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4-Methyl-5-phenyl-1*H*-pyrazol-3-ol

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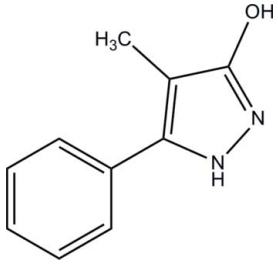
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.059; wR factor = 0.204; data-to-parameter ratio = 21.6.

The title compound, $C_{10}H_{10}N_2O$, crystallizes with two independent molecules in the asymmetric unit, having closely comparable geometries. The dihedral angles between the 1*H*-pyrazole and benzene rings in the two molecules are 39.57 (14) and 41.95 (13)°. The two molecules are each connected to neighbouring molecules by pairs of intermolecular O—H···N hydrogen bonds, forming dimers with $R_2^2(8)$ ring motifs. These dimers are further linked into $R_4^4(10)$ ring motifs by intermolecular N—H···O hydrogen bonds, forming chains along [101]. The crystal structure is further stabilized by a C—H···π interaction.

Related literature

For the biological activity of 4-methyl-3-phenyl-1*H*-pyrazol-5-ol, see: Brogden (1986); Gursoy *et al.* (2000); Ragavan *et al.* (2009, 2010); Watanabe *et al.* (1984); Kawai *et al.* (1997); Wu *et al.* (2002). For related structures, see: Shahani *et al.* (2009, 2010*a*,*b*,*c*). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For bond-length data, see: Allen *et al.* (1987). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{10}H_{10}N_2O$
M_r = 174.20
Monoclinic, $C2/c$
a = 26.4082 (19) Å
b = 11.0972 (8) Å
c = 14.1245 (10) Å
β = 118.996 (1)°
V = 3620.4 (4) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.35 × 0.14 × 0.08 mm

Data collection

Bruker APEXII DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.970, T_{max} = 0.993
19166 measured reflections
5255 independent reflections
2907 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.204
S = 1.13
5255 reflections
243 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

*Cg*1 is the centroid of the C1*B*–C6*B* benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
O1*A*—H1*OA*···N2*A*^{i}	0.83	1.85	2.673 (2)	171
O1*B*—H1*OB*···N2*B*^{ii}	0.83	1.84	2.670 (2)	177
N1*B*—H1*NB*···O1*A*^{iii}	1.00 (3)	1.85 (3)	2.836 (3)	171 (3)
N1*A*—H1*NA*···O1*B*^{iv}	0.97 (3)	1.88 (3)	2.844 (2)	173 (2)
C10*A*—H10*C*···*Cg*1^{v}	0.96	2.77	3.575 (3)	142

Symmetry codes: (i) $-x+\frac{1}{2}, -y+\frac{5}{2}, -z+1$; (ii) $-x, y, -z-\frac{1}{2}$; (iii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x, -y+2, -z$; (v) $x, -y, z-\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2561).

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supporting information

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4-Methyl-5-phenyl-1*H*-pyrazol-3-ol

Tara Shahani, Hoong-Kun Fun, R. Venkat Ragavan, V. Vijayakumar and S. Sarveswari

S1. Comment

Pyrazolone derivatives have a broad spectrum of biological activities being used as analgesic, antipyretic and anti-inflammatory therapeutical drugs (Brogden, 1986; Gursoy *et al.*, 2000). A class of new compounds with the pyrazolone moiety was synthesized and reported for their antibacterial and antifungal activities by Ragavan *et al.* (2009, 2010). A new pyrazolone derivative, edaravone (3-methyl-1-phenyl-2-pyrazoline-5-one), is being used as a drug in clinical practice for brain ischemia (Watanabe *et al.*, 1984; Kawai *et al.*, 1997) and the same has been found to be effective against myocardial ischemia (Wu *et al.*, 2002).

There are two independent molecules (A and B) in the asymmetric unit (Fig. 1). The maximum deviations in 1*H*-pyrazole ring (N1/N2/C7–C9) for molecules A and B are 0.006 (2) and 0.011 (2) Å, respectively, at atoms C6A and C6B. The dihedral angles formed between the 1*H*-pyrazole ring and benzene ring in molecules A and B are 39.57 (14) and 41.95 (13)°, respectively. The bond lengths (Allen *et al.*, 1987) and angles are within normal ranges and comparable to those closely related structures (Shahani *et al.*, 2009, 2010*a–c*).

