23)	0.3344	0.5000	0.4907	4.0655
C(13)	0.15(1)	0.2528(4)	0.4207(7)	2.8(2)	H(24)	0.2933	0.4800	0.5704	4.0655
C(14)	0.128(10)	0.4176(5)	0.3651(7)	2.7(2)	H(25)	0.3049	0.2600	0.4202	4.0655
C(15)	0.19(1)	0.5500(5)	0.4390(9)	3.4(2)	H(26)	-0.2258	0.4200	0.2809	4.0655
C(16)	0.29(1)	0.4547(5)	0.5004(9)	3.3(2)	H(27)	0.5372	0.0143	-0.0574	-94.7482
C(17)	0.27(1)	0.2643(5)	0.4707(8)	2.9(2)	H(27)	-0.2239	0.2800	0.2930	4.0655
C(18)	-0.24(1)	0.3371(6)	0.239(1)	4.4(3)	H(28)	0.4863	0.2642	-0.1357	-94.7482
C(19)	0.08(1)	0.2373(5)	0.4962(9)	3.2(2)	H(28)	-0.3130	0.3600	0.2003	4.0655
C(20)	0.33(1)	0.1454(5)	0.5554(8)	3.2(2)	H(29)	0.3921	0.4594	-0.0768	-94.7482
C(21)	0.31(1)	-0.0389(6)	0.530(1)	4.2(2)	H(29)	0.0981	0.3200	0.5389	4.0655
C(22)	0.45(1)	0.1930(5)	0.589(1)	4.1(2)	H(30)	0.3802	0.4284	0.0798	-94.7482
C(23)	0.52(2)	0.1054(6)	0.678(1)	5.6(3)(6)	H(30)	0.0129	0.2600	0.4752	4.0655
C(24)	0.64(1)	0.1838(6)	0.714(1)	4.6(3)	H(31)	0.0977	0.1400	0.5255	4.0655
C(25)	0.44(5)	0.188(3)	0.106(4)	10(1)	H(31A)	0.4521	0.0530	0.2194	-118.4352
C(26)	0.49(5)	0.067(3)	0.065(5)	10(1)	H(31B)	0.3457	0.1697	0.1952	-118.4352
C(27)	0.50(8)	0.102(3)	-0.032(6)	10(1)	H(31C)	0.4647	0.2474	0.2401	-118.4352
C(28)	0.47(7)	0.248(3)	-0.075(6)	10(1)	H(32)	0.2909	0.1600	0.6046	4.0655
C(29)	0.42(7)	0.362(3)	-0.038(5)	9(1)	H(32A)	0.5636	-0.1656	0.0895	-118.4352
C(30)	0.41(5)	0.339(2)	0.052(4)	9(1)	H(32B)	0.4664	-0.1400	0.1402	-118.4352
C(31)	0.42(5)	0.164(2)	0.196(3)	10(1)	H(32C)	0.5834	-0.0545	0.1830	-118.4352
C(32)	0.53(9)	-0.087(4)	0.129(5)	13(1)	H(33)	0.3493	-0.1200	0.5691	4.0655
H(1)	-0.1086	0.3400	-0.1435	6.1065	H(34)	0.2344	-0.0600	0.5028	4.0655
H(2)	0.0571	0.7600	0.1825	0.0008	H(35)	0.3451	-0.0800	0.4762	4.0655
H(3)	0.1707	0.1800	0.2468	4.3655	H(36)	0.4635	0.2600	0.6247	4.0655
H(4)	0.7678	0.1092	0.7814	6.5479	H(37)	0.4881	0.1600	0.5557	4.0655
H(4)	0.7678	0.1092	0.7814	6.5479	H(38)	0.4821	0.0400	0.7014	4.0655
H(5)	-0.2628	0.2400	0.0668	4.0655	H(39)	0.4949	0.2400	0.7019	4.0655
H(6)	-0.0597	0.2400	0.0399	4.0655					

CA·63

atom	x	y	z	Beq	atom	x	y	z	Beq
O(1)	-0.1086(4)	-0.1319(7)	0.4002(4)	4.1(1)	H(3)	0.0507	-0.3400	0.4140	2.8551
O(2)	0.2373(4)	-0.3578(6)	0.6204(3)	3.08(9)	H(4)	0.1027	-0.2400	0.4954	2.8551
O(3)	0.2972(4)	0.1756(7)	0.7112(3)	3.20(9)	H(6)	0.0043	0.1400	0.3512	2.9396
O(4)	0.7147(7)	-0.0523(9)	1.1729(4)	6.1(2)	H(7)	0.0639	0.0600	0.4716	2.9396
O(5)	0.7793(5)	0.1984(8)	1.2165(4)	4.3(1)	H(8)	0.1524	0.0600	0.3432	3.0548
H(5)	0.765(7)	0.174(5)	1.262(2)	4.3150	H(9)	0.2193	0.1600	0.3979	3.0548
C(1)	0.1717(6)	0.067(1)	0.3989(4)	3.1(1)	H(10)	0.2363	-0.0400	0.5735	2.4177
C(2)	0.0510(6)	0.0501(9)	0.4104(4)	2.9(1)	H(11)	0.2445	-0.4800	0.4608	3.1591
C(3)	0.0000(6)	-0.118(1)	0.3828(5)	3.2(1)	H(12)	0.3574	-0.3600	0.4584	3.1591
C(4)	0.0838(6)	-0.2462(9)	0.4350(4)	2.9(1)	H(13)	0.1929	-0.4600	0.5940	3.0848
C(5)	0.2086(6)	-0.2366(10)	0.4285(4)	2.7(1)	H(14)	0.3999	-0.4400	0.6080	2.7398
C(6)	0.2858(6)	-0.3703(9)	0.4824(5)	3.2(1)	H(15)	0.4538	-0.1600	0.5854	2.4682
C(7)	0.3289(6)	-0.3422(9)	0.5826(4)	2.7(1)	H(16)	0.3070	0.2400	0.5601	2.7343
C(8)	0.3840(5)	-0.1712(9)	0.6051(4)	2.5(1)	H(17)	0.4252	0.1400	0.5582	2.7343
C(9)	0.3014(6)	-0.0332(9)	0.5532(4)	2.4(1)	H(18)	0.3982	0.0800	0.4137	3.7070
C(10)	0.2624(6)	-0.0623(9)	0.4514(4)	2.5(1)	H(19)	0.3481	-0.0600	0.3543	3.7070
C(11)	0.3576(6)	0.1349(9)	0.5837(4)	2.7(1)	H(20)	0.3574	-0.1400	0.7222	2.4358
C(12)	0.3984(6)	0.1648(9)	0.6842(4)	2.8(1)	H(21)	0.5688	-0.2800	0.7458	3.6218
C(13)	0.4845(5)	0.0283(9)	0.7342(4)	2.4(1)	H(22)	0.4618	-0.3600	0.7599	3.6218
C(14)	0.4219(6)	-0.1363(8)	0.7043(4)	2.4(1)	H(23)	0.6344(7)	-0.181(1)	0.8766(4)	3.7647
C(15)	0.5010(7)	-0.2639(10)	0.7663(5)	3.6(2)	H(24)	0.5180(7)	-0.217(1)	0.8973(4)	3.7647
C(16)	0.5496(7)	-0.172(1)	0.8538(4)	3.8(2)	H(25)	0.4436	0.2600	0.6992	2.8053
C(17)	0.5131(5)	0.0111(9)	0.8360(4)	2.5(1)	H(27)	0.4405	0.0200	0.8440	2.4942
C(18)	0.3687(7)	-0.045(1)	0.4159(5)	3.7(1)	H(28)	0.5898	0.0400	0.6604	3.2491
C(19)	0.5981(6)	0.040(1)	0.7122(5)	3.2(1)	H(29)	0.6551	-0.0400	0.7219	3.2491
C(20)	0.6054(6)	0.127(1)	0.8995(4)	3.4(1)	H(30)	0.6236	0.1600	0.7324	3.2491
C(21)	0.5750(9)	0.306(1)	0.8836(6)	5.3(2)	H(31)	0.4959	0.3400	0.8840	5.3170
C(22)	0.6182(6)	0.080(1)	0.9956(5)	4.0(2)	H(32)	0.6032	0.3800	0.9261	5.3170
C(23)	0.7283(8)	0.144(2)	1.0642(5)	5.7(3)	H(33)	0.6816	0.1200	0.8845	3.4236
C(24)	0.7398(7)	0.083(1)	1.1567(5)	3.8(2)	H(34)	0.7974	0.1600	1.0430	5.7323
C(25)	0.916(1)	0.480(2)	0.9795(9)	7.0(2)	H(35)	0.6668	-0.0200	1.0036	3.9984
C(26)	0.989(1)	0.430(2)	1.0648(9)	6.7(2)	H(36)	0.4187	-0.1200	0.4524	3.7070
H(26)	1.0523	0.3627	1.0678	6.7019	H(37)	0.5615	0.3200	0.8228	5.3170
C(27)	0.974(1)	0.471(1)	1.1419(9)	6.3(2)	H(38)	0.7190	0.3000	1.0722	5.7323
C(28)	0.879(1)	0.566(2)	1.140(1)	7.2(2)	H(39)	0.5464	0.0600	1.0094	3.9984
C(29)	0.800(1)	0.620(2)	1.060(1)	7.5(3)	H(40)	0.7605	0.5800	0.9224	7.8854
C(30)	0.823(1)	0.582(2)	0.982(1)	7.9(3)	H(41)	0.7238	0.6800	1.0552	7.5277
C(31)	0.930(2)	0.431(3)	0.895(1)	10.7(5)	H(44)	0.8630	0.6000	1.2143	7.2238
H(31A)	1.000(5)	0.37(1)	0.907(1)	10.7058	H(45)	1.113(5)	0.497(5)	1.256(3)	8.8842
H(31B)	0.934(8)	0.526(3)	0.862(3)	10.7058	H(46)	1.098(6)	0.316(7)	1.220(1)	8.8842
H(31C)	0.864(5)	0.365(10)	0.862(3)	10.7058	H(47)	1.014(2)	0.39(1)	1.269(2)	8.8842
C(32)	1.057(1)	0.412(2)	1.2297(9)	8.9(4)	H(48)	0.3192	0.2400	0.7605	3.2041
H(1)	-0.1461	-0.2200	0.3605	4.0931	H(49)	0.1949	-0.2200	0.3646	2.6853
H(2)	-0.0228	-0.1200	0.3158	3.2064					

CA·64

atom	x	y	z	Beq	atom	x	y	z	Beq
O(1)	0.5929(4)	0.2917(6)	0.6219(3)	4.81(8)	H(9)	0.6877	0.5551	0.4000	4.3150
O(2)	0.4055(3)	0.0637(5)	0.2727(3)	3.36(5)	H(10)	0.7806	0.3183	0.3300	5.0256
O(3)	0.3282(3)	0.5944(6)	0.1940(3)	4.04(6)	H(11)	0.7136	0.4400	0.2600	5.0256
O(4)	-0.1671(4)	0.3530(8)	-0.1474(5)	6.90(9)	H(12)	0.7017	0.2533	0.2400	5.0256
O(5)	-0.1917(3)	0.6077(6)	-0.1937(4)	4.95(6)	H(13)	0.4559	-0.0187	0.1800	3.3770
C(1)	0.6883(5)	0.4607(9)	0.4297(5)	4.32(8)	H(14)	0.6411	0.0264	0.2700	3.9557
C(2)	0.6380(5)	0.4568(8)	0.5068(4)	4.07(9)	H(15)	0.6089	-0.0550	0.3600	3.9557
C(3)	0.6483(5)	0.2915(8)	0.5541(4)	3.82(9)	H(16)	0.4295	-0.0191	0.3200	3.3636
C(4)	0.6015(5)	0.1670(8)	0.4721(4)	3.75(8)	H(17)	0.4871	0.3666	0.3100	2.8519
C(5)	0.6482(4)	0.1663(8)	0.3910(5)	3.61(7)	H(18)	0.5209	0.2240	0.1400	2.7951
C(6)	0.5973(5)	0.0347(8)	0.3091(5)	3.96(8)	H(19)	0.3271	0.2850	0.1500	2.6719
C(7)	0.4835(5)	0.0727(7)	0.2299(4)	3.38(7)	H(20)	0.5213	0.6371	0.2700	3.5657
C(8)	0.4782(4)	0.2389(7)	0.1821(4)	2.80(6)	H(21)	0.5455	0.5405	0.1700	3.5657
C(9)	0.5245(4)	0.3735(7)	0.2646(4)	2.85(6)	H(22)	0.2894	0.0620	0.0600	3.6881
C(10)	0.6432(4)	0.3354(8)	0.3409(5)	3.68(6)	H(23)	0.3397	0.1261	-0.0200	3.6881
C(11)	0.5086(4)	0.5388(7)	0.2139(4)	3.57(7)	H(24)	0.1961	0.2744	-0.1200	3.9660
C(12)	0.3922(5)	0.5780(7)	0.1359(4)	3.48(8)	H(25)	0.1394	0.2227	-0.0700	3.9660
C(13)	0.3491(4)	0.4462(7)	0.0529(4)	3.07(6)	H(26)	0.1897	0.4405	0.0300	3.0462
C(14)	0.3641(4)	0.2822(6)	0.1091(4)	2.67(6)	H(27)	0.3849	0.6809	0.0900	3.4804
C(15)	0.3014(5)	0.1625(8)	0.0225(4)	3.69(8)	H(28)	0.3456	0.5374	0.2500	4.0410
C(16)	0.2054(5)	0.2627(8)	-0.0511(5)	3.97(8)	H(29)	0.4039	0.5639	-0.0500	4.2281
C(17)	0.2248(4)	0.4395(7)	-0.0141(4)	3.05(6)	H(30)	0.3816	0.3793	-0.0700	4.2281
C(18)	0.7190(5)	0.340(1)	0.2850(5)	5.03(8)	H(31)	0.4865	0.4383	0.0200	4.2281
C(19)	0.4109(5)	0.4542(9)	-0.0172(5)	4.23(7)	H(32)	0.2075	0.5465	-0.1500	3.8728
C(20)	0.1700(5)	0.5595(8)	-0.1040(4)	3.87(7)	H(33)	0.2635	0.7724	-0.0500	4.9198
C(21)	0.1909(6)	0.7345(9)	-0.0735(6)	4.9(1)	H(34)	0.1660	0.8129	-0.1300	4.9198
C(22)	0.0485(5)	0.5235(9)	-0.1606(5)	4.31(7)	H(35)	0.1713	0.7631	-0.0200	4.9198
C(23)	-0.0129(5)	0.5272(10)	-0.0906(5)	4.64(8)	H(36)	0.0248	0.4074	-0.2100	4.3079
C(24)	-0.1307(5)	0.4850(8)	-0.1476(5)	3.92(8)	H(37)	0.0214	0.6207	-0.2200	4.3079
C(25)	0.0808(6)	0.4634(9)	-0.6949(6)	5.36(10)	H(38)	0.0227	0.4653	-0.0300	4.6363
C(26)	0.1544(8)	0.374(1)	-0.6194(7)	7.2(1)	H(39)	0.0019	0.6266	-0.0500	4.6363
C(27)	0.1521(9)	0.362(1)	-0.5229(8)	8.8(2)	H(40)	-0.2675	0.6146	-0.2300	4.9522
C(28)	0.0762(10)	0.443(1)	-0.5000(7)	7.7(2)	H(41)	0.2075(8)	0.319(1)	-0.6321(7)	7.1543
C(29)	0.0028(8)	0.526(2)	-0.5775(7)	7.7(1)	H(42)	0.2028(9)	0.297(1)	-0.4726(8)	8.8068
C(30)	0.0036(8)	0.534(1)	-0.6718(7)	7.2(1)	H(43)	0.140(1)	0.369(2)	-0.3493(9)	12.6181
C(31)	0.0834(9)	0.484(1)	-0.7991(7)	7.5(1)	H(44)	-0.0509(8)	0.581(2)	-0.5660(7)	7.7283
C(32)	0.082(1)	0.438(2)	-0.3914(9)	12.6(3)	H(45)	0.1434(9)	0.425(1)	-0.8009(7)	7.5009
H(2)	0.7275	0.2920	0.5900	3.8199	H(46)	0.0910(9)	0.596(1)	-0.8111(7)	7.5009
H(3)	0.6764	0.5396	0.5600	4.0694	H(47)	0.6191	0.2069	0.6700	4.8093
H(4)	0.5598	0.4694	0.4700	4.0694	H(48)	0.015(1)	0.396(2)	-0.3934(9)	12.6181
H(5)	0.6068	0.0613	0.5000	3.7481	H(49)	0.094(1)	0.544(2)	-0.3628(9)	12.6181
H(6)	0.5354	0.1773	0.4400	3.7481	H(50)	-0.0513(8)	0.591(1)	-0.7233(7)	7.2317
H(7)	0.7289	0.1571	0.4400	3.6131	H(51)	0.0173(9)	0.444(1)	-0.8518(7)	7.5009
H(8)	0.7601	0.4573	0.4600	4.3150					

CA·62+63 (1:1)

atom	x	y	z	Beq	atom	x	y	z	Beq
O(1)	0.3908(5)	0.1991(7)	0.3995(4)	5.4(1)	H(27)	1.0208(8)	0.289(1)	0.8976(6)	5.2151
H(34)	0.3577	0.3000	0.4040	5.3730	H(38)	1.1360(8)	0.250(1)	0.8764(6)	5.2151
O(2)	0.7381(4)	0.4279(7)	0.6196(3)	4.6(1)	C(17)	1.0132(7)	0.054(1)	0.8379(5)	4.5(2)
H(35)	0.6765	0.5000	0.6206	4.5503	H(26)	0.9192	0.0600	0.8354	4.4595
O(3)	0.7996(4)	-0.1066(7)	0.7127(3)	4.9(1)	C(18)	0.8676(7)	0.117(1)	0.4156(6)	5.3(2)
H(40)	0.7497	-0.1200	0.6692	4.8945	H(9)	0.8992	0.0000	0.4226	5.3272
O(4)	1.2135(7)	0.121(1)	1.1739(5)	7.6(2)	H(10)	0.8487	0.1200	0.3362	5.3272
O(5)	1.2774(6)	-0.1296(9)	1.2173(4)	6.0(1)	H(11)	0.9314	0.2000	0.4404	5.3272
H(5A)	1.2826	-0.0940	1.2664	5.9936	C(19)	1.0995(7)	0.027(1)	0.7130(5)	4.9(2)
C(1)	0.6692(7)	0.004(1)	0.3990(5)	4.4(2)	H(20)	1.0963	0.0600	0.6504	4.8993
H(7)	0.6585(7)	0.014(1)	0.3362(5)	4.3971	H(21)	1.1343	-0.1000	0.7383	4.8993
H(8)	0.6998(7)	-0.105(1)	0.4176(5)	4.3971	H(22)	1.1648	0.1000	0.7388	4.8993
C(2)	0.5509(7)	0.018(1)	0.4101(6)	4.6(2)	C(20)	1.1050(7)	-0.058(1)	0.8985(5)	4.8(2)
H(1)	0.4984(7)	-0.064(1)	0.3738(6)	4.5700	H(30)	1.1971	-0.0400	0.8912	4.7793
H(2)	0.5584(7)	-0.002(1)	0.4717(6)	4.5700	C(21)	1.073(1)	-0.234(1)	0.8815(7)	7.2(3)
C(3)	0.5003(7)	0.188(1)	0.3827(5)	4.4(2)	H(31)	1.133(1)	-0.301(1)	0.9212(7)	7.2427
H(3)	0.4861	0.2000	0.3038	4.3663	H(32)	1.064(1)	-0.261(1)	0.8212(7)	7.2427
C(4)	0.5843(6)	0.3156(10)	0.4359(6)	4.3(2)	H(33)	1.000(1)	-0.254(1)	0.8912(7)	7.2427
H(4)	0.5912(6)	0.3040(10)	0.4979(6)	4.3458	C(22)	1.1194(7)	-0.010(1)	0.9962(5)	5.3(2)
H(5)	0.5519(6)	0.4232(10)	0.4165(6)	4.3458	H(28)	1.1197(7)	0.109(1)	1.0006(5)	5.2996
C(5)	0.7078(7)	0.306(1)	0.4283(5)	4.0(2)	H(29)	1.0518(7)	-0.050(1)	1.0099(5)	5.2996
H(6)	0.6930	0.2800	0.3616	4.0173	C(23)	1.2278(9)	-0.074(2)	1.0641(5)	7.2(3)
C(6)	0.7862(7)	0.439(1)	0.4823(5)	4.7(2)	H(36)	1.2956(9)	-0.039(2)	1.0492(5)	7.1606
H(13)	0.7435(7)	0.542(1)	0.4699(5)	4.7429	H(37)	1.2259(9)	-0.193(2)	1.0624(5)	7.1606
H(14)	0.8534(7)	0.450(1)	0.4625(5)	4.7429	C(24)	1.2413(8)	-0.017(2)	1.1586(6)	5.7(2)
C(7)	0.8312(7)	0.412(1)	0.5834(6)	4.6(2)	C(25)	0.526(1)	0.100(2)	-0.142(1)	8.9(3)
H(16)	0.8891	0.5200	0.5917	4.6111	C(26)	0.510(1)	0.142(2)	-0.062(1)	10.3(4)
C(8)	0.8866(7)	0.241(1)	0.6056(5)	4.0(2)	H(26A)	0.4446	0.2072	-0.0609	10.3291
H(17)	0.9624	0.2400	0.5812	3.9976	C(27)	0.588(1)	0.087(2)	0.021(1)	10.5(4)
C(9)	0.8022(7)	0.1047(10)	0.5539(5)	3.6(1)	C(28)	0.676(1)	-0.004(2)	0.017(1)	10.9(4)
H(15)	0.7172	0.1200	0.5688	3.5886	H(28A)	0.7300	-0.0437	0.0692	10.9332
C(10)	0.7632(7)	0.131(1)	0.4502(5)	4.2(2)	C(29)	0.697(2)	-0.047(2)	-0.062(2)	12.2(5)
C(11)	0.8575(7)	-0.064(1)	0.5838(5)	4.4(2)	H(29A)	0.7588	-0.1121	-0.0606	12.1538
H(12)	0.9227(7)	-0.078(1)	0.5619(5)	4.4011	C(30)	0.618(1)	0.008(2)	-0.140(1)	11.0(4)
H(18)	0.7997(7)	-0.147(1)	0.5558(5)	4.4011	H(30A)	0.6302	-0.0178	-0.1935	10.9600
C(12)	0.9019(7)	-0.095(1)	0.6839(5)	4.2(2)	C(31)	0.443(1)	0.163(3)	-0.227(1)	13.8(6)
H(19)	0.9533	-0.2200	0.6954	4.1950	H(31A)	0.3812	0.2277	-0.2158	13.8427
C(13)	0.9858(6)	0.042(1)	0.7339(5)	3.7(2)	H(31B)	0.4065	0.0746	-0.2658	13.8427
C(14)	0.9222(6)	0.2076(9)	0.7046(5)	3.6(1)	H(31C)	0.4830	0.2329	-0.2561	13.8427
H(24)	0.8325	0.2000	0.7129	3.5633	C(32)	0.576(2)	0.138(3)	0.105(1)	13.8(6)
C(15)	1.0026(8)	0.332(1)	0.7667(6)	5.5(2)	H(32A)	0.5081	0.2050	0.0963	13.7985
H(23)	1.0650(8)	0.365(1)	0.7449(6)	5.4630	H(32B)	0.6451	0.2047	0.1390	13.7985
H(25)	0.9590(8)	0.428(1)	0.7730(6)	5.4630	H(32C)	0.5736	0.0457	0.1412	13.7985
C(16)	1.0512(8)	0.242(1)	0.8540(6)	5.2(2)					

CA·62+64 (1:1)

atom	x	y	z	Beq	atom	x	y	z	Beq
O(1)	-0.0919(8)	0.172(1)	-0.1238(7)	5.6(3)	H(16A)	0.3557	0.2757	0.6200	4.9893
H(1O)	0.0014	0.2227	-0.0900	5.5736	H(16B)	0.3490	0.1795	0.5200	4.9893
O(2)	0.0935(7)	0.403(1)	0.2270(6)	4.1(2)	C(17)	0.2764(10)	0.021(2)	0.5152(9)	3.6(3)
H(2O)	0.1605	0.3066	0.2200	4.1271	H(17)	0.3003	-0.0094	0.4600	3.6296
O(3)	0.1721(8)	-0.134(1)	0.3050(7)	5.1(2)	C(18)	-0.219(1)	0.127(3)	0.215(1)	5.4(4)
H(3O)	0.1814	-0.0250	0.2900	5.1077	H(18A)	-0.2912	0.1490	0.1665	5.4054
O(4)	0.6911(9)	-0.145(2)	0.6917(10)	6.7(3)	H(18B)	-0.1963	0.2123	0.2669	5.4054
H(4)	0.7529	-0.1113	0.7232	6.7405	H(18C)	-0.2169	0.0267	0.2493	5.4054
O(5)	0.666(1)	0.106(2)	0.653(1)	9.3(4)	C(19)	0.088(1)	0.010(2)	0.519(1)	5.6(4)
C(1)	-0.189(1)	0.004(2)	0.071(1)	4.9(4)	H(19A)	0.1162	0.0714	0.5800	5.6375
H(1A)	-0.2325	-0.0773	0.1100	4.8606	H(19B)	0.0148	0.0529	0.5000	5.6375
H(23B)	-0.1839	-0.1408	0.0800	4.8606	H(32)	0.0920	-0.1421	0.5300	5.6375
C(2)	-0.136(1)	0.009(2)	-0.007(1)	4.8(4)	C(20)	0.328(1)	-0.100(2)	0.604(1)	4.8(4)
H(2A)	-0.0463	-0.0103	0.0500	4.7540	H(20)	0.2833	-0.0833	0.6600	4.7564
H(2B)	-0.1625	-0.1111	-0.0300	4.7540	C(21)	0.309(1)	-0.270(2)	0.569(1)	6.4(5)
C(3)	-0.150(1)	0.172(2)	-0.055(1)	3.9(3)	H(21A)	0.3455	-0.3402	0.6289	6.3560
H(3)	-0.2266	0.1922	-0.0956	3.9392	H(21B)	0.3393	-0.2916	0.5199	6.3560
C(4)	-0.103(1)	0.297(2)	0.026(1)	3.8(3)	H(21C)	0.2341	-0.2946	0.5399	6.3560
H(4A)	-0.0128	0.2620	0.0900	3.8128	C(22)	0.450(1)	-0.057(2)	0.6604(10)	5.4(4)
H(4B)	-0.0964	0.4222	0.0100	3.8128	H(22A)	0.5021	0.0271	0.7300	5.4141
C(5)	-0.150(1)	0.292(2)	0.110(1)	4.5(4)	H(22B)	0.4588	-0.1739	0.7100	5.4141
H(5)	-0.2366	0.2762	0.0900	4.4595	C(23)	0.514(1)	-0.066(2)	0.590(1)	5.6(4)
C(6)	-0.098(1)	0.428(2)	0.192(1)	5.3(4)	H(19C)	0.4932	-0.1595	0.5200	5.5925
H(6A)	-0.1462	0.4200	0.2400	5.2877	H(23A)	0.4657	0.0111	0.5200	5.5925
H(6B)	-0.1252	0.5395	0.1700	5.2877	C(24)	0.628(1)	-0.029(3)	0.648(2)	6.5(5)
C(7)	0.015(1)	0.387(2)	0.2695(10)	3.9(3)	C(25)	-0.420(2)	0.499(3)	-0.197(2)	8.2(6)
H(7)	0.0190	0.4866	0.3100	3.9210	C(26)	-0.488(2)	0.419(4)	-0.169(2)	13.7(9)
C(8)	0.022(1)	0.222(2)	0.3198(10)	3.8(3)	H(26)	-0.5342	0.3458	-0.2110	13.6959
H(8)	-0.0283	0.2176	0.3700	3.7702	C(27)	-0.491(2)	0.449(5)	-0.079(3)	14(1)
C(9)	-0.024(1)	0.090(2)	0.2327(10)	3.6(3)	H(27)	-0.5555	0.4108	-0.0679	14.2999
H(9)	0.0447	0.0957	0.2000	3.6202	C(28)	-0.420(3)	0.521(4)	0.003(2)	11.8(9)
C(10)	-0.141(1)	0.122(2)	0.1601(10)	3.8(3)	C(29)	-0.349(3)	0.609(4)	-0.022(3)	13(1)
C(11)	-0.011(1)	-0.080(2)	0.288(1)	4.2(3)	H(29)	-0.2942	0.6778	0.0198	13.9588
H(11A)	-0.0739	-0.0805	0.3300	4.1823	C(30)	-0.343(2)	0.592(4)	-0.120(3)	12.9(9)
H(11B)	0.0159	-0.1900	0.2600	4.1823	H(30)	-0.2878	0.6356	-0.1374	12.8708
C(12)	0.110(1)	-0.114(2)	0.362(1)	5.1(4)	C(31)	-0.412(2)	0.477(3)	-0.298(2)	11.5(8)
H(12)	0.0930	-0.2203	0.4000	5.1053	H(31A)	-0.4712	0.4086	-0.3473	11.5482
C(13)	0.149(1)	0.014(2)	0.444(1)	4.2(3)	H(31B)	-0.3451	0.4212	-0.2911	11.5482
C(14)	0.136(1)	0.180(2)	0.392(1)	3.2(3)	H(31C)	-0.4145	0.5767	-0.3344	11.5482
H(14)	0.1823	0.1802	0.3400	3.2254	C(32)	-0.420(4)	0.533(6)	0.106(2)	25(2)
C(15)	0.201(1)	0.298(2)	0.479(1)	4.2(3)	H(32A)	-0.4802	0.4713	0.1064	25.3688
H(15A)	0.1456	0.3412	0.5100	4.1871	H(32B)	-0.4331	0.6466	0.1232	25.3688
H(15B)	0.2083	0.4334	0.4900	4.1871	H(32C)	-0.3550	0.4985	0.1610	25.3688
C(16)	0.294(1)	0.198(2)	0.555(1)	5.0(4)					

CA·63+64 (3:1)

atom	x	y	z	Beq	atom	x	y	z	Beq
O(1)	0.3895(4)	0.5925(6)	0.3998(3)	4.3(1)	H(19A)	1.1391	0.3134	0.7354	3.6881
H(1)	0.3755	0.5081	0.4223	4.2826	H(19B)	1.1569	0.5031	0.7473	3.6881
O(2)	0.7393(4)	0.8188(6)	0.6195(3)	3.57(9)	H(19C)	1.0896	0.4298	0.6536	3.6881
H(2)	0.7652	0.8029	0.6731	3.5744	C(20)	1.1059(6)	0.3359(9)	0.9008(4)	3.6(1)
O(3)	0.7993(4)	0.2863(6)	0.7141(3)	3.87(10)	H(20)	1.1816	0.3515	0.8911	3.5815
H(3)	0.7389	0.2984	0.6715	3.8705	C(21)	1.0714(8)	0.158(1)	0.8845(5)	5.9(2)
O(4)	1.2179(6)	0.5170(8)	1.1739(4)	7.2(2)	H(21A)	1.1316	0.0898	0.9243	5.8997
O(5)	1.2770(5)	0.2659(7)	1.2165(3)	5.3(1)	H(21B)	1.0616	0.1280	0.8247	5.8997
H(5)	1.2812	0.3022	1.2649	5.2735	H(21C)	0.9979	0.1387	0.8955	5.8997
C(1)	0.6716(6)	0.3917(8)	0.4014(4)	3.3(1)	C(22)	1.1199(6)	0.383(1)	0.9971(4)	4.5(2)
H(1A)	0.6614	0.3977	0.3388	3.3399	H(22A)	1.1194	0.5027	1.0008	4.5179
H(1B)	0.7018	0.2828	0.4218	3.3399	H(22B)	1.0520	0.3442	1.0106	4.5179
C(2)	0.5517(6)	0.4106(8)	0.4126(4)	3.4(1)	C(23)	1.2286(7)	0.324(1)	1.0660(4)	5.9(2)
H(2A)	0.4980	0.3283	0.3782	3.3833	H(23A)	1.2274	0.2042	1.0644	5.8697
H(2B)	0.5599	0.3939	0.4746	3.3833	H(23B)	1.2966	0.3591	1.0514	5.8697
C(3)	0.4999(5)	0.5762(9)	0.3849(4)	3.3(1)	C(24)	1.2406(6)	0.379(1)	1.1570(4)	4.2(1)
H(3A)	0.4868	0.5909	0.3216	3.3225	C(25)	0.591(6)	0.487(7)	0.023(4)	8.1(6)
C(4)	0.5848(5)	0.7062(8)	0.4366(4)	3.1(1)	C(26)	0.511(2)	0.536(2)	-0.063(1)	6.9(4)
H(4A)	0.5919	0.6980	0.4986	3.1298	H(26)	0.4458	0.6098	-0.0674	6.8724
H(4B)	0.5526	0.8133	0.4157	3.1298	C(27)	0.522(4)	0.489(5)	-0.142(3)	6.4(6)
C(5)	0.7086(6)	0.6926(8)	0.4291(4)	3.0(1)	C(28)	0.622(3)	0.388(3)	-0.139(2)	9.6(7)
H(5A)	0.6993	0.7126	0.3665	3.0169	H(28)	0.6322	0.3516	-0.1887	9.6193
C(6)	0.7893(6)	0.8297(9)	0.4835(4)	3.7(1)	C(29)	0.697(2)	0.341(2)	-0.058(1)	7.8(5)
H(6A)	0.8572	0.8401	0.4642	3.7244	H(29)	0.7615	0.2700	-0.0520	7.8341
H(6B)	0.7463	0.9324	0.4708	3.7244	C(30)	0.677(4)	0.381(5)	0.018(3)	8.8(7)
C(7)	0.8326(5)	0.8011(8)	0.5837(4)	2.9(1)	H(30)	0.7329	0.3583	0.0769	8.8282
H(7)	0.8932	0.8828	0.6115	2.9096	C(31)	0.566(2)	0.535(4)	0.104(2)	10.8(7)
C(8)	0.8868(5)	0.6298(8)	0.6057(4)	2.9(1)	H(31A)	0.6287	0.4943	0.1538	10.7823
H(8)	0.9585	0.6268	0.5893	2.9309	H(31B)	0.4920	0.4968	0.1046	10.7823
C(9)	0.8045(5)	0.4933(8)	0.5550(4)	2.8(1)	H(31C)	0.5664	0.6565	0.1102	10.7823
H(9)	0.7331	0.4998	0.5713	2.7603	C(32)	0.439(2)	0.544(4)	-0.227(2)	11.5(8)
C(10)	0.7641(5)	0.5209(8)	0.4526(4)	2.9(1)	H(32A)	0.4648	0.5008	-0.2759	11.4614
C(11)	0.8603(5)	0.3246(8)	0.5849(4)	2.9(1)	H(32B)	0.4414	0.6619	-0.2313	11.4614
H(11A)	0.8027	0.2418	0.5562	2.9419	H(32C)	0.3634	0.5066	-0.2348	11.4614
H(11B)	0.9272	0.3122	0.5648	2.9419	C(33)	0.540(9)	0.477(10)	-0.152(7)	7(1)
C(12)	0.9011(5)	0.2964(8)	0.6854(4)	2.9(1)	C(34)	0.474(4)	0.546(5)	-0.105(3)	9.1(9)
H(12)	0.9432	0.1914	0.6977	2.8930	H(34)	0.3880	0.6024	-0.1435	9.0800
C(13)	0.9868(5)	0.4328(8)	0.7347(4)	2.9(1)	C(35)	0.493(4)	0.554(5)	-0.014(3)	9.3(8)
C(14)	0.9242(5)	0.5982(8)	0.7050(4)	2.8(1)	H(35)	0.4348	0.5894	0.0090	9.3311
H(14)	0.8514	0.5959	0.7203	2.7769	C(36)	0.59(1)	0.48(1)	0.027(7)	8.8(10)
C(15)	1.0053(6)	0.7228(9)	0.7669(4)	4.0(1)	C(37)	0.670(8)	0.400(9)	0.000(5)	8(1)
H(15A)	0.9622	0.8202	0.7725	4.0481	H(37)	0.7339	0.3482	0.0282	8.1965
H(15B)	1.0693	0.7539	0.7459	4.0481	C(38)	0.626(5)	0.410(5)	-0.106(3)	8.2(9)
C(16)	1.0519(7)	0.6318(10)	0.8550(4)	4.4(2)	H(38)	0.6871	0.3612	-0.1243	8.2131
H(16A)	1.1374	0.6405	0.8786	4.4034	C(39)	0.485(6)	0.538(8)	-0.251(4)	20(2)
H(16B)	1.0195	0.6793	0.8972	4.4034	H(39A)	0.5316	0.4807	-0.2902	20.9883
C(17)	1.0145(6)	0.4505(9)	0.8376(4)	3.3(1)	H(39B)	0.4836	0.6482	-0.2687	20.9883
H(17)	0.9403	0.4377	0.8496	3.2830	H(39C)	0.4024	0.4929	-0.2880	20.9883
C(18)	0.8708(6)	0.504(1)	0.4188(4)	4.4(2)	C(40)	0.631(5)	0.489(8)	0.132(3)	12(1)
H(18A)	0.9056	0.3962	0.4345	4.3608	H(40A)	0.7014	0.4250	0.1675	12.8336
H(18B)	0.9290	0.5849	0.4465	4.3608	H(40B)	0.5693	0.4455	0.1616	12.8336
H(18C)	0.8454	0.5160	0.3560	4.3608	H(40C)	0.6444	0.5996	0.1566	12.8336
C(19)	1.1037(6)	0.4187(9)	0.7155(4)	3.7(1)					

