Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

cis-Cyclohexane-1,4-dicarboxylic acid

Yan-Qin Wang* and Jia-Bao Weng

Fujian Provincial Key Laboratory for Polymer Materials, College of Chemistry and Materials Science, Fujian Normal University, Fuzhou, Fujian 350007, People's Republic of China
Correspondence e-mail: yqwang@fjnu.edu.cn

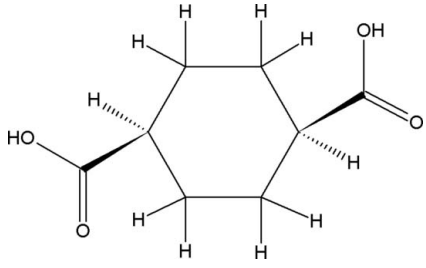
Received 8 March 2009; accepted 29 April 2009

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.055; wR factor = 0.129; data-to-parameter ratio = 16.3.

In the title compound, $C_8H_{12}O_4$, the two carboxyl groups are on the same side of the cyclohexane ring and the ring adopts a chair conformation. Adjacent molecules related by an inversion centre are linked by pairs of O—H···O hydrogen bonds, forming a zigzag chain along [1$\bar{1}\bar{1}$].

Related literature

For related structures, see: Bi *et al.* (2003, 2004); Chen *et al.* (2006); Du *et al.* (2006); Dunitz & Strickler (1966); Kurmoo *et al.* (2003, 2006); Luger *et al.* (1972).



Experimental

Crystal data

$C_8H_{12}O_4$
M_r = 172.18
Triclinic, $P\bar{1}$
a = 5.2912 (6) Å
b = 6.2611 (6) Å
c = 13.1851 (18) Å
α = 82.505 (10)°
β = 80.309 (11)°
γ = 81.875 (10)°
V = 423.70 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 296 K
0.24 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.979, T_{max} = 0.989
9807 measured reflections
1925 independent reflections
1222 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.129
S = 1.05
1925 reflections
118 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H1···O1^{i}	0.88 (4)	1.81 (4)	2.684 (2)	178 (4)
O3—H8···O4^{ii}	1.01 (4)	1.65 (4)	2.658 (2)	175 (4)

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $-x+2, -y, -z+1$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors are grateful for funding support from the National Natural Science Foundation of China (20471015; 20874012) and the Foundation for Key Programs of the Ministry of Education, China (DB–O57).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2399).

References

Bi, W., Cao, R., Sun, D., Yuan, D., Li, X. & Hong, M. (2003). *Inorg. Chem. Commun.* **6**, 1426–1428.
Bi, W., Cao, R., Sun, D., Yuan, D., Li, X., Wang, Y., Li, X. & Hong, M. (2004). *Chem. Commun.* pp. 2104–2105.
Bruker (2007). *SMART* and *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, B., Fronczek, F. R., Courtney, B. H. & Zapata, F. (2006). *Cryst. Growth Des.* **6**, 825–828.
Du, M., Zhang, Z. & Zhao, X. (2006). *Cryst. Growth Des.* **6**, 390–396.
Dunitz, J. D. & Strickler, P. (1966). *Helv. Chim. Acta*, **49**, 2505–2515.
Kurmoo, M., Kumagai, H., Akita-Tanaka, M., Inoue, K. & Takagi, S. (2006). *Inorg. Chem.* **45**, 1627–1637.
Kurmoo, M., Kumagai, H., Hughes, S. M. & Kepert, C. J. (2003). *Inorg. Chem.* **42**, 6709–6722.
Luger, P., Plieth, K. & Ruban, G. (1972). *Acta Cryst.* B**28**, 706–710.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2009). E**65**, o1293 [doi:10.1107/S1600536809016110]

cis-Cyclohexane-1,4-dicarboxylic acid

Yan-Qin Wang and Jia-Bao Weng

S1. Comment

According to the literatures, there are a few structures incorporating 1,4-*cis*-Cyclohexane dicarboxylic acid (Bi *et al.*, 2004). Although the structures of its isomer in *trans* conformation have been described for more than 40 years (Dunitz & Strickler, 1996; Luger *et al.*, 1972), the structure of the title compound, (I), has only been reported as a co-crystal by Du *et al.* (2006).

