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N^2,$N^{2'}$-Bis(3-nitrobenzylidene)pyridine-2,6-dicarbohydrazide dimethylformamide disolvate trihydrate

Cuixia Cheng and Haowen Liu*

Key Laboratory of Catalysis and Materials Science of Hubei Provence, College of Chemistry and Materials Science, South Central University of Nationalities, Wuhan 430074, People's Republic of China
Correspondence e-mail: liuhwchem@mail.scuec.edu.cn

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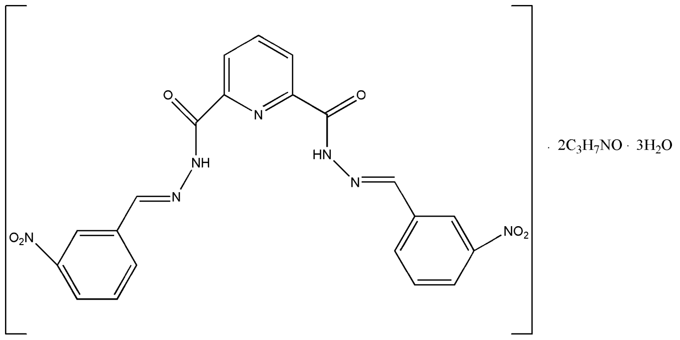
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.003 Å; disorder in solvent or counterion; R factor = 0.049; wR factor = 0.169; data-to-parameter ratio = 11.7.

In the title compound, $C_{21}H_{15}N_7O_6{\cdot}2C_3H_7NO{\cdot}3H_2O$, the N^2,$N^{2'}$-bis(3-nitrobenzylidene)pyridine-2,6-dicarbohydrazide and one water molecule are located on a twofold rotation axis. The molecules are connected by hydrogen bonds. One dimethylformamide molecule is disordered over two positions; the site occupancy factors are *ca* 0.8 and 0.2.

Related literature

Tridentate ligands with 2,6-dipicolinoyhydrazone have been intensively studied due to their interesting coordination modes (Paolucci *et al.*, 1985; Chen *et al.*, 1996, 1997).



Experimental

Crystal data

$C_{21}H_{15}N_7O_6{\cdot}2C_3H_7NO{\cdot}3H_2O$
M_r = 661.64
Monoclinic, $C2/c$
a = 24.704 (3) Å
b = 10.4815 (12) Å
c = 14.4792 (16) Å
β = 120.355 (2)°
V = 3235.2 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 273 (2) K
0.22 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.977, T_{max} = 0.979
9211 measured reflections
3170 independent reflections
2222 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.169
S = 1.08
3170 reflections
272 parameters
51 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O6^{i}	0.833 (16)	1.864 (17)	2.692 (2)	173 (3)
C9—H9···O4^{ii}	0.93	2.60	3.438 (10)	150
N2—H2A···O5	0.90 (2)	2.03 (2)	2.9082 (19)	166.4 (19)
O6—H6A···O1	0.799 (18)	2.05 (2)	2.834 (2)	167 (4)
O6—H6B···O4	0.843 (18)	1.89 (2)	2.728 (7)	175 (4)
C5—H5···O5	0.93	2.48	3.2860 (18)	145

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Bruker, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2593).

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supplementary materials

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N^2,$N^{2'}$-Bis(3-nitrobenzylidene)pyridine-2,6-dicarbohydrazide dimethylformamide disolvate trihydrate

C. Cheng and **H. Liu**

Comment

In recent years, hydrazones, possessing different donor atoms or cavities, have been investigated due to their coordinating capability and some biological activities, especially in bis-arylhydrazones. (Paolucci *et al.*, 1985; Chen *et al.*, 1996, 1997) 2,6-dipicolinoylhydrazine as a multidentate ligand is very useful for the research of coordination modes. As part of our continuing studies of the structures of hydrazones, we report here the synthesis and crystal structure of a novel tridentate ligand. One water molecule is inserted in the cavity of the hydrazone, each of the remaining water molecules and dimethylformamide solvents are located at the two sides of pyridyl ring. N, *N*-dimethylformamide molecules are disordered over two sites with unequal occupancy (Figure 1). In the title compound (I), the two spacer units (one is from atom C1 to C6, another is from atom C1a to C6a.) adopt a nearly planar all-*trans* conformation. The pyridyl ring is effectively coplanar with two spacer units. The two independent aryl rings are essentially coplanar with these spacer units, while the nitro-groups are slightly twisted out of the plane of these spacer units. The independent molecular components are linked by hydrogen bonds.

