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5-(4,5-Dimethoxy-2-nitrophenyl)-1,3-diphenyl-2-pyrazoline

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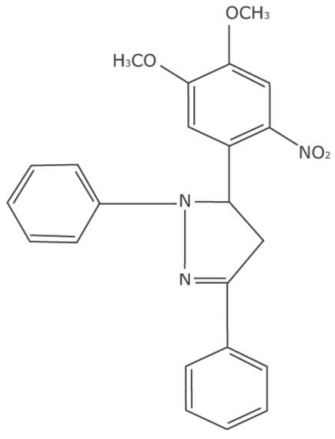
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; disorder in main residue; R factor = 0.040; wR factor = 0.113; data-to-parameter ratio = 12.7.

In the title compound, $C_{23}H_{21}N_3O_4$, the central pyrazoline ring shows a slight envelope distortion from planarity. The aromatic ring substituents at the 1 and 5 positions of the central ring exhibit a *gauche* conformation. In the crystal structure, the molecules are linked by weak C—H···O and C—H···N interactions. The O atoms of the nitro group are disordered over two sites in approximately the ratio 2:1.

Related literature

For related literature, see: Gilchrist (1998); Nakamichi *et al.* (2002); Rurack *et al.* (2000); Taylor *et al.* (1992); Ge (2006).



Experimental

Crystal data

$C_{23}H_{21}N_3O_4$
M_r = 403.43
Monoclinic, $C2/c$
a = 36.0919 (7) Å
b = 13.4372 (1) Å
c = 8.8190 (2) Å
β = 104.099 (1)°
V = 4148.15 (13) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 (2) K
0.35 × 0.30 × 0.20 mm

Data collection

Bruker CCD diffractometer
Absorption correction: none
9555 measured reflections
3721 independent reflections
2605 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.114
S = 0.99
3721 reflections
292 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.10 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15···O1B^{i}	0.93	2.55	3.467 (6)	170
C20—H20···N2^{ii}	0.93	2.54	3.364 (2)	149

Symmetry codes: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, -y+1, z+\frac{1}{2}$.

Data collection: *APEX* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2376).

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  doi:10.1107/S1600536807030504

supplementary materials

Acta Cryst. (2007). E**63**, o3402 [**doi:10.1107/S1600536807030504**]

5-(4,5-Dimethoxy-2-nitrophenyl)-1,3-diphenyl-2-pyrazoline

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Comment

Five- and six-membered heterocyclic compounds are important constituents that often exist in biologically active natural products and synthetic compounds of medicinal interest (Gilchrist, 1998). In this series, 1,3,5–trisubstituted pyrazolines, prepared from phenylhydrazine and chalcone derivatives (Nakamichi *et al.*, 2002) have been used as antitumour (Taylor *et al.*, 1992) agents. Here we report the structure of the title compound, (I), a new derivative of pyrazoline.

In the pyrazoline ring (Fig. 1), the C12═N2 [1.287 (3) Å] and N1—N2 [1.382 (3) Å] bond lengths are shorter than those found in similar structures reported by Rurack *et al.* (2000) and Ge (2006). [C═N = 1.291 (2) Å, 1.293 (3)Å and N—N = 1.394 (3) Å, 1.384 (2)Å respectively]. The C3—C11—N1—C18 torsion angle in (I) of 85.48 (16)° indicates a *gauche* conformation for the substituents. The pyrazoline ring shows a slightly distorted envelope conformation with C9 deviating by 0.036 (3)Å from the plane of C10, C11, N1 and N2. The dihedral angle between the pyrazoline ring and the 3–phenyl ring is 4.6 (1)°, marking their near co-planarity with a maximum deviation of 0.068 (3)Å for atom C(17). The 5–phenyl ring is almost perpendicular to the pyrazoline ring as the dihedral angle between them is 75.4 (1)°.

The molecular packing is stabilized by weak C—H···O and C—H···N interactions (Table 1, Fig. 2).

