Table 2. *Bond lengths* (Å) *and angles* (°) *with their estimated standard deviations*

C(1)–C(2)	1·401 (8)	C(9)–C(10)	1·398 (8)
C(1)–C(13)	1·362 (8)	C(9)–C(21)	1·401 (8)
C(1)–N	1·490 (7)	C(10)–C(11)	1·365 (8)
C(2)–C(3)	1·346 (9)	C(11)–C(12)	1·403 (7)
C(3)–C(15)	1·425 (9)	C(12)–C(13)	1·481 (7)
C(4)–C(5)	1·381 (8)	C(12)–C(17)	1·411 (7)
C(4)–C(15)	1·402 (8)	C(13)–C(14)	1·445 (8)
C(5)–C(6)	1·397 (8)	C(14)–C(15)	1·418 (7)
C(6)–C(16)	1·388 (8)	C(14)–C(16)	1·396 (7)
C(7)–C(16)	1·477 (8)	C(18)–C(19)	1·373 (10)
C(7)–C(17)	1·477 (8)	C(19)–C(20)	1·414 (9)
C(7)–O(1)	1·225 (7)	C(20)–C(21)	1·343 (9)
C(8)–C(9)	1·433 (8)	N–O(2)	1·219 (7)
C(8)–C(17)	1·424 (7)	N–O(3)	1·233 (6)
C(8)–C(18)	1·437 (9)		

C(2)–C(1)–C(13)	125·5 (6)	C(1)–C(13)–C(12)	127·4 (5)
C(2)–C(1)–N	112·9 (5)	C(1)–C(13)–C(14)	115·3 (5)
C(13)–C(1)–N	121·5 (5)	C(12)–C(13)–C(14)	117·1 (5)
C(1)–C(2)–C(3)	118·0 (6)	C(13)–C(14)–C(15)	120·5 (5)
C(2)–C(3)–C(15)	121·6 (6)	C(13)–C(14)–C(16)	119·8 (5)
C(5)–C(4)–C(15)	120·1 (6)	C(15)–C(14)–C(16)	119·6 (5)
C(4)–C(5)–C(6)	119·6 (6)	C(3)–C(15)–C(4)	122·0 (6)
C(5)–C(6)–C(16)	121·6 (6)	C(3)–C(15)–C(14)	118·3 (6)
C(16)–C(7)–C(17)	116·4 (5)	C(4)–C(15)–C(14)	119·7 (5)
C(16)–C(7)–O(1)	120·3 (6)	C(6)–C(16)–C(7)	120·2 (5)
C(17)–C(7)–O(1)	123·3 (6)	C(6)–C(16)–C(14)	119·1 (5)
C(9)–C(8)–C(17)	119·1 (5)	C(7)–C(16)–C(14)	120·6 (5)
C(9)–C(8)–C(18)	117·3 (6)	C(7)–C(17)–C(8)	121·7 (5)
C(17)–C(8)–C(18)	123·1 (6)	C(7)–C(17)–C(12)	117·7 (5)
C(8)–C(9)–C(10)	118·7 (5)	C(8)–C(17)–C(12)	120·6 (5)
C(8)–C(9)–C(21)	119·6 (5)	C(8)–C(18)–C(19)	119·8 (6)
C(10)–C(9)–C(21)	121·7 (6)	C(18)–C(19)–C(20)	121·8 (7)
C(9)–C(10)–C(11)	121·2 (6)	C(19)–C(20)–C(21)	118·9 (6)
C(10)–C(11)–C(12)	122·4 (6)	C(9)–C(21)–C(20)	122·4 (6)
C(11)–C(12)–C(13)	120·3 (5)	C(1)–N–O(2)	118·7 (5)
C(11)–C(12)–C(17)	117·9 (5)	C(1)–N–O(3)	117·6 (5)
C(13)–C(12)–C(17)	121·3 (5)	O(2)–N–O(3)	123·5 (5)

