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4-[(3,5-Diphenyl-1*H*-pyrazol-4-yl)-methyl]benzonitrile ethanol hemisolvate

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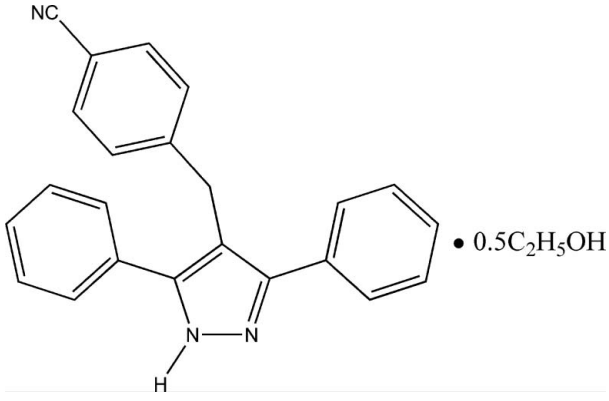
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; R factor = 0.079; wR factor = 0.213; data-to-parameter ratio = 17.6.

In the title compound, $C_{23}H_{17}N_3{\cdot}0.5C_2H_6O$, two pyrazole molecules are bridged by one ethanol molecule through N—H···O and O—H···N hydrogen bonds. The ethanol solvent molecule is located on a mirror plane. These trimolecular units are linked by C—H···N, N—H···O and hydrogen bonds involving the nitrile groups and ethanol OH as acceptors and C—H···π stacking interactions between phenyl groups.

Related literature

For related literature, see: Haghiri *et al.* (2003); Huang *et al.* (2007).



Experimental

Crystal data

$C_{23}H_{17}N_3{\cdot}0.5C_2H_6O$
M_r = 358.43
Monoclinic, $P2_1/m$
a = 6.1301 (12) Å
b = 34.541 (7) Å
c = 9.4459 (19) Å
β = 104.52 (3)°
V = 1936.2 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 291 (2) K
0.25 × 0.18 × 0.15 mm

Data collection

Rigaku RAXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.98, T_{max} = 0.99
5538 measured reflections
4500 independent reflections
3819 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.214
S = 1.08
4500 reflections
256 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2	0.77	2.53	2.786 (2)	102
O1—H1···N2^{i}	0.77	2.53	2.786 (2)	102
N2—H2···O1	0.91	1.91	2.786 (2)	160
C15—H15···N3^{ii}	0.93	2.70	3.470 (3)	141
C6—H6···$Cg1^{iii}$	0.93	2.72	3.601 (2)	159

Symmetry codes: (i) $x, -y+\frac{1}{2}, z$; (ii) $-x+1, -y, -z+1$; (iii) $x-1, y, z-1$. $Cg1$ is the centroid of the C10–C15 ring.

Data collection: *RAPID-AUTO* (Rigaku, 1999); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2234).

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supplementary materials

Acta Cryst. (2007). E**63**, o2863 [**doi:10.1107/S1600536807021812**]

4-[(3,5-Diphenyl-1*H*-pyrazol-4-yl)methyl]benzonitrile ethanol hemisolvate

M. Yu

Comment

Substituted pyrazole tends to form cyclic poly-membered clusters through intermolecular N—H···N hydrogen bonds (Haghiri *et al.*, 2003). Huang *et al.* report a 4-benzyl substituted 3,5-diphenyl-1*H*-pyrazole, in which two pyrazole molecules are connected by N—H···N hydrogen bonds (Huang *et al.*, 2007). In the present paper, we report another substituted pyrazole, 4-((3,5-diphenyl-1*H*-pyrazol-4-yl)methyl)benzonitrile (Fig. 1). In the unit cell, two pyrazole molecules are bridged by one ethanol molecule through N—H···O and O–H···N hydrogen bonds forming a dimer. These dimers are linked by C—H···N hydrogen bonds between the phenyl group and benzonitrile, C—H···π hydrogen bonds between the phenyl groups and π···π interactions between benzonitrile planes as showed in Fig.2. The centroid-centroid contact between two benzonitrile molecules is 4.320 (1) Å.