Experimental

A mixture of 1-aryl-3-(3,4-dimethoxy −6-nitrophenyl) −2-propene-1-ones (0.01 mol) and phenylhydrazine (0.01 mol) in glacial acetic acid (5 ml) was taken in a conical flask and irradiated in a microwave oven for 5 minutes. The resultant solution was poured into a beaker containing crushed ice and the solid separated was collected by filtration, washed with water, dried and recrystallized from formacetic acid. Red blocks of (I) were grown from ethanol by slow evaporation at room temperature.

Refinement

The O atoms of the nitro group are disordered over two sites in a 0.68 (2):0.32 (2) ratio (sum constrained to unity). All the H atoms were fixed geometrically (C—H = 0.93=0.97 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier).

Figures

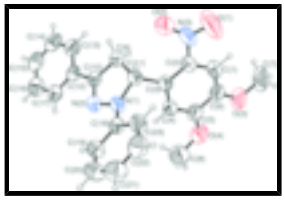

Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids (arbitrary spheres for the H atoms).

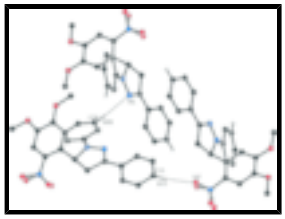

Fig. 2. Hydrogen bonding interactions in (I) shown as dashed lines.

5-(4,5-Dimethoxy-2-nitrophenyl)-1,3-diphenyl-2-pyrazoline

Crystal data

$C_{23}H_{21}N_3O_4$	F_{000} = 1696
M_r = 403.43	D_x = 1.292 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 55 reflections
a = 36.0919 (7) Å	θ = 5–11º
b = 13.4372 (1) Å	μ = 0.09 mm^{-1}
c = 8.8190 (2) Å	*T* = 296 (2) K
β = 104.099 (1)º	Block, red
V = 4148.15 (13) Å^3	0.35 × 0.30 × 0.20 mm
Z = 8	

Data collection

Bruker SMART CCD diffractometer	R_{int} = 0.033
ω scans	θ_{max} = 25.3º
Absorption correction: none	θ_{min} = 1.2º
9555 measured reflections	*h* = −42→31
3721 independent reflections	*k* = −16→16
2605 reflections with $I > 2\sigma(I)$	*l* = −7→10

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0637P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.040	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.114	$\Delta\rho_{max}$ = 0.10 e Å^{-3}
S = 0.99	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
3721 reflections	Extinction correction: none
292 parameters	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.04766 (4)	0.15292 (14)	0.6636 (2)	0.0745 (5)	
H1	0.0341	0.0973	0.618	0.089*	
C2	0.08305 (4)	0.14080 (11)	0.77009 (19)	0.0653 (4)	
C3	0.10437 (4)	0.22122 (10)	0.84411 (16)	0.0522 (4)	
C4	0.08773 (4)	0.31481 (11)	0.80876 (17)	0.0559 (4)	
H4	0.1005	0.3702	0.8592	0.067*	
C5	0.05307 (4)	0.32859 (12)	0.70193 (18)	0.0627 (4)	
C6	0.03303 (4)	0.24523 (13)	0.62634 (19)	0.0674 (4)	
C7	−0.02062 (5)	0.1837 (2)	0.4375 (3)	0.1142 (8)	
H7A	−0.0045	0.1479	0.3845	0.171*	
H7B	−0.0428	0.2074	0.3624	0.171*	
H7C	−0.0284	0.1403	0.5105	0.171*	
C8	0.05319 (6)	0.50507 (15)	0.7358 (3)	0.1170 (8)	
H8A	0.0543	0.5001	0.8453	0.175*	
H8B	0.0382	0.562	0.6928	0.175*	
H8C	0.0786	0.5122	0.7216	0.175*	
C9	0.17542 (4)	0.21164 (10)	0.85409 (18)	0.0570 (4)	
H9A	0.192	0.1543	0.8812	0.068*	
H9B	0.1639	0.211	0.7426	0.068*	
C10	0.19683 (4)	0.30695 (10)	0.90319 (16)	0.0500 (3)	
C11	0.14472 (4)	0.21363 (10)	0.94876 (17)	0.0528 (4)	
H11	0.147	0.1544	1.0152	0.063*	
C12	0.22849 (4)	0.34477 (11)	0.84239 (16)	0.0528 (4)	
C13	0.24274 (4)	0.28957 (13)	0.73612 (19)	0.0665 (4)	
H13	0.2315	0.2289	0.7005	0.08*	
C14	0.27354 (5)	0.32351 (14)	0.6821 (2)	0.0749 (5)	
H14	0.2829	0.2853	0.6117	0.09*	
C15	0.29022 (5)	0.41318 (14)	0.7324 (2)	0.0753 (5)	
H15	0.3108	0.436	0.6962	0.09*	
C16	0.27623 (5)	0.46919 (13)	0.8368 (2)	0.0729 (5)	
H16	0.2874	0.5303	0.8702	0.087*	
C17	0.24589 (4)	0.43598 (12)	0.89252 (18)	0.0618 (4)	
H17	0.237	0.4744	0.9638	0.074*	
C18	0.14669 (4)	0.31886 (10)	1.18989 (16)	0.0489 (3)	
C19	0.16297 (4)	0.39793 (11)	1.28447 (17)	0.0588 (4)	
H19	0.1795	0.4413	1.2512	0.071*	
C20	0.15472 (5)	0.41225 (13)	1.42746 (18)	0.0712 (5)	
H20	0.1659	0.4651	1.4903	0.085*	