According to the results of single X-ray diffraction analysis, there is one complete molecule in the asymmetric unit, and the molecule is in a general position (Fig. 1). The geometry of the molecule is similar to the one observed by Du *et al.* (2006). The bond lengths are comparable to those in its isomers in *trans* conformations (Bi *et al.*, 2003; Chen *et al.*, 2006; Kurmoo *et al.*, 2003, 2006).

Strong hydrogen bonds between two adjacent carboxylate groups link molecules into a zigzag chain along the $[1\overline{1}1]$ direction. The zigzag chains are packed into three-dimensional motif (Fig. 2).

S2. Experimental

$C_8H_{12}O_4$ (1 mmol, 172 mg; mixture of *trans*- and *cis*-ACROS) was disloved into 50 ml of CD_3OD. The solution was stirring and refluxing for 12 h, and the clear solution was allowed to evaporate slowly in the inert atmosphere. Nice plate crystals of the title compound were obtained after 5 days. The crystals were filtered, washed by cool EtOH and dried in the air.

S3. Refinement

H atoms on O atoms were located in a difference Fourier map and were refined freely. Other H atoms were refined as riding, with C—H = 0.97 or 0.98 Å, and with U_{iso}(H) = 1.2U_{eq}(C).

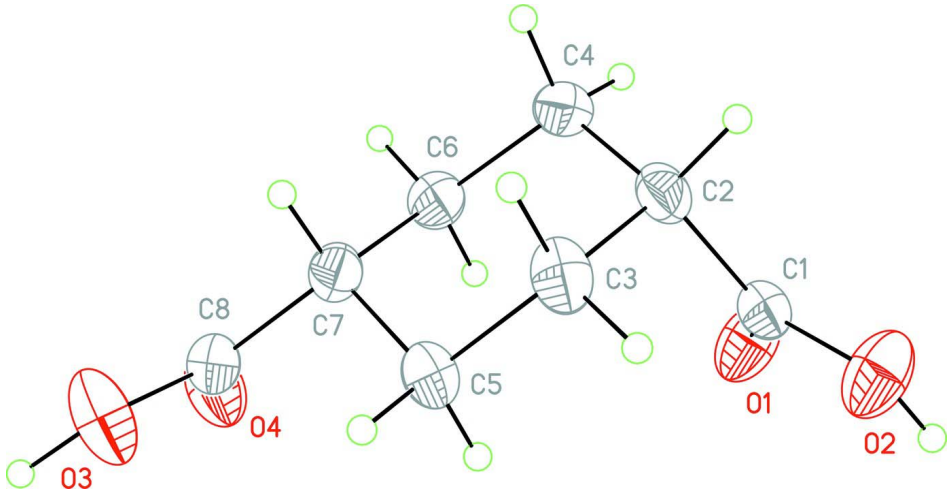


Figure 1

Molecular structure showing 50% probability displacement ellipsoids.

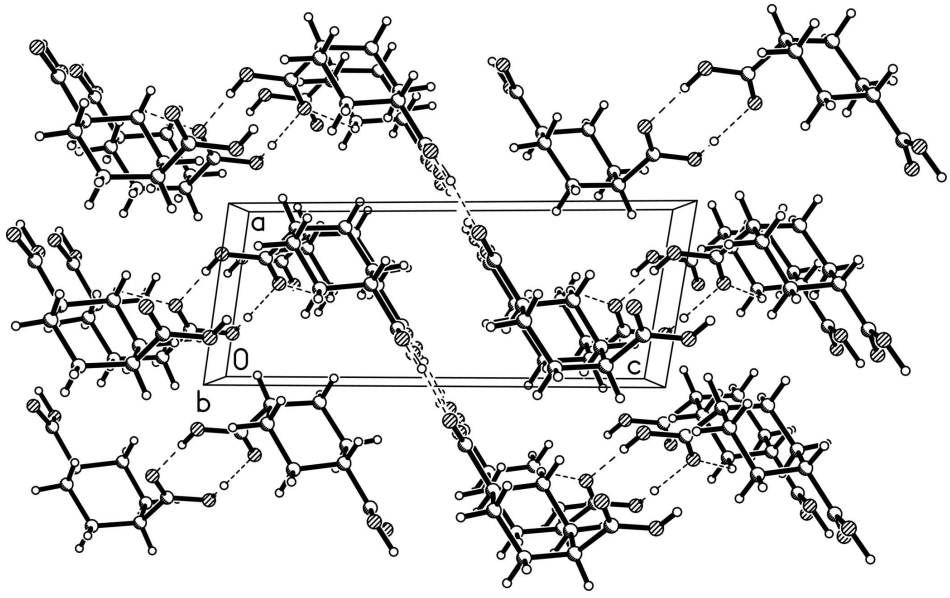


Figure 2

Packing diagram viewed down the *b* axis, The H-bonds are shown as dotted lines.

