Small-Ring Inclusion Hosts. 4.* X-Ray Crystal Structures of *trans*-3,3-Bis(4-methylphenyl)cyclopropane-1,2-dicarboxylic Acid and of Its Inclusion Complex with Dimethyl Sulphoxide (1:2)

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Abstract. The crystal structures of the unsolvated *trans*-3,3-bis(4-methylphenyl)cyclopropane-1,2-dicarboxylic acid (**1**) and of its inclusion compound with dimethyl sulphoxide, **1**·DMSO (1:2), have been studied by X-ray diffraction. Crystals of **1** show triclinic symmetry ($P\bar{1}$) with $Z = 4$ and the unit cell dimensions $a = 7.617(2)$, $b = 15.321(4)$, $c = 15.297(3)$ Å, $\alpha = 109.76(2)$, $\beta = 103.47(1)$, $\gamma = 89.87(2)°$. Final $R = 0.037$ for 3601 reflections collected at $T = 153(1)$ K. Crystals of **1**·DMSO (1:2) are monoclinic ($P2_1/n$) with $Z = 4$ and cell dimensions $a = 10.744(1)$, $b = 10.806(1)$, $c = 21.302(2)$ Å, $\beta = 101.68(1)°$. The clathrate structure was refined to $R = 0.034$ for 1671 reflections obtained at $T = 173(1)$ K. In the unsolvated host compound cyclic pairs of O—H···O bonds, commonly observed in carboxylic acids, couple the carboxylic functions two by two, thus giving rise to endless chains due to the bifunctionality and the *trans* position of the acid groups of **1**. The complex with DMSO as guest, however, consists of distinct hydrogen-bonded 1:2 host–guest associates, held together by weak intermolecular interactions.

Key words. X-ray structure analysis, cyclopropanedicarboxylic acid host, dimethyl sulphoxide, crystalline complex, hydrogen bonding.

Supplementary Data relating to this article have been deposited with the British Library at Boston Spa, Wetherby, West Yorkshire, U.K., as Supplementary Publication No. SUP 82139 (32 pages).

1. Introduction

Engineering of supramolecular crystalline complexes is an important problem [2] connected with the development of new technologies [3–5] including chemical sensor devices [6] and nonlinear optical materials [7]. This involves specific interaction and orientation of molecules in particular aggregate patterns [8]. Searching for the rules which govern the interaction of groups between different molecules in different geometric environments is perhaps the most promising approach. A microstructure involving such interactions may be based on H bonds between particular H donor and acceptor groups of a host and a guest component to form a crystalline inclusion compound [9–11]. In this connection we have studied the

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potential interaction modes between small-ring carboxylic acid hosts and guest molecules with different functional groups attached [1,12–14]. Here we report on the X-ray crystal structures of the free host compound *trans*-3,3-bis(4-methylphenyl)cyclopropane-1,2-dicarboxylic acid (**1**) and of its inclusion complex with dimethyl sulphoxide (DMSO), **1·DMSO** (1:2).

1
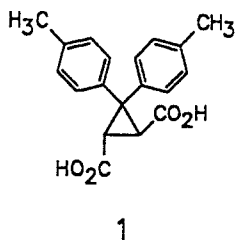
2. Experimental

2.1. SAMPLE PREPARATION

The host compound **1** was prepared as previously described [13]. Crystals of the inclusion compound were grown by dissolving the host in DMSO and saturating the solution by slow evaporation at room temperature.

2.2. X-RAY DATA COLLECTION AND PROCESSING

X-ray data were collected on a STOE/AED2 diffractometer, with graphite-monochromated $MoK\alpha$ radiation, using the $\omega-2\theta$ scan technique. The colourless, irregularly shaped single crystals were sealed in epoxy glue. Five standard reflections for each compound, measured once every hour during the data collections, showed an intensity decrease of $\sim 6\%$ for **1** and less than 5% for the inclusion compound. Data reductions included corrections for background, decay, Lorentz and polarization effects, but the relatively modest absorption effects (*cf.* Table I) were ignored. The unit cell dimensions were refined against θ values of 44 ($10.2 < 2\theta < 21.3°$) and 56 ($10.8 < 2\theta < 29.1°$) carefully centered reflections for **1** and **1·DMSO** (1:2), respectively. Crystal data and selected experimental details are given in Table I.