In the crystal packing (Fig. 2), pairs of intermolecular O1A—H1OA···N2A and O1B—H1OB···N2B hydrogen bonds (Table 1) form dimers with neighbouring molecules, generating $R_2^2(8)$ ring motifs (Bernstein *et al.*, 1995). These dimers are further linked into $R_4^4(10)$ ring motifs by additional intermolecular N1A—H1NA···O1B and N1B—H1NB···O1A hydrogen bonds (Table 1), forming one dimensional chains along the [101] direction. The crystal structure is further stabilized by C—H···π interaction (Table 1), involving the C1B—C6B benzene ring (centroid *Cg*1).

S2. Experimental

The compound 4-methyl-5-phenyl-1-*H*-pyrazol-3-ol has been synthesized using the method available in the literature (Ragavan *et al.*, 2009, 2010) and recrystallized using the ethanol (white solid). *m.p.* 278.5–493 K.

S3. Refinement

The H atoms bound to O atoms were located in a difference map and constrained to ride with their parent atoms, with U_{iso}(H) = 1.5U_{eq}(O) (O—H = 0.83 Å). The H atoms bound to N atoms were located in a difference map and were refined freely [refined N—H lengths, 1.00 (3) and 0.97 (2) Å]. All other H atoms were positioned geometrically (C—H = 0.93–0.96 Å], with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

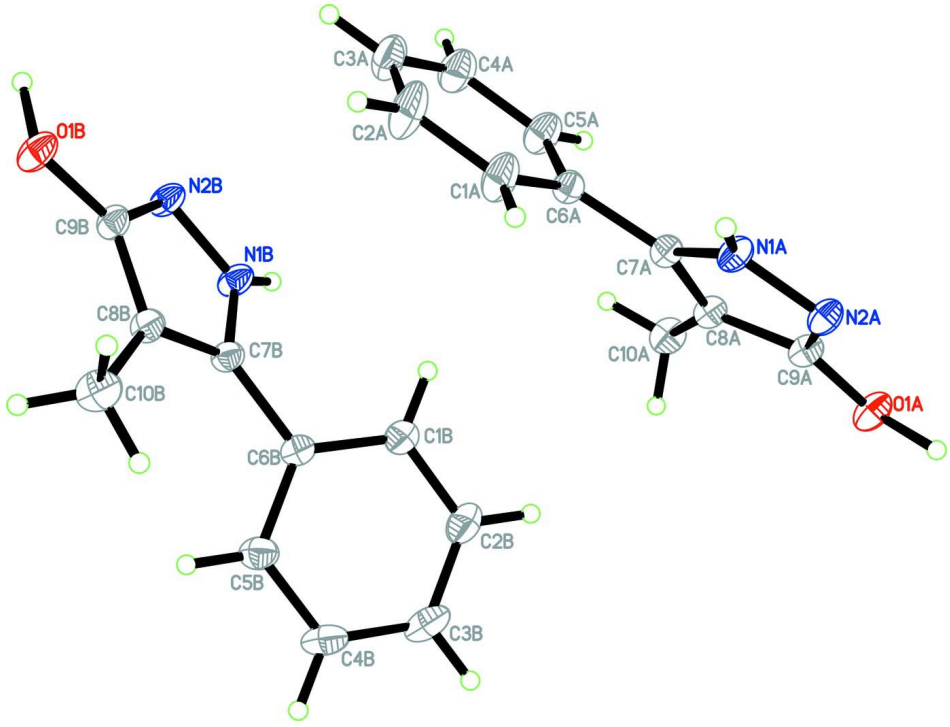

Figure 1

The molecular structure of the title compound, showing 20% probability displacement ellipsoids and the atom numbering scheme.

