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4-[Bis(3-phenyl-1*H*-pyrazol-1-yl)methyl]-benzene-1,2-diol

Florian Blasberg, Hans-Wolfram Lerner and Michael Bolte*

Institut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, Germany
Correspondence e-mail: bolte@chemie.uni-frankfurt.de

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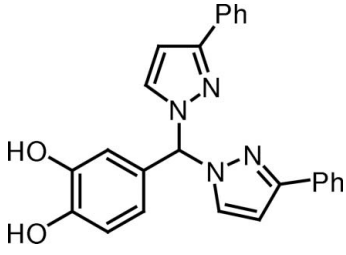
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.007 Å; R factor = 0.069; wR factor = 0.121; data-to-parameter ratio = 12.2.

The title compound, $C_{25}H_{20}N_4O_2$, is a ditopic *ortho*-hydroquinone-based bis(pyrazol-1-yl)methane ligand. The dihedral angles between the planes of the pyrazole rings and their attached phenyl rings are 17.4 (3) and 5.9 (4)°. The pyrazole rings make a dihedral angle of 87.84 (16)°. One of the two hydroxy groups forms an intramolecular hydrogen bond to the other hydroxy group, whereas the second is involved in an intermolecular O—H···N hydrogen bond. As a result of these intermolecular hydrogen bonds, helical chains running along the *b* axis are formed.

Related literature

For the synthesis, structural characterization and coordination behavior of ditopic *ortho*-hydroquinone-based bis(pyrazol-1-yl)methane ligands, see: Blasberg *et al.* (2011).



Experimental

Crystal data

$C_{25}H_{20}N_4O_2$
M_r = 408.45
Monoclinic, $P2_1/n$
a = 13.493 (3) Å
b = 5.6288 (11) Å
c = 26.309 (5) Å
β = 100.87 (3)°
V = 1962.3 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 173 K
0.40 × 0.15 × 0.10 mm

Data collection

Stoe IPDS II two-circle diffractometer
16343 measured reflections
3450 independent reflections
1434 reflections with $I > 2\sigma(I)$
R_{int} = 0.111

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.121
S = 0.82
3450 reflections
282 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O23—H23···O24	0.84	2.21	2.646 (5)	113
O24—H24···N12^{i}	0.84	2.08	2.853 (5)	153

Symmetry code: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2261).

References

Blasberg, F., Bolte, M., Wagner, M. & Lerner, H.-W. (2011). *J. Organomet. Chem.* doi:10.1016/j.jorganchem.2011.08.002.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Stoe & Cie (2001). *X-AREA*. Stoe & Cie, Darmstadt, Germany.

supporting information

Acta Cryst. (2011). E**67**, o2741 [https://doi.org/10.1107/S1600536811037949]

4-[Bis(3-phenyl-1*H*-pyrazol-1-yl)methyl]benzene-1,2-diol

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S1. Comment

Very recently we have reported on the synthesis, structural characterization, and coordination behavior of ditopic *ortho*-hydroquinone-based bis(pyrazol-1-yl)methane ligands (Blasberg *et al.*, 2011). In this report, we have already noted *ortho*-$(OH)_2C_6H_3$-4-CH(3-Phpz)$_2$, but metric parameters will be discussed here. The bis(pyrazol-1-yl)methane derivative (I) was prepared in a three-step one-pot procedure as shown in Fig. 1.

The dihedral angles between the planes of the pyrazol rings and the attached phenyl rings are 20.9 (3)° and 5.9 (4)°. One of the two hydroxy groups forms an intramolecular hydrogen bond to the other hydroxy group, whereas the second one is involved in an intermolecular O—H···N hydrogen bond. As a result of these intermolecular hydrogen bonds, helical chains running along the *b* axis are formed.

