

2-(2,4-Dichlorophenyl)-1-(1*H*-1,2,4-triazol-1-yl)-
hexan-2-ol (hexaconazole)Deepak Chopra,^{a*} T. P. Mohan,^b
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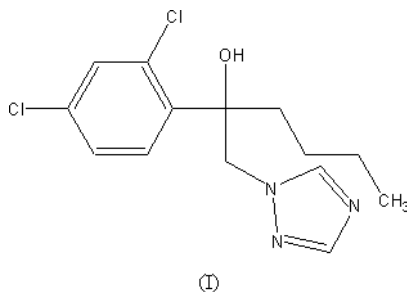
Key indicators

Single-crystal X-ray study
T = 293 K
Mean $\sigma(C-C)$ = 0.003 Å
R factor = 0.038
wR factor = 0.100
Data-to-parameter ratio = 11.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The title compound (also known as hexaconazole), $C_{14}H_{17}Cl_2N_3O$, is a potent agrochemical exhibiting fungicidal activity. The molecular conformation is stabilized by two intramolecular C—H...Cl interactions. Molecules are linked via O—H...N hydrogen bonds, forming zigzag chains along the *b* axis.

Comment

An important aspect in the rational design of bioactive molecules involves relating chemical structure to biological activity (Lewis *et al.*, 1991). The conformation of the molecule is found to influence the levels of biological activity. Correlation of the results obtained from X-ray crystallography with biological activity has aided in the chemical design of few active agrochemicals. 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). Hexaconazole, (I), which is non-phytotoxic, is used in the control of fungi in the growth of bananas and pepper.



The skew conformation of (I) is stabilized by two intramolecular C—H...Cl interactions (Fig. 1 and Table 2). The pseudo-six-membered ring locks the molecular conformation [Etter symbol *S*(6); Bernstein *et al.*, 1995]. The O—H...N hydrogen bond stabilizes the crystal structure, forming molecular chains [Etter symbol *C*(7)] around the twofold screw axis parallel to the *b* axis (Fig. 2).

Experimental

Compound (I) was obtained from Rallis India, Bangalore. Single crystals were grown by slow evaporation of a dichloromethane/hexane solution at 278 K.

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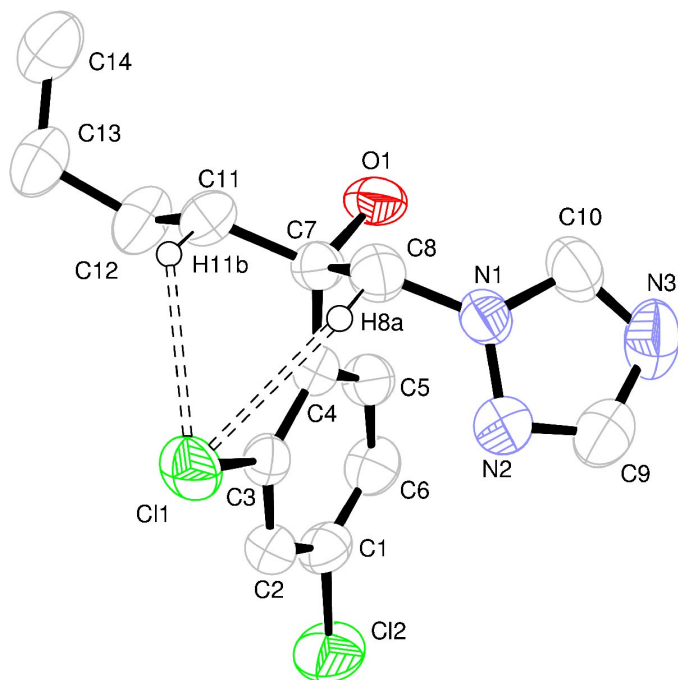


Figure 1
The molecular structure of (I), showing 50% probability ellipsoids. Broken lines represent C—H...Cl interactions. H atoms have been omitted for clarity, except for those involved in the C—H...Cl interactions.

