necessary to establish the general conformational trends for the silacyclohexane ring.

Related literature. Subsequent syntheses of less-substituted systems, also prepared *via* a cyclic hydroboration sequence, have been reported (Soderquist, Shiau & Lemesh, 1984; Soderquist & Negron, 1989).

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Structure of 4-Amino-5-phenyl-4*H*-1,2,4-triazole-3-thione

By Ng Seik Weng

Institute of Advanced Studies, University of Malaya, 59100 *Kuala Lumpur, Malaysia*

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Abstract. $C_8H_8N_4S$, $M_r = 192.24$, triclinic, $P\bar{1}$, $a = 6.1917\,(8)$, $b = 7.1417\,(6)$, $c = 9.9643\,(8)$ Å, $\alpha = 81.822\,(7)$, $\beta = 84.638\,(8)$, $\gamma = 78.682\,(9)°$, $V = 426.67\,(8)$ Å^3, $Z = 2$, $D_x = 1.496$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0.71073$ Å, $\mu = 3.17$ cm^{-1}, $F(000) = 200$, $T = 298$ K, $R = 0.033$ for 1250 reflections $[I \geq 3\sigma(I)]$. The molecule exists in the tautomeric thione form. The dihedral angle between the triazolyl and phenyl rings is 1(2)°; the S and exocyclic amino N atoms deviate from the least-squares plane of the triazolyl ring by 0.0409 (7) and 0.002 (2) Å, respectively.

Experimental. The compound was prepared in a multi-step synthesis from benzhydrazide, carbon disulfide and hydrazine (Reid & Heindel, 1976) and crystals were obtained on crystallization from ethanol. The cubic crystal measuring 0.22 × 0.22 × 0.22 mm was mounted on an Enraf–Nonius CAD-4 diffractometer fitted with Mo $K\alpha$ radiation. Unit-cell constants were fixed from the 25 most intense reflections in the $13 \leq \theta \leq 15°$ thin shell. The 1652 unique data which were collected by using the $\theta/2\theta$-scan technique to $2\theta_{\max} = 50$ consisted of 1250 reflections with $I \geq 3\sigma(I)$ (collection range: h 0–7, k −8–8, l −11–11). Three reflections ($10\bar{6}$, $2\bar{3}2$ and $3\bar{2}2$), monitored hourly, showed negligible variations in intensity. The data set was corrected for absorption by using ψ-scan data (minimum/maximum transmission factors 0.9788/0.9997, average 0.9885). The structure was solved by a combination of direct and heavy-atom methods. The H atoms were located from a difference Fourier map, and were refined with a thermal factor $B = 5$ Å^2. The non-H atoms were refined anisotropically; 142 variables were refined. The weighting scheme $w = [\sigma(F)^2 + (0.02F)^2 + 1]^{-1}$ was used. Full-matrix least-squares refinement based on F converged at $R = 0.033$, $wR = 0.039$; $S = 0.564$; $(\Delta/\sigma) \leq 0.01$ for all atoms. The largest $\Delta\rho$ was 0.14 (2) e Å^{-3}. Scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV, Tables 2.2B and 2.3.1). All computations were performed using the *MolEN* structure determination package (Fair, 1990) on a DEC MicroVAX minicomputer. The atomic coordinates are listed in Table 1;* bond dimensions are gathered in Table 2. Fig. 1 shows the atomic labelling scheme.

Related literature. Katritzky, Bird, Boulton, Cheeseman, Lagowski, Lwowski, McKillop, Potts & Rees (1985) have reviewed the literature on heterocyclic chemistry. Their review contains references to

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* Lists of structure factors, anisotropic thermal parameters and H-atom positional parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55303 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AS0566]

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Table 1. *Positional parameters and equivalent isotropic thermal parameters* (Å^2)

$$B_{eq} = (4/3)[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)].$$

	x	y	z	B_{eq}
S	0.1735 (1)	0.1780 (1)	0.43890 (6)	4.00 (1)
N1	0.3304 (3)	0.2367 (3)	0.1768 (2)	2.56 (3)
N2	0.6871 (3)	0.1354 (3)	0.1797 (2)	3.30 (4)
N3	0.5846 (3)	0.1183 (3)	0.3083 (2)	3.47 (4)
N4	0.1214 (3)	0.3113 (3)	0.1292 (2)	3.88 (5)
C1	0.5640 (3)	0.2527 (3)	−0.0480 (2)	2.56 (4)
C2	0.3977 (4)	0.3337 (4)	−0.1333 (2)	4.01 (6)
C3	0.4443 (4)	0.3712 (4)	−0.2718 (3)	4.60 (6)
C4	0.6556 (5)	0.3284 (4)	−0.3268 (2)	4.18 (6)
C5	0.8226 (4)	0.2475 (4)	−0.2435 (3)	4.34 (6)
C6	0.7783 (4)	0.2088 (4)	−0.1051 (2)	3.53 (5)
C7	0.5272 (3)	0.2094 (3)	0.1003 (2)	2.49 (4)
C8	0.3672 (3)	0.1760 (3)	0.3108 (2)	2.84 (4)

