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4-Methylcyclohexyl *p*-toluenesulfonate

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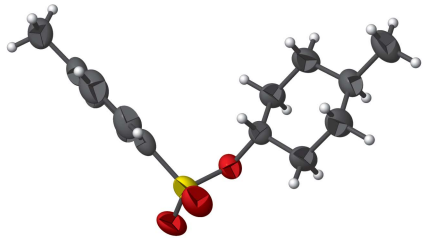
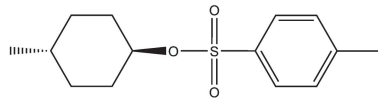
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{14}H_{20}O_3S$, demonstrates a *trans* conformation. The cyclohexyl ring in the structure exhibits a flattening, with average C—C—C angles of 111.2° and average C—C—C—C torsion angles of 55.6°. No significant intermolecular interactions are noted in the solid state.

3D view



Chemical scheme



Structure description

Substituted cyclohexane rings often exhibit a flattening from the ideal chair configuration where average C—C—C angles of 109.5° and average C—C—C—C torsion angles of 60° should exist. The parent cyclohexyl-*p*-toluenesulfonate demonstrates a slight flattening, with angles of 109.7 and 57.5°, respectively, being reported (James & McConnell, 1971). The structure of *trans*-4-*tert*-butylcyclohexyl *p*-toluenesulfonate has been reported from both X-ray (Johnson *et al.*, 1972) and neutron (James & Moore, 1975) studies and exhibits a greater flattening, with angles of 110.9 and 56.3°, respectively. Surprisingly, the title compound, *trans*-4-methylcyclohexyl-*p*-toluenesulfonate (Fig. 1) shows an even greater flattening, with average angles of 111.2 and 55.6°, respectively. Otherwise the three structures exhibit very similar bond lengths and angles. No significant intermolecular interactions are observed in the solid state.

Synthesis and crystallization

The title compound was prepared from 4-methylcyclohexanol and tosyl anhydride in a procedure similar to that published in Comagic & Schirrmacher (2004). A sample suitable for single-crystal X-ray analysis was grown from the slow evaporation of its 4-methylcyclohexanol solution.

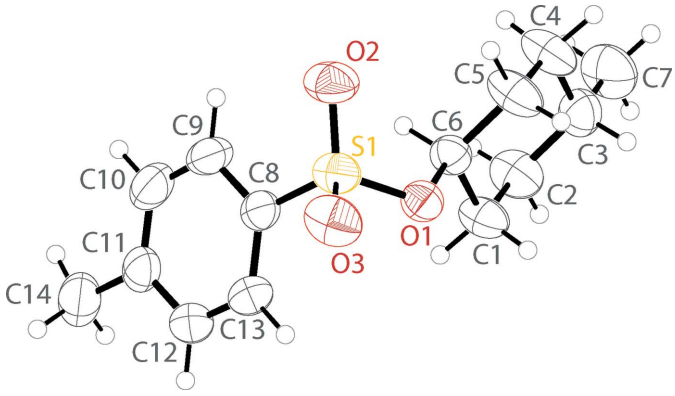


Figure 1
The molecular structure of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radius.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{20}O_3S$
M_r	268.36
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	200
a, b, c (Å)	11.390 (2), 10.9935 (18), 12.5613 (19)
β (°)	113.790 (9)
V (Å^3)	1439.3 (4)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.99
Crystal size (mm)	0.3 × 0.1 × 0.04
Data collection	
Diffractometer	Bruker D8 Venture CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.635, 0.753
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17339, 2730, 1976
R_{int}	0.071
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.612
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.151, 1.09
No. of reflections	2730
No. of parameters	165
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.34

Computer programs: *APEX2* (Bruker, 2014), *SAINT* (Bruker, 2014), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), OLEX2 (Dolomanov *et al.*, 2009), *publCIF* (Westrip, 2010).

