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Host channel framework determined by C–H⋯π interaction in the inclusion crystal of 2,5-bis(diphenylmethyl)hydroquinone and benzaldehyde

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Abstract

A new kind of host compound, 2,5-bis(diphenylmethyl)hydroquinone is designed and prepared. The crystal structure of the inclusion compound formed by the host with benzaldehyde was determined by single crystal X-ray diffraction. The result shows that the host exhibits a stable conformation through intramolecular CH⋯π interactions in the inclusion crystal, and benzaldehyde guest molecules are accommodated in the channel which is constructed by the hosts, in which intermolecular C–H⋯π interactions between the hosts, play an important role in the architecture of channel framework besides van der Waal's forces. The complex structure is further stabilized by strong hydrogen bonding (O1–H1⋯O1′) and two weak C–H⋯O interactions (C5′–H5′⋯O1, C3–H3⋯O1′) between the host and guest.

Keywords: 2,5-Bis(diphenylmethyl)hydroquinone; Inclusion compound; Hydrogen bonding; Inter- and intra-C–H⋯π interactions

1. Introduction

In past years, there has been increasing interest in the study of weak intra- and inter-molecular interactions, because of their important roles played in the various fields of chemistry and biochemistry, such as crystal engineering, supramolecular chemistry, molecular recognition and self-assembly of molecules [1]. Interactions such as C–H⋯X (X: the proton acceptor, such as O, N) systems are commonly recognized as weak hydrogen bonds. Of all the weak hydrogen bonds, the CH⋯π interaction could be regarded as the weakest [2]. In recent years, much attention has been paid to the CH⋯π interaction as an important factor in the crystal packing and in determining the structure of clathrate compounds [3]. Crystalline inclusion compounds, in particular, organic molecules with many functional groups that can form strong and stable intra- and inter-molecular interactions, provide a lot of useful models to study the function of weak CH⋯π interactions in the aggregation of molecules [4].

Herein, we report a crystal structure of an inclusion compound, in which 2,5-bis(diphenylmethyl) hydroquinone is a new host molecule that conforms to Weber's rules for host design [5], bearing hydroquinone as the core fragment, diphenylmethyl fragment as a large bulky space group, and hydroxyl moieties as hydrogen-bonding donors. The result of structural analysis of the inclusion crystal formed by the title compound shows that this host molecule facilitates the formation of a channel type host framework by the interaction of CH⋯π between hosts, which is obviously different from the layer type structures constructed by 2,5-bis(2,4-dimethylphenyl) hydroquinone [6] and 2,5-diphenyl hydroquinone [7]. The new evidence, i.e. weak inter- and intra-molecular CH⋯π interaction playing an indispensable role in the crystal packing and in

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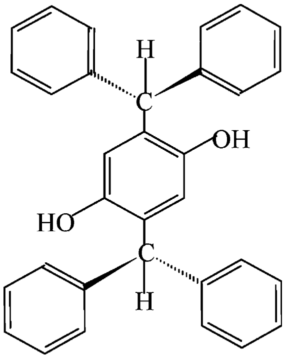
determining the structure of the lattice clathrate, is provided in this paper.



2. Experimental section

2.1. General methods

The ^1H NMR and ^{13}C NMR spectra were recorded on a Varian YH 300 MB instrument in DMSO-d6. The IR spectra were obtained with KBr pellets on a Perkin–Elmer 983 FT infrared spectrophotometer.

2.2. Synthesis

Diphenylmethanol (8.0 g, 0.49 mol), hydroquinone (2.2 g, 0.2 mol), and *p*-toluenesulfonic acid (1.0 g) and 70 ml toluene were added into a tri-neck-flask and stirred and refluxed for 4 h under the protection of N_2. The product was recrystallized from ethyl acetate to obtain the white crystals of pure host 8.2 g, m.p. 278–279 °C, yield 87%.

^1H NMR: δ(DMSO-d6): 8.6 (2H, s, OH), 7.0–7.3 (20H, m, ArH, substituted), 6.3 (2H, s, ArH, framework), 5.7 (2H, m, C–H); δ 8.6 peak disappeared after being exchanged for D_2O.

