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2-(1,1,2,2-Tetrachloroethylsulfanyl)-3a,4,7,7a-tetrahydro-1*H*-isoindole-1,3(2*H*)-dione

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The title compound (also known as captafol), $C_{10}H_9Cl_4NO_2S$, exhibits fungicidal activity. The six-membered ring exists in a boat conformation. The crystal packing is stabilized by weak intermolecular C—H···O and C—H···Cl interactions.

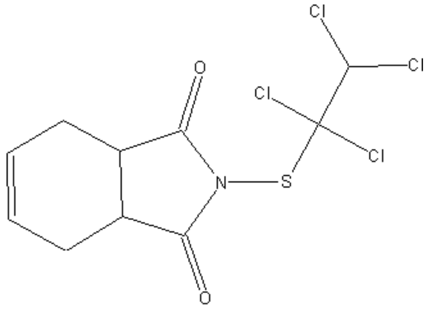
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.016 Å
R factor = 0.097
wR factor = 0.231
Data-to-parameter ratio = 14.7

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

Comment

An important aspect of the rational design of bioactive molecules involves the search for structure–activity relationships (Lewis *et al.*, 1991). The conformation of the molecule is found to influence the level of biological activity of the proper compound (Baughman & Jacobson, 1978). The correlations found between the crystal structures of some compounds and their biological activity have aided in the chemical design of few active agrochemicals (Rohrbaugh & Jacobson, 1978). Earlier, the activity of a series of triazolyl ketone herbicides (Anderson *et al.*, 1983) has been investigated along with the fungicidal activities of *N*-phenylsuccinamides (Zenei *et al.*, 1988).



(I)

We present here the crystal structure of the title compound, (I) (Fig. 1), which posesses fungicidal activity. Atoms H4 and H5 at the fused ring junction have a *cis* relationship. The puckering parameters (Cremer & Pople, 1975), generated by *PLATON* (Spek, 2003), for the six-membered cyclohexene ring are q_2 = 0.557 (13) Å, φ_2 = 117.3 (12)° and τ = 91.7 (12)°, indicating a boat conformation. The crystal structure is stabilized by weak intermolecular C—H···O and C—H···Cl interactions (Table 1) which link the molecules into linear chains along the c axis (Fig. 2).

Experimental

The title compound was obtained from Rallis India, Bangalore. Single crystals were grown by slow evaporation of a mixture of ethyl acetate/benzene at 278 K.

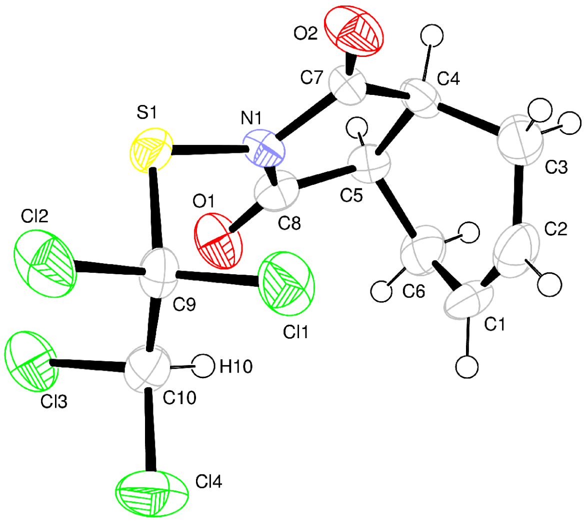


Figure 1
View of (I), shown with 50% probability displacement ellipsoids.

Crystal data

$C_{10}H_9Cl_4NO_2S$
$M_r = 349.04$
Monoclinic, $P2_1/c$
$a = 10.567\ (8)$ Å
$b = 6.674\ (5)$ Å
$c = 19.427\ (15)$ Å
$\beta = 91.715\ (12)^\circ$
$V = 1369.6\ (18)$ Å^3
$Z = 4$
$D_x = 1.683$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 675 reflections
$\theta = 2.2–26.4^\circ$
$\mu = 1.01$ mm^{-1}
$T = 293\ (2)$ K
Rod, colorless
$0.22 \times 0.07 \times 0.06$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.809$, $T_{\max} = 0.942$
8949 measured reflections
2449 independent reflections
2158 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.039$
$\theta_{\max} = 25.4^\circ$
$h = -11 \rightarrow 12$
$k = -8 \rightarrow 8$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.097$
$wR(F^2) = 0.231$
$S = 1.17$
2449 reflections
167 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0809P)^2 + 27.5824P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 1.05$ e Å^{-3}
$\Delta\rho_{\min} = -0.53$ e Å^{-3}

Table 1
Intermolecular contacts (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C2—H2$\cdots$O2$^{\rm i}$	0.93	2.65	3.545 (15)	163 (1)
C3—H3$A\cdots$Cl2$^{\rm ii}$	0.97	2.88	3.616 (13)	134 (1)

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

All H atoms were placed in idealized positions (0.93–0.98 Å) and refined as riding, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The maximum positive peak in the difference Fourier map was located 1.15 Å from atom S1.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2003).

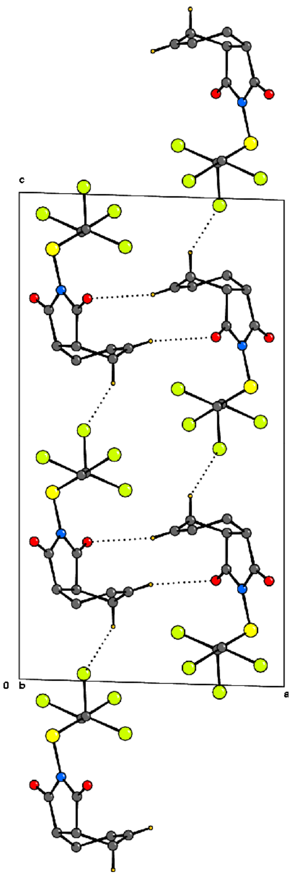


Figure 2
Packing diagram of (I), showing the intermolecular C—H$\cdots$O and C—H$\cdots$Cl contacts (dashed lines).

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References

Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
Anderson, N. H., Heritage, K. J. & Branch, S. K. (1983). *Quantitative Approaches to Drug Design*, edited by J. C. Dearden, p. 47. Amsterdam: Elsevier.
Baughman, R. G. & Jacobson, R. A. (1978). *J. Agric. Food Chem.* **26**, 403–407.
Bruker (2000). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Lewis, R. J., Camilleri, P., Kirby, A. J., Marby, C. A., Slawin, A. A. & Williams, D. J. (1991). *J. Chem. Soc. Perkin Trans.* 2, pp. 1625–1631.
Rohrbaugh, W. J. & Jacobson, R. A. (1978). *J. Agric.* Food *Chem.* **26**, 1120–1124.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Watkin, D. M., Pearce, L. & Prout, C. K. (1993). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, England.
Zenei, T., Takayami, C. & Terada, H. (1988). *J. Chem. Soc. Perkin Trans.* 2, pp. 1439–1445.

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