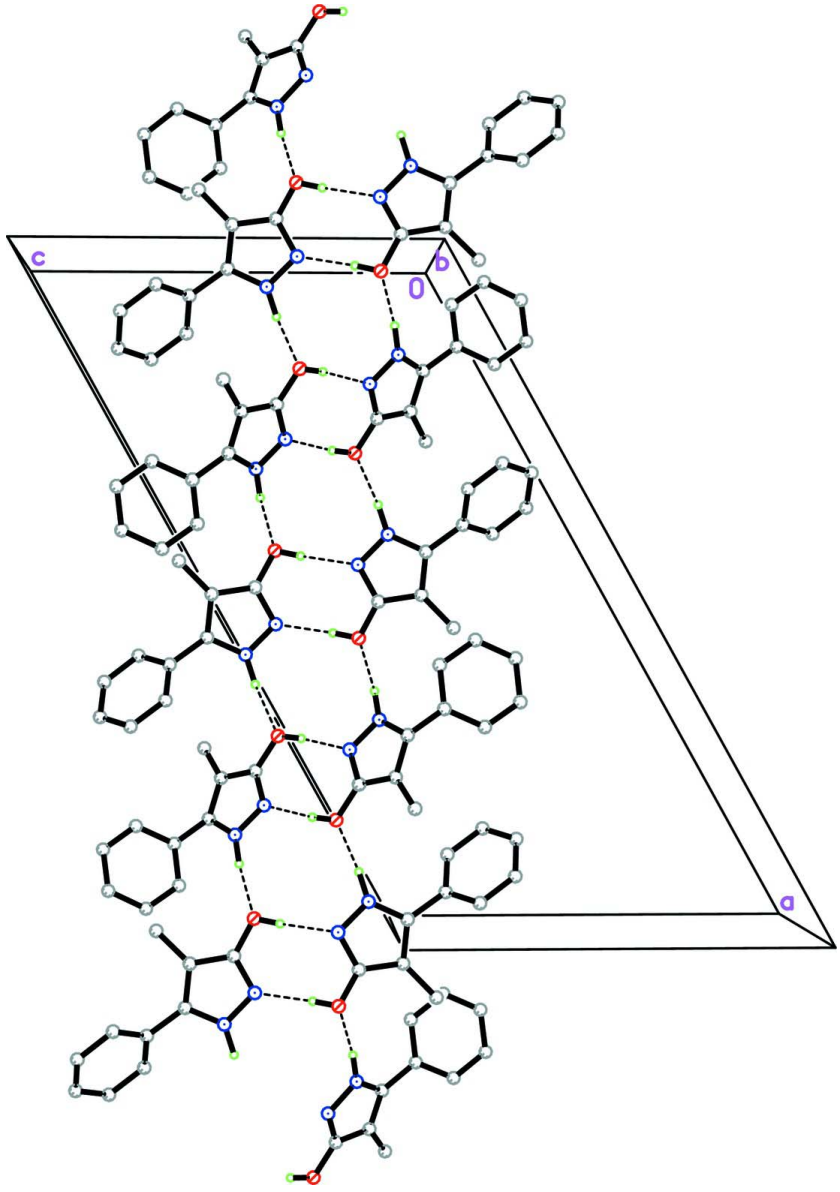

Figure 2

The crystal packing of the title compound, viewed approximately along the *b* axis, showing a one-dimensional chain.

4-Methyl-5-phenyl-1*H*-pyrazol-3-ol

Crystal data

$C_{10}H_{10}N_2O$
$M_r = 174.20$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 26.4082\ (19)$ Å
$b = 11.0972\ (8)$ Å
$c = 14.1245\ (10)$ Å
$\beta = 118.996\ (1)°$
$V = 3620.4\ (4)$ Å^3
$Z = 16$

$F(000) = 1472$
$D_x = 1.278$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3052 reflections
$\theta = 3.3–27.2°$
$\mu = 0.09$ mm^{-1}
$T = 100$ K
Block, colourless
0.35 × 0.14 × 0.08 mm

Data collection

Bruker APEXII DUO CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.970, T_{max} = 0.993
19166 measured reflections
5255 independent reflections
2907 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 30.0°, θ_{min} = 2.0°
h = −37→28
k = −15→13
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.204
S = 1.13
5255 reflections
243 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0985P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cyrosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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.