S2. Experimental

Neat 3-phenylpyrazole (2.00 g, 13.87 mmol) was added to NaH (0.33 g, 13.87 mmol) suspended in THF (60 ml) at r.t. After 30 min $SOCl_2$ (0.50 ml, 0.83 g, 6.94 mmol) was added in one portion and the resulting mixture stirred at r.t. for 5 min. After 3,4-dihydroxybenzaldehyde (0.96 g, 6.94 mmol) and pyridine (5.60 ml, 4.78 g, 60.40 mmol) were added, the reaction mixture was kept at reflux temperature for 16 h. H_2O (50 ml) was added and the aqueous phase extracted into CH_2Cl_2 (3×50 ml). The combined organic extracts were washed with brine, dried ($MgSO_4$), filtered, and the filtrate was evaporated to dryness in vacuo. The crude product was purified by column chromatography (silica gel; $CHCl_3$/EtOAc 1:1) and all product-containing fractions were concentrated by rotary evaporation at 40°C to ca. half of the original volume. Upon cooling to r.t. colorless crystals of the title compound precipitated, which were isolated by filtration and washed with Et_2O. Yield: 1.53 g (54%). Single crystals suitable for X-ray diffraction were obtained by repeatedly dissolving the compound in refluxing MeCN and letting the clear colorless solution cool to room temperature. After three cycles needles of sufficient size were obtained. R</f = 0.63 (silica gel, $CHCl_3$/EtOAc 1:1). ^{1}H NMR (400.1 MHz, d_6-DMSO) δ = 6.48 (dd, $^3J_{HH}$ = 8.3, $^4J_{HH}$ = 2.0, 1 H; HQ—H6), 6.66 (d, $^4J_{HH}$ = 2.0, 1 H; HQ—H2), 6.76 (d, $^3J_{HH}$ = 8.3, 1 H; HQ—H5), 6.84 (d, $^3J_{HH}$ = 2.5, 2 H; pz-H4), 7.31 (m, 2 H; Ph—H4), 7.41 (m, 4 H; Ph—H3), 7.82 (m, 4 H; Ph—H2), 7.91 (s, 1H, CH), 7.94 (d, $^3J_{HH}$ = 2.5, 2 H; pz-H5), 9.15 (bs, 2 H; OH). ^{13}C NMR (100.6 MHz, d_6-DMSO) δ = 76.7 (Cpz$_2$), 103.5 (pz-C4), 114.4 (HQ—C2), 115.5 (HQ—C5), 118.2 (HQ—C6), 125.3 (Ph—C2), 127.2 (HQ—C1), 127.8 (Ph—C4), 128.7 (Ph—C3), 131.9 (pz-C5), 132.8 (Ph—C1), 145.3, 146.1 (HQ—C3,4), 151.0 (pz-C3). ESI-MS: m/z (%) 263 (67) [M—Phpz]$^-$, 408 (100) [M—H]$^-$. Anal. Calcd (%) for $C_{25}H_{20}N_4O_2$ (408.45): C 73.51, H 4.94, N 13.72. Found: C 73.22, H 4.86, N 13.67.

S3. Refinement

All H atoms were geometrically positioned and refined using a riding model with fixed individual displacement parameters [U(H) = 1.2 U_{eq}(C) or U(H) = 1.5 U_{eq}(O, C_{methyl})] using a riding model with O—H = 0.84 Å, C—H(aromatic)

= 0.95Å or C—H(methine) = 1.00 Å, respectively. The H—O—C—C torsions angles of the hydroxy groups were refined.

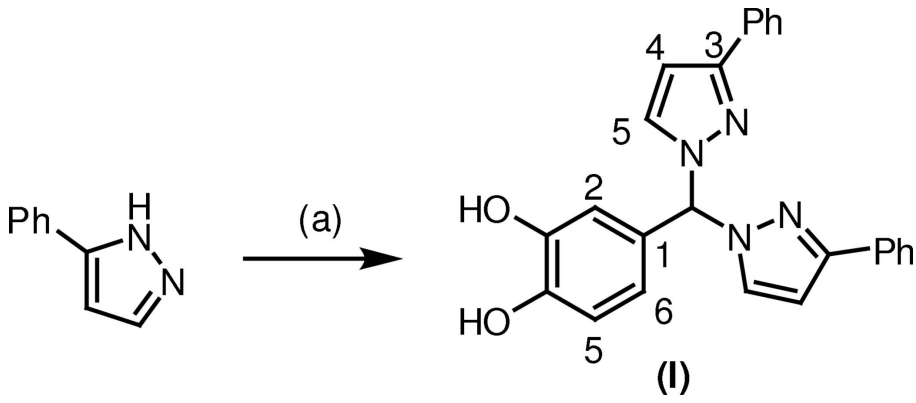

Figure 1

Synthesis and numbering scheme of *ortho*-hydroquinone-based bis(pyrazol-1-yl)methane ligand (I). (*a*) (i) NaH, THF, 30 min; (ii) $SOCl_2$, THF, 5 min; (iii) 3,4-dihydroxybenzaldehyde, pyridine, THF, reflux, over night.