CA·63+64 (2:1)

atom	x	y	z	Beq	atom	x	y	z	Beq
O(1)	0.6106(2)	0.5071(4)	0.5982(2)	4.22(7)	H(19A)	-0.1592	0.4186	0.2527	3.3746
H(1)	0.6395	0.5975	0.6144	4.2179	H(19B)	-0.0899	0.3442	0.3457	3.3746
O(2)	0.2581(2)	0.7339(4)	0.3794(2)	3.33(6)	H(19C)	-0.1406	0.2289	0.2637	3.3746
H(2)	0.2886	0.8249	0.3914	3.3336	C(20)	-0.1055(4)	0.2527(6)	0.0981(3)	3.57(9)
O(3)	0.2006(2)	0.2051(4)	0.2865(2)	3.77(6)	H(20)	-0.1825	0.2660	0.1070	3.5657
H(3)	0.2606	0.2163	0.3297	3.7662	C(21)	-0.0704(6)	0.0736(8)	0.1134(3)	5.8(1)
O(4)	-0.2195(4)	0.4358(6)	-0.1746(2)	7.1(1)	H(21A)	-0.1296	0.0060	0.0727	5.8460
O(5)	-0.2745(3)	0.1836(5)	-0.2165(2)	5.23(8)	H(21B)	-0.0619	0.0432	0.1727	5.8460
H(5)	-0.2793	0.2207	-0.2651	5.2254	H(21C)	0.0042	0.0571	0.1039	5.8460
C(1)	0.3281(4)	0.3085(6)	0.5977(3)	3.10(8)	C(22)	-0.1211(4)	0.3026(8)	0.0027(3)	4.7(1)
H(1A)	0.3384	0.3175	0.6601	3.0991	H(22A)	-0.1205	0.4215	-0.0003	4.6845
H(1B)	0.2977	0.2003	0.5784	3.0991	H(22B)	-0.0533	0.2634	-0.0115	4.6845
C(2)	0.4489(3)	0.3261(5)	0.5868(3)	3.12(8)	C(23)	-0.2308(5)	0.2421(9)	-0.0663(3)	6.0(1)
H(2A)	0.5020	0.2436	0.6220	3.1204	H(23A)	-0.2315	0.1237	-0.0652	5.9936
H(2B)	0.4407	0.3085	0.5254	3.1204	H(23B)	-0.2995	0.2804	-0.0526	5.9936
C(3)	0.5000(4)	0.4924(6)	0.6149(3)	3.22(8)	C(24)	-0.2417(4)	0.2986(8)	-0.1574(3)	4.3(1)
H(3A)	0.5138	0.5070	0.6781	3.2222	C(25)	0.475(4)	0.397(5)	0.144(3)	7.0(5)
C(4)	0.4149(4)	0.6230(5)	0.5628(3)	2.85(7)	C(26)	0.493(2)	0.446(3)	0.066(2)	7.5(5)
H(4A)	0.4079	0.6141	0.5010	2.8496	H(26)	0.5592	0.5151	0.0715	7.4519
H(4B)	0.4473	0.7296	0.5836	2.8496	C(27)	0.410(6)	0.401(7)	-0.021(3)	8.7(7)
C(5)	0.2906(4)	0.6100(5)	0.5697(3)	2.85(8)	C(28)	0.317(5)	0.294(6)	-0.016(3)	9.9(9)
H(5A)	0.2995	0.6297	0.6319	2.8527	H(28)	0.2674	0.2744	-0.0764	9.8554
C(6)	0.2102(3)	0.7456(5)	0.5161(3)	3.08(8)	C(29)	0.299(2)	0.262(2)	0.055(2)	7.8(5)
H(6A)	0.1421	0.7563	0.5357	3.0817	H(29)	0.2328	0.1917	0.0508	7.7686
H(6B)	0.2530	0.8484	0.5285	3.0817	C(30)	0.367(3)	0.298(4)	0.142(2)	10.3(7)
C(7)	0.1654(4)	0.7172(5)	0.4161(3)	2.91(7)	H(30)	0.3613	0.2707	0.1883	10.3212
H(7)	0.1042	0.7990	0.3885	2.9143	C(31)	0.564(2)	0.463(5)	0.231(2)	11.9(9)
C(8)	0.1111(3)	0.5479(5)	0.3931(3)	2.66(7)	H(31A)	0.5419	0.4243	0.2783	11.8791
H(8)	0.0400	0.5441	0.4099	2.6585	H(31B)	0.5651	0.5791	0.2289	11.8791
C(9)	0.1945(3)	0.4115(5)	0.4440(2)	2.39(7)	H(31C)	0.6404	0.4201	0.2343	11.8791
H(9)	0.2661	0.4182	0.4277	2.3869	C(32)	0.430(3)	0.458(5)	-0.108(2)	12.2(10)
C(10)	0.2348(3)	0.4377(5)	0.5462(2)	2.73(7)	H(32A)	0.3730	0.4095	-0.1538	12.2051
C(11)	0.1386(4)	0.2415(5)	0.4136(3)	2.89(8)	H(32B)	0.5103	0.4178	-0.1051	12.2051
H(11A)	0.1964	0.1581	0.4418	2.8859	H(32C)	0.4319	0.5733	-0.1095	12.2051
H(11B)	0.0714	0.2276	0.4334	2.8859	C(33)	0.461(4)	0.404(5)	0.148(3)	10.3(8)
C(12)	0.0974(4)	0.2142(5)	0.3133(3)	2.84(7)	C(34)	0.531(3)	0.479(3)	0.105(2)	10.6(7)
H(12)	0.0558	0.1093	0.3004	2.8377	H(34)	0.6019	0.5317	0.1406	10.5621
C(13)	0.0113(3)	0.3495(5)	0.2637(2)	2.60(7)	C(35)	0.504(2)	0.480(3)	0.014(2)	10.3(6)
C(14)	0.0734(4)	0.5156(5)	0.2943(3)	2.75(8)	H(35)	0.5504	0.5326	-0.0120	10.2983
H(14)	0.1465	0.5133	0.2796	2.7477	C(36)	0.404(6)	0.408(7)	-0.039(3)	10.8(9)
C(15)	-0.0074(4)	0.6408(6)	0.2327(3)	3.72(9)	C(37)	0.330(4)	0.324(5)	-0.004(3)	9.3(7)
H(15A)	-0.0707	0.6735	0.2541	3.7212	H(37)	0.2610	0.2652	-0.0325	9.3074
H(15B)	0.0368	0.7372	0.2271	3.7212	C(38)	0.373(3)	0.322(3)	0.102(2)	8.8(6)
C(16)	-0.0556(5)	0.5494(6)	0.1452(3)	4.3(1)	H(38)	0.3125	0.2643	0.1201	8.7911
H(16A)	-0.0256	0.5977	0.1018	4.2976	C(39)	0.510(3)	0.428(5)	0.247(2)	18(1)
H(16B)	-0.1418	0.5562	0.1224	4.2976	H(39A)	0.4590	0.3637	0.2701	18.3219
C(17)	-0.0161(4)	0.3674(6)	0.1618(3)	3.03(8)	H(39B)	0.5063	0.5372	0.2569	18.3219
H(17)	0.0590	0.3561	0.1504	3.0264	H(39C)	0.5879	0.3832	0.2677	18.3219
C(18)	0.1288(4)	0.4189(7)	0.5796(3)	3.82(9)	C(40)	0.372(3)	0.410(5)	-0.138(2)	15(1)
H(18A)	0.1552	0.4348	0.6423	3.8191	H(40A)	0.3008	0.3489	-0.1622	15.0168
H(18B)	0.0952	0.3117	0.5654	3.8191	H(40B)	0.4358	0.3658	-0.1494	15.0168
H(18C)	0.0698	0.4997	0.5514	3.8191	H(40C)	0.3595	0.5225	-0.1513	15.0168
C(19)	-0.1050(4)	0.3341(6)	0.2836(3)	3.37(9)					

CA·63+64 (1:1)

atom	x	y	z	Beq	atom	x	y	z	Beq
O(1)	1.1112(4)	-0.2161(7)	0.5976(3)	4.2(1)	H(19B)	0.3994	-0.3600	0.3391	6.2092
H(1O)	1.1569	-0.1600	0.6386	6.2092	H(19C)	0.3581	-0.5200	0.2648	6.2092
O(2)	0.7579(4)	0.0118(6)	0.3797(3)	3.42(9)	C(20)	0.3936(6)	-0.4712(10)	0.0978(4)	3.8(1)
H(2O)	0.8430	0.0200	0.3668	6.2092	H(20)	0.3169	-0.4400	0.1098	6.2092
O(3)	0.7018(4)	-0.5153(6)	0.2871(3)	3.68(9)	C(21)	0.4319(10)	-0.647(1)	0.1116(6)	6.3(2)
H(3O)	0.6747	-0.5800	0.2407	6.2092	H(21A)	0.3781	-0.7200	0.0708	6.2092
O(4)	0.2267(6)	-0.5398(8)	-0.2169(4)	5.5(1)	H(21B)	0.3987	-0.6400	0.1681	6.2092
H(4)	0.2225(6)	-0.5039(8)	-0.2654(4)	8.2857	H(21C)	0.5039	-0.6800	0.1269	6.2092
O(5)	0.2779(8)	-0.284(1)	-0.1753(4)	7.7(2)	C(22)	0.3761(7)	-0.417(1)	0.0013(4)	4.9(2)
C(1)	0.8280(6)	-0.4167(9)	0.5961(4)	3.2(1)	H(22A)	0.3936	-0.2800	0.0008	6.2092
H(1A)	0.7886	-0.5200	0.5755	6.2092	H(22B)	0.4435	-0.3800	-0.0123	6.2092
H(1B)	0.8371	-0.4000	0.6601	6.2092	C(23)	0.2684(9)	-0.477(2)	-0.0675(5)	6.3(3)
C(2)	0.9497(6)	-0.4007(9)	0.5852(4)	3.3(1)	H(23A)	0.2185	-0.5400	-0.0563	6.2092
H(2A)	0.9997	-0.5000	0.6187	6.2092	H(23B)	0.2773	-0.6200	-0.0611	6.2092
H(2B)	0.9440	-0.4400	0.5244	6.2092	C(24)	0.2580(7)	-0.422(1)	-0.1584(5)	4.5(2)
C(3)	0.9993(6)	-0.2324(9)	0.6139(4)	3.3(1)	C(25)	0.103(5)	-0.825(5)	0.028(2)	8.8(8)
H(3)	1.0097	-0.2200	0.6712	6.2092	C(26)	-0.003(2)	-0.750(3)	-0.014(2)	8.7(5)
C(4)	0.9140(6)	-0.1028(8)	0.5620(4)	3.1(1)	H(26)	-0.051(2)	-0.699(3)	0.013(2)	10.3931
H(4A)	0.8921	-0.1000	0.5000	6.2092	C(27)	-0.028(3)	-0.763(4)	-0.105(3)	10.1(8)
H(4B)	0.9436	0.0200	0.5845	6.2092	H(27)	-0.099(3)	-0.717(4)	-0.141(3)	12.1594
C(5)	0.7901(6)	-0.1162(9)	0.5694(4)	2.8(1)	C(28)	0.037(7)	-0.832(6)	-0.145(5)	8.1(7)
H(5)	0.8022	-0.1000	0.6344	6.2092	C(29)	0.134(3)	-0.903(4)	-0.096(2)	9.0(6)
C(6)	0.7102(6)	0.0207(9)	0.5159(4)	3.4(1)	H(29)	0.182(3)	-0.956(4)	-0.122(2)	10.7958
H(6A)	0.6397	0.0200	0.5370	6.2092	C(30)	0.179(9)	-0.900(9)	0.020(8)	9.4(9)
H(6B)	0.7569	0.1400	0.5432	6.2092	H(30)	0.244(9)	-0.946(9)	0.063(8)	11.2221
C(7)	0.6639(6)	-0.0047(9)	0.4162(4)	3.1(1)	C(31)	0.132(4)	-0.804(6)	0.142(2)	15(1)
H(7)	0.6122	0.1000	0.3992	6.2092	H(31A)	0.206(4)	-0.858(6)	0.173(2)	22.7719
C(8)	0.6092(5)	-0.1766(8)	0.3927(4)	2.6(1)	H(31B)	0.069(4)	-0.854(6)	0.157(2)	22.7719
H(8)	0.5384	-0.1800	0.4128	6.2092	H(31C)	0.138(4)	-0.690(6)	0.157(2)	22.7719
C(9)	0.6937(5)	-0.3137(8)	0.4432(4)	2.5(1)	C(32)	0.012(4)	-0.843(5)	-0.244(2)	14(1)
H(9)	0.7653	-0.3000	0.4283	6.2092	H(32A)	0.074(4)	-0.904(5)	-0.255(2)	22.2943
C(10)	0.7337(5)	-0.2882(8)	0.5449(4)	2.8(1)	H(32B)	0.009(4)	-0.735(5)	-0.268(2)	22.2943
C(11)	0.6374(6)	-0.4829(8)	0.4127(4)	3.0(1)	H(32C)	-0.063(4)	-0.897(5)	-0.272(2)	22.2943
H(11A)	0.5733	-0.5000	0.4381	6.2092	C(33)	0.084(9)	-0.811(10)	0.046(6)	9(1)
H(11B)	0.6903	-0.5600	0.4330	6.2092	C(34)	0.008(7)	-0.765(7)	-0.063(6)	9.6(10)
C(12)	0.5964(6)	-0.5090(8)	0.3124(4)	2.9(1)	H(34)	-0.060(7)	-0.701(7)	-0.075(6)	11.4930
H(12)	0.5514	-0.6000	0.2950	6.2092	C(35)	0.04(1)	-0.81(1)	-0.13(1)	9(1)
C(13)	0.5099(5)	-0.3736(8)	0.2627(4)	2.7(1)	C(36)	0.118(6)	-0.909(8)	-0.148(5)	10(1)
C(14)	0.5733(6)	-0.2074(8)	0.2947(4)	2.9(1)	H(36)	0.126(6)	-0.936(8)	-0.202(5)	12.4870
H(14)	0.6546	-0.2200	0.2805	6.2092	C(37)	0.197(9)	-0.965(9)	-0.056(6)	10(1)
C(15)	0.4905(6)	-0.0831(9)	0.2325(5)	3.9(1)	H(37)	0.258(9)	-1.038(9)	-0.031(6)	12.3544
H(15A)	0.4413	-0.0400	0.2534	6.2092	C(38)	0.16(2)	-0.91(2)	-0.04(2)	9(1)
H(15B)	0.5349	0.0000	0.2289	6.2092	H(38)	0.14(2)	-0.83(2)	-0.09(2)	11.7669
C(16)	0.4424(7)	-0.173(1)	0.1453(5)	4.4(2)	C(39)	0.064(7)	-0.765(8)	0.105(5)	11(1)
H(16A)	0.4636	-0.1200	0.1005	6.2092	H(39A)	0.120(7)	-0.809(8)	0.158(5)	17.3129
H(16B)	0.3621	-0.1800	0.1205	6.2092	H(39B)	-0.015(7)	-0.800(8)	0.101(5)	17.3129
C(17)	0.4830(6)	-0.3537(9)	0.1614(4)	3.2(1)	H(39C)	0.068(7)	-0.648(8)	0.107(5)	17.3129
H(17)	0.5587	-0.3600	0.1571	6.2092	C(40)	-0.057(4)	-0.759(6)	-0.230(3)	9(1)
C(18)	0.6272(6)	-0.306(1)	0.5782(5)	3.9(1)	H(40A)	-0.033(4)	-0.807(6)	-0.275(3)	14.0867
H(18A)	0.6040	-0.4200	0.5780	6.2092	H(40B)	-0.057(4)	-0.642(6)	-0.235(3)	14.0867
H(19A)	0.3274	-0.3200	0.2368	6.2092	H(40C)	-0.135(4)	-0.796(6)	-0.236(3)	14.0867

CA·63+64 (1:2)

atom	x	y	z	Beq	atom	x	y	z	Beq
O(1)	-0.1120(1)	-0.1566(3)	0.4029(1)	3.09(3)	H(8)	0.1653	-0.3400	0.3383	2.4895
O(2)	0.2435(1)	0.0702(2)	0.6217(1)	2.71(3)	H(9)	0.2016	0.1600	0.6091	2.7074
O(3)	0.2985(1)	-0.4586(3)	0.7125(1)	3.02(3)	H(10)	0.1980	-0.0600	0.3681	2.3355
O(4)	0.7244(3)	-0.2247(4)	1.1762(2)	5.74(6)	H(11)	0.2437	0.1800	0.4640	2.6680
O(5)	0.7738(2)	-0.4823(3)	1.2173(1)	4.17(4)	H(12)	0.3618	0.0800	0.4691	2.6680
C(1)	0.1731(2)	-0.3574(3)	0.4042(2)	2.49(4)	H(13)	0.3583	-0.2200	0.3644	3.0888
C(2)	0.0508(2)	-0.3416(3)	0.4152(2)	2.65(4)	H(14)	0.4171	-0.3600	0.4372	3.0888
C(3)	-0.0005(2)	-0.1719(3)	0.3864(2)	2.56(4)	H(15)	0.4402	-0.1800	0.4513	3.0888
C(4)	0.0863(2)	-0.0440(3)	0.4390(2)	2.38(4)	H(16)	0.3922	0.1400	0.6132	2.3971
C(5)	0.2117(2)	-0.0571(3)	0.4317(1)	2.34(4)	H(17)	0.4587	-0.1200	0.5880	2.2392
C(6)	0.2926(2)	0.0788(3)	0.4850(2)	2.67(4)	H(18)	0.2378	-0.2400	0.5718	1.9755
C(7)	0.3370(2)	0.0527(3)	0.5840(2)	2.40(4)	H(19)	0.3051	-0.5000	0.5664	2.3924
C(8)	0.3921(2)	-0.1185(3)	0.6076(1)	2.24(3)	H(20)	0.4352	-0.4400	0.5699	2.3924
C(9)	0.3070(2)	-0.2555(3)	0.5573(1)	1.98(3)	H(21)	0.3556	-0.1600	0.7200	2.2471
C(10)	0.2674(2)	-0.2307(3)	0.4560(1)	2.25(4)	H(22)	0.4526	-0.5600	0.7037	2.3869
C(11)	0.3644(2)	-0.4238(3)	0.5881(1)	2.39(4)	H(23)	0.4674	0.0600	0.7676	3.2143
C(12)	0.4050(2)	-0.4518(3)	0.6886(1)	2.39(4)	H(24)	0.5762	0.0000	0.7432	3.2143
C(13)	0.4912(2)	-0.3152(3)	0.7380(1)	2.25(4)	H(25)	0.6034	-0.3200	0.6577	2.8985
C(14)	0.4288(2)	-0.1500(3)	0.7064(1)	2.25(4)	H(26)	0.6605	-0.2600	0.7484	2.8985
C(15)	0.5101(2)	-0.0232(4)	0.7671(2)	3.21(5)	H(26A)	1.0551(8)	-0.6390(10)	0.9908(5)	7.1116
C(16)	0.5578(3)	-0.1137(4)	0.8554(2)	3.41(5)	H(27)	0.6416	-0.4400	0.7354	2.8985
C(17)	0.5178(2)	-0.2960(3)	0.8391(1)	2.57(4)	H(27A)	1.0992(7)	-0.649(1)	1.1399(6)	7.1266
C(18)	0.3742(2)	-0.2499(4)	0.4221(2)	3.09(5)	H(28)	0.6493	-0.1000	0.8726	3.4062
C(19)	0.6094(2)	-0.3325(4)	0.7189(2)	2.90(4)	H(29)	0.5195	-0.0600	0.8945	3.4062
C(20)	0.6074(2)	-0.4111(4)	0.9035(2)	2.95(4)	H(29A)	0.8124(10)	-0.897(1)	1.1167(8)	7.5427
C(21)	0.5685(3)	-0.5876(5)	0.8892(2)	4.83(7)	H(30)	0.4378	-0.3000	0.8462	2.5716
C(22)	0.6238(3)	-0.3577(5)	0.9989(2)	3.90(6)	H(30A)	0.764(1)	-0.900(2)	0.972(1)	8.6229
C(23)	0.7323(3)	-0.4230(6)	1.0677(2)	5.10(9)	H(31)	0.3160	-0.5200	0.7500	3.0240
C(24)	0.7428(2)	-0.3645(4)	1.1587(2)	3.50(5)	H(31A)	0.795(1)	-0.804(2)	0.8323(6)	14.2675
C(25)	0.900(1)	-0.762(1)	0.9574(7)	7.6(3)	H(31B)	0.931(1)	-0.797(2)	0.8433(6)	14.2675
C(26)	1.0033(8)	-0.6920(10)	1.0139(5)	7.1(2)	H(31C)	0.860(1)	-0.635(2)	0.8442(6)	14.2675
C(27)	1.0302(7)	-0.700(1)	1.1039(6)	7.1(2)	H(32)	0.5868	-0.6200	0.8381	4.8258
C(28)	0.960(2)	-0.778(2)	1.1415(9)	7.4(3)	H(32A)	1.057(1)	-0.731(2)	1.2724(8)	14.4207
C(29)	0.8625(10)	-0.846(1)	1.0912(8)	7.5(2)	H(32B)	0.986(1)	-0.897(2)	1.2600(8)	14.4207
C(30)	0.833(1)	-0.844(2)	1.005(1)	8.6(3)	H(32C)	0.919(1)	-0.730(2)	1.2540(8)	14.4207
C(31)	0.869(1)	-0.748(2)	0.8608(6)	14.3(6)	H(33)	0.4792	-0.5800	0.8885	4.8258
C(32)	0.983(1)	-0.785(2)	1.2414(8)	14.4(6)	H(33A)	0.752(3)	-0.868(6)	0.928(2)	7.2703
C(33)	0.810(3)	-0.847(6)	0.982(2)	7.3(7)	H(34)	0.6137	-0.6400	0.9359	4.8258
C(34)	0.911(2)	-0.755(4)	0.988(2)	7.0(6)	H(35)	0.6844	-0.4000	0.8908	2.9514
C(35)	0.989(2)	-0.715(4)	1.070(1)	7.7(6)	H(35A)	1.059(2)	-0.660(4)	1.074(1)	7.6722
C(36)	0.967(4)	-0.752(6)	1.147(2)	7.1(9)	H(36)	0.6266(3)	-0.2392(5)	1.0015(2)	3.9013
C(37)	0.869(3)	-0.851(4)	1.140(2)	9.5(8)	H(37)	0.5545(3)	-0.3924(5)	1.0129(2)	3.9013
C(38)	0.798(2)	-0.906(3)	1.058(2)	9.7(7)	H(37A)	0.851(3)	-0.880(4)	1.190(2)	9.5238
C(39)	0.927(2)	-0.712(4)	0.902(2)	10(1)	H(38)	0.8022(3)	-0.3890(6)	1.0543(2)	5.1030
C(40)	1.049(2)	-0.718(5)	1.234(1)	9.8(10)	H(38A)	0.741(2)	-0.985(3)	1.054(2)	9.7014
H(1)	-0.1565	-0.0800	0.3649	3.0880	H(39)	0.7296(3)	-0.5416(6)	1.0665(2)	5.1030
H(2)	-0.0100	-0.1600	0.3250	2.5590	H(39A)	0.861(2)	-0.753(4)	0.854(2)	10.4760
H(3)	0.0977	-0.0400	0.4997	2.3813	H(39B)	1.000(2)	-0.760(4)	0.900(2)	10.4760
H(4)	0.0578	0.0600	0.4182	2.3813	H(39C)	0.931(2)	-0.595(4)	0.897(2)	10.4760
H(5)	0.0084	-0.4200	0.3836	2.6458	H(40A)	1.112(2)	-0.650(5)	1.230(1)	9.8270
H(5A)	0.7790	-0.4456	1.2658	4.1705	H(40B)	1.081(2)	-0.819(5)	1.263(1)	9.8270
H(6)	0.0561	-0.3600	0.4756	2.6458	H(40C)	1.007(2)	-0.663(5)	1.268(1)	9.8270
H(7)	0.2112	-0.4400	0.4187	2.4895					

CA·63+64 (1:3)

atom	x	y	z	Beq	atom	x	y	z	Beq
O(1)	-0.1114(4)	-0.0766(7)	-0.0978(4)	4.7(1)	H(21)	0.5934	0.1000	0.1557	4.1129
H(38)	-0.152(3)	-0.149(7)	-0.129(4)	4.6506	H(22)	0.6469	0.2200	0.2233	4.1129
O(2)	0.2440(4)	-0.3032(7)	0.1213(3)	3.7(1)	H(23)	0.6754	0.0200	0.2653	4.1129
H(25)	0.1829	-0.4200	0.0973	3.7276	C(20)	0.6086(7)	0.177(1)	0.4045(5)	4.0(2)
O(3)	0.2988(4)	0.2261(7)	0.2128(3)	4.0(1)	H(29)	0.7077	0.1400	0.3934	3.9992
H(39)	0.282(4)	0.134(2)	0.226(5)	3.9692	C(21)	0.5682(10)	0.353(1)	0.3899(6)	6.3(3)
O(4)	0.7692(6)	0.2430(9)	0.7161(4)	6.5(2)	H(30)	0.6065	0.4200	0.4572	6.2842
H(37)	0.795(7)	0.2012(10)	0.7650(4)	6.4508	H(31)	0.5621	0.4200	0.3304	6.2842
O(5)	0.7261(7)	-0.013(1)	0.6762(4)	7.9(2)	H(32)	0.4787	0.3600	0.3935	6.2842
C(1)	0.1734(6)	0.1250(10)	-0.0960(4)	3.1(1)	C(22)	0.6235(7)	0.125(1)	0.4990(5)	5.0(2)
H(4)	0.1413	0.1400	-0.1712	3.0746	H(22A)	0.5558	0.1507	0.5124	5.0288
H(5)	0.2115	0.2400	-0.0679	3.0746	H(22B)	0.6335	0.0041	0.5014	5.0288
C(2)	0.0514(6)	0.1083(10)	-0.0847(5)	3.7(2)	C(23)	0.7312(8)	0.186(1)	0.5676(5)	6.3(3)
H(1)	0.0542	0.1400	-0.0214	3.7181	H(35)	0.7303(8)	0.304(1)	0.5669(5)	6.2976
H(2)	0.0147	0.2400	-0.1044	3.7181	H(36)	0.8007(8)	0.150(1)	0.5544(5)	6.2976
C(3)	-0.0002(7)	-0.0608(10)	-0.1151(4)	3.4(2)	C(24)	0.7418(7)	0.129(1)	0.6564(6)	4.9(2)
H(3)	-0.0077	-0.0800	-0.1817	3.3817	C(25)	0.041(2)	1.043(2)	0.359(1)	8.2(5)
C(4)	0.0856(6)	-0.1878(10)	-0.0612(5)	3.5(2)	C(26)	-0.031(2)	0.967(2)	0.396(1)	9.3(5)
H(6)	0.0972	-0.1800	0.0065	3.4575	H(26A)	-0.1030	0.9230	0.3582	9.2948
H(7)	0.0531	-0.3000	-0.0782	3.4575	C(27)	-0.004(2)	0.956(2)	0.486(1)	9.0(5)
C(5)	0.2122(6)	-0.175(1)	-0.0686(4)	3.3(2)	H(27A)	-0.0548	0.9052	0.5085	8.9529
H(8)	0.1820	-0.1800	-0.1440	3.3146	C(28)	0.101(2)	1.020(3)	0.540(1)	8.8(5)
C(6)	0.2908(6)	-0.311(1)	-0.0160(5)	3.9(2)	C(29)	0.172(2)	1.100(2)	0.501(1)	8.9(5)
H(11)	0.2639	-0.4200	-0.0308	3.8610	H(29A)	0.2438	1.1482	0.5359	8.8558
H(12)	0.3756	-0.3400	-0.0293	3.8610	C(30)	0.138(2)	1.112(2)	0.414(1)	9.1(5)
C(7)	0.3370(6)	-0.2854(10)	0.0839(4)	3.2(1)	H(30A)	0.1854	1.1691	0.3869	9.1187
H(13)	0.3832	-0.4000	0.1181	3.1630	C(31)	0.015(2)	1.053(3)	0.260(1)	14.0(9)
C(8)	0.3915(6)	-0.1133(10)	0.1072(4)	2.9(1)	H(31A)	-0.059(2)	0.998(3)	0.230(1)	14.0148
H(14)	0.4623	-0.1000	0.0824	2.9277	H(31B)	0.078(2)	1.001(3)	0.245(1)	14.0148
C(9)	0.3066(6)	0.0231(10)	0.0570(4)	2.8(1)	H(31C)	0.009(2)	1.165(3)	0.242(1)	14.0148
H(15)	0.2322	0.0000	0.0782	2.8322	C(32)	0.133(2)	1.017(3)	0.639(1)	14.1(8)
C(10)	0.2653(6)	-0.0023(10)	-0.0444(4)	3.1(2)	H(32A)	0.073(2)	0.957(3)	0.653(1)	14.1317
C(11)	0.3625(6)	0.1903(10)	0.0884(4)	3.3(2)	H(32B)	0.137(2)	1.126(3)	0.661(1)	14.1317
H(16)	0.3336	0.3000	0.0567	3.2593	H(32C)	0.208(2)	0.964(3)	0.665(1)	14.1317
H(17)	0.4382	0.2200	0.0640	3.2593	C(33)	0.019(7)	1.000(9)	0.356(5)	9(1)
C(12)	0.4057(6)	0.218(1)	0.1887(4)	3.2(1)	C(34)	-0.004(7)	0.95(1)	0.441(3)	10(1)
H(24)	0.4551	0.3600	0.2083	3.2262	H(34A)	-0.0752	0.8702	0.4410	10.0094
C(13)	0.4903(6)	0.0833(10)	0.2384(4)	3.1(2)	C(35)	0.074(6)	1.018(9)	0.531(5)	9(1)
C(14)	0.4290(6)	-0.0848(9)	0.2058(5)	3.1(1)	C(36)	0.179(6)	1.130(9)	0.535(4)	9(1)
H(18)	0.3422	-0.0600	0.2180	3.0517	H(36A)	0.2352	1.1602	0.5926	9.4993
C(15)	0.5109(7)	-0.209(1)	0.2679(5)	4.3(2)	C(37)	0.196(6)	1.190(8)	0.451(4)	9(1)
H(19)	0.5668	-0.2600	0.2389	4.2897	H(37A)	0.2642	1.2574	0.4542	9.8720
H(20)	0.4652	-0.3000	0.2722	4.2897	C(38)	0.120(6)	1.121(8)	0.361(5)	9(1)
C(16)	0.5593(8)	-0.119(1)	0.3554(5)	4.6(2)	H(38A)	0.1265	1.1454	0.3028	9.5964
H(27)	0.6456(8)	-0.126(1)	0.3780(5)	4.6134	C(39)	-0.053(6)	0.930(9)	0.271(5)	12(2)
H(28)	0.5289(8)	-0.169(1)	0.3979(5)	4.6134	H(39A)	-0.112(6)	0.858(9)	0.279(5)	12.9213
C(17)	0.5197(6)	0.0622(10)	0.3406(4)	3.2(2)	H(39B)	-0.002(6)	0.870(9)	0.247(5)	12.9213
H(26)	0.4240	0.1000	0.3417	3.1709	H(39C)	-0.091(6)	1.016(9)	0.231(5)	12.9213
C(18)	0.3719(7)	0.014(1)	-0.0789(5)	4.5(2)	C(40)	0.054(6)	0.97(1)	0.612(5)	12(2)
H(18A)	0.4312	-0.0668	-0.0461	4.4650	H(40A)	-0.015(6)	0.91(1)	0.600(5)	12.2762
H(18B)	0.4047	0.1197	-0.0654	4.4650	H(40B)	0.042(6)	1.07(1)	0.641(5)	12.2762
H(18C)	0.3456	-0.0100	-0.1387	4.4650	H(40C)	0.123(6)	0.92(1)	0.650(5)	12.2762
C(19)	0.6095(6)	0.098(1)	0.2199(4)	4.1(2)					

CA·63+64 (1:4)

atom	x	y	z	Beq	atom	x	y	z	Beq
O(1)	-0.1119(3)	0.1037(5)	-0.0975(2)	3.93(7)	H(22)	0.6643	0.0000	0.2604	3.3438
H(35)	-0.1567	0.1800	-0.1461	3.9336	H(23)	0.6406	-0.1800	0.2286	3.3438
O(2)	0.2449(3)	0.3320(4)	0.1214(2)	3.27(6)	H(24)	0.6148	-0.0400	0.1691	3.3438
H(20)	0.2095	0.4400	0.1061	3.2728	C(20)	0.6073(4)	-0.1495(7)	0.4037(3)	3.54(9)
O(3)	0.2984(3)	-0.1947(5)	0.2129(2)	3.56(6)	H(33)	0.6863	-0.1400	0.3917	3.5436
H(27)	0.3167	-0.2600	0.2602	3.5641	C(21)	0.5660(6)	-0.3241(9)	0.3898(4)	5.8(2)
O(4)	0.7268(5)	0.0404(7)	0.6757(3)	7.4(1)	H(25)	0.5840	-0.3800	0.3476	5.7852
O(5)	0.7718(4)	-0.2173(6)	0.7165(3)	5.44(9)	H(26)	0.6131	-0.4000	0.4232	5.7852
H(37)	0.7651	-0.1800	0.7644	5.4433	H(32)	0.4849	-0.3200	0.3872	5.7852
C(1)	0.1726(4)	-0.0973(6)	-0.0951(3)	3.06(8)	C(22)	0.6231(5)	-0.0935(9)	0.4984(3)	4.6(1)
H(6)	0.1605	-0.1000	-0.1592	3.0612	H(34)	0.6264(5)	0.0249(9)	0.5004(3)	4.6245
H(7)	0.2142	-0.1800	-0.0889	3.0612	H(36)	0.5533(5)	-0.1267(9)	0.5120(3)	4.6245
C(2)	0.0507(4)	-0.0802(6)	-0.0853(3)	3.10(8)	C(23)	0.7310(5)	-0.159(1)	0.5679(3)	5.9(2)
H(4)	0.0584	-0.1000	-0.0324	3.1022	H(23A)	0.8012(5)	-0.125(1)	0.5549(3)	5.8531
H(5)	0.0125	-0.1800	-0.1225	3.1022	H(23B)	0.7279(5)	-0.277(1)	0.5666(3)	5.8531
C(3)	-0.0001(4)	0.0869(6)	-0.1138(3)	2.94(8)	C(24)	0.7424(5)	-0.1008(8)	0.6582(3)	4.3(1)
H(3)	-0.0224	0.1000	-0.1819	2.9419	C(25)	0.102(2)	0.001(2)	0.544(1)	9.1(4)
C(4)	0.0860(4)	0.2159(6)	-0.0612(3)	2.76(8)	C(26)	-0.005(1)	0.068(2)	0.4862(9)	8.6(3)
H(1)	0.0972	0.2000	0.0041	2.7635	H(26A)	-0.0583	0.1215	0.5069	8.5921
H(2)	0.0550	0.3200	-0.0783	2.7635	C(27)	-0.028(1)	0.054(2)	0.3959(9)	8.8(3)
C(5)	0.2105(4)	0.2039(6)	-0.0682(3)	2.86(8)	H(27A)	-0.1010	0.0969	0.3595	8.7532
H(8)	0.1984	0.2000	-0.1381	2.8630	C(28)	0.041(1)	-0.013(2)	0.356(1)	8.2(3)
C(6)	0.2917(4)	0.3403(6)	-0.0153(3)	3.14(8)	C(29)	0.139(1)	-0.081(2)	0.411(1)	8.7(4)
H(15)	0.3756	0.3400	-0.0306	3.1370	H(29A)	0.1884	-0.1376	0.3870	8.6931
H(16)	0.2450	0.4600	-0.0424	3.1370	C(30)	0.172(2)	-0.075(2)	0.499(1)	9.3(4)
C(7)	0.3383(4)	0.3138(5)	0.0838(3)	2.66(7)	H(30A)	0.2427	-0.1226	0.5317	9.2585
H(19)	0.3984	0.4000	0.1150	2.6616	C(31)	0.130(2)	0.013(3)	0.6406(10)	15.4(9)
C(8)	0.3928(4)	0.1426(5)	0.1083(3)	2.52(7)	H(31A)	0.205(2)	-0.040(3)	0.6702(10)	15.4037
H(18)	0.4659	0.1400	0.0898	2.5219	H(31B)	0.068(2)	-0.041(3)	0.6562(10)	15.4037
C(9)	0.3068(4)	0.0063(5)	0.0571(3)	2.34(7)	H(31C)	0.134(2)	0.125(3)	0.6577(10)	15.4037
H(14)	0.2358	0.0200	0.0756	2.3387	C(32)	0.013(2)	-0.019(3)	0.2591(10)	14.5(8)
C(10)	0.2670(4)	0.0311(6)	-0.0444(3)	2.68(8)	H(32A)	-0.061(2)	0.037(3)	0.2304(10)	14.5407
C(11)	0.3633(4)	-0.1627(6)	0.0883(3)	2.76(8)	H(32B)	0.006(2)	-0.131(3)	0.2400(10)	14.5407
H(12)	0.3152	-0.2600	0.0636	2.7635	H(32C)	0.076(2)	0.033(3)	0.2442(10)	14.5407
H(13)	0.4359	-0.1800	0.0717	2.7635	C(33)	0.110(6)	-0.090(7)	0.361(4)	10(1)
C(12)	0.4047(4)	-0.1893(6)	0.1889(3)	2.68(7)	H(33A)	0.1211	-0.1279	0.3090	10.7302
H(17)	0.4486	-0.3000	0.2040	2.6830	C(34)	0.021(5)	0.028(7)	0.360(4)	9(1)
C(13)	0.4913(4)	-0.0532(6)	0.2384(3)	2.56(8)	C(35)	0.003(5)	0.079(7)	0.437(3)	8(1)
C(14)	0.4298(4)	0.1124(5)	0.2066(3)	2.58(8)	H(35A)	-0.0540	0.1516	0.4349	8.7224
H(21)	0.3495	0.1000	0.2178	2.5827	C(36)	0.076(7)	0.017(10)	0.521(4)	8(1)
C(15)	0.5116(5)	0.2380(6)	0.2676(3)	3.75(10)	C(37)	0.166(7)	-0.10(1)	0.521(4)	9(1)
H(28)	0.5654	0.2800	0.2393	3.7489	H(37A)	0.2247	-0.1334	0.5760	9.5411
H(29)	0.4799	0.3400	0.2732	3.7489	C(38)	0.183(6)	-0.147(8)	0.446(4)	10(1)
C(16)	0.5593(5)	0.1482(7)	0.3548(3)	4.1(1)	H(38A)	0.2484	-0.2230	0.4482	10.5139
H(30)	0.5282	0.2000	0.3931	4.0639	C(39)	0.060(5)	0.070(8)	0.619(4)	9(1)
H(38)	0.6439	0.1600	0.3764	4.0639	H(39A)	-0.006(5)	0.144(8)	0.608(4)	9.8435
C(17)	0.5182(4)	-0.0331(6)	0.3390(3)	3.04(8)	H(39B)	0.131(5)	0.123(8)	0.656(4)	9.8435
H(31)	0.4381	-0.0400	0.3467	3.0398	H(39C)	0.046(5)	-0.026(8)	0.648(4)	9.8435
C(18)	0.3725(4)	0.0115(7)	-0.0776(3)	3.60(9)	C(40)	-0.061(7)	0.11(1)	0.257(5)	16(2)
H(9)	0.4019	-0.1000	-0.0793	3.5996	H(40A)	-0.036(7)	0.06(1)	0.213(5)	16.3409
H(10)	0.4362	0.0800	-0.0523	3.5996	H(40B)	-0.047(7)	0.23(1)	0.258(5)	16.3409
H(11)	0.3549	0.0400	-0.1328	3.5996	H(40C)	-0.144(7)	0.09(1)	0.245(5)	16.3409
C(19)	0.6099(4)	-0.0717(7)	0.2203(3)	3.34(9)					