^{13}C NMR: δ (DMSO-d6) (ppm): 146.7 (Ar, 1,4-C), 143.9 (Ar, 2,5-C), 116.5 (Ar, 3,6-C), 128.5 (4 substituted phenyls 1′-C), 128.1 (4 substituted phenyls *o*-C), 125.9 (4 substituted phenyls *m*-C), 120.9 (4 substituted phenyls *p*-C), 48.9 (CH_2–C). There are eight chemical shifts for carbon atoms, also confirming the symmetry of the host. IR: ν_{max} (KBr): 3531 (s, OH), 3059 (w, ArH), 1598, 1491, 1448 (s, Ar), 1166 (s, ArO) cm^{-1}.

2.3. Inclusion complexes preparation

Potential guest solvents, such as methanol, ethanol, 1-propanol, 2-propanol, cyclopentanol, formaldehyde, acetaldehyde, benzaldehyde, acetone, cyclopentanone, acetophenone, 2,5-hexanedione, *N*-methyl-2-pyrrolidone, ethyl acetate, methyl benzoate, THF, 1,4-dioxane, pyridine, cyclohexylamine, 1-chloro-2,3-epoxypropane), DMSO, and DMF, were used to dissolve the host by stirring or heating. After cooling and standing for a few days, five inclusion compounds with DMF, DMSO, THF, Benzaldehyde and acetophenone were crystallized, and the pure crystalline materials were obtained by further recrystallization as the same crystalline condition. The components and ratios of the complexes were confirmed by measurement of m.p., IR and ^1H NMR data.

2.4. Crystal structure determination of host with benzaldehyde

Crystals suitable for X-ray investigation were obtained by slow evaporation at room temperature. X-ray single crystal determination was obtained using a Bruker Axs P4 X-ray diffractometer with graphite monochromated Mo Kα radiation ($\lambda = 0.71073$ Å) with $\theta/2\theta$ scan mode in the range $2.15° < \theta < 25°$, $-1 \le h \le 8$, $-11 \le k \le 11$, $-11 \le l \le 11$. Three standard intensities were monitored after each group of 100 reflections and no evidence of crystal decay was observed. The structure was solved by direct methods and refined on F^2 by full-matrix least-squares calculation. All non-hydrogen atoms refined with anisotropic thermal displacement parameters. All of the hydrogen atoms were located in difference electron density map and their positions were allowed to refine together with individual isotropic temperature factors. The detailed data and structure refinement are listed in Table 1. Selected bonds and angles are listed in Table 2.

Table 1
Crystallographic data for host with benzaldehyde

Empirical formula	$(C_{32}H_{26}O_2)_{1/2}\cdot C_7H_6O$
Formula weight	327.40
Crystal color, habit	Yellow, block
Crystal dimensions (mm)	0.4×0.4×0.3
Crystal temperature (K)	293
Crystal system	Triclinic
Space group	*P*-1
Z	2
a (Å)	9.394(8)
b (Å)	10.099(8)
c (Å)	10.838(9)
α (°)	106.62(4)
β (°)	112.48(5)
γ (°)	94.09(5)
V (Å^3)	891.2(13)
D_x (g cm^{-3})	1.224
μ (mm^{-1})	0.077
F(000)	348
R_{int}	0.027
No. of collected data (unique)	2794
No. of data with $I > 2\sigma(I)$	1913
No. of parameters varied	302
S	1.012
R_f/wR_f	0.0463/0.1148
All data R_f/wR_f	0.0731/0.1309

Table 2
Selected bond lengths (Å) and angles (°)