Experimental

Hydrazine hydrate (85%) (7.06 g, 12.0 mmol) was added to a solution of 4-(2-benzoyl-3-oxo-3-phenylpropyl)benzonitrile (3.40 g, 10.0 mmol) in 20 ml e thanol. The mixture was refluxed for two hours, then cooled to room temperature to give colourless microcrystals. The crystals were filtered, washed with a minimum amount of cold ethanol and dried under vacuum (yield, of 3.2 g). Crystals were obtained by slow evaporation of a ethanol solution of the title compound. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.25 (3⟨i⟩H, t, J=7.0 Hz, CH_3), 3.73 (3*H*, q, J=7.0 Hz, CH_2), 4.16 (2⟨i⟩H, s, CH_2), 7.22 (4*H*, d, J=8.0 Hz, benzonitrile-H), 7.36 (12*H*, m, Ph—H), 7.41 (8*H*, m,Ph—H), 7.54 (4*H*, d, J=8.0 Hz, benzonitrile-H), 10.5 (2*H*,br, N—H) p.p.m.

Refinement

The imino H atom was located in a difference Fourier map and refined as riding on N2, with N–H = 0.91 Å and U_{iso}(H) = 1.2U_{eq}(N2). The hydroxy H atom was located in a difference Fourier map and refined as riding on O1, with O–H = 0.77 Å and U_{iso}(H) = 1.2U_{eq}(O1). The aromatic H atoms were constrained to an ideal geometry, with C—H distances of 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C). The methyl H atoms were rotated to fit the electron density, with C—H distances of 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C). The methylene H atoms were constrained to ideal geometry, with C—H distances of 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C).The largest peak and deepest hole on the final difference Fourier map corresponded to 0.33 and -0.45 e.Å^{-3}, and were located 0.56 and 1.55 Å from the C24 and H1 atom, respectively.

Figures

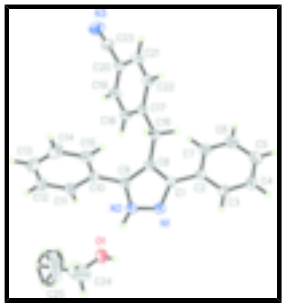

Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom numbering scheme.

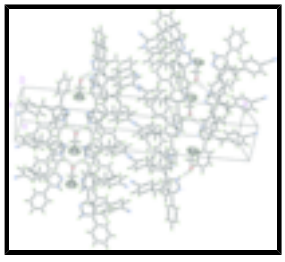

Fig. 2. Crystal packing for title compound.

4-[(3,5-Diphenyl-1*H*-pyrazol-4-yl)methyl]benzonitrile ethanol hemisolvate

Crystal data

$C_{23}H_{17}N_3 \cdot 0.5C_2H_6O$	F_{000} = 756
M_r = 358.43	D_x = 1.230 Mg m^{-3}
Monoclinic, $P2_1/m$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yb	Cell parameters from 582 reflections
a = 6.1301 (12) Å	θ = 1.2–27.5º
b = 34.541 (7) Å	μ = 0.08 mm^{-1}
c = 9.4459 (19) Å	T = 291 (2) K
β = 104.52 (3)º	Block, colorless
V = 1936.2 (7) Å^3	0.25 × 0.18 × 0.15 mm
Z = 4	

Data collection

Rigaku RAXIS RAPID IP diffractometer	4500 independent reflections
Radiation source: Rotating Anode	3819 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.038
T = 291(2) K	θ_{max} = 27.5º
Oscillation scans	θ_{min} = 1.2º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	h = −7→7
T_{min} = 0.98, T_{max} = 0.99	k = 0→44
5538 measured reflections	l = 0→12

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.079$

$wR(F^2) = 0.214$

$S = 1.08$

4500 reflections

256 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.199P)^2 + 0.1P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.33$ e Å^{-3}

