J Chem Crystallogr (2011) 41:929–935
DOI 10.1007/s10870-011-0020-z

ORIGINAL PAPER

Hydrogen-Bonded Molecular Ladders and Interlaced Networks in Complexes Built of V-Shaped Molecules 4,4′-Isopropylidenediphenol or 4,4′-Oxydibenzoic Acid with 4,4′-Bipyridine

Yunxia Yang · Qi Li

Received: 9 December 2010 / Accepted: 1 February 2011 / Published online: 10 February 2011

Abstract The title compounds, $C_{10}H_8N_2 \cdot C_{15}H_{16}O_2$ (**1**) and $C_{10}H_8N_2 \cdot C_{14}H_{10}O_5$ (**2**), were synthesized by 4,4′-bipyridyl and two similar V-shaped molecules. The two complexes both crystallized in the same space group $P2_1/n$ with the crystal cell parameters: $a = 16.0536(3)$ Å, $b = 6.42730(1)$ Å, $c = 21.2717(4)$ Å, $\beta = 102.330°$, $V = 2144.21(7)$ Å^3, $Z = 4$ in compound **1** and $a = 7.45020(10)$ Å, $b = 10.0784(2)$ Å, $c = 26.9430(5)$ Å, $\beta = 92.1140(10)°$, $V = 2021.67(6)$ Å^3, $Z = 4$ in compound **2**. Compound **1** forms regular molecular chains containing alternative 4,4′-bipyridyl and 4,4′-isopropylidenediphenol units; the molecular components are linked by two types of O–H···N hydrogen bonds. Additionally, every two neighboring chains are connected to be a ladder structure by means of weak C–H···O interactions. In compound **2**, 4,4′-bipyridyl and 4,4′-oxydibenzoic acid first construct one-dimensional architecture by strong O–H···N hydrogen bonds, which are similar with the interactions in compound **1**. Secondly, two types of weak C–H···O contacts formed between 4,4′-bipyridyl and the acid link one-dimensional chains to be interlaced three-dimensional hydrogen-bonded networks.

Keywords 4,4′-Bipyridyl · 4,4′-Isopropylidenediphenol · 4,4′-Oxydibenzoic acid · Hydrogen bond · Cocrystal

Introduction

Cocrystal formation is of high effectiveness in construction of organic solid-state materials that exhibit customized properties (e.g., optical, photo, electrical, mechanical, pharmaceutical property) [1–8]. Recognizing that crystal engineering is the solid-state supramolecular equivalent of organic synthesis, supramolecular synthons are ‘structural units within supermolecules formed and/or assembled by known or conceivable intermolecular interactions’. The O–H···N hydrogen bond is a robust and versatile synthon in terms of crystal engineering [9–11]. The bisphenolic compound, 4,4′-isopropylidenediphenol, which has been widely used in many areas including biochemistry [12–15] and environmental chemistry [16, 17], could form several adducts with different amines, e.g., 1,4-diazabicyclo[2.2.2]octane [18], hexamethyltetramine [19], methylhydrazine [20], quinoline [21] and pyridine [22]. Among these structures, it is obvious that the bisphenol is a good double hydrogen-bond donor resembling V-shape. Similarly, 4,4′-oxydibenzoic acid, which is generally employed to construct different MOFs [23–27], also exists as an analogical V-configuration molecule with terminal carboxyl groups acting as good hydrogen-bond acceptors and donors. It is well known that 4,4′-bipyridyl is a double hydrogen-bond acceptor. 4,4′-isopropylidenediphenol and 4,4′-oxydibenzoic acid molecules both display in the configuration of V-shape, but the terminal functional groups are very different.