O(1)–C(2)	1.369(3)	C(11)–C(12)	1.387(3)
C(1)–C(3)	1.390(3)	C(11)–C(16)	1.391(3)
C(1)–C(2)	1.398(3)	C(12)–C(13)	1.386(4)
C(1)–C(4)	1.526(3)	C(13)–C(14)	1.377(4)
C(2)–C(3)#1	1.393(3)	C(14)–C(15)	1.374(5)
C(3)–C(2)#1	1.393(3)	C(15)–C(16)	1.386(4)
C(4)–C(11)	1.524(3)	O(1′)–C(1′)	1.219(3)
C(4)–C(5)	1.530(3)	C(1′)–C(2′)	1.464(4)
C(5)–C(6)	1.382(3)	C(2′)–C(7′)	1.381(4)
C(5)–C(10)	1.385(3)	C(2′)–C(3′)	1.389(4)
C(6)–C(7)	1.393(4)	C(3′)–C(4′)	1.373(5)
C(7)–C(8)	1.356(4)	C(4′)–C(5′)	1.370(5)
C(8)–C(9)	1.377(4)	C(5′)–C(6′)	1.380(5)
C(9)–C(10)	1.381(4)	C(6′)–C(7′)	1.368(5)
C(3)–C(1)–C(2)	117.35(18)	C(12)–C(11)–C(16)	117.8(2)
C(3)–C(1)–C(4)	122.94(18)	C(12)–C(11)–C(4)	121.7(2)
C(2)–C(1)–C(4)	119.70(18)	C(16)–C(11)–C(4)	120.4(2)
O(1)–C(2)–C(3)#1	120.97(19)	C(13)–C(12)–C(11)	121.0(3)
O(1)–C(2)–C(1)	117.87(18)	C(14)–C(13)–C(12)	120.4(3)
C(3)#1–C(2)–C(1)	121.16(18)	C(15)–C(14)–C(13)	119.3(3)
C(1)–C(3)–C(2)#1	121.48(19)	C(14)–C(15)–C(16)	120.5(3)
C(11)–C(4)–C(1)	112.33(17)	C(15)–C(16)–C(11)	120.9(3)
C(11)–C(4)–C(5)	112.00(17)	O(1′)–C(1′)–C(2′)	124.9(3)
C(1)–C(4)–C(5)	113.68(17)	C(7′)–C(2′)–C(3′)	119.8(3)
C(6)–C(5)–C(10)	117.6(2)	C(7′)–C(2′)–C(1′)	121.2(3)
C(6)–C(5)–C(4)	123.83(19)	C(3′)–C(2′)–C(1′)	119.0(3)
C(10)–C(5)–C(4)	118.53(19)	C(4′)–C(3′)–C(2′)	120.2(3)
C(5)–C(6)–C(7)	120.9(2)	C(5′)–C(4′)–C(3′)	119.8(4)
C(8)–C(7)–C(6)	120.6(3)	C(4′)–C(5′)–C(6′)	120.1(4)
C(7)–C(8)–C(9)	119.2(3)	C(7′)–C(6′)–C(5′)	120.8(4)
C(8)–C(9)–C(10)	120.5(3)	C(6′)–C(7′)–C(2′)	119.3(3)
C(9)–C(10)–C(5)	121.1(2)		

Symmetry transformation used to generate equivalent atoms: #1 $1-x$, $-y$, $-z$.

3. Results and discussion

3.1. Inclusion property of host

The molar ratio of host/guest in each inclusion complex was measured by ^{1}H NMR, the molar ratio results and the melting points were listed in Table 3.

The melting points of complexes are generally lower than the host itself (278–279 °C), indicating that the new inclusion compounds with different crystal lattices from the host are formed.

IR absorption peaks of both host and guest are also found in each inclusion compound, in which the hydroxyl group absorption of the hosts was red shifted in each complex to some extent: (h)·DMF: 71 cm^{-1}; (h)·DMSO: 375 cm^{-1}; (h)·THF: 269 cm^{-1}; (h)·Benzaldehyde: 111 cm^{-1}; (h)·acetophenone: 240 cm^{-1}; (h)·2,5-hexanedione: 149 cm^{-1}, showing that hydrogen bond interactions between the host hydroxyl and the functional group of the guests may be involved in the crystal.

Table 3
Molar ratio of host/guest and melting points of complex structures

Inclusion complex	Molar ratio	m.p. (°C)
(h):DMF	1:2	267–268
(h):DMSO	1:2	274–275
(h):THF	1:1	270–271
(h):Benzaldehyde	1:2	258–259
(h):Acetophenone	1:2	262–263

3.2. Crystal structure of host with benzaldehyde

A perspective view of the complex crystal is depicted in Fig. 1. The host is a symmetric molecule, and its symmetry centre occupies a crystallographic symmetry centre, which results in the asymmetric unit comprising half a host and one guest, and the ratio of host and guest in the crystal is 1:2.