2.3. STRUCTURE ANALYSIS AND REFINEMENT

Direct methods using the SHELXS program system [15] resulted in a reasonable model for the clathrate with DMSO as guest but not for the unsolvated host. This latter structure was finally solved using the MULTAN80 system [16]. A randomly oriented and positioned host molecule from the clathrate structure was used in the calculation of the normalized structure factors (E). 350 E values ($E > 2.2$) and 1265 phase relationships between them were used to calculate 512 different phase sets by the tangent formula [16]. Set No. 457, having the best figure of merit, yielded more or less reasonable positions for all but one of the non-hydrogen atoms of the two crystallographically independent host molecules. This very approximate model was then used as input to a combination of reycling procedures and weighted Fourier

Table I. Crystal data and selected experimental details. The esds are given in parentheses

Compound	1	1·DMSO (1:2)
Formula	$C_{19}H_{18}O_4$	$C_{19}H_{18}O_4 \cdot 2(C_2H_6OS)$
Formula weight	310.35	466.61
Space group	$P\bar{1}$	$P2_1/n$
a, Å	7.617(2)	10.744(1)
b, Å	15.321(4)	10.806(1)
c, Å	15.297(3)	21.302(2)
α, deg.	109.76(2)	90.0
β, deg.	103.47(1)	101.68(1)
γ, deg.	89.87(2)	90.0
V_c, Å^3	1628.1(8)	2721.9(4)
Z	4	4
$F(000)$	656	992
D_c, g cm^{-3}	1.2661(6)	1.2797(2)
μ, cm^{-1}	0.82	2.43
Radiation/λ, Å	MoK_α/0.71069	MoK_α/0.71069
Temperature, K	153(1)	173(1)
Approximate crystal size	$0.58 \times 0.34 \times 0.30$	$0.32 \times 0.32 \times 0.32$
No. of collected reflections	7621	8771
θ limit, deg.	27.5	25
Range of h, k, l	$-9 \Rightarrow 9, -19 \Rightarrow 19,$ $0 \Rightarrow 19$	$-12 \Rightarrow 12, -12 \Rightarrow 12,$ $0 \Rightarrow 25$
No. of unique non-zero reflections	6421	3982
No. of significantly observed reflections	3601	1734
Criterion of significance	$I/\sigma(I) > 3$	$I/\sigma(I) > 2.5$
No. of refined variables	461	345
$R = \Sigma|\Delta F|/\Sigma|F_o|$	0.037	0.034
$wR = [\Sigma w|\Delta F|^2/\Sigma|F_o|^2]^{1/2}$	0.045	0.036
Weighting: $w = [\sigma^2(F) + g \cdot F^2]^{-1}$		
with g	0.00650	0.00025
wR_{tot}	0.060	0.049
Final $\Delta\rho_{max}/\Delta\rho_{min}$, e$^-$Å^{-3}	0.08/$-$0.13	0.20/$-$0.20

syntheses [16] to yield the final solution comprising acceptable positions for all O and C atoms of the crystallographic asymmetric unit.

The structure models were refined by full-matrix least-squares calculations (SHELX) [17]. All hydrogen positions in the clathrate structure as well as those of the carboxyl H atoms and the hydrogens bonded to the cyclopropane ring in the free host structure were derived from $\Delta\rho$ maps. The (C)—H atoms in 1, except the four mentioned above, were assumed to have geometrically predicted positions (C—H = 1.00 Å), which were recalculated after each refinement cycle.