CA·63+64 (1:5)

atom	x	y	z	Beq	atom	x	y	z	Beq
O(1)	0.6120(2)	0.0585(4)	0.5976(2)	3.67(6)	H(22)	-0.1450(3)	-0.2217(6)	0.2592(3)	3.2562
H(37)	0.6606	0.1400	0.6345	3.6707	H(23)	-0.1642(3)	-0.0321(6)	0.2515(3)	3.2562
O(2)	0.2552(2)	0.2854(4)	0.3786(2)	3.13(5)	H(24)	-0.0938(3)	-0.1110(6)	0.3428(3)	3.2562
H(17)	0.2985	0.3800	0.3921	3.1298	C(20)	-0.1068(4)	-0.1946(6)	0.0957(2)	3.46(9)
O(3)	0.2013(2)	-0.2411(4)	0.2867(2)	3.49(6)	H(33)	-0.1826	-0.2000	0.1092	3.4583
H(20)	0.1853	-0.3000	0.2396	3.4899	C(21)	-0.0671(6)	-0.3717(8)	0.1111(4)	5.6(1)
O(4)	-0.2707(4)	-0.2637(5)	-0.2166(2)	5.27(8)	H(30)	-0.1245(6)	-0.4401(8)	0.0693(4)	5.6004
H(36)	-0.2807	-0.2000	-0.2666	5.2712	H(31)	-0.0610(6)	-0.4034(8)	0.1696(4)	5.6004
O(5)	-0.2256(5)	-0.0070(6)	-0.1757(3)	7.4(1)	H(32)	0.0093(6)	-0.3837(8)	0.1040(4)	5.6004
C(1)	0.3273(3)	-0.1429(5)	0.5950(2)	2.90(7)	C(22)	-0.1238(4)	-0.1389(8)	0.0014(2)	4.5(1)
H(8)	0.2821	-0.2200	0.5910	2.8953	H(22A)	-0.1271(4)	-0.0205(8)	-0.0003(2)	4.5100
H(9)	0.3363	-0.1400	0.6622	2.8953	H(22B)	-0.0542(4)	-0.1718(8)	-0.0126(2)	4.5100
C(2)	0.4492(3)	-0.1265(5)	0.5852(3)	3.03(7)	C(23)	-0.2314(5)	-0.203(1)	-0.0677(3)	6.0(2)
H(2)	0.4906	-0.2200	0.6146	3.0296	H(23A)	-0.3016(5)	-0.169(1)	-0.0547(3)	5.9573
H(3)	0.4431	-0.1400	0.5316	3.0296	H(23B)	-0.2288(5)	-0.321(1)	-0.0665(3)	5.9573
C(3)	0.5001(3)	0.0416(5)	0.6134(3)	2.94(7)	C(24)	-0.2431(4)	-0.1447(7)	-0.1593(3)	4.05(9)
H(1)	0.5187	0.0400	0.6811	2.9372	C(25)	0.4557(9)	-0.060(1)	0.1418(7)	8.4(2)
C(4)	0.4137(3)	0.1703(5)	0.5613(2)	2.77(7)	C(26)	0.5290(9)	0.013(2)	0.1060(7)	9.1(2)
H(4)	0.4046	0.1600	0.4981	2.7666	H(26A)	0.6007	0.0583	0.1436	9.0856
H(5)	0.4393	0.2800	0.5790	2.7666	C(27)	0.5065(9)	0.023(1)	0.0167(6)	8.3(2)
C(5)	0.2890(3)	0.1578(5)	0.5680(2)	2.73(7)	H(27A)	0.5628	0.0755	-0.0033	8.2834
H(7)	0.2974	0.1800	0.6335	2.7335	C(28)	0.4010(10)	-0.043(1)	-0.0423(7)	8.7(2)
C(6)	0.2076(3)	0.2939(6)	0.5152(3)	3.14(7)	C(29)	0.3299(9)	-0.123(1)	-0.0001(8)	9.0(2)
H(6)	0.2502	0.4000	0.5403	3.1393	H(29A)	0.2598	-0.1698	-0.0358	9.0050
H(10)	0.1288	0.3000	0.5390	3.1393	C(30)	0.3597(9)	-0.127(1)	0.0877(8)	8.6(2)
C(7)	0.1621(3)	0.2683(5)	0.4162(2)	2.67(7)	H(30A)	0.3100	-0.1824	0.1122	8.6284
H(38)	0.1005	0.3600	0.3858	2.6687	C(31)	0.487(1)	-0.062(2)	0.2417(8)	14.5(5)
C(8)	0.1070(3)	0.0965(5)	0.3920(2)	2.44(6)	H(31A)	0.4277	-0.1148	0.2581	14.5265
H(18)	0.0331	0.1000	0.4121	2.4398	H(31B)	0.4967	0.0504	0.2642	14.5265
C(9)	0.1932(3)	-0.0403(5)	0.4428(2)	2.28(6)	H(31C)	0.5638	-0.1162	0.2697	14.5265
H(11)	0.2655	-0.0400	0.4247	2.2755	C(32)	0.377(1)	-0.026(2)	-0.1395(8)	15.1(5)
C(10)	0.2330(3)	-0.0159(5)	0.5439(2)	2.46(6)	H(32A)	0.3027	-0.0767	-0.1720	15.0658
C(11)	0.1358(3)	-0.2092(5)	0.4113(2)	2.69(7)	H(32B)	0.4403	-0.0774	-0.1550	15.0658
H(12)	0.1873	-0.3000	0.4342	2.6861	H(32C)	0.3740	0.0881	-0.1554	15.0658
H(13)	0.0701	-0.2400	0.4351	2.6861	C(33)	0.385(3)	-0.143(5)	0.134(2)	8.7(6)
C(12)	0.0950(3)	-0.2355(5)	0.3106(2)	2.67(7)	H(33A)	0.3783	-0.1964	0.1775	8.7413
H(19)	0.0524	-0.3400	0.2958	2.6672	C(34)	0.490(3)	-0.030(4)	0.151(3)	7.9(6)
C(13)	0.0082(3)	-0.0982(5)	0.2614(2)	2.41(6)	C(35)	0.519(4)	0.044(6)	0.075(2)	8.4(6)
C(14)	0.0708(3)	0.0655(5)	0.2937(2)	2.60(7)	H(35A)	0.5837	0.1253	0.0884	8.4002
H(21)	0.1451	0.0600	0.2771	2.6016	C(36)	0.441(4)	0.005(8)	-0.019(3)	7.9(5)
C(15)	-0.0106(4)	0.1931(6)	0.2329(3)	3.65(9)	C(37)	0.338(4)	-0.110(8)	-0.037(3)	8.6(6)
H(25)	-0.0743(4)	0.2255(6)	0.2540(3)	3.6486	H(37A)	0.3111	-0.1459	-0.0915	8.6245
H(26)	0.0342(4)	0.2892(6)	0.2279(3)	3.6486	C(38)	0.308(5)	-0.179(8)	0.040(3)	8.3(6)
C(16)	-0.0599(4)	0.1032(6)	0.1450(3)	4.04(9)	H(38A)	0.2476	-0.2401	0.0271	8.2589
H(27)	-0.0301(4)	0.1530(6)	0.1022(3)	4.0394	C(39)	0.564(5)	0.007(7)	0.239(3)	7(1)
H(28)	-0.1464(4)	0.1092(6)	0.1227(3)	4.0394	H(39A)	0.5379	-0.0458	0.2831	7.4456
C(17)	-0.0188(3)	-0.0782(6)	0.1607(2)	2.95(7)	H(39B)	0.5581	0.1307	0.2533	7.4456
H(29)	0.0591	-0.1000	0.1494	2.9467	H(39C)	0.6479	-0.0095	0.2537	7.4456
C(18)	0.1273(4)	-0.0352(7)	0.5778(2)	3.45(8)	C(40)	0.470(5)	0.074(9)	-0.091(3)	8.9(7)
H(14)	0.0655(4)	0.0411(7)	0.5479(2)	3.4544	H(40A)	0.5396	0.1648	-0.0687	8.8550
H(15)	0.1540(4)	-0.0142(7)	0.6399(2)	3.4544	H(40B)	0.4065	0.1457	-0.1304	8.8550
H(16)	0.0965(4)	-0.1445(7)	0.5666(2)	3.4544	H(40C)	0.4981	0.0046	-0.1238	8.8550
C(19)	-0.1099(3)	-0.1176(6)	0.2806(3)	3.26(8)					

CA·62+63+64 (1:1:1)

atom	x	y	z	Beq	atom	x	y	z	Beq
O(1)	0.3880(1)	0.6222(2)	0.4030(1)	3.12(3)	H(8)	0.6942	0.5200	0.3704	2.4137
O(2)	0.7427(1)	0.3958(2)	0.6216(1)	2.76(3)	H(9)	0.8540	0.6800	0.3704	3.1567
O(3)	0.7991(1)	0.9257(2)	0.7120(1)	3.11(3)	H(10)	0.9406	0.6400	0.4500	3.1567
O(4)	1.2207(3)	0.6940(4)	1.1758(1)	5.92(6)	H(11)	0.9182	0.8200	0.4347	3.1567
O(5)	1.2747(2)	0.9499(3)	1.2177(1)	4.20(4)	H(12)	0.7410	0.3000	0.4656	2.7390
C(1)	0.6727(2)	0.8230(3)	0.4033(1)	2.58(3)	H(13)	0.8584	0.3800	0.4671	2.7390
C(2)	0.5505(2)	0.8070(3)	0.4142(1)	2.66(3)	H(14)	0.8953	0.3200	0.6107	2.4729
C(3)	0.4992(2)	0.6370(3)	0.3859(1)	2.59(3)	H(15)	0.9585	0.6000	0.5868	2.3419
C(4)	0.5861(2)	0.5091(3)	0.4387(1)	2.51(3)	H(16)	0.7353	0.7200	0.5728	2.0608
C(5)	0.7106(2)	0.5220(3)	0.4311(1)	2.41(3)	H(17)	0.9360	0.9000	0.5706	2.4208
C(6)	0.7921(2)	0.3859(3)	0.4850(1)	2.74(3)	H(18)	0.8130	0.9800	0.5625	2.4208
C(7)	0.8362(2)	0.4131(3)	0.5841(1)	2.47(3)	H(19)	0.9470	1.0200	0.6979	2.4208
C(8)	0.8912(2)	0.5842(3)	0.6074(1)	2.34(3)	H(20)	0.8116	0.9800	0.7520	3.1125
C(9)	0.8063(2)	0.7213(3)	0.5567(1)	2.06(3)	H(21)	0.8584	0.6200	0.7205	2.3892
C(10)	0.7668(2)	0.6950(3)	0.4548(1)	2.31(3)	H(22)	1.0974	0.7800	0.6623	2.9925
C(11)	0.8636(2)	0.8898(3)	0.5872(1)	2.42(3)	H(23)	1.1615	0.7200	0.7490	2.9925
C(12)	0.9045(2)	0.9184(3)	0.6877(1)	2.42(3)	H(24)	1.1397	0.9000	0.7346	2.9925
C(13)	0.9905(2)	0.7817(3)	0.7374(1)	2.31(3)	H(25)	0.9634	0.4000	0.7681	3.1796
C(14)	0.9284(2)	0.6161(3)	0.7061(1)	2.39(3)	H(26)	1.0701	0.4800	0.7458	3.1796
C(15)	1.0090(2)	0.4892(3)	0.7675(2)	3.18(4)	H(26A)	0.5964	0.0981	1.1391	7.5191
C(16)	1.0566(2)	0.5801(4)	0.8555(2)	3.57(5)	H(27)	1.1369	0.5800	0.8818	3.5736
C(17)	1.0178(2)	0.7630(3)	0.8387(1)	2.70(4)	H(27A)	0.5566	0.1047	0.9890	7.6367
C(18)	0.8734(2)	0.7139(4)	0.4212(1)	3.16(4)	H(28)	1.0198	0.5200	0.8977	3.5736
C(19)	1.1086(2)	0.7983(3)	0.7182(1)	2.99(4)	H(29)	0.9404	0.7800	0.8448	2.6956
C(20)	1.1079(2)	0.8792(4)	0.9028(1)	3.12(4)	H(29A)	0.2652	0.3673	0.9694	7.8325
C(21)	1.0713(3)	1.0565(5)	0.8876(2)	5.18(7)	H(30)	1.0825	1.1000	0.8332	5.1835
C(22)	1.1226(2)	0.8260(4)	0.9982(1)	3.93(5)	H(30A)	0.3150	0.3595	1.1199	7.1440
C(23)	1.2314(3)	0.8935(5)	1.0679(2)	5.13(8)	H(31)	0.9795	1.0600	0.8885	5.1835
C(24)	1.2418(2)	0.8316(4)	1.1583(2)	3.69(5)	H(31A)	0.5577	0.1897	1.2747	13.5956
C(25)	0.464(2)	0.240(3)	1.144(1)	7.1(3)	H(31B)	0.4200	0.1951	1.2561	13.5956
C(26)	0.5289(9)	0.158(1)	1.1028(7)	7.5(2)	H(31C)	0.4911	0.3585	1.2611	13.5956
C(27)	0.5016(9)	0.154(1)	1.0140(6)	7.6(2)	H(32)	1.1073	1.1200	0.9303	5.1835
C(28)	0.400(2)	0.233(3)	0.9603(8)	8.0(3)	H(32A)	0.2911	0.2763	0.8351	14.5446
C(29)	0.333(3)	0.310(5)	1.006(1)	7.8(3)	H(32B)	0.3554	0.1071	0.8404	14.5446
C(30)	0.368(1)	0.311(1)	1.0939(8)	7.1(2)	H(32C)	0.4250	0.2703	0.8410	14.5446
C(31)	0.491(2)	0.245(2)	1.2425(8)	13.6(6)	H(33)	1.1829	0.8800	0.8898	3.1196
C(32)	0.367(2)	0.217(2)	0.8608(8)	14.5(6)	H(33A)	0.2668	0.3610	0.9272	8.1855
C(33)	0.319(4)	0.320(8)	0.982(2)	8.2(4)	H(34)	1.0506	0.8400	1.0102	3.9336
C(34)	0.302(1)	0.367(2)	1.061(1)	8.5(4)	H(34A)	0.2445	0.4324	1.0561	8.4650
C(35)	0.374(1)	0.316(2)	1.144(1)	7.6(3)	H(35)	1.2342	0.8000	1.0503	5.1275
C(36)	0.472(3)	0.219(5)	1.146(2)	7.8(5)	H(35A)	0.3584	0.3523	1.1878	7.5925
C(37)	0.488(1)	0.185(2)	1.068(1)	7.1(3)	H(36)	1.2796	0.9800	1.0604	5.1275
C(38)	0.413(3)	0.220(5)	0.985(2)	7.6(4)	H(37)	0.3467	0.5600	0.3660	3.1156
C(39)	0.552(1)	0.170(3)	1.231(1)	9.3(5)	H(37A)	0.5572	0.1194	1.0688	7.0737
C(40)	0.429(2)	0.180(3)	0.900(2)	9.5(4)	H(38)	0.7030	0.3000	0.6040	2.7611
H(1)	0.4828	0.6200	0.3269	2.5858	H(39)	1.1388	0.7000	1.0096	3.9336
H(2)	0.5599	0.8400	0.4741	2.6601	H(39A)	0.5213	0.2209	1.2761	9.2743
H(3)	0.5028	0.9000	0.3886	2.6601	H(39B)	0.6303	0.2140	1.2424	9.2743
H(4)	0.7123	0.9200	0.4184	2.5787	H(39C)	0.5514	0.0579	1.2365	9.2743
H(5)	0.6591	0.8200	0.3448	2.5787	H(40A)	0.3616	0.2203	0.8470	9.5435
H(5A)	1.2692	0.9178	1.2645	4.1966	H(40B)	0.4211	0.0565	0.8912	9.5435
H(6)	0.5565	0.4200	0.4239	2.5053	H(40C)	0.5002	0.2103	0.8917	9.5435
H(7)	0.5990	0.5200	0.4995	2.5053					

CA·66 (crossing)

atom	x	y	z	U	atom	x	y	z	U
O(1)	-0.8124(3)	0.1023(2)	-0.4868(3)	0.065(1)	H(7)	-0.8203	-0.0746	-0.4967	0.0532
O(2)	-0.6698(2)	-0.1896(2)	-0.1775(2)	0.0372(9)	H(8)	-1.0159	-0.0829	-0.5000	0.0545
O(3)	-0.3766(3)	-0.5937(2)	-0.1407(3)	0.071(1)	H(9)	-0.9464	-0.1865	-0.6153	0.0545
O(4)	-0.3800(2)	-0.6169(2)	0.0357(3)	0.056(1)	H(10)	-1.0080	-0.2249	-0.5421	0.0456
O(5)	-0.7704(2)	-0.2205(2)	-0.5439(2)	0.0394(10)	H(11)	-0.8744	-0.3125	-0.5242	0.0494
O(6)	-0.7250(3)	0.2250(3)	-0.2631(3)	0.113(2)	H(12)	-0.9015	-0.3082	-0.3678	0.0431
O(7)	-0.6642(3)	0.1913(2)	-0.4188(3)	0.063(1)	H(13)	-0.8046	-0.1424	-0.3498	0.0393
C(1)	-0.9541(4)	-0.0352(3)	-0.2935(4)	0.049(2)	H(14)	-0.8460	-0.1316	-0.1610	0.0443
C(2)	-0.8786(4)	0.0299(3)	-0.3302(4)	0.051(2)	H(15)	-0.9126	-0.2086	-0.1775	0.0443
C(3)	-0.8884(4)	0.0438(3)	-0.4515(4)	0.051(2)	H(16)	-0.7584	-0.2502	-0.0867	0.0380
C(4)	-0.8804(4)	-0.0414(3)	-0.5126(4)	0.044(2)	H(17)	-0.7019	-0.2751	-0.3697	0.0367
C(5)	-0.9550(3)	-0.1101(3)	-0.4729(4)	0.043(2)	H(18)	-0.7211	-0.4126	-0.4722	0.0494
C(6)	-0.9460(3)	-0.1950(3)	-0.5344(4)	0.049(2)	H(19)	-0.7983	-0.4298	-0.3983	0.0494
C(7)	-0.8608(4)	-0.2524(3)	-0.5034(4)	0.041(1)	H(20)	-0.6036	-0.4509	-0.3526	0.0443
C(8)	-0.8531(3)	-0.2633(3)	-0.3802(3)	0.035(1)	H(21)	-0.6882	-0.4968	-0.2933	0.0443
C(9)	-0.8597(3)	-0.1753(3)	-0.3214(4)	0.034(1)	H(22)	-0.6082	-0.3353	-0.2467	0.0393
C(10)	-0.9521(3)	-0.1237(3)	-0.3492(4)	0.038(1)	H(23)	-0.8985	-0.3596	-0.1826	0.0507
C(11)	-0.8465(3)	-0.1877(3)	-0.1981(4)	0.038(1)	H(24)	-0.8254	-0.3900	-0.1064	0.0507
C(12)	-0.7570(3)	-0.2405(3)	-0.1649(3)	0.032(1)	H(25)	-0.8355	-0.4400	-0.2222	0.0507
C(13)	-0.7527(3)	-0.3278(3)	-0.2245(3)	0.029(1)	H(26)	-1.0585	-0.1681	-0.2372	0.0697
C(14)	-0.7604(3)	-0.3102(3)	-0.3460(3)	0.031(1)	H(27)	-1.0400	-0.2358	-0.3278	0.0697
C(15)	-0.7363(3)	-0.3986(3)	-0.3965(3)	0.043(2)	H(28)	-1.1031	-0.1543	-0.3507	0.0697
C(16)	-0.6638(3)	-0.4409(3)	-0.3179(4)	0.040(1)	H(29)	-0.6740	-0.4699	-0.1001	0.0469
C(17)	-0.6553(3)	-0.3783(3)	-0.2185(3)	0.031(1)	H(30)	-0.5866	-0.3116	-0.0359	0.0633
C(18)	-0.8354(3)	-0.3853(3)	-0.1823(4)	0.043(1)	H(31)	-0.6828	-0.3483	0.0095	0.0633
C(19)	-1.0443(3)	-0.1729(3)	-0.3148(4)	0.056(2)	H(32)	-0.5852	-0.3913	0.0410	0.0633
C(20)	-0.6268(3)	-0.4250(3)	-0.1150(3)	0.035(1)	H(33)	-0.4811	-0.4272	-0.1562	0.0456
C(21)	-0.6224(4)	-0.3661(3)	-0.0174(4)	0.056(2)	H(34)	-0.5332	-0.5121	-0.1912	0.0456
C(22)	-0.5294(3)	-0.4710(3)	-0.1322(3)	0.037(1)	H(35)	-0.4712	-0.4706	0.0186	0.0507
C(23)	-0.4908(3)	-0.5162(3)	-0.0315(4)	0.043(2)	H(36)	-0.5420	-0.5537	-0.0005	0.0507
C(24)	-0.4096(3)	-0.5794(3)	-0.0546(4)	0.040(2)	H(37)	-0.8340	0.1329	-0.5485	0.0760
C(25)	-0.6651(4)	0.2365(4)	-0.3299(4)	0.054(2)	H(38)	-0.6670	-0.1624	-0.2460	0.0431
C(26)	-0.5869(4)	0.3013(4)	-0.3213(5)	0.074(2)	H(39)	-0.3576	-0.6762	0.0173	0.0646
H(1)	-1.0082	0.0027	-0.3174	0.0595	H(40)	-0.7725	-0.2243	-0.6256	0.0456
H(2)	-0.9561	-0.0379	-0.2145	0.0595	H(41)	-0.5404	0.3055	-0.3842	0.0849
H(3)	-0.8201	-0.0044	-0.3219	0.0608	H(42)	-0.5436	0.2979	-0.2595	0.0849
H(4)	-0.8680	0.0851	-0.2998	0.0608	H(43)	-0.6091	0.3649	-0.3181	0.0849
H(5)	-0.9406	0.0816	-0.4742	0.0608	H(44)	-0.7261	0.1753	-0.4414	0.0709
H(6)	-0.8833	-0.0380	-0.5906	0.0532					

CA·66 (bilayer)

atom	x	y	z	U	atom	x	y	z	U
O(1)	-0.0916(2)	-0.1259	-0.4454(2)	0.038(1)	H(7)	-0.0211	-0.0274	-0.5822	0.0329
O(2)	0.1817(2)	-0.4480(6)	-0.6711(2)	0.0353(10)	H(8)	-0.2258	-0.0036	-0.7466	0.0355
O(3)	0.3736(3)	-0.3080(6)	-1.0684(3)	0.043(1)	H(9)	-0.1025	0.2112	-0.7422	0.0380
O(4)	0.4898(3)	-0.4846(7)	-1.0899(3)	0.084(2)	H(10)	-0.1479	0.1212	-0.8475	0.0380
O(5)	0.0879(2)	0.0937(6)	-0.6622(2)	0.0340(10)	H(11)	0.0305	0.1491	-0.8107	0.0329
O(6)	-0.3077(3)	-0.3572(8)	-0.4285(4)	0.100(2)	H(12)	-0.0199	-0.1091	-0.8786	0.0291
O(7)	-0.3628(3)	-0.0998(9)	-0.4303(4)	0.095(2)	H(13)	0.0228	-0.2269	-0.6787	0.0279
O(8)	-0.5776(4)	-0.3908(8)	-0.2851(3)	0.081(2)	H(14)	-0.0249	-0.4837	-0.7487	0.0367
O(9)	-0.6833(3)	-0.1975(6)	-0.2629(3)	0.055(1)	H(15)	-0.0514	-0.4150	-0.8589	0.0367
C(1)	-0.1850(4)	-0.3250(8)	-0.7084(3)	0.033(2)	H(16)	0.1142	-0.5491	-0.8092	0.0380
C(2)	-0.1321(4)	-0.3146(7)	-0.5914(3)	0.032(1)	H(17)	0.1797	-0.1440	-0.7167	0.0291
C(3)	-0.1471(4)	-0.1436(8)	-0.5565(3)	0.030(1)	H(18)	0.2260	0.0758	-0.7919	0.0291
C(4)	-0.1005(4)	-0.0180(7)	-0.6075(3)	0.028(1)	H(19)	0.1527	0.0205	-0.9023	0.0380
C(5)	-0.1498(4)	-0.0290(7)	-0.7267(3)	0.029(1)	H(20)	0.3610	-0.0833	-0.7947	0.0393
C(6)	-0.1018(4)	0.1052(7)	-0.7740(3)	0.031(1)	H(21)	0.2936	-0.1188	-0.9101	0.0393
C(7)	0.0131(4)	0.0693(7)	-0.7666(3)	0.027(1)	H(22)	0.3161	-0.3227	-0.7424	0.0329
C(8)	0.0238(4)	-0.1027(7)	-0.8038(3)	0.024(1)	H(23)	0.1081	-0.2384	-0.9887	0.0380
C(9)	-0.0210(3)	-0.2363(7)	-0.7523(3)	0.023(1)	H(24)	0.0945	-0.4248	-0.9779	0.0380
C(10)	-0.1407(4)	-0.2010(7)	-0.7658(3)	0.026(1)	H(25)	0.0108	-0.3041	-0.9651	0.0380
C(11)	-0.0039(4)	-0.4087(7)	-0.7881(3)	0.029(1)	H(26)	-0.1911	-0.1354	-0.9223	0.0469
C(12)	0.1120(4)	-0.4438(7)	-0.7792(3)	0.030(1)	H(27)	-0.2135	-0.3179	-0.9081	0.0469
C(13)	0.1530(3)	-0.3113(7)	-0.8340(3)	0.022(1)	H(28)	-0.2883	-0.1838	-0.8932	0.0469
C(14)	0.1391(4)	-0.1440(7)	-0.7896(3)	0.024(1)	H(29)	0.2768	-0.4116	-0.9473	0.0380
C(15)	0.1988(4)	-0.0242(7)	-0.8336(3)	0.030(1)	H(30)	0.3505	-0.6201	-0.7725	0.0507
C(16)	0.2942(4)	-0.1267(8)	-0.8395(4)	0.033(2)	H(31)	0.2360	-0.6336	-0.8584	0.0507
C(17)	0.2758(4)	-0.3065(7)	-0.8150(3)	0.027(1)	H(32)	0.3371	-0.6766	-0.8825	0.0507
C(18)	0.0867(3)	-0.3237(7)	-0.9509(3)	0.031(1)	H(33)	0.4789	-0.4226	-0.7819	0.0456
C(19)	-0.2167(4)	-0.2153(8)	-0.8820(3)	0.039(2)	H(34)	0.4469	-0.2748	-0.8567	0.0456
C(20)	0.3202(4)	-0.4291(8)	-0.8730(3)	0.031(1)	H(35)	0.4670	-0.5888	-0.9242	0.0507
C(21)	0.3070(4)	-0.6083(8)	-0.8456(4)	0.042(2)	H(36)	0.5616	-0.4644	-0.8932	0.0507
C(22)	0.4394(4)	-0.3915(8)	-0.8540(3)	0.038(2)	H(37)	-0.0943	-0.2418	-0.4165	0.0456
C(23)	0.4835(4)	-0.4772(8)	-0.9263(4)	0.041(2)	H(38)	0.1488	-0.5271	-0.6407	0.0418
C(24)	0.4427(4)	-0.4138(8)	-1.0355(4)	0.042(2)	H(39)	0.4530	-0.4708	-1.1652	0.1013
C(25)	-0.3708(5)	-0.248(1)	-0.4647(4)	0.051(2)	H(40)	0.1650	0.0923	-0.6457	0.0418
C(26)	-0.4705(5)	-0.273(1)	-0.5603(4)	0.079(2)	H(41)	-0.4697	-0.1981	-0.6184	0.0950
C(27)	-0.6408(5)	-0.2786(10)	-0.3182(5)	0.062(3)	H(42)	-0.4765	-0.3789	-0.5883	0.0950
C(28)	-0.6802(6)	-0.225(1)	-0.4273(5)	0.087(3)	H(43)	-0.5367	-0.2444	-0.5528	0.0950
H(1)	-0.1779	-0.4308	-0.7314	0.0393	H(44)	-0.2864	-0.0586	-0.4027	0.1140
H(2)	-0.2622	-0.3031	-0.7276	0.0393	H(45)	-0.6517	-0.2803	-0.4694	0.1039
H(3)	-0.0536	-0.3309	-0.5710	0.0380	H(46)	-0.6694	-0.1047	-0.4371	0.1039
H(4)	-0.1576	-0.3925	-0.5581	0.0380	H(47)	-0.7617	-0.2325	-0.4635	0.1039
H(5)	-0.2242	-0.1210	-0.5768	0.0367	H(48)	-0.6541	-0.2334	-0.1906	0.0646
H(6)	-0.1099	0.0965	-0.5846	0.0329					

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atom	x	y	z	U	atom	x	y	z	U
O(1)	0.167(1)	0.616(1)	0.530(1)	0.076(7)	H(6)	0.1002	0.4752	0.4281	0.0554
O(2)	0.2282(10)	0.2900(10)	0.4680(10)	0.052(5)	H(7)	0.1739	0.4443	0.5105	0.0554
O(3)	0.3198(9)	0.3175(8)	0.8284(10)	0.038(4)	H(8)	-0.0138	0.4091	0.5217	0.0555
O(4)	0.628(1)	-0.082(1)	0.844(1)	0.094(7)	H(9)	0.0036	0.2678	0.4909	0.0609
O(5)	0.623(1)	-0.116(1)	1.018(1)	0.092(8)	H(10)	0.0590	0.3150	0.4013	0.0609
O(6)	0.238(1)	0.282(1)	1.253(1)	0.116(8)	H(11)	0.1394	0.1948	0.4754	0.0557
O(7)	0.183(1)	0.306(1)	1.093(1)	0.081(6)	H(12)	0.1009	0.2008	0.6445	0.0521
C(1)	0.042(1)	0.464(1)	0.717(1)	0.049(7)	H(13)	0.1883	0.3629	0.6641	0.0526
C(2)	0.109(2)	0.534(2)	0.682(2)	0.060(8)	H(14)	0.1553	0.3666	0.8439	0.0513
C(3)	0.105(2)	0.551(2)	0.560(2)	0.068(8)	H(15)	0.0991	0.2806	0.8361	0.0513
C(4)	0.112(1)	0.464(1)	0.502(2)	0.046(7)	H(16)	0.2352	0.2444	0.9132	0.0497
C(5)	0.047(2)	0.389(2)	0.537(2)	0.046(7)	H(17)	0.2916	0.2305	0.6439	0.0467
C(6)	0.056(2)	0.303(1)	0.476(2)	0.051(7)	H(18)	0.2184	0.0665	0.5980	0.0534
C(7)	0.144(2)	0.251(2)	0.508(2)	0.046(6)	H(19)	0.2960	0.1143	0.5350	0.0534
C(8)	0.151(1)	0.237(1)	0.624(2)	0.043(6)	H(20)	0.3258	0.0072	0.6983	0.0717
C(9)	0.139(1)	0.326(2)	0.687(1)	0.044(6)	H(21)	0.4016	0.0645	0.6452	0.0717
C(10)	0.048(2)	0.373(2)	0.661(2)	0.050(6)	H(22)	0.3910	0.1688	0.7708	0.0488
C(11)	0.152(1)	0.311(1)	0.810(2)	0.043(6)	H(23)	0.1139	0.1294	0.8037	0.0480
C(12)	0.240(2)	0.258(1)	0.839(2)	0.041(6)	H(24)	0.1809	0.0529	0.7791	0.0480
C(13)	0.248(1)	0.172(1)	0.778(2)	0.038(5)	H(25)	0.1813	0.0962	0.8918	0.0480
C(14)	0.243(1)	0.191(1)	0.659(1)	0.039(6)	H(26)	-0.0934	0.3489	0.6713	0.0745
C(15)	0.270(1)	0.104(1)	0.604(1)	0.045(7)	H(27)	-0.0366	0.2637	0.6587	0.0745
C(16)	0.343(2)	0.065(1)	0.679(1)	0.060(9)	H(28)	-0.0396	0.3112	0.7687	0.0745
C(17)	0.346(1)	0.125(1)	0.783(2)	0.041(7)	H(29)	0.3369	0.0247	0.8896	0.0663
C(18)	0.174(1)	0.106(1)	0.817(2)	0.040(6)	H(30)	0.3873	0.0934	1.0440	0.0872
C(19)	-0.039(1)	0.319(1)	0.693(2)	0.062(8)	H(31)	0.4125	0.1760	0.9782	0.0872
C(20)	0.378(2)	0.073(1)	0.882(2)	0.055(7)	H(32)	0.3096	0.1488	0.9915	0.0872
C(21)	0.371(2)	0.128(2)	0.983(2)	0.073(10)	H(33)	0.4780	0.0026	0.8042	0.0470
C(22)	0.476(2)	0.036(1)	0.868(1)	0.039(6)	H(34)	0.5179	0.0839	0.8621	0.0470
C(23)	0.510(2)	-0.020(1)	0.958(2)	0.061(9)	H(35)	0.5239	0.0159	1.0179	0.0735
C(24)	0.596(2)	-0.074(2)	0.932(2)	0.070(9)	H(36)	0.4614	-0.0594	0.9770	0.0735
C(25)	0.051(2)	0.178(2)	1.136(2)	0.11(1)	H(37)	0.1666	0.6222	0.4538	0.0915
C(26)	0.103(2)	0.202(2)	1.207(2)	0.08(1)	H(38)	0.2295	0.2860	0.3918	0.0619
C(27)	0.182(2)	0.267(2)	1.187(2)	0.065(9)	H(39)	0.3094(10)	0.3684(10)	0.8703(10)	0.0453
H(1)	0.0512	0.4541	0.7921	0.0584	H(40)	0.6827	-0.1402	1.0060	0.1100
H(2)	-0.0192	0.4854	0.7062	0.0584	H(41)	0.0026	0.1381	1.1513	0.1364
H(3)	0.0942	0.5862	0.7191	0.0721	H(42)	0.0581	0.2001	1.0647	0.1364
H(4)	0.1699	0.5160	0.7004	0.0721	H(43)	0.0945	0.1794	1.2770	0.1013
H(5)	0.0445	0.5732	0.5459	0.0813	H(44)	0.2316	0.3484	1.0924	0.0969

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atom	x	y	z	U	atom	x	y	z	U
O(1)	0.4787(4)	0.3159(6)	0.5987(4)	0.081(2)	H(7)	0.4902	0.3191	0.4425	0.0668
O(2)	0.5289(4)	0.2699(5)	0.2963(3)	0.053(2)	H(8)	0.4791	0.5324	0.4243	0.0674
O(3)	0.1724(4)	0.1629(5)	0.3207(3)	0.054(2)	H(9)	0.5079	0.5216	0.2926	0.0674
O(4)	0.1500(4)	-0.1070(7)	-0.0884(5)	0.094(3)	H(10)	0.5940	0.4544	0.3324	0.0674
O(5)	-0.0187(4)	-0.1016(6)	-0.1124(4)	0.083(2)	H(11)	0.5189	0.3795	0.2163	0.0596
O(6)	0.2614(4)	-0.2270(7)	0.1909(5)	0.115(3)	H(12)	0.3500	0.4199	0.2270	0.0508
O(7)	0.0986(4)	-0.1906(6)	0.2087(5)	0.089(2)	H(13)	0.3389	0.3096	0.3693	0.0554
C(1)	0.2910(6)	0.4646(8)	0.4717(5)	0.065(3)	H(14)	0.1654	0.3431	0.3805	0.0692
C(2)	0.3258(6)	0.3819(9)	0.5314(5)	0.064(3)	H(15)	0.1675	0.4129	0.3048	0.0692
C(3)	0.4431(6)	0.3943(9)	0.5442(6)	0.067(2)	H(16)	0.0915	0.2667	0.2642	0.0608
C(4)	0.5010(5)	0.3867(7)	0.4639(5)	0.055(2)	H(17)	0.3563	0.2075	0.2436	0.0464
C(5)	0.4625(6)	0.4664(7)	0.4020(6)	0.057(2)	H(18)	0.3926	0.3076	0.0996	0.0614
C(6)	0.5215(6)	0.4591(7)	0.3213(5)	0.057(2)	H(19)	0.4535	0.2140	0.1344	0.0614
C(7)	0.4895(5)	0.3680(7)	0.2674(5)	0.050(2)	H(20)	0.2895	0.2001	0.0367	0.0596
C(8)	0.3713(5)	0.3612(6)	0.2583(5)	0.044(2)	H(21)	0.3451	0.1068	0.0767	0.0596
C(9)	0.3142(5)	0.3666(7)	0.3395(5)	0.049(2)	H(22)	0.2323	0.1000	0.1774	0.0565
C(10)	0.3426(6)	0.4647(7)	0.3894(5)	0.056(2)	H(23)	0.1687	0.4079	0.1788	0.0601
C(11)	0.1948(5)	0.3524(7)	0.3286(5)	0.052(2)	H(24)	0.2325	0.3688	0.1056	0.0601
C(12)	0.1641(5)	0.2590(7)	0.2761(5)	0.048(2)	H(25)	0.1179	0.3324	0.1179	0.0601
C(13)	0.2207(5)	0.2575(7)	0.1950(5)	0.046(2)	H(26)	0.3318	0.6238	0.3752	0.0845
C(14)	0.3388(4)	0.2658(6)	0.2112(5)	0.040(2)	H(27)	0.3394	0.5677	0.2931	0.0845
C(15)	0.3866(5)	0.2454(7)	0.1291(5)	0.053(2)	H(28)	0.2348	0.5673	0.3403	0.0845
C(16)	0.3114(5)	0.1710(7)	0.0861(5)	0.052(2)	H(29)	0.0991	0.1862	0.0646	0.0646
C(17)	0.2164(5)	0.1566(7)	0.1425(5)	0.048(2)	H(30)	0.0123	0.1711	0.1844	0.0892
C(18)	0.1814(6)	0.3510(7)	0.1447(5)	0.055(2)	H(31)	-0.0355	0.0948	0.1227	0.0892
C(19)	0.3082(7)	0.5655(7)	0.3455(7)	0.071(3)	H(32)	0.0405	0.0546	0.1883	0.0892
C(20)	0.1165(5)	0.1290(7)	0.0978(5)	0.053(2)	H(33)	0.1934	0.0475	0.0106	0.0673
C(21)	0.0245(6)	0.1104(9)	0.1539(6)	0.077(3)	H(34)	0.1472	-0.0239	0.0765	0.0673
C(22)	0.1343(6)	0.0338(7)	0.0437(5)	0.056(2)	H(35)	-0.0128	-0.0168	0.0209	0.0934
C(23)	0.0436(7)	0.0084(9)	-0.0112(6)	0.079(3)	H(36)	0.0221	0.0693	-0.0382	0.0934
C(24)	0.0660(6)	-0.0725(8)	-0.0746(6)	0.061(2)	H(37)	0.5531	0.3232	0.6067	0.0916
C(25)	0.1380(9)	-0.100(1)	0.3592(7)	0.103(4)	H(38)	0.4992	0.2783	0.3578	0.0940
C(26)	0.2199(7)	-0.119(1)	0.3006(7)	0.092(4)	H(39)	0.2435	0.1537	0.3417	0.0940
C(27)	0.1972(6)	-0.1854(9)	0.2276(6)	0.070(3)	H(40)	-0.0404	-0.1866	-0.1435	0.0940
H(1)	0.2176	0.4550	0.4633	0.0778	H(41)	0.1634	-0.0546	0.3998	0.1166
H(2)	0.3029	0.5298	0.4951	0.0778	H(42)	0.0786	-0.0711	0.3344	0.1166
H(3)	0.2909	0.3909	0.5816	0.0769	H(43)	0.1186	-0.1642	0.3844	0.1166
H(4)	0.3117	0.3146	0.5116	0.0769	H(44)	0.2412	-0.0537	0.2813	0.1074
H(5)	0.4569	0.4597	0.5674	0.0816	H(45)	0.2761	-0.1515	0.3281	0.1074
H(6)	0.5737	0.3967	0.4732	0.0668	H(46)	0.0731	-0.2521	0.1564	0.0940

CA·69

atom	x	y	z	U	atom	x	y	z	U
O(1)	-1.0925(7)	-0.246(1)	-0.6222(6)	0.033(3)	H(7)	-1.0285	-0.3406	-0.4306	0.0626
O(2)	-0.9175(7)	-0.472(1)	-0.2764(6)	0.031(3)	H(8)	-1.2515	-0.3947	-0.4379	0.0773
O(3)	-0.8299(7)	0.070(1)	-0.2025(6)	0.040(3)	H(9)	-1.1613	-0.5053	-0.2761	0.0183
O(4)	-0.3402(9)	-0.180(2)	0.1499(8)	0.061(3)	H(10)	-1.1120	-0.5974	-0.3443	0.0183
O(5)	-0.2986(8)	0.089(1)	0.2062(7)	0.037(3)	H(11)	-0.9875	-0.5453	-0.1848	0.0240
C(1)	-1.200(1)	-0.045(2)	-0.4388(10)	0.032(4)	H(12)	-1.0333	-0.2766	-0.1421	0.0325
C(2)	-1.142(1)	-0.069(2)	-0.5104(10)	0.029(4)	H(13)	-0.9888	-0.1564	-0.3055	0.0309
C(3)	-1.157(1)	-0.238(2)	-0.5574(10)	0.029(4)	H(14)	-1.0311	0.1157	-0.2633	0.0473
C(4)	-1.109(1)	-0.370(2)	-0.476(1)	0.039(4)	H(15)	-1.0564	0.0415	-0.1742	0.0473
C(5)	-1.167(1)	-0.363(2)	-0.3958(10)	0.046(4)	H(16)	-0.8838	0.1544	-0.1056	0.0464
C(6)	-1.1128(9)	-0.492(2)	-0.3097(9)	0.022(3)	H(17)	-0.8231	-0.2395	-0.1518	0.0395
C(7)	-1.0019(10)	-0.463(2)	-0.2368(9)	0.020(3)	H(18)	-0.8625	-0.3899	0.0055	0.0415
C(8)	-0.993(1)	-0.285(2)	-0.1884(9)	0.024(3)	H(19)	-0.7949	-0.4645	-0.0523	0.0415
C(9)	-1.0342(10)	-0.152(2)	-0.2682(9)	0.017(3)	H(20)	-0.7045	-0.2748	0.1121	0.0505
C(10)	-1.152(1)	-0.183(2)	-0.344(1)	0.031(3)	H(21)	-0.6466	-0.3122	0.0383	0.0505
C(11)	-1.014(1)	0.027(2)	-0.2159(10)	0.036(4)	H(22)	-0.6913	-0.0651	-0.0385	0.0347
C(12)	-0.897(1)	0.052(2)	-0.1473(10)	0.030(4)	H(23)	-0.9106	0.0381	0.0405	0.0366
C(13)	-0.853(1)	-0.076(2)	-0.0580(9)	0.023(3)	H(24)	-0.9971	-0.0836	-0.0341	0.0366
C(14)	-0.873(1)	-0.248(2)	-0.1135(9)	0.024(3)	H(25)	-0.8968	-0.1531	0.0588	0.0366
C(15)	-0.811(1)	-0.370(2)	-0.0273(9)	0.028(4)	H(26)	-1.2513	-0.0424	-0.2786	0.0638
C(16)	-0.709(1)	-0.270(2)	0.0471(9)	0.031(4)	H(27)	-1.3208	-0.1831	-0.3506	0.0638
C(17)	-0.7245(10)	-0.085(2)	0.0115(9)	0.023(3)	H(28)	-1.2364	-0.2263	-0.2409	0.0638
C(18)	-0.921(1)	-0.070(2)	0.0096(9)	0.035(4)	H(29)	-0.7146	0.0158	0.1373	0.0464
C(19)	-1.245(1)	-0.163(2)	-0.295(1)	0.039(4)	H(30)	-0.6804	0.2941	0.1272	0.0642
C(20)	-0.677(1)	0.033(2)	0.0979(9)	0.032(3)	H(31)	-0.6568	0.2670	0.0297	0.0642
C(21)	-0.699(1)	0.223(2)	0.071(1)	0.049(5)	H(32)	-0.7765	0.2474	0.0242	0.0642
C(22)	-0.550(1)	0.000(3)	0.158(1)	0.061(5)	H(33)	-0.5229	0.0675	0.2195	0.0932
C(23)	-0.485(1)	0.024(2)	0.096(1)	0.047(4)	H(34)	-0.5426	-0.1167	0.1826	0.0932
C(24)	-0.361(1)	-0.030(2)	0.1529(10)	0.031(3)	H(35)	-0.5171	-0.0372	0.0352	0.0682
H(1)	-1.1925	0.0692	-0.4146	0.0452	H(36)	-0.4877	0.1414	0.0802	0.0682
H(2)	-1.2806	-0.0607	-0.4782	0.0452	H(37)	-1.1090	-0.3632	-0.6389	0.0641
H(3)	-1.1702	0.0107	-0.5642	0.0433	H(38)	-0.9165	-0.5828	-0.3011	0.0437
H(4)	-1.0660	-0.0454	-0.4703	0.0433	H(39)	-0.7537	0.1077	-0.1578	0.0490
H(5)	-1.2304	-0.2628	-0.5911	0.0459	H(40)	-0.2370	0.1072	0.1880	0.0528
H(6)	-1.1067	-0.4745	-0.5021	0.0626					

