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) $1 - x, -y, 1 - z$.

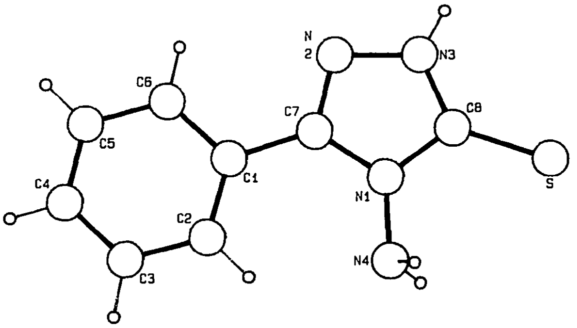

Fig. 1. The numbering scheme for the title compound.

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

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1-Acetyl-7-methoxy-2-naphthol

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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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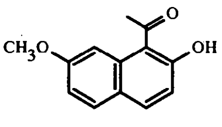
Experimental. The title compound, (1), was prepared by the selective demethylation of 1-acetyl-2,7-dimethoxynaphthalene with aluminium chloride in dichloroethane at room temperature. Pale yellow plates of (1), m.p. 408–409 K, were recrystallized from methanol. A crystal of size 0.20 × 0.37 × 0.45 mm was mounted in a capillary in random orientation on an Enraf–Nonius CAD-4 diffractometer equipped with a graphite monochromator and Cu $K\alpha$ radiation. Cell dimensions were determined from setting angles of 25 reflections having $25 < \theta < 29°$. Space group was determined to be $Pna2_1$ from systematic absences $0kl$ with $k + l$ odd, $h0l$ with h odd, and successful refinement of a non-centrosymmetric model.



(1)

An octant of data having $2 < 2\theta < 150°$, $0 \le h \le 9$, $0 \le k \le 16$, $0 \le l \le 13$ was collected using ω–2θ scans designed for $I = 50\sigma(I)$, subject to a maximum scan time of 120 s, with scan rates varied by 0.46–3.30° min^{-1}. Three reflections (400, 040, 006) were measured every 166 min, and their intensities exhibited only random fluctuations during data collection. Lorentz and polarization corrections were applied. An empirical absorption correction based on a series of ψ scans was applied to the data. Relative transmission coefficients ranged from 0.9990 to 0.9667 with an average value of 0.9833. The extinction coefficient was refined in the least squares to $g = 3.9\,(4) \times 10^{-6}$, where the correction factor $(1 + gI_c)^{-1}$ was applied to F_c. The structure was solved by direct methods using *RANTAN* (Yao, 1981), and successive difference Fourier syntheses. The structure was refined by weighted full-matrix least squares. Non-H atoms were refined anisotropically. H atoms were located in difference maps, and those on C atoms were included as fixed contributions with C—H distance 0.95 Å and $B = 1.3B_{\rm eq}$ for C. Refinement of the OH H atom was unsuccessful, and it was fixed in the position indicated by difference maps.

The function $\sum w(|F_o| - |F_c|)^2$ was minimized {weights were assigned as $w = 4F_o{}^2\mathrm{Lp}[S^2(C + R^2B) + (0.02F_o{}^2)^2]^{-1}$, where S = scan rate, C = total integrated peak count, R = scan time/background counting time, B = total background count, and Lp = Lorentz–polarization factor} using the Enraf–Nonius *SDP* (Frenz & Okaya, 1980), scattering factors of Cromer & Waber (1974), and anomalous coefficients of Cromer (1974). Of 1191 unique data, 1028 reflections having $I > 3\sigma(I)$ were used in the refinement. The final cycle included 145 variables and converged (largest $\Delta/\sigma = 0.02$) with $R = 0.043$, $wR = 0.055$, R(all) = 0.052, and $S = 3.230$. The maximum and minimum residual densities were 0.16 and −0.19 e Å^{-3}, respectively. Table 1 presents the final coordinates[*] and equivalent isotropic thermal parameters; Table 2 presents bond distances and angles. Fig. 1 illustrates the molecule and the numbering scheme; Fig. 2 shows the unit cell.

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

$$B_{\rm eq} = (8\pi^2/3)\textstyle\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$
O1	0.9557 (4)	0.1842 (2)	0†	7.74 (6)
O2	0.9092 (4)	0.3359 (2)	−0.6463 (2)	8.10 (7)
O3	0.9411 (3)	0.4680 (1)	−0.4902 (3)	6.65 (5)
C1	0.9248 (4)	0.1715 (2)	−0.1224 (3)	5.66 (7)
C2	0.8792 (4)	0.0736 (3)	−0.1581 (4)	6.34 (7)
C3	0.8531 (4)	0.0521 (2)	−0.2782 (4)	6.18 (7)
C4	0.8677 (4)	0.1263 (2)	−0.3696 (3)	5.02 (6)
C5	0.8501 (4)	0.1023 (2)	−0.4957 (4)	6.32 (7)
C6	0.8678 (5)	0.1718 (3)	−0.5844 (4)	6.74 (8)
C7	0.8973 (5)	0.2711 (2)	−0.5513 (3)	5.81 (7)
C8	0.9054 (3)	0.3012 (2)	−0.4287 (3)	4.43 (5)
C9	0.9016 (3)	0.2259 (2)	−0.3347 (3)	4.33 (5)
C10	0.9379 (4)	0.2445 (2)	−0.2086 (3)	4.73 (5)
C11	0.9807 (7)	0.2850 (4)	0.0434 (4)	8.7 (1)
C12	0.9040 (4)	0.4095 (2)	−0.4067 (3)	4.82 (6)
C13	0.8435 (5)	0.4546 (2)	−0.2889 (3)	6.26 (7)

† Coordinate fixed to define origin of structure in non-centrosymmetric space group.