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x160390 [doi:10.1107/S2414314616003904]

4-Methylcyclohexyl *p*-toluenesulfonate

Cyrenus T. Paquin, Donald W. Boerth, James A. Golen and David R. Manke

4-Methylcyclohexyl 4-methylbenzenesulfonate

Crystal data

$C_{14}H_{20}O_3S$
M_r = 268.36
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 11.390 (2) Å
b = 10.9935 (18) Å
c = 12.5613 (19) Å
β = 113.790 (9)°
V = 1439.3 (4) Å^3
Z = 4
$F(000)$ = 576
D_x = 1.238 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 6338 reflections
θ = 4.2–70.0°
μ = 1.99 mm^{-1}
T = 200 K
Needle, colourless
0.3 × 0.1 × 0.04 mm

Data collection

Bruker D8 Venture CMOS diffractometer
Radiation source: Cu
HELIOS MX monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2014)
T_{min} = 0.635, T_{max} = 0.753
17339 measured reflections
2730 independent reflections
1976 reflections with $I > 2\sigma(I)$
R_{int} = 0.071
θ_{max} = 70.5°, θ_{min} = 4.2°
h = −13→13
k = −13→13
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.151
S = 1.09
2730 reflections
165 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0764P)^2 + 0.3146P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Special details

Experimental. Absorption correction: *SADABS2014*/4 (Bruker,2014/4) was used for absorption correction. wR2(int) was 0.1521 before and 0.0777 after correction. The Ratio of minimum to maximum transmission is 0.8423. The $\lambda/2$ correction factor is 0.00150.

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.21794 (7)	0.40952 (6)	0.43539 (5)	0.0555 (2)
O1	0.33075 (16)	0.38628 (14)	0.55667 (13)	0.0504 (4)
O2	0.2587 (2)	0.38475 (19)	0.34409 (16)	0.0721 (6)
O3	0.1735 (2)	0.52791 (17)	0.44614 (18)	0.0726 (6)
C1	0.4404 (3)	0.2253 (2)	0.6879 (2)	0.0591 (7)
H1A	0.3592	0.1980	0.6914	0.071*
H1B	0.4795	0.2877	0.7488	0.071*
C2	0.5313 (3)	0.1179 (3)	0.7097 (3)	0.0679 (8)
H2A	0.5518	0.0857	0.7888	0.081*
H2B	0.4878	0.0526	0.6533	0.081*
C3	0.6544 (3)	0.1515 (3)	0.6987 (2)	0.0602 (7)
H3	0.6994	0.2131	0.7602	0.072*
C4	0.6252 (3)	0.2108 (3)	0.5822 (3)	0.0719 (9)
H4A	0.5870	0.1494	0.5200	0.086*
H4B	0.7064	0.2391	0.5794	0.086*
C5	0.5332 (3)	0.3185 (3)	0.5586 (3)	0.0691 (8)
H5A	0.5748	0.3847	0.6146	0.083*
H5B	0.5118	0.3500	0.4791	0.083*
C6	0.4134 (2)	0.2788 (2)	0.5703 (2)	0.0467 (6)
H6	0.3672	0.2178	0.5085	0.056*
C7	0.7438 (3)	0.0438 (3)	0.7188 (3)	0.0852 (10)
H7A	0.7639	0.0101	0.7965	0.128*
H7B	0.8231	0.0703	0.7131	0.128*
H7C	0.7021	−0.0187	0.6600	0.128*
C8	0.1017 (2)	0.3018 (2)	0.42833 (18)	0.0490 (6)
C9	0.0655 (3)	0.2116 (3)	0.3445 (2)	0.0626 (8)
H9	0.1055	0.2058	0.2913	0.075*
C10	−0.0284 (3)	0.1308 (3)	0.3385 (2)	0.0685 (8)
H10	−0.0529	0.0692	0.2806	0.082*
C11	−0.0887 (2)	0.1364 (2)	0.4146 (2)	0.0553 (7)
C12	−0.0512 (3)	0.2275 (3)	0.4980 (2)	0.0612 (7)
H12	−0.0909	0.2330	0.5513	0.073*
C13	0.0425 (3)	0.3102 (3)	0.5051 (2)	0.0603 (7)
H13	0.0663	0.3726	0.5623	0.072*
C14	−0.1925 (3)	0.0476 (3)	0.4064 (3)	0.0712 (8)
H14A	−0.1995	−0.0150	0.3486	0.107*
H14B	−0.2744	0.0908	0.3829	0.107*
H14C	−0.1712	0.0093	0.4824	0.107*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0583 (4)	0.0607 (4)	0.0519 (4)	0.0160 (3)	0.0268 (3)	0.0123 (3)
O1	0.0476 (10)	0.0512 (9)	0.0523 (9)	0.0085 (8)	0.0202 (8)	−0.0014 (7)
O2	0.0769 (14)	0.0932 (15)	0.0572 (10)	0.0193 (12)	0.0385 (10)	0.0190 (10)

