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1-[4-(Iodomethyl)cyclohexyl]-4-methylbenzene

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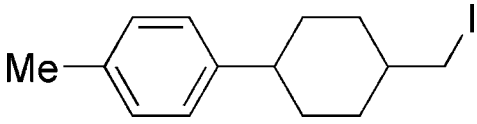
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.004 Å; R factor = 0.028; wR factor = 0.074; data-to-parameter ratio = 16.5.

In the title compound, $C_{14}H_{19}I$, the cyclohexane ring adopts a chair conformation and the substituents are in equatorial sites. The dihedral angle between the mean planes of the cyclohexane and benzene rings is 67.23 (13)°.

Related literature

The title compound is an intermediate in the praparation of liquid crystals. For background to liquid crystals, see: Demus & Hauser (1990). For the synthesis, see: Kozhushkov *et al.* (2004).



Experimental

Crystal data

$C_{14}H_{19}I$
M_r = 314.19
Monoclinic, $P2_1/c$
a = 17.593 (4) Å
b = 5.7722 (12) Å
c = 13.319 (3) Å
β = 105.71 (3)°
V = 1302.0 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.43 mm^{-1}
T = 113 K
0.20 × 0.18 × 0.12 mm

Data collection

Rigaku Saturn CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.642, T_{max} = 0.759
8233 measured reflections
2264 independent reflections
2077 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.074
S = 1.13
2264 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −1.49 e Å^{-3}

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *CrystalStructure* (Rigaku/MSC, 2005).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5876).

References

Demus, D. & Hauser, A. (1990). *Selected Topics in Liquid Crystal Research*, edited by H.-D. Koswig, p. 19. Berlin: Akademie-Verlag.
Kozhushkov, S. I., Langer, R. & Yufit, D. S. (2004). *Eur. J. Org. Chem.* pp. 289–303.
Rigaku/MSC (2005). *CrystalClear* and *CrystalStructure*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

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1-[4-(Iodomethyl)cyclohexyl]-4-methylbenzene

Juan Wang, Erhong Duan, Erpeng Zhou, Qingguo Yao and Wenna Zhang

S1. Comment

The title compound, (I), is an intermediate of liquid crystal compounds (Demus *et al.*,1990), which is synthesized from 1-bromo- 4-methylbenzene and 1-bromo-4-(iodomethyl)cyclohexane using diethyl ether as solvent (Kozhushkov *et al.*,2004). Herein, we report the title compound crystal structure.

In the molecule, Fig 1, a cyclohexane ring was attached at the *para* position of a benzene ring. The cyclohexyl ring has a typical chair conformation, with the tosion angles C3/C4/C5/C6 and C4/C5/C6/C7 being 56.7 (3) ° and -56.4 (3)°. No significant H-bonding or stacking interactions occur in the molecule packing.

S2. Experimental

1-(4-(Iodomethyl)cyclohexyl)-4-methylbenzene was synthesized according to the method described by Kozhushkov *et al.* (2004). Colourless prisms of (I) were obtained by evaporation from its ethanoic solution at room temperature (m.p. 318–319 K).

S3. Refinement

All H atoms were positioned geometrically and constrained to ride on their parent atoms [C—H distances are 0.95, 0.99 and 1.0Å with U_{iso}(H) = 1.2 U_{eq}(C) for aromatic and other aliphatic atoms, 0.98Å with U_{iso} = 1.5U_{eq} (C) for CH_3 atoms].