of the two naphthalene moieties [(*a,b*) and (*d,e*) rings in Fig. 2] make an angle of 25·7 (2)°. The central *c* ring shows the quinonoid structure. The steric repulsion is also relieved by an enlargement of the C(1)–C(13)–C(12) angle [127·4 (5)°]. Moreover, the C–NO_2 and C=O bonds are bent from the mean planes of the *e* and *c* rings, respectively. The twisting angle of C(1)–N and C(12)–C(11) around the line of C(1)···C(12) and that of C(7)–O(1) and C(8)–C(18) around C(7)···C(8) become 30·0 (6) and 23·5 (5)°, respectively. The N···H(11) distance is 2·33 (5) Å, which is significantly shorter than the sum of van der Waals radii. The NO_2 group rotates around the C(1)–N bond from the coplanar conformation. The torsion angle O(3)–N–C(1)–C(13) is 45·7 (3)°. The O(3)···H(11) distance becomes 2·51 (5) Å. Although the original 8,9-BzBT molecule without the NO_2 group also deviates from a planar conformation, the degree of deviation is smaller than in the present nitro compound (Fujisawa, Sato & Saito, 1981). The twisting angle of O–C(7)···C(8)–C(18) is 6 (1)°. This indicates that the distortion of the present molecule is caused mainly by the steric repulsion of the NO_2 group.

It is interesting to consider why the NO_2 group is substituted on the C(1) atom in spite of the large steric repulsion. The reaction mechanism will be discussed in detail elsewhere.

References

Fujisawa, S., Sato, S. & Saito, Y. (1981). *Acta Cryst.* **B37**, 2194–2198.

International Tables for X-ray Crystallography (1974). Vol. IV, pp. 71–151. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

Main, P., Hull, S. E., Lessinger, L., Germain, G., Declercq, J.-P. & Woolfson, M. M. (1978). *MULTAN78. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univs. of York, England, and Louvain, Belgium.

Ohashi, Y. (1975). Unpublished version of original *HBLS* program by T. Ashida.

Acta Cryst. (1987). C**43**, 256–259

Structure of 5-Tritylamino-1,4-dihydronaphthalene

By C. W. Holzapfel, G. J. Kruger and M. S. Van Dyk

Department of Chemistry, Rand Afrikaans University, PO Box 524, *Johannesburg* 2000, *Republic of South Africa*

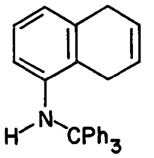
(*Received* 16 *April* 1986; *accepted* 21 *August* 1986)

Abstract. $C_{29}H_{25}N$, $M_r = 387{\cdot}53$, monoclinic, $C2/c$, $a = 14{\cdot}214\,(5)$, $b = 13{\cdot}691\,(4)$, $c = 22{\cdot}095\,(7)$ Å, $\beta = 97{\cdot}97\,(3)°$, $V = 4258{\cdot}11$ Å^3, $Z = 8$, $D_x = 1{\cdot}209$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71073$ Å, $\mu(\text{Mo } K\alpha) = 0{\cdot}35$ mm^{-1}, $F(000) = 1648$, $T = 253$ K, final $R = 0{\cdot}073$, $wR = 0{\cdot}044$ for 1342 $[I > 3\sigma(I)]$ independent reflections. The dihydro ring has a flattened, slightly distorted boat conformation. There are no unusual bond distances or angles.

