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# Structure of a Tetrazole

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**Abstract.** 2-Phenyl-1,2,3,4-tetrazole-5-carbonitrile, $C_8H_5N_5$, $M_r = 171{\cdot}1$, monoclinic, $P2_1/a$, $a = 10{\cdot}028$ (1), $b = 11{\cdot}747$ (1), $c = 7{\cdot}205$ (1) Å, $\beta = 102{\cdot}94$ (1)°, $V = 827{\cdot}1$ (1) Å$^3$, $Z = 4$, $D_x = 1{\cdot}374$ Mg m$^{-3}$, $\lambda$(Cu $K\alpha_1$) = 1·54050 Å, $\mu = 0{\cdot}78$ mm$^{-1}$, $F(000) = 352$, $T = 293$ K, final $R = 0{\cdot}059$ for 730 reflexions. The dihedral angle between the phenyl and tetrazole rings is 1·9 (5)°. Bond lengths and planarity indicate extensive electron delocalization in the tetrazole ring.

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters*

$B_{eq} = (1/3)\sum_i\sum_j B_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

| | $x$ | $y$ | $z$ | $B_{eq}$(Å$^2$) |
|---|---|---|---|---|
| N(1) | 0·4563 (3) | 0·2743 (3) | 0·2259 (4) | 5·92 (28) |
| N(2) | 0·5360 (3) | 0·3632 (2) | 0·2789 (4) | 5·41 (28) |
| N(3) | 0·6629 (3) | 0·3358 (3) | 0·3690 (5) | 7·09 (29) |
| N(4) | 0·6661 (3) | 0·2233 (4) | 0·3773 (5) | 7·56 (30) |
| C(5) | 0·5401 (4) | 0·1896 (4) | 0·2887 (7) | 6·15 (29) |
| C(6) | 0·5024 (4) | 0·0722 (5) | 0·2658 (7) | 7·78 (32) |
| N(7) | 0·4723 (5) | −0·0209 (4) | 0·2457 (7) | 11·31 (33) |
| C(8) | 0·4906 (3) | 0·4783 (3) | 0·2462 (5) | 5·06 (28) |
| C(9) | 0·3566 (4) | 0·4974 (4) | 0·1572 (6) | 6·06 (30) |
| C(10) | 0·3135 (5) | 0·6089 (4) | 0·1259 (6) | 6·93 (32) |
| C(11) | 0·4015 (5) | 0·6975 (4) | 0·1793 (7) | 7·17 (31) |
| C(12) | 0·5354 (5) | 0·6764 (4) | 0·2696 (8) | 7·10 (31) |
| C(13) | 0·5805 (4) | 0·5655 (4) | 0·3024 (6) | 6·15 (30) |

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

| | | | |
|---|---|---|---|
| N(1)—C(5) | 1·316 (6) | | |
| N(1)—N(2) | 1·318 (5) | C(8)—C(9) | 1·372 (6) |
| N(2)—N(3) | 1·332 (5) | C(9)—C(10) | 1·382 (7) |
| N(3)—N(4) | 1·323 (6) | C(10)—C(11) | 1·364 (7) |
| N(4)—C(5) | 1·342 (6) | C(11)—C(12) | 1·376 (7) |
| C(5)—C(6) | 1·429 (8) | C(12)—C(13) | 1·383 (7) |
| C(6)—N(7) | 1·135 (8) | C(13)—C(8) | 1·364 (6) |
| N(2)—C(8) | 1·429 (5) | | |

| | | | |
|---|---|---|---|
| N(1)—N(2)—N(3) | 113·6 (3) | N(3)—N(2)—C(8) | 122·9 (3) |
| N(2)—N(3)—N(4) | 105·9 (3) | N(2)—C(8)—C(13) | 119·7 (3) |
| N(3)—N(4)—C(5) | 105·2 (3) | N(2)—C(8)—C(9) | 118·3 (3) |
| N(4)—C(5)—N(1) | 113·6 (4) | C(8)—C(9)—C(10) | 118·0 (4) |
| C(5)—N(1)—N(2) | 101·5 (3) | C(9)—C(10)—C(11) | 121·1 (4) |
| C(5)—C(6)—N(7) | 179·2 (7) | C(10)—C(11)—C(12) | 119·8 (4) |
| N(4)—C(5)—C(6) | 122·4 (4) | C(11)—C(12)—C(13) | 119·8 (4) |
| N(1)—C(5)—C(6) | 123·9 (4) | C(12)—C(13)—C(8) | 119·2 (4) |
| N(1)—N(2)—C(8) | 123·4 (3) | C(13)—C(8)—C(9) | 121·9 (4) |