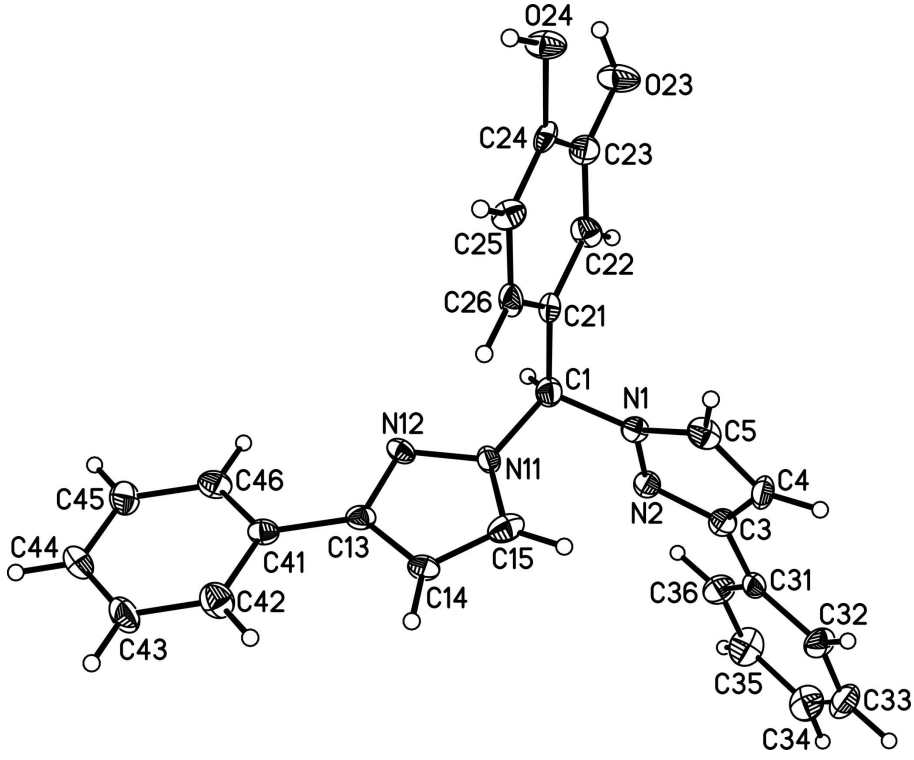

Figure 2

Perspective view of the title compound with displacement ellipsoids drawn at the 50% probability level.

4-[Bis(3-phenyl-1*H*-pyrazol-1-yl)methyl]benzene-1,2-diol

Crystal data

$C_{25}H_{20}N_4O_2$
M_r = 408.45
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 13.493 (3) Å
b = 5.6288 (11) Å

c = 26.309 (5) Å
β = 100.87 (3)°
V = 1962.3 (7) Å^3
Z = 4
F(000) = 856
D_x = 1.383 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 2882 reflections
θ = 3.7–25.8°
μ = 0.09 mm^{-1}
T = 173 K
Needle, colourless
0.40 × 0.15 × 0.10 mm

Data collection

Stoe IPDS II two-circle diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
16343 measured reflections
3450 independent reflections

1434 reflections with $I > 2\sigma(I)$
R_{int} = 0.111
θ_{max} = 25.0°, θ_{min} = 3.7°
h = −16→16
k = −6→6
l = −31→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.121
S = 0.82
3450 reflections
282 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.003P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Special details