Introduction. An investigation into the possible factors determining the regioselectivity observed in the cycloaddition reactions of vinylnitrosonium ions with various 5-substituted 1,4-dihydronaphthalenes (Holzapfel, Koekemoer & Van Dyk, 1985) required, amongst others, information on the conformation and puckering amplitude of the dihydro ring in these compounds. NMR conformational analysis of 1,4-dihydro-1-naphthoic acid (based on the ratios of $^5J_{cis}/^5J_{trans}$ for the

0108-2701/87/020256-04$01.50

proton–proton and carbon–proton homoallylic coupling constants) (Marshall, Faehl, McDaniel & Ledford, 1977) indicated that the dihydro ring has a flattened boat conformation. This conclusion has, however, not been confirmed thus far by X-ray structure determination of this acid or any closely related compound. In addition, the possibility of differences between 1- and 5-substituted 1,4-dihydronaphthalenes still exists. Various derivatives of 5-amino-1,4-dihydronaphthalene were therefore prepared with a view to X-ray structure determination. Only the title compound (I), obtained by the reaction of 5-amino-1,4-dihydronaphthalene with trityl chloride in pyridine, yielded crystals (m.p. 455–457 K) suitable for this purpose.


(I)

Experimental. Single crystal, crystallized from dichloromethane–hexane solution, as a colourless prism with approximate dimensions 0·30 x 0·25 x 0·25 mm used for intensity-data collection. Lattice parameters refined using 25 reflections in the range $5 < \theta < 15°$. Enraf–Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$ radiation, $\omega/2\theta$ mode, $2\theta_{\max} = 50°$ ($h \leq 16$, $k \leq 16$, $-26 \leq l \leq 26$). Three standard reflections ($\bar{1}\bar{3}5$, 040 and $\bar{2}0\bar{6}$) monitored every 3600 s showed a total loss in intensity of 2·9% over the total exposure time of 30·9 h. 3912 independent reflections measured. The data are of relatively poor quality (hence high R) with a large number of weak reflections: 1990 with $I > \sigma(I)$, 1342 with $I > 3\sigma(I)$. The data were corrected for Lorentz and polarization effects and for absorption (North, Phillips & Mathews, 1968).

The structure was solved by direct methods as applied for centrosymmetric space groups in the *EEES* routine of *SHELX76* (Sheldrick, 1976). Scattering factors from *International Tables for X-ray Crystallography* (1974). The structure was refined by full-matrix least-squares procedure minimizing the function $\sum w(|F_o| - |F_c|)^2$ with $w = [\sigma(F)]^{-2}$. The full-matrix least-squares program *SHELX76* (Sheldrick, 1976) was used. Since a difference Fourier synthesis did not reveal the positions of all the hydrogen atoms, only the hydrogen atoms bonded to N(1), C(2) and C(3) were refined individually. The rest were refined in calculated positions at 1·08 Å, and with a common isotropic temperature factor. Refinement with non-hydrogen atoms treated anisotropically and hydrogen atoms isotropically produced convergence with $R = 0{\cdot}073$ and $wR = 0{\cdot}044$. $(\Delta/\sigma)_{\max} = 0{\cdot}04$. A final difference Fourier synthesis showed $\Delta\rho = \pm 0{\cdot}5$ e Å^{-3}.

Discussion. The final positional and isotropic thermal parameters are given in Table 1.* The atomic numbering scheme, and selected bond lengths and angles for the 1,4-dihydronaphthalene fragment are shown in Fig. 1. Fig. 2 shows a perspective drawing of one molecule of the dihydronaphthalene (I).

Table 1. *Positional parameters* ($\times 10^4$ *for non-hydrogen atoms*, $\times 10^3$ *for hydrogen atoms*) *and isotropic thermal parameters* (Å^2 $\times 10^3$)

For the non-hydrogen atoms U_{eq} is defined as the geometric mean of the diagonal elements of the diagonalized matrix of $U(ij)$.

