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(*Z*)-1-(1,3-Diphenyl-1*H*-pyrazol-4-yl)-*N*-phenylmethanimine *N*-oxide

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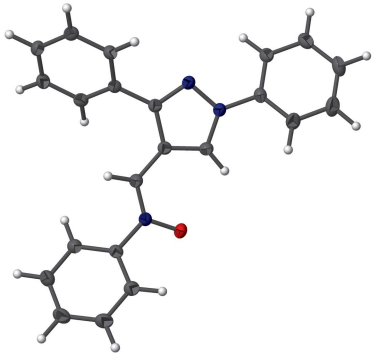
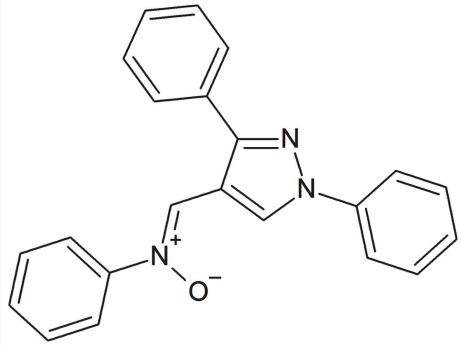
Structural data: full structural data are available from iucrdata.iucr.org

In the title nitrone, $C_{22}H_{17}N_3O$, the dihedral angles between the central pyrazole ring and pendant N-bound, C-bound and nitrone-bound phenyl rings are 20.93 (6), 41.27 (6), and 32.57 (6)°, respectively. In the crystal, (101) layers are generated by C—H···O hydrogen bonds coupled with C—H···π(ring) and offset π–π stacking interactions.

3D view



Chemical scheme



Structure description

Nitrones have various uses including as spin-trap reagents (Villamena *et al.*, 2007) and therapeutic agents (Piperno *et al.*, 2010). They react in [3 + 2] dipolar cycloadditions with carious dipolarophiles to construct functionalized isoxazolidines, which are useful intermediates in organic synthesis (Dell, 1998). As part of our studies in this area, we report herein the synthesis and crystal structure of the title compound (Fig. 1).

The dihedral angle between the pyrazole and the C4–C9 rings is 41.27 (6)°; those between the pyrazole and the C11–C16 and C17–C22 rings are, respectively, 32.57 (6) and 20.93 (6)°.

In the crystal, zigzag chains along the *c*-axis direction are generated by C6—H6···O1 and C7—H7···O1 hydrogen bonds (Table 1 and Figs. 2 and 3). These are connected into layers parallel to the *ac* plane by C5—H5···O1 hydrogen bonds, three C—H···π(ring) interactions (Table 1) and offset π–π stacking interactions between inversion-related C17–C22 rings [centroid–centroid distance = 3.6187 (8) Å](Figs. 2 and 3).

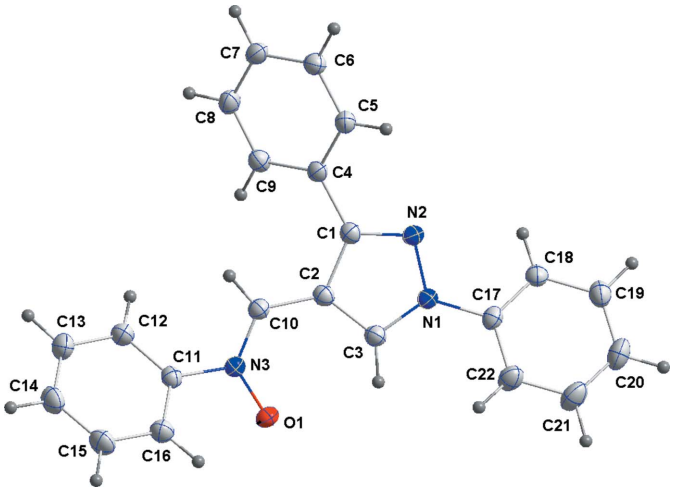


Figure 1
The title molecule, shown with 50% probability displacement ellipsoids.

Synthesis and crystallization

A solution of (20 g, 0.08 mol) 1,3-diphenyl 4-formyl pyrazole in ethanol (20 ml) was added to a solution of (9.0 g, 0.08 mol) *N*-phenylhydroxyamine in ethanol (50 ml) and the mixture was heated under reflux for 2 h. The product was separated in 92% yield (25 g) and recrystallized from ethanol solution to afford colourless slabs; m.p. 431 K.