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atom	x	y	z	U	atom	x	y	z	U
O(1)	0.1096	-0.2867	0.3750	0.038(1)	H(13)	-0.0154	-0.5922	0.2787	0.0291
O(2)	-0.1745(5)	-0.6798(4)	0.0439(7)	0.036(1)	H(14)	0.0591	-0.7323	0.1190	0.0317
O(3)	-0.6996(5)	-1.1853(4)	-0.1064(7)	0.040(1)	H(15)	0.0355	-0.6402	0.0397	0.0317
O(4)	-0.6873(5)	-1.1091(4)	0.1315(7)	0.042(1)	H(16)	-0.1027	-0.7701	-0.0483	0.0304
O(5)	-0.0893(5)	-0.6076(4)	0.5902(6)	0.030(1)	H(17)	-0.1712	-0.7121	0.3477	0.0253
O(6)	-0.0802(5)	-0.5111(4)	-0.1262(7)	0.033(1)	H(18)	-0.1721	-0.8959	0.5043	0.0317
O(7)	0.1758(5)	-0.1329(4)	-0.3940(7)	0.033(1)	H(19)	-0.2237	-0.8068	0.5617	0.0317
O(8)	0.6689(5)	0.2935(4)	-0.2387(7)	0.044(1)	H(20)	-0.3207	-0.9728	0.3839	0.0405
O(9)	0.6963(5)	0.3599(4)	-0.4826(7)	0.033(1)	H(21)	-0.3769	-0.8881	0.4018	0.0405
O(10)	0.0889(5)	-0.1785(4)	0.1199(6)	0.033(1)	H(22)	-0.3235	-0.8256	0.1666	0.0279
O(11)	-0.5270(7)	-0.3329(5)	-0.0412(10)	0.094(2)	H(23)	-0.1308	-0.9572	0.2689	0.0380
O(12)	-0.6758(6)	-0.3605(5)	-0.2125(8)	0.068(2)	H(24)	-0.0919	-0.9293	0.0955	0.0380
O(13)	0.5265(6)	0.5126(5)	-0.5323(10)	0.082(2)	H(25)	-0.0184	-0.8773	0.2454	0.0380
O(14)	0.6845(5)	0.5345(5)	-0.6586(8)	0.055(2)	H(26)	0.2117	-0.6944	0.4185	0.0418
C(1)	0.2020(6)	-0.4965(5)	0.2081(9)	0.032(2)	H(27)	0.2218	-0.6842	0.2325	0.0418
C(2)	0.1513(6)	-0.4109(5)	0.2080(9)	0.032(2)	H(28)	0.3077	-0.6115	0.3500	0.0418
C(3)	0.1636(6)	-0.3650(5)	0.3763(9)	0.031(2)	H(29)	-0.2960	-1.0123	0.0751	0.0329
C(4)	0.1100(6)	-0.4407(5)	0.4977(8)	0.027(2)	H(30)	-0.2262	-0.9160	-0.1129	0.0380
C(5)	0.1621(6)	-0.5296(5)	0.4980(8)	0.029(2)	H(31)	-0.3418	-0.8900	-0.1602	0.0380
C(6)	0.1095(6)	-0.6042(5)	0.6272(8)	0.030(2)	H(32)	-0.3227	-0.9932	-0.1766	0.0380
C(7)	-0.0090(6)	-0.6656(5)	0.5831(8)	0.028(1)	H(33)	-0.4818	-1.0010	0.1968	0.0418
C(8)	-0.0200(6)	-0.7125(5)	0.4145(8)	0.027(1)	H(34)	-0.5002	-0.9544	0.0315	0.0418
C(9)	0.0288(6)	-0.6372(5)	0.2822(8)	0.024(1)	H(35)	-0.4874	-1.1462	0.0714	0.0507
C(10)	0.1543(6)	-0.5790(5)	0.3284(9)	0.027(1)	H(36)	-0.4942	-1.1002	-0.0978	0.0507
C(11)	0.0129(6)	-0.6886(5)	0.1168(8)	0.029(2)	H(37)	0.1332	-0.2357	0.4551	0.0418
C(12)	-0.1089(6)	-0.7487(5)	0.0672(8)	0.028(2)	H(38)	-0.2385	-0.7028	-0.0288	0.0405
C(13)	-0.1557(6)	-0.8246(5)	0.1971(8)	0.025(1)	H(39)	-0.7637	-1.1385	0.1253	0.0481
C(14)	-0.1416(6)	-0.7684(5)	0.3623(8)	0.024(1)	H(40)	-0.0806	-0.5689	0.6851	0.0329
C(15)	-0.2084(6)	-0.8447(5)	0.4767(9)	0.030(2)	H(41)	-0.2807	-0.3487	-0.2850	0.0418
C(16)	-0.3103(6)	-0.9031(5)	0.3680(9)	0.034(2)	H(42)	-0.1951	-0.2889	-0.4033	0.0418
C(17)	-0.2863(6)	-0.8744(5)	0.1890(8)	0.026(1)	H(43)	-0.1713	-0.4456	-0.3715	0.0329
C(18)	-0.0931(6)	-0.9036(5)	0.2012(8)	0.030(2)	H(44)	-0.0626	-0.3666	-0.3101	0.0329
C(19)	0.2323(6)	-0.6477(5)	0.3311(9)	0.036(2)	H(45)	-0.2240	-0.4772	-0.1123	0.0380
C(20)	-0.3347(6)	-0.9601(5)	0.0693(9)	0.030(1)	H(46)	-0.0279	-0.3388	0.0026	0.0342
C(21)	-0.3070(7)	-0.9352(6)	-0.1051(9)	0.037(2)	H(47)	-0.1224	-0.3979	0.1090	0.0342
C(22)	-0.4644(6)	-0.9972(5)	0.0819(9)	0.038(2)	H(48)	-0.2412	-0.3101	0.0183	0.0329
C(23)	-0.5162(7)	-1.1006(6)	0.0075(10)	0.042(2)	H(49)	-0.1670	-0.1667	0.1478	0.0380
C(24)	-0.6420(6)	-1.1360(5)	0.0042(9)	0.032(2)	H(50)	-0.1083	-0.2387	0.2318	0.0380
C(25)	-0.2041(6)	-0.3180(5)	-0.3015(9)	0.035(2)	H(51)	0.0153	-0.0805	0.1801	0.0342
C(26)	-0.1398(6)	-0.3951(5)	-0.2931(9)	0.030(2)	H(52)	-0.0483	-0.0513	-0.0710	0.0291
C(27)	-0.1478(6)	-0.4416(5)	-0.1303(9)	0.031(2)	H(53)	0.0060	-0.2177	-0.1825	0.0279
C(28)	-0.1054(6)	-0.3649(5)	0.0046(9)	0.032(2)	H(54)	-0.0709	-0.0941	-0.3923	0.0317
C(29)	-0.1637(6)	-0.2805(5)	-0.0038(9)	0.030(2)	H(55)	-0.0410	-0.1889	-0.4449	0.0317
C(30)	-0.1164(6)	-0.2048(5)	0.1312(8)	0.032(2)	H(56)	0.1043	-0.0443	-0.5030	0.0405
C(31)	-0.0005(6)	-0.1325(5)	0.1016(9)	0.030(1)	H(57)	0.1683	-0.0710	-0.0865	0.0253
C(32)	0.0020(6)	-0.0905(5)	-0.0692(9)	0.026(1)	H(58)	0.1259	0.0970	0.0331	0.0380
C(33)	-0.0387(6)	-0.1726(5)	-0.2001(8)	0.024(1)	H(59)	0.2006	0.0371	0.1157	0.0380
C(34)	-0.1619(6)	-0.2352(5)	-0.1739(9)	0.028(1)	H(60)	0.2777	0.1844	-0.0842	0.0380
C(35)	-0.0201(6)	-0.1325(5)	-0.3726(9)	0.032(2)	H(61)	0.3461	0.1131	-0.0250	0.0380
C(36)	0.1009(6)	-0.0708(5)	-0.3983(8)	0.029(2)	H(62)	0.3058	0.0231	-0.2474	0.0279
C(37)	0.1374(6)	0.0159(5)	-0.2740(8)	0.024(1)	H(63)	0.0984	0.1482	-0.2474	0.0443
C(38)	0.1209(6)	-0.0277(5)	-0.1022(8)	0.024(1)	H(64)	0.0650	0.1017	-0.4196	0.0443
C(39)	0.1767(6)	0.0598(5)	0.0125(9)	0.033(2)	H(65)	-0.0086	0.0602	-0.2755	0.0443
C(40)	0.2777(6)	0.1178(5)	-0.0814(9)	0.033(2)	H(66)	-0.2328	-0.1266	-0.0984	0.0494
C(41)	0.2656(6)	0.0715(5)	-0.2556(8)	0.025(1)	H(67)	-0.2374	-0.1380	-0.2858	0.0494
C(42)	0.0671(6)	0.0892(5)	-0.3086(9)	0.037(2)	H(68)	-0.3214	-0.2142	-0.1851	0.0494
C(43)	-0.2455(7)	-0.1709(6)	-0.186(1)	0.042(2)	H(69)	0.2883	0.2002	-0.3738	0.0355
C(44)	0.3198(6)	0.1475(5)	-0.3822(9)	0.031(1)	H(70)	0.2230	0.0927	-0.5847	0.0545
C(45)	0.3011(7)	0.1063(6)	-0.5559(9)	0.045(2)	H(71)	0.3212	0.0452	-0.5559	0.0545
C(46)	0.4458(6)	0.1865(5)	-0.3350(9)	0.034(2)	H(72)	0.3448	0.1512	-0.6218	0.0545
C(47)	0.5090(7)	0.2758(6)	-0.4251(9)	0.039(2)	H(73)	0.4547	0.2016	-0.2187	0.0380
C(48)	0.6323(6)	0.3097(5)	-0.3709(9)	0.032(1)	H(74)	0.4802	0.1328	-0.3495	0.0380
C(49)	-0.5913(8)	-0.3858(6)	-0.136(1)	0.052(2)	H(75)	0.4762	0.3256	-0.4072	0.0443
C(50)	-0.5906(8)	-0.4889(6)	-0.1791(10)	0.053(2)	H(76)	0.5047	0.2569	-0.5353	0.0443
C(51)	-0.5149(8)	-0.5303(7)	-0.077(1)	0.067(3)	H(77)	-0.1183	-0.5810	-0.1055	0.0380
C(52)	-0.5349(9)	-0.6092(7)	-0.006(1)	0.070(3)	H(78)	0.1989	-0.1421	-0.2774	0.0380
C(53)	-0.4622(10)	-0.6555(7)	0.099(1)	0.072(3)	H(79)	0.7711	0.3615	-0.4638	0.0380
C(54)	0.5955(8)	0.5619(6)	-0.614(1)	0.049(2)	H(80)	0.1018	-0.2051	0.2194	0.0380
C(55)	0.5933(7)	0.6601(7)	-0.6846(10)	0.054(2)	H(81)	-0.5642	-0.4878	-0.2837	0.0659
C(56)	0.5223(8)	0.7100(7)	-0.600(1)	0.068(3)	H(82)	-0.6647	-0.5310	-0.1758	0.0659
C(57)	0.5393(9)	0.7994(7)	-0.565(1)	0.070(3)	H(83)	-0.4417	-0.4932	-0.0524	0.0823
C(58)	0.4657(9)	0.8513(7)	-0.489(1)	0.069(3)	H(84)	-0.6141	-0.6513	-0.0185	0.0823
H(1)	0.2789	-0.4683	0.2498	0.0380	H(85)	-0.3895	-0.6248	0.0812	0.0887
H(2)	0.1937	-0.5266	0.0971	0.0380	H(86)	-0.4790	-0.6463	0.2113	0.0887
H(3)	0.1790	-0.3583	0.1283	0.0380	H(87)	-0.4833	-0.7240	0.0762	0.0887
H(4)	0.0714	-0.4280	0.1666	0.0380	H(88)	-0.6780	-0.2971	-0.1671	0.0823
H(5)	0.2419	-0.3408	0.4057	0.0380	H(89)	0.6670	0.6992	-0.6796	0.0659
H(6)	0.1231	-0.4111	0.6071	0.0304	H(90)	0.5636	0.6452	-0.7916	0.0659
H(7)	0.0302	-0.4643	0.4782	0.0304	H(91)	0.4518	0.6678	-0.5661	0.0861
H(8)	0.2350	-0.4876	0.5379	0.0317	H(92)	0.6096	0.8392	-0.5914	0.0874
H(9)	0.1563	-0.6482	0.6497	0.0317	H(93)	0.4516	0.8992	-0.5550	0.0887
H(10)	0.1090	-0.5694	0.7291	0.0317	H(94)	0.5019	0.8807	-0.3859	0.0887
H(11)	-0.0240	-0.7149	0.6647	0.0317	H(95)	0.3958	0.8044	-0.4622	0.0887
H(12)	0.0080	-0.7713	0.4023	0.0291	H(96)	0.6935	0.4691	-0.6010	0.0659

CA·77

atom	x	y	z	U	atom	x	y	z	U
O(1)	1.3989(4)	0.1014(4)	0.3356(4)	0.075(2)	H(7)	1.2187	0.0780	0.2886	0.0253
O(2)	1.0735(4)	0.0224(3)	0.2160(3)	0.061(1)	H(8)	1.1908	0.2701	0.2844	0.0253
O(3)	1.0572(3)	-0.0647(3)	0.6115(4)	0.048(1)	H(9)	1.0294	0.2316	0.2310	0.0253
O(4)	0.6867(5)	-0.3884(4)	0.5659(6)	0.092(2)	H(10)	1.1022	0.1843	0.1400	0.0253
O(5)	0.6138(8)	-0.3663(4)	0.7414(5)	0.131(3)	H(11)	0.9679	0.1005	0.2038	0.0253
O(7)	0.0475(5)	0.0190(4)	0.9875(5)	0.095(2)	H(12)	0.9521	0.1362	0.3906	0.0253
C(1)	1.2132(4)	0.2092(4)	0.5096(5)	0.046(1)	H(13)	1.1243	0.0607	0.4429	0.0253
C(2)	1.2930(5)	0.1459(5)	0.4815(5)	0.054(2)	H(14)	1.1016	0.0980	0.6329	0.0253
C(3)	1.3233(5)	0.1586(5)	0.3571(5)	0.054(2)	H(15)	1.0072	0.1419	0.6030	0.0253
C(4)	1.2407(5)	0.1402(4)	0.2777(5)	0.049(2)	H(16)	0.9763	0.0159	0.6914	0.0253
C(5)	1.1566(6)	0.1997(4)	0.3060(5)	0.050(1)	H(17)	0.9977	-0.0479	0.3936	0.0253
C(6)	1.0748(6)	0.1837(4)	0.2229(5)	0.054(2)	H(18)	0.8284	0.0247	0.3131	0.0253
C(7)	1.0233(5)	0.1008(4)	0.2499(6)	0.054(2)	H(19)	0.8887	-0.0500	0.2600	0.0253
C(8)	0.9955(5)	0.0917(4)	0.3761(6)	0.044(1)	H(20)	0.7556	-0.0755	0.4147	0.0253
C(9)	1.0786(5)	0.1067(4)	0.4571(5)	0.043(1)	H(21)	0.8226	-0.1485	0.3708	0.0253
C(10)	1.1259(5)	0.1955(4)	0.4356(5)	0.044(1)	H(22)	0.9111	-0.1564	0.5278	0.0253
C(11)	1.0507(5)	0.0947(4)	0.5853(5)	0.043(1)	H(23)	0.8710	0.1229	0.5600	0.0253
C(12)	0.9975(4)	0.0095(4)	0.6120(5)	0.043(1)	H(24)	0.7930	0.0674	0.5028	0.0253
C(13)	0.9114(5)	-0.0029(3)	0.5306(5)	0.040(1)	H(25)	0.8146	0.0556	0.6330	0.0253
C(14)	0.9511(5)	0.0040(3)	0.4065(5)	0.045(1)	H(26)	1.0932	0.3301	0.4380	0.0253
C(15)	0.8669(5)	-0.0257(4)	0.3338(6)	0.058(2)	H(27)	1.0078	0.2705	0.4128	0.0253
C(16)	0.8192(5)	-0.0951(4)	0.4081(6)	0.058(2)	H(28)	1.0478	0.2835	0.5522	0.0253
C(17)	0.8663(5)	-0.0954(4)	0.5268(6)	0.048(1)	H(29)	0.7523	-0.0764	0.6265	0.0253
C(18)	0.8422(5)	0.0684(4)	0.5589(6)	0.051(2)	H(30)	0.8022	-0.1267	0.8017	0.0253
C(19)	1.0621(5)	0.2746(4)	0.4608(6)	0.056(2)	H(31)	0.8940	-0.1606	0.7474	0.0253
C(20)	0.8010(5)	-0.1213(4)	0.6242(6)	0.055(2)	H(32)	0.8749	-0.0597	0.7556	0.0253
C(21)	0.8439(5)	-0.1147(4)	0.7436(7)	0.058(2)	H(33)	0.7366	-0.2118	0.5313	0.0253
C(22)	0.7627(8)	-0.2118(5)	0.6056(8)	0.095(3)	H(34)	0.8080	-0.2516	0.6171	0.0253
C(23)	0.6915(9)	-0.2455(6)	0.6660(10)	0.104(3)	H(35)	0.7096	-0.2365	0.7436	0.0253
C(24)	0.6700(9)	-0.3397(6)	0.6527(9)	0.117(3)	H(36)	0.6401	-0.2105	0.6471	0.0253
C(25)	-0.0489(8)	0.2081(6)	0.8880(10)	0.095(3)	H(37)	1.4237	0.0887	0.2808	0.0961
C(26)	-0.028(1)	0.1396(6)	0.9119(8)	0.178(5)	H(38)	1.0679	0.0131	0.1355	0.0729
C(27)	-0.0378(8)	0.0468(8)	0.9592(9)	0.102(3)	H(39)	1.0923	-0.0698	0.5677	0.0253
H(1)	1.1887	0.2147	0.6106	0.0253	H(40)	0.5883	-0.4398	0.7466	0.0253
H(2)	1.2357	0.2657	0.4976	0.0253	H(41)	-0.0673	0.2682	0.8680	0.1095
H(3)	1.3420	0.1565	0.5305	0.0253	H(42)	-0.0686	0.0083	0.9021	0.1267
H(4)	1.2702	0.0852	0.4944	0.0253	H(43)	-0.0813	0.0466	1.0252	0.1267
H(5)	1.3554	0.2215	0.3557	0.0253	H(44)	0.0732	-0.0153	0.9217	0.1390
H(6)	1.2567	0.1461	0.2003	0.0253					

CA·79

atom	x	y	z	U	atom	x	y	z	U
O(1)	0.8244(4)	0.6334(4)	0.4299(4)	0.046(2)	H(8)	1.0173	0.4399	0.4568	0.0329
O(2)	0.7798(3)	0.3167(3)	0.5441(4)	0.031(1)	H(9)	1.0041	0.3009	0.5210	0.0342
O(3)	0.6728(3)	0.3045(3)	0.1575(4)	0.029(1)	H(10)	0.9447	0.3573	0.6041	0.0342
O(4)	0.3602(4)	-0.0721(4)	0.1699(5)	0.044(2)	H(11)	0.8928	0.2271	0.5516	0.0380
O(5)	0.3886(4)	-0.1365(4)	-0.0009(4)	0.049(2)	H(12)	0.9055	0.2129	0.3666	0.0304
O(6)	0.6999(5)	-0.3021(4)	0.2743(5)	0.070(2)	H(13)	0.8168	0.3836	0.3111	0.0291
O(7)	0.5243(5)	-0.2142(5)	0.2821(6)	0.087(3)	H(14)	0.8277	0.3596	0.1325	0.0291
C(1)	0.9494(5)	0.4712(5)	0.2431(6)	0.029(2)	H(15)	0.8933	0.2694	0.1420	0.0291
C(2)	0.8797(5)	0.5430(5)	0.2778(6)	0.028(2)	H(16)	0.7735	0.2486	0.0685	0.0279
C(3)	0.8927(6)	0.5687(5)	0.4019(6)	0.033(2)	H(17)	0.7045	0.2369	0.3574	0.0279
C(4)	0.8845(5)	0.4873(5)	0.4783(6)	0.031(2)	H(18)	0.7989	0.0861	0.4339	0.0380
C(5)	0.9541(5)	0.4159(5)	0.4459(5)	0.030(2)	H(19)	0.7199	0.1334	0.4997	0.0380
C(6)	0.9488(5)	0.3358(5)	0.5253(6)	0.033(2)	H(20)	0.7038	0.0154	0.3333	0.0342
C(7)	0.8643(6)	0.2769(5)	0.5034(6)	0.031(2)	H(21)	0.6157	0.0465	0.3922	0.0342
C(8)	0.8528(5)	0.2510(5)	0.3773(6)	0.028(2)	H(22)	0.6126	0.1633	0.2465	0.0279
C(9)	0.8574(5)	0.3332(4)	0.2995(6)	0.026(2)	H(23)	0.8403	0.0606	0.2488	0.0317
C(10)	0.9478(5)	0.3875(5)	0.3167(5)	0.027(2)	H(24)	0.8170	0.0771	0.1206	0.0317
C(11)	0.8429(5)	0.3064(5)	0.1720(6)	0.025(2)	H(25)	0.8885	0.1367	0.1828	0.0317
C(12)	0.7564(5)	0.2513(5)	0.1477(5)	0.022(2)	H(26)	1.0383	0.2780	0.3288	0.0431
C(13)	0.7530(5)	0.1697(4)	0.2279(6)	0.024(2)	H(27)	1.0391	0.3172	0.2059	0.0431
C(14)	0.7630(5)	0.2022(5)	0.3535(6)	0.027(2)	H(28)	1.0920	0.3646	0.3040	0.0431
C(15)	0.7410(5)	0.1193(5)	0.4245(6)	0.033(2)	H(29)	0.6728	0.0095	0.1317	0.0291
C(16)	0.6700(5)	0.0674(5)	0.3516(6)	0.033(2)	H(30)	0.5911	0.0741	-0.0326	0.0557
C(17)	0.6594(5)	0.1188(5)	0.2362(6)	0.026(2)	H(31)	0.6900	0.1099	-0.0098	0.0557
C(18)	0.8307(5)	0.1068(5)	0.1909(6)	0.029(2)	H(32)	0.6044	0.1636	0.0301	0.0557
C(19)	1.0345(5)	0.3339(5)	0.2867(7)	0.038(2)	H(33)	0.4850	0.0666	0.1532	0.0469
C(20)	0.6300(5)	0.0592(5)	0.1379(6)	0.029(2)	H(34)	0.5264	-0.0020	0.2376	0.0469
C(21)	0.6308(6)	0.1059(6)	0.0220(7)	0.046(2)	H(35)	0.5199	-0.0275	0.0013	0.0494
C(22)	0.5335(6)	0.0191(5)	0.1595(7)	0.037(2)	H(36)	0.5555	-0.0969	0.0885	0.0494
C(23)	0.5053(6)	-0.0540(6)	0.0792(7)	0.044(2)	H(37)	0.8308	0.6401	0.5152	0.0557
C(24)	0.4125(6)	-0.0876(6)	0.0906(7)	0.039(2)	H(38)	0.7962	0.3499	0.6108	0.0317
C(25)	0.6823(7)	-0.2169(6)	0.3083(8)	0.052(2)	H(39)	0.6686	0.3462	0.2292	0.0317
C(26)	0.5899(7)	-0.2030(8)	0.3652(8)	0.069(3)	H(40)	0.3208	-0.1667	-0.0028	0.0595
H(1)	0.9441	0.4558	0.1627	0.0380	H(41)	0.7377	-0.1969	0.3634	0.0633
H(2)	1.0139	0.4964	0.2489	0.0380	H(42)	0.6922	-0.1730	0.2469	0.0633
H(3)	0.8201	0.5191	0.2653	0.0304	H(43)	0.5847	-0.1465	0.4082	0.1051
H(4)	0.8878	0.5934	0.2284	0.0304	H(44)	0.5839	-0.2475	0.4302	0.1051
H(5)	0.9581	0.5795	0.4045	0.0380	H(45)	0.7630	-0.3362	0.3090	0.0861
H(6)	0.8846	0.5153	0.5540	0.0380	H(46)	0.4600	-0.1933	0.3128	0.1115
H(7)	0.8261	0.4650	0.4535	0.0380					

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aatom	x	y	z	U	atom	x	y	z	U
O(1)	-0.1848(1)	0.0338(1)	-0.8239(4)	0.0480(6)	H(9)	-0.5336	0.0504	-1.0296	0.0362
O(2)	-0.4564(2)	-0.1030(1)	-0.9275(2)	0.0388(6)	H(10)	-0.4572	0.0073	-1.0959	0.0362
O(3)	-0.4720(1)	-0.0872(1)	-0.4147(2)	0.0326(5)	H(11)	-0.5665	-0.0609	-0.9784	0.0367
O(4)	-0.7975(2)	-0.3706(1)	-0.2546(4)	0.0563(7)	H(12)	-0.5981	0.0030	-0.7789	0.0300
O(5)	-0.6592(1)	-0.3989(1)	-0.2157(2)	0.0361(5)	H(13)	-0.4288	-0.0144	-0.6713	0.0290
O(6)	-0.4672(2)	-0.1828(1)	-0.1832(2)	0.0508(7)	H(14)	-0.4613	0.0447	-0.4588	0.0330
C(1)	-0.3821(2)	0.1256(1)	-0.6740(3)	0.0317(6)	H(15)	-0.5542	0.0611	-0.5152	0.0330
C(2)	-0.2946(2)	0.0878(2)	-0.6705(4)	0.0347(7)	H(16)	-0.5646	-0.0268	-0.3398	0.0316
C(3)	-0.2631(2)	0.0749(2)	-0.8287(4)	0.0333(7)	H(17)	-0.5274	-0.1204	-0.6657	0.0334
C(4)	-0.3300(2)	0.0332(2)	-0.9155(3)	0.0315(7)	H(18)	-0.6870	-0.1128	-0.8089	0.0433
C(5)	-0.4202(2)	0.0671(1)	-0.9162(3)	0.0295(6)	H(19)	-0.6183	-0.1724	-0.8242	0.0433
C(6)	-0.4839(2)	0.0213(2)	-1.0058(3)	0.0345(7)	H(20)	-0.7486	-0.1749	-0.6262	0.0466
C(7)	-0.5172(2)	-0.0451(2)	-0.9257(3)	0.0314(7)	H(21)	-0.6739	-0.2299	-0.6296	0.0466
C(8)	-0.5488(2)	-0.0274(1)	-0.7687(3)	0.0266(6)	H(22)	-0.6013	-0.1762	-0.4479	0.0329
C(9)	-0.4801(2)	0.0144(1)	-0.6775(3)	0.0237(6)	H(23)	-0.6762	0.0201	-0.5829	0.0422
C(10)	-0.4543(2)	0.0850(1)	-0.7581(3)	0.0270(6)	H(24)	-0.7395	-0.0437	-0.5919	0.0422
C(11)	-0.5088(2)	0.0263(1)	-0.5146(3)	0.0273(6)	H(25)	-0.7141	-0.0124	-0.4381	0.0422
C(12)	-0.5435(2)	-0.0400(1)	-0.4353(3)	0.0276(6)	H(26)	-0.5484	0.1497	-0.6763	0.0434
C(13)	-0.6171(2)	-0.0742(1)	-0.5271(3)	0.0247(6)	H(27)	-0.5127	0.1756	-0.8283	0.0434
C(14)	-0.5784(2)	-0.0921(1)	-0.6826(3)	0.0281(6)	H(28)	-0.5768	0.1123	-0.8223	0.0434
C(15)	-0.6463(2)	-0.1400(2)	-0.7541(4)	0.0391(8)	H(29)	-0.7630	-0.1214	-0.3773	0.0347
C(16)	-0.6869(2)	-0.1811(2)	-0.6230(4)	0.0381(8)	H(30)	-0.6349	-0.1509	-0.1697	0.0424
C(17)	-0.6502(2)	-0.1489(1)	-0.4766(3)	0.0255(6)	H(31)	-0.6635	-0.0750	-0.2151	0.0424
C(18)	-0.6938(2)	-0.0224(2)	-0.5367(4)	0.0354(7)	H(32)	-0.7270	-0.1241	-0.1295	0.0424
C(19)	-0.5310(2)	0.1358(2)	-0.7721(4)	0.0378(7)	H(33)	-0.8000	-0.2261	-0.2572	0.0377
C(20)	-0.7176(2)	-0.1521(1)	-0.3500(3)	0.0297(6)	H(34)	-0.7767	-0.2439	-0.4211	0.0377
C(21)	-0.6831(2)	-0.1230(2)	-0.2019(3)	0.0382(8)	H(35)	-0.6420	-0.2838	-0.3477	0.0462
C(22)	-0.7543(2)	-0.2276(1)	-0.3272(3)	0.0300(6)	H(36)	-0.6622	-0.2634	-0.1839	0.0462
C(23)	-0.6874(2)	-0.2810(2)	-0.2758(4)	0.0408(8)	H(37)	-0.1393	0.0553	-0.8377	0.0606
C(24)	-0.7224(2)	-0.3542(2)	-0.2473(3)	0.0323(6)	H(38)	-0.4182	-0.0923	-0.8683	0.0606
C(25)	-0.4397(3)	-0.2850(3)	-0.3211(7)	0.077(1)	H(39)	-0.4774	-0.1176	-0.3387	0.0606
C(26)	-0.4255(5)	-0.2451(3)	-0.1854(8)	0.138(3)	H(40)	-0.6822	-0.4433	-0.2107	0.0606
C(27)	-0.3597(4)	-0.2622(3)	-0.0825(6)	0.074(1)	H(41)	-0.4997	-0.2885	-0.3548	0.0809
H(1)	-0.4013	0.1341	-0.5762	0.0377	H(42)	-0.4082	-0.2603	-0.3943	0.0809
H(2)	-0.3747	0.1702	-0.7246	0.0377	H(43)	-0.4186	-0.3341	-0.3198	0.0809
H(3)	-0.2541	0.1171	-0.6182	0.0401	H(44)	-0.4775	-0.2771	-0.1162	0.1025
H(4)	-0.3008	0.0442	-0.6190	0.0401	H(45)	-0.3489	-0.3122	-0.0756	0.0782
H(5)	-0.2539	0.1195	-0.8794	0.0415	H(46)	-0.3122	-0.2404	-0.1318	0.0782
H(6)	-0.3102	0.0295	-1.0137	0.0326	H(47)	-0.3689	-0.2428	0.0109	0.0782
H(7)	-0.3333	-0.0115	-0.8692	0.0326	H(48)	-0.4734	-0.1624	-0.0964	0.0606
H(8)	-0.4148	0.1111	-0.9659	0.0328					

CA·82

atom	x	y	z	U	atom	x	y	z	U
O(1)	-0.1679(3)	0.1392(2)	-0.5816(2)	0.0846(10)	H(7)	-0.1085	0.0082	-0.4528	0.0596
O(2)	-0.2293(2)	-0.1774(2)	-0.4676(2)	0.0509(7)	H(8)	0.0075	-0.0655	-0.5338	0.0380
O(3)	-0.3152(2)	-0.1930(2)	-0.8570(2)	0.0478(6)	H(9)	-0.0642	-0.1633	-0.3977	0.0380
O(4)	-0.6267(2)	-0.5746(3)	-0.8208(3)	0.087(1)	H(10)	-0.0144	-0.2038	-0.4805	0.0380
O(5)	-0.6085(2)	-0.6295(3)	-0.9955(3)	0.110(1)	H(11)	-0.1230	-0.2726	-0.4619	0.0380
O(6)	-0.0737(6)	-0.2555(5)	-1.0796(5)	0.224(3)	H(12)	-0.1072	-0.2869	-0.6417	0.0499
O(7)	-0.2304(3)	-0.2083(3)	-1.2439(3)	0.120(1)	H(13)	-0.1977	-0.1286	-0.6910	0.0380
C(1)	-0.0457(3)	-0.0304(2)	-0.7533(3)	0.0486(9)	H(14)	-0.1446	-0.1450	-0.8817	0.0380
C(2)	-0.1124(3)	0.0436(2)	-0.7263(3)	0.052(1)	H(15)	-0.1000	-0.2284	-0.8454	0.0380
C(3)	-0.1038(3)	0.0691(3)	-0.6042(3)	0.059(1)	H(16)	-0.2290	-0.2560	-0.9352	0.0380
C(4)	-0.1175(3)	-0.0100(3)	-0.5284(3)	0.0499(10)	H(17)	-0.2893	-0.2508	-0.6403	0.0380
C(5)	-0.0521(2)	-0.0855(2)	-0.5553(3)	0.0466(9)	H(18)	-0.2793	-0.3552	-0.5077	0.0380
C(6)	-0.0648(2)	-0.1630(3)	-0.4753(3)	0.0506(10)	H(19)	-0.2177	-0.4118	-0.5624	0.0380
C(7)	-0.1476(2)	-0.2214(2)	-0.5013(3)	0.0452(9)	H(20)	-0.3973	-0.4208	-0.6229	0.0649
C(8)	-0.1549(2)	-0.2468(2)	-0.6257(3)	0.0418(8)	H(21)	-0.3225	-0.4845	-0.6656	0.0649
C(9)	-0.1434(2)	-0.1662(2)	-0.7036(3)	0.0372(7)	H(22)	-0.3823	-0.3241	-0.7734	0.0380
C(10)	-0.0541(2)	-0.1136(2)	-0.6812(3)	0.0420(8)	H(23)	-0.1774	-0.4154	-0.8790	0.0599
C(11)	-0.1533(2)	-0.1944(2)	-0.8277(3)	0.0418(8)	H(24)	-0.1783	-0.4460	-0.7544	0.0599
C(12)	-0.2374(2)	-0.2483(2)	-0.8540(2)	0.0398(8)	H(25)	-0.1153	-0.3692	-0.7918	0.0599
C(13)	-0.2474(2)	-0.3282(2)	-0.7773(3)	0.0376(7)	H(26)	0.0323	-0.1850	-0.7834	0.0708
C(14)	-0.2419(2)	-0.2937(2)	-0.6537(2)	0.0388(8)	H(27)	0.0256	-0.2256	-0.6638	0.0708
C(15)	-0.2708(3)	-0.3760(3)	-0.5834(3)	0.053(1)	H(28)	0.0824	-0.1404	-0.6839	0.0708
C(16)	-0.3393(3)	-0.4241(3)	-0.6564(3)	0.054(1)	H(29)	-0.3255	-0.4875	-0.8690	0.0611
C(17)	-0.3403(2)	-0.3760(2)	-0.7734(3)	0.0412(8)	H(30)	-0.3023	-0.3782	-0.9996	0.0861
C(18)	-0.1726(3)	-0.3962(2)	-0.8031(3)	0.050(1)	H(31)	-0.4002	-0.3444	-0.9841	0.0861
C(19)	0.0297(2)	-0.1716(3)	-0.7054(3)	0.059(1)	H(32)	-0.3826	-0.4365	-1.0389	0.0861
C(20)	-0.3661(3)	-0.4387(3)	-0.8693(3)	0.0510(9)	H(33)	-0.5036	-0.4276	-0.8575	0.0846
C(21)	-0.3627(4)	-0.3954(3)	-0.9836(3)	0.072(1)	H(34)	-0.4650	-0.4965	-0.7732	0.0846
C(22)	-0.4621(3)	-0.4751(3)	-0.8483(4)	0.070(1)	H(35)	-0.4852	-0.5263	-0.9991	0.0911
C(23)	-0.4889(3)	-0.5480(3)	-0.9236(4)	0.075(1)	H(36)	-0.4472	-0.5952	-0.9145	0.0911
C(24)	-0.5825(3)	-0.5844(3)	-0.9062(4)	0.073(1)	H(37)	-0.1713	0.1472	-0.5012	0.0380
C(25)	-0.0566(8)	-0.3358(7)	-1.1130(7)	0.185(4)	H(38)	-0.2291	-0.1646	-0.3891	0.0380
C(26)	-0.0937(7)	-0.2875(6)	-1.1849(7)	0.167(3)	H(39)	-0.3300	-0.1570	-0.7857	0.0843
C(27)	-0.1925(6)	-0.2871(5)	-1.2072(5)	0.138(3)	H(40)	-0.6758	-0.6339	-0.9785	0.1677
H(1)	-0.0485	-0.0401	-0.8326	0.0380	H(41)	-0.0873	-0.3844	-1.0839	0.2163
H(2)	0.0159	-0.0114	-0.7436	0.0380	H(42)	0.0060	-0.3521	-1.1256	0.2163
H(3)	-0.1731	0.0254	-0.7392	0.0380	H(43)	-0.0556	-0.2652	-1.2446	0.2023
H(4)	-0.0929	0.0902	-0.7749	0.0380	H(44)	-0.2211	-0.3029	-1.1388	0.1624
H(5)	-0.0435	0.0971	-0.5936	0.0380	H(45)	-0.2038	-0.3309	-1.2625	0.1624
H(6)	-0.1772	-0.0311	-0.5375	0.0596	H(46)	-0.2766	-0.1836	-1.1895	0.0843