	x	y	z	U_{eq} or U_{iso}
N(1)	2127 (4)	3833 (5)	1938 (3)	39 (4)
C(1)	1537 (6)	3544 (7)	4082 (3)	62 (6)
C(1*A*)	1948 (5)	4067 (6)	3573 (3)	47 (5)
C(2)	910 (7)	2713 (7)	3871 (4)	63 (7)
C(3)	830 (6)	2346 (7)	3318 (4)	55 (6)
C(4)	1315 (5)	2762 (5)	2815 (3)	46 (5)
C(4*A*)	1843 (5)	3713 (6)	2978 (3)	44 (5)
C(5)	2218 (5)	4228 (6)	2528 (3)	38 (5)
C(6)	2708 (5)	5104 (5)	2667 (3)	43 (5)
C(7)	2807 (5)	5451 (6)	3260 (4)	53 (5)
C(8)	2432 (5)	4946 (6)	3714 (3)	49 (5)
C(9)	2045 (5)	4418 (5)	1364 (3)	39 (4)
C(11)	1417 (5)	5318 (5)	1443 (3)	37 (4)
C(12)	522 (5)	5155 (5)	1614 (3)	43 (5)
C(13)	−54 (5)	5916 (6)	1738 (3)	47 (5)
C(14)	257 (5)	6873 (6)	1680 (3)	51 (5)
C(15)	1138 (5)	7055 (6)	1507 (3)	52 (5)
C(16)	1715 (5)	6273 (5)	1380 (3)	44 (5)
C(21)	3039 (5)	4676 (5)	1203 (3)	41 (5)
C(22)	3111 (5)	5154 (5)	654 (3)	49 (5)
C(23)	3998 (6)	5379 (6)	483 (4)	54 (6)
C(24)	4811 (6)	5107 (6)	866 (4)	56 (6)
C(25)	4746 (5)	4624 (6)	1401 (4)	55 (6)
C(26)	3864 (5)	4395 (5)	1575 (4)	49 (5)
C(31)	1590 (5)	3745 (5)	850 (3)	39 (5)
C(32)	1918 (5)	2795 (6)	812 (3)	45 (5)
C(33)	1556 (5)	2179 (6)	341 (3)	49 (5)
C(34)	864 (5)	2504 (6)	−105 (3)	50 (5)
C(35)	532 (5)	3458 (6)	−84 (3)	53 (5)
C(36)	892 (5)	4079 (6)	387 (3)	50 (5)
H(1N)	173 (5)	326 (5)	190 (3)	93 (32)
H(1*A*)	133	406	430	76 (6)
H(1*B*)	212	328	441	76 (6)
H(2)	59 (4)	238 (4)	421 (3)	43 (20)
H(3)	38 (5)	171 (6)	310 (3)	118 (36)
H(4*A*)	182	223	269	76 (6)
H(4*B*)	78	290	243	76 (6)
H(6)	300	550	232	76 (6)
H(7)	318	613	337	76 (6)
H(8)	251	523	417	76 (6)
H(12)	27	441	165	76 (6)
H(13)	−74	577	188	76 (6)
H(14)	−19	748	177	76 (6)
H(15)	138	780	174	76 (6)
H(16)	239	642	123	76 (6)
H(22)	247	535	36	76 (6)
H(23)	405	576	6	76 (6)
H(24)	550	528	74	76 (6)
H(25)	539	442	169	76 (6)
H(26)	382	400	199	76 (6)
H(32)	247	253	116	76 (6)
H(33)	182	144	32	76 (6)
H(34)	57	202	−47	76 (6)
H(35)	−1	372	−44	76 (6)
H(36)	63	482	40	76 (6)

---

* Lists of structure factors, anisotropic thermal parameters and a list of bond lengths and angles (not including the aromatic H atoms) have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43346 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

The use of a compound with such a large substituent as the trityl group as a representative example of 5-substituted 1,4-dihydronaphthalenes in general was questionable. The phenyl rings of the trityl group are, however, far removed from the naphthalene system and the shortest distance between one of these groups and the naphthalene fragment is 2·51 Å between H(6) and H(26). No atoms belonging to any of the phenyl rings are within 3 Å from the dihydro ring.