cis-Cyclohexane-1,4-dicarboxylic acid

Crystal data

$C_8H_{12}O_4$
$M_r = 172.18$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.2912\ (6)$ Å
$b = 6.2611\ (6)$ Å
$c = 13.1851\ (18)$ Å
$\alpha = 82.505\ (10)°$
$\beta = 80.309\ (11)°$
$\gamma = 81.875\ (10)°$
$V = 423.70\ (9)$ Å^3
$Z = 2$
$F(000) = 184$
$D_x = 1.350$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3560 reflections
$\theta = 2.6–26.9°$
$\mu = 0.11$ mm^{-1}

T = 296 K
Plate, colorless

0.24 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.979, T_{max} = 0.989

9807 measured reflections
1925 independent reflections
1222 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 27.5°, θ_{min} = 3.5°
h = −6→6
k = −7→8
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.129
S = 1.05
1925 reflections
118 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.038P)^2 + 0.2496P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.057 (12)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
O1	0.4359 (3)	0.5154 (3)	0.88398 (12)	0.0583 (5)
O2	0.2703 (4)	0.2964 (3)	1.01503 (13)	0.0620 (5)
O3	0.7370 (4)	−0.1284 (3)	0.57741 (15)	0.0709 (6)
O4	0.8260 (3)	0.2120 (3)	0.55122 (14)	0.0632 (5)
C1	0.2929 (4)	0.3798 (3)	0.91784 (16)	0.0386 (5)
C2	0.1278 (4)	0.2898 (4)	0.85544 (16)	0.0420 (5)
H2	−0.0488	0.3021	0.8932	0.050*
C3	0.2176 (4)	0.0476 (3)	0.84796 (17)	0.0457 (6)
H3A	0.2410	−0.0240	0.9161	0.055*
H3B	0.0853	−0.0174	0.8242	0.055*
C4	0.1185 (4)	0.4153 (4)	0.74843 (17)	0.0493 (6)
H4A	−0.0264	0.3782	0.7208	0.059*

H4B	0.0878	0.5694	0.7557	0.059*
C5	0.4695 (4)	0.0121 (3)	0.77409 (16)	0.0411 (5)
H5A	0.5175	−0.1420	0.7694	0.049*
H5B	0.6056	0.0664	0.8006	0.049*
C6	0.3638 (4)	0.3713 (4)	0.67093 (17)	0.0457 (6)
H6A	0.3350	0.4396	0.6028	0.055*
H6B	0.5029	0.4346	0.6907	0.055*
C7	0.4420 (4)	0.1286 (3)	0.66664 (16)	0.0411 (5)
H7	0.3028	0.0710	0.6423	0.049*
C8	0.6862 (4)	0.0769 (4)	0.59270 (16)	0.0432 (5)
H1	0.369 (7)	0.355 (6)	1.048 (3)	0.106 (12)*
H8	0.898 (8)	−0.163 (6)	0.526 (3)	0.128 (13)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0785 (12)	0.0610 (11)	0.0431 (9)	−0.0335 (10)	−0.0145 (8)	−0.0002 (8)
O2	0.0795 (13)	0.0717 (12)	0.0413 (10)	−0.0360 (10)	−0.0111 (9)	0.0020 (8)
O3	0.0759 (13)	0.0525 (11)	0.0741 (13)	−0.0054 (9)	0.0251 (10)	−0.0191 (9)
O4	0.0571 (11)	0.0595 (11)	0.0685 (12)	−0.0124 (9)	0.0167 (9)	−0.0190 (9)
C1	0.0371 (11)	0.0377 (11)	0.0396 (12)	−0.0004 (9)	−0.0016 (9)	−0.0091 (9)
C2	0.0299 (10)	0.0512 (13)	0.0452 (12)	−0.0048 (9)	0.0017 (9)	−0.0163 (10)
C3	0.0454 (12)	0.0447 (13)	0.0476 (13)	−0.0145 (10)	0.0045 (10)	−0.0131 (10)
C4	0.0422 (12)	0.0544 (14)	0.0531 (14)	0.0066 (10)	−0.0150 (10)	−0.0168 (11)
C5	0.0437 (12)	0.0358 (11)	0.0422 (12)	−0.0034 (9)	0.0003 (9)	−0.0084 (9)
C6	0.0490 (13)	0.0490 (13)	0.0378 (12)	0.0017 (10)	−0.0098 (10)	−0.0038 (10)
C7	0.0377 (11)	0.0491 (13)	0.0383 (11)	−0.0058 (9)	−0.0051 (9)	−0.0122 (9)
C8	0.0450 (12)	0.0483 (14)	0.0366 (11)	−0.0024 (10)	−0.0057 (9)	−0.0097 (10)