C21	0.13019 (5)	0.34949 (13)	1.4787 (2)	0.0769 (5)	
H21	0.1245	0.3601	1.5748	0.092*	
C22	0.11419 (5)	0.27102 (14)	1.3861 (2)	0.0749 (5)	
H22	0.0978	0.2279	1.4206	0.09*	
C23	0.12210 (4)	0.25515 (12)	1.24222 (19)	0.0640 (4)	
H23	0.111	0.2018	1.1805	0.077*	
N1	0.15523 (3)	0.30319 (9)	1.04577 (13)	0.0530 (3)	
N2	0.18567 (3)	0.35337 (8)	1.01177 (13)	0.0512 (3)	
N3	0.09614 (6)	0.03865 (13)	0.8015 (3)	0.1039 (6)	
O1A	0.1226 (6)	0.0251 (11)	0.856 (2)	0.217 (11)	0.32 (2)
O2A	0.0810 (7)	−0.0219 (9)	0.692 (3)	0.150 (9)	0.32 (2)
O1B	0.13056 (17)	0.0181 (4)	0.8620 (6)	0.0994 (18)	0.68 (2)
O2B	0.07079 (11)	−0.0280 (3)	0.7954 (18)	0.133 (3)	0.68 (2)
O3	−0.00013 (3)	0.26599 (10)	0.51909 (15)	0.0943 (4)	
O4	0.03612 (3)	0.41708 (9)	0.65777 (15)	0.0895 (4)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0562 (9)	0.0791 (12)	0.0831 (12)	−0.0132 (9)	0.0070 (8)	−0.0252 (9)
C2	0.0544 (9)	0.0571 (10)	0.0805 (11)	−0.0057 (7)	0.0090 (8)	−0.0163 (8)
C3	0.0465 (7)	0.0560 (9)	0.0544 (8)	−0.0053 (7)	0.0128 (6)	−0.0076 (6)
C4	0.0499 (8)	0.0585 (9)	0.0583 (9)	−0.0052 (7)	0.0116 (7)	−0.0080 (7)
C5	0.0521 (9)	0.0721 (10)	0.0634 (9)	0.0034 (8)	0.0128 (7)	−0.0007 (8)
C6	0.0439 (8)	0.0927 (13)	0.0627 (9)	−0.0030 (8)	0.0078 (7)	−0.0117 (9)
C7	0.0633 (11)	0.171 (2)	0.0927 (15)	−0.0215 (13)	−0.0106 (10)	−0.0300 (15)
C8	0.1029 (16)	0.0712 (13)	0.158 (2)	0.0177 (12)	−0.0050 (15)	−0.0059 (14)
C9	0.0481 (8)	0.0579 (9)	0.0623 (9)	0.0015 (6)	0.0082 (7)	−0.0064 (7)
C10	0.0467 (7)	0.0532 (8)	0.0468 (8)	0.0045 (6)	0.0048 (6)	0.0021 (6)
C11	0.0497 (7)	0.0487 (8)	0.0570 (8)	−0.0034 (6)	0.0069 (6)	−0.0037 (6)
C12	0.0458 (7)	0.0607 (9)	0.0486 (8)	0.0045 (6)	0.0051 (6)	0.0070 (7)
C13	0.0605 (9)	0.0757 (11)	0.0636 (10)	0.0038 (8)	0.0158 (8)	−0.0013 (8)
C14	0.0638 (10)	0.0997 (13)	0.0652 (10)	0.0148 (10)	0.0236 (8)	0.0080 (9)
C15	0.0552 (9)	0.0993 (14)	0.0731 (11)	0.0025 (9)	0.0192 (8)	0.0248 (10)
C16	0.0645 (10)	0.0762 (11)	0.0779 (11)	−0.0064 (8)	0.0171 (9)	0.0142 (9)
C17	0.0572 (9)	0.0654 (10)	0.0624 (9)	−0.0007 (7)	0.0138 (7)	0.0054 (7)
C18	0.0444 (7)	0.0515 (8)	0.0492 (8)	0.0016 (6)	0.0084 (6)	0.0038 (6)
C19	0.0679 (9)	0.0545 (9)	0.0550 (8)	−0.0081 (7)	0.0165 (7)	−0.0002 (7)
C20	0.0940 (12)	0.0650 (10)	0.0565 (9)	−0.0043 (9)	0.0218 (9)	−0.0042 (8)
C21	0.0960 (13)	0.0823 (12)	0.0604 (10)	0.0022 (10)	0.0344 (9)	0.0049 (9)
C22	0.0743 (11)	0.0834 (12)	0.0750 (11)	−0.0091 (9)	0.0334 (9)	0.0107 (9)
C23	0.0586 (9)	0.0666 (10)	0.0681 (10)	−0.0126 (7)	0.0181 (8)	−0.0028 (8)
N1	0.0488 (6)	0.0571 (7)	0.0529 (7)	−0.0123 (5)	0.0121 (5)	−0.0067 (5)
N2	0.0488 (6)	0.0538 (7)	0.0490 (6)	−0.0051 (5)	0.0081 (5)	0.0020 (5)
N3	0.0774 (12)	0.0602 (11)	0.1527 (17)	−0.0077 (10)	−0.0133 (11)	−0.0300 (11)
O1A	0.116 (9)	0.062 (5)	0.39 (2)	0.029 (6)	−0.092 (11)	−0.055 (7)
O2A	0.157 (9)	0.057 (4)	0.189 (14)	−0.003 (4)	−0.046 (10)	−0.039 (6)
O1B	0.059 (2)	0.067 (2)	0.159 (4)	0.0116 (14)	−0.001 (2)	−0.0281 (18)