Table 2. *Conformational parameters describing the dihydro ring*

(*a*) Endocyclic torsion angles (°)	
C(21)–C(1)–C(1*A*)–C(4*A*)	−8 (1)
C(1)–C(1*A*)–C(4*A*)–C(4)	−1 (1)
C(1*A*)–C(4*A*)–C(4)–C(3)	8 (1)
C(4*A*)–C(4)–C(3)–C(2)	−6 (1)
C(4)–C(3)–C(2)–C(1)	4 (1)
C(3)–C(2)–C(1)–C(1*A*)	10 (1)

(*b*) Puckering parameters	
Q (Å)	0·108
q_2 (Å)	0·108
q_3 (Å)	−0·009
θ (°)	94·613
φ_2 (°)	192·655

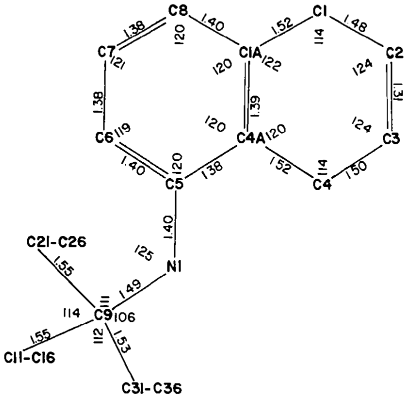


Fig. 1. Schematic drawing of the 1,4-dihydronaphthalene (I) showing the atom labelling and intramolecular bond lengths (Å) and angles (°) (mean e.s.d.'s 0·01 Å and 1°). The C—C bond lengths and C—C—C angles in the phenyl rings range from 1·37 (1) to 1·40 (1) Å [mean 1·39 (1) Å] and from 118 (1) to 122 (1)° [mean 120 (1)°], respectively.

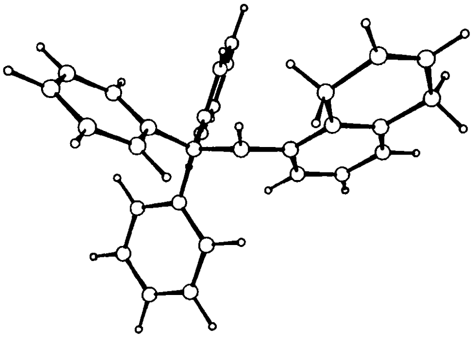


Fig. 2. A perspective drawing of one molecule of the 1,4-dihydronaphthalene (I).

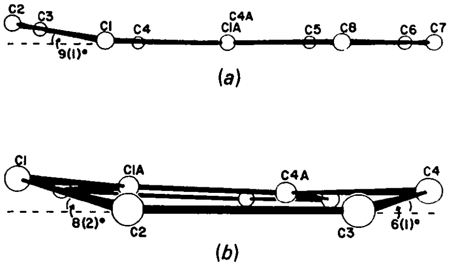


Fig. 3. Drawings of the dihydronaphthalene moiety showing the relevant planes and interplanar angles.

As can be seen in Fig. 3(*a*), C(1) and C(4) are coplanar with the aromatic ring [C(1*A*), C(4*A*), C(5), C(6), C(7) and C(8)], with deviations from the plane all smaller than one standard deviation of 0·01 Å. A second plane is formed by C(1), C(2), C(3) and C(4). The angle between this plane and a second plane through C(1), C(2), C(3) and C(4), as shown in Fig. 3(*a*), is 9 (1)°. Marshall, Faehl, McDaniel & Ledford (1977) define the puckering of dihydro rings in terms of puckering angle, α, which in a symmetric system is the angle between the plane formed by C(1*A*), C(1) and C(2) [or by C(4*A*), C(4) and C(3)] and the plane formed by C(1*A*), C(2), C(3) and C(4*A*) (Fig. 3*b*). Their calculations predict an approximate puckering angle, α, of 10° for their 1,4-dihydro-1-naphthoic acid system. As can be seen in Fig. 3(*b*) two puckering angles of 8 (2) and 6 (1)° are obtained for the present 5-substituted 1,4-dihydronaphthalene (I).