Experimental

To a solution of 3-nitrobenzaldehyde (1.66 g, 11 mmol) in absolute ethanol (40 ml) a suspension of 2,6-dipicolinoyhydrazine in the same solvent (50 ml) was added at 353 K. The mixture was left to react at reflux for 10 h, then the pale yellow product was filtered, washed with hot ethanol (20 ml portion) three times and dried *in vacuo*. Crystals suitable for X-ray diffraction were obtained from dimethylformamide-methanol (3:1 *v*/*v*) over a period of about three weeks. Melting point: 601 K.

Refinement

Corresponding distances and angles of the disordered DMF molecule, were restrained to be equal. Their anisotropic displacement parameters were restrained to an isotropic shape. Refinement of the site-occupancy factors for the two components gave values of 0.78 (1) and 0.22 (1) for the major and minor components. All the H atoms bonded to C atoms were set to ideal geometrical positions with C–H ranging from 0.93Å to 0.96Å and with $U_{\rm iso}$(H) =1.2$U_{\rm eq}$(aromatic C) or 1.5$U_{\rm eq}$(methyl C). Coordinates of the H atoms bonded to N or O atoms were refined with $U_{\rm iso}$(H) =1.2$U_{\rm eq}$(N) or 1.5$U_{\rm eq}$(O), respectively.

Figures

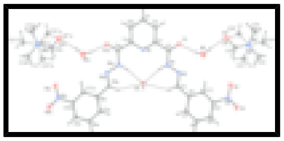


Fig. 1. The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level. Dashed lines indicate hydrogen bonds.

N^2,*N*$^{2'}$—Bis(3-nitrobenzylidene)pyridine-2,6-dicarbohydrazide dimethylformamide disolvate trihydrate

Crystal data

$C_{21}H_{15}N_7O_6 \cdot 2C_3H_7NO \cdot 3H_2O$

$M_r = 661.64$

Monoclinic, *C*2/*c*

Hall symbol: -C 2yc

$a = 24.704$ (3) Å

$b = 10.4815$ (12) Å

$c = 14.4792$ (16) Å

$\beta = 120.355$ (2)°

$V = 3235.2$ (6) Å^3

$Z = 4$

$F_{000} = 1392$

$D_x = 1.358$ Mg m^{-3}

Mo *K*α radiation
$\lambda = 0.71073$ Å

Cell parameters from 2433 reflections

$\theta = 2.4$–24.1°

$\mu = 0.11$ mm^{-1}

$T = 273$ (2) K

Block, pale yellow

0.22 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 273(2)$ K

phi and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2001)

$T_{min} = 0.977$, $T_{max} = 0.979$

9211 measured reflections

3170 independent reflections

2222 reflections with $I > 2\sigma(I)$

$R_{int} = 0.018$

$\theta_{max} = 26.0°$

$\theta_{min} = 2.2°$

$h = -30 \rightarrow 30$

$k = -12 \rightarrow 12$

$l = -17 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.049$

$wR(F^2) = 0.169$

$S = 1.08$

3170 reflections

272 parameters

51 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

$w = 1/[\sigma^2(F_o^2) + (0.1056P)^2 + 0.1192P]$
where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.43$ e Å^{-3}

$\Delta\rho_{min} = -0.17$ e Å^{-3}

Extinction correction: none

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.