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
O1A	0.30484 (5)	1.15234 (15)	0.48624 (10)	0.0513 (4)
H1OA	0.3021	1.1865	0.5356	0.077*
N1A	0.17011 (7)	1.19165 (16)	0.26752 (12)	0.0419 (4)
N2A	0.21137 (6)	1.22060 (17)	0.36985 (11)	0.0416 (4)
C1A	0.09436 (9)	1.0463 (3)	0.07114 (18)	0.0643 (7)
H1AA	0.0772	1.0599	0.1142	0.077*
C2A	0.06077 (11)	1.0113 (3)	−0.0353 (2)	0.0835 (10)
H2AA	0.0211	1.0019	−0.0634	0.100*
C3A	0.08503 (12)	0.9902 (3)	−0.09985 (19)	0.0704 (8)
H3AA	0.0621	0.9665	−0.1715	0.084*
C4A	0.14342 (12)	1.0042 (3)	−0.05821 (19)	0.0676 (7)
H4AA	0.1603	0.9906	−0.1017	0.081*
C5A	0.17726 (10)	1.0384 (3)	0.04793 (17)	0.0605 (6)
H5AA	0.2170	1.0462	0.0758	0.073*

C6A	0.15335 (8)	1.06126 (19)	0.11381 (14)	0.0412 (4)
C7A	0.18926 (8)	1.10453 (19)	0.22525 (14)	0.0386 (4)
C8A	0.24504 (8)	1.07398 (19)	0.30334 (14)	0.0406 (4)
C9A	0.25656 (7)	1.1493 (2)	0.39179 (14)	0.0404 (4)
C10A	0.28424 (9)	0.9785 (2)	0.30003 (17)	0.0526 (5)
H10A	0.2662	0.9409	0.2300	0.079*
H10B	0.2914	0.9190	0.3545	0.079*
H10C	0.3202	1.0143	0.3135	0.079*
O1B	−0.05992 (5)	0.70768 (16)	−0.21038 (10)	0.0515 (4)
H1OB	−0.0528	0.7049	−0.2616	0.077*
N1B	0.08261 (7)	0.69465 (18)	−0.01528 (12)	0.0468 (4)
N2B	0.04080 (6)	0.70277 (17)	−0.12057 (12)	0.0455 (4)
C1B	0.14424 (9)	0.7478 (2)	0.21872 (16)	0.0564 (6)
H1BA	0.1524	0.8034	0.1787	0.068*
C2B	0.17998 (11)	0.7390 (3)	0.32909 (18)	0.0725 (8)
H2BA	0.2123	0.7887	0.3631	0.087*
C3B	0.16837 (12)	0.6580 (3)	0.38904 (18)	0.0708 (8)
H3BA	0.1925	0.6531	0.4635	0.085*
C4B	0.12108 (10)	0.5843 (3)	0.33917 (17)	0.0630 (7)
H4BA	0.1134	0.5285	0.3797	0.076*
C5B	0.08471 (9)	0.5923 (2)	0.22872 (16)	0.0520 (5)
H5BA	0.0524	0.5426	0.1954	0.062*
C6B	0.09620 (8)	0.67397 (19)	0.16757 (14)	0.0409 (4)
C7B	0.05896 (8)	0.68061 (19)	0.04958 (14)	0.0400 (4)
C8B	−0.00068 (8)	0.6800 (2)	−0.01460 (14)	0.0411 (5)
C9B	−0.00976 (8)	0.69654 (19)	−0.12047 (14)	0.0406 (4)
C10B	−0.04620 (9)	0.6615 (3)	0.01754 (18)	0.0598 (6)
H10D	−0.0283	0.6528	0.0947	0.090*
H10E	−0.0679	0.5901	−0.0167	0.090*
H10F	−0.0717	0.7298	−0.0047	0.090*
H1NB	0.1235 (11)	0.687 (3)	0.0001 (19)	0.073 (8)*
H1NA	0.1316 (11)	1.224 (2)	0.2420 (18)	0.064 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0298 (6)	0.0806 (12)	0.0370 (7)	0.0088 (6)	0.0112 (5)	−0.0066 (7)
N1A	0.0321 (7)	0.0554 (11)	0.0348 (7)	0.0049 (7)	0.0134 (6)	−0.0018 (7)
N2A	0.0299 (7)	0.0569 (11)	0.0336 (7)	0.0034 (7)	0.0120 (6)	−0.0038 (7)
C1A	0.0429 (11)	0.093 (2)	0.0548 (12)	−0.0142 (12)	0.0221 (10)	−0.0223 (12)
C2A	0.0463 (13)	0.126 (3)	0.0661 (15)	−0.0210 (15)	0.0174 (12)	−0.0364 (17)
C3A	0.0739 (17)	0.079 (2)	0.0488 (12)	−0.0139 (14)	0.0223 (12)	−0.0220 (12)
C4A	0.0755 (16)	0.082 (2)	0.0516 (12)	−0.0043 (14)	0.0357 (12)	−0.0183 (12)
C5A	0.0478 (11)	0.0854 (19)	0.0496 (11)	−0.0037 (12)	0.0245 (10)	−0.0106 (12)
C6A	0.0393 (9)	0.0436 (12)	0.0394 (9)	−0.0020 (8)	0.0180 (8)	−0.0021 (8)
C7A	0.0342 (8)	0.0461 (12)	0.0385 (9)	−0.0015 (8)	0.0199 (7)	−0.0007 (8)
C8A	0.0330 (8)	0.0515 (13)	0.0383 (9)	0.0012 (8)	0.0181 (7)	−0.0002 (8)
C9A	0.0295 (8)	0.0549 (13)	0.0363 (9)	0.0031 (8)	0.0157 (7)	0.0020 (8)

