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N-Methyl-*N*-[(*Z*)-2-phenylpropenyl]-thiobenzamide

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

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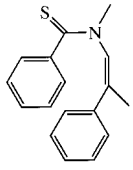
The crystal structure of the title thiobenzamide, $C_{17}H_{17}NS$, was determined to investigate the relationship between the photoreactivity in solid state and the structure. The geometry was confirmed to be the *Z* isomer.



(I)

Experimental

The title compound, (I), 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 benzene solution.

Crystal data

$C_{17}H_{17}NS$
M_r = 267.39
Monoclinic, $P2_1/c$
a = 10.057 (3) Å
b = 8.344 (3) Å
c = 17.962 (4) Å
β = 100.13 (2)°
V = 1483.8 (7) Å^3
Z = 4
D_x = 1.197 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 14.3–15.0°
μ = 0.204 mm^{-1}
T = 298 (1) K
Prism, yellow
0.6 × 0.6 × 0.3 mm

Data collection

Rigaku AFC-7*R* diffractometer
θ–2θ scans
3585 measured reflections
3396 independent reflections
2232 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.5°
$h = -13 \rightarrow 0$
$k = 0 \rightarrow 10$
$l = -23 \rightarrow 23$
3 standard reflections
every 150 reflections
intensity decay: none

Refinement

Refinement on F^2
$R(F)$ = 0.066
$wR(F^2)$ = 0.175
S = 1.02
3396 reflections
172 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 2.0P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected geometric parameters (Å).

S1—C3	1.661 (3)	N2—C11	1.428 (4)
N2—C3	1.351 (4)	C11—C12	1.327 (5)

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.
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.