3.2.1. Strong hydrogen bond and weak C–H···O interactions between host and guest in the inclusion crystal

As one of the most important factors in maintaining the stability of the inclusion compound and decreasing the crystal energy, a strong hydrogen bond between the host and guest is involved in this crystal. Atom O1 of the host at (x, y, z) acts as hydrogen bonding donor to the atom O1′ of the guest at $(x,\ y-1,\ z-1)$, with the length of 2.785 Å and hydrogen bond angle of 171.07° (O1–H1 = 0.884 Å, H1···O1′ = 1.908 Å).

Apart from the conventional hydrogen bonding, the inclusion complex is also further stabilized by two evident C–H···O weak interactions between the host and guest. The first C–H···O weak interaction occurs between the atom C5′ of the guest molecule and O atom of hydroxyl group in the host. The atom C5′ of the guest molecule acts as hydrogen bonding donor to the atom O1 of the host at $(1-x,\ 1-y,\ -z)$, C5′–O1 = 3.590 Å, C5′–H5′ = 0.988 Å, H5′···O1 = 2.799 Å, and the angle of D–H···A is 137.44°. Meanwhile, the C3 atom in the core hydroquinone ring of the host, which is located beside the hydroxyl group and O1′ of carbonyl group in the guest, is also linked by C–H···O interaction, with the length of C3 and O1′ is 3.538 Å, H3···O1′: 2.903 Å, C3–H3: 0.953 Å, and the bond angle of C3–H···O1′ is 125.16°. Although the directionality of the moderate and weak hydrogen bonds is much softer than that of strong hydrogen bonding, it can still be identified by the orientation of the lone electron pair. The oxygen lone electron pair of carbonyl groups are located in the R2C = O plane and form weak hydrogen bond angles of about 120° with C=O bond [8]. Here, the bond angle of H3···O1′–C1′ is 134.25° and the torsion angle of H3–O1′–C1–C2′ is 11.65°, showing that H3 is connected with lone electron pair of sp^2 orbital at O1′ atom. The deviation of directionality of this weak C–H···O interaction is 11.65° from the R2C=O plane, and 14.25° from the criterion of 120° of normal contacting with sp^2 orbital. The strong hydrogen bond and the two weak C–H···O interactions between host and guest in the inclusion complex are shown in Fig. 2 (Table 4).

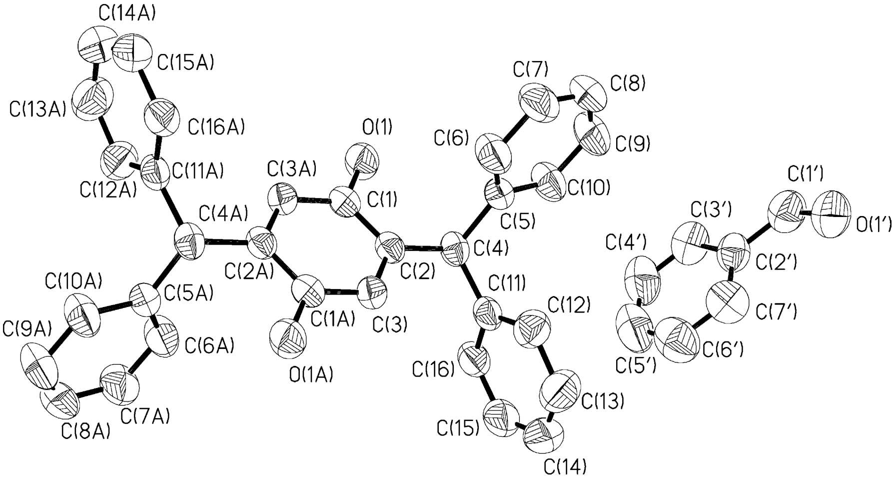


Fig. 1. Perspective view of the inclusion complex.

3.2.2. C–H···π interaction motif of host framework

Although the C–H···π interaction could be the weakest hydrogen bond, it has been found in this complex crystal to be an important contributive force to the formation of the host framework besides the weak van der Waal's force.