The torsion angles for the dihydro ring are given in Table 2(*a*). From the interplanar angles and the torsion angles it is evident that the dihydro ring has a slightly puckered, slightly distorted boat conformation. This is confirmed by the Cremer & Pople (1975) puckering parameters given in Table 2(*b*) (the parameters for the nearest ideal boat are $\theta = 90°$, $\varphi = 180°$ and $Q > 0$ Å). A search of the 1984 version of the Cambridge Crystallographic Data Base (Allen *et al.*, 1979) yielded one example of a 1,4-dihydrophenanthrene system as part of a tricarbonyl(1,4-dihydrophenanthrene)-chromium(0) complex (Guss & Mason, 1973). In this case the bond lengths for the dihydro ring are indistinguishable from those of the aromatic rings, but the dihydro ring has a more puckered, more distorted, boat conformation with puckering constants $Q = 0{\cdot}228$ Å, $\varphi = 201{\cdot}07°$ and $\theta = 102{\cdot}20°$.

References

Allen, F. H., Bellard, S., Brice, M. D., Cartwright, B. A., Doubleday, A., Higgs, H., Hummelink, T., Hummelink-Peters, B. G., Kennard, O., Motherwell, W. D. S., Rodgers, J. R. & Watson, D. G. (1979). *Acta Cryst.* B**35**, 2331–2339.

Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.

Guss, J. M. & Mason, R. (1973). *J. Chem. Soc. Dalton Trans.* pp. 1834–1840.

Holzapfel, C. W., Koekemoer, J. M. & Van Dyk, M. S. (1985). *Abstracts.* 10th International Congress of Heterocyclic Chemistry, Waterloo, Ontario, *P*1–*P*11.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

Marshall, J. L., Faehl, L. G., McDaniel, C. R. Jr & Ledford, N. D. (1977). *J. Am. Chem. Soc.* **99**, 321–325.

North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.

Sheldrick, G. M. (1976). *SHELX*76. Program for crystal structure determination. Univ. of Cambridge, England.

Acta Cryst. (1987). C**43**, 259–260

Structure of 3,4-Dimethylthiazole-2-thione

By F. Ugozzoli and G. D. Andreetti

*Institute of Structural Chemistry of the University and Centro di Studio per la Strutturistica Diffrattometrica del CNR, Viale delle Scienze, I-*43100 *Parma, Italy*

(*Received* 11 *April* 1986; *accepted* 15 *August* 1986)

Abstract. $C_5H_7NS_2$, $M_r = 145{\cdot}2$, orthorhombic, $Pna2_1$, $a = 7{\cdot}555\ (4)$, $b = 7{\cdot}513\ (4)$, $c = 12{\cdot}003\ (7)$ Å, $V = 681{\cdot}3\ (7)$ Å^3, $Z = 4$, $D_m = 1{\cdot}42\ (1)$, $D_x = 1{\cdot}42\ (1)$ Mg m^{-3}, $\lambda(\text{Cu}\ K\alpha) = 1{\cdot}5418$ Å, $\mu = 61{\cdot}3$ mm^{-1}, $F(000) = 304$, $T = 298$ K, final $R = 0{\cdot}069$ for 479 observed independent reflections. The heterocyclic ring is planar and bond distances and angles are mainly as expected, but some C—S and C—N bond distances slightly deviate from the values given in the literature for similar compounds.

Introduction. The reaction of *N*-alkylthiazolium halides with potassium superoxide has recently been reported by Dondoni, Galliani & Mastellari (1985). The reaction products *N*-alkylthiazol-2-one and the corresponding thio-analogue have been characterized by spectroscopic techniques and their structures were assigned on the basis of the X-ray analysis reported in this paper.

Experimental. Crystal 0·55 × 0·46 × 0·28 mm. D_m determined pycnometrically. Orthorhombic, Laue class *mm*2, systematic extinctions $h0l$, $h + l = 2n + 1$, $hk0$, $k = 2n + 1$, space group $Pna2_1$.