$\Delta\rho_{min} = -0.45$ e Å^{-3}

Extinction correction: none

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.1507 (2)	0.17406 (4)	0.55204 (15)	0.0431 (3)	
C2	−0.0612 (3)	0.17793 (4)	0.43839 (15)	0.0448 (4)	
C3	−0.2417 (3)	0.19860 (5)	0.45897 (18)	0.0503 (4)	
H3	−0.2270	0.2121	0.5460	0.060*	
C4	−0.4435 (3)	0.20000 (6)	0.3553 (2)	0.0627 (5)	
H4	−0.5630	0.2141	0.3731	0.075*	
C5	−0.4694 (4)	0.18040 (7)	0.2239 (2)	0.0689 (5)	
H5	−0.6062	0.1809	0.1536	0.083*	
C6	−0.2842 (4)	0.15971 (7)	0.1993 (2)	0.0692 (5)	
H6	−0.2973	0.1473	0.1102	0.083*	
C7	−0.0844 (3)	0.15756 (6)	0.30514 (18)	0.0599 (5)	
H7	0.0345	0.1429	0.2894	0.072*	
C8	0.2659 (2)	0.14007 (5)	0.60830 (15)	0.0441 (3)	
C9	0.4582 (2)	0.15295 (4)	0.71101 (15)	0.0434 (3)	
C10	0.6524 (3)	0.13115 (4)	0.80378 (16)	0.0454 (4)	
C11	0.8684 (3)	0.14761 (5)	0.83408 (16)	0.0493 (4)	

H11	0.8897	0.1717	0.7959	0.059*	
C12	1.0487 (3)	0.12795 (6)	0.92064 (19)	0.0601 (5)	
H12	1.1910	0.1392	0.9421	0.072*	
C13	1.0214 (4)	0.09147 (7)	0.9765 (2)	0.0699 (6)	
H13	1.1441	0.0782	1.0338	0.084*	
C14	0.8116 (4)	0.07567 (7)	0.9456 (3)	0.0749 (6)	
H14	0.7921	0.0513	0.9826	0.090*	
C15	0.6261 (3)	0.09482 (5)	0.86047 (19)	0.0568 (4)	
H15	0.4843	0.0834	0.8413	0.068*	
C16	0.1811 (3)	0.09973 (5)	0.56892 (16)	0.0469 (4)	
H16B	0.0213	0.1013	0.5220	0.056*	
H16C	0.1967	0.0853	0.6590	0.056*	
C17	0.2924 (2)	0.07649 (4)	0.47008 (14)	0.0435 (3)	
C18	0.4823 (3)	0.08927 (5)	0.42526 (18)	0.0506 (4)	
H18	0.5419	0.1136	0.4548	0.061*	
C19	0.5828 (3)	0.06676 (5)	0.33870 (19)	0.0568 (4)	
H19	0.7059	0.0761	0.3083	0.068*	
C20	0.4983 (3)	0.03003 (5)	0.29748 (18)	0.0532 (4)	
C21	0.3082 (3)	0.01678 (5)	0.3381 (2)	0.0601 (5)	
H21	0.2481	−0.0074	0.3076	0.072*	
C22	0.2100 (3)	0.03981 (5)	0.42376 (19)	0.0554 (4)	
H22	0.0844	0.0306	0.4516	0.066*	
C23	0.6143 (3)	0.00582 (6)	0.2168 (2)	0.0618 (5)	
N1	0.2632 (2)	0.20491 (4)	0.62334 (13)	0.0475 (3)	
N2	0.4512 (2)	0.19150 (4)	0.71881 (13)	0.0475 (3)	
H2	0.5363	0.2094	0.7792	0.105 (10)*	
N3	0.7146 (4)	−0.01378 (7)	0.1585 (2)	0.0833 (6)	
O1	0.7504 (4)	0.2500	0.8444 (3)	0.0823 (7)	
H1	0.6334	0.2500	0.8613	0.18 (3)*	
C24	0.8776 (18)	0.2500	0.9996 (6)	0.163 (3)	
H24A	0.8465	0.2729	1.0505	0.196*	0.50
H24B	0.8465	0.2271	1.0505	0.196*	0.50
C25	1.1059 (16)	0.2500	0.9826 (17)	0.303 (9)	
H25A	1.1067	0.2398	0.8881	0.455*	0.50
H25B	1.1993	0.2342	1.0572	0.455*	0.50
H25C	1.1631	0.2760	0.9911	0.455*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0417 (8)	0.0438 (8)	0.0423 (7)	−0.0021 (5)	0.0078 (5)	−0.0025 (5)
C2	0.0454 (8)	0.0420 (7)	0.0467 (7)	−0.0016 (6)	0.0110 (5)	−0.0011 (5)
C3	0.0501 (9)	0.0412 (8)	0.0571 (8)	0.0015 (6)	0.0088 (6)	0.0014 (5)
C4	0.0541 (10)	0.0592 (11)	0.0710 (10)	0.0064 (8)	0.0084 (7)	0.0025 (8)
C5	0.0619 (12)	0.0676 (13)	0.0693 (11)	−0.0075 (9)	0.0015 (8)	0.0009 (8)
C6	0.0777 (14)	0.0682 (13)	0.0570 (9)	−0.0025 (10)	0.0080 (8)	−0.0080 (8)
C7	0.0664 (11)	0.0596 (11)	0.0527 (9)	0.0001 (8)	0.0129 (7)	−0.0047 (7)
C8	0.0424 (8)	0.0438 (8)	0.0458 (7)	−0.0031 (5)	0.0106 (5)	−0.0035 (5)