Geometric parameters (Å, º)

O1—C1	1.209 (2)	C3—H3B	0.9700
O2—C1	1.312 (3)	C4—C6	1.527 (3)
O2—H1	0.88 (4)	C4—H4A	0.9700
O3—C8	1.310 (3)	C4—H4B	0.9700
O3—H8	1.01 (4)	C5—C7	1.526 (3)
O4—C8	1.217 (3)	C5—H5A	0.9700
C1—C2	1.503 (3)	C5—H5B	0.9700
C2—C4	1.528 (3)	C6—C7	1.523 (3)
C2—C3	1.534 (3)	C6—H6A	0.9700
C2—H2	0.9800	C6—H6B	0.9700
C3—C5	1.520 (3)	C7—C8	1.505 (3)
C3—H3A	0.9700	C7—H7	0.9800
C1—O2—H1	110 (2)	H4A—C4—H4B	107.6
C8—O3—H8	114 (2)	C3—C5—C7	110.71 (18)
O1—C1—O2	121.6 (2)	C3—C5—H5A	109.5
O1—C1—C2	124.7 (2)	C7—C5—H5A	109.5

O2—C1—C2	113.66 (19)	C3—C5—H5B	109.5
C1—C2—C4	113.11 (18)	C7—C5—H5B	109.5
C1—C2—C3	109.99 (18)	H5A—C5—H5B	108.1
C4—C2—C3	111.41 (17)	C7—C6—C4	111.18 (19)
C1—C2—H2	107.3	C7—C6—H6A	109.4
C4—C2—H2	107.3	C4—C6—H6A	109.4
C3—C2—H2	107.3	C7—C6—H6B	109.4
C5—C3—C2	111.67 (17)	C4—C6—H6B	109.4
C5—C3—H3A	109.3	H6A—C6—H6B	108.0
C2—C3—H3A	109.3	C8—C7—C6	113.13 (18)
C5—C3—H3B	109.3	C8—C7—C5	109.85 (18)
C2—C3—H3B	109.3	C6—C7—C5	111.08 (17)
H3A—C3—H3B	107.9	C8—C7—H7	107.5
C6—C4—C2	114.13 (18)	C6—C7—H7	107.5
C6—C4—H4A	108.7	C5—C7—H7	107.5
C2—C4—H4A	108.7	O4—C8—O3	122.7 (2)
C6—C4—H4B	108.7	O4—C8—C7	123.5 (2)
C2—C4—H4B	108.7	O3—C8—C7	113.8 (2)
O1—C1—C2—C4	−10.6 (3)	C2—C4—C6—C7	51.0 (2)
O2—C1—C2—C4	169.74 (18)	C4—C6—C7—C8	−178.86 (18)
O1—C1—C2—C3	114.7 (2)	C4—C6—C7—C5	−54.8 (2)
O2—C1—C2—C3	−65.0 (2)	C3—C5—C7—C8	−175.50 (17)
C1—C2—C3—C5	−74.0 (2)	C3—C5—C7—C6	58.6 (2)
C4—C2—C3—C5	52.3 (2)	C6—C7—C8—O4	9.4 (3)
C1—C2—C4—C6	74.9 (2)	C5—C7—C8—O4	−115.3 (2)
C3—C2—C4—C6	−49.6 (2)	C6—C7—C8—O3	−171.16 (19)
C2—C3—C5—C7	−57.3 (2)	C5—C7—C8—O3	64.1 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1···O1^{i}	0.88 (4)	1.81 (4)	2.684 (2)	178 (4)
O3—H8···O4^{ii}	1.01 (4)	1.65 (4)	2.658 (2)	175 (4)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+2; (ii) −*x*+2, −*y*, −*z*+1.