

***r*-1,*c*-2,*c*-3,*t*-4,5-Pentachloro-6-phenyltetralin**

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Key indicators

Single-crystal X-ray study

$T = 298$ K

Mean $\sigma(\text{C}-\text{C}) = 0.006$ Å

Disorder in main residue

R factor = 0.047

wR factor = 0.127

Data-to-parameter ratio = 12.1

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, $\text{C}_{16}\text{H}_{11}\text{Cl}_5$, is an asymmetric tetrachloro-tetralin showing disorder of the alicyclic moiety, which has a boat conformation in the crystalline state and half-chair in solution.

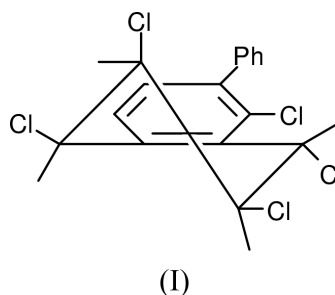
Received 13 September 2001

Accepted 9 October 2001

Online 13 October 2001

Comment

Preliminary results were presented at a National Conference (Bombieri *et al.*, 1984). The results obtained from X-ray crystal structure analysis show that the stereochemistry of this adduct in the solid state is different from that in solution, as found from NMR studies. In fact, the asymmetric distribution of Cl atoms results in severe steric interactions within the alicyclic moiety of the molecule; these are released in solution, where the molecule is more flexible, by a distortion of the basic half-chair conformation. In the solid state, the very strict steric rigidity requirement of the system does not allow such an accommodation and the dissymmetric adduct is forced to assume a boat conformation, which minimizes steric strain and seems to better accommodate the otherwise strongly interacting *c*-2, *c*-3 and *t*-4 chlorine atoms. The molecule shows a disorder problem within the alicyclic ring owing to the conformational fluxionality.

**Experimental**

The title compound was prepared according to the procedure of Aversa *et al.* (1982). Crystals suitable for X-ray diffraction analysis were obtained by slow cooling of a light petroleum solution.

Crystal data

$\text{C}_{16}\text{H}_{11}\text{Cl}_5$
 $M_r = 380.50$
 Monoclinic, $P2_1/c$
 $a = 13.321$ (3) Å
 $b = 9.101$ (2) Å
 $c = 14.279$ (3) Å
 $\beta = 112.77$ (3)°
 $V = 1596.2$ (6) Å³
 $Z = 4$
 $D_x = 1.583$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 30 reflections
 $\theta = 13.0$ – 30.0°
 $\mu = 0.90$ mm⁻¹
 $T = 298$ (2) K
 Regular prismatic, colourless
 $0.31 \times 0.20 \times 0.14$ mm
 Crystal source: chemical synthesis

Data collection

Siemens R3m/V diffractometer
 ω -2 θ scans
 Absorption correction: none
 2652 measured reflections
 2652 independent reflections
 1977 reflections with $I > 2\sigma(I)$
 $\theta_{\max} = 24.9^\circ$

$h = -15 \rightarrow 14$
 $k = 0 \rightarrow 10$
 $l = 0 \rightarrow 16$
 3 standard reflections
 every 197 reflections
 intensity decay: 1.3%

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.127$
 $S = 1.04$
 2651 reflections
 219 parameters
 H atoms treated by a mixture of
 independent and constrained
 refinement

$w = 1/[\sigma^2(F_o^2) + (0.0788P)^2 + 1.7180P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.097$
 $\Delta\rho_{\max} = 0.52 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.41 \text{ e } \text{\AA}^{-3}$

Data collection: P3/V (Siemens, 1989); cell refinement: P3/V; data reduction: XDISK (Siemens, 1990); program(s) used to solve structure: SHELXS86 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: XPW (Siemens, 1996); software used to prepare material for publication: PARST95 (Nardelli, 1995) and SHELXL97.

We would like to express our gratitude, for support and aid, to the Italian MURST and to the 'Centro Interdipartimentale di Servizi per la Diffrazione a Raggi X' of the University of Messina.

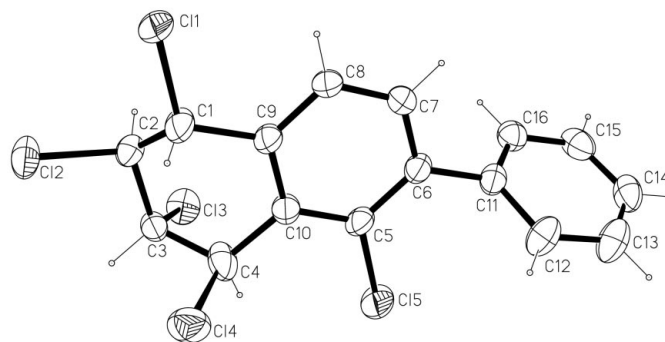


Figure 1
 ORTEP (Johnson, 1976) drawing of the title molecule with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% level.

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