O2B	0.100 (2)	0.0738 (17)	0.202 (7)	−0.0342 (14)	−0.010 (3)	−0.005 (2)
O3	0.0558 (7)	0.1252 (11)	0.0873 (9)	−0.0017 (7)	−0.0105 (6)	−0.0107 (8)
O4	0.0699 (7)	0.0812 (9)	0.1052 (10)	0.0147 (7)	−0.0018 (7)	0.0063 (7)

Geometric parameters (Å, °)

C1—C6	1.357 (2)	C12—C17	1.399 (2)
C1—C2	1.399 (2)	C13—C14	1.389 (2)
C1—H1	0.93	C13—H13	0.93
C2—C3	1.3933 (19)	C14—C15	1.371 (2)
C2—N3	1.456 (2)	C14—H14	0.93
C3—C4	1.396 (2)	C15—C16	1.377 (2)
C3—C11	1.5258 (19)	C15—H15	0.93
C4—C5	1.383 (2)	C16—C17	1.379 (2)
C4—H4	0.93	C16—H16	0.93
C5—O4	1.3505 (19)	C17—H17	0.93
C5—C6	1.410 (2)	C18—C19	1.3897 (19)
C6—O3	1.361 (2)	C18—C23	1.3902 (19)
C7—O3	1.424 (2)	C18—N1	1.3949 (17)
C7—H7A	0.96	C19—C20	1.378 (2)
C7—H7B	0.96	C19—H19	0.93
C7—H7C	0.96	C20—C21	1.376 (2)
C8—O4	1.430 (2)	C20—H20	0.93
C8—H8A	0.96	C21—C22	1.372 (2)
C8—H8B	0.96	C21—H21	0.93
C8—H8C	0.96	C22—C23	1.384 (2)
C9—C10	1.5040 (19)	C22—H22	0.93
C9—C11	1.541 (2)	C23—H23	0.93
C9—H9A	0.97	N1—N2	1.3829 (15)
C9—H9B	0.97	N3—O1A	0.98 (2)
C10—N2	1.2867 (17)	N3—O1B	1.257 (7)
C10—C12	1.467 (2)	N3—O2B	1.272 (4)
C11—N1	1.4717 (17)	N3—O2A	1.282 (10)
C11—H11	0.98	O2A—O2B	1.07 (3)
C12—C13	1.388 (2)		
C6—C1—C2	120.45 (15)	C14—C13—H13	119.5
C6—C1—H1	119.8	C15—C14—C13	120.18 (16)
C2—C1—H1	119.8	C15—C14—H14	119.9
C3—C2—C1	122.30 (15)	C13—C14—H14	119.9
C3—C2—N3	121.69 (14)	C14—C15—C16	119.55 (16)
C1—C2—N3	116.00 (14)	C14—C15—H15	120.2
C2—C3—C4	115.82 (13)	C16—C15—H15	120.2
C2—C3—C11	124.64 (13)	C15—C16—C17	120.90 (17)
C4—C3—C11	119.39 (12)	C15—C16—H16	119.5
C5—C4—C3	122.78 (13)	C17—C16—H16	119.5
C5—C4—H4	118.6	C16—C17—C12	120.35 (15)
C3—C4—H4	118.6	C16—C17—H17	119.8
O4—C5—C4	125.83 (14)	C12—C17—H17	119.8
O4—C5—C6	114.77 (14)	C19—C18—C23	118.84 (13)