FTIR (KBr) (cm^{-1}): 3150 (Ar. C—H), 3050 (H—C═N+), 1597 (C═N), 1579 (C═N^+). ^{1}H-NMR spectrum: δ p.p.m. (400 MHz, $CDCl_3$) 7.3–8.1 (*m*, 16H, Ar H), 9.9 (*s*, 1H, CH═N^+). Proton decoupled ^{13}C NMR spectrum: δ (100.5 MHz, $CDCl_3$) 113.2, 119.5, 127.2, 128.9, 129.0, 129.1, 129.3, 129.6, 129.8, 129.8, 132.3, 139.6, 147.9, 153.8 (15 Ar C). Mass spectrum (electron impact): *e*/*m* (%) 339.2 (1/2), 286.8 (100), 219.1 (58). Analysis calculated for ($C_{22}H_{17}N_3O$) (%): C 77.86, H 5.05, N 12.38. Found; C 77.27, H 5.02, N 12.38.

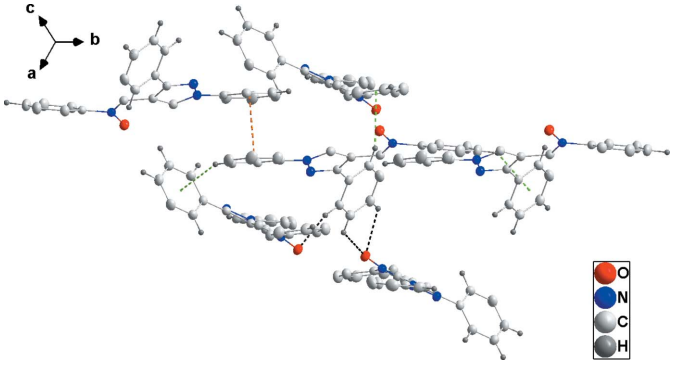


Figure 2
Details of the intermolecular interactions. C—H···O hydrogen bonds are shown by black dashed lines while C—H···π(ring) and offset π–π stacking interactions are shown, respectively, by green and orange dashed lines.

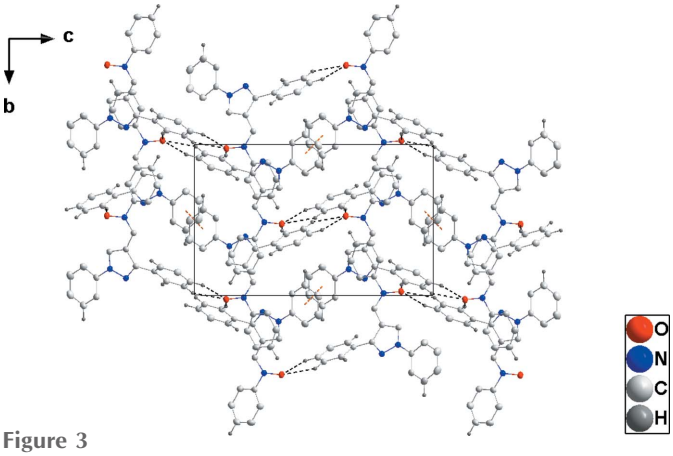


Figure 3
Packing viewed along the *a*-axis direction, with intermolecular interactions shown as depicted in Fig. 2.

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

*Cg*2 and *Cg*3 are, respectively, the centroids of the C4–C9 and C11–C16 benzene rings.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1^{i}	0.979 (15)	2.303 (15)	3.2561 (14)	164.1 (11)
C6—H6···O1^{ii}	0.988 (15)	2.514 (15)	3.1746 (14)	124.1 (11)
C7—H7···O1^{ii}	1.003 (15)	2.544 (15)	3.1837 (14)	121.4 (11)
C9—H9···*Cg*3^{iii}	0.975 (14)	2.764 (14)	3.6409 (13)	152.8 (11)
C14—H14···*Cg*2^{iv}	0.988 (17)	2.884 (16)	3.6249 (14)	132.5 (12)
C19—H19···*Cg*2^{i}	1.003 (17)	2.678 (17)	3.6128 (14)	155.3 (12)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{17}N_3O$
M_r	339.38
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, *b*, *c* (Å)	9.1084 (8), 10.8314 (9), 17.2226 (14)
β (°)	94.060 (3)
V (Å^3)	1694.9 (2)
Z	4
Radiation type	Cu *K*α
μ (mm^{-1})	0.66
Crystal size (mm)	0.24 × 0.21 × 0.10
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.85, 0.94
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12691, 3366, 3115
R_{int}	0.028
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.035, 0.086, 1.06
No. of reflections	3366
No. of parameters	304
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.19

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2016* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Refinement

Crystal and refinement details are presented in Table 2.