C9	0.0427 (8)	0.0419 (7)	0.0459 (7)	−0.0031 (5)	0.0118 (5)	−0.0037 (5)
C10	0.0461 (8)	0.0409 (7)	0.0480 (7)	0.0044 (5)	0.0099 (5)	−0.0078 (5)
C11	0.0436 (8)	0.0556 (9)	0.0483 (7)	−0.0001 (6)	0.0105 (5)	−0.0020 (6)
C12	0.0439 (9)	0.0719 (12)	0.0602 (9)	0.0070 (7)	0.0048 (6)	−0.0058 (7)
C13	0.0653 (12)	0.0716 (13)	0.0684 (11)	0.0233 (10)	0.0085 (8)	0.0016 (8)
C14	0.0811 (15)	0.0581 (12)	0.0815 (12)	0.0106 (10)	0.0128 (10)	0.0108 (9)
C15	0.0584 (10)	0.0460 (9)	0.0627 (9)	−0.0032 (7)	0.0089 (7)	−0.0034 (6)
C16	0.0397 (8)	0.0448 (8)	0.0521 (8)	−0.0028 (5)	0.0037 (5)	−0.0045 (5)
C17	0.0407 (8)	0.0377 (7)	0.0477 (7)	−0.0010 (5)	0.0030 (5)	−0.0011 (5)
C18	0.0523 (9)	0.0401 (8)	0.0589 (8)	−0.0070 (6)	0.0128 (6)	−0.0081 (5)
C19	0.0620 (10)	0.0465 (9)	0.0630 (9)	−0.0055 (7)	0.0179 (7)	−0.0041 (7)
C20	0.0582 (10)	0.0408 (8)	0.0577 (8)	0.0018 (7)	0.0088 (6)	−0.0055 (6)
C21	0.0592 (10)	0.0435 (9)	0.0736 (10)	−0.0090 (7)	0.0090 (7)	−0.0153 (7)
C22	0.0515 (9)	0.0458 (9)	0.0671 (9)	−0.0064 (7)	0.0116 (6)	−0.0069 (6)
C23	0.0682 (12)	0.0465 (9)	0.0722 (10)	0.0033 (8)	0.0201 (8)	−0.0055 (7)
N1	0.0451 (7)	0.0426 (7)	0.0512 (7)	−0.0005 (5)	0.0053 (5)	−0.0063 (5)
N2	0.0458 (7)	0.0431 (7)	0.0509 (7)	−0.0007 (5)	0.0070 (5)	−0.0068 (5)
N3	0.0951 (16)	0.0631 (12)	0.0988 (13)	0.0049 (10)	0.0375 (11)	−0.0144 (10)
O1	0.0603 (14)	0.0570 (13)	0.1096 (17)	0.000	−0.0159 (10)	0.000
C24	0.250 (10)	0.109 (5)	0.098 (3)	0.000	−0.015 (4)	0.000
C25	0.108 (6)	0.219 (12)	0.469 (19)	0.000	−0.142 (9)	0.000