C4—C5—C6	119.38 (15)	C19—C18—N1	120.48 (12)
C1—C6—O3	125.44 (15)	C23—C18—N1	120.68 (13)
C1—C6—C5	119.17 (14)	C20—C19—C18	120.12 (14)
O3—C6—C5	115.39 (15)	C20—C19—H19	119.9
O3—C7—H7A	109.5	C18—C19—H19	119.9
O3—C7—H7B	109.5	C21—C20—C19	120.98 (16)
H7A—C7—H7B	109.5	C21—C20—H20	119.5
O3—C7—H7C	109.5	C19—C20—H20	119.5
H7A—C7—H7C	109.5	C22—C21—C20	119.12 (15)
H7B—C7—H7C	109.5	C22—C21—H21	120.4
O4—C8—H8A	109.5	C20—C21—H21	120.4
O4—C8—H8B	109.5	C21—C22—C23	120.89 (15)
H8A—C8—H8B	109.5	C21—C22—H22	119.6
O4—C8—H8C	109.5	C23—C22—H22	119.6
H8A—C8—H8C	109.5	C22—C23—C18	120.04 (15)
H8B—C8—H8C	109.5	C22—C23—H23	120
C10—C9—C11	102.46 (11)	C18—C23—H23	120
C10—C9—H9A	111.3	N2—N1—C18	119.19 (11)
C11—C9—H9A	111.3	N2—N1—C11	112.24 (10)
C10—C9—H9B	111.3	C18—N1—C11	124.77 (11)
C11—C9—H9B	111.3	C10—N2—N1	109.52 (11)
H9A—C9—H9B	109.2	O1A—N3—O1B	4.4 (13)
N2—C10—C12	121.14 (13)	O1A—N3—O2B	119.9 (10)
N2—C10—C9	113.28 (12)	O1B—N3—O2B	119.3 (4)
C12—C10—C9	125.54 (13)	O1A—N3—O2A	116.1 (10)
N1—C11—C3	111.70 (11)	O1B—N3—O2A	112.2 (8)
N1—C11—C9	102.22 (10)	O2B—N3—O2A	49.5 (12)
C3—C11—C9	112.31 (12)	O1A—N3—C2	120.1 (9)
N1—C11—H11	110.1	O1B—N3—C2	121.9 (3)
C3—C11—H11	110.1	O2B—N3—C2	117.3 (2)
C9—C11—H11	110.1	O2A—N3—C2	113.3 (6)
C13—C12—C17	118.03 (14)	O2B—O2A—N3	64.7 (11)
C13—C12—C10	120.76 (14)	O2A—O2B—N3	65.7 (5)
C17—C12—C10	121.19 (13)	C6—O3—C7	116.90 (16)
C12—C13—C14	120.99 (16)	C5—O4—C8	118.52 (14)
C12—C13—H13	119.5		
C6—C1—C2—C3	1.2 (3)	N1—C18—C19—C20	−179.27 (13)
C6—C1—C2—N3	−179.87 (17)	C18—C19—C20—C21	−0.4 (2)
C1—C2—C3—C4	1.7 (2)	C19—C20—C21—C22	0.8 (3)
N3—C2—C3—C4	−177.18 (15)	C20—C21—C22—C23	−0.7 (3)
C1—C2—C3—C11	−173.75 (14)	C21—C22—C23—C18	0.3 (3)