In the basic unit of the host framework, there are altogether four host molecules constructing the host framework as shown in Fig. 3(a), in which the intermolecular C–H···π interactions between C13 in substituted phenyl ring (C11–C16) of one host molecule and C8 in phenyl ring (C5–C10) of another host molecule ($1-x$, $1-y$, $1-z$) form half of the host framework. Due to the symmetry of the host, the other half host framework is formed by the symmetry. Here, cg′ is the centroid of the phenyl ring of C5–C10, atom C13 aggregates at (x, y, z) acts as hydrogen bonding donor to the centroid cg′ of another

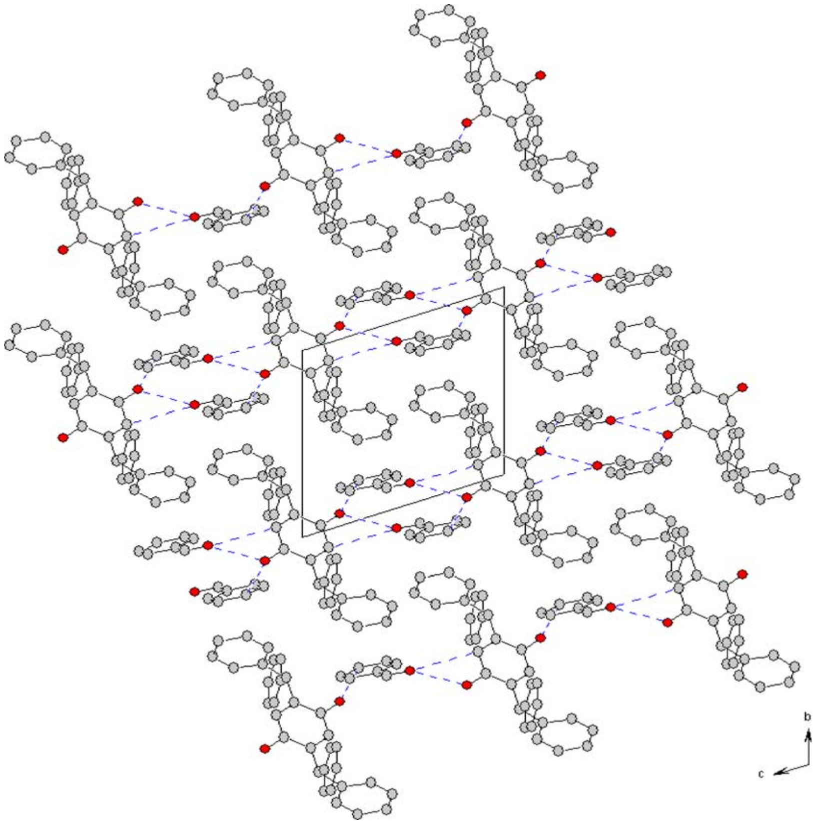


Fig. 2. Packing diagram along the *a* axis of the inclusion complex, showing the O–H···O hydrogen bonding and C–H···O weak interactions between the host and guest.

Table 4
Intermolecular O–H⋯O, C–H⋯O and C–H⋯π contacts for the complex structure

	D⋯A	D–H	H⋯A	D–H⋯A (°)	Symmetry code
Host–Guest					
O1–H1⋯O1′	2.785	0.884	1.908	171.07	$x, y-1, z-1$
C5′–H5′⋯O1	3.590	0.988	2.799	137.44	$1-x, 1-y, -z$
C3–H3⋯O1′	3.538	0.953	2.903	125.16	$1-x, 1-y, 1-z$
Host–Host					
C13–H13⋯cg′	3.975	0.906	3.171	149.02	$1-x, 1-y, 1-z$
C13–H13⋯C8	3.775	0.906	3.070	136.08	$1-x, 1-y, 1-z$

Note: cg′ designates the centroid of the phenyl ring (C5–C10).