Geometric parameters (Å, °)

C1—N1	1.354 (2)	C14—H14	0.9300
C1—C8	1.404 (2)	C15—H15	0.9300
C1—C2	1.469 (2)	C16—C17	1.517 (2)
C2—C3	1.371 (2)	C16—H16B	0.9700
C2—C7	1.418 (2)	C16—H16C	0.9700
C3—C4	1.372 (2)	C17—C22	1.393 (2)
C3—H3	0.9300	C17—C18	1.406 (2)
C4—C5	1.387 (3)	C18—C19	1.380 (2)
C4—H4	0.9300	C18—H18	0.9300
C5—C6	1.410 (4)	C19—C20	1.389 (2)
C5—H5	0.9300	C19—H19	0.9300
C6—C7	1.375 (3)	C20—C21	1.393 (3)
C6—H6	0.9300	C20—C23	1.434 (2)
C7—H7	0.9300	C21—C22	1.376 (3)
C8—C9	1.398 (2)	C21—H21	0.9300
C8—C16	1.501 (2)	C22—H22	0.9300
C9—N2	1.335 (2)	C23—N3	1.144 (3)
C9—C10	1.493 (2)	N1—N2	1.355 (2)
C10—C15	1.390 (2)	N2—H2	0.910
C10—C11	1.403 (2)	O1—C24	1.478 (6)
C11—C12	1.378 (2)	O1—H1	0.77
C11—H11	0.9300	C24—C25	1.448 (15)
C12—C13	1.393 (3)	C24—H24A	0.9700
C12—H12	0.9300	C24—H24B	0.9700
C13—C14	1.359 (4)	C25—H25A	0.9600

C13—H13	0.9300	C25—H25B	0.9600
C14—C15	1.385 (3)	C25—H25C	0.9600
N1—C1—C8	108.95 (13)	C10—C15—H15	120.1
N1—C1—C2	122.61 (13)	C8—C16—C17	117.6 (1)
C8—C1—C2	128.41 (13)	C8—C16—H16B	107.9
C3—C2—C7	118.65 (16)	C17—C16—H16B	107.9
C3—C2—C1	122.74 (13)	C8—C16—H16C	107.9
C7—C2—C1	118.50 (14)	C17—C16—H16C	107.9
C2—C3—C4	122.14 (16)	H16B—C16—H16C	107.2
C2—C3—H3	118.9	C22—C17—C18	116.97 (14)
C4—C3—H3	118.9	C22—C17—C16	119.40 (14)
C3—C4—C5	120.13 (19)	C18—C17—C16	123.60 (13)
C3—C4—H4	119.9	C19—C18—C17	121.86 (15)
C5—C4—H4	119.9	C19—C18—H18	119.1
C4—C5—C6	118.58 (19)	C17—C18—H18	119.1
C4—C5—H5	120.7	C18—C19—C20	119.35 (17)
C6—C5—H5	120.7	C18—C19—H19	120.3
C7—C6—C5	121.01 (18)	C20—C19—H19	120.3
C7—C6—H6	119.5	C19—C20—C21	120.14 (16)
C5—C6—H6	119.5	C19—C20—C23	118.81 (17)
C6—C7—C2	119.43 (18)	C21—C20—C23	121.03 (16)
C6—C7—H7	120.3	C22—C21—C20	119.45 (16)
C2—C7—H7	120.3	C22—C21—H21	120.3
C9—C8—C1	104.66 (14)	C20—C21—H21	120.3
C9—C8—C16	130.29 (14)	C21—C22—C17	122.19 (16)
C1—C8—C16	124.91 (14)	C21—C22—H22	118.9
N2—C9—C8	108.83 (14)	C17—C22—H22	118.9
N2—C9—C10	120.16 (13)	N3—C23—C20	176.7 (2)
C8—C9—C10	131.01 (14)	C1—N1—N2	107.7 (1)
C15—C10—C11	118.84 (15)	C9—N2—N1	109.7 (1)
C15—C10—C9	121.93 (15)	C9—N2—H2	134
C11—C10—C9	119.23 (14)	N1—N2—H2	116
C12—C11—C10	119.81 (17)	C24—O1—H1	95
C12—C11—H11	120.1	C25—C24—O1	100.0 (7)
C10—C11—H11	120.1	C25—C24—H24A	111.8
C11—C12—C13	121.05 (18)	O1—C24—H24A	111.8
C11—C12—H12	119.5	C25—C24—H24B	111.8
C13—C12—H12	119.5	O1—C24—H24B	111.8
C14—C13—C12	118.64 (19)	H24A—C24—H24B	109.5
C14—C13—H13	120.7	C24—C25—H25A	109.5
C12—C13—H13	120.7	C24—C25—H25B	109.5
C13—C14—C15	121.9 (2)	H25A—C25—H25B	109.5
C13—C14—H14	119.1	C24—C25—H25C	109.5
C15—C14—H14	119.1	H25A—C25—H25C	109.5
C14—C15—C10	119.80 (19)	H25B—C25—H25C	109.5
C14—C15—H15	120.1		
N1—C1—C2—C3	−51.3 (2)	C10—C11—C12—C13	1.4 (3)
C8—C1—C2—C3	126.61 (17)	C11—C12—C13—C14	−0.9 (3)