Experimental. ;
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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
N1	0.6081 (3)	0.2494 (7)	0.30782 (15)	0.0162 (10)
C1	0.5052 (4)	0.2507 (9)	0.31608 (19)	0.0199 (12)
H1	0.4873	0.0847	0.3245	0.024*
N2	0.6784 (3)	0.1200 (7)	0.34051 (15)	0.0181 (9)
C3	0.7672 (4)	0.1933 (8)	0.33129 (19)	0.0189 (12)
C4	0.7529 (4)	0.3725 (8)	0.29212 (19)	0.0216 (12)
H4	0.8037	0.4530	0.2782	0.026*
C5	0.6523 (4)	0.4033 (9)	0.27902 (19)	0.0224 (12)
H5	0.6184	0.5127	0.2542	0.027*
N11	0.4994 (3)	0.4008 (7)	0.36107 (14)	0.0171 (9)

N12	0.4236 (3)	0.3584 (6)	0.38778 (15)	0.0165 (10)
C13	0.4318 (4)	0.5389 (8)	0.42204 (18)	0.0171 (12)
C14	0.5103 (4)	0.6909 (8)	0.4161 (2)	0.0214 (12)
H14	0.5308	0.8302	0.4356	0.026*
C15	0.5517 (4)	0.6011 (9)	0.37699 (19)	0.0239 (12)
H15	0.6064	0.6659	0.3635	0.029*
C21	0.4313 (4)	0.3296 (8)	0.26841 (19)	0.0179 (12)
C22	0.4107 (4)	0.1733 (8)	0.22619 (19)	0.0209 (12)
H22	0.4464	0.0273	0.2272	0.025*
C23	0.3402 (4)	0.2291 (9)	0.1838 (2)	0.0214 (12)
O23	0.3195 (3)	0.0753 (6)	0.14321 (13)	0.0287 (9)
H23	0.2640	0.1116	0.1245	0.043*
C24	0.2880 (4)	0.4488 (8)	0.18097 (19)	0.0168 (11)
O24	0.2181 (3)	0.4800 (6)	0.13669 (13)	0.0237 (9)
H24	0.1816	0.5976	0.1402	0.036*
C25	0.3102 (4)	0.6034 (8)	0.22209 (18)	0.0196 (12)
H25	0.2768	0.7525	0.2206	0.024*
C26	0.3800 (4)	0.5442 (8)	0.26527 (19)	0.0193 (12)
H26	0.3935	0.6523	0.2935	0.023*
C31	0.8626 (4)	0.0957 (8)	0.36075 (19)	0.0190 (11)
C32	0.9534 (4)	0.2161 (8)	0.3623 (2)	0.0238 (13)
H32	0.9540	0.3577	0.3427	0.029*
C33	1.0414 (4)	0.1348 (9)	0.3913 (2)	0.0312 (14)
H33	1.1021	0.2212	0.3919	0.037*
C34	1.0433 (4)	−0.0750 (10)	0.4203 (2)	0.0317 (14)
H34	1.1042	−0.1318	0.4409	0.038*
C35	0.9530 (5)	−0.1962 (9)	0.4177 (2)	0.0332 (15)
H35	0.9531	−0.3406	0.4364	0.040*
C36	0.8634 (4)	−0.1155 (9)	0.38900 (19)	0.0249 (13)
H36	0.8027	−0.2021	0.3884	0.030*
C41	0.3634 (4)	0.5541 (8)	0.45945 (19)	0.0176 (12)
C42	0.3673 (4)	0.7591 (9)	0.4918 (2)	0.0263 (13)
H42	0.4139	0.8830	0.4891	0.032*
C43	0.3040 (4)	0.7773 (9)	0.5268 (2)	0.0272 (14)
H43	0.3078	0.9133	0.5485	0.033*
C44	0.2345 (4)	0.6001 (9)	0.53102 (19)	0.0239 (12)
H44	0.1905	0.6154	0.5551	0.029*
C45	0.2296 (4)	0.4007 (9)	0.49981 (19)	0.0248 (12)
H45	0.1820	0.2790	0.5023	0.030*
C46	0.2950 (4)	0.3786 (8)	0.46467 (19)	0.0223 (12)
H46	0.2922	0.2396	0.4440	0.027*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.019 (3)	0.014 (2)	0.016 (2)	−0.0032 (19)	0.0029 (19)	0.0009 (17)
C1	0.019 (3)	0.021 (3)	0.021 (3)	−0.001 (2)	0.006 (2)	−0.003 (2)
N2	0.019 (2)	0.017 (2)	0.019 (2)	−0.0002 (19)	0.0042 (19)	−0.0018 (18)