In the last stage of the refinements, the non-hydrogen positions were refined together with their anisotropic displacement parameters. The sites of the carboxylic H atoms, and of those bonded to the cyclopropane ring in both compounds and of the hydrogens belonging to the DMSO guests in the clathrate crystal were refined together with their isotropic thermal motion parameters. Furthermore, isotropic displacement parameters were refined for the calculated hydrogen positions of 1, whereas for the remaining H atoms in the clathrate structure, located from $\Delta\rho$ maps

Table II. Fractional atomic coordinates and equivalent isotropic temperature factors of the non-hydrogen atoms with esds given in parentheses

Atom	x/a	y/b	z/c	$U_{eq}^{a}(Å^2)$
1 (*Free Host*)				
C(1)	0.8076(3)	0.0073(2)	0.2770(2)	0.018(1)
C(2)	0.9114(3)	0.0563(2)	0.3819(2)	0.017(1)
C(3)	0.7693(3)	−0.0208(2)	0.3588(2)	0.019(1)
C(4)	0.9036(3)	−0.0598(2)	0.2095(2)	0.021(1)
C(5)	0.9788(4)	−0.0277(2)	0.1497(2)	0.035(1)
C(6)	1.0676(4)	−0.0870(2)	0.0866(2)	0.042(2)
C(7)	1.0865(4)	−0.1782(2)	0.0806(2)	0.032(1)
C(71)	1.1812(5)	−0.2420(3)	0.0098(3)	0.054(2)
C(8)	1.0125(4)	−0.2093(2)	0.1400(2)	0.034(1)
C(9)	0.9214(4)	−0.1514(2)	0.2032(2)	0.028(1)
C(10)	0.6844(3)	0.0652(2)	0.2315(2)	0.019(1)
C(11)	0.5362(4)	0.0235(2)	0.1556(2)	0.036(1)
C(12)	0.4358(4)	0.0759(2)	0.1066(2)	0.044(2)
C(13)	0.4785(4)	0.1700(2)	0.1307(2)	0.029(1)
C(131)	0.3696(4)	0.2259(3)	0.0757(3)	0.044(2)
C(14)	0.6251(4)	0.2110(2)	0.2067(2)	0.032(1)
C(15)	0.7258(4)	0.1599(2)	0.2566(2)	0.026(1)
C(16)	1.1073(3)	0.0425(2)	0.4050(2)	0.018(1)
O(17)	1.1687(2)	−0.0290(1)	0.4119(2)	0.023(1)
O(18)	1.2074(2)	0.1164(1)	0.4121(2)	0.025(1)
C(19)	0.5950(3)	0.0023(2)	0.3858(2)	0.019(1)
O(20)	0.5487(2)	0.0808(1)	0.4131(2)	0.024(1)
O(21)	0.4947(3)	−0.0730(1)	0.3737(2)	0.030(1)
C(1′)	0.4391(3)	0.3789(2)	0.6655(2)	0.016(1)
C(2′)	0.3231(3)	0.3218(2)	0.5661(2)	0.018(1)
C(3′)	0.4805(3)	0.2808(2)	0.6125(2)	0.018(1)
C(4′)	0.3759(3)	0.3926(2)	0.7555(2)	0.018(1)
C(5′)	0.2587(4)	0.4600(2)	0.7833(2)	0.028(1)
C(6′)	0.2124(4)	0.4788(2)	0.8705(2)	0.030(1)
C(7′)	0.2821(3)	0.4317(2)	0.9319(2)	0.026(1)
C(71′)	0.2368(4)	0.4529(2)	1.0273(2)	0.034(1)
C(8′)	0.3984(4)	0.3637(2)	0.9032(2)	0.033(1)
C(9′)	0.4452(4)	0.3444(2)	0.8162(2)	0.028(1)
C(10′)	0.5484(3)	0.4634(2)	0.6706(2)	0.018(1)
C(11′)	0.4668(3)	0.5250(2)	0.6275(2)	0.023(1)
C(12′)	0.5596(4)	0.6079(2)	0.6402(2)	0.026(1)
C(13′)	0.7367(4)	0.6318(2)	0.6963(2)	0.025(1)
C(132)	0.8361(4)	0.7234(2)	0.7119(2)	0.039(2)
C(14′)	0.8186(4)	0.5690(2)	0.7376(2)	0.025(1)
C(15′)	0.7263(3)	0.4860(2)	0.7258(2)	0.021(1)
C(16′)	0.1352(3)	0.2891(2)	0.5588(2)	0.019(1)
O(17′)	0.0974(2)	0.2386(1)	0.6004(2)	0.024(1)
O(18′)	0.0148(3)	0.3243(2)	0.5063(2)	0.028(1)
C(19′)	0.6514(3)	0.2698(2)	0.5807(2)	0.018(1)
O(20′)	0.6828(2)	0.2980(1)	0.5197(1)	0.023(1)
O(21′)	0.7673(3)	0.2300(2)	0.6302(2)	0.026(1)