N3—C2—C3—C11	7.3 (3)	C19—C18—C23—C22	0.0 (2)
C2—C3—C4—C5	−2.8 (2)	N1—C18—C23—C22	179.35 (14)
C11—C3—C4—C5	172.92 (13)	C19—C18—N1—N2	13.30 (19)
C3—C4—C5—O4	−177.22 (14)	C23—C18—N1—N2	−165.99 (12)
C3—C4—C5—C6	1.0 (2)	C19—C18—N1—C11	169.58 (13)
C2—C1—C6—O3	176.69 (16)	C23—C18—N1—C11	−9.7 (2)
C2—C1—C6—C5	−3.0 (3)	C3—C11—N1—N2	−116.82 (12)
O4—C5—C6—C1	−179.59 (15)	C9—C11—N1—N2	3.46 (14)

C4—C5—C6—C1	2.0 (2)	C3—C11—N1—C18	85.48 (16)
O4—C5—C6—O3	0.7 (2)	C9—C11—N1—C18	−154.24 (12)
C4—C5—C6—O3	−177.77 (14)	C12—C10—N2—N1	179.09 (11)
C11—C9—C10—N2	5.23 (15)	C9—C10—N2—N1	−3.25 (16)
C11—C9—C10—C12	−177.23 (12)	C18—N1—N2—C10	158.75 (11)
C2—C3—C11—N1	−163.01 (14)	C11—N1—N2—C10	−0.33 (15)
C4—C3—C11—N1	21.66 (18)	C3—C2—N3—O1A	−14.5 (15)
C2—C3—C11—C9	82.81 (18)	C1—C2—N3—O1A	166.5 (15)
C4—C3—C11—C9	−92.52 (15)	C3—C2—N3—O1B	−19.2 (4)
C10—C9—C11—N1	−4.77 (13)	C1—C2—N3—O1B	161.9 (3)
C10—C9—C11—C3	115.09 (12)	C3—C2—N3—O2B	147.0 (8)
N2—C10—C12—C13	173.82 (13)	C1—C2—N3—O2B	−31.9 (9)
C9—C10—C12—C13	−3.5 (2)	C3—C2—N3—O2A	−158 (2)
N2—C10—C12—C17	−4.5 (2)	C1—C2—N3—O2A	23 (2)
C9—C10—C12—C17	178.15 (13)	O1A—N3—O2A—O2B	108.2 (15)
C17—C12—C13—C14	0.5 (2)	O1B—N3—O2A—O2B	110.4 (10)
C10—C12—C13—C14	−177.84 (13)	C2—N3—O2A—O2B	−106.8 (8)
C12—C13—C14—C15	−0.6 (2)	O1A—N3—O2B—O2A	−100.1 (14)
C13—C14—C15—C16	0.1 (2)	O1B—N3—O2B—O2A	−95.1 (9)
C14—C15—C16—C17	0.5 (2)	C2—N3—O2B—O2A	98.3 (7)
C15—C16—C17—C12	−0.6 (2)	C1—C6—O3—C7	−1.3 (3)
C13—C12—C17—C16	0.1 (2)	C5—C6—O3—C7	178.40 (16)
C10—C12—C17—C16	178.44 (13)	C4—C5—O4—C8	−5.7 (3)
C23—C18—C19—C20	0.0 (2)	C6—C5—O4—C8	175.99 (17)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···O1B^{i}	0.93	2.55	3.467 (6)	170
C20—H20···N2^{ii}	0.93	2.54	3.364 (2)	149