Funding information

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full crystallographic data

IUCrData (2018). **3**, x180208 [https://doi.org/10.1107/S2414314618002080]

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Crystal data

$C_{22}H_{17}N_3O$
M_r = 339.38
Monoclinic, $P2_1/c$
a = 9.1084 (8) Å
b = 10.8314 (9) Å
c = 17.2226 (14) Å
β = 94.060 (3)°
V = 1694.9 (2) Å^3
Z = 4
$F(000)$ = 712
D_x = 1.330 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9914 reflections
θ = 4.8–74.6°
μ = 0.66 mm^{-1}
T = 150 K
Slab, colourless
0.24 × 0.21 × 0.10 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.85, T_{max} = 0.94
12691 measured reflections
3366 independent reflections
3115 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 74.6°, θ_{min} = 4.8°
h = −10→9
k = −13→12
l = −21→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.086
S = 1.06
3366 reflections
304 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0366P)^2 + 0.5699P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL2016* (Sheldrick, 2015*b*), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0046 (4)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.28419 (9)	0.52663 (7)	0.36611 (4)	0.0258 (2)
N1	0.47211 (10)	0.17352 (8)	0.35347 (5)	0.0215 (2)
N2	0.43135 (10)	0.11254 (8)	0.28595 (5)	0.0224 (2)
N3	0.24264 (10)	0.51508 (8)	0.29270 (5)	0.0204 (2)
C1	0.34438 (12)	0.19128 (10)	0.24500 (6)	0.0210 (2)
C2	0.32853 (12)	0.30422 (10)	0.28615 (6)	0.0213 (2)
C3	0.41176 (12)	0.28765 (10)	0.35573 (6)	0.0225 (2)
H3	0.4284 (15)	0.3403 (13)	0.4012 (8)	0.033 (4)*
C4	0.28057 (12)	0.15709 (10)	0.16696 (6)	0.0209 (2)
C5	0.36634 (12)	0.09282 (10)	0.11610 (7)	0.0233 (2)
H5	0.4686 (16)	0.0721 (13)	0.1323 (8)	0.030 (4)*
C6	0.30717 (13)	0.06002 (10)	0.04264 (7)	0.0248 (2)
H6	0.3662 (16)	0.0143 (14)	0.0062 (9)	0.033 (4)*
C7	0.16261 (13)	0.08928 (11)	0.01886 (7)	0.0264 (3)
H7	0.1217 (16)	0.0663 (13)	−0.0348 (9)	0.032 (4)*
C8	0.07650 (13)	0.15151 (11)	0.06946 (7)	0.0278 (3)
H8	−0.0281 (17)	0.1681 (14)	0.0528 (9)	0.037 (4)*
C9	0.13483 (12)	0.18579 (10)	0.14310 (7)	0.0242 (2)
H9	0.0741 (16)	0.2279 (13)	0.1793 (8)	0.030 (3)*
C10	0.25703 (12)	0.41252 (10)	0.25391 (6)	0.0221 (2)
H10	0.2241 (15)	0.4182 (12)	0.1985 (8)	0.026 (3)*
C11	0.18754 (12)	0.62568 (10)	0.25287 (6)	0.0211 (2)
C12	0.07684 (13)	0.62002 (11)	0.19349 (7)	0.0266 (3)
H12	0.0327 (17)	0.5402 (15)	0.1778 (9)	0.041 (4)*
C13	0.02996 (15)	0.72902 (12)	0.15667 (7)	0.0320 (3)
H13	−0.0492 (18)	0.7239 (15)	0.1140 (10)	0.044 (4)*
C14	0.09319 (15)	0.84091 (12)	0.17922 (8)	0.0328 (3)
H14	0.0611 (18)	0.9174 (15)	0.1518 (9)	0.046 (4)*
C15	0.20296 (15)	0.84466 (11)	0.23889 (8)	0.0329 (3)
H15	0.2490 (18)	0.9228 (16)	0.2557 (9)	0.046 (4)*
C16	0.25028 (13)	0.73711 (11)	0.27657 (7)	0.0275 (3)
H16	0.3280 (16)	0.7378 (13)	0.3209 (9)	0.033 (4)*
C17	0.57182 (12)	0.11615 (10)	0.40996 (6)	0.0222 (2)
C18	0.58624 (13)	−0.01172 (11)	0.40974 (7)	0.0246 (2)
H18	0.5275 (16)	−0.0599 (13)	0.3711 (8)	0.030 (4)*