C3	0.019 (3)	0.016 (2)	0.022 (3)	0.000 (2)	0.005 (2)	−0.004 (2)
C4	0.016 (3)	0.026 (3)	0.025 (3)	−0.002 (2)	0.010 (2)	0.001 (2)
C5	0.031 (3)	0.018 (3)	0.019 (3)	−0.003 (2)	0.004 (2)	0.004 (2)
N11	0.019 (2)	0.019 (2)	0.016 (2)	−0.005 (2)	0.0077 (19)	−0.0038 (18)
N12	0.021 (3)	0.014 (2)	0.014 (2)	0.0026 (18)	0.0023 (19)	−0.0035 (17)
C13	0.018 (3)	0.019 (3)	0.013 (3)	−0.002 (2)	0.000 (2)	0.002 (2)
C14	0.022 (3)	0.019 (3)	0.023 (3)	−0.005 (2)	0.004 (2)	−0.012 (2)
C15	0.020 (3)	0.022 (3)	0.027 (3)	−0.006 (2)	−0.001 (2)	0.002 (2)
C21	0.015 (3)	0.023 (3)	0.018 (3)	−0.002 (2)	0.008 (2)	0.000 (2)
C22	0.027 (3)	0.015 (2)	0.021 (3)	−0.002 (2)	0.006 (3)	−0.006 (2)
C23	0.021 (3)	0.020 (3)	0.024 (3)	−0.005 (2)	0.005 (2)	−0.009 (2)
O23	0.032 (2)	0.024 (2)	0.025 (2)	0.0058 (18)	−0.0061 (18)	−0.0090 (17)
C24	0.009 (3)	0.020 (3)	0.023 (3)	0.005 (2)	0.005 (2)	0.002 (2)
O24	0.026 (2)	0.0201 (19)	0.022 (2)	0.0082 (16)	−0.0056 (17)	−0.0014 (14)
C25	0.018 (3)	0.016 (2)	0.024 (3)	0.002 (2)	0.000 (2)	0.001 (2)
C26	0.020 (3)	0.017 (3)	0.024 (3)	−0.002 (2)	0.011 (2)	−0.008 (2)
C31	0.020 (3)	0.020 (2)	0.018 (3)	−0.005 (2)	0.008 (2)	−0.007 (2)
C32	0.025 (3)	0.021 (3)	0.025 (3)	−0.010 (2)	0.004 (3)	0.005 (2)
C33	0.020 (3)	0.036 (3)	0.038 (4)	−0.007 (3)	0.008 (3)	0.000 (3)
C34	0.022 (3)	0.037 (3)	0.034 (3)	0.012 (3)	0.002 (3)	0.006 (3)
C35	0.034 (4)	0.027 (3)	0.039 (4)	0.003 (3)	0.007 (3)	0.012 (3)
C36	0.024 (3)	0.020 (3)	0.029 (3)	−0.002 (2)	0.003 (3)	−0.001 (2)
C41	0.020 (3)	0.014 (3)	0.019 (3)	−0.001 (2)	0.001 (2)	−0.002 (2)
C42	0.032 (3)	0.022 (3)	0.027 (3)	−0.001 (3)	0.008 (3)	−0.002 (2)
C43	0.032 (4)	0.025 (3)	0.027 (3)	0.001 (3)	0.012 (3)	−0.010 (2)
C44	0.030 (3)	0.026 (3)	0.017 (3)	0.002 (3)	0.008 (2)	−0.002 (2)
C45	0.026 (3)	0.028 (3)	0.022 (3)	−0.006 (3)	0.010 (2)	0.003 (3)
C46	0.027 (3)	0.016 (2)	0.024 (3)	−0.005 (2)	0.003 (2)	−0.006 (2)

Geometric parameters (Å, º)