In recent years, multiple systematic studied on construction of new inclusion compounds and the hydrogen-bonding

---

Y. Yang · Q. Li (✉)
College of Chemistry, Beijing Normal University,
Beijing 100875, China
e-mail: qili@bnu.edu.cn

Y. Yang
Key Laboratory of Eco-Environment-Related Polymer Materials,
Ministry of Education, College of Chemistry and Chemical
Engineering, Northwest Normal University, Lanzhou 730070,
Gansu, China

modes within their crystal structures were undertaken by our researchers. A number of novel inclusion compounds have been synthesized based on multi-carboxylato aliphatic or aromatic rings, with or without participation of urea or thiourea molecules [28]. As a part of our ongoing investigation on properties and molecular packing of inclusion compounds based on multi-carboxylato aromatic rings, some new cocrystals have been prepared in successive way. For ongoing work, preparation and X-ray crystallographic analyses of two complexes, 4,4′-bipyridyl·4,4′-isopropylidenediphenol (**1**) and 4,4′-bipyridyl·4,4′-oxydibenzoic acid (**2**) were reported in this paper.

Experiment

Synthesis of 4,4′-Bipyridyl·4,4′-isopropylidenediphenol ($C_{10}H_8N_2 \cdot C_{15}H_{16}O_2$, **1**) and 4,4′-Bipyridyl·4,4′-oxydibenzoic acid ($C_{10}H_8N_2 \cdot C_{14}H_{10}O_5$, **2**)

0.25 mmol 4,4′-bipyridyl (0.039 g) and 0.25 mmol 4,4′-isopropylidenediphenol (0.057 g) were separately dissolved in a small amount of water–ethanol (50/50 v/v). The mixture were stirred for half an hour and set aside to crystallize, after 7 days, finally yielding colorless prism-shaped crystals suitable for single crystal X-ray diffraction. Compound **2** was prepared with the same procedure with 0.25 mmol 4,4′-oxydibenzoic acid (0.065 g), and the resulting solution was set aside and allowed to slowly evaporate at room temperature. After 7 days, colorless prism-shaped crystals of compound **2** suitable for single crystal X-ray diffraction were obtained.

X-ray data Collection and Structure Determination

Crystals were mounted on glass fibers for intensity data collection with a Bruker SMART Apex II CCD area detector [29] at room temperature. All data were collected using graphite-monochromated Mo–Kα radiation ($\lambda = 0.71073$ Å). The structure was solved with direct methods and refined by full matrix least square methods based on F^2, using the structure determination and graphics package SHELXTL based on SHELX97 [30]. All non-hydrogen atoms were refined with anisotropic displacement parameters, and all the hydrogen atoms bonded to carbon atoms were introduced into idealized dispositions. The hydrogen atoms bonded to oxygen atoms were placed in difference map with fixed distance of 0.86 Å. The final reliability indices together with crystal data of the refinement calculations were given in Table 1 and the selected geometric parameters of two crystal structures were listed in Table 2.

Table 1 Crystallographic data

Formula	$C_{10}H_8N_2 \cdot C_{15}H_{16}O_2$	$C_{10}H_8N_2 \cdot C_{14}H_{10}O_5$
Formula weight	384.46	414.40
Crystal color	Colorless	Colorless
Crystal shape	Prism	Prism
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/n$
Crystal size/mm	0.68 × 0.48 × 0.53	0.60 × 0.27 × 0.21
a/Å	16.0536(3)	7.45020(10)
b/Å	6.42730(1)	10.0784(2)
c/Å	21.2717(4)	26.9430(5)
β/°	102.330	92.1140(10)
V/Å^3	2144.21(7)	2021.67(6)
Z	4	4
Dc/(mg cm^{-3})	1.191	1.362
μ/mm^{-1}	0.076	0.097
θ range for data collection	1.79–27.62	2.52–27.65
Reflection number	13355	9645
Independent reflections	4972	4687
$R_1, wR_2[I > 2\sigma(I)]$	0.0462, 0.1267	0.0430, 0.1165
R_1, wR_2(all data)	0.0621, 0.1420	0.0607, 0.1300
S	1.041	1.025

Results

Crystal Structure of 4,4′-Bipyridyl-4,4′-isopropylidenediphenol (1)