host at $(1-x, 1-y, 1-z)$, C13–cg′: 3.975 Å, C13–H13⋯cg′ = 149.02°, H13–cg′ = 3.171 Å. The nearest atom in this phenyl ring from C13 is C8: C13–C8: 3.775 Å, H13–C8: 3.070 Å, C13–H13⋯C8: 136.08°. The second nearest atom from C13 is C9, C13–C9 = 3.922 Å, C13–H13⋯C9 = 160.16°. The presence of C–H⋯π interaction is also confirmed by the evaluation method proposed by Nishio [3c] ($D_{\text{lin}} = 2.988$ Å $< D_{\max}$ (3.05 Å), $\theta = 34.34° < 60°$, $\omega = 87.56°$), showing C–H⋯π weak interaction between the hosts belongs to type 'region 1' [3e], namely, the hydrogen atom is above the π-plane. The diagram of intermolecular C–H⋯π interaction between the hosts is shown in Fig. 3(b).

In the lattice crystal, the equivalent isotropic displacement parameters (U_{eq}) values of C8, C7 and C9 as acceptor atoms are 0.076, 0.080 and 0.080 Å^2, respectively, generally, the U_{eq} value of C atom located in the *p*-position of substituted phenyl ring is a little higher than that of the *o*-position and *m*-position due to the comparably far distance from the substituted position and it exhibits more obvious thermal instability. However, here, atom C8 which is located in the *p*-position has a comparably lower U_{eq} value instead, which also indicates from another angle that C8 is restricted and stabilized by C–H⋯π interaction, and its disordered thermal motion is weakened to an extent. This evidence further confirms the presence of the C–H⋯π interaction between hosts.

As shown in Fig. 2, we can roughly observe two distinct contact gaps between the hosts, which could be due to the existence result of van der Waal's forces. The nearest distance of 3.991 Å between C16 in the phenyl rings (C11–C16) and C16A in the rings (C11A–C16A) confirms the existence of van der Waal's forces. Therefore, the dispersion force also plays a necessary role in the architecture of host framework.

3.2.3. Structure and intra-molecular C–H⋯π interactions in the host

Compared with compounds of similar structure [6,7], the title host molecule forms a channel host framework, while the latter form layer host frameworks. What factors could cause this difference? The type of host framework may be closely connected with the structure of the host. In the title host of the inclusion crystal, the substituted phenyl rings are connected to the core hydroquinone ring by C4 and C4A (C^3_{sp}), with the bond angles about C4 (C4A) 112.33(17), 112.00(17) and 113.68(17)°, respectively, which all are close to the standard tetrahedral bond angle of 109.5°. More importantly, the two substituted phenyl rings on the same side which are linked by C4 (C4A) are almost perpendicular with the dihedral angle of 93.22(1)°, and such conformation is much more beneficial for the aromatic edge-face contact in the host. Furthermore, when the host forms its inclusion

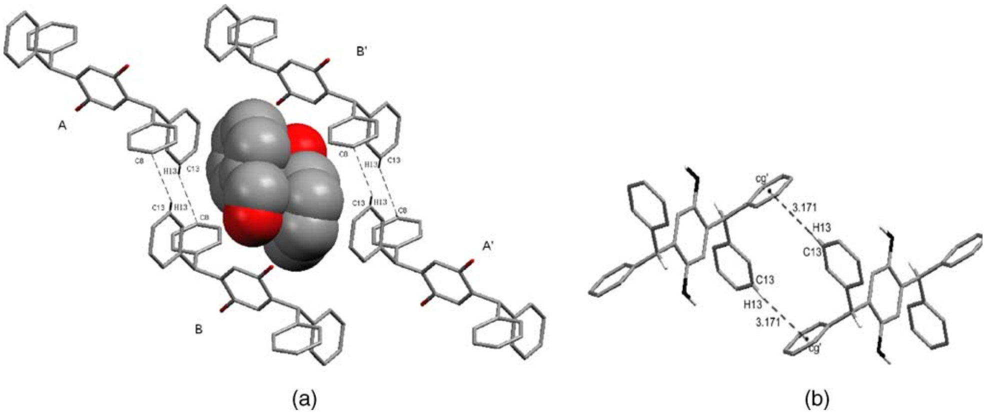


Fig. 3. (a) Guest molecules which are accommodated in the channel hole formed by intermolecular C–H⋯π interaction; (b) intermolecular C–H⋯π interaction in the host framework.