Table II. *Continued*

Atom	x/a	y/b	z/c	$U_{eq}^a (Å^2)$
1·DMSO *(1:2)*				
C(1)	0.3829(4)	0.7678(4)	1.1104(2)	0.024(2)
C(2)	0.3286(4)	0.7437(4)	1.0401(2)	0.028(2)
C(3)	0.3946(4)	0.6406(4)	1.0808(2)	0.027(2)
C(4)	0.2953(4)	0.7749(4)	1.1577(2)	0.022(2)
C(5)	0.3024(4)	0.6875(4)	1.2062(2)	0.028(2)
C(6)	0.2256(4)	0.6969(4)	1.2508(2)	0.032(2)
C(7)	0.1405(4)	0.7936(4)	1.2489(2)	0.030(2)
C(71)	0.0552(4)	0.8020(5)	1.2975(2)	0.047(2)
C(8)	0.1337(4)	0.8804(4)	1.2004(2)	0.033(2)
C(9)	0.2104(4)	0.8723(4)	1.1555(2)	0.029(2)
C(10)	0.4974(4)	0.8518(4)	1.1268(2)	0.024(2)
C(11)	0.5970(4)	0.8227(4)	1.1765(2)	0.033(2)
C(12)	0.7002(4)	0.9018(4)	1.1937(2)	0.035(2)
C(13)	0.7040(4)	1.0147(4)	1.1629(2)	0.028(2)
C(131)	0.8166(4)	1.1003(4)	1.1815(3)	0.044(2)
C(14)	0.6029(4)	1.0436(4)	1.1138(2)	0.033(2)
C(15)	0.5013(4)	0.9638(4)	1.0957(2)	0.030(2)
C(16)	0.1883(4)	0.7400(4)	1.0167(2)	0.028(2)
O(17)	0.1189(3)	0.6656(3)	1.0340(2)	0.037(1)
O(18)	0.1502(3)	0.8331(3)	0.9771(2)	0.036(2)
C(19)	0.5212(4)	0.5953(4)	1.0730(2)	0.029(2)
O(20)	0.5903(3)	0.6508(3)	1.0441(2)	0.041(2)
O(21)	0.5505(4)	0.4909(3)	1.1040(2)	0.045(2)
S	0.8972(1)	0.4768(1)	1.1140(1)	0.039(1)
O(D)	0.7779(3)	0.4022(3)	1.1112(2)	0.050(2)
C(D1)	0.8824(7)	0.6079(6)	1.1627(4)	0.056(3)
C(D2)	1.0168(6)	0.3979(6)	1.1697(3)	0.051(3)
S′	−0.2014(1)	0.8140(1)	0.9521(1)	0.040(1)
O(D′)	−0.0882(3)	0.8530(3)	0.9244(2)	0.038(1)
C(D1′)	−0.1625(8)	0.8498(6)	1.0350(3)	0.057(3)
C(D2′)	−0.1954(6)	0.6504(5)	0.9577(3)	0.040(2)

^{a} $U_{eq} = \frac{1}{3} \Sigma_i \Sigma_j U_{ij} \mathbf{a}_i^* \mathbf{a}_j^* a_i a_j$

and kept riding on their 'mother atoms', only one common isotropic vibration parameter was refined. Three strong low-θ reflections with considerably larger F_c than F_o, in all probability due to extinction effects, were excluded from the last refinement calculation of **1·DMSO** (1:2). Final reliability factors and details of the refinement calculations are given in Table I. The wR_{tot} values were calculated for the final models using all unique non-zero reflections. The refined fractional atomic coordinates and equivalent isotropic displacement parameters for the non-hydrogen atoms in both compounds are listed in Table II.