Compound **1** crystallizes in $P2_1/n$ with one molecule of bipyridyl and one molecule of bisphenol lying in the general positions, thus giving a 1:1 molar ratio of bipyridyl to bisphenol, and it is explicitly observed that the hydroxyl hydrogen atoms are fully ordered and there is no evidence for any proton transfer from bisphenol to pyridyl (Fig. 1a). Within the asymmetric unit, the oxygen atoms of bisphenol, O1 and O2, both act as hydrogen-bond donors to interact with the nitrogen atoms N1 and N2 belonged to bipyridyl, which form two types of O–H···N hydrogen bonds (Fig. 2a). The O–H···N interactions between two components give an infinite molecular chain along the [101] orientation, and these chains translated by n glide plane are regularly arranged in b axis (Fig. 2a). Notably, thinking of weak C–H···O hydrogen bond formed between carbon atom C7 of bipyridyl and hydroxyl oxygen atom O1 of bisphenol (Figs. 1a, 2b) as the rungs of the ladder structure, two neighboring molecular chains related by 2_1 screw axis are connected to be the molecular ladder stretching toward the [101] orientation, and the bordering ladders are arranged in the direction $[10\bar{1}]$to acquire final three-dimensional crystal structure (Fig. 2b).

Table 2 Selected geometric parameters (fl. Å)

1	
Bond distance	
C(1)–N(1)	1.327(2)
C(3)–C(6)	1.484(2)
C(5)–N(1)	1.316(2)
C(8)–N(2)	1.325(2)
C(9)–N(2)	1.329(2)
C(11)–O(1)	1.3609(2)
C(14)–C(17)	1.5351(2)
C(17)–C(18)	1.5311(2)
C(17)–C(24)	1.5363(2)
C(17)–C(25)	1.5380(2)
Bond angle	
N(1)–C(1)–C(2)	123.91(16)
C(2)–C(3)–C(6)	122.64(12)
C(4)–C(3)–C(6)	121.33(14)
N(1)–C(5)–C(4)	124.36(16)
C(10)–C(6)–C(3)	122.05(12)
C(7)–C(6)–C(3)	121.89(13)
N(2)–C(8)–C(7)	124.22(14)
N(2)–C(9)–C(10)	123.28(14)
O(1)–C(11)–C(16)	118.37(13)
O(1)–C(11)–C(12)	123.31(13)
C(15)–C(14)–C(17)	123.88(11)
C(13)–C(14)–C(17)	120.11(11)
C(18)–C(17)–C(14)	109.33(10)
C(18)–C(17)–C(24)	112.23(10)
C(14)–C(17)–C(24)	108.29(11)
C(18)–C(17)–C(25)	107.54(11)
C(14)–C(17)–C(25)	112.02(11)
C(24)–C(17)–C(25)	107.47(12)
O(2)–C(21)–C(20)	118.55(13)
O(2)–C(21)–C(22)	123.09(13)
2	
Bond distance	
O(1)–C(21)	1.3726(15)
O(1)–C(14)	1.3948(15)
O(3)–C(17)	1.3153(17)
O(2)–C(17)	1.2075(16)
O(4)–C(24)	1.3158(18)
O(5)–C(24)	1.2052(18)
N(1)–C(5)	1.3249(19)
N(1)–C(1)	1.3275(19)
N(2)–C(10)	1.321(2)
N(2)–C(6)	1.333(2)
C(3)–C(8)	1.4882(17)
C(11)–C(17)	1.4948(17)
C(18)–C(24)	1.4880(18)
Bond angle	
C(21)–O(1)–C(14)	120.39(10)
C(5)–N(1)–C(1)	117.13(12)
C(10)–N(2)–C(6)	117.07(13)
C(2)–C(3)–C(8)	121.17(13)
C(4)–C(3)–C(8)	121.41(12)
C(9)–C(8)–C(3)	120.61(13)
C(7)–C(8)–C(3)	121.47(13)
N(1)–C(5)–C(4)	123.48(13)
N(2)–C(10)–C(9)	123.60(15)
N(1)–C(1)–C(2)	123.45(14)
N(2)–C(6)–C(7)	123.73(17)
C(15)–C(14)–O(1)	117.14(13)
C(13)–C(14)–O(1)	120.82(12)
O(1)–C(21)–C(22)	125.05(11)
O(1)–C(21)–C(20)	114.37(12)
O(2)–C(17)–O(3)	123.76(12)
O(2)–C(17)–C(11)	122.74(13)
O(3)–C(17)–C(11)	113.48(11)
O(5)–C(24)–O(4)	123.15(13)
O(5)–C(24)–C(18)	123.61(13)
O(4)–C(24)–C(18)	113.23(13)