C10A	0.0426 (10)	0.0601 (15)	0.0530 (11)	0.0109 (10)	0.0214 (9)	−0.0005 (10)
O1B	0.0298 (6)	0.0862 (12)	0.0357 (7)	0.0068 (7)	0.0135 (6)	−0.0007 (6)
N1B	0.0305 (8)	0.0740 (14)	0.0338 (7)	−0.0012 (8)	0.0139 (6)	0.0038 (7)
N2B	0.0291 (7)	0.0713 (13)	0.0316 (7)	0.0007 (7)	0.0113 (6)	0.0029 (7)
C1B	0.0556 (12)	0.0620 (16)	0.0418 (10)	−0.0101 (11)	0.0160 (9)	0.0013 (10)
C2B	0.0650 (15)	0.088 (2)	0.0436 (12)	−0.0171 (14)	0.0097 (11)	−0.0075 (12)
C3B	0.0685 (16)	0.102 (2)	0.0352 (10)	0.0073 (15)	0.0196 (11)	0.0036 (12)
C4B	0.0648 (14)	0.0853 (19)	0.0455 (11)	0.0113 (13)	0.0320 (11)	0.0194 (11)
C5B	0.0494 (11)	0.0626 (15)	0.0466 (10)	0.0015 (10)	0.0253 (9)	0.0098 (10)
C6B	0.0398 (9)	0.0474 (12)	0.0349 (8)	0.0043 (8)	0.0176 (8)	0.0034 (8)
C7B	0.0369 (9)	0.0481 (12)	0.0351 (9)	−0.0006 (8)	0.0174 (8)	0.0021 (8)
C8B	0.0338 (9)	0.0519 (13)	0.0384 (9)	−0.0004 (8)	0.0180 (8)	0.0009 (8)
C9B	0.0308 (8)	0.0524 (13)	0.0363 (9)	0.0002 (8)	0.0145 (7)	−0.0011 (8)
C10B	0.0405 (11)	0.0886 (19)	0.0561 (12)	0.0052 (11)	0.0280 (10)	0.0070 (12)

Geometric parameters (Å, º)