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

O1—C1	1.360 (4)	C4—C9	1.415 (4)
O1—C11	1.446 (5)	C5—C6	1.348 (5)
O2—C7	1.353 (4)	C6—C7	1.400 (5)
O3—C12	1.232 (4)	C7—C8	1.394 (4)
C1—C2	1.413 (5)	C8—C9	1.437 (4)
C1—C10	1.360 (4)	C8—C12	1.475 (4)
C2—C3	1.350 (6)	C9—C10	1.419 (4)
C3—C4	1.410 (5)	C12—C13	1.487 (5)
C4—C5	1.414 (5)		

C1—O1—C11	117.3 (3)	O2—C7—C8	122.6 (3)
O1—C1—C2	115.2 (3)	C6—C7—C8	121.9 (3)
O1—C1—C10	124.8 (3)	C7—C8—C9	118.3 (2)
C2—C1—C10	120.0 (3)	C7—C8—C12	116.1 (3)
C1—C2—C3	119.9 (3)	C9—C8—C12	125.4 (3)
C2—C3—C4	121.2 (3)	C4—C9—C8	118.7 (3)
C3—C4—C5	120.9 (3)	C4—C9—C10	117.4 (3)
C3—C4—C9	119.6 (3)	C8—C9—C10	123.9 (2)
C5—C4—C9	119.5 (3)	C1—C10—C9	121.6 (3)
C4—C5—C6	121.7 (3)	O3—C12—C8	120.6 (3)
C5—C6—C7	119.5 (3)	O3—C12—C13	116.3 (2)
O2—C7—C6	115.3 (3)	C8—C12—C13	122.9 (3)

C11—O1—C1—C10	8.7 (5)
O2—C7—C8—C12	7.8 (4)
C12—C8—C9—C10	−15.4 (4)
C7—C8—C12—O3	−18.4 (4)
C9—C8—C12—C13	−19.3 (4)

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[*] Lists of H-atom coordinates, torsion angles, anisotropic thermal parameters, least-squares planes and structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55301 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: ST0581]

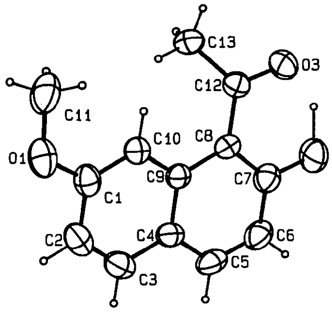

Fig. 1. Numbering scheme and thermal ellipsoids drawn at the 40% probability level. H atoms are drawn as circles with arbitrary radius.

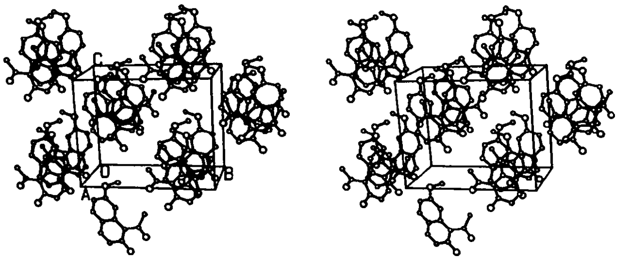

Fig. 2. Stereoview of the unit cell.

Related literature. The literature contains seven crystal structures of organic compounds containing the 2-hydroxyacetophenone fragment, and forming an intramolecular hydrogen bond between the hydroxy group and the acetyl O atom (Cohen *et al.*, 1989; Li, Li, Yang, You, Huang & Wang, 1986; Nowshad & Ul-Haque, 1976; Ray & Sen Gupta, 1981; Schlemper, 1986; Wajsman, Grabowski, Stępień & Cygler, 1978; Wu, Wang, Jong, McPhail, McPhail & Lee, 1989). The average O···O distance is 2.52 Å.

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Structure of 2-Phenylpyrimidinium 1-Oxide

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Abstract. $C_{10}H_8N_2O$, $M_r = 172.2$, orthorhombic, $P2_12_12_1$, $a = 7.189\,(1)$, $b = 10.141\,(2)$, $c = 11.302\,(2)$ Å, $V = 824.0\,(3)$ Å^3, $Z = 4$, $D_x = 1.388$ g cm^{-3}, Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å, $\mu = 0.87$ cm^{-1}, $F(000) = 360$, $T = 293\,(2)$ K, final $R = 0.058$ and $wR = 0.064$ for 1104 observed reflections. The benzene and pyrimidine rings are planar to within 0.020 (2) and 0.007 (3) Å respectively. The dihedral angle between the rings is 25.0 (5)°. The bond lengths and angles agree with expected values.

Experimental. A prismatic single crystal (0.63 × 0.50 × 0.47 mm) was used for X-ray data collection. Cell dimensions were determined from the angular settings of 25 reflections with $10 < \theta < 12°$, measured on an Enraf–Nonius CAD-4 diffractometer. Space