Crystal Structure of 4,4′-Bipyridyl-4,4′-oxydibenzoic acid (**2**)

Compound **2** exhibits the same space group of $P2_1/n$, and the asymmetric unit is constituted by one molecule of bipyridyl and one molecule of oxydibenzoic acid in general positions. Similarly, hydroxyl hydrogen atoms of the acid are fully ordered and there is no proton transfer from acid to pyridyl (Fig. 1b). Seen from Fig. 3a, the hydroxyl oxygen atoms in carboxyl groups of 4,4′-oxydibenzoic acid, O3 and O4, separately interact with nitrogen atoms N1 and N2 of bipyridyl to form one-dimensional chains by using two conventional O–H···N hydrogen bonds that are similar with the hydrogen bonding in compound **1**. Interestingly, the chains extend to become two-dimensional layers along *a* axis generated from the linkage of C–H···O hydrogen bonding between carbon atom of bipyridyl and carbonyl oxygen atom located in the acid, e.g., C9–H9A···O5B (Fig. 3a). Moreover, another carbonyl oxygen atom O2 of 4,4′-oxydibenzoic acid is also able to generate C–H···O hydrogen bond with the carbon atom adjacent to N1 atom of pyridyl ring and this weak contact changes the forgoing layers into three-dimensional interlaced hydrogen-bonded networks shown in block diagram of compound **2** (Fig. 3b).

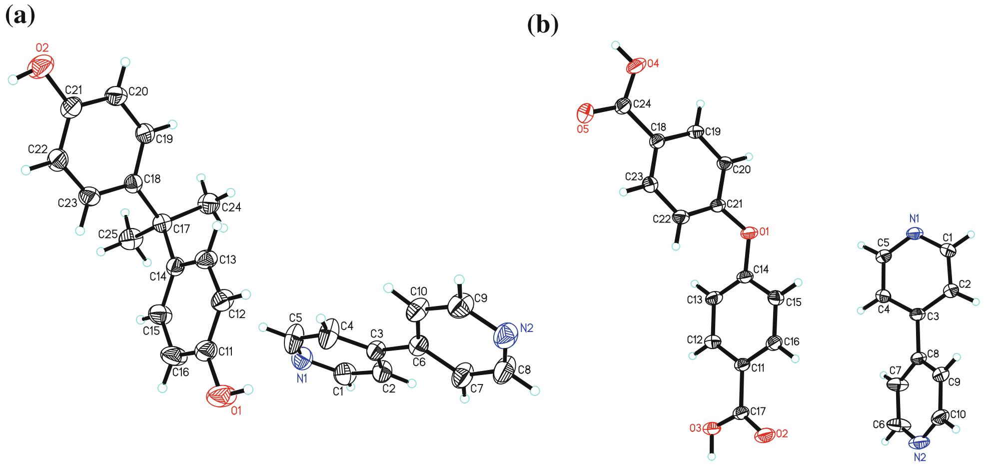

Fig. 1 A view of the unique molecular components of compound **1** (**a**) and **2** (**b**). Displacement ellipsoids are drawn at 30% probability level