**Experimental.** A colorless prism, 0·15 × 0·10 × 0·45 mm, by recrystallization from $C_2H_5OC_2H_5$/$C_6H_{14}$. Rigaku AFC5 four-circle diffractometer used with $\theta$–$2\theta$-scan method, $\omega$-scan width (1·3 + 0·41 tan$\theta$)° and scan speed 16° min$^{-1}$. Lattice parameters obtained from least-squares analysis of 20 reflexions with $2\theta$ values ranging from 54 to 60°. Out of 1466 reflexions scanned within index range $h$ −11–11, $k$ 0–13, $l$ 0–8 up to $(\sin\theta)/\lambda = 0{\cdot}56$ Å$^{-1}$ including 112 equivalent reflexions ($R_{int} = 0{\cdot}014$), 1229 unique reflexions classified as observed. Three standard reflexions measured every 120 reflexions, no significant intensity variation. Intensities corrected for Lorentz and polarization factors, but absorption correction not applied. Structure solved using the program package *SAPI*85 (Yao, Zheng, Qian, Han, Gu & Fan, 1985), a version of *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). The refinement was carried out by the

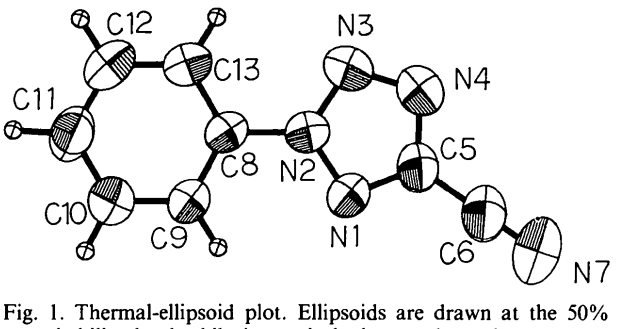


Fig. 1. Thermal-ellipsoid plot. Ellipsoids are drawn at the 50% probability level while isotropic hydrogen thermal parameters are represented by spheres of arbitrary size.

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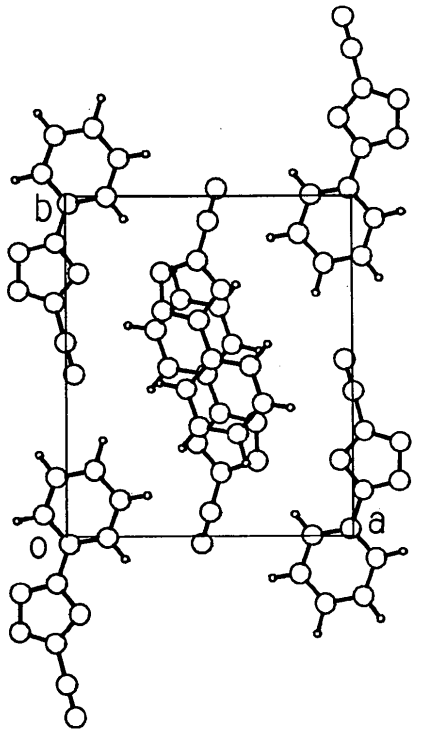


Fig. 2. Projection of the crystal structure along the *c* axis.

full-matrix least-squares method with anisotropic temperature factors for non-H atoms. Function minimized $\sum w(|(|F_o|)^2 - (|F_c|)^2|)^2$ with $w = 1/[\sigma^2(F_o) + 0{\cdot}014(F_o)^2]$, $\sigma(F_o)$ determined from counting statistics. All H atoms located from the difference map and refined, the initial thermal parameters set at equivalent isotropic thermal parameter of each bonded atom. Final discrepancy indices $R = 0{\cdot}059$, $wR = 0{\cdot}050$, $S = 1{\cdot}301$ for 730 reflexions with $F > 3\sigma(F)$. Maximum $\Delta/\sigma = 0{\cdot}17$ in final least-squares cycle. Final difference Fourier map showed no residuals greater than 0·29 e $Å^{-3}$. All calculations performed using Panafacom computer with *RCRYSTAN* (Rigaku Corporation, 1985) X-ray analysis program system. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).

Final atomic parameters are listed in Table 1.* The bond lengths and angles are listed in Table 2. Fig. 1 shows the thermal-ellipsoid plot of the molecule with atomic labelling. Fig. 2 is the crystal structure.

**Related literature.** The title compound is one of the breakdown products from 6-phenyl-[1,2,3]triazolo-[4,5-*e*]-1,2,3,4-tetrazine (Kaihoh, Itoh, Yamaguchi & Ohsawa, 1988). See also Moderhack (1981) for the preparation of related compounds.

* Lists of structure amplitudes, anisotropic thermal parameters and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52565 (8 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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# Structure of a Cyclooctatetraene Derivative

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**Abstract.** 1-Carbamoyl-2-phenyl-9-oxabicyclo[6.1.0]-nona-2,4,6-triene, $C_{15}H_{13}NO_2$, $M_r = 239{\cdot}3$, triclinic, $P\bar{1}$, $a = 8{\cdot}833$ (3), $b = 10{\cdot}754$ (5), $c = 8{\cdot}204$ (1) Å, $\alpha = 93{\cdot}52$ (3), $\beta = 105{\cdot}12$ (3)°, $\gamma = 125{\cdot}20$ (1)°, $V = 592{\cdot}3$ (4) $Å^3$, $Z = 2$, $D_x = 1{\cdot}342$ Mg $m^{-3}$, $\lambda$(Cu $K\alpha_1$) = 1·54050 Å, $\mu = 0{\cdot}733$ $mm^{-1}$, $F(000) = 252$, $T =$

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