Table 2. *Bond distances* (Å) *and angles* (°)

S—C8	1.668 (2)	C1—C2	1.381 (3)
N1—N4	1.398 (3)	C1—C6	1.389 (3)
N1—C7	1.371 (3)	C1—C7	1.472 (3)
N1—C8	1.369 (3)	C2—C3	1.382 (3)
N2—N3	1.376 (2)	C3—C4	1.365 (4)
N2—C7	1.307 (3)	C4—C5	1.371 (4)
N3—C8	1.327 (3)	C5—C6	1.380 (3)
S···N3^i	3.318 (2)		
N4—N1—C7	126.8 (2)	C3—C4—C5	119.5 (2)
N4—N1—C8	123.8 (2)	C4—C5—C6	120.5 (2)
C7—N1—C8	109.4 (2)	C1—C6—C5	120.4 (2)
N3—N2—C7	104.6 (2)	N1—C7—N2	109.4 (2)
N2—N3—C8	113.5 (2)	N1—C7—C1	127.7 (2)
C2—C1—C6	118.3 (2)	N2—C7—C1	122.9 (2)
C2—C1—C7	123.7 (2)	S—C8—N1	125.6 (2)
C6—C1—C7	117.9 (2)	S—C8—N3	131.4 (2)
C1—C2—C3	120.7 (2)	N1—C8—N3	103.1 (2)
C2—C3—C4	120.6 (3)		

Symmetry code: (i) $1 - x, -y, 1 - z$.

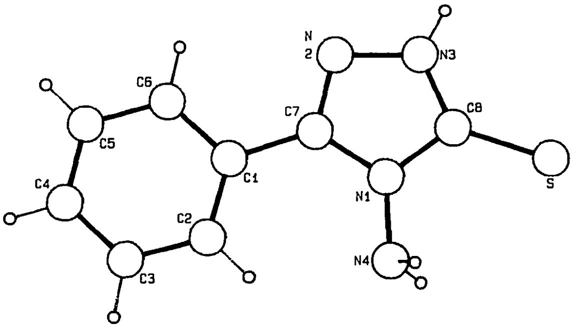

Fig. 1. The numbering scheme for the title compound.

tautomerism in mercapto-substituted heterocyclic compounds, many of which exist predominantly as thiones.

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1-Acetyl-7-methoxy-2-naphthol

BY PHILIPPE PRINCE, FRANK R. FRONCZEK AND RICHARD D. GANDOUR*

Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803-1804, *USA*

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Abstract. $C_{13}H_{12}O_3$, $M_r = 216.2$, orthorhombic, $Pna2_1$, $a = 7.4946\ (10)$, $b = 13.437\ (2)$, $c = 10.8630\ (8)$ Å, $V = 1094.0\ (4)$ Å^3, $Z = 4$, $D_x = 1.313$ g cm^{-3}, $\lambda(\mathrm{Cu}\ K\alpha) = 1.54184$ Å, $\mu = 7.24$ cm^{-1}, $F(000) = 456$, $T = 298$ K, $R = 0.043$ for 1028 observations (of 1191 unique data). The average deviation from planarity is 0.047 (4) Å with a maximum of 0.100 (3) Å for the atoms of the naphthyl ring. The dihedral angle between the naphthalene system and the acetyl group is 155.1 (1)°. This angle compares with 117.91 (6)° which is the value obtained with 1-acetyl-2,7-dimethoxynaphthalene [Prince, Fronczek & Gandour (1989). *Acta Cryst.* C**45**, 1256–1258]. The methoxy group has the methyl *syn* to the neighboring α C atom, and is nearly coplanar with the ring with a C—C—O—C torsion angle of 8.7 (5)°; in the case of 1-acetyl-2,7-dimethoxynaphthalene the methyl is also *syn* with a C—C—O—C torsion angle of −1.3 (3)°. The hydroxy group forms an intramolecular hydrogen bond with the acetyl O atom, with an O···O distance of 2.466 (4) Å.

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* To whom correspondence should be addressed.

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