CA·90

atom	x	y	z	U	atom	x	y	z	U
O(1)	-0.4050(3)	-0.276(1)	-0.3915(2)	0.0550(8)	H(10)	-0.3862	-0.6237	-0.6694	0.0660
O(2)	-0.5822(3)	-0.501(1)	-0.7106(2)	0.0530(8)	H(11)	-0.5190	-0.5718	-0.8173	0.0592
O(3)	-0.6787(3)	0.031(1)	-0.7773(2)	0.0601(9)	H(12)	-0.4696	-0.3140	-0.8579	0.0533
O(4)	-1.1653(4)	-0.180(1)	-1.1940(4)	0.099(2)	H(13)	-0.5162	-0.1841	-0.6908	0.0532
O(5)	-1.2071(3)	0.073(1)	-1.2626(3)	0.076(1)	H(14)	-0.4751	0.0745	-0.7344	0.0594
O(6)	-0.9107	0.0404	-0.7976	0.2586	H(15)	-0.4439	0.0046	-0.8270	0.0594
C(1)	-0.3106(4)	-0.079(1)	-0.5949(3)	0.051(1)	H(16)	-0.6142	0.1315	-0.8772	0.0623
C(2)	-0.3643(4)	-0.094(1)	-0.5121(3)	0.052(1)	H(17)	-0.6751	-0.2743	-0.8220	0.0550
C(3)	-0.3461(4)	-0.264(1)	-0.4650(3)	0.052(1)	H(18)	-0.6397	-0.4346	-0.9864	0.0679
C(4)	-0.3874(4)	-0.396(1)	-0.5435(3)	0.050(1)	H(19)	-0.7097	-0.5010	-0.9168	0.0679
C(5)	-0.3375(4)	-0.385(1)	-0.6307(3)	0.050(1)	H(20)	-0.7935	-0.3194	-1.0741	0.0693
C(6)	-0.3852(4)	-0.523(1)	-0.7047(3)	0.055(1)	H(21)	-0.8564	-0.3569	-0.9938	0.0693
C(7)	-0.5015(4)	-0.491(1)	-0.7664(3)	0.0493(10)	H(22)	-0.8160	-0.1124	-0.9233	0.0583
C(8)	-0.5150(4)	-0.318(1)	-0.8124(3)	0.0444(9)	H(23)	-0.5092	-0.1100	-0.9709	0.0602
C(9)	-0.4715(3)	-0.179(1)	-0.7368(3)	0.0442(9)	H(24)	-0.6114	-0.1812	-1.0486	0.0602
C(10)	-0.3498(4)	-0.209(1)	-0.6778(3)	0.049(1)	H(25)	-0.6000	0.0108	-1.0304	0.0602
C(11)	-0.4928(4)	-0.008(1)	-0.7849(3)	0.049(1)	H(26)	-0.1962	-0.2208	-0.7096	0.0791
C(12)	-0.6116(4)	0.025(1)	-0.8455(3)	0.052(1)	H(27)	-0.2933	-0.2732	-0.7983	0.0791
C(13)	-0.6511(3)	-0.112(1)	-0.9229(3)	0.0466(10)	H(28)	-0.2730	-0.0850	-0.7715	0.0791
C(14)	-0.6313(3)	-0.278(1)	-0.8687(3)	0.0458(10)	H(29)	-0.7996	-0.0247	-1.1095	0.0643
C(15)	-0.6881(4)	-0.404(1)	-0.9463(3)	0.057(1)	H(30)	-0.7383	0.2011	-1.0108	0.0777
C(16)	-0.7900(4)	-0.312(1)	-1.0060(3)	0.058(1)	H(31)	-0.8515	0.2432	-1.0848	0.0777
C(17)	-0.7772(4)	-0.126(1)	-0.9733(3)	0.0485(10)	H(32)	-0.8485	0.2001	-0.9766	0.0777
C(18)	-0.5871(4)	-0.097(1)	-1.0003(3)	0.050(1)	H(33)	-0.9588	-0.1696	-1.1031	0.0760
C(19)	-0.2706(4)	-0.196(1)	-0.7458(4)	0.066(1)	H(34)	-0.9887	-0.0287	-1.0379	0.0760
C(20)	-0.8325(4)	-0.006(1)	-1.0562(3)	0.053(1)	H(35)	-1.0249	0.1504	-1.1640	0.1040
C(21)	-0.8162(5)	0.176(1)	-1.0296(4)	0.065(1)	H(36)	-0.9819	0.0230	-1.2295	0.1040
C(22)	-0.9548(4)	-0.053(1)	-1.0900(4)	0.063(1)	H(37)	-0.3762	-0.3580	-0.3456	0.0944
C(23)	-1.0200(5)	0.034(2)	-1.1789(4)	0.087(2)	H(38)	-0.5737	-0.5867	-0.6911	0.0944
C(24)	-1.1392(5)	-0.037(2)	-1.2157(4)	0.076(1)	H(39)	-0.7210	0.0866	-0.7954	0.0944
C(25)	-0.9825	0.0471	-0.7218	0.3658	H(40)	-1.2794	0.0257	-1.2854	0.0918
C(26)	-0.8931	-0.0708	-0.6477	0.2180	H(41)	-0.9246	-0.1072	-0.3837	0.4000
C(27)	-0.9662	-0.0307	-0.5715	0.2991	H(42)	-1.0225	-0.2224	-0.4373	0.4000
C(28)	-0.8988	-0.1931	-0.5256	0.2130	H(43)	-0.9082	-0.3003	-0.3831	0.4000
C(29)	-0.9435	-0.2073	-0.4209	0.3333	H(44)	-0.9493	0.0703	-0.5349	0.3590
H(1)	-0.3259	0.0302	-0.6225	0.0607	H(45)	-1.0452	-0.0419	-0.5950	0.3590
H(2)	-0.2319	-0.0917	-0.5694	0.0607	H(46)	-0.8183	-0.0294	-0.6298	0.2616
H(3)	-0.3334	-0.0106	-0.4641	0.0625	H(47)	-0.8926	-0.1851	-0.6668	0.2616
H(4)	-0.4427	-0.0745	-0.5360	0.0625	H(48)	-0.8199	-0.1770	-0.5122	0.2555
H(5)	-0.2683	-0.2791	-0.4365	0.0620	H(49)	-0.9195	-0.2887	-0.5666	0.2555
H(6)	-0.3700	-0.5023	-0.5142	0.0601	H(50)	-1.0548	-0.0018	-0.7443	0.4389
H(7)	-0.4665	-0.3839	-0.5666	0.0601	H(51)	-0.9896	0.1563	-0.6969	0.4389
H(8)	-0.2594	-0.4051	-0.6071	0.0597	H(52)	-0.8401	0.0918	-0.7705	0.3104
H(9)	-0.3370	-0.5348	-0.7473	0.0660					

CA·106

atom	x	y	z	U	atom	x	y	z	U
O(1)	0.5893(2)	-0.074(1)	0.6262(2)	0.0556(8)	H(10)	0.5887	-0.4211	0.3480	0.0646
O(2)	0.4010(2)	-0.299(1)	0.2750(2)	0.0494(7)	H(11)	0.4659	-0.3632	0.1792	0.0572
O(3)	0.3405(2)	0.205(1)	0.2134(2)	0.0584(9)	H(12)	0.5271	-0.1340	0.1492	0.0526
O(4)	-0.1488(4)	0.042(1)	-0.2242(6)	0.200(3)	H(13)	0.4875	-0.0068	0.3113	0.0520
O(5)	-0.1855(2)	0.262(1)	-0.1812(3)	0.088(1)	H(14)	0.5408	0.2300	0.2794	0.0626
O(6)	0.8849(4)	-0.253(1)	0.8417(3)	0.105(2)	H(15)	0.5647	0.1648	0.1881	0.0626
C(1)	0.6964(3)	0.072(1)	0.4340(3)	0.057(1)	H(16)	0.4049	0.2953	0.1224	0.0624
C(2)	0.6403(3)	0.076(1)	0.5087(3)	0.052(1)	H(17)	0.3260	-0.0783	0.1539	0.0499
C(3)	0.6452(3)	-0.081(1)	0.5574(3)	0.051(1)	H(18)	0.3543	-0.2197	-0.0097	0.0631
C(4)	0.5968(3)	-0.203(1)	0.4759(3)	0.048(1)	H(19)	0.2815	-0.2764	0.0460	0.0631
C(5)	0.6471(3)	-0.206(1)	0.3950(3)	0.051(1)	H(20)	0.2131	-0.0918	-0.1155	0.0658
C(6)	0.5959(3)	-0.332(1)	0.3141(3)	0.053(1)	H(21)	0.1480	-0.1249	-0.0477	0.0658
C(7)	0.4835(3)	-0.292(1)	0.2335(3)	0.0480(10)	H(22)	0.1983	0.0930	0.0386	0.0570
C(8)	0.4824(3)	-0.131(1)	0.1876(3)	0.0431(10)	H(23)	0.5011	0.0710	0.0371	0.0731
C(9)	0.5302(3)	-0.008(1)	0.2713(3)	0.0432(9)	H(24)	0.4015	0.0149	-0.0574	0.0731
C(10)	0.6485(3)	-0.048(1)	0.3449(3)	0.051(1)	H(25)	0.4184	0.1898	-0.0329	0.0731
C(11)	0.5188(3)	0.155(1)	0.2250(3)	0.052(1)	H(26)	0.7964	-0.0798	0.3363	0.0835
C(12)	0.4040(3)	0.194(1)	0.1517(3)	0.051(1)	H(27)	0.7007	-0.1238	0.2348	0.0835
C(13)	0.3596(3)	0.075(1)	0.0640(3)	0.0453(9)	H(28)	0.7293	0.0485	0.2620	0.0835
C(14)	0.3688(3)	-0.085(1)	0.1139(3)	0.0415(9)	H(29)	0.2304	0.1876	-0.1347	0.0717
C(15)	0.3085(3)	-0.190(1)	0.0238(3)	0.051(1)	H(30)	0.2872	0.3780	-0.0066	0.0942
C(16)	0.2153(3)	-0.091(1)	-0.0474(3)	0.055(1)	H(31)	0.1953	0.4367	-0.1064	0.0942
C(17)	0.2363(3)	0.078(1)	-0.0056(3)	0.0469(9)	H(32)	0.1691	0.3886	-0.0127	0.0942
C(18)	0.4268(3)	0.087(1)	-0.0039(3)	0.060(1)	H(33)	0.0511	0.2434	-0.2139	0.0849
C(19)	0.7260(3)	-0.052(1)	0.2894(4)	0.069(2)	H(34)	0.0651	0.0700	-0.1841	0.0849
C(20)	0.1917(4)	0.199(1)	-0.0915(3)	0.060(1)	H(35)	0.0178	0.1235	-0.0457	0.0965
C(21)	0.2125(5)	0.365(1)	-0.0504(4)	0.076(2)	H(36)	-0.0006	0.2949	-0.0799	0.0965
C(22)	0.0719(4)	0.171(1)	-0.1587(3)	0.070(1)	H(37)	0.6006	-0.1600	0.6868	0.0956
C(23)	-0.0041(4)	0.189(1)	-0.1035(4)	0.079(2)	H(38)	0.3995	-0.3981	0.3091	0.0956
C(24)	-0.1192(4)	0.154(1)	-0.1728(5)	0.085(2)	H(39)	0.2578	0.2091	0.1662	0.0956
C(25)	0.9366(6)	-0.348(1)	0.7950(7)	0.132(3)	H(40)	-0.2598	0.2265	-0.2114	0.0956
C(26)	0.8785(7)	-0.389(2)	0.6888(6)	0.132(3)	H(41)	1.0014	-0.2962	0.8016	0.1597
C(27)	0.9258(8)	-0.484(2)	0.6331(7)	0.151(3)	H(42)	0.9532	-0.4398	0.8340	0.1597
C(28)	0.8803(9)	-0.514(2)	0.5289(8)	0.171(5)	H(43)	0.8141	-0.4378	0.6853	0.1589
C(29)	0.9315(8)	-0.610(2)	0.4763(8)	0.160(4)	H(44)	0.8596	-0.2915	0.6528	0.1589
C(30)	0.883(1)	-0.584(2)	0.3692(9)	0.234(7)	H(45)	0.9946	-0.4342	0.6469	0.1855
H(1)	0.6912	0.1728	0.4039	0.0689	H(46)	0.9381	-0.5784	0.6688	0.1855
H(2)	0.7705	0.0484	0.4714	0.0689	H(47)	0.8115	-0.5606	0.5185	0.2115
H(3)	0.6756	0.1524	0.5605	0.0627	H(48)	0.8663	-0.4149	0.4965	0.2115
H(4)	0.5666	0.1081	0.4723	0.0627	H(49)	1.0060	-0.5840	0.5000	0.1942
H(5)	0.7186	-0.1053	0.5961	0.0623	H(50)	0.9225	-0.7143	0.4884	0.1942
H(6)	0.6074	-0.2989	0.5084	0.0577	H(51)	0.8915	-0.4755	0.3555	0.2776
H(7)	0.5213	-0.1812	0.4419	0.0577	H(52)	0.9168	-0.6440	0.3349	0.2776
H(8)	0.7210	-0.2330	0.4302	0.0613	H(53)	0.8077	-0.6053	0.3439	0.2776
H(9)	0.6423	-0.3488	0.2788	0.0646	H(54)	0.8547	-0.1904	0.7721	0.1896

CA·113

atom	x	y	z	U	atom	x	y	z	U
O(1)	0.4015(3)	0.467(1)	0.3922(2)	0.0507(8)	H(9)	0.3506	0.2148	0.7613	0.0574
O(2)	0.5870(2)	0.240(1)	0.7098(2)	0.0462(7)	H(10)	0.3936	0.1246	0.6795	0.0574
O(3)	0.6910(2)	0.771(1)	0.7786(2)	0.0470(7)	H(11)	0.5292	0.1725	0.8227	0.0529
O(4)	1.1652(3)	0.550(1)	1.2013(3)	0.0668(9)	H(12)	0.4835	0.4280	0.8689	0.0492
O(5)	1.1993(3)	0.800(1)	1.2676(2)	0.0563(8)	H(13)	0.5244	0.5554	0.6929	0.0431
O(6)	1.0302(4)	0.503(2)	0.6127(4)	0.112(2)	H(14)	0.4885	0.8171	0.7443	0.0512
C(1)	0.3210(3)	0.664(1)	0.6089(3)	0.0458(10)	H(15)	0.4610	0.7449	0.8390	0.0512
C(2)	0.3700(3)	0.650(1)	0.5194(3)	0.0438(9)	H(16)	0.6282	0.8650	0.8830	0.0478
C(3)	0.3489(3)	0.478(1)	0.4737(3)	0.0443(9)	H(17)	0.6824	0.4594	0.8209	0.0506
C(4)	0.3932(3)	0.351(1)	0.5501(3)	0.0421(9)	H(18)	0.6504	0.2955	0.9878	0.0626
C(5)	0.3483(3)	0.363(1)	0.6420(3)	0.0418(9)	H(19)	0.7190	0.2342	0.9154	0.0626
C(6)	0.3957(3)	0.225(1)	0.7152(3)	0.048(1)	H(20)	0.7993	0.4126	1.0752	0.0675
C(7)	0.5122(3)	0.255(1)	0.7719(3)	0.0429(9)	H(21)	0.8619	0.3763	0.9937	0.0675
C(8)	0.5257(3)	0.425(1)	0.8199(3)	0.0397(8)	H(22)	0.8225	0.6205	0.9225	0.0513
C(9)	0.4832(3)	0.562(1)	0.7431(3)	0.0366(8)	H(23)	0.6112	0.7458	1.0391	0.0547
C(10)	0.3631(3)	0.536(1)	0.6913(3)	0.0403(8)	H(24)	0.5216	0.6298	0.9804	0.0547
C(11)	0.5065(3)	0.734(1)	0.7930(3)	0.0415(9)	H(25)	0.6201	0.5562	1.0557	0.0547
C(12)	0.6245(3)	0.762(1)	0.8498(3)	0.0400(9)	H(26)	0.2950	0.6609	0.7910	0.0668
C(13)	0.6611(3)	0.625(1)	0.9269(2)	0.0386(8)	H(27)	0.2161	0.5306	0.7319	0.0668
C(14)	0.6426(3)	0.457(1)	0.8711(3)	0.0399(9)	H(28)	0.3112	0.4748	0.8172	0.0668
C(15)	0.6963(4)	0.331(1)	0.9470(3)	0.051(1)	H(29)	0.8050	0.7056	1.1114	0.0512
C(16)	0.7951(4)	0.422(1)	1.0077(3)	0.054(1)	H(30)	0.8612	0.9723	1.0824	0.0704
C(17)	0.7848(3)	0.609(1)	0.9738(2)	0.0412(9)	H(31)	0.8640	0.9238	0.9752	0.0704
C(18)	0.5979(3)	0.640(1)	1.0072(2)	0.046(1)	H(32)	0.7537	0.9334	1.0064	0.0704
C(19)	0.2885(3)	0.552(1)	0.7642(3)	0.054(1)	H(33)	0.9623	0.5547	1.0985	0.0635
C(20)	0.8398(3)	0.721(1)	1.0578(3)	0.0434(9)	H(34)	0.9953	0.7042	1.0418	0.0635
C(21)	0.8281(4)	0.904(1)	1.0288(3)	0.056(1)	H(35)	1.0203	0.8609	1.1789	0.0773
C(22)	0.9586(3)	0.671(1)	1.0918(3)	0.052(1)	H(36)	0.9823	0.7161	1.2361	0.0773
C(23)	1.0189(4)	0.745(1)	1.1869(3)	0.066(1)	H(37)	0.3596	0.3758	0.3342	0.0840
C(24)	1.1341(4)	0.688(1)	1.2188(3)	0.0511(10)	H(38)	0.5729	0.1492	0.6699	0.0840
C(25)	0.9925(6)	0.720(1)	0.7590(6)	0.097(2)	H(39)	0.7455	0.8554	0.7769	0.0840
C(26)	0.9067(5)	0.682(1)	0.6696(6)	0.088(2)	H(40)	1.2739	0.7524	1.2735	0.0917
C(27)	0.9434(5)	0.573(2)	0.5953(5)	0.087(2)	H(41)	1.0206	0.6155	0.7940	0.1126
C(28)	0.8687(7)	0.550(2)	0.5020(6)	0.159(4)	H(42)	1.0539	0.7720	0.7435	0.1126
C(29)	0.9073(7)	0.519(2)	0.4188(7)	0.146(4)	H(43)	0.9665	0.7844	0.8056	0.1126
H(1)	0.3375	0.7718	0.6365	0.0555	H(44)	0.8471	0.6250	0.6886	0.1068
H(2)	0.2445	0.6523	0.5880	0.0555	H(45)	0.8802	0.7817	0.6382	0.1068
H(3)	0.3370	0.7308	0.4722	0.0513	H(46)	0.8183	0.4605	0.5080	0.1729
H(4)	0.4456	0.6691	0.5386	0.0513	H(47)	0.8232	0.6483	0.4866	0.1729
H(5)	0.2724	0.4608	0.4509	0.0525	H(48)	0.9507	0.4156	0.4290	0.1735
H(6)	0.3783	0.2436	0.5214	0.0496	H(49)	0.8519	0.5013	0.3604	0.1735
H(7)	0.4710	0.3643	0.5689	0.0496	H(50)	0.9548	0.6033	0.4072	0.1735
H(8)	0.2716	0.3431	0.6216	0.0519					

CA·120

atom	x	y	z	U	atom	x	y	z	U
O(1)	0.3762(4)	1.4270(3)	0.7315(6)	0.0388(7)	H(27)	0.1593	0.7804	0.6310	0.0426
O(2)	0.1761(4)	1.1148(3)	0.9410(6)	0.0313(6)	H(28)	0.1783	0.7949	0.4458	0.0426
O(3)	0.0952(4)	1.0430(3)	0.3915(6)	0.0362(6)	H(29)	0.2646	0.8564	0.5751	0.0426
O(4)	-0.4093(4)	0.6016(4)	0.4806(6)	0.0449(7)	H(30)	0.4785	1.0198	0.7600	0.0495
O(5)	-0.4132(5)	0.5536(4)	0.2205(6)	0.0440(7)	H(31)	0.5051	1.0460	0.5801	0.0495
O(6)	0.1840(4)	0.2121(3)	0.2280(6)	0.0372(6)	H(32)	0.5792	1.1060	0.7229	0.0495
O(7)	0.3638(4)	0.5372(3)	0.4707(6)	0.0343(6)	H(33)	0.3873	1.3028	0.9618	0.0358
O(8)	0.4446(4)	0.5858(4)	-0.0514(6)	0.0348(6)	H(34)	0.3013	1.2514	0.8231	0.0358
O(9)	0.9321(4)	1.0132(4)	0.1167(6)	0.0454(7)	H(35)	0.4251	1.0709	1.0042	0.0403
O(10)	0.9556(4)	1.0729(4)	-0.1322(6)	0.0374(7)	H(36)	0.3777	1.1474	1.0892	0.0403
O(11)	0.8812(5)	0.5462(4)	-0.2951(6)	0.0613(9)	H(37)	0.5139	1.3749	0.7650	0.0398
O(12)	0.9122(5)	0.3827(4)	-0.3151(6)	0.0561(8)	H(38)	0.1078	0.8393	0.8641	0.0393
O(13)	0.6233(5)	0.2358(4)	-0.8144(6)	0.0619(9)	H(39)	0.0390	0.9085	0.9209	0.0393
O(14)	0.6568(5)	0.0785(4)	-0.7492(6)	0.076(1)	H(40)	-0.0532	0.7565	0.7291	0.0412
C(1)	0.4724(5)	1.2207(4)	0.5622(6)	0.0335(9)	H(41)	-0.1083	0.8410	0.7456	0.0412
C(2)	0.4193(5)	1.3049(4)	0.5639(7)	0.0349(9)	H(42)	-0.2085	0.7337	0.5317	0.0522
C(3)	0.4323(5)	1.3506(4)	0.7331(6)	0.0333(8)	H(43)	-0.2211	0.7717	0.3568	0.0522
C(4)	0.3814(5)	1.2762(4)	0.8553(6)	0.0317(8)	H(44)	0.0552	0.8064	0.2285	0.0509
C(5)	0.4307(4)	1.1884(4)	0.8556(6)	0.0316(8)	H(45)	-0.0610	0.7409	0.1650	0.0509
C(6)	0.3767(5)	1.1163(4)	0.9850(6)	0.0331(8)	H(46)	-0.0489	0.8481	0.2069	0.0509
C(7)	0.2566(5)	1.0571(4)	0.9363(6)	0.0308(8)	H(47)	0.3093	1.0856	0.3843	0.0363
C(8)	0.2485(4)	1.0109(4)	0.7664(6)	0.0260(7)	H(48)	0.3372	0.9959	0.4600	0.0363
C(9)	0.2995(5)	1.0846(4)	0.6351(6)	0.0271(7)	H(49)	0.2381	1.0068	1.0153	0.0365
C(10)	0.4238(5)	1.1404(4)	0.6829(6)	0.0296(8)	H(50)	-0.2047	0.6241	0.2480	0.0446
C(11)	0.2848(5)	1.0354(4)	0.4646(6)	0.0329(8)	H(51)	-0.2014	0.5864	0.4247	0.0446
C(12)	0.1642(5)	0.9769(4)	0.4150(6)	0.0307(8)	H(52)	0.0691	0.4321	-0.0528	0.0407
C(13)	0.1172(5)	0.9018(4)	0.5457(6)	0.0269(7)	H(53)	-0.0129	0.3756	0.0720	0.0407
C(14)	0.1287(5)	0.9567(4)	0.7117(6)	0.0256(7)	H(54)	0.0970	0.2814	-0.0237	0.0398
C(15)	0.0628(5)	0.8813(4)	0.8250(6)	0.0323(9)	H(55)	0.2056	0.3575	0.0398	0.0398
C(16)	-0.0385(5)	0.8243(4)	0.7145(7)	0.0343(8)	H(56)	0.1564	0.3303	0.4688	0.0421
C(17)	-0.0117(5)	0.8523(4)	0.5332(6)	0.0291(7)	H(57)	0.2457	0.3853	0.3521	0.0421
C(18)	0.1846(5)	0.8250(4)	0.5484(6)	0.0349(9)	H(58)	0.1049	0.5556	0.5092	0.0388
C(19)	0.5029(5)	1.0731(4)	0.6856(7)	0.0408(10)	H(59)	0.1640	0.4846	0.5937	0.0388
C(20)	-0.0585(5)	0.7672(4)	0.4127(6)	0.0305(7)	H(60)	0.2304	0.5348	-0.0971	0.0458
C(21)	-0.0268(5)	0.7910(4)	0.2364(6)	0.0378(9)	H(61)	0.1987	0.6259	-0.0362	0.0458
C(22)	-0.1874(5)	0.7305(4)	0.4197(7)	0.0374(9)	H(62)	0.3983	0.8069	0.3945	0.0470
C(23)	-0.2328(5)	0.6274(4)	0.3557(6)	0.0370(8)	H(63)	0.4746	0.7466	0.4710	0.0470
C(24)	-0.3596(5)	0.5905(4)	0.3429(6)	0.0336(8)	H(64)	0.5514	0.8949	0.2731	0.0444
C(25)	0.0636(5)	0.4059(4)	0.0531(6)	0.0363(9)	H(65)	0.6215	0.8241	0.3263	0.0444
C(26)	0.1263(5)	0.3277(4)	0.0582(6)	0.0337(8)	H(66)	0.7256	0.9077	0.1284	0.0474
C(27)	0.1179(5)	0.2823(4)	0.2247(6)	0.0325(8)	H(67)	0.7474	0.8481	-0.0193	0.0474
C(28)	0.1631(5)	0.3580(4)	0.3596(6)	0.0321(8)	H(68)	0.7605	0.9774	-0.1884	0.0550
C(29)	0.1069(5)	0.4421(4)	0.3535(6)	0.0309(8)	H(69)	0.7301	1.0368	-0.0471	0.0550
C(30)	0.1572(5)	0.5173(4)	0.4900(6)	0.0321(8)	H(70)	0.3575	0.8536	0.1258	0.0473
C(31)	0.2724(5)	0.5840(4)	0.4573(6)	0.0297(8)	H(71)	0.3478	0.8264	-0.0593	0.0473
C(32)	0.2743(5)	0.6270(4)	0.2850(6)	0.0271(7)	H(72)	0.2580	0.7705	0.0561	0.0473
C(33)	0.2310(5)	0.5463(4)	0.1528(6)	0.0278(7)	H(73)	0.0493	0.6036	0.2521	0.0511
C(34)	0.1086(5)	0.4876(4)	0.1823(6)	0.0297(8)	H(74)	0.0216	0.5756	0.0682	0.0511
C(35)	0.2473(5)	0.5860(4)	-0.0206(6)	0.0320(8)	H(75)	-0.0476	0.5138	0.2008	0.0511
C(36)	0.3676(5)	0.6468(4)	-0.0485(6)	0.0301(8)	H(76)	0.4836	0.7993	-0.2364	0.0629
C(37)	0.4050(5)	0.7300(4)	0.0787(6)	0.0283(7)	H(77)	0.5961	0.8696	-0.2829	0.0629
C(38)	0.3919(5)	0.6869(4)	0.2502(6)	0.0265(7)	H(78)	0.5955	0.7683	-0.2212	0.0629
C(39)	0.4489(5)	0.7705(4)	0.3660(6)	0.0320(8)	H(79)	0.0417	0.2522	0.2470	0.0427
C(40)	0.5474(5)	0.8286(4)	0.2712(6)	0.0302(8)	H(80)	0.0294	0.4138	0.3749	0.0397
C(41)	0.5335(5)	0.7846(4)	0.0950(6)	0.0273(7)	H(81)	0.2928	0.6370	0.5372	0.0320
C(42)	0.3325(5)	0.8010(4)	0.0484(7)	0.0375(10)	H(82)	0.3668	0.6735	-0.1557	0.0338
C(43)	0.0250(5)	0.5508(4)	0.1717(7)	0.041(1)	H(83)	0.4390	0.6427	0.2586	0.0294
C(44)	0.5849(5)	0.8611(4)	-0.0314(6)	0.0311(8)	H(84)	0.2241	0.6675	0.2823	0.0326
C(45)	0.5625(5)	0.8227(4)	-0.2077(7)	0.047(1)	H(85)	0.5774	0.7376	0.0906	0.0313
C(46)	0.7120(5)	0.8979(4)	0.0115(6)	0.0337(8)	H(86)	0.5507	0.9133	-0.0161	0.0361
C(47)	0.7714(5)	0.9889(4)	-0.0722(6)	0.0384(9)	H(87)	0.2816	0.5013	0.1716	0.0344
C(48)	0.8934(5)	1.0259(4)	-0.0179(6)	0.0334(8)	H(88)	0.7915	0.6353	-0.0807	0.0766
C(49)	0.7362(6)	0.5802(5)	-0.1417(7)	0.064(1)	H(89)	0.7055	0.6094	-0.2304	0.0766
C(50)	0.7986(5)	0.5120(4)	-0.1999(7)	0.0507(10)	H(90)	0.6804	0.5547	-0.0684	0.0766
C(51)	0.7732(5)	0.4164(4)	-0.1558(7)	0.0478(10)	H(91)	0.7501	0.2362	-0.0912	0.0727
C(52)	0.8320(5)	0.3533(4)	-0.2155(7)	0.0468(10)	H(92)	0.7875	0.2099	-0.2600	0.0727
C(53)	0.8077(5)	0.2523(4)	-0.1661(7)	0.061(1)	H(93)	0.8757	0.2385	-0.1134	0.0727
C(54)	0.7256(6)	0.3801(4)	-0.6791(7)	0.063(1)	H(94)	0.7886	0.4029	-0.5954	0.0740
C(55)	0.7039(5)	0.2741(4)	-0.7096(7)	0.0436(9)	H(95)	0.7434	0.4157	-0.7721	0.0740
C(56)	0.7680(5)	0.2218(4)	-0.6269(7)	0.0436(10)	H(96)	0.6609	0.3946	-0.6311	0.0740
C(57)	0.7389(5)	0.1201(4)	-0.6470(7)	0.054(1)	H(97)	0.7430	0.0165	-0.4807	0.0958
C(58)	0.7958(6)	0.0592(5)	-0.5523(8)	0.072(2)	H(98)	0.8271	0.0197	-0.6173	0.0958
H(1)	0.4046	1.4595	0.8363	0.0380	H(99)	0.8559	0.0963	-0.4767	0.0958
H(5)	0.5101	1.2179	0.8943	0.0380	H(100)	0.7831	0.4213	-0.0359	0.0537
H(7)	0.2921	0.9631	0.7604	0.0380	H(101)	0.6952	0.3933	-0.1830	0.0537
H(8)	0.2596	1.1325	0.6528	0.0380	H(102)	0.8442	0.2454	-0.6537	0.0548
H(10)	0.1733	0.9464	0.3119	0.0380	H(103)	0.7644	0.2348	-0.5098	0.0548
H(12)	0.0863	1.0046	0.7252	0.0380	H(104)	0.1923	1.1543	1.0607	0.0587
H(15)	-0.0529	0.9011	0.5263	0.0380	H(105)	0.0386	1.0173	0.3050	0.0587
H(19)	-0.0267	0.7120	0.4335	0.0380	H(107)	-0.5025	0.5679	0.4732	0.0587
H(23)	0.4674	1.1926	0.4569	0.0384	H(109)	0.4713	0.5801	0.0592	0.0587
H(24)	0.5546	1.2450	0.5934	0.0384	H(111)	0.3623	0.5024	0.5366	0.0490
H(25)	0.4531	1.3532	0.4876	0.0423	H(114)	0.1611	0.1694	0.3036	0.0545
H(26)	0.3402	1.2836	0.5344	0.0423	H(116)	1.0104	1.0820	-0.1065	0.0409

CA·125

atom	x	y	z	U	atom	x	y	z	U
O(1)	1.0984(1)	0.4642(9)	0.6209(1)	0.0349(4)	H(8)	1.2422	0.3943	0.4260	0.0315
O(2)	0.9438(1)	0.2324(9)	0.2738(1)	0.0294(4)	H(9)	1.1735	0.2701	0.2673	0.0346
O(3)	0.8049(1)	0.7948(9)	0.1914(1)	0.0289(4)	H(10)	1.1371	0.1558	0.3374	0.0346
O(4)	0.2795(1)	0.7137(9)	-0.1831(2)	0.0577(6)	H(11)	1.0007	0.2037	0.1680	0.0311
O(5)	0.3762(1)	0.4733(9)	-0.1403(2)	0.0453(5)	H(12)	1.0265	0.4833	0.1369	0.0277
O(6)	0.5561(3)	0.6974(10)	0.4136(3)	0.094(1)	H(13)	0.9825	0.5904	0.3039	0.0277
C(1)	1.1765(2)	0.7199(8)	0.4337(2)	0.0293(5)	H(14)	1.0074	0.8704	0.2666	0.0298
C(2)	1.1249(2)	0.6869(8)	0.5097(2)	0.0294(5)	H(15)	1.0343	0.8093	0.1750	0.0298
C(3)	1.1521(2)	0.5063(8)	0.5552(2)	0.0294(5)	H(16)	0.8620	0.9165	0.1021	0.0303
C(4)	1.1184(2)	0.3727(8)	0.4683(2)	0.0273(5)	H(17)	0.8305	0.4802	0.1495	0.0274
C(5)	1.1661(2)	0.4046(8)	0.3886(2)	0.0264(5)	H(18)	0.8588	0.3353	-0.0183	0.0355
C(6)	1.1289(2)	0.2645(8)	0.3036(2)	0.0285(5)	H(19)	0.8027	0.2495	0.0455	0.0355
C(7)	1.0125(2)	0.2813(8)	0.2240(2)	0.0257(5)	H(20)	0.6979	0.4377	-0.1245	0.0355
C(8)	0.9874(2)	0.4649(8)	0.1783(2)	0.0228(5)	H(21)	0.6499	0.3889	-0.0457	0.0355
C(9)	1.0227(2)	0.6071(8)	0.2637(2)	0.0229(5)	H(22)	0.6804	0.6477	0.0270	0.0289
C(10)	1.1442(2)	0.5910(8)	0.3413(2)	0.0255(5)	H(23)	0.9725	0.6927	0.0208	0.0352
C(11)	0.9916(2)	0.7861(8)	0.2124(2)	0.0249(5)	H(24)	0.8768	0.6091	-0.0730	0.0352
C(12)	0.8721(2)	0.8056(8)	0.1352(2)	0.0251(5)	H(25)	0.8773	0.8069	-0.0530	0.0352
C(13)	0.8387(2)	0.6646(8)	0.0501(2)	0.0219(5)	H(26)	1.2904	0.6148	0.3341	0.0434
C(14)	0.8680(2)	0.4863(8)	0.1061(2)	0.0227(5)	H(27)	1.2005	0.5506	0.2287	0.0434
C(15)	0.8155(2)	0.3553(8)	0.0187(2)	0.0297(6)	H(28)	1.2058	0.7444	0.2599	0.0434
C(16)	0.7084(2)	0.4432(8)	-0.0531(2)	0.0294(5)	H(29)	0.6861	0.7357	-0.1626	0.0321
C(17)	0.7158(2)	0.6370(8)	-0.0183(2)	0.0238(5)	H(30)	0.7408	0.9803	-0.0597	0.0399
C(18)	0.8971(2)	0.6959(8)	-0.0206(2)	0.0296(6)	H(31)	0.6298	1.0131	-0.1530	0.0399
C(19)	1.2175(2)	0.6282(8)	0.2860(2)	0.0362(6)	H(32)	0.6364	0.9756	-0.0419	0.0399
C(20)	0.6553(2)	0.7551(8)	-0.1145(2)	0.0266(5)	H(33)	0.5040	0.7674	-0.2338	0.0370
C(21)	0.6665(2)	0.9483(8)	-0.0901(2)	0.0335(6)	H(34)	0.5327	0.5833	-0.1855	0.0370
C(22)	0.5361(2)	0.7023(8)	-0.1702(2)	0.0307(6)	H(35)	0.5132	0.7000	-0.0354	0.0442
C(23)	0.4715(2)	0.7371(8)	-0.1059(2)	0.0365(6)	H(36)	0.4584	0.8581	-0.1061	0.0442
C(24)	0.3655(2)	0.6434(8)	-0.1478(2)	0.0356(5)	H(37)	1.0733	0.5616	0.6406	0.0597
C(25)	0.6532(4)	0.589(1)	0.3189(4)	0.098(2)	H(38)	0.8859	0.2383	0.2380	0.0639
C(26)	0.5902(4)	0.694(1)	0.3330(4)	0.095(2)	H(39)	0.8379	0.8271	0.2455	0.0684
C(27)	0.5984(3)	0.5660(9)	0.4893(4)	0.079(1)	H(40)	0.3041	0.4117	-0.1625	0.0597
C(28)	0.5607(4)	0.596(1)	0.5725(4)	0.102(2)	H(41)	0.7272	0.6170	0.3451	0.1166
H(1)	1.1566	0.8338	0.4056	0.0357	H(42)	0.6259	0.4849	0.2820	0.1166
H(2)	1.2526	0.7152	0.4730	0.0357	H(43)	0.5582	0.7834	0.2829	0.1174
H(3)	1.1508	0.7699	0.5652	0.0352	H(44)	0.5731	0.4570	0.4570	0.0949
H(4)	1.0486	0.6986	0.4730	0.0352	H(45)	0.6748	0.5682	0.5187	0.0949
H(5)	1.2278	0.4989	0.5958	0.0354	H(46)	0.5853	0.7074	0.6042	0.1278
H(6)	1.1414	0.2624	0.4992	0.0329	H(47)	0.4838	0.5957	0.5427	0.1278
H(7)	1.0420	0.3747	0.4320	0.0329	H(48)	0.5877	0.5096	0.6249	0.1278

CA·133

atom	x	y	z	U	atom	x	y	z	U
O(1)	-0.0910(2)	-0.5668	-0.6201(2)	0.0389(7)	H(7)	-0.0260	-0.6659	-0.4339	0.0394
O(2)	0.0862(2)	-0.7966(4)	-0.2710(2)	0.0384(7)	H(8)	-0.2266	-0.6895	-0.4190	0.0423
O(3)	0.1827(2)	-0.2516(4)	-0.1950(2)	0.0364(6)	H(9)	-0.1517	-0.8147	-0.2661	0.0471
O(4)	0.6559(3)	-0.5042(6)	0.1496(3)	0.079(1)	H(10)	-0.1082	-0.9080	-0.3382	0.0471
O(5)	0.7010(2)	-0.2405(6)	0.1995(2)	0.0677(10)	H(11)	0.0262	-0.8554	-0.1697	0.0386
O(7)	-0.5005(6)	0.249(2)	-0.6658(7)	0.238(4)	H(12)	-0.0202	-0.5955	-0.1373	0.0335
O(8)	-0.468(1)	0.109(2)	-0.532(1)	0.330(9)	H(13)	0.0213	-0.4692	-0.3029	0.0320
C(1)	-0.1808(3)	-0.3657(6)	-0.4256(2)	0.0345(9)	H(14)	-0.0180	-0.2053	-0.2630	0.0403
C(2)	-0.1279(3)	-0.3792(5)	-0.5040(2)	0.0332(8)	H(15)	-0.0422	-0.2759	-0.1717	0.0403
C(3)	-0.1468(3)	-0.5523(6)	-0.5517(2)	0.0332(8)	H(16)	0.1227	-0.1497	-0.1033	0.0359
C(4)	-0.1030(3)	-0.6804(5)	-0.4673(2)	0.0309(8)	H(17)	0.1787	-0.5576	-0.1490	0.0334
C(5)	-0.1508(3)	-0.6692(6)	-0.3839(2)	0.0323(8)	H(18)	0.1521	-0.7187	0.0149	0.0414
C(6)	-0.1052(3)	-0.8049(6)	-0.3022(2)	0.0373(9)	H(19)	0.2175	-0.7831	-0.0466	0.0414
C(7)	0.0095(3)	-0.7748(5)	-0.2247(2)	0.0310(8)	H(20)	0.3007	-0.5953	0.1214	0.0444
C(8)	0.0219(3)	-0.6006(5)	-0.1784(2)	0.0270(7)	H(21)	0.3584	-0.6315	0.0478	0.0444
C(9)	-0.0208(2)	-0.4619(5)	-0.2626(2)	0.0259(7)	H(22)	0.3150	-0.3899	-0.0295	0.0345
C(10)	-0.1397(2)	-0.4932(6)	-0.3356(2)	0.0314(8)	H(23)	0.1083	-0.2675	0.0517	0.0443
C(11)	0.0008(3)	-0.2879(6)	-0.2106(2)	0.0321(8)	H(24)	0.0199	-0.3867	-0.0204	0.0443
C(12)	0.1173(3)	-0.2554(5)	-0.1358(2)	0.0302(8)	H(25)	0.1180	-0.4585	0.0718	0.0443
C(13)	0.1563(2)	-0.3915(5)	-0.0510(2)	0.0265(7)	H(26)	-0.2123	-0.3673	-0.2512	0.0565
C(14)	0.1383(2)	-0.5615(5)	-0.1067(2)	0.0269(7)	H(27)	-0.2877	-0.5011	-0.3241	0.0565
C(15)	0.1960(3)	-0.6863(6)	-0.0206(2)	0.0333(8)	H(28)	-0.1950	-0.5548	-0.2212	0.0565
C(16)	0.2955(3)	-0.5889(6)	0.0525(3)	0.0355(8)	H(29)	0.2990	-0.3046	0.1553	0.0412
C(17)	0.2791(2)	-0.4038(5)	0.0156(2)	0.0279(7)	H(30)	0.3464	-0.0314	0.1389	0.0517
C(18)	0.0948(3)	-0.3748(6)	0.0196(2)	0.0354(9)	H(31)	0.3519	-0.0728	0.0333	0.0517
C(19)	-0.2154(3)	-0.4789(7)	-0.2785(3)	0.046(1)	H(32)	0.2419	-0.0735	0.0434	0.0517
C(20)	0.3336(3)	-0.2843(6)	0.1075(2)	0.0333(8)	H(33)	0.4843	-0.2499	0.2227	0.0447
C(21)	0.3162(3)	-0.0990(6)	0.0780(3)	0.0403(9)	H(34)	0.4630	-0.4356	0.1892	0.0447
C(22)	0.4539(3)	-0.3233(6)	0.1644(2)	0.0360(9)	H(35)	0.4836	-0.3637	0.0334	0.0547
C(23)	0.5184(3)	-0.3026(6)	0.0976(3)	0.0439(10)	H(36)	0.5187	-0.1864	0.0789	0.0547
C(24)	0.6315(3)	-0.3625(7)	0.1504(3)	0.0435(8)	H(37)	-0.1285	-0.6562	-0.6795	0.0650
C(30)	-0.4373(6)	0.263(2)	-0.5490(10)	0.160(3)	H(38)	0.0969	-0.7262	-0.3069	0.0650
C(31)	-0.4265(8)	0.210(2)	-0.7111(9)	0.175(4)	H(39)	0.2428	-0.1936	-0.1649	0.0650
C(32)	-0.3623(9)	0.083(2)	-0.6787(9)	0.154(4)	H(40)	0.7769	-0.2915	0.2229	0.0650
C(33)	-0.3361(9)	-0.013(1)	-0.590(1)	0.206(5)	H(41)	-0.3605	0.2854	-0.5219	0.1966
C(34)	-0.415(2)	-0.025(2)	-0.554(1)	0.254(9)	H(42)	-0.4654	0.3493	-0.5145	0.1966
H(1)	-0.1681	-0.2550	-0.3958	0.0432	H(43)	-0.4629	0.1776	-0.7891	0.2184
H(2)	-0.2566	-0.3800	-0.4613	0.0432	H(44)	-0.3776	0.2973	-0.7135	0.2184
H(3)	-0.1551	-0.2979	-0.5566	0.0404	H(45)	-0.3251	0.0311	-0.7171	0.2256
H(4)	-0.0510	-0.3635	-0.4686	0.0404	H(46)	-0.2644	-0.0375	-0.5331	0.3080
H(5)	-0.2229	-0.5690	-0.5892	0.0410	H(47)	-0.3992	-0.1115	-0.5034	0.3579
H(6)	-0.1160	-0.7898	-0.4978	0.0394	H(48)	-0.4726	-0.0812	-0.6191	0.3579

