Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

2-Isopropyl-4-methyl-4-phenyl-1,2,3,4-tetrahydroisoquinoline-1-thione

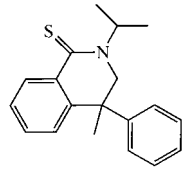
Hiroyuki Hosomi,[a] Shigeru Ohba[a]* and Hiromu Aoyama[b]

[a]Department of Chemistry, Faculty of Science and Technology, Keio University, Hiyoshi 3-14-1, Kohoku-ku, Yokohama 223-8522, Japan, and [b]Department of Material Chemistry, Faculty of Textile Science and Technology, Shinshu University, Tokida 3-15-1, Ueda 386-0081, Japan
Correspondence e-mail: ohba@chem.keio.ac.jp

Received 3 March 2000
Accepted 13 March 2000

Data validation number: IUC0000079

The title compound, $C_{19}H_{21}NS$, is the photoproduct obtained from *N*-isopropyl-*N*-[(*E*)-2-phenylpropenyl]thiobenzamide. Recrystallization showed a spontaneous resolution.



(I)

Experimental

The title compound was prepared by one of the authors (HA) in a study on photocyclization of enamides and thioamides in the solid state (Aoyama, 2000). Crystals were grown from a hexane solution.

Crystal data

$C_{19}H_{21}NS$
M_r = 295.44
Orthorhombic, $P2_12_12_1$
a = 11.166 (1) Å
b = 13.423 (1) Å
c = 10.878 (1) Å
V = 1630.4 (2) Å^3
Z = 4
D_x = 1.204 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 14.0–14.8°
μ = 0.192 mm^{-1}
T = 298 (1) K
Prism, yellow
0.55 × 0.40 × 0.30 mm

Data collection

Rigaku AFC-7*R* diffractometer
θ–2θ scans
Absorption correction: by integration (Coppens *et al.*, 1965)
T_{min} = 0.928, T_{max} = 0.947
3090 measured reflections
2684 independent reflections
1963 reflections with $I > 2\sigma(I)$
R_{int} = 0.006
θ_{max} = 30.0°
$h = 0 \rightarrow 16$
$k = -10 \rightarrow 19$
$l = -8 \rightarrow 16$
3 standard reflections
every 150 reflections
intensity decay: none

Refinement

Refinement on F^2
$R(F)$ = 0.043
$wR(F^2)$ = 0.124
S = 1.06
2684 reflections
190 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.0601P)^2 + 0.1846P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Absolute structure: Flack (1983), no Friedel pairs
Flack parameter = 0.1 (1)

Table 1
Selected geometric parameters (Å).

S1—C3	1.681 (2)	C9—C14	1.510 (3)
N2—C3	1.326 (3)	C13—C14	1.533 (4)
N2—C13	1.470 (3)		

X-ray intensity data were measured for $+h,+k,+l$ ($\theta < 30°$) and for $+h,-k,-l$ ($\theta < 15°$). The chiral space group and Flack parameter of 0.1 (1) suggested a spontaneous resolution of the title compound. All H-atom positional parameters were calculated geometrically and fixed with $U_{iso}(H) = 1.2U_{eq}$(parent atom).

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *TEXSAN*.

References

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Aoyama, H. (2000). To be published.
Coppens, P., Leiserowitz, L. & Rabinovich, D. (1965). *Acta Cryst.* **18**, 1035–1038.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Molecular Structure Corporation (1993). *MSC/AFC Diffractometer Control Software*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Molecular Structure Corporation (1999). *TEXSAN*. Version 1.10. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.