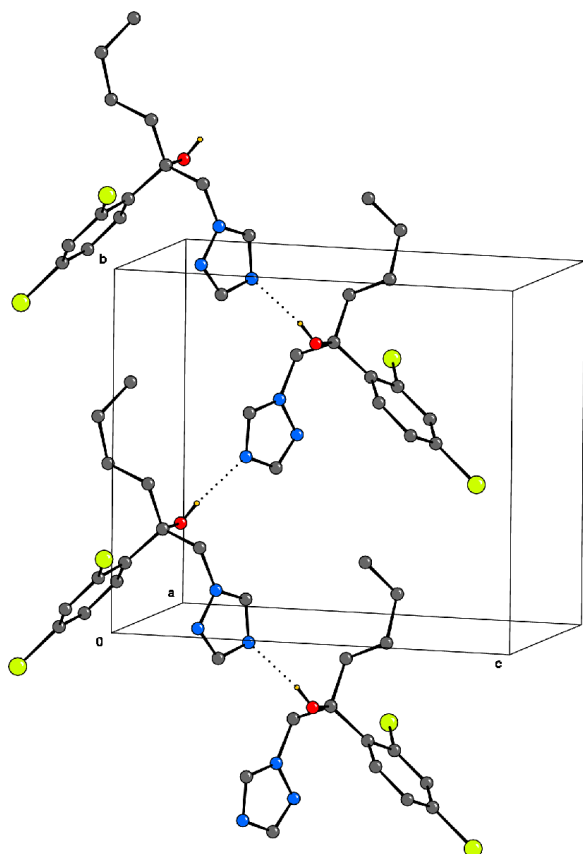


Figure 2
Packing diagram of (I), showing the O—H...N hydrogen bonds (dashed lines) forming molecular chains. H atoms have been omitted for clarity, except for those involved in the O—H...N hydrogen bonds.

Crystal data

$C_{14}H_{17}Cl_2N_3O$
 $M_r = 314.21$
 Monoclinic, $P2_1/c$
 $a = 10.895 (6) \text{ \AA}$
 $b = 11.006 (6) \text{ \AA}$
 $c = 13.595 (8) \text{ \AA}$
 $\beta = 106.526 (9)^\circ$
 $V = 1562.9 (15) \text{ \AA}^3$
 $Z = 4$

$D_x = 1.335 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 Cell parameters from 788 reflections
 $\theta = 1.6\text{--}25.2^\circ$
 $\mu = 0.41 \text{ mm}^{-1}$
 $T = 293 (2) \text{ K}$
 Block, colorless
 $0.30 \times 0.25 \times 0.20 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.886$, $T_{\max} = 0.922$
 11 231 measured reflections

2867 independent reflections
 2509 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.015$
 $\theta_{\max} = 25.4^\circ$
 $h = -13 \rightarrow 13$
 $k = -13 \rightarrow 13$
 $l = -15 \rightarrow 16$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.100$
 $S = 1.05$
 2867 reflections
 249 parameters
 All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 0.5742P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.35 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.33 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

N1—C10	1.321 (3)	N2—C9	1.306 (3)
N1—N2	1.351 (2)	N3—C10	1.319 (3)
N1—C8	1.452 (3)	N3—C9	1.348 (3)
N2—N1—C8—C7	−91.8 (2)	C8—C7—C11—C12	−172.7 (2)
C3—C4—C7—C8	63.9 (2)	C7—C11—C12—C13	−173.4 (2)
N1—C8—C7—C4	54.7 (2)	C11—C12—C13—C14	71.1 (3)

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
O1—H1O...N3 ⁱ	0.77 (2)	2.07 (2)	2.821 (3)	166 (2)
C8—H8A...Cl1	0.96 (2)	2.70 (2)	3.320 (3)	123 (2)
C11—H11B...Cl1	0.95 (3)	2.67 (2)	3.272 (3)	122 (2)

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

All H atoms were located in difference Fourier maps and refined isotropically. C—H bond lengths are in the range 0.91 (2)–1.03 (3) \AA .

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; structure solution: SIR92 (Altomare *et al.*, 1993); structure refinement: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997) and CAMERON (Watkin *et al.*, 1993); software used to prepare material for publication: PLATON (Spek, 2003).

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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.
- Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
- Bruker (2000). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
- 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.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXL97*. 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.