3. Results and Discussion

Perspective views of the crystallographic asymmetric unit of **1** and **1·DMSO** (1:2), with atoms labelled as in the text, are shown in Figures 1 and 2, respectively.

Table III. Distances (Å) and angles (deg.) in (O—)H⋯O hydrogen bonds and in possible (C—)H⋯O interactions. The esds are given in parentheses

Atoms involved	Symmetry	Distances	D—H	H⋯A	Angle
		Donor⋯Acceptor			D—H⋯A
1 (*free host*)					
O(18)—H(18)⋯O(20)	$x + 1, y, z,$	2.652(2)	1.00(4)	1.66(4)	169(4)
O(21')—H(21')⋯O(17')	$x + 1, y, z,$	2.669(3)	0.95(4)	1.73(4)	172(4)
O(18')—H(18')⋯O(20')	$x - 1, y, z,$	2.627(3)	0.86(4)	1.77(4)	169(4)
O(21)—H(21)⋯O(17)	$x - 1, y, z$	2.714(3)	0.97(4)	1.75(4)	175(4)
C(3')—H(3')⋯O(21)	$-x + 1, -y, -z + 1$	3.263(3)	0.93(3)	2.46(3)	144(2)
C(12')—H(12')[a]⋯O(20')	$-x + 1, -y + 1, -z + 1$	3.425(3)	1.00	2.47	159
1·*DMSO* (*1:2*)					
O(18)—H(18)⋯O(D')	x, y, z	2.589(4)	0.88(6)	1.72(5)	168(6)
O(21)—H(21)⋯O(D)	x, y, z	2.600(4)	0.82(5)	1.80(5)	168(5)
C(D1)—H(D11)⋯O(20)	x, y, z	3.637(7)	0.92(4)	2.84(4)	146(3)
C(D1')—H(D14)⋯O(17)	x, y, z	3.624(8)	0.94(6)	2.82(5)	144(5)
C(D2')—H(D24)⋯O(17)	$x, y, z,$	3.442(6)	0.97(4)	2.55(4)	154(3)
C(D2')—H(D25)⋯O(20)	$x - 1, y, z$	3.226(7)	0.95(5)	2.35(5)	153(4)
C(D1')—H(D15)⋯O(18)	$-x, -y + 2, -z + 2$	3.441(7)	1.04(6)	2.41(5)	170(4)
C(D1')—H(D16)⋯O(20)	$x - 1, y, z$	3.453(8)	0.86(5)	2.72(4)	144(4)
C(D2')—H(D24)⋯O(17)	$-x, -y + 1, -z + 2$	3.508(6)	0.97(4)	3.16(4)	103(3)

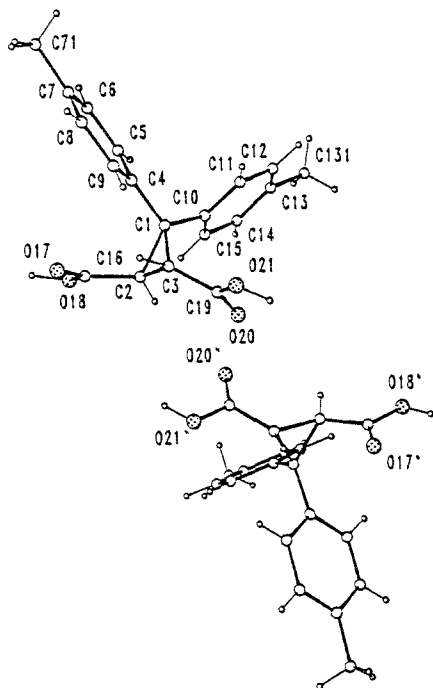[a] The position of H(12') in the structure of the unsolvated **1** was not refined (see text).