N1—C5	1.360 (6)	C24—C25	1.377 (7)
N1—N2	1.364 (5)	O24—H24	0.8400
N1—C1	1.445 (7)	C25—C26	1.373 (7)
C1—N11	1.468 (6)	C25—H25	0.9500
C1—C21	1.515 (6)	C26—H26	0.9500
C1—H1	1.0000	C31—C32	1.394 (7)
N2—C3	1.333 (7)	C31—C36	1.401 (7)
C3—C4	1.429 (7)	C32—C33	1.364 (7)
C3—C31	1.477 (7)	C32—H32	0.9500
C4—C5	1.348 (7)	C33—C34	1.403 (7)
C4—H4	0.9500	C33—H33	0.9500
C5—H5	0.9500	C34—C35	1.387 (8)
N11—C15	1.354 (6)	C34—H34	0.9500
N11—N12	1.367 (6)	C35—C36	1.376 (7)
N12—C13	1.349 (6)	C35—H35	0.9500
C13—C14	1.392 (7)	C36—H36	0.9500
C13—C41	1.473 (7)	C41—C46	1.376 (7)

C14—C15	1.358 (7)	C41—C42	1.430 (7)
C14—H14	0.9500	C42—C43	1.373 (7)
C15—H15	0.9500	C42—H42	0.9500
C21—C26	1.386 (6)	C43—C44	1.388 (7)
C21—C22	1.403 (6)	C43—H43	0.9500
C22—C23	1.360 (7)	C44—C45	1.385 (7)
C22—H22	0.9500	C44—H44	0.9500
C23—O23	1.362 (6)	C45—C46	1.398 (8)
C23—C24	1.418 (6)	C45—H45	0.9500
O23—H23	0.8400	C46—H46	0.9500
C24—O24	1.365 (6)		

C5—N1—N2	111.4 (4)	C25—C24—C23	118.6 (4)
C5—N1—C1	128.0 (4)	C24—O24—H24	109.5
N2—N1—C1	118.7 (4)	C26—C25—C24	120.7 (5)
N1—C1—N11	108.8 (4)	C26—C25—H25	119.7
N1—C1—C21	112.2 (4)	C24—C25—H25	119.7
N11—C1—C21	111.8 (4)	C25—C26—C21	121.2 (4)
N1—C1—H1	107.9	C25—C26—H26	119.4
N11—C1—H1	107.9	C21—C26—H26	119.4
C21—C1—H1	107.9	C32—C31—C36	118.6 (5)
C3—N2—N1	105.2 (4)	C32—C31—C3	120.5 (4)
N2—C3—C4	110.2 (5)	C36—C31—C3	120.8 (5)
N2—C3—C31	120.9 (4)	C33—C32—C31	121.4 (5)
C4—C3—C31	128.8 (5)	C33—C32—H32	119.3
C5—C4—C3	105.5 (5)	C31—C32—H32	119.3
C5—C4—H4	127.2	C32—C33—C34	120.7 (5)
C3—C4—H4	127.2	C32—C33—H33	119.6
C4—C5—N1	107.6 (4)	C34—C33—H33	119.6
C4—C5—H5	126.2	C35—C34—C33	117.5 (5)
N1—C5—H5	126.2	C35—C34—H34	121.3
C15—N11—N12	112.5 (4)	C33—C34—H34	121.3
C15—N11—C1	128.7 (4)	C36—C35—C34	122.6 (5)
N12—N11—C1	118.2 (4)	C36—C35—H35	118.7
C13—N12—N11	103.7 (4)	C34—C35—H35	118.7
N12—C13—C14	110.9 (5)	C35—C36—C31	119.2 (5)
N12—C13—C41	120.5 (4)	C35—C36—H36	120.4
C14—C13—C41	128.7 (4)	C31—C36—H36	120.4
C15—C14—C13	106.7 (4)	C46—C41—C42	118.1 (5)
C15—C14—H14	126.7	C46—C41—C13	122.8 (4)
C13—C14—H14	126.7	C42—C41—C13	119.1 (5)
N11—C15—C14	106.2 (5)	C43—C42—C41	120.1 (5)
N11—C15—H15	126.9	C43—C42—H42	119.9
C14—C15—H15	126.9	C41—C42—H42	119.9
C26—C21—C22	118.5 (5)	C42—C43—C44	121.0 (5)
C26—C21—C1	123.3 (4)	C42—C43—H43	119.5
C22—C21—C1	118.2 (4)	C44—C43—H43	119.5
C23—C22—C21	120.5 (5)	C45—C44—C43	119.5 (5)