C19	0.68443 (14)	−0.06779 (12)	0.46408 (7)	0.0309 (3)
H19	0.6950 (17)	−0.1599 (16)	0.4635 (9)	0.042 (4)*
C20	0.76560 (14)	0.00264 (13)	0.51877 (8)	0.0358 (3)
H20	0.8351 (19)	−0.0370 (16)	0.5572 (10)	0.050 (5)*
C21	0.74840 (15)	0.12980 (13)	0.51930 (8)	0.0369 (3)
H21	0.803 (2)	0.1830 (17)	0.5598 (10)	0.055 (5)*
C22	0.65314 (14)	0.18760 (12)	0.46431 (7)	0.0307 (3)
H22	0.6438 (17)	0.2784 (15)	0.4628 (9)	0.039 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0310 (4)	0.0277 (4)	0.0179 (4)	0.0011 (3)	−0.0025 (3)	−0.0018 (3)
N1	0.0239 (5)	0.0209 (5)	0.0192 (4)	0.0005 (3)	−0.0005 (4)	0.0000 (3)
N2	0.0253 (5)	0.0216 (5)	0.0199 (4)	−0.0002 (3)	−0.0010 (4)	−0.0012 (3)
N3	0.0205 (5)	0.0211 (5)	0.0195 (4)	−0.0004 (3)	0.0009 (3)	0.0003 (3)
C1	0.0217 (5)	0.0199 (5)	0.0214 (5)	−0.0008 (4)	0.0019 (4)	0.0012 (4)
C2	0.0226 (5)	0.0202 (5)	0.0214 (5)	0.0001 (4)	0.0026 (4)	0.0003 (4)
C3	0.0252 (6)	0.0203 (5)	0.0219 (5)	0.0003 (4)	0.0020 (4)	−0.0007 (4)
C4	0.0238 (5)	0.0173 (5)	0.0213 (5)	−0.0013 (4)	0.0000 (4)	0.0015 (4)
C5	0.0227 (6)	0.0225 (5)	0.0245 (5)	0.0023 (4)	−0.0006 (4)	0.0008 (4)
C6	0.0281 (6)	0.0230 (5)	0.0230 (6)	0.0011 (4)	0.0016 (4)	−0.0012 (4)
C7	0.0302 (6)	0.0245 (6)	0.0237 (6)	−0.0018 (4)	−0.0047 (5)	−0.0001 (4)
C8	0.0237 (6)	0.0267 (6)	0.0321 (6)	0.0009 (4)	−0.0052 (5)	0.0000 (5)
C9	0.0229 (6)	0.0221 (5)	0.0278 (6)	0.0008 (4)	0.0022 (4)	−0.0010 (4)
C10	0.0240 (6)	0.0220 (5)	0.0201 (5)	0.0005 (4)	0.0015 (4)	0.0001 (4)
C11	0.0222 (5)	0.0208 (5)	0.0207 (5)	0.0021 (4)	0.0040 (4)	0.0012 (4)
C12	0.0287 (6)	0.0233 (6)	0.0272 (6)	0.0010 (4)	−0.0016 (5)	−0.0012 (4)
C13	0.0363 (7)	0.0300 (6)	0.0287 (6)	0.0057 (5)	−0.0037 (5)	0.0023 (5)
C14	0.0419 (7)	0.0241 (6)	0.0324 (6)	0.0057 (5)	0.0029 (5)	0.0059 (5)
C15	0.0381 (7)	0.0209 (6)	0.0395 (7)	−0.0015 (5)	0.0011 (5)	0.0005 (5)
C16	0.0283 (6)	0.0237 (6)	0.0301 (6)	−0.0009 (4)	−0.0003 (5)	−0.0013 (5)
C17	0.0208 (5)	0.0258 (6)	0.0198 (5)	0.0002 (4)	0.0011 (4)	0.0030 (4)
C18	0.0266 (6)	0.0261 (6)	0.0213 (5)	0.0034 (4)	0.0023 (4)	−0.0007 (4)
C19	0.0327 (7)	0.0313 (7)	0.0287 (6)	0.0086 (5)	0.0026 (5)	0.0037 (5)
C20	0.0297 (7)	0.0442 (7)	0.0323 (7)	0.0036 (5)	−0.0061 (5)	0.0094 (6)
C21	0.0337 (7)	0.0415 (7)	0.0336 (7)	−0.0096 (5)	−0.0102 (5)	0.0044 (6)
C22	0.0321 (6)	0.0283 (6)	0.0307 (6)	−0.0064 (5)	−0.0053 (5)	0.0022 (5)