Siemens AED diffractometer on-line to a General Automation Jumbo 220 microcomputer, Ni-filtered Cu $K\alpha$ radiation, θ–2θ scan, scan width from $(\theta - 0{\cdot}60)$ to $(\theta + 0{\cdot}60 + 0{\cdot}142 + \tan\theta)°$; scan speed 3·0° min^{-1}. Cell dimensions based on 25 (θ,χ,φ) *hkl* measured intensities. 794 symmetry-independent reflections ($0 \le h \le 8$, $0 \le k \le 9$, $0 \le l \le 14$, $3 \le \theta \le 70°$) collected at $T = 298$ K with a modified version (Belletti, Ugozzoli, Cantoni & Pasquinelli, 1979) of the Lehmann & Larsen (1974) procedure. One standard reflection, no significant deviations from the initial intensity. Corrections for Lorentz and polarization, no correction for absorption effects.

Structure solved by direct methods (*MULTAN*, Main, Woolfson, Lessinger, Germain & Declercq, 1974). 479 observed reflections $[I > 2\sigma(I)]$ in full-matrix least-squares refinement; 88 parameters; H(5) from difference electron density map; methyl H atoms were calculated and refined as rigid groups; $\sum w\big||F_o| - |F_c|\big|^2$ minimized; $w = [\sigma^2(F_o) + 0{\cdot}72245F_o^2]^{-1}$, *SHELX*76 system (Sheldrick, 1976); $(\Delta/\sigma)_{\max} = 0{\cdot}090$, $\Delta\rho = -0{\cdot}43$ to $0{\cdot}91$ e Å^{-3}; the latter was found at

Table 1. *Final atomic coordinates* (×10^4) *and equivalent isotropic temperature factors* (×10^4 Å^2) *of the non-hydrogen atoms with e.s.d.'s in parentheses*

$$U_{\rm eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
S1	9201 (4)	4542 (4)	4367	504 (9)
C2	8529 (15)	3829 (24)	3097 (11)	514 (49)
N3	8517 (12)	2034 (19)	3086 (10)	451 (33)
C4	9039 (16)	1195 (22)	4084 (12)	487 (39)
C5	9431 (17)	2371 (23)	4862 (14)	518 (43)
C6	8025 (18)	1006 (26)	2099 (18)	626 (52)
C7	9161 (19)	−767 (24)	4166 (21)	668 (68)
S8	7979 (5)	5206 (6)	2019 (5)	640 (13)

Table 2. *Bond distances* (Å), *bond angles* (°) *and torsion angles* (°) *with e.s.d.'s in parentheses*

S1—C2	1·694 (14)	N3—C4	1·410 (19)
S1—C5	1·745 (17)	N3—C6	1·462 (24)
C2—N3	1·349 (23)	C4—C5	1·319 (23)
C2—S8	1·708 (16)	C4—C7	1·480 (25)
C2—S1—C5	92·3 (8)	C4—N3—C6	121·6 (13)
S1—C2—S8	124·3 (9)	N3—C4—C7	121·3 (13)
S1—C2—N3	109·1 (9)	N3—C4—C5	111·4 (14)
N3—C2—S8	126·6 (11)	C5—C4—C7	127·3 (15)
C2—N3—C6	122·5 (13)	S1—C5—C4	111·3 (12)
C2—N3—C4	115·9 (12)		
C2—S1—C5—C4	1·0 (13)	C2—N3—C4—C5	0·7 (19)
C5—S1—C2—S8	179·8 (11)	C2—N3—C4—C7	−177·2 (14)
C5—S1—C2—N3	−0·6 (11)	C6—N3—C4—C7	1·8 (22)
S1—C2—N3—C4	0·0 (16)	C6—N3—C4—C5	179·7 (14)
S1—C2—N3—C6	−178·9 (12)	N3—C4—C5—S1	−1·1 (17)
S8—C2—N3—C6	0·7 (21)	C7—C4—C5—S1	176·7 (14)
S8—C2—N3—C4	179·6 (11)		