= 1·407 and 1·435 Å, CH—CH [C(2)—C(3) and C(6)—C(5)] = 1·367 and 1·375 Å, CH—CNO_2 [C(3)—C(4) and C(5)—C(4)] = 1·392 and 1·400 Å, and C—NO_2 [C(4)—N(3)] = 1·434 and 1·405 Å.

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Structure of 1-(2,4-Dinitrophenyl)pyrazole

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Abstract. 1-(2,4-Dinitrophenyl)pyrazole, $C_9H_6N_4O_4$, $M_r = 234{\cdot}2$, orthorhombic, *Pbca*, $a = 8{\cdot}958\,(2)$, $b = 19{\cdot}103\,(3)$, $c = 11{\cdot}806\,(3)$ Å, $V = 2020{\cdot}2\,(8)$ Å^3, $Z = 8$, $D_x = 1{\cdot}540$ g cm^{-3}, Cu $K\alpha$, $\lambda = 1{\cdot}54184$ Å, $\mu = 10{\cdot}3$ cm^{-1}, $F(000) = 960$, $T = 299$ K, $R = 0{\cdot}037$ for 1798 observations having $I > 3\sigma(I)$ (of 2077 unique data). The phenyl ring is nearly planar with maximum deviation 0·014 (1) Å. The pyrazole ring is planar and forms a 26·24 (7)° dihedral angle with the phenyl ring. The nitro groups are twisted out of the best plane of the phenyl ring by 69·0 (1) and 9·1 (2)°.

Experimental. 1-(2,4-Dinitrophenyl)pyrazole was prepared by the modification of the procedure described by Shriner, Fuson & Curtin (1970). Crystals were obtained by slow evaporation of a $CDCl_3$ solution, as yellow needles, dimensions 0·30 × 0·40 × 0·48 mm. Space group from absences $0kl$ with k odd, $h0l$ with l odd, $hk0$ with h odd. Enraf–Nonius CAD-4 diffractometer with graphite monochromator, cell dimensions from setting angles of 25 reflections having $30 > \theta > 25°$. Data collection by ω-2θ scans designed for $I = 50\sigma(I)$, subject to max. scan time = 120 s; scan rates varied 0·53–3·30° min^{-1}. Two octants of data having $2 < \theta < 75°$, $0 \le h \le 11$, $-23 \le k \le 23$, $0 \le l \le 14$ were measured, corrected for background, Lorentz–polarization, and absorption by ψ scans, minimum relative transmission 94·1%. Two equivalent octants merged to give 2077 unique data, $R_{\rm int} = 0{\cdot}012$. Standard reflections 400, 0,10,0, 008 displayed only random variation, no decay correction. Structure solved using *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), refinement by full-matrix least squares based on F with weights $w = 4F_o^2[\sigma^2(I) + (0{\cdot}02F_o^2)^2]^{-1}$ with 1798 data for which $I > 3\sigma(I)$ (279 unobserved reflections), using Enraf–Nonius *SDP* (Frenz & Okaya, 1980). Non-H atoms anisotropic; H atoms located by ΔF synthesis and refined isotropically. Atomic scattering factors from Cromer & Waber (1974) and anomalous coefficients from Cromer (1974). Final $R = 0{\cdot}037$, $wR = 0{\cdot}051$, $S = 2{\cdot}814$ for 179 variables, extinction coefficient $g = 8{\cdot}1\,(2) \times 10^{-6}$, where the correction factor $(1 + gI_c)^{-1}$ was applied to F_c, max. shift in final cycle $0{\cdot}05\sigma$, max. residual density 0·21, min. −0·18 e Å^{-3}. Atomic coordinates and equivalent isotropic thermal parameters are given in Table 1,* bond distances and angles in Table 2. Fig. 1 shows the atom-numbering scheme.

