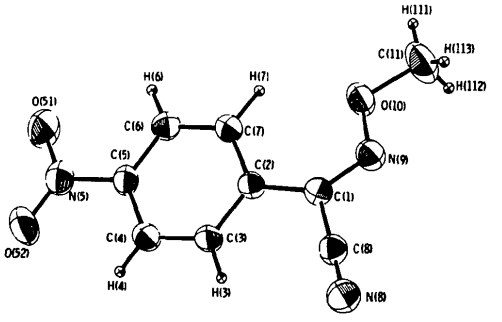

Fig. 1. *ORTEP* (Johnson, 1965) drawing of the molecule.

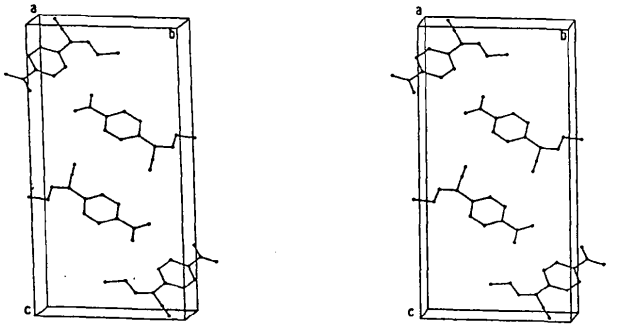

Fig. 2. Stereoscopic view of the packing of the molecules in the unit cell.

Related literature. This compound is one of a series of benzohydroximic acid derivatives that have been prepared for kinetic and stereochemical studies on nucleophilic substitution at the carbon–nitrogen double bond. Previous structures on related compounds include the *Z* and *E* isomers of *O*-methyl-*p*-nitrobenzohydroximoyl chloride, *p*-(NO_2)-$C_6H_4C(Cl)$-$NOCH_3$ (Bertolasi, Sacerdoti & Tassi, 1977; Johnson, Ghafouripour, Haug, Cordes, Pennington & Exner, 1985) and the *Z* and *E* isomers of ethylbenzohydroximate, $C_6H_5C(OC_2H_5)NOH$ (Larsen, 1971).

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2,2′-Azinodi-2-ethanenitrile

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Abstract. $C_{16}H_{10}N_4$, $M_r = 258{\cdot}28$, triclinic, $P\bar{1}$, $a = 10{\cdot}617$ (1), $b = 8{\cdot}264$ (1), $c = 3{\cdot}938$ (1) Å, $\alpha = 92{\cdot}41$ (1), $\beta = 84{\cdot}37$ (1), $\gamma = 106{\cdot}29$ (1)°, $V = 330{\cdot}0$ (1) Å^3, $Z = 1$, $D_x = 1{\cdot}300$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, μ(Mo $K\alpha$) = 0·76 cm^{-1}, $F(000) = 134$, $T = 295$ K. Final $R = 0{\cdot}038$ for 870 observed reflections. The structure shows that the compound is the *Z,Z* isomer. The bond distances N–N, N=C and C–C(phenyl) are 1·396 (2), 1·289 (2) and 1·465 (2) Å, respectively.

Experimental. Crystals of the title compound are orange prisms. Unit-cell parameters by least-squares fit of 15 reflections in the range $15 < 2\theta < 24°$, space group $P\bar{1}$; crystal 0·48 × 0·26 × 0·13 mm, automatic Syntex $P2_1$ diffractometer, graphite-monochromated Mo $K\alpha$ radiation, $\theta/2\theta$ scan mode, 1156 independent reflections in range $3 < 2\theta < 50°$, *hkl* range,

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h −12→12, k −9→9, l 0→4; 874 observed reflections with $I > 3\sigma(I)$, $\sigma(I)$ from counting statistics; three standard reflections (100, 010, 011) remeasured every 100 reflections showed a random variation of less than 3% in intensity; Lorentz–polarization correction, no absorption correction; direct methods, *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), refinement by full-matrix least squares using *SHELX*76 (Sheldrick, 1976), anisotropic, H atoms located in difference Fourier map, isotropic temperature factors for H, $w = 1/(\sigma_F^2 + 0{\cdot}00125F^2)$, $\sum w(|F_o| - |F_c|)^2$ minimized, $R = 0{\cdot}038$, $wR = 0{\cdot}036$ and $S = 1{\cdot}84$. Four low-angle reflections (110, 111, 001 and 200) possibly affected by extinction were taken out during the last refinement. $(\Delta/\sigma)_{max} = 0{\cdot}07$; $(\Delta\rho)_{max,min} = 0{\cdot}13$, $-0{\cdot}14$ e Å^{-3} in final difference Fourier map. Atomic scattering factors used were those stored in *SHELX*76. The final parameters are given in Table 1; bond lengths and angles are listed in Table 2.* The molecule is shown in Fig. 1.