Fig. 1. Perspective view of the asymmetric unit of the structure of the unsolvated host, **1**, with crystallographic labelling of the atoms. O atoms are dotted.
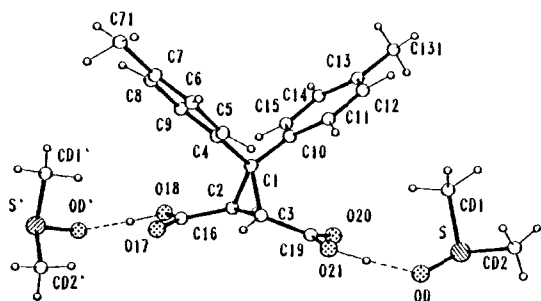

Fig. 2. Perspective view of the asymmetric unit in **1**·DMSO.*Jis*(2), with crystallographic labelling of the atoms. Heteroatoms are shaded. Solid and dashed lines represent covalent and hydrogen bonds, respectively.

Stereo packing illustrations are given in Figures 3 and 4. Hydrogen bonds and possible (C)—H···O interactions are listed in Table III.

3.1. MOLECULAR STRUCTURES

Corresponding covalent bond lengths and bond angles in four crystallographically independent *trans*-3,3-bis(methylphenyl)cyclopropane-1,2-dicarboxylic acid mole-
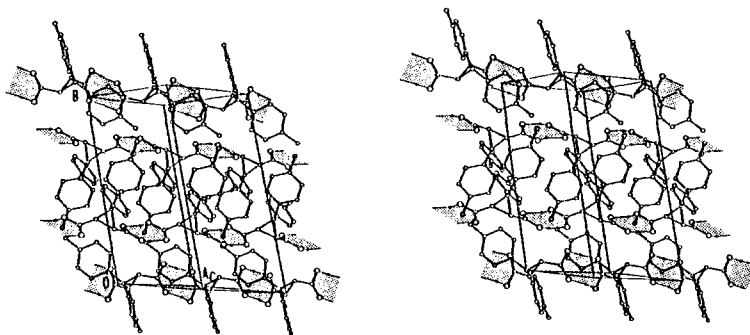
Fig. 3. Stereo packing diagram of the host compound **1**. The carbon-bonded H atoms are omitted for clarity. Thin lines represent hydrogen bonds. Hydrogen-bonded ring systems are marked with dotting.
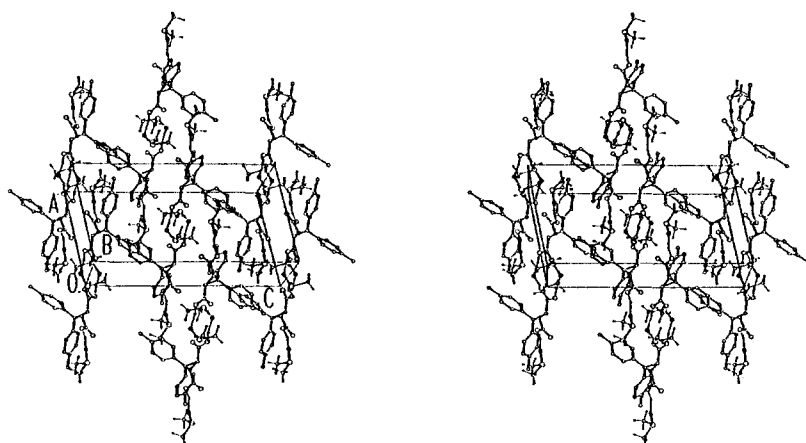

Fig. 4. Stereo packing diagram of the **1·DMSO** (1:2) inclusion complex. The carbon-bonded H atoms of the host are omitted for clarity. O atoms of the DMSO molecules are filled. Thin lines represent hydrogen bonds.

cules [the unprimed and primed molecules of unsolvated **1**, and the hosts in **1·DMSO** (1:2) and in the recently studied complex **1·EtOH** (1:2)] [18] agree with each other within experimental errors. Comparison of the dihedral angles between least-squares (LS) planes through different planar fragments of the host molecule **1** (Table IV in the supplementary material) indicates, however, that the diphenyl-cyclopropane-dicarboxylic acid skeleton is not strictly rigid. Its conformation varies somewhat, most likely depending on differences in intermolecular interactions (*e.g.* hydrogen bonds) and in packing forces. The inclination angle between the LS planes of the two *trans*-positioned —COO(H) groups is 25.9(3) and 23.0(4)° in the unprimed and primed molecules, respectively.