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atom	x	y	z	U	atom	x	y	z	U
O(1)	1.5975(5)	-0.2641(4)	-1.4193(6)	0.0442(5)	H(14)	1.6023	0.1535	-1.6841	0.0478
O(2)	1.8502(5)	0.1151(4)	-1.6922(6)	0.0425(5)	H(15)	1.6341	0.0600	-1.7390	0.0478
O(3)	1.7743(5)	0.0635(4)	-1.1731(6)	0.0379(5)	H(16)	1.7699	0.2044	-1.7925	0.0445
O(4)	2.3439(5)	0.5421(4)	-1.5287(6)	0.0497(6)	H(17)	1.8487	0.1724	-1.3873	0.0378
O(5)	2.3653(5)	0.5998(4)	-1.7786(6)	0.0446(5)	H(18)	1.8102	0.3379	-1.2478	0.0473
O(6)	1.7881(5)	0.9571(4)	-0.9117(6)	0.0468(6)	H(19)	1.8905	0.2779	-1.1775	0.0473
O(7)	1.5857(5)	0.6394(4)	-0.7057(6)	0.0367(5)	H(20)	1.9526	0.4288	-1.3744	0.0440
O(8)	1.5056(5)	0.5682(4)	-1.2534(6)	0.0406(5)	H(21)	2.0287	0.3617	-1.3191	0.0440
O(9)	0.9873(5)	0.0679(4)	-1.4284(6)	0.0576(7)	H(22)	1.9823	0.2685	-1.5440	0.0392
O(10)	1.0006(5)	0.1221(4)	-1.1709(6)	0.0541(6)	H(23)	1.6625	0.2990	-1.5803	0.0498
O(11)	1.088(2)	0.691(2)	-1.524(3)	0.56(1)	H(24)	1.7481	0.3569	-1.6976	0.0498
O(12)	1.1665(7)	0.7466(5)	-1.3031(9)	0.131(2)	H(25)	1.7637	0.3853	-1.5136	0.0498
O(13)	1.143(1)	1.0962(9)	-0.773(1)	0.276(6)	H(26)	1.3600	0.0376	-1.4520	0.0645
O(14)	1.1927(7)	0.9585(6)	-0.864(1)	0.198(3)	H(27)	1.4308	0.1024	-1.5788	0.0645
C(1)	1.4712(5)	-0.0705(4)	-1.5898(7)	0.0445(7)	H(28)	1.4584	0.1286	-1.3945	0.0645
C(2)	1.5353(5)	-0.1490(4)	-1.5868(6)	0.0411(7)	H(29)	1.9595	0.4469	-1.6596	0.0436
C(3)	1.5306(5)	-0.1960(4)	-1.4228(7)	0.0403(7)	H(30)	1.8850	0.3309	-1.8696	0.0579
C(4)	1.5765(5)	-0.1184(4)	-1.2885(6)	0.0377(6)	H(31)	1.9964	0.4031	-1.9180	0.0579
C(5)	1.5186(5)	-0.0351(4)	-1.2927(7)	0.0405(7)	H(32)	1.9968	0.2994	-1.8589	0.0579
C(6)	1.5703(5)	0.0419(4)	-1.1568(6)	0.0425(7)	H(33)	2.1325	0.4450	-1.5141	0.0468
C(7)	1.6859(5)	0.1112(4)	-1.1863(7)	0.0378(6)	H(34)	2.1527	0.3788	-1.6531	0.0468
C(8)	1.6856(5)	0.1546(4)	-1.3565(6)	0.0347(6)	H(35)	2.1445	0.5720	-1.6967	0.0532
C(9)	1.6398(5)	0.0739(4)	-1.4890(6)	0.0329(6)	H(36)	2.1707	0.5058	-1.8308	0.0532
C(10)	1.5175(5)	0.0122(4)	-1.4619(7)	0.0394(7)	H(37)	1.9617	0.7717	-1.0431	0.0482
C(11)	1.6540(5)	0.1140(4)	-1.6616(6)	0.0398(7)	H(38)	1.8712	0.7186	-1.1788	0.0482
C(12)	1.7738(5)	0.1758(4)	-1.6870(6)	0.0370(6)	H(39)	1.8689	0.8811	-1.1465	0.0462
C(13)	1.8135(5)	0.2611(4)	-1.5593(6)	0.0325(6)	H(40)	1.7528	0.8110	-1.1107	0.0462
C(14)	1.8029(5)	0.2159(4)	-1.3901(6)	0.0316(6)	H(41)	1.9204	0.9067	-0.8727	0.0489
C(15)	1.8619(5)	0.3009(4)	-1.2725(6)	0.0395(7)	H(42)	1.8013	0.8351	-0.6816	0.0449
C(16)	1.9581(5)	0.3629(4)	-1.3681(7)	0.0365(6)	H(43)	1.7100	0.7824	-0.8167	0.0449
C(17)	1.9423(5)	0.3165(4)	-1.5428(6)	0.0326(6)	H(44)	1.9170	0.7402	-0.7476	0.0455
C(18)	1.7409(5)	0.3322(4)	-1.5891(7)	0.0416(7)	H(45)	1.8307	0.5981	-0.6388	0.0488
C(19)	1.4345(5)	0.0763(4)	-1.4713(7)	0.0539(9)	H(46)	1.7837	0.6770	-0.5590	0.0488
C(20)	1.9921(5)	0.3931(4)	-1.6681(6)	0.0363(6)	H(47)	1.6438	0.5312	-0.6349	0.0418
C(21)	1.9658(5)	0.3528(4)	-1.8440(7)	0.0482(8)	H(48)	1.6991	0.4887	-0.8710	0.0382
C(22)	2.1208(5)	0.4299(4)	-1.6257(6)	0.0389(7)	H(49)	1.6646	0.6565	-1.0133	0.0380
C(23)	2.1800(5)	0.5211(4)	-1.7155(7)	0.0442(7)	H(50)	1.7406	0.5175	-1.1736	0.0417
C(24)	2.3031(5)	0.5556(4)	-1.6621(7)	0.0376(6)	H(51)	1.7160	0.6099	-1.2513	0.0417
C(25)	1.8837(5)	0.7474(4)	-1.0705(6)	0.0402(7)	H(52)	1.5732	0.4666	-1.3291	0.0422
C(26)	1.8319(5)	0.8335(4)	-1.0725(6)	0.0384(7)	H(53)	1.4940	0.5288	-0.9534	0.0360
C(27)	1.8433(5)	0.8799(4)	-0.9043(6)	0.0408(7)	H(54)	1.5115	0.3621	-0.7879	0.0448
C(28)	1.7902(5)	0.8049(4)	-0.7852(6)	0.0375(7)	H(55)	1.4438	0.4344	-0.7389	0.0448
C(29)	1.8398(4)	0.7160(4)	-0.7807(7)	0.0379(6)	H(56)	1.3541	0.2788	-0.9278	0.0506
C(30)	1.7860(5)	0.6421(4)	-0.6555(6)	0.0405(7)	H(57)	1.2995	0.3651	-0.9149	0.0506
C(31)	1.6659(5)	0.5824(4)	-0.7078(6)	0.0348(6)	H(58)	1.3563	0.4243	-1.1498	0.0405
C(32)	1.6575(5)	0.5356(4)	-0.8763(6)	0.0318(6)	H(59)	1.6665	0.3765	-1.0660	0.0455
C(33)	1.7083(5)	0.6096(4)	-1.0053(6)	0.0316(6)	H(60)	1.5803	0.3150	-1.1997	0.0455
C(34)	1.8333(5)	0.6669(4)	-0.9510(7)	0.0348(6)	H(61)	1.5585	0.2995	-1.0176	0.0455
C(35)	1.6937(4)	0.5602(4)	-1.1725(6)	0.0347(6)	H(62)	1.9856	0.6343	-0.9077	0.0606
C(36)	1.5732(5)	0.5002(4)	-1.2275(6)	0.0351(6)	H(63)	1.9112	0.5702	-1.0497	0.0606
C(37)	1.5249(4)	0.4249(4)	-1.0998(6)	0.0308(6)	H(64)	1.8837	0.5470	-0.8713	0.0606
C(38)	1.5356(5)	0.4807(4)	-0.9359(6)	0.0300(6)	H(65)	1.3785	0.2369	-1.2036	0.0434
C(39)	1.4686(5)	0.4041(4)	-0.8259(6)	0.0373(7)	H(66)	1.3450	0.3625	-1.4512	0.0514
C(40)	1.3668(5)	0.3473(4)	-0.9384(7)	0.0421(7)	H(67)	1.4562	0.3316	-1.4167	0.0514
C(41)	1.3938(5)	0.3751(4)	-1.1173(6)	0.0337(6)	H(68)	1.3456	0.2543	-1.4814	0.0514
C(42)	1.5894(5)	0.3465(4)	-1.0939(7)	0.0380(7)	H(69)	1.1823	0.2894	-1.3025	0.0521
C(43)	1.9118(5)	0.5980(4)	-0.9427(7)	0.0504(9)	H(70)	1.1971	0.2527	-1.1276	0.0521
C(44)	1.3473(5)	0.2880(4)	-1.2364(7)	0.0360(6)	H(71)	1.1954	0.1385	-1.4059	0.0574
C(45)	1.3771(5)	0.3113(4)	-1.4117(7)	0.0428(7)	H(72)	1.2016	0.1021	-1.2293	0.0574
C(46)	1.2177(5)	0.2491(4)	-1.2345(7)	0.0433(7)	H(73)	1.0395	0.8703	-1.5101	0.2143
C(47)	1.1722(5)	0.1429(4)	-1.2980(7)	0.0478(8)	H(74)	1.0337	0.8473	-1.3267	0.2143
C(48)	1.0437(5)	0.1069(4)	-1.3069(7)	0.0427(7)	H(75)	1.1476	0.9046	-1.3916	0.2143
C(49)	1.0806(9)	0.854(1)	-1.414(1)	0.179(3)	H(76)	1.1008	0.6106	-1.3228	0.2839
C(50)	1.108(1)	0.762(1)	-1.444(2)	0.234(5)	H(77)	1.2222	0.6455	-1.3810	0.2839
C(51)	1.177(2)	0.6521(10)	-1.295(2)	0.241(7)	H(78)	1.1999	0.5474	-1.1915	0.3008
C(52)	1.214(2)	0.616(1)	-1.173(2)	0.251(9)	H(79)	1.2925	0.6458	-1.1559	0.3008
C(53)	1.3176(9)	1.0884(7)	-0.916(2)	0.165(4)	H(80)	1.1762	0.6282	-1.0824	0.3008
C(54)	1.2040(8)	1.0570(6)	-0.852(1)	0.179(2)	H(81)	1.3132	1.0606	-1.0245	0.1980
C(55)	1.269(2)	0.928(2)	-0.978(3)	0.38(2)	H(82)	1.3401	1.1579	-0.9227	0.1980
C(56)	1.237(1)	0.833(2)	-0.893(2)	0.32(1)	H(83)	1.3696	1.0666	-0.8487	0.1980
H(1)	1.3932	-0.1012	-1.5736	0.0534	H(84)	1.2436	0.9254	-1.0922	0.4547
H(2)	1.4738	-0.0424	-1.6961	0.0534	H(85)	1.3464	0.9633	-0.9652	0.4547
H(3)	1.5006	-0.1976	-1.6708	0.0494	H(86)	1.1555	0.8075	-0.9039	0.3826
H(4)	1.6112	-0.1196	-1.6085	0.0494	H(87)	1.2691	0.7872	-0.9422	0.3826
H(5)	1.4532	-0.2297	-1.4084	0.0484	H(88)	1.2619	0.8431	-0.7825	0.3826
H(6)	1.5651	-0.1491	-1.1886	0.0453	H(89)	1.5737	-0.3109	-1.3414	0.0724
H(7)	1.6542	-0.0908	-1.3007	0.0453	H(90)	1.8724	0.1145	-1.5997	0.0724
H(8)	1.4407	-0.0634	-1.2737	0.0485	H(91)	1.7680	0.0196	-1.0845	0.0724
H(9)	1.5180	0.0805	-1.1457	0.0511	H(92)	2.4387	0.6015	-1.7561	0.0724
H(10)	1.5777	0.0083	-1.0612	0.0511	H(93)	1.8063	1.0105	-0.8305	0.0724
H(11)	1.7021	0.1635	-1.1095	0.0454	H(94)	1.6381	0.7011	-0.6646	0.0724
H(12)	1.6357	0.1964	-1.3617	0.0418	H(95)	1.4398	0.5531	-1.3358	0.0724
H(13)	1.6852	0.0303	-1.4785	0.0394	H(96)	0.9190	0.1038	-1.1890	0.0650

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atom	x	y	z	U	atom	x	y	z	U
O(1)	1.0208(2)	0.2755	0.3944(2)	0.0452(8)	H(7)	0.8376	0.3936	0.5718	0.0020
O(2)	0.8382(2)	0.0483(5)	0.6157(2)	0.0391(7)	H(9)	0.6381	0.6279	0.5788	-0.0007
O(3)	0.8889(2)	0.6072(5)	0.7298(2)	0.0408(7)	H(10)	0.7343	0.7263	0.7320	0.0072
O(4)	1.0289(3)	0.5324(7)	1.2047(2)	0.086(1)	H(12)	0.8312	0.2876	0.7298	-0.0185
O(5)	0.9824(3)	0.2863(6)	1.1309(2)	0.073(1)	H(13)	0.6820	0.2489	0.9007	0.0359
O(6)	0.5365(3)	0.2740(7)	0.0233(2)	0.094(1)	H(14)	0.8664	0.4671	0.8703	0.0305
O(7)	0.6398(4)	0.2112(7)	0.1612(2)	0.083(1)	H(15)	0.6446	0.5451	0.9284	0.0426
C(1)	0.7598(3)	0.5271(7)	0.4066(2)	0.0338(10)	H(16)	0.7773	0.4168	1.0371	0.0529
C(2)	0.8847(3)	0.4941(6)	0.4151(2)	0.0355(9)	H(17)	0.6879	0.8023	0.8761	0.1247
C(3)	0.9017(3)	0.3142(7)	0.3813(2)	0.0344(9)	H(18)	0.8641	-0.1373	0.1728	0.1177
C(4)	0.8538(3)	0.1840(7)	0.4343(3)	0.0333(10)	H(19)	0.9178	0.5869	0.3776	0.0756
C(5)	0.7272(3)	0.2123(6)	0.4287(2)	0.0316(9)	H(20)	0.8767	0.0730	0.4137	0.0266
C(6)	0.6826(3)	0.0721(7)	0.4814(2)	0.0348(10)	H(21)	0.7615	0.6859	0.5787	0.0101
C(7)	0.7199(3)	0.0920(7)	0.5845(2)	0.0325(8)	H(22)	0.8574	0.0330	0.6680	0.1033
C(8)	0.6968(3)	0.2740(6)	0.6140(2)	0.0277(8)	H(23)	0.5482	0.4073	0.3649	0.0341
C(9)	0.7456(3)	0.4153(6)	0.5635(2)	0.0270(8)	H(24)	0.6240	0.1541	0.7581	0.0290
C(10)	0.7025(3)	0.3975(7)	0.4581(2)	0.0288(8)	H(25)	0.5391	0.4865	0.6684	0.0381
C(11)	0.7237(3)	0.5930(6)	0.5994(2)	0.0294(9)	H(26)	0.5610	0.6201	0.7509	0.0648
C(12)	0.7663(3)	0.6162(6)	0.7034(2)	0.0309(8)	H(27)	0.6029	0.0707	0.4598	0.0717
C(13)	0.7155(3)	0.4760(6)	0.7520(2)	0.0278(8)	H(28)	0.7073	-0.0454	0.4574	0.0249
C(14)	0.7438(3)	0.2993(6)	0.7159(2)	0.0276(9)	H(29)	0.9019	0.1777	0.5023	0.0578
C(15)	0.7096(4)	0.1694(7)	0.7797(3)	0.041(1)	H(30)	0.5476	0.5581	0.4330	0.0420
C(16)	0.7444(4)	0.2563(7)	0.8729(3)	0.040(1)	H(31)	0.5250	0.3636	0.4653	0.0511
C(17)	0.7707(3)	0.4489(6)	0.8568(2)	0.0296(9)	H(32)	0.7550	0.6698	0.4209	0.0100
C(18)	0.5884(3)	0.5065(7)	0.7354(3)	0.041(1)	H(33)	0.5581	0.4471	0.7639	0.0623
C(19)	0.5737(3)	0.4310(7)	0.4264(2)	0.043(1)	H(34)	0.8186	0.2051	0.9216	0.1130
C(20)	0.7346(3)	0.5677(7)	0.9263(2)	0.0338(9)	H(35)	0.7349	0.0426	0.7781	0.0156
C(21)	0.7977(3)	0.5154(7)	1.0251(2)	0.041(1)	H(36)	0.8256	0.7667	0.9054	0.0706
C(22)	0.9240(4)	0.5434(8)	1.0494(3)	0.048(1)	H(37)	0.9600	0.5024	1.0061	0.0423
C(23)	0.9840(4)	0.4548(8)	1.1372(3)	0.049(1)	H(38)	0.7634	0.6019	1.0727	0.0549
C(24)	0.7498(4)	0.7586(7)	0.9120(3)	0.049(1)	H(39)	0.9548	0.6802	1.0450	0.0841
C(25)	0.5485(5)	0.4785(9)	0.1416(4)	0.081(2)	H(40)	1.0182	0.2387	1.1742	0.1493
C(26)	0.5719(4)	0.3108(9)	0.1010(3)	0.061(1)	H(41)	0.9259	0.6355	0.6853	0.1276
C(27)	0.6697(7)	0.045(1)	0.1261(5)	0.113(3)	H(42)	1.0494	0.3474	0.4112	0.1140
C(28)	0.744(1)	-0.041(1)	0.1937(7)	0.198(4)	H(43)	0.6189	0.5395	0.1714	0.1689
C(29)	0.8339(9)	-0.102(1)	0.2153(6)	0.156(4)	H(44)	0.5049	0.5697	0.1107	0.1522
H(1)	0.7183	0.5331	0.3407	0.0201	H(45)	0.5146	0.4293	0.1945	0.1748
H(2)	0.9288	0.5083	0.4813	0.0454	H(46)	0.5967	-0.0038	0.0947	0.1166
H(3)	0.8563	0.3240	0.3016	-0.0059	H(47)	0.7269	0.0162	0.0973	0.2248
H(4)	0.6822	0.1950	0.3597	0.0182	H(48)	0.8810	-0.1500	0.2540	0.3020
H(5)	0.6801	0.0074	0.6130	0.0123	H(49)	0.7383	0.8552	0.9727	0.1033
H(6)	0.6024	0.2807	0.5973	-0.0102	H(50)	0.7078	-0.0711	0.2163	0.3703

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atom	x	y	z	U	atom	x	y	z	U
O(1)	-0.2458(6)	0.2328(4)	-0.2789(7)	0.0390(7)	H(15)	-0.2975	-0.1132	-0.6060	0.0412
O(2)	-0.4387(5)	-0.0852(4)	-0.0688(7)	0.0316(6)	H(16)	-0.4439	-0.2578	-0.6839	0.0370
O(3)	-0.5121(5)	-0.1582(4)	-0.6188(7)	0.0380(7)	H(17)	-0.5266	-0.1960	-0.3201	0.0335
O(4)	-1.0490(6)	-0.6497(4)	-0.8006(7)	0.0457(7)	H(18)	-0.5784	-0.2915	-0.1068	0.0400
O(5)	-1.0274(5)	-0.5981(4)	-0.5455(7)	0.0490(7)	H(19)	-0.5109	-0.3615	-0.1543	0.0400
O(6)	-1.4253(6)	-0.9896(4)	0.2170(7)	0.0371(7)	H(20)	-0.7235	-0.3596	-0.2902	0.0464
O(7)	-1.2541(5)	-0.6592(4)	0.4621(7)	0.0339(6)	H(21)	-0.6717	-0.4455	-0.2985	0.0464
O(8)	-1.1913(5)	-0.6090(4)	-0.0581(7)	0.0364(6)	H(22)	-0.6622	-0.3023	-0.5194	0.0384
O(9)	-0.6801(6)	-0.1924(4)	0.1031(7)	0.0451(7)	H(23)	-0.4385	-0.4082	-0.5547	0.0448
O(10)	-0.6610(5)	-0.1332(4)	-0.1428(7)	0.0382(7)	H(24)	-0.4618	-0.4224	-0.3760	0.0448
O(11)	0.1331(9)	-0.9554(6)	-1.921(1)	0.161(3)	H(25)	-0.3520	-0.3450	-0.4204	0.0448
O(12)	0.0332(8)	-0.9316(5)	-1.7376(10)	0.133(2)	H(26)	-0.1037	-0.1410	-0.3946	0.0509
O(13)	0.2416(7)	-0.6345(5)	-1.3211(8)	0.097(2)	H(27)	-0.1324	-0.1638	-0.2197	0.0509
O(14)	0.1129(6)	-0.6844(5)	-1.1466(8)	0.072(1)	H(28)	-0.0306	-0.0745	-0.2526	0.0509
C(1)	-0.1367(5)	0.0320(5)	-0.4211(8)	0.0363(9)	H(29)	-0.6461	-0.4894	-0.5688	0.0376
C(2)	-0.1925(5)	0.1135(4)	-0.4293(7)	0.0364(8)	H(30)	-0.6696	-0.4735	-0.8448	0.0522
C(3)	-0.1852(5)	0.1610(4)	-0.2651(8)	0.0349(8)	H(31)	-0.5598	-0.3935	-0.7750	0.0522
C(4)	-0.2372(5)	0.0850(5)	-0.1458(7)	0.0316(8)	H(32)	-0.6721	-0.3670	-0.8199	0.0522
C(5)	-0.1828(5)	0.0019(4)	-0.1375(8)	0.0324(8)	H(33)	-0.8367	-0.4330	-0.6749	0.0446
C(6)	-0.2359(5)	-0.0728(4)	-0.0142(7)	0.0344(9)	H(34)	-0.8254	-0.4711	-0.5030	0.0446
C(7)	-0.3565(5)	-0.1387(4)	-0.0690(7)	0.0311(8)	H(35)	-0.8309	-0.6206	-0.6086	0.0479
C(8)	-0.3636(5)	-0.1852(4)	-0.2364(8)	0.0293(7)	H(36)	-0.8392	-0.5827	-0.7810	0.0479
C(9)	-0.3107(5)	-0.1098(4)	-0.3611(8)	0.0287(7)	H(37)	-0.2237	0.2810	-0.2004	0.0640
C(10)	-0.1861(5)	-0.0484(4)	-0.3045(8)	0.0330(8)	H(38)	-0.4381	-0.0425	0.0417	0.0640
C(11)	-0.3219(5)	-0.1614(5)	-0.5269(8)	0.0336(8)	H(39)	-0.5821	-0.1954	-0.6755	0.0640
C(12)	-0.4448(5)	-0.2239(4)	-0.5861(7)	0.0290(8)	H(40)	-1.1003	-0.6109	-0.5460	0.0640
C(13)	-0.4947(5)	-0.2987(4)	-0.4609(7)	0.0298(8)	H(41)	-1.6399	-0.8415	0.0563	0.0432
C(14)	-0.4847(5)	-0.2430(4)	-0.3003(7)	0.0287(8)	H(42)	-1.5586	-0.7795	-0.0601	0.0432
C(15)	-0.5538(5)	-0.3200(4)	-0.1931(8)	0.0332(9)	H(43)	-1.4176	-0.8464	0.0315	0.0418
C(16)	-0.6560(6)	-0.3770(5)	-0.3083(8)	0.0384(9)	H(44)	-1.5269	-0.9291	-0.0310	0.0418
C(17)	-0.6265(6)	-0.3503(5)	-0.4845(8)	0.0314(8)	H(45)	-1.5725	-0.9605	0.2301	0.0403
C(18)	-0.4304(5)	-0.3764(5)	-0.4518(8)	0.0364(9)	H(46)	-1.3706	-0.8153	0.3330	0.0394
C(19)	-0.1046(5)	-0.1126(5)	-0.2906(8)	0.042(1)	H(47)	-1.4561	-0.8757	0.4459	0.0394
C(20)	-0.6746(5)	-0.4387(4)	-0.6036(8)	0.0317(8)	H(48)	-1.5886	-0.7985	0.3616	0.0410
C(21)	-0.6403(6)	-0.4163(5)	-0.7738(8)	0.0420(10)	H(49)	-1.4505	-0.7205	0.5700	0.0432
C(22)	-0.8057(6)	-0.4748(5)	-0.6085(8)	0.0371(9)	H(50)	-1.5154	-0.6541	0.4854	0.0432
C(23)	-0.8593(6)	-0.5786(5)	-0.6738(8)	0.0400(9)	H(51)	-1.3289	-0.5617	0.5206	0.0373
C(24)	-0.9865(6)	-0.6126(4)	-0.6805(8)	0.0353(8)	H(52)	-1.4019	-0.5349	0.2723	0.0333
C(25)	-1.5624(5)	-0.8072(4)	0.0458(8)	0.0352(9)	H(53)	-1.3456	-0.6951	0.1547	0.0333
C(26)	-1.4943(5)	-0.8800(4)	0.0527(8)	0.0345(9)	H(54)	-1.4398	-0.5762	-0.0376	0.0417
C(27)	-1.4950(5)	-0.9248(4)	0.2150(8)	0.0333(8)	H(55)	-1.4113	-0.6674	-0.1003	0.0417
C(28)	-1.4489(5)	-0.8460(5)	0.3474(8)	0.0331(9)	H(56)	-1.2745	-0.5231	-0.1567	0.0365
C(29)	-1.5115(5)	-0.7674(4)	0.3415(8)	0.0338(8)	H(57)	-1.1855	-0.5518	0.2452	0.0346
C(30)	-1.4602(5)	-0.6888(5)	0.4765(8)	0.0347(9)	H(58)	-1.1384	-0.4469	0.4543	0.0443
C(31)	-1.3459(5)	-0.6151(4)	0.4453(7)	0.0309(8)	H(59)	-1.2175	-0.3875	0.3852	0.0443
C(32)	-1.3503(5)	-0.5742(4)	0.2787(8)	0.0287(7)	H(60)	-0.9998	-0.3667	0.3106	0.0426
C(33)	-1.3958(5)	-0.6557(4)	0.1468(8)	0.0291(7)	H(61)	-1.0728	-0.2984	0.2600	0.0426
C(34)	-1.5174(5)	-0.7226(5)	0.1763(8)	0.0347(8)	H(62)	-1.0544	-0.4570	0.0906	0.0363
C(35)	-1.3881(5)	-0.6143(4)	-0.0208(8)	0.0327(8)	H(63)	-1.2887	-0.3704	-0.0592	0.0473
C(36)	-1.2682(5)	-0.5505(4)	-0.0510(7)	0.0311(8)	H(64)	-1.2691	-0.3422	0.1230	0.0473
C(37)	-1.2232(5)	-0.4660(4)	0.0758(8)	0.0310(8)	H(65)	-1.3735	-0.4285	0.0567	0.0473
C(38)	-1.2321(5)	-0.5099(4)	0.2431(8)	0.0277(7)	H(66)	-1.6112	-0.6405	0.0579	0.0558
C(39)	-1.1692(6)	-0.4246(5)	0.3601(8)	0.0365(9)	H(67)	-1.5850	-0.6131	0.2402	0.0558
C(40)	-1.0720(5)	-0.3650(5)	0.2674(8)	0.0334(8)	H(68)	-1.6800	-0.7079	0.1810	0.0558
C(41)	-1.0936(5)	-0.4099(4)	0.0929(8)	0.0293(8)	H(69)	-1.0728	-0.2793	-0.0189	0.0373
C(42)	-1.2947(5)	-0.3951(5)	0.0495(8)	0.0377(9)	H(70)	-1.0442	-0.3214	-0.2773	0.0518
C(43)	-1.6058(6)	-0.6659(5)	0.1660(8)	0.047(1)	H(71)	-1.1571	-0.3930	-0.2299	0.0518
C(44)	-1.0434(5)	-0.3337(4)	-0.0317(8)	0.0313(8)	H(72)	-1.0468	-0.4251	-0.2240	0.0518
C(45)	-1.0743(6)	-0.3719(5)	-0.2037(8)	0.0426(10)	H(73)	-0.8846	-0.3506	-0.0169	0.0456
C(46)	-0.9127(6)	-0.2983(5)	0.0097(8)	0.0362(9)	H(74)	-0.8983	-0.2828	0.1203	0.0456
C(47)	-0.8485(6)	-0.2099(5)	-0.0783(8)	0.0418(10)	H(75)	-0.8796	-0.1574	-0.0576	0.0527
C(48)	-0.7218(6)	-0.1780(4)	-0.0289(8)	0.0344(8)	H(76)	-0.8627	-0.2253	-0.1923	0.0527
C(49)	0.1779(7)	-1.1731(5)	-1.5408(9)	0.068(2)	H(77)	-1.4750	-1.0552	0.2334	0.0640
C(50)	0.1518(9)	-1.0960(6)	-1.631(1)	0.129(3)	H(78)	-1.2465	-0.7014	0.5646	0.0640
C(51)	0.113(1)	-1.0574(6)	-1.706(1)	0.172(4)	H(79)	-1.1721	-0.6298	0.0402	0.0640
C(52)	0.0968(7)	-0.9764(6)	-1.789(1)	0.105(2)	H(80)	-0.5697	-0.1218	-0.1249	0.0640
C(53)	0.0225(8)	-0.8445(6)	-1.803(1)	0.101(2)	H(81)	0.1425	-1.2342	-1.5941	0.0825
C(54)	0.288(1)	-0.9221(7)	-1.325(1)	0.131(3)	H(82)	0.1480	-1.1720	-1.4393	0.0825
C(55)	0.2637(7)	-0.8254(6)	-1.326(1)	0.083(2)	H(83)	0.2579	-1.1614	-1.5243	0.0825
C(56)	0.1989(7)	-0.7973(6)	-1.2371(10)	0.075(2)	H(84)	0.1944	-1.1071	-1.7223	0.1627
C(57)	0.1870(6)	-0.6984(5)	-1.2420(9)	0.063(1)	H(85)	0.1995	-1.0450	-1.5675	0.1627
C(58)	0.0930(7)	-0.5904(6)	-1.1478(9)	0.073(2)	H(86)	0.0624	-1.0494	-1.6159	0.1845
H(1)	-0.0578	0.0602	-0.3912	0.0453	H(87)	0.0619	-1.1084	-1.7723	0.1845
H(2)	-0.1468	0.0030	-0.5283	0.0453	H(88)	0.0934	-0.7950	-1.7938	0.1200
H(3)	-0.2702	0.0883	-0.4730	0.0448	H(89)	-0.0318	-0.8220	-1.7498	0.1200
H(4)	-0.1533	0.1620	-0.5012	0.0448	H(90)	-0.0060	-0.8546	-1.9159	0.1200
H(5)	-0.1077	0.1918	-0.2299	0.0407	H(91)	0.2158	-0.9725	-1.3590	0.1617
H(6)	-0.3185	0.0585	-0.1793	0.0400	H(92)	0.3164	-0.9349	-1.2256	0.1617
H(7)	-0.2286	0.1161	-0.0436	0.0400	H(93)	0.3391	-0.9258	-1.4051	0.1617
H(8)	-0.1039	0.0304	-0.1033	0.0389	H(94)	0.2392	-0.8149	-1.4377	0.0986
H(9)	-0.2400	-0.0382	0.0814	0.0426	H(95)	0.3398	-0.7772	-1.3042	0.0986
H(10)	-0.1881	-0.1133	0.0087	0.0426	H(96)	0.2220	-0.8055	-1.1300	0.0897
H(11)	-0.3769	-0.1895	0.0028	0.0357	H(97)	0.1224	-0.8402	-1.2655	0.0897
H(12)	-0.3199	-0.2296	-0.2296	0.0349	H(98)	0.1626	-0.5399	-1.1217	0.0883
H(13)	-0.3568	-0.0660	-0.3736	0.0340	H(99)	0.0395	-0.5877	-1.0756	0.0883
H(14)	-0.2746	-0.2027	-0.5231	0.0412	H(100)	0.0624	-0.5796	-1.2551	0.0883

CA·162

atom	x	y	z	U	atom	x	y	z	U
O(1)	0.5177(2)	0.2768(10)	-0.1059(2)	0.0412(7)	H(7)	0.3581	0.0744	-0.0918	0.0369
O(2)	0.3373(2)	0.0459(10)	0.1124(2)	0.0356(7)	H(8)	0.1855	0.2138	-0.1358	0.0366
O(3)	0.3906(2)	0.6077(10)	0.2304(2)	0.0363(7)	H(9)	0.2075	-0.0352	-0.0379	0.0385
O(4)	0.5305(3)	0.531(1)	0.7070(2)	0.065(1)	H(10)	0.1027	0.0769	-0.0403	0.0385
O(5)	0.4872(3)	0.286(1)	0.6282(2)	0.0547(9)	H(11)	0.1821	0.0327	0.1175	0.0363
O(6)	-0.1038(8)	0.454(2)	0.367(1)	0.285(7)	H(12)	0.1190	0.2954	0.1003	0.0319
O(7)	-0.1662(6)	0.698(1)	0.3821(8)	0.201(4)	H(13)	0.3266	0.4184	0.0785	0.0315
C(1)	0.2605(3)	0.534(1)	-0.0940(2)	0.0329(9)	H(14)	0.2654	0.6834	0.0701	0.0347
C(2)	0.3853(3)	0.500(1)	-0.0842(3)	0.0344(9)	H(15)	0.1495	0.6235	0.0794	0.0347
C(3)	0.4006(3)	0.320(1)	-0.1189(3)	0.0329(8)	H(16)	0.2529	0.7351	0.2226	0.0348
C(4)	0.3508(3)	0.186(1)	-0.0675(3)	0.0327(9)	H(17)	0.3219	0.3088	0.2212	0.0347
C(5)	0.2269(3)	0.217(1)	-0.0732(2)	0.0307(9)	H(18)	0.2493	0.0623	0.2761	0.0421
C(6)	0.1819(3)	0.0755(10)	-0.0216(3)	0.0335(9)	H(19)	0.1322	0.1478	0.2581	0.0421
C(7)	0.2197(3)	0.094(1)	0.0815(3)	0.0318(8)	H(20)	0.3104	0.2000	0.4067	0.0454
C(8)	0.1985(3)	0.277(1)	0.1114(2)	0.0281(8)	H(21)	0.1866	0.2477	0.3987	0.0454
C(9)	0.2461(3)	0.420(1)	0.0616(3)	0.0275(8)	H(22)	0.3520	0.4540	0.3633	0.0345
C(10)	0.2033(3)	0.404(1)	-0.0441(3)	0.0308(8)	H(23)	0.0589	0.4243	0.2630	0.0444
C(11)	0.2274(3)	0.601(1)	0.0984(2)	0.0300(8)	H(24)	0.0785	0.6220	0.2549	0.0444
C(12)	0.2690(3)	0.6199(10)	0.2018(2)	0.0302(8)	H(25)	0.0566	0.5047	0.1693	0.0444
C(13)	0.2180(3)	0.480(1)	0.2509(2)	0.0296(8)	H(26)	0.0364	0.3601	-0.0479	0.0436
C(14)	0.2449(3)	0.301(1)	0.2142(2)	0.0297(8)	H(27)	0.0606	0.5544	-0.0621	0.0436
C(15)	0.2106(3)	0.169(1)	0.2761(3)	0.037(1)	H(28)	0.0503	0.4229	-0.1409	0.0436
C(16)	0.2459(3)	0.256(1)	0.3697(3)	0.0395(10)	H(29)	0.1594	0.5522	0.4164	0.0354
C(17)	0.2730(3)	0.452(1)	0.3550(2)	0.0305(8)	H(30)	0.2248	0.8288	0.4545	0.0470
C(18)	0.0913(3)	0.511(1)	0.2330(3)	0.0382(10)	H(31)	0.2091	0.7991	0.3514	0.0470
C(19)	0.0755(3)	0.440(1)	-0.0769(3)	0.038(1)	H(32)	0.3279	0.7927	0.4178	0.0470
C(20)	0.2381(3)	0.568(1)	0.4245(2)	0.0318(9)	H(33)	0.2890	0.3921	0.5294	0.0416
C(21)	0.2504(3)	0.763(1)	0.4110(3)	0.040(1)	H(34)	0.2693	0.5765	0.5633	0.0416
C(22)	0.3012(3)	0.516(1)	0.5225(3)	0.0368(9)	H(35)	0.4407	0.6681	0.5554	0.0495
C(23)	0.4276(3)	0.548(1)	0.5497(3)	0.043(1)	H(36)	0.4579	0.5034	0.5021	0.0495
C(24)	0.4866(3)	0.459(1)	0.6361(3)	0.0419(9)	H(37)	0.5678	0.3889	-0.1040	0.0474
C(25)	-0.323(1)	0.356(2)	0.2793(7)	0.194(6)	H(38)	0.3601	0.0591	0.1685	0.0410
C(26)	-0.3042(8)	0.489(2)	0.3225(8)	0.124(3)	H(39)	0.4124	0.6524	0.1946	0.0419
C(27)	-0.186(1)	0.560(2)	0.343(1)	0.158(5)	H(40)	0.5345	0.2176	0.6860	0.0643
C(28)	-0.0600(7)	0.774(2)	0.4160(7)	0.138(3)	H(41)	-0.4091	0.2514	0.2528	0.2265
C(29)	-0.0589(9)	0.927(2)	0.3656(7)	0.157(5)	H(42)	-0.2452	0.2783	0.2734	0.2265
H(1)	0.2523	0.6482	-0.0706	0.0386	H(43)	-0.3717	0.5979	0.3090	0.1459
H(2)	0.2204	0.5339	-0.1574	0.0386	H(44)	-0.0494	0.8248	0.4797	0.1641
H(3)	0.4265	0.5087	-0.0228	0.0394	H(45)	0.0034	0.7118	0.4178	0.1641
H(4)	0.4137	0.5823	-0.1197	0.0394	H(46)	-0.1233	0.9913	0.3656	0.1854
H(5)	0.3746	0.2983	-0.1820	0.0378	H(47)	0.0058	0.9833	0.3838	0.1854
H(6)	0.3914	0.1895	-0.0054	0.0369	H(48)	-0.0698	0.8786	0.3040	0.1854