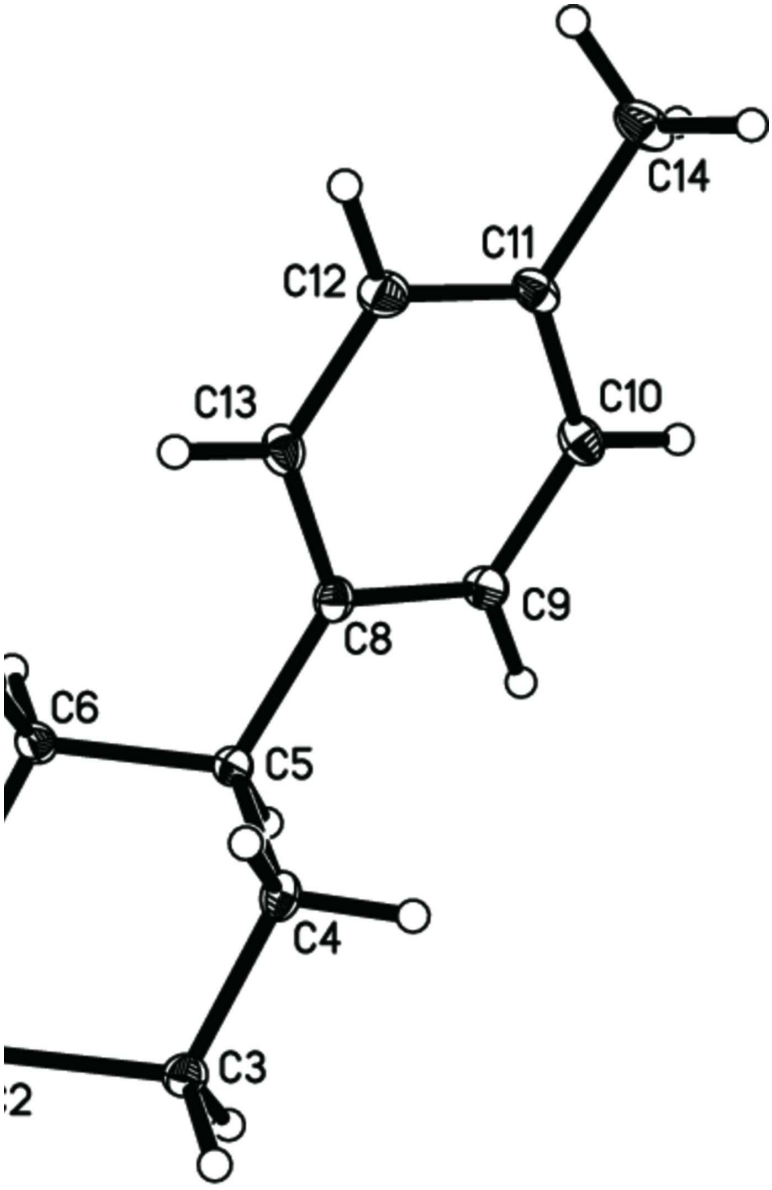

Figure 1

The molecular structure of (I) with 50% probability displacement ellipsoids.

1-[4-(Iodomethyl)cyclohexyl]-4-methylbenzene

Crystal data

$C_{14}H_{19}I$
$M_r = 314.19$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 17.593$ (4) Å
$b = 5.7722$ (12) Å
$c = 13.319$ (3) Å
$\beta = 105.71$ (3)°
$V = 1302.0$ (5) Å^3
$Z = 4$
$F(000) = 624$
$D_x = 1.603$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4209 reflections
$\theta = 2.4$–27.9°
$\mu = 2.43$ mm^{-1}
$T = 113$ K
Prism, colourless
0.20 × 0.18 × 0.12 mm

Data collection

Rigaku Saturn CCD diffractometer
Radiation source: rotating anode
Confocal monochromator
Detector resolution: 7.31 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.642, T_{max} = 0.759
8233 measured reflections
2264 independent reflections
2077 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.0°, θ_{min} = 2.4°
h = −20→19
k = −5→6
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.074
S = 1.13
2264 reflections
137 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0482P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −1.49 e Å^{-3}

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
I1	0.069728 (10)	1.27167 (3)	0.586560 (14)	0.02224 (11)
C1	0.08795 (15)	0.9476 (4)	0.6716 (2)	0.0203 (6)
H1A	0.0358	0.8786	0.6681	0.024*
H1B	0.1162	0.8396	0.6364	0.024*
C2	0.13409 (14)	0.9681 (4)	0.78479 (19)	0.0141 (5)
H2	0.1054	1.0764	0.8205	0.017*
C3	0.13670 (19)	0.7272 (4)	0.8348 (2)	0.0189 (6)
H3A	0.0821	0.6747	0.8291	0.023*
H3B	0.1610	0.6158	0.7961	0.023*
C4	0.18367 (18)	0.7284 (4)	0.9493 (2)	0.0182 (6)
H4A	0.1856	0.5694	0.9777	0.022*
H4B	0.1567	0.8288	0.9892	0.022*
C5	0.26817 (15)	0.8169 (4)	0.9629 (2)	0.0153 (5)
H5	0.2931	0.7121	0.9211	0.018*
C6	0.26524 (15)	1.0592 (4)	0.9148 (2)	0.0192 (6)
H6A	0.3197	1.1131	0.9206	0.023*