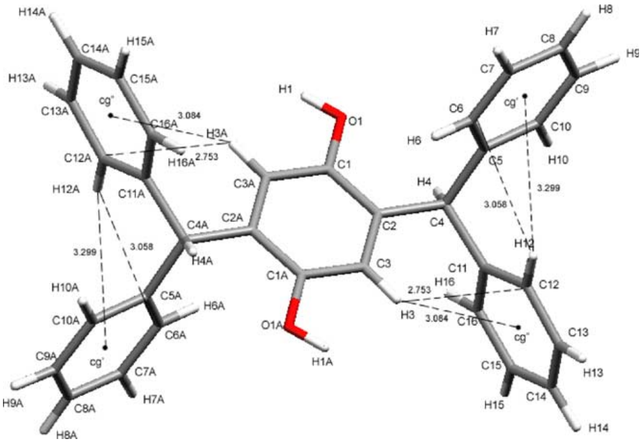


Fig. 4. Intramolecular C–H···π interactions in the host.

complex with benzaldehyde guest molecules, although the strong hydrogen bonding and weak C–H···O interactions between the host and guest are found in the crystals, the host molecules still maintain a stable conformation, which could indicate the possible existence of C–H···π interactions in the host.

In the host, two kinds of intramolecular C–H···π interactions are investigated. Firstly, C–H···π interaction is found between the core hydroquinone ring and substituted phenyl ring (C11–C16), here, cg$''$ designates the centroid of the phenyl ring (C11–C16), C3 atom which is located in the rich electron hydroquinone ring acts as hydrogen bond donor, via H3, to the centroid cg$''$, C3–cg$''$ = 3.741 Å, C3–H3···cg$''$ = 127.49°, H3–cg$''$ = 3.084 Å. The distance between C3 and C12 of ring (C11–C16) is 3.391 Å, H3–C12 = 2.753 Å, C3–H12···C12 = 125.07°. This C–H···π interaction fixes the orientation of substituted phenyl rings (C11–C16) with the dihedral angle between this substituted phenyl and core hydroquinone of 94.66(1)°. At the same time, the fixed orientation of phenyl ring C11–C16 results in another C–H···π interactions between this ring and another substituted phenyl ring (C5–C10). C12 atoms of phenyl ring (C11–C16), as hydrogen bond donor, is linked with cg$'$ (the centroid of C5–C10), with the length of C12–cg$'$ is 3.842 Å, and the angle of C12–H12···cg$'$ is 118.90°. The distance from C12 of ring (C11–C16) to C6 of ring (C5–C10) is 3.665 Å, and the angle of C12–H12···C6 is 123.79°. This C–H···π interaction gives rise to the dihedral angle between this substituted phenyl (C5–C10) and core hydroquinone of 98.66(1)°. Therefore, due to the two C–H···π interactions between the two substituted phenyl rings and substituted phenyl ring and core hydroquinone, the conformation of the host is further stabilized in the complex. The two intramolecular C–H···π interactions in the host are shown in Fig. 4.

The corresponding equivalent isotropic displacement parameters (U_{eq}) of atoms in the intramolecular C–H···π interaction are also been tested to validate the existence of intramolecular C–H···π interactions in the host. The results show that these values are comparably lower than that of other atoms with no C–H···π interaction involved, which indicates that the disordered thermal motions of these C atoms, as hydrogen bonding acceptors, have been decreased to some extent by the restriction of the C–H···π interaction.

4. Conclusion

In the complex structure channel host framework depicted here, conventional strong hydrogen bonding and weak intermolecular C–H···O interaction play a very important role in the decreasing the crystal energy and fixing the guest molecules in the inclusion compound. The C–H···π weak interactions are another important contribution to determining the shape of host framework and dominating the structure of inclusion compounds. The orientations of substituted phenyls of the host favour the formation of both intra- and inter-molecular C–H···π weak interactions.

5. Supplementary material

Crystallographic data for this article have been deposited in the Cambridge Crystallographic Data Centre as supplementary publication No. 231489. Copies of this information may be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge CB21 EZ, UK (fax: +44 1223 336 033; email: deposit@ccdc.cam.ac.uk or www: http://ccdc.cam.ac.uk).

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