CA·169

atom	x	y	z	U	atom	x	y	z	U
O(1)	-0.0183(3)	-0.2399	-0.8984(2)	0.0305(9)	H(7)	0.1206	-0.3261	-0.9999	0.0304
O(2)	0.1605(3)	-0.4695(6)	-1.1124(2)	0.0270(9)	H(8)	0.3128	-0.3206	-0.8635	0.0279
O(3)	0.1039(3)	0.0884(6)	-1.2265(2)	0.0249(8)	H(9)	0.3047	-0.5638	-0.9757	0.0279
O(4)	-0.0330(3)	0.0073(8)	-1.7058(2)	0.055(1)	H(10)	0.3981	-0.4260	-0.9544	0.0279
O(5)	0.0281(3)	-0.2385(7)	-1.6325(2)	0.045(1)	H(11)	0.3163	-0.5074	-1.1134	0.0253
O(6)	-0.4645(4)	-0.2826(9)	-1.3665(3)	0.074(2)	H(12)	0.3807	-0.2191	-1.0912	0.0253
O(7)	-0.3208(4)	-0.1372(8)	-1.3907(3)	0.062(1)	H(13)	0.1706	-0.0913	-1.0718	0.0228
C(1)	0.2410(4)	0.0130(8)	-0.9054(3)	0.025(1)	H(14)	0.2344	0.1639	-1.0695	0.0253
C(2)	0.1164(4)	-0.0227(8)	-0.9151(3)	0.026(1)	H(15)	0.3532	0.0962	-1.0818	0.0253
C(3)	0.0997(4)	-0.2001(8)	-0.8833(3)	0.025(1)	H(16)	0.2470	0.2194	-1.2133	0.0279
C(4)	0.1475(4)	-0.3318(8)	-0.9342(3)	0.025(1)	H(17)	0.1707	-0.2098	-1.2271	0.0228
C(5)	0.2730(4)	-0.3047(8)	-0.9277(3)	0.024(1)	H(18)	0.2528	-0.4599	-1.2716	0.0329
C(6)	0.3166(4)	-0.4416(8)	-0.9779(3)	0.025(1)	H(19)	0.3686	-0.3677	-1.2530	0.0329
C(7)	0.2781(4)	-0.4245(8)	-1.0806(3)	0.023(1)	H(20)	0.3071	-0.2642	-1.3964	0.0329
C(8)	0.2992(4)	-0.2421(8)	-1.1091(3)	0.020(1)	H(21)	0.1838	-0.3182	-1.4046	0.0329
C(9)	0.2515(4)	-0.1010(8)	-1.0600(3)	0.019(1)	H(22)	0.1406	-0.0729	-1.3567	0.0253
C(10)	0.2980(4)	-0.1174(8)	-0.9549(3)	0.023(1)	H(23)	0.4170	0.1018	-1.2575	0.0304
C(11)	0.2707(4)	0.0816(8)	-1.0957(3)	0.022(1)	H(24)	0.4378	-0.0960	-1.2580	0.0304
C(12)	0.2261(4)	0.1011(8)	-1.1993(3)	0.022(1)	H(25)	0.4430	-0.0023	-1.1680	0.0304
C(13)	0.2761(4)	-0.0388(8)	-1.2472(3)	0.021(1)	H(26)	0.4432	0.0366	-0.9239	0.0355
C(14)	0.2516(4)	-0.2169(7)	-1.2111(3)	0.020(1)	H(27)	0.4643	-0.1438	-0.9599	0.0355
C(15)	0.2869(4)	-0.3461(8)	-1.2727(3)	0.028(1)	H(28)	0.4571	-0.1244	-0.8617	0.0355
C(16)	0.2493(4)	-0.2594(8)	-1.3653(3)	0.028(1)	H(29)	0.3337	0.0329	-1.4046	0.0304
C(17)	0.2212(4)	-0.0666(8)	-1.3509(3)	0.023(1)	H(30)	0.2897	0.2951	-1.3595	0.0405
C(18)	0.4035(4)	-0.0048(8)	-1.2292(3)	0.028(1)	H(31)	0.2301	0.3060	-1.4624	0.0405
C(19)	0.4250(4)	-0.0819(9)	-0.9227(3)	0.032(1)	H(32)	0.1609	0.2620	-1.3957	0.0405
C(20)	0.2548(4)	0.0524(8)	-1.4194(3)	0.025(1)	H(33)	0.2214	-0.1249	-1.5223	0.0304
C(21)	0.2332(5)	0.2440(9)	-1.4072(3)	0.036(1)	H(34)	0.2319	0.0561	-1.5571	0.0304
C(22)	0.1972(4)	-0.0045(8)	-1.5175(3)	0.027(1)	H(35)	0.0527	0.1404	-1.5496	0.0393
C(23)	0.0711(4)	0.0195(9)	-1.5489(3)	0.034(1)	H(36)	0.0393	-0.0292	-1.4999	0.0393
C(24)	0.0171(4)	-0.0670(9)	-1.6377(3)	0.035(1)	H(37)	-0.0590	-0.1574	-0.8692	0.0342
C(25)	-0.4240(6)	-0.207(1)	-1.4159(5)	0.056(2)	H(38)	0.1370	-0.5111	-1.1712	0.0291
C(26)	-0.4770(6)	-0.171(1)	-1.5148(4)	0.060(2)	H(39)	0.0802	0.1538	-1.1830	0.0279
C(27)	-0.5703(6)	-0.235(1)	-1.5589(4)	0.071(2)	H(40)	-0.0254	-0.3082	-1.6801	0.0532
C(28)	-0.6243(7)	-0.203(1)	-1.6596(4)	0.079(3)	H(41)	-0.4389	-0.0976	-1.5502	0.0697
C(29)	-0.2533(6)	-0.166(1)	-1.3035(4)	0.065(2)	H(42)	-0.6130	-0.2991	-1.5252	0.0899
C(30)	-0.1480(7)	-0.123(1)	-1.2801(5)	0.085(3)	H(43)	-0.5762	-0.2459	-1.6922	0.0937
H(1)	0.2803	0.0039	-0.8412	0.0304	H(44)	-0.6347	-0.0799	-1.6713	0.0937
H(2)	0.2508	0.1263	-0.9243	0.0304	H(45)	-0.6963	-0.2566	-1.6801	0.0937
H(3)	0.0967	0.0673	-0.8792	0.0291	H(46)	-0.2914	-0.2066	-1.2572	0.0773
H(4)	0.0760	-0.0110	-0.9792	0.0291	H(47)	-0.1121	-0.0827	-1.3255	0.1013
H(5)	0.1389	-0.2087	-0.8208	0.0304	H(48)	-0.0965	-0.1399	-1.2199	0.1013
H(6)	0.1315	-0.4462	-0.9162	0.0304					

CA·185 (crossing)

atom	x	y	z	U	atom	x	y	z	U
O(1)	-0.1634(5)	-1.0600(5)	-0.301(1)	0.037(3)	H(6)	-0.2637	-1.0619	-0.0633	0.0317
O(2)	-0.4643(4)	-0.9118(4)	-0.6002(10)	0.027(2)	H(7)	-0.3058	-1.0184	-0.1742	0.0317
O(3)	-0.8486(6)	-0.6663(6)	-0.585(1)	0.061(4)	H(8)	-0.3558	-1.1653	-0.1174	0.0380
O(4)	-0.8811(5)	-0.6922(5)	-0.830(1)	0.045(3)	H(9)	-0.4022	-1.0821	0.0744	0.0304
O(5)	-0.4165(5)	-0.9451(4)	-0.0813(9)	0.029(2)	H(10)	-0.4605	-1.1231	-0.0332	0.0304
N(1)	-0.6209(8)	-1.0953(6)	-0.901(2)	0.1023	H(11)	-0.5092	-0.9939	-0.0050	0.0342
C(1)	-0.3489(8)	-1.1555(6)	-0.431(2)	0.033(4)	H(12)	-0.5368	-1.0648	-0.2355	0.0291
C(2)	-0.2747(7)	-1.1080(6)	-0.445(2)	0.025(4)	H(13)	-0.3978	-1.0148	-0.3600	0.0253
C(3)	-0.2341(7)	-1.1059(7)	-0.287(2)	0.025(4)	H(14)	-0.4298	-1.0421	-0.5928	0.0380
C(4)	-0.2873(7)	-1.0719(7)	-0.169(2)	0.026(4)	H(15)	-0.5060	-1.0933	-0.5610	0.0380
C(5)	-0.3682(7)	-1.1155(7)	-0.153(2)	0.033(4)	H(16)	-0.5420	-0.9857	-0.6837	0.0380
C(6)	-0.4251(7)	-1.0801(7)	-0.027(1)	0.025(4)	H(17)	-0.5084	-0.9061	-0.3030	0.0266
C(7)	-0.4677(7)	-1.0095(7)	-0.076(2)	0.029(4)	H(18)	-0.5908	-0.8824	-0.1153	0.0317
C(8)	-0.5051(8)	-1.0177(7)	-0.243(1)	0.023(4)	H(19)	-0.6445	-0.9514	-0.1538	0.0317
C(9)	-0.4443(6)	-1.0465(7)	-0.363(1)	0.022(4)	H(20)	-0.6563	-0.8108	-0.2852	0.0329
C(10)	-0.4090(6)	-1.1243(6)	-0.312(2)	0.023(4)	H(21)	-0.7149	-0.8774	-0.3114	0.0329
C(11)	-0.4775(7)	-1.0464(7)	-0.530(2)	0.032(4)	H(22)	-0.5772	-0.8482	-0.4925	0.0317
C(12)	-0.5196(8)	-0.9730(7)	-0.579(2)	0.032(4)	H(23)	-0.6985	-1.0137	-0.4058	0.0329
C(13)	-0.5861(7)	-0.9550(7)	-0.463(1)	0.021(3)	H(24)	-0.6658	-1.0225	-0.5706	0.0329
C(14)	-0.5464(6)	-0.9459(6)	-0.297(1)	0.022(3)	H(25)	-0.6287	-1.0682	-0.4606	0.0329
C(15)	-0.6122(7)	-0.9130(7)	-0.196(2)	0.027(4)	H(26)	-0.5185	-1.1680	-0.2377	0.0431
C(16)	-0.6611(7)	-0.8628(7)	-0.314(2)	0.028(4)	H(27)	-0.4957	-1.1986	-0.4028	0.0431
C(17)	-0.6267(7)	-0.8751(7)	-0.479(1)	0.027(4)	H(28)	-0.4553	-1.2315	-0.2536	0.0431
C(18)	-0.6481(7)	-1.0177(7)	-0.463(1)	0.027(4)	H(29)	-0.7243	-0.9090	-0.5962	0.0380
C(19)	-0.4764(7)	-1.1847(7)	-0.299(2)	0.036(4)	H(30)	-0.6759	-0.8406	-0.8439	0.0697
C(20)	-0.6898(7)	-0.8660(7)	-0.607(2)	0.032(4)	H(31)	-0.5997	-0.8755	-0.7723	0.0697
C(21)	-0.6558(10)	-0.8780(9)	-0.776(2)	0.059(5)	H(32)	-0.6713	-0.9272	-0.8124	0.0697
C(22)	-0.7279(8)	-0.7865(7)	-0.598(2)	0.036(4)	H(33)	-0.6907	-0.7487	-0.6278	0.0418
C(23)	-0.7999(8)	-0.7790(8)	-0.707(2)	0.046(5)	H(34)	-0.7440	-0.7774	-0.4914	0.0418
C(24)	-0.8435(7)	-0.7065(8)	-0.698(2)	0.029(4)	H(35)	-0.7851	-0.7870	-0.8100	0.0507
C(25)	-0.6147(5)	-1.1453(6)	-0.813(1)	0.1023	H(36)	-0.8379	-0.8182	-0.6754	0.0507
C(26)	-0.6068(8)	-1.2088(8)	-0.702(1)	0.1023	H(37)	-0.1241	-1.0744	-0.2264	0.0418
C(27)	-0.5493(9)	-1.2661(7)	-0.729(2)	0.1023	H(38)	-0.4211	-0.9130	-0.5148	0.0317
H(1)	-0.3717	-1.1673	-0.5322	0.0380	H(39)	-0.8821	-0.6366	-0.8547	0.0532
H(2)	-0.3337	-1.2076	-0.4054	0.0380	H(40)	-0.3870	-0.9356	0.0180	0.0342
H(3)	-0.2401	-1.1313	-0.5230	0.0304	H(41)	-0.645(2)	-1.212(1)	-0.598(3)	0.1023
H(4)	-0.2880	-1.0590	-0.4806	0.0304	H(42)	-0.543(1)	-1.3148(8)	-0.644(2)	0.1023
H(5)	-0.2287	-1.1566	-0.2368	0.0304	H(43)	-0.510(2)	-1.262(1)	-0.836(3)	0.1023

CA·185 (bilayer)

atom	x	y	z	U	atom	x	y	z	U
O(1)	0.4035	0.0411	-0.1035	0.0563	H(7)	0.4605	-0.0727	0.0608	0.0649
O(2)	0.5656	-0.1899	0.2099	0.0540	H(8)	0.2559	-0.0805	0.1098	0.0482
O(3)	0.6850	0.3505	0.2762	0.0528	H(9)	0.3230	-0.2183	0.2442	0.0487
O(4)	1.1532	0.1109	0.7067	0.0782	H(10)	0.3737	-0.3067	0.1683	0.0487
O(5)	1.1971	0.3682	0.7580	0.0782	H(11)	0.5090	-0.2500	0.3194	0.0517
C(1)	0.3044	0.2613	0.0955	0.0455	H(12)	0.4590	0.0194	0.3580	0.0538
C(2)	0.3621	0.2342	0.0150	0.0678	H(13)	0.5093	0.1410	0.1887	0.0483
C(3)	0.3391	0.0552	-0.0356	0.0564	H(14)	0.4751	0.4146	0.2413	0.0735
C(4)	0.3818	-0.0800	0.0406	0.0541	H(15)	0.4508	0.3373	0.3337	0.0735
C(5)	0.3334	-0.0604	0.1341	0.0401	H(16)	0.6119	0.4624	0.3702	0.0583
C(6)	0.3726	-0.2054	0.2040	0.0406	H(17)	0.6646	0.0348	0.3167	0.0555
C(7)	0.4918	-0.1693	0.2684	0.0430	H(18)	0.6411	-0.1368	0.4820	0.0510
C(8)	0.5030	0.0117	0.3127	0.0449	H(19)	0.7143	-0.1903	0.4139	0.0510
C(9)	0.4660	0.1517	0.2345	0.0402	H(20)	0.7822	0.0108	0.5707	0.0573
C(10)	0.3394	0.1226	0.1799	0.0514	H(21)	0.8544	-0.0388	0.5010	0.0573
C(11)	0.4950	0.3277	0.2886	0.0612	H(22)	0.8230	0.2118	0.4212	0.0441
C(12)	0.6065	0.3548	0.3396	0.0486	H(23)	0.6159	0.3251	0.5370	0.0522
C(13)	0.6560	0.2114	0.4220	0.0886	H(24)	0.5148	0.2352	0.4688	0.0522
C(14)	0.6255	0.0347	0.3658	0.0462	H(25)	0.6055	0.1295	0.5395	0.0522
C(15)	0.6879	-0.0969	0.4436	0.0425	H(26)	0.2698	0.2617	0.2718	0.0801
C(16)	0.7862	0.0108	0.5051	0.0478	H(27)	0.1860	0.1342	0.2101	0.0801
C(17)	0.7818	0.1985	0.4683	0.0368	H(28)	0.2780	0.0707	0.2982	0.0801
C(18)	0.5921	0.2268	0.4990	0.0435	H(29)	0.7860	0.2768	0.5976	0.0555
C(19)	0.2608	0.1499	0.2464	0.0667	H(30)	0.8489	0.5574	0.5901	0.0615
C(20)	0.8241	0.3021	0.5495	0.0463	H(31)	0.8610	0.5271	0.4859	0.0615
C(21)	0.8189	0.4997	0.5308	0.0512	H(32)	0.7438	0.5332	0.5052	0.0615
C(22)	0.9610	0.2508	0.5929	0.0589	H(33)	0.9665	0.1309	0.5975	0.0707
C(23)	1.0147	0.3217	0.6880	0.0830	H(34)	0.9999	0.2903	0.5480	0.0707
C(24)	1.1369	0.2435	0.7250	0.0441	H(35)	1.0196	0.4413	0.6831	0.0996
H(1)	0.3234	0.3705	0.1226	0.0546	H(36)	0.9723	0.2943	0.7326	0.0996
H(2)	0.2263	0.2552	0.0687	0.0546	H(37)	0.3929	-0.0678	-0.1327	0.0676
H(3)	0.3372	0.3191	-0.0328	0.0814	H(38)	0.5585	-0.3011	0.1836	0.0649
H(4)	0.4399	0.2456	0.0416	0.0814	H(39)	0.7587	0.3682	0.3144	0.0634
H(5)	0.2623	0.0402	-0.0656	0.0677	H(40)	1.2421	0.3959	0.7155	0.0938
H(6)	0.3609	-0.1880	0.0124	0.0649					

CA·187 (bilayer)

atom	x	y	z	U	atom	x	y	z	U
O(1)	-0.6689	-1.3385	0.2325	0.0302(7)	H(12)	-0.6281	-0.8751	0.2855	0.0266
O(2)	-0.4204(3)	-0.9562(2)	-0.0382(4)	0.0292(7)	H(13)	-0.5762	-1.0466	0.1790	0.0266
O(3)	0.0861(3)	-0.5313(3)	0.1259(4)	0.0415(8)	H(14)	-0.6659	-0.9218	-0.0306	0.0317
O(4)	0.1074(3)	-0.4774(2)	-0.1243(4)	0.0341(7)	H(15)	-0.6339	-1.0148	-0.0852	0.0317
O(5)	-0.4921(3)	-1.0053(2)	0.4815(4)	0.0267(7)	H(16)	-0.4949	-0.8669	-0.1644	0.0329
O(6)	0.5122(3)	-0.1146(2)	-0.2621(4)	0.0312(7)	H(17)	-0.4149	-0.9109	0.2572	0.0253
O(7)	0.2449(3)	-0.5080(2)	-0.5977(4)	0.0323(7)	H(18)	-0.4500	-0.7282	0.4052	0.0342
O(8)	-0.2917(3)	-1.0126(3)	-0.7756(4)	0.0391(8)	H(19)	-0.3728	-0.7881	0.4796	0.0342
O(9)	-0.2702(3)	-0.9515(3)	-0.5217(4)	0.0387(8)	H(20)	-0.3027	-0.6370	0.2873	0.0317
O(10)	0.3265(3)	-0.4345(2)	-0.0501(4)	0.0269(7)	H(21)	-0.2323	-0.7076	0.3392	0.0317
N(1)	0.0564(5)	-1.0311(5)	-0.3146(8)	0.102(2)	H(22)	-0.2848	-0.7976	0.1109	0.0291
N(2)	-0.134(1)	-0.341(1)	-0.798(2)	0.257(7)	H(23)	-0.5174	-0.7137	-0.0423	0.0380
C(1)	-0.7978(3)	-1.1498(3)	0.0585(5)	0.0306(10)	H(24)	-0.4900	-0.6791	0.1398	0.0380
C(2)	-0.7335(4)	-1.2269(3)	0.0628(5)	0.0290(10)	H(25)	-0.5975	-0.7664	0.0840	0.0380
C(3)	-0.7369(3)	-1.2716(3)	0.2276(5)	0.0278(9)	H(26)	-0.8301	-0.9691	0.0769	0.0418
C(4)	-0.6918(4)	-1.1925(3)	0.3626(5)	0.0261(9)	H(27)	-0.8128	-0.9522	0.2646	0.0418
C(5)	-0.7484(3)	-1.1094(3)	0.3563(5)	0.0279(10)	H(28)	-0.9080	-1.0430	0.1849	0.0418
C(6)	-0.6958(4)	-1.0301(3)	0.4935(5)	0.0289(10)	H(29)	-0.3049	-0.6182	0.0007	0.0304
C(7)	-0.5807(4)	-0.9575(3)	0.4642(5)	0.0235(9)	H(30)	-0.3805	-0.7324	-0.2140	0.0431
C(8)	-0.5810(3)	-0.9162(3)	0.2949(5)	0.0221(8)	H(31)	-0.2766	-0.7724	-0.1999	0.0431
C(9)	-0.6274(3)	-0.9994(3)	0.1611(5)	0.0213(8)	H(32)	-0.2638	-0.6659	-0.2573	0.0431
C(10)	-0.7503(3)	-1.0634(3)	0.1876(5)	0.0261(9)	H(33)	-0.1281	-0.6217	0.1446	0.0380
C(11)	-0.6149(4)	-0.9592(3)	-0.0086(5)	0.0269(9)	H(34)	-0.1121	-0.6911	0.0074	0.0367
C(12)	-0.4952(3)	-0.8946(3)	-0.0345(5)	0.0261(9)	H(35)	-0.1078	-0.4945	-0.0343	0.0456
C(13)	-0.4521(3)	-0.8088(3)	0.0931(5)	0.0226(9)	H(36)	-0.0922	-0.5639	-0.1719	0.0456
C(14)	-0.4616(3)	-0.8533(3)	0.2635(5)	0.0212(8)	H(37)	-0.6785	-1.3855	0.3056	0.0380
C(15)	-0.4007(4)	-0.7657(3)	0.3814(5)	0.0287(10)	H(38)	-0.4154	-0.9723	0.0808	0.0380
C(16)	-0.3029(4)	-0.7041(3)	0.2887(5)	0.0270(9)	H(39)	0.1803	-0.4706	-0.1001	0.0405
C(17)	-0.3225(3)	-0.7508(3)	0.1119(5)	0.0239(9)	H(40)	-0.4895	-1.0364	0.5793	0.0317
C(18)	-0.5211(4)	-0.7354(3)	0.0658(5)	0.031(1)	H(41)	0.6083	-0.3495	-0.5214	0.0367
C(19)	-0.8330(4)	-1.0006(3)	0.1783(6)	0.036(1)	H(42)	0.6984	-0.2896	-0.3859	0.0367
C(20)	-0.2720(3)	-0.6752(3)	-0.0130(5)	0.0259(9)	H(43)	0.5974	-0.1875	-0.4929	0.0329
C(21)	-0.3005(4)	-0.7160(3)	-0.1883(5)	0.036(1)	H(44)	0.4845	-0.2635	-0.4557	0.0329
C(22)	-0.1428(4)	-0.6384(3)	0.0306(5)	0.0296(10)	H(45)	0.6524	-0.1543	-0.2215	0.0355
C(23)	-0.0791(4)	-0.5479(3)	-0.0577(5)	0.036(1)	H(46)	0.5433	-0.2293	-0.0242	0.0317
C(24)	0.0465(4)	-0.5182(3)	-0.0070(5)	0.0289(10)	H(47)	0.4476	-0.2881	-0.1539	0.0317
C(25)	0.6195(3)	-0.3186(3)	-0.4141(5)	0.0298(10)	H(48)	0.6574	-0.3210	-0.0913	0.0342
C(26)	0.5630(3)	-0.2363(3)	-0.4200(5)	0.0271(9)	H(49)	0.5755	-0.4633	0.0271	0.0380
C(27)	0.5737(3)	-0.1868(3)	-0.2538(5)	0.0286(10)	H(50)	0.5254	-0.3855	0.0997	0.0380
C(28)	0.5276(4)	-0.2625(3)	-0.1298(5)	0.0270(9)	H(51)	0.3879	-0.5412	0.0235	0.0317
C(29)	0.5786(3)	-0.3489(3)	-0.1258(5)	0.0277(10)	H(52)	0.4403	-0.5838	-0.2143	0.0279
C(30)	0.5280(4)	-0.4236(3)	0.0018(5)	0.031(1)	H(53)	0.4041	-0.4171	-0.3538	0.0266
C(31)	0.4075(4)	-0.4897(3)	-0.0515(5)	0.0269(9)	H(54)	0.4780	-0.5563	-0.5152	0.0304
C(32)	0.3984(3)	-0.5379(3)	-0.2202(5)	0.0235(9)	H(55)	0.4538	-0.4646	-0.5932	0.0304
C(33)	0.4481(3)	-0.4622(3)	-0.3475(5)	0.0221(8)	H(56)	0.3083	-0.6117	-0.6713	0.0329
C(34)	0.5726(3)	-0.4001(3)	-0.2945(5)	0.0259(9)	H(57)	0.2360	-0.5475	-0.2950	0.0253
C(35)	0.4312(4)	-0.5154(3)	-0.5164(5)	0.0270(9)	H(58)	0.2533	-0.7141	-0.1319	0.0355
C(36)	0.3092(4)	-0.5769(3)	-0.5711(5)	0.0261(9)	H(59)	0.1881	-0.6419	-0.0815	0.0355
C(37)	0.2612(3)	-0.6527(3)	-0.4455(5)	0.0219(9)	H(60)	0.0927	-0.8014	-0.2733	0.0380
C(38)	0.2759(3)	-0.5957(3)	-0.2802(5)	0.0213(8)	H(61)	0.0401	-0.7152	-0.2585	0.0380
C(39)	0.2089(4)	-0.6730(3)	-0.1713(5)	0.0287(10)	H(62)	0.0944	-0.6551	-0.4923	0.0291
C(40)	0.1052(4)	-0.7320(3)	-0.2851(5)	0.033(1)	H(63)	0.2840	-0.7852	-0.3762	0.0380
C(41)	0.1304(3)	-0.7040(3)	-0.4636(5)	0.0242(9)	H(64)	0.3217	-0.7582	-0.5478	0.0380
C(42)	0.3225(4)	-0.7328(3)	-0.4407(5)	0.030(1)	H(65)	0.3985	-0.7053	-0.3943	0.0380
C(43)	0.6520(4)	-0.4665(3)	-0.2865(6)	0.039(1)	H(66)	0.6240	-0.5206	-0.2223	0.0456
C(44)	0.0789(3)	-0.7927(3)	-0.5859(5)	0.0264(9)	H(67)	0.6548	-0.4903	-0.3957	0.0456
C(45)	0.1063(4)	-0.7682(3)	-0.7588(5)	0.034(1)	H(68)	0.7260	-0.4283	-0.2449	0.0456
C(46)	-0.0509(4)	-0.8311(3)	-0.5807(5)	0.032(1)	H(69)	0.1103	-0.8440	-0.5533	0.0329
C(47)	-0.1037(4)	-0.9381(3)	-0.6488(6)	0.035(1)	H(70)	0.0708	-0.8249	-0.8290	0.0431
C(48)	-0.2316(4)	-0.9722(3)	-0.6577(5)	0.0287(10)	H(71)	0.1859	-0.7497	-0.7633	0.0431
C(49)	-0.0111(5)	-1.0366(5)	-0.2289(7)	0.063(2)	H(72)	0.0789	-0.7148	-0.7919	0.0431
C(50)	-0.0983(4)	-1.0409(4)	-0.1238(6)	0.047(1)	H(73)	-0.0663	-0.8286	-0.4673	0.0380
C(51)	-0.1304(5)	-1.1194(5)	-0.0298(7)	0.064(2)	H(74)	-0.0852	-0.7888	-0.6379	0.0380
C(52)	-0.1464(5)	-0.9575(4)	-0.1277(6)	0.056(2)	H(75)	-0.0810	-0.9420	-0.7544	0.0456
C(53)	-0.088(1)	-0.3523(9)	-0.675(2)	0.167(6)	H(76)	-0.0752	-0.9812	-0.5807	0.0456
C(54)	-0.0337(7)	-0.3693(7)	-0.531(1)	0.097(3)	H(77)	0.5351	-0.0680	-0.1811	0.0380
C(55)	-0.005(1)	-0.2969(7)	-0.404(1)	0.181(5)	H(78)	0.1844	-0.5240	-0.6896	0.0380
C(56)	-0.0116(8)	-0.4570(8)	-0.5203(9)	0.126(4)	H(79)	-0.3449	-0.9565	-0.5369	0.0456
H(1)	-0.8747	-1.1818	0.0740	0.0367	H(80)	0.3307	-0.4059	0.0626	0.0444
H(2)	-0.7948	-1.1218	-0.0468	0.0367	H(81)	-0.1870	-1.1238	0.0415	0.0786
H(3)	-0.7673	-1.2775	-0.0187	0.0329	H(82)	-0.0945	-1.1707	-0.0332	0.0786
H(4)	-0.6567	-1.1954	0.0441	0.0329	H(83)	-0.0885	-0.8974	-0.1001	0.0669
H(5)	-0.8175	-1.3091	0.2328	0.0329	H(84)	-0.1798	-0.9538	-0.2372	0.0669
H(6)	-0.7036	-1.2239	0.4639	0.0304	H(85)	-0.2032	-0.9675	-0.0565	0.0669
H(7)	-0.6127	-1.1640	0.3572	0.0304	H(86)	0.0340	-0.3104	-0.3014	0.2226
H(8)	-0.8221	-1.1391	0.3808	0.0329	H(87)	-0.0202	-0.2352	-0.4081	0.2226
H(9)	-0.7469	-0.9941	0.5094	0.0380	H(88)	-0.0799	-0.5062	-0.5331	0.1510
H(10)	-0.6850	-1.0645	0.5899	0.0380	H(89)	0.0366	-0.4587	-0.5981	0.1510
H(11)	-0.5548	-0.9001	0.5791	0.0291	H(90)	0.0256	-0.4551	-0.4128	0.1510

CA·187 (crossing)

atom	x	y	z	U	atom	x	y	z	U
O(1)	0.1578(2)	-0.0599(2)	-0.2268(3)	0.0350(9)	H(7)	0.2987	-0.0217	-0.3081	0.0329
O(2)	0.4638(2)	0.0884(2)	0.0748(3)	0.0261(8)	H(8)	0.3431	-0.1648	-0.3764	0.0329
O(3)	0.8447(4)	0.3445(3)	0.2406(6)	0.156(3)	H(9)	0.3952	-0.0756	-0.5779	0.0380
O(4)	0.8890(2)	0.2937(2)	0.0338(4)	0.050(1)	H(10)	0.4704	-0.1067	-0.5001	0.0380
O(5)	0.4159(2)	0.0562(2)	-0.4430(4)	0.0359(9)	H(11)	0.5019	0.0051	-0.5165	0.0329
N(1)	0.8784(3)	0.0932(3)	0.8828(6)	0.058(2)	H(12)	0.5424	-0.0567	-0.2902	0.0291
C(1)	0.3467(3)	-0.1519(2)	-0.0821(5)	0.026(1)	H(13)	0.3960	-0.0147	-0.1416	0.0253
C(2)	0.2700(3)	-0.1064(2)	-0.0716(5)	0.027(1)	H(14)	0.5110	-0.0875	0.0307	0.0253
C(3)	0.2308(3)	-0.1038(3)	-0.2300(5)	0.028(1)	H(15)	0.4342	-0.0520	0.0910	0.0253
C(4)	0.2858(3)	-0.0707(3)	-0.3498(5)	0.028(1)	H(16)	0.5421	0.0161	0.1665	0.0279
C(5)	0.3666(3)	-0.1134(3)	-0.3603(5)	0.028(1)	H(17)	0.5063	0.0909	-0.1997	0.0279
C(6)	0.4228(3)	-0.0788(3)	-0.4812(5)	0.032(1)	H(18)	0.5892	0.1189	-0.3984	0.0329
C(7)	0.4670(3)	-0.0082(3)	-0.4300(5)	0.028(1)	H(19)	0.6431	0.0496	-0.3687	0.0329
C(8)	0.5048(3)	-0.0165(3)	-0.2710(5)	0.024(1)	H(20)	0.7147	0.1107	-0.1997	0.0329
C(9)	0.4425(2)	-0.0455(2)	-0.1515(5)	0.021(1)	H(21)	0.6607	0.1880	-0.2213	0.0329
C(10)	0.4080(3)	-0.1224(2)	-0.2014(5)	0.026(1)	H(22)	0.5862	0.1620	-0.0231	0.0279
C(11)	0.4749(3)	-0.0450(2)	0.0151(5)	0.020(1)	H(23)	0.6718	-0.0201	0.0526	0.0329
C(12)	0.5195(3)	0.0261(2)	0.0646(5)	0.023(1)	H(24)	0.6906	-0.0058	-0.1207	0.0329
C(13)	0.5855(2)	0.0453(2)	-0.0526(5)	0.021(1)	H(25)	0.6253	-0.0634	-0.0742	0.0329
C(14)	0.5459(2)	0.0538(3)	-0.2127(5)	0.023(1)	H(26)	0.5023	-0.1887	-0.1176	0.0405
C(15)	0.6114(3)	0.0880(3)	-0.3144(5)	0.027(1)	H(27)	0.5127	-0.1689	-0.2911	0.0405
C(16)	0.6629(3)	0.1357(3)	-0.2020(6)	0.028(1)	H(28)	0.4523	-0.2304	-0.2418	0.0405
C(17)	0.6277(2)	0.1231(2)	-0.0342(5)	0.023(1)	H(29)	0.7323	0.0931	0.0708	0.0317
C(18)	0.6487(3)	-0.0169(2)	-0.0491(6)	0.028(1)	H(30)	0.6544	0.0642	0.2623	0.0405
C(19)	0.4740(3)	-0.1825(3)	-0.2139(6)	0.034(1)	H(31)	0.6192	0.1482	0.2960	0.0405
C(20)	0.6930(3)	0.1322(2)	0.0910(5)	0.026(1)	H(32)	0.7000	0.1249	0.3353	0.0405
C(21)	0.6618(3)	0.1166(3)	0.2533(5)	0.034(1)	H(33)	0.6840	0.2442	0.0995	0.0342
C(22)	0.7301(3)	0.2108(2)	0.0813(5)	0.029(1)	H(34)	0.7368	0.2269	-0.0276	0.0342
C(23)	0.8032(3)	0.2201(3)	0.1851(6)	0.046(2)	H(35)	0.8320	0.1726	0.1670	0.0545
C(24)	0.8473(3)	0.2921(3)	0.1601(6)	0.045(2)	H(36)	0.7966	0.2067	0.2970	0.0545
C(25)	0.8915(3)	0.1427(3)	0.8026(7)	0.041(2)	H(37)	0.1292	-0.0549	-0.1273	0.0418
C(26)	0.9098(3)	0.2056(3)	0.7018(6)	0.043(2)	H(38)	0.4303	0.0870	0.1668	0.0304
C(27)	0.8561(4)	0.2265(3)	0.5995(7)	0.062(2)	H(39)	0.9290	0.3329	0.0313	0.0608
C(28)	0.9900(4)	0.2421(3)	0.7230(8)	0.065(2)	H(40)	0.3872	0.0774	-0.3570	0.0431
H(1)	0.3744	-0.1607	0.0119	0.0317	H(41)	0.8582	0.2699	0.5252	0.0760
H(2)	0.3326	-0.2007	-0.1208	0.0317	H(42)	0.8015	0.2012	0.5897	0.0760
H(3)	0.2831	-0.0531	-0.0637	0.0317	H(43)	0.9989	0.2606	0.8317	0.0798
H(4)	0.2314	-0.1159	0.0085	0.0317	H(44)	1.0357	0.2064	0.7109	0.0798
H(5)	0.2150	-0.1527	-0.2687	0.0329	H(45)	1.0031	0.2838	0.6591	0.0798
H(6)	0.2613	-0.0633	-0.4492	0.0329					

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atom	x	y	z	U	atom	x	y	z	U
O(1)	1.3362(2)	-0.0579(2)	0.1913(5)	0.0509(10)	H(6)	1.2357	-0.0707	0.4299	0.0452
O(2)	1.0798(2)	0.0522(2)	0.4145(4)	0.0419(8)	H(7)	1.1971	-0.0207	0.3007	0.0452
O(3)	1.0333(2)	0.0831(2)	-0.1075(4)	0.0395(8)	H(8)	1.1432	-0.1639	0.3818	0.0423
O(4)	0.6465(4)	0.3347(3)	-0.0760(5)	0.083(2)	H(9)	1.0356	-0.1192	0.4979	0.0472
O(5)	0.6172(3)	0.3137(2)	-0.3266(5)	0.0497(10)	H(10)	1.1054	-0.0694	0.5587	0.0472
O(6)	0.8926(5)	-0.1440(4)	-0.3392(9)	0.115(2)	H(11)	0.9860	-0.0023	0.4924	0.0477
O(7)	0.8382(4)	-0.1943(4)	-0.1390(8)	0.102(2)	H(12)	0.9477	-0.0582	0.2669	0.0339
N(1)	0.8900(4)	-0.1927(4)	-0.2430(8)	0.079(2)	H(13)	1.0942	-0.0136	0.1332	0.0399
C(1)	1.1488(3)	-0.1547(3)	0.0628(6)	0.041(1)	H(14)	1.0594	-0.0567	-0.1112	0.0490
C(2)	1.2241(3)	-0.1082(3)	0.0477(6)	0.042(1)	H(15)	0.9787	-0.0880	-0.0477	0.0490
C(3)	1.2653(3)	-0.1033(3)	0.2086(6)	0.041(1)	H(16)	0.9493	0.0155	-0.1850	0.0399
C(4)	1.2088(3)	-0.0716(3)	0.3309(6)	0.037(1)	H(17)	0.9908	0.0864	0.1880	0.0398
C(5)	1.1297(3)	-0.1155(3)	0.3448(6)	0.036(1)	H(18)	0.8502	0.0490	0.3493	0.0560
C(6)	1.0733(3)	-0.0822(3)	0.4692(6)	0.040(1)	H(19)	0.9065	0.1161	0.3836	0.0560
C(7)	1.0279(3)	-0.0113(3)	0.4184(6)	0.038(1)	H(20)	0.7787	0.1205	0.1894	0.0510
C(8)	0.9888(3)	-0.0207(2)	0.2553(6)	0.0323(10)	H(21)	0.8374	0.1864	0.2175	0.0510
C(9)	1.0504(3)	-0.0479(3)	0.1315(6)	0.0314(9)	H(22)	0.9108	0.1599	0.0017	0.0412
C(10)	1.0871(3)	-0.1250(3)	0.1813(7)	0.038(1)	H(23)	0.8017	-0.0023	0.1024	0.0542
C(11)	1.0166(3)	-0.0482(3)	-0.0372(6)	0.040(1)	H(24)	0.8208	-0.0182	-0.0741	0.0542
C(12)	0.9754(3)	0.0237(3)	-0.0856(5)	0.034(1)	H(25)	0.8653	-0.0620	0.0580	0.0542
C(13)	0.9090(3)	0.0453(3)	0.0338(5)	0.0315(9)	H(26)	0.9814	-0.1686	0.2716	0.0611
C(14)	0.9483(3)	0.0507(3)	0.1966(5)	0.0314(9)	H(27)	0.9962	-0.1925	0.0975	0.0611
C(15)	0.8835(3)	0.0863(3)	0.3004(6)	0.045(1)	H(28)	1.0433	-0.2308	0.2335	0.0611
C(16)	0.8349(3)	0.1364(3)	0.1868(6)	0.042(1)	H(29)	0.7644	0.1006	-0.0949	0.0496
C(17)	0.8694(3)	0.1239(3)	0.0177(6)	0.0347(10)	H(30)	0.8630	0.0756	-0.2860	0.0729
C(18)	0.8428(3)	-0.0148(3)	0.0289(7)	0.042(1)	H(31)	0.7974	0.1281	-0.3543	0.0729
C(19)	1.0207(3)	-0.1853(3)	0.1976(8)	0.050(1)	H(32)	0.8795	0.1606	-0.3009	0.0729
C(20)	0.8062(3)	0.1363(3)	-0.1123(6)	0.039(1)	H(33)	0.7535	0.2253	0.0062	0.0499
C(21)	0.8391(4)	0.1230(4)	-0.2779(7)	0.057(2)	H(34)	0.8057	0.2513	-0.1355	0.0499
C(22)	0.7684(3)	0.2153(3)	-0.1001(6)	0.040(1)	H(35)	0.7073	0.2124	-0.3104	0.0726
C(23)	0.6928(4)	0.2222(3)	-0.2001(8)	0.061(2)	H(36)	0.6554	0.1838	-0.1703	0.0726
C(24)	0.6508(3)	0.2963(3)	-0.1919(8)	0.048(1)	H(37)	1.3701	-0.0616	0.2991	0.0736
C(25)	0.9475(7)	-0.2520(5)	-0.239(2)	0.121(4)	H(38)	1.1185	0.0576	0.5147	0.0736
H(1)	1.1228	-0.1581	-0.0376	0.0518	H(39)	1.0583	0.1090	-0.0226	0.0736
H(2)	1.1642	-0.2043	0.0947	0.0518	H(40)	0.5999	0.3716	-0.3251	0.0736
H(3)	1.2597	-0.1307	-0.0288	0.0543	H(41)	0.9240	-0.3008	-0.2381	0.1495
H(4)	1.2103	-0.0595	0.0092	0.0543	H(42)	0.9871	-0.2506	-0.3213	0.1495
H(5)	1.2811	-0.1514	0.2417	0.0500	H(43)	0.9797	-0.2498	-0.1383	0.1495

References

Introduction

[1] a) J.-M. Lehn, *Supramolecular Chemistry*, VCH, Weinhheim, **1995**. b) J.-M. Lehn, J. L. Atwood, J. E. D. Davies, D. D. MacNicol, F. Vögtle, *Comprehensive Supramolecular Chemistry*, Pergamon, New York, **1996**.