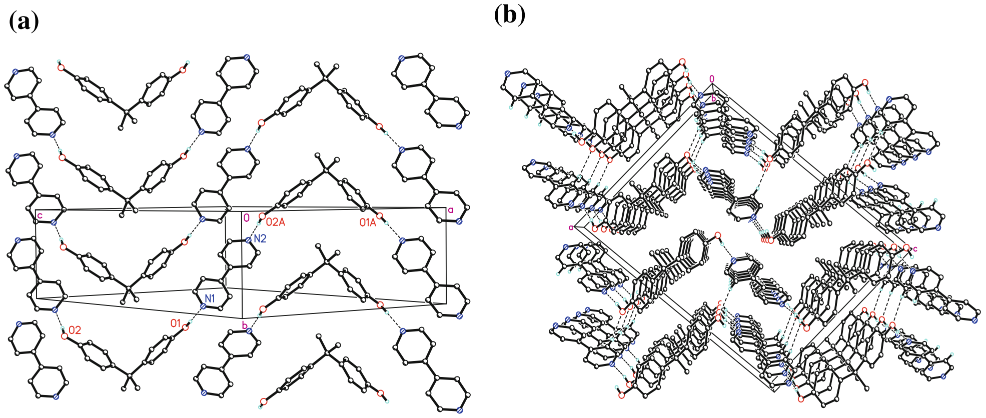

Fig. 2 **a** Part of the crystal structure of compound **1** showing the infinite chains arranged in the *b* axis. [*Symmetry codes*: A 1/2 + *x*, −*y* + 2/3, −1/2 + *z*]. **b** Depiction of the 3-D nature of the hydrogen bonding networks of compound **1** viewed down the *b*-axis, with the *a*-axis pointing to the southwest direction. For the sake of clarity, all the hydrogen atoms bond to carbon are omitted in **a** but the ones that involve in the hydrogen bonds are signified in **b**

Discussion

Complex **1** forms regular molecular chains containing alternative 4,4′-bipyridyl and 4,4′-isopropylidenediphenol units which are linked with O–H···N hydrogen bonds. Interestingly, every two neighboring chains are further connected to be a ladder structure by weak C–H···O interactions. Meanwhile, in compound **2**, 4,4′-bipyridyl and 4,4′-oxydibenzoic acid form one-dimensional architecture firstly; the molecular components are connected by strong O–H···N contacts. Additionally, two kinds of weak C–H···O hydrogen bonds formed between 4,4′-bipyridyl and the acid link one-dimensional chains to be interlaced three-dimensional hydrogen-bonded networks. Obviously, the conventional O–H···N hydrogen bonds play a significant role in the formation of two cocrystals, but to some extent, weak C–H···O interaction causes distinction to exist between these two crystal structures.

In compounds **1** and **2**, O–H···N hydrogen bonds and weak C–H···O contacts are essential interactions to yield ultimate crystal structures. Seen from Table 3, in compound **1**, the distance of O···N varies from 2.7424 to 2.7663 Å, and angle of O–H···N from 170° to 171°, whereas the corresponding distances from 2.6718 to 2.6729 Å, and the angles from 176° to 174° in compound **2**. Apparently, the O–H···N hydrogen bonds of compound **2** are stronger than those in compound **1**. Compared with the related parameters of O–H···N hydrogen bonds formed by V-shaped analogues and bipyridyl as well as its derivatives [31–34], the changes of the O···N distances and the corresponding angles of compound **1** and **2** are within the range of relevant values (The distance of O···N varies from 2.629 to 2.792 Å and the angles from 162° to 176°). From the two structures of this paper and other analogous structures in the literatures, it can be speculated that O–H···N hydrogen bond is a kind of efficient interaction to