N1—C1—C2—C7	132.54 (17)	C12—C13—C14—C15	0.1 (3)
C8—C1—C2—C7	−49.6 (2)	C13—C14—C15—C10	0.3 (3)
C7—C2—C3—C4	0.3 (3)	C11—C10—C15—C14	0.2 (2)
C1—C2—C3—C4	−175.85 (17)	C9—C10—C15—C14	179.78 (16)
C2—C3—C4—C5	−0.6 (3)	C9—C8—C16—C17	−78.51 (19)
C3—C4—C5—C6	−0.9 (3)	C1—C8—C16—C17	106.47 (16)
C4—C5—C6—C7	2.6 (3)	C8—C16—C17—C22	−176.18 (14)
C5—C6—C7—C2	−2.9 (3)	C8—C16—C17—C18	6.1 (2)
C3—C2—C7—C6	1.4 (3)	C22—C17—C18—C19	0.3 (2)
C1—C2—C7—C6	177.75 (17)	C16—C17—C18—C19	178.05 (15)
N1—C1—C8—C9	−3.01 (16)	C17—C18—C19—C20	−1.7 (3)
C2—C1—C8—C9	178.87 (13)	C18—C19—C20—C21	2.7 (3)
N1—C1—C8—C16	173.06 (13)	C18—C19—C20—C23	−175.38 (17)
C2—C1—C8—C16	−5.1 (2)	C19—C20—C21—C22	−2.3 (3)
C1—C8—C9—N2	2.43 (15)	C23—C20—C21—C22	175.70 (17)
C16—C8—C9—N2	−173.35 (14)	C20—C21—C22—C17	0.9 (3)
C1—C8—C9—C10	−177.27 (14)	C18—C17—C22—C21	0.1 (2)
C16—C8—C9—C10	7.0 (2)	C16—C17—C22—C21	−177.77 (16)
N2—C9—C10—C15	145.60 (15)	C8—C1—N1—N2	2.50 (16)
C8—C9—C10—C15	−34.7 (2)	C2—C1—N1—N2	−179.25 (12)
N2—C9—C10—C11	−34.83 (19)	C8—C9—N2—N1	−1.00 (16)
C8—C9—C10—C11	144.84 (15)	C10—C9—N2—N1	178.74 (12)
C15—C10—C11—C12	−1.0 (2)	C1—N1—N2—C9	−0.93 (16)
C9—C10—C11—C12	179.42 (14)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.77	2.53	2.786 (2)	102
O1—H1···N2^{i}	0.77	2.53	2.786 (2)	102
N2—H2···O1	0.91	1.91	2.786 (2)	160
C15—H15···N3^{ii}	0.93	2.70	3.470 (3)	141
C6—H6···Cg1^{iii}	0.93	2.72	3.601 (2)	159