Geometric parameters (Å, º)

O1—N3	1.2999 (11)	C10—H10	0.982 (14)
N1—C3	1.3546 (14)	C11—C16	1.3845 (16)
N1—N2	1.3657 (12)	C11—C12	1.3857 (16)
N1—C17	1.4257 (13)	C12—C13	1.3927 (16)
N2—C1	1.3316 (14)	C12—H12	0.983 (16)
N3—C10	1.3076 (14)	C13—C14	1.3855 (18)
N3—C11	1.4523 (13)	C13—H13	0.994 (16)

C1—C2	1.4262 (15)	C14—C15	1.3828 (18)
C1—C4	1.4733 (14)	C14—H14	0.988 (17)
C2—C3	1.3836 (15)	C15—C16	1.3872 (17)
C2—C10	1.4343 (15)	C15—H15	0.980 (17)
C3—H3	0.973 (15)	C16—H16	1.003 (15)
C4—C9	1.3966 (16)	C17—C22	1.3875 (16)
C4—C5	1.3997 (16)	C17—C18	1.3912 (16)
C5—C6	1.3859 (16)	C18—C19	1.3878 (16)
C5—H5	0.979 (14)	C18—H18	0.976 (15)
C6—C7	1.3877 (17)	C19—C20	1.3846 (19)
C6—H6	0.988 (15)	C19—H19	1.003 (17)
C7—C8	1.3878 (17)	C20—C21	1.386 (2)
C7—H7	1.002 (14)	C20—H20	0.982 (17)
C8—C9	1.3903 (16)	C21—C22	1.3876 (17)
C8—H8	0.992 (15)	C21—H21	1.009 (18)
C9—H9	0.975 (14)	C22—H22	0.987 (16)

C3—N1—N2	112.30 (9)	C16—C11—C12	121.32 (10)
C3—N1—C17	128.19 (9)	C16—C11—N3	117.27 (10)
N2—N1—C17	119.47 (9)	C12—C11—N3	121.41 (10)
C1—N2—N1	104.89 (9)	C11—C12—C13	118.82 (11)
O1—N3—C10	123.09 (9)	C11—C12—H12	120.3 (9)
O1—N3—C11	116.56 (8)	C13—C12—H12	120.9 (9)
C10—N3—C11	120.21 (9)	C14—C13—C12	120.39 (11)
N2—C1—C2	111.32 (9)	C14—C13—H13	121.4 (9)
N2—C1—C4	120.24 (10)	C12—C13—H13	118.2 (9)
C2—C1—C4	128.43 (10)	C15—C14—C13	119.89 (11)
C3—C2—C1	104.51 (9)	C15—C14—H14	120.4 (9)
C3—C2—C10	130.34 (10)	C13—C14—H14	119.7 (9)
C1—C2—C10	124.64 (10)	C14—C15—C16	120.49 (12)
N1—C3—C2	106.98 (9)	C14—C15—H15	121.2 (10)
N1—C3—H3	121.2 (8)	C16—C15—H15	118.4 (10)
C2—C3—H3	131.8 (8)	C11—C16—C15	119.08 (11)
C9—C4—C5	119.18 (10)	C11—C16—H16	119.0 (8)
C9—C4—C1	121.19 (10)	C15—C16—H16	121.9 (8)
C5—C4—C1	119.62 (10)	C22—C17—C18	120.74 (11)
C6—C5—C4	120.04 (10)	C22—C17—N1	120.07 (10)
C6—C5—H5	120.1 (8)	C18—C17—N1	119.19 (10)
C4—C5—H5	119.8 (8)	C19—C18—C17	119.36 (11)
C5—C6—C7	120.69 (11)	C19—C18—H18	121.5 (8)
C5—C6—H6	120.9 (8)	C17—C18—H18	119.2 (8)
C7—C6—H6	118.4 (8)	C20—C19—C18	120.35 (12)
C6—C7—C8	119.49 (11)	C20—C19—H19	120.5 (9)
C6—C7—H7	119.9 (8)	C18—C19—H19	119.1 (9)
C8—C7—H7	120.6 (8)	C19—C20—C21	119.78 (12)
C7—C8—C9	120.41 (11)	C19—C20—H20	120.4 (10)
C7—C8—H8	118.7 (9)	C21—C20—H20	119.8 (10)
C9—C8—H8	120.9 (9)	C20—C21—C22	120.61 (12)