O3	0.0795 (14)	0.0564 (11)	0.0892 (14)	0.0250 (10)	0.0416 (12)	0.0210 (10)
C1	0.0592 (17)	0.0634 (16)	0.0668 (15)	0.0077 (13)	0.0380 (14)	0.0132 (12)
C2	0.070 (2)	0.0675 (17)	0.0731 (17)	0.0121 (15)	0.0358 (16)	0.0227 (14)
C3	0.0520 (16)	0.0625 (16)	0.0598 (15)	0.0076 (13)	0.0160 (13)	−0.0005 (12)
C4	0.0604 (19)	0.079 (2)	0.094 (2)	0.0158 (16)	0.0498 (17)	0.0214 (16)
C5	0.0624 (18)	0.0694 (18)	0.093 (2)	0.0152 (15)	0.0496 (17)	0.0295 (15)
C6	0.0462 (14)	0.0460 (13)	0.0491 (12)	0.0059 (11)	0.0204 (11)	0.0001 (10)
C7	0.074 (2)	0.092 (2)	0.088 (2)	0.034 (2)	0.0324 (19)	0.0216 (18)
C8	0.0439 (14)	0.0593 (14)	0.0389 (11)	0.0150 (11)	0.0116 (10)	0.0013 (10)
C9	0.0622 (18)	0.085 (2)	0.0410 (12)	0.0151 (16)	0.0211 (12)	−0.0077 (12)
C10	0.0656 (19)	0.0777 (19)	0.0516 (14)	0.0050 (16)	0.0128 (14)	−0.0207 (13)
C11	0.0424 (14)	0.0618 (15)	0.0514 (13)	0.0089 (12)	0.0083 (11)	−0.0077 (11)
C12	0.0540 (16)	0.0747 (18)	0.0586 (14)	−0.0014 (14)	0.0267 (13)	−0.0179 (13)
C13	0.0594 (17)	0.0699 (17)	0.0544 (14)	−0.0028 (14)	0.0259 (13)	−0.0203 (12)
C14	0.0567 (18)	0.0742 (19)	0.0695 (17)	−0.0004 (15)	0.0117 (14)	−0.0111 (14)

Geometric parameters (Å, º)

S1—O1	1.5677 (17)	C5—C6	1.496 (4)
S1—O2	1.4265 (19)	C6—H6	1.0000
S1—O3	1.4226 (19)	C7—H7A	0.9800
S1—C8	1.752 (3)	C7—H7B	0.9800
O1—C6	1.477 (3)	C7—H7C	0.9800
C1—H1A	0.9900	C8—C9	1.383 (4)
C1—H1B	0.9900	C8—C13	1.385 (3)
C1—C2	1.520 (4)	C9—H9	0.9500
C1—C6	1.502 (3)	C9—C10	1.369 (4)
C2—H2A	0.9900	C10—H10	0.9500
C2—H2B	0.9900	C10—C11	1.385 (4)
C2—C3	1.510 (4)	C11—C12	1.386 (3)
C3—H3	1.0000	C11—C14	1.505 (4)
C3—C4	1.511 (4)	C12—H12	0.9500
C3—C7	1.514 (4)	C12—C13	1.376 (4)
C4—H4A	0.9900	C13—H13	0.9500
C4—H4B	0.9900	C14—H14A	0.9800
C4—C5	1.529 (4)	C14—H14B	0.9800
C5—H5A	0.9900	C14—H14C	0.9800
C5—H5B	0.9900		