H6B	0.2407	1.1686	0.9540	0.023*
C7	0.21762 (14)	1.0587 (4)	0.79919 (19)	0.0183 (6)
H7A	0.2152	1.2184	0.7713	0.022*
H7B	0.2450	0.9606	0.7589	0.022*
C8	0.31731 (17)	0.8004 (4)	1.0745 (2)	0.0176 (6)
C9	0.36274 (15)	0.6031 (4)	1.1085 (2)	0.0196 (6)
H9	0.3623	0.4812	1.0605	0.024*
C10	0.40846 (15)	0.5803 (5)	1.2105 (2)	0.0219 (6)
H10	0.4389	0.4438	1.2307	0.026*
C11	0.41059 (18)	0.7517 (4)	1.2830 (3)	0.0202 (7)
C12	0.36493 (16)	0.9486 (4)	1.2509 (2)	0.0236 (6)
H12	0.3654	1.0694	1.2995	0.028*
C13	0.31856 (15)	0.9713 (4)	1.1484 (2)	0.0213 (6)
H13	0.2872	1.1063	1.1287	0.026*
C14	0.4619 (2)	0.7254 (5)	1.3942 (3)	0.0281 (7)
H14A	0.4348	0.6273	1.4337	0.042*
H14B	0.4719	0.8782	1.4272	0.042*
H14C	0.5123	0.6535	1.3935	0.042*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.02506 (16)	0.01680 (15)	0.02078 (17)	−0.00064 (6)	−0.00077 (11)	0.00342 (6)
C1	0.0228 (15)	0.0154 (13)	0.0209 (15)	−0.0007 (11)	0.0028 (12)	0.0017 (11)
C2	0.0136 (13)	0.0133 (13)	0.0153 (14)	0.0027 (9)	0.0037 (11)	−0.0018 (10)
C3	0.0193 (16)	0.0200 (14)	0.0175 (17)	−0.0035 (10)	0.0053 (13)	0.0004 (10)
C4	0.0207 (16)	0.0166 (14)	0.0201 (17)	−0.0014 (10)	0.0100 (13)	0.0026 (10)
C5	0.0156 (14)	0.0148 (12)	0.0155 (14)	0.0024 (10)	0.0044 (11)	−0.0013 (10)
C6	0.0158 (14)	0.0206 (14)	0.0191 (15)	−0.0035 (11)	0.0012 (11)	0.0038 (11)
C7	0.0175 (14)	0.0179 (13)	0.0193 (15)	−0.0023 (10)	0.0044 (11)	0.0045 (10)
C8	0.0168 (15)	0.0171 (13)	0.0198 (16)	−0.0007 (10)	0.0067 (12)	0.0019 (11)
C9	0.0193 (15)	0.0191 (14)	0.0197 (15)	0.0047 (11)	0.0038 (12)	−0.0021 (11)
C10	0.0192 (15)	0.0253 (14)	0.0212 (16)	0.0062 (11)	0.0051 (12)	0.0035 (11)
C11	0.0167 (16)	0.0292 (16)	0.0153 (17)	−0.0044 (10)	0.0050 (13)	0.0038 (10)
C12	0.0293 (16)	0.0245 (14)	0.0187 (16)	−0.0012 (12)	0.0092 (13)	−0.0032 (11)
C13	0.0267 (16)	0.0186 (13)	0.0194 (15)	0.0071 (11)	0.0079 (12)	0.0020 (11)
C14	0.0184 (17)	0.046 (2)	0.0187 (18)	−0.0042 (12)	0.0027 (14)	0.0033 (12)

Geometric parameters (Å, º)

I1—C1	2.165 (3)	C6—H6B	0.9900
C1—C2	1.511 (3)	C7—H7A	0.9900
C1—H1A	0.9900	C7—H7B	0.9900
C1—H1B	0.9900	C8—C13	1.389 (4)
C2—C7	1.522 (3)	C8—C9	1.394 (3)
C2—C3	1.537 (3)	C9—C10	1.385 (4)
C2—H2	1.0000	C9—H9	0.9500
C3—C4	1.525 (4)	C10—C11	1.376 (4)