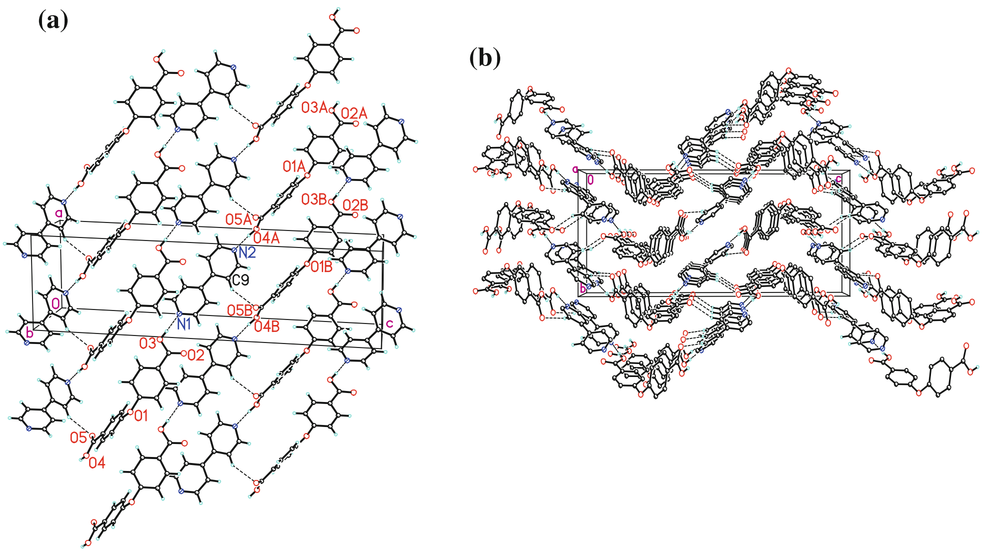

Fig. 3 **a** Part of the crystal structure of compound **2** showing the two-dimensional layer along the *a*-axis. [*Symmetry codes*: A 5/2 + *x*, −1 + *y*, 1/2 + *z*; B 3/2 + *x*, −1 + *y*, 1/2 + *z*]. **b** Projection of the 3-D nature of the interlaced networks of **2** viewed down the *a*-axis. All the hydrogen atoms but the ones that involve in the hydrogen bonds are omitted for clarity in **b**

Table 3 Hydrogen bonding geometry

Hydrogen bond	Distance (Å)	Angle (°)
Compound **1**		
O1···N1	2.7663	171
O2···N2	2.7424	170
C7···O1	3.3646	160
Compound **2**		
O3···N1	2.6729	174
O4···N2	2.6718	176
C2···O2	3.2920	155
C9···O5	3.3290	145

synthesize crystal structures. Thus it can be seen, it is useful to pre-design some interesting structures if the linkage models of different hydrogen bonds can be obtained.

Although two structures mentioned above form one-dimensional architecture by O–H···N hydrogen bonds, the final packing modes of two compounds are not identical for the influence of weak C–H···O interactions. There is only one type of weak C–H···O hydrogen bond in compound **1**, in which the related distance reaches 3.3646 Å and the angle 160°, whereas there exist two C–H···O hydrogen bonds in compound **2** (The corresponding distances are 3.2920 and 3.3290 Å, and the angles 155° and 145°). C–H···O contact is not a classic hydrogen bond, but many properties of C–H···O interaction have been discussed because weak and less common types of hydrogen bonds have been major topics in hydrogen bond research [35, 36]. Obviously, the related distances and angles of C–H···O hydrogen bonds in these two cocrystals are comparable with normal values (3.35(2) Å and 127(1)°) [36].

In crystal structure of compound **1**, the dihedral angle of two benzenes of 4,4′-isopropylidenediphenol is 87.5°, close to right-angle. Comparatively, the relevant angle of 4,4′-oxydibenzoic acid is 66.6° in compound **2**. Evidently, the interplanar angle of 4,4′-isopropylidenediphenol in compound **1** is greater than 4,4′-oxydibenzoic acid. That is to say, the repulsion of unshared pair electrons belonged to bridged oxygen atom of 4,4′-oxydibenzoic acid is not as strong as that yielded by two methyls in 4,4′-isopropylidenediphenol. Thus 4,4′-oxydibenzoic acid exhibits a gentle V-shaped structure compared with 4,4′-isopropylidenediphenol. Analyzing the crystal structures of 4,4′-sulfonyldiphenol·4,4′-bipyridyl (**3**) [34], 4,4′-bipyridyl·4,4′-thiodiphnol (**4**) [32] and 4,4′-dihydroxybenzophenone·4,4′-bipyridyl (**5**) [33], these three compounds are all constructed by similar V-shaped molecules with terminal hydroxyl groups and 4,4′-bipyridyl, but the central bridge atoms or groups of the V-shaped components are very different. In compound **3**, the dihedral angle of two benzenes connected by O=S=O group is 88.8°, whereas in complexes **4** and **5**, which are linked by S atom and C=O group separately, the corresponding values are 75.8° and 63.0°. Obviously, according to torsion angles, the sequence should be **3** > **1** > **4** > **2** > **5**. That is to say, if it is expressed by the central bridge atoms or groups, the order should be O=S=O > Me–C–Me > S > O > C=O. Conclusion can be made that the repulsions of O=S=O and Me–C–Me are similar and they are both stronger than forces generated by unshared pair electrons of single S or O atom. Regarding C=O group, V-shaped molecule having a smaller torsion angle compared with other analogues in compound **5** is possibly due to its planarity .