O1—S1—C8	104.21 (10)	O1—C6—C1	107.19 (18)
O2—S1—O1	110.19 (11)	O1—C6—C5	108.6 (2)
O2—S1—C8	108.35 (13)	O1—C6—H6	109.6
O3—S1—O1	103.91 (11)	C1—C6—H6	109.6
O3—S1—O2	119.66 (12)	C5—C6—C1	112.2 (2)
O3—S1—C8	109.43 (13)	C5—C6—H6	109.6
C6—O1—S1	118.50 (14)	C3—C7—H7A	109.5
H1A—C1—H1B	108.2	C3—C7—H7B	109.5
C2—C1—H1A	109.7	C3—C7—H7C	109.5

C2—C1—H1B	109.7	H7A—C7—H7B	109.5
C6—C1—H1A	109.7	H7A—C7—H7C	109.5
C6—C1—H1B	109.7	H7B—C7—H7C	109.5
C6—C1—C2	109.6 (2)	C9—C8—S1	120.7 (2)
C1—C2—H2A	109.1	C9—C8—C13	119.9 (3)
C1—C2—H2B	109.1	C13—C8—S1	119.35 (19)
H2A—C2—H2B	107.8	C8—C9—H9	120.2
C3—C2—C1	112.6 (2)	C10—C9—C8	119.5 (2)
C3—C2—H2A	109.1	C10—C9—H9	120.2
C3—C2—H2B	109.1	C9—C10—H10	119.1
C2—C3—H3	107.5	C9—C10—C11	121.8 (2)
C2—C3—C4	110.1 (2)	C11—C10—H10	119.1
C2—C3—C7	112.3 (3)	C10—C11—C12	117.8 (3)
C4—C3—H3	107.5	C10—C11—C14	121.3 (2)
C4—C3—C7	111.7 (2)	C12—C11—C14	121.0 (3)
C7—C3—H3	107.5	C11—C12—H12	119.3
C3—C4—H4A	109.0	C13—C12—C11	121.4 (2)
C3—C4—H4B	109.0	C13—C12—H12	119.3
C3—C4—C5	112.8 (2)	C8—C13—H13	120.2
H4A—C4—H4B	107.8	C12—C13—C8	119.5 (2)
C5—C4—H4A	109.0	C12—C13—H13	120.2
C5—C4—H4B	109.0	C11—C14—H14A	109.5
C4—C5—H5A	109.7	C11—C14—H14B	109.5
C4—C5—H5B	109.7	C11—C14—H14C	109.5
H5A—C5—H5B	108.2	H14A—C14—H14B	109.5
C6—C5—C4	109.6 (2)	H14A—C14—H14C	109.5
C6—C5—H5A	109.7	H14B—C14—H14C	109.5
C6—C5—H5B	109.7		

S1—O1—C6—C1	−139.75 (19)	C2—C3—C4—C5	53.4 (4)
S1—O1—C6—C5	98.8 (2)	C3—C4—C5—C6	−55.0 (4)
S1—C8—C9—C10	−178.0 (2)	C4—C5—C6—O1	175.4 (2)
S1—C8—C13—C12	178.4 (2)	C4—C5—C6—C1	57.1 (3)
O1—S1—C8—C9	−116.6 (2)	C6—C1—C2—C3	56.1 (3)
O1—S1—C8—C13	65.7 (2)	C7—C3—C4—C5	179.0 (3)
O2—S1—O1—C6	−40.9 (2)	C8—S1—O1—C6	75.12 (18)
O2—S1—C8—C9	0.7 (2)	C8—C9—C10—C11	−0.1 (4)
O2—S1—C8—C13	−177.0 (2)	C9—C8—C13—C12	0.7 (4)
O3—S1—O1—C6	−170.28 (17)	C9—C10—C11—C12	0.2 (4)
O3—S1—C8—C9	132.7 (2)	C9—C10—C11—C14	179.5 (3)
O3—S1—C8—C13	−44.9 (2)	C10—C11—C12—C13	0.2 (4)
C1—C2—C3—C4	−54.0 (3)	C11—C12—C13—C8	−0.7 (4)
C1—C2—C3—C7	−179.2 (2)	C13—C8—C9—C10	−0.4 (4)
C2—C1—C6—O1	−177.0 (2)	C14—C11—C12—C13	−179.1 (3)
C2—C1—C6—C5	−57.8 (3)		