Symmetry codes: (i) −*x*+1/2, *y*+1/2, −*z*+3/2; (ii) *x*, −*y*+1, *z*+1/2.

Fig. 1

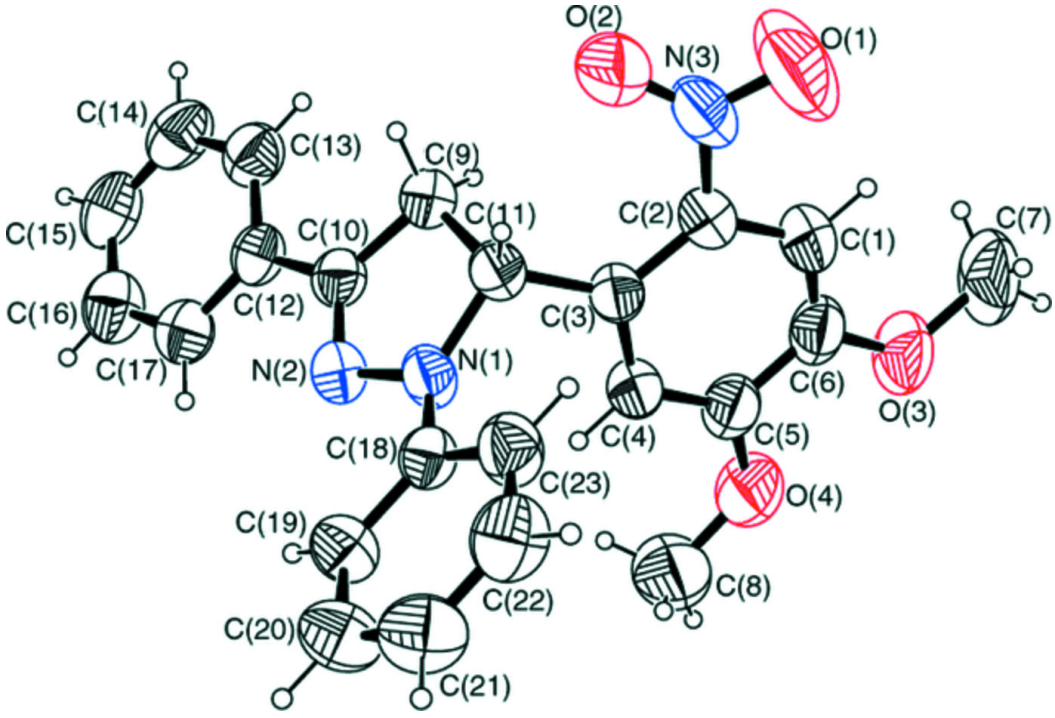
O(2)
N(3)
O(1)
C(14)
C(13)
C(9)
C(15)
C(10)
C(11)
C(2)
C(1)
C(7)
C(16)
C(12)
C(3)
C(17)
N(2)
N(1)
C(6)
O(3)
C(4)
C(5)
C(18)
C(23)
O(4)
C(19)
C(22)
C(8)
C(20)
C(21)

Fig. 2