Meanwhile, it can be found that the dihedral angle of two pyridyls is 19.3° in compound **1** and 37.5° in **2**. Calculating the optimized configuration of a single 4,4′-bipyridyl molecule using the Hartree–Fock method based on the 3-21G basis set by the program Gaussian03 W [37], the result shows that the dihedral angle of two pyridyl rings is up to 49.2°. In other words, 4,4′-bipyridyl distorts to greater extent in compound **1** compared with optimized structure of itself. In compounds **3**, **4** and **5**, the V-shaped molecules all have terminal hydroxyl groups and the corresponding angles of bipyridyls are 24.4°, 25.8° and 12.7°, compared with the related values in compound **1**. As we have calculated the relevant interplanar angles of the V-shaped molecules in those five cocrystals, it is evident that the configuration of 4,4′-oxydibenzoic acid in compound **2** is comparatively gentle and its terminal carboxyl groups can subtly adjust their torsion angles (The dihedral angles between the carboxyl groups and the related benzene rings amount to 5.8° and 7.3°) to access pyridyl rings of 4,4′-bipyridyl. Thus 4,4′-bipyridyl of **2** doesn't need too much distortion to match 4,4′-oxydibenzoic acid. On the contrary, in complexes **1**, **3**, **4** and **5**, the terminal groups of the V-shaped components are all hydroxyl groups rotating along single C–O bond. To adapt the configuration of bisphenol and to generate hydrogen bonds as many as possible, 4,4′-bipyridyl in these four compounds contorts at least 23° from its optimized structure, thus builds final crystal structures.

The similar V-shaped molecules with the specified functional groups, e.g., hydroxyl and carboxyl groups, acting as interesting host molecule, can construct various hydrogen-bonded crystal structures. From the literatures, it can be found a series of adducts formed by V-shaped molecules and diamines, e.g., 4,4′-bipyridyl or its neutral derivatives. For example, in cocrystals of 4,4′-sulfonyldiphenol·1,2-bis(4-pyridyl)ethane (**6**) [31], 4,4′-dihydroxybenzophenone·1,2-bis(4-pyridyl)ethylene (**7**) [33], 4,4′-diazastilbene·4,4′-oxydibenzoic acid (**8**) [34], 1,3-bis(4-pyridyl)propane·4,4′-oxydibenzoic acid (**9**) [38] and complexes **3**, **4**, and **5**, all the V-shaped molecules can combine with diamines almost by the same linking model to generate one-dimensional molecular strings or spirals, in which the V-shaped molecules act as double donors of hydrogen bonds and the neutral diamines as double acceptors. Notably, there exist different weak interactions such as C–H···O interactions in compounds **3**, **6** and **7**, aromatic $\pi \cdots \pi$ stacking interactions in **4** and so on to generate the corresponding crystal structures.

Examination on structures with PLATON [39] shows that the total potential solvent area volume in compound **1** reaches 36.7 Å^3, accounting for approximately 1.7% in the unit cell volume, and the percent of filled space of compound **2** realizes 68.4% and the unit cell contains no residual solvent accessible void. Clearly, the V-shaped molecules and 4,4′-bipyridyl pack so tightly that no guest molecules can be included within them.

Supplementary Materials

CCDC 710200 and 747454 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data request/cif, by e-mailing data request@ccdc.cam.ac.uk, or by contracting the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0)1223-336033.

Acknowledgments Support from the National Nature Science Foundation of China (Grant No. 20871019) is gratefully acknowledged.