C23—C22—H22	119.7	C45—C44—H44	120.3
C21—C22—H22	119.7	C43—C44—H44	120.3
C22—C23—O23	120.3 (5)	C44—C45—C46	119.9 (5)
C22—C23—C24	120.6 (4)	C44—C45—H45	120.0
O23—C23—C24	119.1 (4)	C46—C45—H45	120.0
C23—O23—H23	109.5	C41—C46—C45	121.4 (5)
O24—C24—C25	127.0 (4)	C41—C46—H46	119.3
O24—C24—C23	114.4 (4)	C45—C46—H46	119.3

C5—N1—C1—N11	−88.4 (5)	C22—C23—C24—O24	−178.9 (5)
N2—N1—C1—N11	74.6 (5)	O23—C23—C24—O24	1.8 (7)
C5—N1—C1—C21	35.9 (6)	C22—C23—C24—C25	−0.2 (8)
N2—N1—C1—C21	−161.0 (4)	O23—C23—C24—C25	−179.6 (5)
C5—N1—N2—C3	−0.7 (5)	O24—C24—C25—C26	177.4 (5)
C1—N1—N2—C3	−166.4 (4)	C23—C24—C25—C26	−1.1 (8)
N1—N2—C3—C4	0.1 (5)	C24—C25—C26—C21	1.0 (8)
N1—N2—C3—C31	178.5 (4)	C22—C21—C26—C25	0.4 (8)
N2—C3—C4—C5	0.6 (6)	C1—C21—C26—C25	−176.9 (5)
C31—C3—C4—C5	−177.7 (5)	N2—C3—C31—C32	−161.3 (5)
C3—C4—C5—N1	−1.0 (6)	C4—C3—C31—C32	16.8 (8)
N2—N1—C5—C4	1.1 (5)	N2—C3—C31—C36	16.7 (7)
C1—N1—C5—C4	165.2 (4)	C4—C3—C31—C36	−165.2 (5)
N1—C1—N11—C15	34.3 (6)	C36—C31—C32—C33	−1.3 (8)
C21—C1—N11—C15	−90.2 (6)	C3—C31—C32—C33	176.8 (5)
N1—C1—N11—N12	−155.2 (4)	C31—C32—C33—C34	0.6 (9)
C21—C1—N11—N12	80.2 (5)	C32—C33—C34—C35	0.7 (9)
C15—N11—N12—C13	−1.2 (5)	C33—C34—C35—C36	−1.4 (9)
C1—N11—N12—C13	−173.1 (4)	C34—C35—C36—C31	0.7 (9)
N11—N12—C13—C14	0.7 (5)	C32—C31—C36—C35	0.6 (8)
N11—N12—C13—C41	−178.6 (4)	C3—C31—C36—C35	−177.4 (5)
N12—C13—C14—C15	0.0 (6)	N12—C13—C41—C46	5.9 (7)
C41—C13—C14—C15	179.3 (5)	C14—C13—C41—C46	−173.3 (5)
N12—N11—C15—C14	1.2 (5)	N12—C13—C41—C42	−173.9 (4)
C1—N11—C15—C14	172.1 (5)	C14—C13—C41—C42	6.8 (8)
C13—C14—C15—N11	−0.7 (5)	C46—C41—C42—C43	−0.1 (8)
N1—C1—C21—C26	−110.4 (6)	C13—C41—C42—C43	179.7 (5)
N11—C1—C21—C26	12.2 (7)	C41—C42—C43—C44	−0.8 (8)
N1—C1—C21—C22	72.2 (6)	C42—C43—C44—C45	0.7 (8)
N11—C1—C21—C22	−165.1 (5)	C43—C44—C45—C46	0.4 (8)
C26—C21—C22—C23	−1.7 (8)	C42—C41—C46—C45	1.2 (7)
C1—C21—C22—C23	175.8 (5)	C13—C41—C46—C45	−178.6 (5)
C21—C22—C23—O23	−179.1 (5)	C44—C45—C46—C41	−1.4 (8)
C21—C22—C23—C24	1.6 (8)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O23—H23···O24	0.84	2.21	2.646 (5)	113

O24—H24···N12^{i}	0.84	2.08	2.853 (5)	153

Symmetry code: (i) $-x+1/2, y+1/2, -z+1/2$.