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

Fig. 1

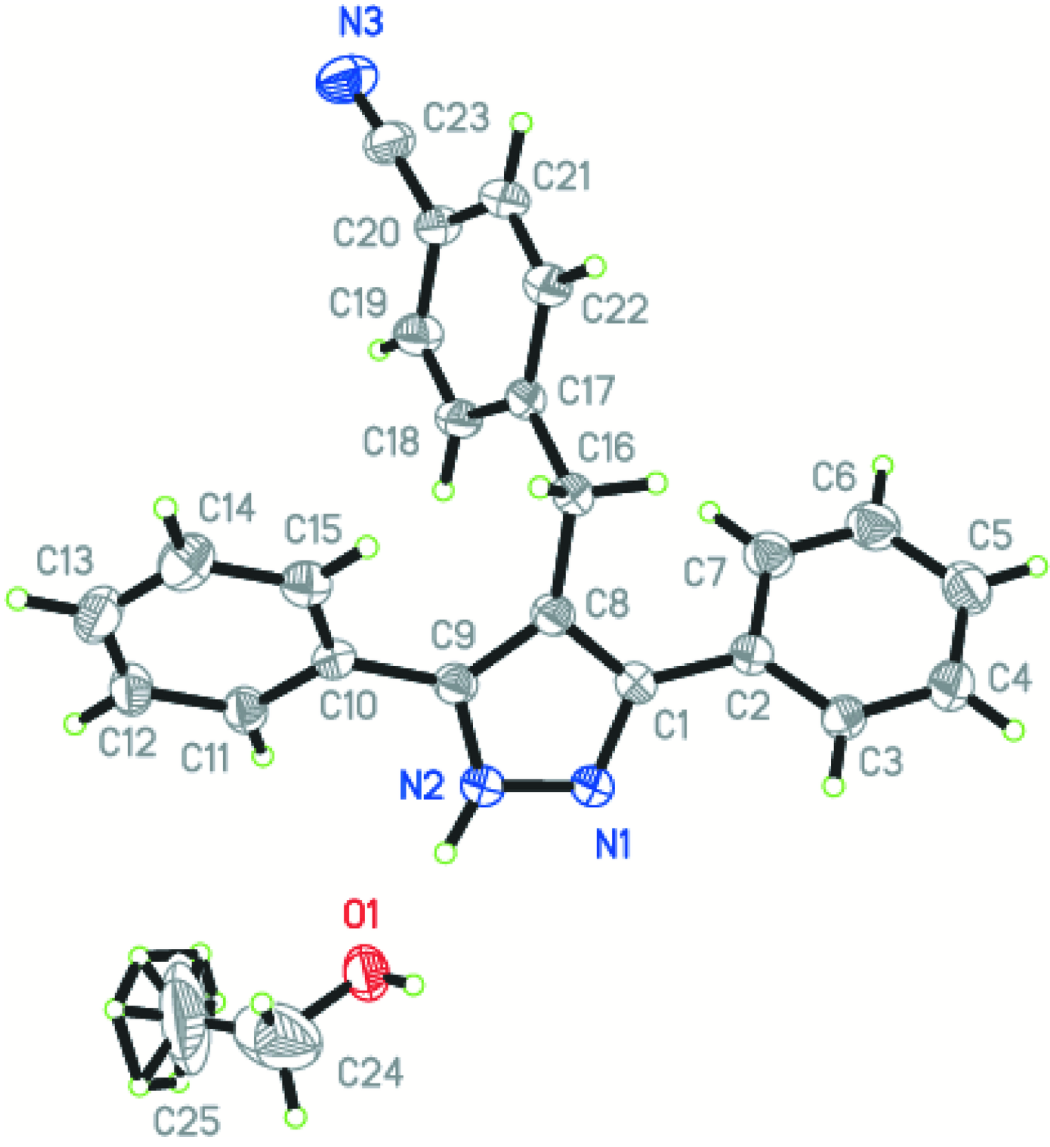
N3
C23
C21
C20
C22
C19
C17
C18
C16
C6
C14
C15
C5
C13
C7
C8
C9
C4
C10
C1
C2
C12
C11
C3
N2
N1
O1
C24
C25

Fig. 2