O1A—C9A	1.326 (2)	O1B—C9B	1.323 (2)
O1A—H1OA	0.8273	O1B—H1OB	0.8317
N1A—C7A	1.356 (3)	N1B—C7B	1.345 (2)
N1A—N2A	1.3612 (19)	N1B—N2B	1.359 (2)
N1A—H1NA	0.97 (2)	N1B—H1NB	1.00 (3)
N2A—C9A	1.337 (2)	N2B—C9B	1.338 (2)
C1A—C2A	1.380 (3)	C1B—C2B	1.380 (3)
C1A—C6A	1.381 (3)	C1B—C6B	1.384 (3)
C1A—H1AA	0.9300	C1B—H1BA	0.9300
C2A—C3A	1.365 (4)	C2B—C3B	1.368 (4)
C2A—H2AA	0.9300	C2B—H2BA	0.9300
C3A—C4A	1.367 (4)	C3B—C4B	1.368 (4)
C3A—H3AA	0.9300	C3B—H3BA	0.9300
C4A—C5A	1.375 (3)	C4B—C5B	1.383 (3)
C4A—H4AA	0.9300	C4B—H4BA	0.9300
C5A—C6A	1.378 (3)	C5B—C6B	1.383 (3)
C5A—H5AA	0.9300	C5B—H5BA	0.9300
C6A—C7A	1.470 (2)	C6B—C7B	1.470 (2)
C7A—C8A	1.388 (2)	C7B—C8B	1.385 (2)
C8A—C9A	1.409 (3)	C8B—C9B	1.407 (3)
C8A—C10A	1.498 (3)	C8B—C10B	1.491 (3)
C10A—H10A	0.9600	C10B—H10D	0.9600
C10A—H10B	0.9600	C10B—H10E	0.9600
C10A—H10C	0.9600	C10B—H10F	0.9600
C9A—O1A—H1OA	115.1	C9B—O1B—H1OB	106.7
C7A—N1A—N2A	111.00 (15)	C7B—N1B—N2B	110.74 (15)
C7A—N1A—H1NA	130.4 (15)	C7B—N1B—H1NB	130.8 (14)
N2A—N1A—H1NA	117.7 (14)	N2B—N1B—H1NB	117.7 (14)
C9A—N2A—N1A	105.76 (15)	C9B—N2B—N1B	106.09 (15)
C2A—C1A—C6A	120.2 (2)	C2B—C1B—C6B	120.0 (2)

C2A—C1A—H1AA	119.9	C2B—C1B—H1BA	120.0
C6A—C1A—H1AA	119.9	C6B—C1B—H1BA	120.0
C3A—C2A—C1A	120.9 (2)	C3B—C2B—C1B	120.7 (2)
C3A—C2A—H2AA	119.5	C3B—C2B—H2BA	119.7
C1A—C2A—H2AA	119.5	C1B—C2B—H2BA	119.7
C2A—C3A—C4A	119.3 (2)	C4B—C3B—C2B	119.8 (2)
C2A—C3A—H3AA	120.3	C4B—C3B—H3BA	120.1
C4A—C3A—H3AA	120.3	C2B—C3B—H3BA	120.1
C3A—C4A—C5A	120.1 (2)	C3B—C4B—C5B	120.2 (2)
C3A—C4A—H4AA	119.9	C3B—C4B—H4BA	119.9
C5A—C4A—H4AA	119.9	C5B—C4B—H4BA	119.9
C4A—C5A—C6A	121.3 (2)	C4B—C5B—C6B	120.3 (2)
C4A—C5A—H5AA	119.4	C4B—C5B—H5BA	119.9
C6A—C5A—H5AA	119.4	C6B—C5B—H5BA	119.9
C5A—C6A—C1A	118.19 (18)	C1B—C6B—C5B	119.03 (18)
C5A—C6A—C7A	120.97 (18)	C1B—C6B—C7B	120.16 (18)
C1A—C6A—C7A	120.81 (18)	C5B—C6B—C7B	120.79 (18)
N1A—C7A—C8A	107.63 (16)	N1B—C7B—C8B	108.12 (15)
N1A—C7A—C6A	121.31 (16)	N1B—C7B—C6B	120.11 (16)
C8A—C7A—C6A	131.04 (18)	C8B—C7B—C6B	131.71 (17)
C7A—C8A—C9A	104.45 (17)	C7B—C8B—C9B	104.41 (16)
C7A—C8A—C10A	129.14 (17)	C7B—C8B—C10B	129.08 (17)
C9A—C8A—C10A	126.32 (17)	C9B—C8B—C10B	126.47 (17)
O1A—C9A—N2A	122.24 (17)	O1B—C9B—N2B	121.95 (16)
O1A—C9A—C8A	126.60 (17)	O1B—C9B—C8B	127.43 (17)
N2A—C9A—C8A	111.16 (15)	N2B—C9B—C8B	110.60 (15)
C8A—C10A—H10A	109.5	C8B—C10B—H10D	109.5
C8A—C10A—H10B	109.5	C8B—C10B—H10E	109.5
H10A—C10A—H10B	109.5	H10D—C10B—H10E	109.5
C8A—C10A—H10C	109.5	C8B—C10B—H10F	109.5
H10A—C10A—H10C	109.5	H10D—C10B—H10F	109.5
H10B—C10A—H10C	109.5	H10E—C10B—H10F	109.5