Related literature. This compound is one of the unexpected byproducts obtained by UV irradiation of *O*-methylbenzohydroximoyl cyanide, $C_6H_5C(CN)NOCH_3$. It has also been prepared by oxidation of triazolopyridazines (Gilchrist, Gymer & Rees, 1975). Previous azine structural studies include those of benzalazine (Burke-Laing & Laing, 1976) and 1,2-dibenzilidene hydrazinium hexafluoroarsenate (Noltemeyer, Schmidt & Sheldrick, 1983).

* Lists of anisotropic temperature factors, structure factors and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43131 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

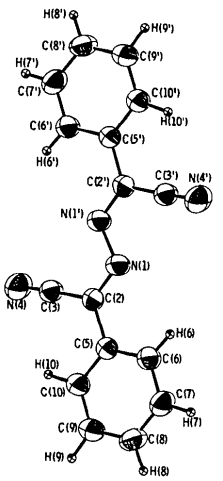

Fig. 1. *ORTEP* (Johnson, 1965) drawing of the molecule. Thermal ellipsoids scaled at the 50% probability level. H atoms shown as spheres of arbitrary radius.

Table 1. *Fractional atomic coordinates with equivalent isotropic thermal parameters for the non-*H *and isotropic for the* H *atoms (e.s.d.'s in parentheses)*

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

	x	y	z	U_{eq}/U(Å^2)
N(1)	0·4776 (1)	0·0677 (1)	0·4580 (3)	0·0545 (3)
C(2)	0·3570 (1)	0·0515 (2)	0·5743 (3)	0·0428 (3)
C(3)	0·2820 (1)	−0·0953 (2)	0·7719 (4)	0·0498 (3)
N(4)	0·2196 (1)	−0·2053 (2)	0·9319 (4)	0·0695 (3)
C(5)	0·2911 (1)	0·1800 (2)	0·5138 (3)	0·0422 (3)
C(6)	0·3614 (1)	0·3293 (2)	0·3530 (4)	0·0511 (3)
C(7)	0·2999 (2)	0·4498 (2)	0·2971 (4)	0·0598 (4)
C(8)	0·1679 (2)	0·4236 (2)	0·3958 (4)	0·0645 (4)
C(9)	0·0971 (1)	0·2772 (2)	0·5553 (4)	0·0625 (4)
C(10)	0·1584 (1)	0·1555 (2)	0·6157 (4)	0·0511 (3)
H(6)	0·453 (1)	0·348 (2)	0·292 (3)	0·050 (4)
H(7)	0·350 (1)	0·553 (2)	0·195 (4)	0·073 (4)
H(8)	0·124 (1)	0·507 (2)	0·363 (3)	0·066 (4)
H(9)	0·003 (2)	0·258 (2)	0·635 (4)	0·084 (5)
H(10)	0·111 (1)	0·054 (2)	0·722 (3)	0·062 (4)

Table 2. *Bond lengths* (Å) *and bond angles* (°)

N(1)–N(1′)	1·396 (2)	C(5)–C(10)	1·387 (2)
N(1)–C(2)	1·289 (2)	C(6)–C(7)	1·370 (2)
C(2)–C(3)	1·458 (2)	C(7)–C(8)	1·375 (3)
C(2)–C(5)	1·465 (2)	C(8)–C(9)	1·373 (2)
C(3)–N(4)	1·136 (2)	C(9)–C(10)	1·382 (2)
C(5)–C(6)	1·392 (2)		
N(1′)–N(1)–C(2)	112·5 (1)	C(6)–C(5)–C(10)	119·0 (1)
N(1)–C(2)–C(3)	121·0 (1)	C(5)–C(6)–C(7)	120·2 (1)
N(1)–C(2)–C(5)	121·2 (1)	C(6)–C(7)–C(8)	120·4 (2)
C(3)–C(2)–C(5)	117·9 (1)	C(7)–C(8)–C(9)	120·2 (2)
C(2)–C(3)–N(4)	176·7 (2)	C(8)–C(9)–C(10)	120·0 (1)
C(2)–C(5)–C(6)	120·2 (1)	C(5)–C(10)–C(9)	120·3 (1)
C(2)–C(5)–C(10)	120·8 (1)		

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