C3—H3A	0.9900	C10—H10	0.9500
C3—H3B	0.9900	C11—C12	1.391 (4)
C4—C5	1.536 (4)	C11—C14	1.519 (5)
C4—H4A	0.9900	C12—C13	1.393 (4)
C4—H4B	0.9900	C12—H12	0.9500
C5—C8	1.507 (4)	C13—H13	0.9500
C5—C6	1.533 (3)	C14—H14A	0.9800
C5—H5	1.0000	C14—H14B	0.9800
C6—C7	1.541 (3)	C14—H14C	0.9800
C6—H6A	0.9900		

C2—C1—I1	114.67 (17)	C5—C6—H6B	109.4
C2—C1—H1A	108.6	C7—C6—H6B	109.4
I1—C1—H1A	108.6	H6A—C6—H6B	108.0
C2—C1—H1B	108.6	C2—C7—C6	111.81 (19)
I1—C1—H1B	108.6	C2—C7—H7A	109.3
H1A—C1—H1B	107.6	C6—C7—H7A	109.3
C1—C2—C7	113.1 (2)	C2—C7—H7B	109.3
C1—C2—C3	107.8 (2)	C6—C7—H7B	109.3
C7—C2—C3	110.0 (2)	H7A—C7—H7B	107.9
C1—C2—H2	108.6	C13—C8—C9	116.9 (3)
C7—C2—H2	108.6	C13—C8—C5	123.3 (2)
C3—C2—H2	108.6	C9—C8—C5	119.8 (2)
C4—C3—C2	111.9 (2)	C10—C9—C8	121.7 (2)
C4—C3—H3A	109.2	C10—C9—H9	119.1
C2—C3—H3A	109.2	C8—C9—H9	119.1
C4—C3—H3B	109.2	C11—C10—C9	121.2 (2)
C2—C3—H3B	109.2	C11—C10—H10	119.4
H3A—C3—H3B	107.9	C9—C10—H10	119.4
C3—C4—C5	111.4 (2)	C10—C11—C12	117.9 (3)
C3—C4—H4A	109.3	C10—C11—C14	120.6 (2)
C5—C4—H4A	109.3	C12—C11—C14	121.6 (2)
C3—C4—H4B	109.3	C11—C12—C13	121.0 (3)
C5—C4—H4B	109.3	C11—C12—H12	119.5
H4A—C4—H4B	108.0	C13—C12—H12	119.5
C8—C5—C6	114.5 (2)	C8—C13—C12	121.3 (2)
C8—C5—C4	112.0 (2)	C8—C13—H13	119.4
C6—C5—C4	109.4 (2)	C12—C13—H13	119.4
C8—C5—H5	106.8	C11—C14—H14A	109.5
C6—C5—H5	106.8	C11—C14—H14B	109.5
C4—C5—H5	106.8	H14A—C14—H14B	109.5
C5—C6—C7	111.3 (2)	C11—C14—H14C	109.5
C5—C6—H6A	109.4	H14A—C14—H14C	109.5
C7—C6—H6A	109.4	H14B—C14—H14C	109.5

I1—C1—C2—C7	−61.9 (2)	C4—C5—C8—C13	−85.8 (3)
I1—C1—C2—C3	176.26 (17)	C6—C5—C8—C9	−142.4 (2)
C1—C2—C3—C4	178.9 (2)	C4—C5—C8—C9	92.3 (3)

C7—C2—C3—C4	55.1 (3)	C13—C8—C9—C10	−1.5 (4)
C2—C3—C4—C5	−56.9 (3)	C5—C8—C9—C10	−179.7 (2)
C3—C4—C5—C8	−175.25 (19)	C8—C9—C10—C11	0.4 (4)
C3—C4—C5—C6	56.7 (3)	C9—C10—C11—C12	0.3 (4)
C8—C5—C6—C7	177.0 (2)	C9—C10—C11—C14	−179.2 (2)
C4—C5—C6—C7	−56.4 (3)	C10—C11—C12—C13	0.0 (4)
C1—C2—C7—C6	−175.4 (2)	C14—C11—C12—C13	179.5 (2)
C3—C2—C7—C6	−54.8 (3)	C9—C8—C13—C12	1.8 (4)
C5—C6—C7—C2	56.8 (3)	C5—C8—C13—C12	180.0 (2)
C6—C5—C8—C13	39.4 (3)	C11—C12—C13—C8	−1.1 (4)