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* Tables of H-atom parameters, distances and angles involving H atoms, anisotropic thermal parameters and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52085 (19 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Positional parameters and their e.s.d.'s*

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

	x	y	z	$B_{\rm eq}$(Å^2)
O1	0·8152 (1)	0·07319 (6)	0·41330 (7)	4·68 (2)
O2	0·6654 (1)	0·16124 (5)	0·42765 (7)	4·96 (2)
O3	0·9169 (2)	0·23643 (5)	−0·06998 (7)	5·36 (2)
O4	0·9313 (2)	0·28780 (5)	0·09200 (9)	6·17 (3)
N1	0·5927 (1)	0.01204 (5)	0·23429 (8)	3·18 (2)
N2	0·5284 (1)	0·01928 (5)	0·33833 (8)	3·76 (2)
N3	0·7353 (1)	0·11838 (5)	0·37298 (8)	3·38 (2)
N4	0·8913 (1)	0·23961 (5)	0·03173 (9)	4·32 (2)
C1	0·6651 (1)	0·06923 (6)	0·18438 (8)	2·97 (2)
C2	0·7289 (1)	0·12258 (6)	0·24855 (9)	3·05 (2)
C3	0·7993 (1)	0·17940 (6)	0·20101 (9)	3·43 (2)
C4	0·8096 (1)	0·18128 (6)	0·08385 (9)	3·46 (2)
C5	0·7482 (2)	0·12990 (6)	0·01629 (9)	3·68 (2)
C6	0·6745 (1)	0·07461 (6)	0·06637 (9)	3·50 (2)
C7	0·4694 (2)	−0·04278 (7)	0·3589 (1)	4·08 (2)
C8	0·4932 (2)	−0·09004 (7)	0·2701 (1)	4·21 (2)
C9	0·5729 (2)	−0·05361 (6)	0·1915 (1)	3·80 (2)

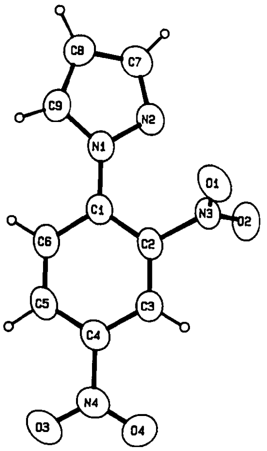

Fig. 1. Numbering scheme with thermal ellipsoids drawn at the 40% probability level. H atoms have arbitrary radius.

Related literature. 1-(2,4-Dinitrophenyl)pyrazole: mass spectral data (Atmani & Aubagnac, 1978). UV–vis. (Elguero, Jacquier & Tien Duc, 1966). NMR (Wilshire, 1966). Crystal structures of 1-(2,4-dinitrophenyl)-4-bromopyrazole (Galigne & Falgueirettes 1969); 1-(2,4-dinitrophenyl)-4-chloropyrazole (Galigne & Falgueirettes, 1970).

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

O1—N3	1·2180 (9)	N4—C4	1·468 (1)
O2—N3	1·2161 (9)	C1—C2	1·393 (1)
O3—N4	1·2246 (9)	C1—C6	1·4001 (9)
O4—N4	1·217 (1)	C2—C3	1·375 (1)
N1—N2	1·3642 (8)	C3—C4	1·3871 (9)
N1—C1	1·4000 (9)	C4—C5	1·379 (1)
N1—C9	1·363 (1)	C5—C6	1·378 (1)
N2—C7	1·320 (1)	C7—C8	1·400 (1)
N3—C2	1·4729 (9)	C8—C9	1·363 (1)
N2—N1—C1	119·71 (6)	N3—C2—C1	121·27 (6)
N2—N1—C9	111·86 (6)	N3—C2—C3	115·63 (6)
C1—N1—C9	128·42 (6)	C1—C2—C3	122·92 (6)
N1—N2—C7	104·13 (6)	C2—C3—C4	117·27 (7)
O1—N3—O2	124·88 (7)	N4—C4—C3	118·09 (7)
O1—N3—C2	116·85 (6)	N4—C4—C5	119·74 (6)
O2—N3—C2	118·22 (6)	C3—C4—C5	122·16 (7)
O3—N4—O4	123·76 (8)	C4—C5—C6	119·18 (7)
O3—N4—C4	117·86 (7)	C1—C6—C5	120·82 (7)
O4—N4—C4	118·37 (7)	N2—C7—C8	112·31 (7)
N1—C1—C2	122·12 (6)	C7—C8—C9	105·16 (7)
N1—C1—C6	120·29 (6)	N1—C9—C8	106·54 (7)
C2—C1—C6	117·59 (7)		
N2—N1—C1—C2	27·2 (2)	O2—N3—C2—C3	69·13 (14)
O1—N3—C2—C1	66·9 (2)	O3—N4—C4—C3	170·66 (13)
O1—N3—C2—C3	−108·43 (13)	O4—N4—C4—C3	−8·4 (2)
O2—N3—C2—C1	−115·53 (13)	N1—C1—C2—N3	5·6 (2)

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