References

1. Imai Y, Tajima N, Sato T, Kuroda R (2006) Org Lett 8:2941
2. Kuroda R, Imai Y, Tajima N (2002) Chem Commun 2842
3. Friščić T, MacGillivray LR (2005) Chem Commun 5748
4. Shan N, Jones W (2003) Tetrahedron Lett 44:3687
5. Sokolov AN, Friščić T, MacGillivray L (2006) R J Am Chem Soc 128:2806
6. Sun CC, Hou H (2008) Cryst Growth Des 8:1575
7. Trask AV (2007) Mol Pharm 4:301
8. Chekal BP, Campeta AM, Abramov YA, Feeder N, Glynn PP, McLaughlin RW, Meenan PA, Singer RA (2009) Org Process Res Dev 13:1327
9. Desiraju GR (1995) Angew Chem Int Ed Engl 34:2311
10. Fan E, Vincent C, Geib SJ, Hamilton AD (1994) Chem Mater 6:1113
11. Subramanian S, Zaworotko MJ (1994) Coord Chem Rev 137:357–401
12. Abad MC, Askari H, O'Neill J, Klinger AL, Milligan C, Lewandowski F, Springer B, Spurlino J, Rentzeperis D (2008) J Steroid Biochem 108:44
13. Matsushima A, Teramoto T, Okada H, Liu XH, Tokunaga T, Kakuta Y, Shimohigashi Y (2008) Biochem Biophys Res Commun 373:408
14. Sumbayev VV, Jensen JK, Hansen JA, Andreasen PA (2008) Mol Cell Endocrinol 287:30
15. Kawamura A, Westwood I, Wakefield L, Long H, Zhang NX, Walters K, Redfield C, Sim E (2008) Biochem Pharmcol 75:1550
16. Li FB, Li XZ, Liu CS, Liu TX (2007) J Hazard Mater 149:199
17. Li FB, Li XZ, Li XM, Liu TX, Dong J (2007) J Colloid Interface Sci 311:481
18. Ferguson G, Coupar PI, Glidewell C (1997) Acta Cryst B53:513
19. Coupar PI, Glidewell C, Ferguson G (1997) Acta Cryst B53:521
20. Toda F, Tanaka K, Hyoda T, Mak TCW (1988) Chem Lett 1 107
21. Hatano B, Aikawa A, Tagaya H, Takahashiy H (2004) Chem Lett 33(10):1276
22. Takahashi I, Takahashi M, Kitajima H, Wagi M, Takahashi Y, Sabi M, Hatanaka M, Yamano A, Ohta T, Hosoi S (2003) Heterocyc 59(2):517

23. Mahata P, Prabu M, Natarajan S (2008) Inorg Chem 47(19):8451
24. Zhang J, Chen S, Bu X (2008) Angew Chem Int Ed 47(29):5434
25. Lan YQ, Li SL, Fu YM, Xu YH, Li L, Su ZM, Fu Q (2008) Dalton Trans (47): 6796
26. Martin DP, Supkowski RM, LaDuca RL (2007) Inorg Chem 46(19):7917
27. Kondo M, Irie Y, Miyazawa M, Kawaguchi H, Yasue S, Maeda K, Uchida F (2007) J Organomet Chem 692:136
28. Yang Y, Yin B, Li Q, Englert UJ (2009) Mol Struct 920:401
29. SMART APEX software (5.624) for SMART APEX detector, Bruker Axs Inc. Madison, WI
30. Sheldrick GM (1997) SHELXS97 and SHELXL97. University of Göttingen, Germany
31. Ferguson G, Glidewell C, Gregsonb RM, Lavender ES (1999) Acta Cryst B55:573
32. Lough AJ, Gregson RM, Ferguson G, Glidewell C (1999) Acta Cryst C55:1890
33. Wang J, Ding LY, Yang CQ (2007) CrystEngComm 9:591
34. Ma ZC, Ma AQ, Wang GP (2006) Acta Cryst E62:o1165
35. Van Den Berg JA, Seddon KR (2003) Cryst Growth Des 3(5):643
36. Steiner T (2002) Angew Chem Int Ed 41:48
37. Frisch MJ et al (2004) Gaussian03, ReVision B.04. Gaussian Inc, Wallingford, CT
38. Li G, Salim C, Hinode H (2008) Acta Cryst E64:o2251
39. Spek AL (1995) *PLATON*. Molecular geometry program. University of Utrecht, Utrecht, The Netherlands