The bond distances and bond angles in the two pyramid-shaped DMSO guests in the **1·DMSO** (1:2) inclusion compound generally conform to the expected values. The sum of the angles around the S atoms is 308.9 and 311.3° for the unprimed and primed molecule, respectively.

3.2. PACKING RELATIONS AND HOST-GUEST INTERACTIONS

Unsolvated compound **1** crystallizes as a typical *trans*-dicarboxylic acid. It forms infinite chains in which the carboxyl groups are interlinked by hydrogen bonds into cyclic pairs (Figure 3), a pattern which is observed to occur frequently in carboxylic acids [19–21]. It is noteworthy, that in the present centrosymmetric ($P\bar{1}$) structure the hydrogen bonded ring of carboxyl groups does not lie on an inversion centre. Instead, molecules related by translation in the x direction are H-bonded to each other, thus giving rise to chains which are chiral. Molecules related by the center of symmetry or by translation in the two other directions belong to different chains. H-bonded endless chiral chains were found also in the crystal structure of the related 3,3′-diphenyl-*cis*-1,2-dicarboxylic acid [13]. The *cis*-acid molecules are interlinked by the catemer motif [19] achieved by translation in the x direction. Nevertheless, the chains in this latter case are arranged so as to yield the enantiomorphous $P2_1$ space group symmetry [13], whereas the packing of the chains formed by the *trans*-acid is centrosymmetric. Investigation of the intermolecular contacts in the crystals of the present *trans*-dicarboxylic acid gives indication of possible (C—)H⋯O interactions (*cf.* Table III). However, the shortest (C—)H⋯O distance, surprisingly, is to a hydroxy oxygen, O(21). This makes it seem likely that the C⋯O contacts, listed in Table III for the unsolvated host **1**, are effects of an electrostatically favourable packing of the H-bonded chains in this structure.

Earlier X-ray investigations of DMSO inclusion compounds by different carboxylic host molecules [12, 22, 23] revealed largely identical patterns for the host–guest interaction in the studied compounds. The shortest distance from one of the (S)-methyl carbons of each guest to the nearest (C)=O group of a host was less than 3.3 Å in all cases, thus suggesting the presence of a weak (C—)H⋯O type interaction [24–28] between host and guest besides the usual (O—)H⋯O(=S) hydrogen bond. Inspection of the contact distances between host and guest in the present DMSO clathrate indicates several possible C(H)⋯O type of bonds between them, but the two guests seem to have different modes of interaction with the host matrix (Figure 4). Both guests are ordinary proton acceptors in a hydrogen bond from the host (Table III), but only the primed DMSO molecule may be involved in (C—)H⋯O type of bonds, probably with both of its (S)-methyl groups (Table III), if the geometric criterion recommended by Bertolasi *et al.* [C⋯O < 3.5 Å, H⋯O < 2.7 Å, 120° < C—H⋯O < 180°, Ref. 27] is applied. The shortest distances observed for the (S)-methyl⋯O contact from the unprimed guest molecule [C⋯O = 3.637(7), H...O = 2.83 Å, *cf.* Table III] is in the range of common van der Waals' contact. Nevertheless, according to the suggestion of Desiraju [28] even long C⋯O separations of 3.5–4.0 Å may have to be considered seriously as C(H)⋯O bonds, because this type of contact is not really a van der Waals' interaction but is primarily electrostatic, falling off much more slowly with distance. Moreover, there is one more host-guest distance worth mentioning, *viz.* C(16)⋯O(D)$_{1-x,1-y,2-z}$ = 3.218(6) Å. Examination of the stereo packing diagram (Figure 4), however, reveals that this latest short approach between centrosymmetrically related units is probably a packing effect. The unprimed DMSO guest seems to be forced to turn around its H-bond and take a somewhat peculiar position in order to avoid collision with the nearest symmetry related primed guest molecule.

In summary, the pattern of host–guest interaction in the present DMSO inclusion compound differs somewhat from those studied earlier [12, 22, 23], indicating the current problems in predicting a reliable model for molecular recognition and organization in hetero-molecular crystals. We are still at the data-gathering level with regard to the classification of specific interaction modes that define supramolecular structures.

Acknowledgements

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