C8—C9—C4	120.19 (11)	C20—C21—H21	121.5 (10)
C8—C9—H9	120.7 (8)	C22—C21—H21	117.9 (10)
C4—C9—H9	119.1 (8)	C17—C22—C21	119.14 (12)
N3—C10—C2	123.79 (10)	C17—C22—H22	119.8 (9)
N3—C10—H10	114.1 (8)	C21—C22—H22	121.1 (9)
C2—C10—H10	121.8 (8)		

C3—N1—N2—C1	0.49 (12)	C3—C2—C10—N3	−10.05 (19)
C17—N1—N2—C1	−177.46 (9)	C1—C2—C10—N3	179.52 (11)
N1—N2—C1—C2	0.02 (12)	O1—N3—C11—C16	33.72 (14)
N1—N2—C1—C4	179.05 (9)	C10—N3—C11—C16	−142.14 (11)
N2—C1—C2—C3	−0.49 (13)	O1—N3—C11—C12	−146.36 (10)
C4—C1—C2—C3	−179.42 (11)	C10—N3—C11—C12	37.78 (15)
N2—C1—C2—C10	171.98 (10)	C16—C11—C12—C13	0.83 (18)
C4—C1—C2—C10	−6.94 (18)	N3—C11—C12—C13	−179.08 (10)
N2—N1—C3—C2	−0.81 (13)	C11—C12—C13—C14	−0.01 (19)
C17—N1—C3—C2	176.91 (10)	C12—C13—C14—C15	−0.3 (2)
C1—C2—C3—N1	0.76 (12)	C13—C14—C15—C16	−0.1 (2)
C10—C2—C3—N1	−171.12 (11)	C12—C11—C16—C15	−1.28 (18)
N2—C1—C4—C9	138.67 (11)	N3—C11—C16—C15	178.64 (11)
C2—C1—C4—C9	−42.49 (17)	C14—C15—C16—C11	0.91 (19)
N2—C1—C4—C5	−40.22 (15)	C3—N1—C17—C22	−19.80 (17)
C2—C1—C4—C5	138.62 (12)	N2—N1—C17—C22	157.78 (11)
C9—C4—C5—C6	0.95 (16)	C3—N1—C17—C18	160.22 (11)
C1—C4—C5—C6	179.86 (10)	N2—N1—C17—C18	−22.20 (15)
C4—C5—C6—C7	−0.57 (17)	C22—C17—C18—C19	−0.72 (17)
C5—C6—C7—C8	−0.32 (18)	N1—C17—C18—C19	179.27 (10)
C6—C7—C8—C9	0.81 (18)	C17—C18—C19—C20	1.00 (18)
C7—C8—C9—C4	−0.42 (18)	C18—C19—C20—C21	0.1 (2)
C5—C4—C9—C8	−0.46 (17)	C19—C20—C21—C22	−1.6 (2)
C1—C4—C9—C8	−179.35 (10)	C18—C17—C22—C21	−0.69 (19)
O1—N3—C10—C2	−4.28 (17)	N1—C17—C22—C21	179.32 (11)
C11—N3—C10—C2	171.30 (10)	C20—C21—C22—C17	1.8 (2)

Hydrogen-bond geometry (Å, º)

Cg2 and Cg3 are, respectively, the centroids of the C4–C9 and C11–C16 benzene rings.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1^{i}	0.979 (15)	2.303 (15)	3.2561 (14)	164.1 (11)
C6—H6···O1^{ii}	0.988 (15)	2.514 (15)	3.1746 (14)	124.1 (11)
C7—H7···O1^{ii}	1.003 (15)	2.544 (15)	3.1837 (14)	121.4 (11)
C9—H9···*Cg*3^{iii}	0.975 (14)	2.764 (14)	3.6409 (13)	152.8 (11)
C14—H14···*Cg*2^{iv}	0.988 (17)	2.884 (16)	3.6249 (14)	132.5 (12)
C19—H19···*Cg*2^{i}	1.003 (17)	2.678 (17)	3.6128 (14)	155.3 (12)

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