C7A—N1A—N2A—C9A	−0.7 (2)	C7B—N1B—N2B—C9B	1.5 (2)
C6A—C1A—C2A—C3A	0.3 (5)	C6B—C1B—C2B—C3B	−0.2 (4)
C1A—C2A—C3A—C4A	0.0 (5)	C1B—C2B—C3B—C4B	0.4 (5)
C2A—C3A—C4A—C5A	0.4 (5)	C2B—C3B—C4B—C5B	−0.7 (4)
C3A—C4A—C5A—C6A	−1.2 (4)	C3B—C4B—C5B—C6B	0.8 (4)
C4A—C5A—C6A—C1A	1.4 (4)	C2B—C1B—C6B—C5B	0.2 (4)
C4A—C5A—C6A—C7A	−176.4 (2)	C2B—C1B—C6B—C7B	−178.2 (2)
C2A—C1A—C6A—C5A	−1.0 (4)	C4B—C5B—C6B—C1B	−0.5 (3)
C2A—C1A—C6A—C7A	176.8 (3)	C4B—C5B—C6B—C7B	178.0 (2)
N2A—N1A—C7A—C8A	0.7 (2)	N2B—N1B—C7B—C8B	−0.3 (2)
N2A—N1A—C7A—C6A	−177.51 (17)	N2B—N1B—C7B—C6B	−177.91 (18)
C5A—C6A—C7A—N1A	138.9 (2)	C1B—C6B—C7B—N1B	39.6 (3)
C1A—C6A—C7A—N1A	−38.9 (3)	C5B—C6B—C7B—N1B	−138.8 (2)
C5A—C6A—C7A—C8A	−38.9 (3)	C1B—C6B—C7B—C8B	−137.3 (2)
C1A—C6A—C7A—C8A	143.3 (2)	C5B—C6B—C7B—C8B	44.2 (3)

N1A—C7A—C8A—C9A	−0.5 (2)	N1B—C7B—C8B—C9B	−0.9 (2)
C6A—C7A—C8A—C9A	177.5 (2)	C6B—C7B—C8B—C9B	176.3 (2)
N1A—C7A—C8A—C10A	176.4 (2)	N1B—C7B—C8B—C10B	177.0 (2)
C6A—C7A—C8A—C10A	−5.6 (4)	C6B—C7B—C8B—C10B	−5.9 (4)
N1A—N2A—C9A—O1A	−179.23 (17)	N1B—N2B—C9B—O1B	176.63 (19)
N1A—N2A—C9A—C8A	0.4 (2)	N1B—N2B—C9B—C8B	−2.1 (2)
C7A—C8A—C9A—O1A	179.64 (19)	C7B—C8B—C9B—O1B	−176.7 (2)
C10A—C8A—C9A—O1A	2.7 (3)	C10B—C8B—C9B—O1B	5.3 (4)
C7A—C8A—C9A—N2A	0.1 (2)	C7B—C8B—C9B—N2B	1.9 (2)
C10A—C8A—C9A—N2A	−176.89 (19)	C10B—C8B—C9B—N2B	−176.1 (2)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C1B–C6B benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*A*—H1*OA*···N2*A*^{i}	0.83	1.85	2.673 (2)	171
O1*B*—H1*OB*···N2*B*^{ii}	0.83	1.84	2.670 (2)	177
N1*B*—H1*NB*···O1*A*^{iii}	1.00 (3)	1.85 (3)	2.836 (3)	171 (3)
N1*A*—H1*NA*···O1*B*^{iv}	0.97 (3)	1.88 (3)	2.844 (2)	173 (2)
C10*A*—H10*C*···*Cg*1^{v}	0.96	2.77	3.575 (3)	142

Symmetry codes: (i) −*x*+1/2, −*y*+5/2, −*z*+1; (ii) −*x*, *y*, −*z*−1/2; (iii) −*x*+1/2, *y*−1/2, −*z*+1/2; (iv) −*x*, −*y*+2, −*z*; (v) *x*, −*y*, *z*−1/2.