[2] a) G. W. Gokel, *Crown Ethers and Cryptands*, Royal Society of Chemistry, Cambridge, **1994**. b) *Comprehensive Supramolecular Chemistry, Molecular Recognition: Receptors for Cationic Guests, Vol. 1,* (Eds.: G. W. Gokel), Pergamon, New York, **1996**.

[3] a) D. J. Cram, *Science*, **1994**, *219*, 1177-1183. b) D. J. Cram, *Nature*, **1992**, *356*, 29-36. c) A. Jasat, J. C. Sherman, *Chemical Reviews*, **1999**, *99*, 931-967. d) *Comprehensive Supramolecular Chemistry, Molecular Recognition: Receptors for Molecular Guests, Vol. 2,* (Eds.: F. Vögtle), Pergamon, New York, **1996**.

[4] a) K. A. Connors, *Chemical Reviews*, **1997**, *97*, 1325-1357. b) *Comprehensive Supramolecular Chemistry, Cyclodextrins, Vol. 3,* (Eds.: J. Szejtli, T. Osa), Pergamon, New York, **1996**.

[5] a) S. Ibach, V. Prautzsch, F. Vögtle, C. Chartroux, K. Gloe, *Acc. Chem. Res.*, **1999**, *32*, 729-740. b) A. Ikeda, S. Shinkai, *Chemical Reviews*, **1997**, *97*, 1713-1734.

[6] a) A. I. Kitaigorodskii, *Molecular Crystals and Molecules*, Academic Press, New York, **1973**. b) G. R. Desiraju, *Crystal Engineering: The Design of Organic Solids*, Elsevier, New York, **1989**. c) A. Gavezzotti, *Acc. Chem. Res.*, **1994**, *27*, 309-314.

[7] a) D. D. MacNicol, J. J. McKendrick, D. R. Wilson, *Chem. Soc. Rev.*, **1978**, *7*, 66-87. b) J. E. D. Davies, W. Kemula, H. M. Powell, N. O. Smith, *J. Incl. Phenom.,* **1983**, *1*, 3-44. c) *Top. Curr. Chem.,* **1988**, *140* and **1988**, *149*. d) *Inclusion Compounds, Vol. 1-3* and *4-5,* (Eds.: J. L. Atwood, J. E. D. Davies, D. D. MacNicol), Academic Press, London, **1984**, and Oxford Press, Oxford, **1991**. e) *Comprehensive Supramolecular Chemistry, Solid-State Supramolecular Chemistry: Crystal Engineering, Vol. 6,* (Eds.: D. D. MacNicol, F. Toda, R. Bishop), Pergamon, New York, **1996**. f) R. Bishop, *Chem. Soc. Rev.* **1996**, 311-319.

[8] D. Lawton, H. M. Powell, *J., Am. Chem. Soc.*, **1958**, 2339-2357.

[9] M. Miyata, K. Sada, *Comprehensive Supramolecular Chemistry, Solid-state Supramolecular Chemistry: Crystal Engineering, Vol. 6* (Eds.: D. D. MacNicol, F. Toda, R. Bishop), Pergamon, Oxford, **1996**, 147-176.

[10] K. Nakano, Y. Kurozumi, K. Sada, M. Miyata, *Chem. Eur. J.*, **2001**, *7*, 209-220.

[11] a) A. P. Davis, *Chem. Soc. Rev.* **1993**, *22*, 243-253. b) A. P. Davis, R. P. Bonar-law, J. K. M. Sanders, *Comprehesive Supramolecular Chemistry, Supramolecular Reactivity and Transport: Bioorganic Systems, Vol. 4,* (Eds.: Y. Murakami), Pergamon, New York, **1996**,

257-286. c) Y. Li, J. R. Dias, *Chem. Rev.*, **1997**, *97*, 283-304. d) P. Wallimann, T. Marti, A. Fürer, F. Diederich, *Chem. Rev.* **1997**, *97*, 1567-1608.

[12] a) P. Latschinoff, *Chem. Ber.* **1885**, *18*, 3039. b) P. L. Johnson, J. P. Schaefer, *Acta Crystallogr.*, **1972**, *B28*, 3083-3088. c) E. L. Jones, L. R. Nassimbeni, *Acta Crystallogr.*, **1990**, *B46*, 399-405.

[13] a) M. Miyata, M. Shibakami, W. Goonewardena, K. Takemoto, *Chem. Lett.*, **1987**, 605-608. b) K. Miki, A. Masui, N. Kasai. M. Miyata, M. Shibakami, K. Takemoto, *J. Am. Chem. Soc.*, **1988**, *110*, 6594-6596. c) K. Miki, N. Kasai, M. Shibakami, K. Takemoto, M. Miyata, *J. Chem. Soc., Chem. Commun.*, **1991**, 1757-1759.

[14] a) M. R. Caira, L. R. Nassimbeni, J. L. Scott, *J. Chem. Soc., Chem. Commun.*, **1993**, 612-613. b) M. R. Caira, L. R. Nassimbeni, J. L. Scott, *J. Chem. Soc., Perkin Trans.2*, **1994**, 623-628. c) M. R. Caira, L. R. Nassimbeni, J. L. Scott, *J. Chem. Soc., Perkin Trans.2*, **1994**, 1403-1405.

Chapter 1

[1] a) E. Giglio, *Inclusion Compounds, Vol. 2*, (Eds.: J. L. Atwood, J. E. D. Davies, D. D. MacNicol), Academic Press, **1984**, 207-229. b) K. Padmanabhan, K. Venkatesan, V. Ramamurthy, *Can. J. Chem.*, **1984**, *62*, 2025-2028. c) E. Giglio, F. Mazza, L. Scaramuzza, *J. Inclu. Phenom.*, **1985**, *3*, 437. d) R. Popovitz-Biro, C. P. Tang, H. C. Chang, M. Lahav, L. Leiserowitz, *J. Am. Chem. Soc.*, **1985**, *107*, 4043-4058. e) C. P. Tang, H. C. Chang, R. Popovitz-Biro, F. Frolow, M. Lahav, L. Leiserowitz, R. K. McMullan, *J. Am. Chem. Soc.*, **1985**, *107*, 4058-4070. f) L. R. Nassimbeni, M. L. Niven, D. A. Stuart, K. J. Zemke, *J. Crystallogr. Spectrosc. Res.*, **1986**, *16*, 557-567. g) H. C. Chang, R. Popovitz-Biro, M. Lahav, L. Leiserowitz, *J. Am. Chem. Soc.*, **1987**, *109*, 3883-3893. h) T. Oguchi, S. Limmatvapirat, C. takahashi, S. Sungthongjeen, W. S. Choi, E. Yonemochi, K. Yamamoto, *Bull. Chem. Soc. Jpn.*, **1998**, *71*, 1573-1579.

[2] a) M. Miyata, *Nippon Kagaku Kaishi*, **1993**, 128-138. b) M. Miyata, *Seibutu Buturi*, **1992**, *32*, 169-173.

[3] K. Miki, A. Masui, N. Kasai, M. Miyata, M. Shibakami, K. Takemoto, *J. Am. Chem. Soc.*, **1988**, *110*, 6594-6596.

[4] M. Miyata, K. Sada, S. Hori, K. Miki, *Mol. Cryst. Liq. Cryst.*, **1992**, *219*, 71-74.

[5] M. Miyata, M. Shibakami, S. Chirachanchai, K. Takemoto, N. Kasai, K. Miki, *Nature*, **1990**, *343*, 446-447.

[6] K. Miki, N. Kasai, M. Shibakami, K. Takemoto, M. Miyata, *J. Chem. Soc., Chem. Commun.*, **1991**, 1757-1759.

[7] M. Miyata, M. Shibakami, K. Takemoto, *J. Chem. Soc., Chem. Commun.*, **1988**, 655-656.

[8] M. Miyata, M. Shibakami, W. Goonewardena, K. Takemoto, *Chem. Lett.*, **1987**, 605-608.

[9] TEXSAN, XRAY Structure Analysis Package; Molecular Structure Corporation: The Woodlands, TX, **1985**.

[10] a) P. L. Johnson, J. P. Schaefer, *Acta Crystallogr.*, **1972**, *B28*, 3083-3088. b) E. L. Jones, L. R. Nassimbeni, *Acta Crystallogr.*, **1990**, *B46*, 399-405.

[11] K. Sada, T. Kondo, M. Miyata, K. Miki, *J. Chem. Soc., Chem. Commun.*, **1993**, 753-755.

[12] M. R. Caira, L. R. Nassimbeni, J. L. Scott, *J. Chem. Soc., Chem. Commun.*, **1993**, 612-613.

[13] a) M. Miyata, *Polymerization in Organized Media*, (Eds.: C. M. Paleos), Gordon and Breach, New York, **1992**, 327. b) W. Goonewardena, M. Miyata, K. Takemoto, *Polym. J.*, **1993**, *25*, 731-740.

Chapter 2

[1] a) S. Ibach, V. Prautzsch, F. Vögtle, *Acc. Chem. Res.*, **1999**, *32*, 729-740. b) A. Jasat, J. C. Sherman, *Chem. Rev.*, **1999**, *99*, 931-967. c) K. A. Connors, *Chem. Rev.*, **1997**, *97*, 1325-1357. d) M. M. Conn, J. Jr. Rebek, *Chem. Rev.*, **1997**, *97*, 1647-1668. e) A. Ikeda, S. Shinkai, *Chem. Rev.*, **1997**, *97*, 1713-1734. f) *Comprehesive Supramolecular Chemistry, Vol. 1-3*, (Eds.: J.-M. Lehn, J. L. Atwood, J. E. D. Davies, D. D. MacNicol, F. Vögtle), Pergamon, New York, **1996**.

[2] S. Mecozzi, J. Jr. Rebek, *Chem. Eur. J.*, **1998**, *4*, 1016-1022.

[3] a) Y. Ohashi, K. Yanagi, T. Kurihara, Y. Sasada, Y. Ohgo, *J. Am. Chem. Soc.*, **1981**, *103*, 5805-58121. b) Y. Ohashi, *Acc. Chem. Res.* **1988**, *21*, 268-274. c) Y. Ohahsi, in *Reactivity in Molecular Crystals*, Kodansha, Tokyo, **1993**, 115-153. d) T. Yamada, Y. Ohashi, *Bull. Chem. Soc. Jpn.* **1998**, *72*, 2527-2537.

[4] a) R. Arad-Yellin, B. S. Green, M. Knossow, G. Tsoucaris, *J. Am. Chem. Soc.* **1983**, *105*, 4561-4571. b) R. Gerdil, *Top. Curr. Chem.*, **1987**, 140, 72-105, c) R. Gerdil, *Comprehesive Supramolecular Chemistry, Solid-State Supramolecular Chemistry: Crystal Engineering, Vol. 6*, (Eds.: D. D. MacNicol, F. Toda, R. Bishop), Pergamon, New York, **1996**, 239-280.

[5] a) D. D. MacNicol, J. J. McKendrick, D. R. Wilson, *Chem. Soc. Rev.*, **1978**, *7*, 66-87. b) J. E. D. Davies, W. Kemula, H. M. Powell, N. O. Smith, *J. Incl. Phenom.*, **1983**, *1*, 3-44. c) *Top. Curr. Chem.*, **1988**, *140* and **1988**, *149*. d) *Inclusion Compounds, Vol. 1-3* and *4-5*, (Eds.: J. L. Atwood, J. E. D. Davies, D. D. MacNicol), Academic Press, London, **1984**, and Oxford Press, Oxford, **1991**. e) *Comprehesive Supramolecular Chemistry, Solid-State Supramolecular Chemistry: Crystal Engineering, Vol. 6*, (Eds.: D. D. MacNicol, F. Toda, R. Bishop), Pergamon, New York, **1996**. f) R. Bishop, *Chem. Soc. Rev.*, **1996**, 311-319.

[6] D. Lawton, H. M. Powell, *J. Chem. Soc.*, **1958**, 2339-2357.

[7] K. Biradha, D. Dennis, V. A. MacKinnon, C. V. K. Sharma, M. J. Zaworotko, *J. Am. Chem.*

Soc. **1998**, *120,* 11894-11903.

[8] M. D. Hollingsworth, D. B. Santarsiero, K. D. M. Harris, *Angew. Chem. Int. Ed. Engl.*, **1994**, *33*, 649-652.

[9] A. T. Ung, D. Gizachew, R. Bishop, M. L. Scudder, I. G. Dance, D. C. Craig, *J. Am. Chem. Soc.* **1995**, *117*, 8745-8756.

[10] Y. Endo, T. Ezuhara, M. Koyanagi, H. Masuda, Y. Aoyama, *J. Am. Chem. Soc.,* **1997**, *119*, 499-505.

[11] M. P. Byrn, C. J. Curtis, Y. Hsiou, S. I. Khan, P. A. Sawin, S. K. Tendick, A. Terzis, C. E. Strouse, *J. Am. Chem. Soc.*, **1993**, *115*, 9480-9497.

[12] M. Gdaniec, B. T. Ibragimov, S. A. Talipov, *Comprehesive Supramolecular Chemistry*, *Solid-State Supramolecular Chemistry: Crystal Engineering*, *Vol. 6*, (Eds.: D. D. MacNicol, F. Toda, R. Bishop), Pergamon, New York, **1996**,117-145.

[13] a) K. Beketov, E. Weber, J. Seidel, K. Köhnke, K. Makhkamov, B. Ibragimov, *J. Chem. Soc., Chem. Commun.*, **1999**, 91-92. b) B. Ibragimov, K. Beketov, K. Makhkamov, E. Weber, *J. Chem. Soc., Perkin Trans.2*, **1997**, 1349-1352.

[14] a) V. A. Russell, C. C. Evans, W. Li, M. D. Ward, *Science*, **1997**, *276*, 575-579. b) J. A. Swift, A. M. Pivovar, A. M. Reynolds, M. D. Ward, *J. Am. Chem. Soc.,* **1998**, *120*, 5887-5897. c) C. C. Evans, L. Sukarto, M. D. Ward, *J. Am. Chem. Soc.,* **1999**, *121*, 320-325.

[15] a) M. Miyata, K. Sada, *Comprehesive Supramolecular Chemistry*, *Solid-State Supramolecular Chemistry: Crystal Engineering*, *Vol. 6*, (Eds.: D. D. MacNicol, F. Toda, R. Bishop), Pergamon, New York, **1996**, 147-176. b) M. Miyata, K. Sada, K. Hirayama, Y. Yasuda, K. Miki, *Supramol. Chem.*, **1993**, *2*, 283-288. c) K. Nakano, K. Sada, M. Miyata, *J. Chem. Soc., Chem. Commun.*, **1996**, 989-990. d) K. Nakano, K. Sada, M. Miyata, *Progr. Colloid Polym. Sci.*, **1997**, *106*, 249-251.

[16] a) M. Miyata, M. Shibakami, W. Goonewardena, K. Takemoto, *Chem. Lett.,* **1987**, 605-608. b) K. Miki, A. Masui, N. Kasai, M. Miyata, M. Shibakami, K. Takemoto, *J. Am. Chem. Soc.*, **1988**, *110*, 6594-6596. c) K. Miki, N. Kasai, M. Shibakami, K. Takemoto, M. Miyata, *J. Chem. Soc., Chem. Commun.*, **1991**, 1757-1759. d) K. Nakano, K. Sada, M. Miyata, *Chem. Lett.*, **1994**, 137-140. e) K. Nakano, K. Sada, M. Miyata, *J. Chem. Soc., Chem. Commun.*, **1995**, 953-954. f) K. Nakano, K. Sada, M. Miyata, *Mol. Cryst. Liq. Cryst.,* **1996**, *276*, 129-132.

[17] a) M. Shibakami, A. Sekiya, *J. Chem. Soc., Chem. Commun.*, **1994**, 429-430. b) M. Shibakami, A. Sekiya, *J. Incl. Phenom.*, **1994**, *18*, 397-412. c) M. Shibakami, M. Tamura, A. Sekiya, *J. Incl. Phenom.*, **1995**, *22,* 155-168. d) M. Shibakami, M. Tamura, A. Sekiya, *J. Incl. Phenom.*, **1995**, *22,* 299-311. e) M. Shibakami, M. Tamura, A. Sekiya, *J. Am. Chem. Soc.*, **1995**, *117*, 4499-4505.

[18] a) M. R. Caira, L. R. Nassimbeni, J. L. Scott, *J. Chem. Soc., Chem. Commun.*, **1993**, 612-613. b) M. R. Caira, L. R. Nassimbeni, J. L. Scott, *J. Chem. Soc., Perkin Trans.2*, **1994**, 623-628. c) M. R. Caira, L. R. Nassimbeni, J. L. Scott, *J. Chem. Soc., Perkin Trans.2*, **1994**, 1403-1405. d) J. L. Scott, *J. Chem. Soc., Perkin Trans.2*, **1995**, 495-502. e) J. L. Scott, *Supramol. Chem.*, **1996**, *7*, 201-207.

[19] a) M. Gdaniec, T. Polonski, *J. Am. Chem. Soc.*, **1998**, *120*, 7353-7354. b) M. Gdaniec, M. Milewska, T. Polonski, *Angew. Chem. Int. Ed. Engl.*, **1999**, *38*, 392-395.

[20] TEXSAN, XRAY Structure Analysis Package; Molecular Structure Corporation: The Woodlands, TX, **1985**.

[21] H. Nakano, *Molecular Graphics*, Science House, Tokyo, **1987**.

[22] R. Voorintholt, M. T. Kosters, G. Vegter, G. Vriend, W. G. J. Hol, *J. Mol. Graphics*, **1989**, 7, 243-245.

[23] Cerius^2, Molecular Simulation Software; Molecular Simulation Inc.

[24] The mean values of the host cavities in α–*gauche* lattice and β–*trans* lattice are 247±11Å^3 and 307±10Å^3, when the cavity volume was calculated using 1.0Å radius probe.

[25] a) A. I. Kitaigorodskii, *Molecular Crystals and Molecules*, Academic Press, New York, **1973**. b) G. R. Desiraju, *Crystal Engineering: The Design of Organic Solids*, Elsevier, New York, **1989**, c) A. Gavezzotti, *Acc. Chem. Res.*, **1994**, *27*, 309-314.

[26] a) M. H. Klapper, *Biochim. Biophys. Acta*, **1971**, *229*, 557-566. b) F. M. Richards, *Ann. Rev. Biophys. Bioeng.*, **1977**, *6*, 151-176. c) F. M. Richards, *J. Mol. Biol.*, **1974**, *82*, 1-14.

Chapter 3

[1] a) D. D. MacNicol, J. J. McKendrick, D. R. Wilson, *Chem. Soc. Rev.*, **1978**, *7*, 66-87. b) J. E. D. Davies, W. Kemula, H. M. Powell, N. O. Smith, *J. Incl. Phenom.*, **1983**, *1*, 3-44. c) *Top. Curr. Chem.*, **1988**, *140* and **1988**, *149*. d) *Inclusion Compounds*, *Vol. 1-3* and *4-5*, (Eds.: J. L. Atwood, J. E. D. Davies, D. D. MacNicol), Academic Press, London, **1984**, and Oxford Press, Oxford, **1991**. e) *Comprehesive Supramolecular Chemistry*, *Solid-State Supramolecular Chemistry: Crystal Engineering*, *Vol. 6*, (Eds.: D. D. MacNicol, F. Toda, R. Bishop), Pergamon, New York, **1996**. f) R. Bishop, *Chem. Soc. Rev.*, **1996**, 311-319.

[2] a) F. Toda, *Comprehesive Supramolecular Chemistry*, *Solid-State Supramolecular Chemistry: Crystal Engineering*, *Vol. 6*, (Eds.: D. D. MacNicol, F. Toda, R. Bishop), Pergamon, New York, **1996**, 43-69. b) F. Toda in *Advances in Supramolecular Chemistry*, *Vol. 2* (Eds.; G. W. Gokel), JAI Press, London, **1992**, 141-191. c) G. Kaupp, *Angew. Chem. Int. Ed. Engl.*, **1994**, *33*, 728-729. d) A. Mravik, Z. Boöcskei, K. Simon, F. Elekes, Z. Izsaki, *Chem. Eur. J.*, **1998**, *4*, 1621-1627. e) M. Gdaniec, M. J. Milewska, T. Polonski, *Angew. Chem. Int. Ed.*, **1999**, *38*, 392-395.

[3] a) P. Brunet, M. Simard, J. D. Wuest, *J. Am. Chem. Soc.*, **1997**, *119*, 2737-2738. b) R. Bhyrappa, S. R. Wilson, K. S. Suslick, *J. Am. Chem. Soc.*, **1997**, *119*, 8492-8502. c) K. Kobayashi, M. Koyanagi, K. Endo, Y. Aoyama, *Chem. Eur. J.*, **1998**, *4*, 417-424. d) K. Biradha, D. Dennis, V. A. MacKinnon, C. V. K. Sharma, M. J. Zaworotko, *J. Am. Chem. Soc.*, **1998**, *120*, 11894-11903. e) C. C. Evans, L. Sukarto, M. D. Ward, *J. Am. Chem. Soc.* **1999**, *121*, 320-325. f) K. Kobayashi, T. Shirasaka, A. Sato, E. Horn, N. Furukawa, *Angew. Chem. Int. Ed.*, **1999**, *38*, 3483-3486. g) S. V. Kolotuchin, P. A. Thiessen, E. E. Fenlon, S. R. Wilson, C. J. Loweth, S. C. Zimmerman, *Chem. Eur. J.*, **1999**, *5*, 2537-2547.

[4] a) D. Lawton, H. M. Powell, *J. Chem. Soc.*, **1958**, 2339-2357. b) E. Weber, I. Csoöregh, B. M. Czugler, *J. Am. Chem. Soc.*, **1984**, *106*, 3297-3306. c) M. P. Byrn, C. J. Curtis, Y. Hsiou, S. I. Khan, P. A. Sawin, S. K. Tendick, A. Terzis, C. E. Strouse, *J. Am. Chem. Soc.*, **1993**, *115*, 9480-9497. d) M. D. Hollingsworth, D. B. Santarsiero, K. D. M. Harris, *Angew. Chem. Int. Ed. Engl.*, **1994**, *33*, 649-652. e) A. T. Ung, D. Gizachew, R. Bishop, M. L. Scudder, I. G. Dance, D. C. Craig, *J. Am. Chem. Soc.*, **1995**, *117*, 8745-8756. f) Y. Endo, T. Ezuhara, M. Koyanagi, H. Masuda, Y. Aoyama, *J. Am. Chem. Soc.*, **1997**, *119*, 499-505. g) J. A. Swift, A. M. Pivovar, A. M. Reynolds, M. D. Ward, *J. Am. Chem. Soc.*, **1998**, *120*, 5887-5897. h) M. Gdaniec, B. T. Ibragimov, S. A. Talipov, *Comprehesive Supramolecular Chemistry*, *Solid-State Supramolecular Chemistry: Crystal Engineering*, *Vol. 6*, (Eds.: D. D. MacNicol, F. Toda, R. Bishop), Pergamon, New York, **1996**, 117-145. i) R. Gerdil, *Comprehesive Supramolecular Chemistry*, *Solid-State Supramolecular Chemistry: Crystal Engineering*, *Vol. 6*, (Eds.: D. D. MacNicol, F. Toda, R. Bishop), Pergamon, New York, **1996**, 239-280.

[5] K. Nakano, K. Sada, Y. Kurozumi, M. Miyata, *Chem. Eur. J.*, **2001**, *7*, 209-220.

[6] S. Mecozzi, J. Jr. Rebek, *Chem. Eur. J.*, **1998**, *4*, 1016-1022.

[7] TEXSAN, X-ray Structure Analysis Package; Molecular Structure Corporation: The Woodlands, TX, **1985**.

[8] H. Nakano, *Molecular Graphics*, Science House, Tokyo, **1987**.

[9] R. Voorintholt, M. T. Kosters, G. Vegter, G. Vriend, W. G. J. Hol, *J. Mol. Graphics*, **1989**, *7*, 243-245.

[10] Cerius2, Molecular Simulation Software; Molecular Simulation Inc.

[11] a) K. Nakano, K. Sada, M. Miyata, *J. Chem. Soc., Chem. Commun.*, **1995**, 953-954. b) M. Miyata, K. Sada, *Comprehesive Supramolecular Chemistry*, *Solid-State Supramolecular Chemistry: Crystal Engineering*, *Vol. 6*, (Eds.: D. D. MacNicol, F. Toda, R. Bishop), Pergamon, New York, **1996**, 147-176. c) K. Nakano, K. Sada, M. Miyata, *Chem. Commun.*, **1996**, 989-990. d) K. Nakano, K. Sada, M. Miyata, *Progr. Colloid Polym. Sci.*, **1997**, *106*, 249-251.

[12] E. Giglio, *Inclusion Compounds, Vol. 2*, (Eds.: J. L. Atwood, J. E. D. Davies, D. D. MacNicol), Academic Press, **1984**, 207-229.

[13] a) A. Gavezzotti, G. Fillippini, *J. Am. Chem. Soc.*, **1995**, *117*, 12299-12305. b) L. Yu, G. A. Stephenson, C. A. Mitchell, C. A. Bunnell, S. V. Snorek, J. J. Bowyer, T. B. Borchardt, J. G. Stowell, S. R. Byrn, *J. Am. Chem. Soc.*, **2000**, *122*, 585-591.

Chapter 4

[1] K. Nakano, K. Sada, M. Miyata, *Chem. Eur. J.*, **2001**, *7*, 209-220.

[2] C. C. Evans, L. Sukarto, M. D. Ward, *J. Am. Chem. Soc.*, **1999**, *121*, 320-325.

[3] Y. Endo, T. Ezuhara, M. Koyanagi, H. Masuda, Y. Aoyama, *J. Am. Chem. Soc.*, **1997**, *119*, 499-505.

[4] K. Biradha, D. Dennis, V. A. MacKinnon, C. V. Krishnamohan Sharma, M. J. Zawaromotrko, *J. Am. Chem. Soc.*, **1998**, *120*, 499-505.

[5] R. Gerdil, *Top. Curr. Chem.*, **1987**, *140*, 11894-11903.

[6] a) P. L. Johnson, J. P. Schaefer, *Acta Crystallogr.*, **1972**, *B28*, 3083-3088. b) E. L. Jones, L. R. Nassimbeni, *Acta Crystallogr.*, **1990**, *B46*, 399-405.

[7] A. Gavezzotti and G. Filippini, *J. Am. Chem. Soc.*, **1995**, *117*, 12299-12305.

[8] J. Bernstein, *Organic Solid State Chemistry, Vol. 32*, (Eds.: G. Desiraju), Elsevier, Amsterdam, **1987**, 471-518.

[9] J. Bernstein, A. T. Hagler, *J. Am. Chem. Soc.*, **1978**, *100*, 673-681.

[10] L. Yu, G. A. Stephenson, C. A. Mitchell, C. A. Bunnell, S. V. Snorek, J. J. Bowyer, T. B. Borchardt, J. G. Stowell, S. R. Byrn, *J. Am. Chem. Soc.*, **2000**, *122*, 585-591.

[11] M. D. Hollingsworth, D. B. Santarsiero, K. D. M. Harris, *Angew. Chem. Int. Ed. Engl.*, **1994**, *33*, 649-652.

[12] TEXSAN, X-ray Structure Analysis Package; Molecular Structure Corporation: The Woodlands, TX, **1985**.

[13] H. Nakano, *Molecular Graphics*, Science House, Tokyo, **1987**.

[14] R. Voorintholt, M. T. Kosters, G. Vegter, G. Vriend, W. G. J. Hol, *J. Mol. Graphics*, **1989**, *7*, 243-245.

[15] Cerius^2, Molecular Simulation Software; Molecular Simulation Inc.

[16] a) J. L. Scott, *J. Chem. Soc., Perkin Trans.2*, **1995**, 495-502. b) M. R. Caira, L. R. Nassimbeni, J. L. Scott, *J. Chem. Soc., Perkin Trans.2*, **1994**, 623-628.

[17] a) K. Miki, N. Kasai, M. Shibakami, K. Takemoto, M. Miyata, *J. Chem. Soc., Chem. Commun.*, **1991**, 1757-1759. b) K. Sada, K. Nakano, K. Hirayama, M. Miyata, S. Sasaki, K. Takemoto, N. Kasai, K. Kato, M. Shigesato, K. Miki, *Supramol. Chem.*, in printing.

[18] S. Mecozzi, J. Jr. Rebek, *Chem. Eur. J.*, **1998**, *6*, 1016-1022.

[19] K. Nakano, E. Mochizuki, N. Yasui, K. Morioka, Y. Yamauchi, N. Kanehisa, Y. Kai, N. Yoswathananont, K. Sada, M. Miyata, *Chem. Eur. J.*, submitted.

[20] a) M. Miyata, K. Sada, *Comprehesive Supramolecular Chemistry*, *Solid-state Supramolecular Chemistry: Crystal Engineering*, *Vol. 6*, (Eds.: D. D. MacNicol, F. Toda, R. Bishop), Pergamon, Oxford, **1996**, 147-176.

Chapter 5

[1] a) D. W. Breck, *Zeolite Molecular Sieves, Structure, Chemistry, and Use*, Jone Willy and Sons, New York, **1974**. b) F. Liebau, *Structural Chemistry of Silicates*, Springer-Verlag, Berlin, **1985**.

[2] a) M. Miyata, M. Shibakami, S. Chirachanchai, K. Takemoto, N. Kasai, K. Miki, *Nature*, **1990**, *343*, 446-447. b) M. Miyata, K. Sada, S. Hori, K. Miki, *Mol. Cryst. Liq. Cryst.*, **1992**, *219*, 71-74.

[3] M. Shibakami, M. Tamura, A. Sekiya, *J. Am. Chem. Soc.*, **1995**, *117*, 4499-4505.

[4] G. B. Gardner, D. Venkataraman, J. S. Moore, S. Lee, *Nature*, **1995**, *374*, 792-795.

[5] H. Noguchi, K. Yamamura, I. Tabushi, T. Higuchi, K. Hirotsu, *Bull. Chem. Soc. Jpn.*, **1992**, *65*, 805-811.

[6] Y. Endo, T. Sawaki, M. Koyanagi, K. Kobayashi, H. Masuda, Y. Aoyama, *J. Am. Chem. Soc.*, **1995**, *117*, 8341-8352.

[7] a) K. Nakano, K. Sada, M. Miyata, *J. Chem. Soc., Chem. Commun.*, **1996**, 989-990. b) K. Nakano, K. Sada, M. Miyata, *Progr. Colloid Polym. Sci.*, **1997**, *106*, 249-251. c) K. Nakano, M. Katsuta, K. Sada, M. Miyata, *CrystEngComm*, in press.

[8] K. Nakano, Y. Kurozumi, K. Sada, M. Miyata, *Chem. Eur. J.*, **2001**, *7*, 209-220.

[9] K. Miki, N. Kasai, M. Shibakami, K. Takemoto, M. Miyata, *J. Chem. Soc., Chem. Commun.*, **1991**, 1757-1759.

[10] K. Nakano, E. Mochizuki, N. Yasui, K. Morioka, Y. Yamauchi, N. Kanehisa, Y. Kai, N. Yoswathananont, K. Sada, M. Miyata, *Chem. Eur. J.*, submitted.

Chapter 6

[1] H. Ringsdorf, B. Schlarb, J. Venzmer, *Angew. Chem., Int. Ed. Engl.*, **1988**, *27*, 113-158.

[2] C. A. Guymon, E. N. Hoggan, N. A. Clark, T. P. Rirker, D. M. Walba, C. N. Bowman, *Science*, **1997**, *275*, 57-59.

[3] M. Loos, J. Esch, I. Stokroos, R. M. Kellog, B. L. Feringa, *J. Am. Chem. Soc.*, **1997**, *119*, 12675-12676.

[4] A. Matsumoto, T. Odani, M. Chikada, K. Sada, M. Miyata, *J. Am. Chem. Soc.*, **1999**, *121*, 11122-11129.

[5] M. Miyata, *Comprehensive Supramolecular Chemistry: Inclusion Polymerization, Vol. 10*, (Eds.: D. Reinhoudt), Pergamon, Oxford, **1996**, 557-582.

[6] J. F. Brown, Jr., D. M. White, *J. Am. Chem. Soc.*, **1960**, *82*, 5671-5678.

[7] D. M. White, *J. Am. Chem. Soc.*, **1960**, *82*, 5678-5685.

[8] M. Farina, G. Natta, G. Allegra, M. Löffelholz, *J. Polym. Sci. C*, **1967**, *16*, 2517.

[9] M. Farina, G.Audisio, M. T. Gramegna, *Macromolecules*, **1972**, *5*, 617.

[10] M. Miyata, K. Morioka, K. Takemoto, *J. Polym. Sci., Polym. Chem. Ed.*, **1977**, *15*, 2987-2996.

[11] M. Miyata, T. Tsuzuki, F. Noma, K. Takemoto, *Makromol. Chem. Rapid Commun.*, **1988**, *9*, 45.

[12] M. Miyata, Y. Kitahara, Y. Osaki, K. Takemoto, *J. Inclusion Phenom.*, **1984**, *2*, 391-398.

[13] W. Goonewardena, M. Miyata, K. Takemoto, *Polym. J.*, **1991**, *23*, 1405-1408.

[14] W. Goonewardena, M. Miyata, K. Takemoto, *Polym. J.*, **1993**, *25*, 731-740.

[15] M. Chikada, K. Sada, M. Miyata, *Polym. J.*, **1999**, *31*, 1061-1064.

[16] M. Miyata and K.Sada, *Comprehensive Supramolecular Chemistry: Deoxycholic Acid and related Hosts, Vol. 6*, (Eds.: D. D. MacNicol, F. Toda, R. Bishop), Pergamon, Oxford, **1996**, 147-176.

[17] M. Miyata, M. Shibakami, S. Chirachanchai, K. Takemoto, N. Kasi, K. Miki, *Nature*, **1990**, *343*, 446-447.

[18] M. Miyata, K. Sada, S. Hori, K. Miki, *Mol. Cryst. Liq. Cryst.*, **1992**, *219*, 71-74.

[19] K. Nakano, K. Sada, M. Miyata, *Mol. Cryst. Liq. Cryst.*, **1996**, *276*, 129-132.

[20] K. Nakano, K. Sada, M. Miyata, *Progr. Colloid Polym. Sci.*, **1997**, *106*, 249-251.

[21] K. Nakano, K. Sada, M. Miyata, *J. Chem. Soc., Chem. Commun.*, **1996**, 989-990.

[22] H. Nakano, *Molecular Graphics*, Science House, Tokyo, **1987**.

[23] K. Miki, A. Masui, N. Kasai, M. Miyata, M. Shibakami, K. Takemoto, *J. Am. Chem. Soc.*, **1988**, *110*, 6594-6596.

[24] P. L. Johnson, J. P. Schaefer, *Acta Crystallogr.*, **1972**, *B28*, 3083-3088.

[25] K. Miki, N. Kasai, M. Shibakami, K. Takemoto, M. Miyata, *J. Chem. Soc., Chem. Commun.*, **1991**, 1757-1759.

[26] D. Blondin, J. Regis, J. Prud'homme, *Macromolecules*, **1974**, *7*, 187-189.

[27] E. Giglio, *Inclusion Compounds, Vol. 2*, (Eds.: J. L. Atwood, J. E. D. Davies, D. D. MacNicol), Academic Press, **1984**, 207-229.

[28] R. Popovitz-Biro, C.-P. Tang, H. C. Chang, M. Lahav, L. Leiserowitz, *J. Am. Chem. Soc.*, **1985**, *107*, 4043-4058.

[29] P. J. Rizkallah, M. M. Harding, P. F. Lindley, A. Aigner, A. Bauer, *Acta. Cryst.*, **1990**, *B46*, 262.

List of Publications

[1] Inclusion Compounds of Cholic Acid with Various Hydrocarbons and the Crystal Structure of a 1:1 Complex of Cholic Acid and Benzene.
Kazunori Nakano, Kazuki Sada, and Mikiji Miyata
Chem. Lett., **1994**, 137-140.

[2] Guest-participating Reversion of Molecular Arrangements in Asymmetric Multibilayers of Cholic Acid Inclusion Crystals.
Kazunori Nakano, Kazuki Sada, and Mikiji Miyata
J. Chem. Soc., Chem. Commun., **1995**, 953-954.

[3] Novel Additive Effect on Polymorphs of Inclusion Crystals; Cholic Acid Crystals Involving Different Hydrogen-Bonded Networks in Spite of the Same Organic Guest.
Kazunori Nakano, Kazuki Sada, and Mikiji Miyata
J. Chem. Soc., Chem. Commun., **1996**, 989-990.

[4] Reversible Layer Sliding in Cholic Acid Crystals
Kazunori Nakano, Kazuki Sada, and Mikiji Miyata
Mol. Cryst. Liq. Cryst., **1996**, *276*, 129-132.

[5] Molecular Architectures of Steroidal Acids and their Derivatives: Selective Acquisition of Polymorphic Inclusion Crystals of Cholic Acid.
Kazunori Nakano, Kanae Tani, Kazuki Sada, and Mikiji Miyata
Progr. Colloid Polym. Sci., **1997**, *106*, 249-251.

[6] Importance of Packing Coefficients of Host Cavities to Isomerization of Open Host Frameworks. Guest Size Dependent Isomerizations in Cholic Acid Inclusion Crystals with Monosubstituted Benzenes.
Kazunori Nakano, Yukio Kurozumi, Kazuki Sada, and Mikiji Miyata
Chem. Eur. J., **2001**, *7*, 209-220.

[7] Inclusion Polymerization in Polymorphic Crystals of Cholic Acid.
Kazunori Nakano, Kazuki Sada, and Mikiji Miyata,
Polym. J., **2001**, *33*, 172-176.

[8] Conformational Polymorphism in Inclusion Crystals of Cholic Acid with Ethyl Acetate.
Kazunori Nakano, Masanori Katsuta, Kazuki Sada, and Mikiji Miyata
CrystEngComm, **2001**, *11*, 1-2.

[9] Molecular Recognitions of Xylenes by Cholic Acid Host Lattice. Selective Inclusions vs. "Clathrate Solid Solution" of Cholic Acid and Mixed Xylenes.
Kazunori Nakano, Eiko Mochizuki, Nobuyoshi Yasui, Kyoichi Morioka, Yukinori Yamauchi, Nobuko Kanehisa, Yasushi Kai, Nungruethai Yoswathananont, Kazuki Sada, and Mikiji Miyata
Chem. Eur. J., submitted.

List of Related Papers

[1] Functionalization of Inclusion Cavities of Bile Acid Hosts. Channel-Type Inclusion Compounds of Cholamide
Kazuki Sada, Takashi Kondo, Masahiko Ushioda, Kazunori Nakano, Mikiji Miyata, Taro Tamada, and Kunio Miki
Bull. Chem. Soc. Jpn., **1998**, *71*, 1931-1937.

[2] Novel Gelators of Bile Acid-alkylamine Salt Prepared through a Combinatorial Library Approach.
Kazunori Nakano, Yukio Hishikawa, Kazuki Sada, Mikiji Miyata, and Kenji Hanabusa
Chem. Lett., **2000**, 1170-1171.

[3] Molecular Recognition of Medium-size Lactones by Enclathration of Cholic Acid.
Kazuki Sada, Kazunari Nakano, Kiyoshi Hirayama, Mikiji Miyata, Satoshi Sasaki, Kiichi Takemoto, Nobutami Kasai, Kazuaki Kato, Masashi Shigesato, and Kunio Miki
Supramol. Chem., in printing.

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