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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	0.02389 (8)	0.81428 (16)	0.20004 (15)	0.0577 (5)	
C2	0.02453 (11)	0.94590 (19)	0.1985 (2)	0.0813 (7)	
H2	0.0415	0.9888	0.1627	0.098*	
C3	0.0000	1.0127 (3)	0.2500	0.0923 (11)	
H3	0.0000	1.1015	0.2500	0.111*	
C4	0.05053 (9)	0.74204 (17)	0.14262 (16)	0.0583 (5)	
C5	0.07425 (8)	0.42180 (18)	0.11595 (15)	0.0603 (5)	
H5	0.0574	0.3909	0.1562	0.072*	
C6	0.09827 (8)	0.33080 (17)	0.06894 (15)	0.0563 (5)	
C7	0.09512 (10)	0.20133 (19)	0.08487 (19)	0.0724 (6)	
H7	0.0777	0.1746	0.1255	0.087*	
C8	0.11679 (11)	0.11154 (19)	0.0428 (2)	0.0797 (7)	
H8	0.1135	0.0253	0.0543	0.096*	
C9	0.14336 (10)	0.1483 (2)	−0.01612 (18)	0.0739 (6)	
H9	0.1585	0.0882	−0.0447	0.089*	
C10	0.14703 (8)	0.27662 (19)	−0.03173 (15)	0.0601 (5)	
C11	0.12441 (8)	0.36987 (18)	0.00764 (15)	0.0562 (5)	
H11	0.1265	0.4558	−0.0062	0.067*	
N1	0.0000	0.74859 (17)	0.2500	0.0504 (5)	
N2	0.05128 (7)	0.61435 (14)	0.15307 (13)	0.0569 (4)	
H2A	0.0369 (9)	0.573 (2)	0.1909 (17)	0.068*	
N3	0.07557 (7)	0.54085 (15)	0.10391 (12)	0.0569 (4)	
N4	0.17601 (8)	0.3184 (2)	−0.09403 (15)	0.0781 (5)	
O1	0.06961 (7)	0.79807 (14)	0.09078 (13)	0.0815 (5)	
O2	0.18130 (10)	0.4303 (2)	−0.10546 (17)	0.1116 (7)	
O3	0.19383 (10)	0.2370 (2)	−0.13148 (17)	0.1126 (7)	
O5	0.0000	0.44674 (18)	0.2500	0.0710 (6)	
H5A	0.0265 (11)	0.402 (2)	0.3000 (19)	0.107*	
O6	0.07737 (13)	0.7056 (2)	−0.08613 (17)	0.1214 (8)	
H6A	0.070 (2)	0.726 (4)	−0.040 (3)	0.182*	
H6B	0.1015 (18)	0.756 (3)	−0.094 (4)	0.182*	
C12	0.18750 (15)	0.7702 (3)	−0.1301 (2)	0.0744 (9)	0.781 (4)
H12A	0.1756	0.6860	−0.1300	0.089*	0.781 (4)

C13	0.2617 (2)	0.6854 (4)	−0.1750 (4)	0.1137 (14)	0.781 (4)
H13A	0.2487	0.6065	−0.1586	0.171*	0.781 (4)
H13B	0.3065	0.6928	−0.1325	0.171*	0.781 (4)
H13C	0.2491	0.6871	−0.2495	0.171*	0.781 (4)
C14	0.2445 (2)	0.9163 (4)	−0.1734 (4)	0.1282 (17)	0.781 (4)
H14A	0.2229	0.9772	−0.1541	0.192*	0.781 (4)
H14B	0.2301	0.9235	−0.2484	0.192*	0.781 (4)
H14C	0.2888	0.9327	−0.1330	0.192*	0.781 (4)
O4	0.1592 (3)	0.8575 (10)	−0.1098 (8)	0.096 (2)	0.781 (4)
N5	0.2325 (5)	0.7922 (5)	−0.1510 (10)	0.073 (2)	0.781 (4)
C12'	0.1999 (5)	0.8886 (10)	−0.1353 (9)	0.082 (3)	0.219 (4)
H12B	0.2177	0.9686	−0.1109	0.099*	0.219 (4)
C13'	0.2179 (6)	0.6684 (10)	−0.1392 (10)	0.095 (4)	0.219 (4)
H13D	0.1813	0.6642	−0.1324	0.142*	0.219 (4)
H13E	0.2544	0.6488	−0.0716	0.142*	0.219 (4)
H13F	0.2141	0.6078	−0.1919	0.142*	0.219 (4)
C14'	0.2747 (6)	0.8196 (17)	−0.1897 (12)	0.121 (6)	0.219 (4)
H14D	0.2748	0.9089	−0.2045	0.181*	0.219 (4)
H14E	0.2695	0.7707	−0.2497	0.181*	0.219 (4)
H14F	0.3137	0.7973	−0.1272	0.181*	0.219 (4)
O4'	0.1497 (12)	0.849 (4)	−0.142 (3)	0.099 (8)	0.219 (4)
N5'	0.2237 (16)	0.7926 (15)	−0.171 (3)	0.062 (6)	0.219 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0639 (10)	0.0489 (10)	0.0711 (12)	−0.0025 (8)	0.0420 (10)	0.0030 (8)
C2	0.1114 (17)	0.0489 (11)	0.1180 (19)	−0.0064 (10)	0.0832 (16)	0.0050 (10)
C3	0.136 (3)	0.0412 (15)	0.138 (3)	0.000	0.097 (3)	0.000
C4	0.0662 (11)	0.0531 (11)	0.0706 (12)	−0.0024 (8)	0.0455 (10)	0.0034 (8)
C5	0.0680 (11)	0.0576 (11)	0.0738 (13)	0.0000 (8)	0.0493 (10)	0.0025 (9)
C6	0.0582 (10)	0.0519 (10)	0.0657 (11)	0.0016 (8)	0.0363 (9)	0.0012 (8)
C7	0.0847 (13)	0.0597 (12)	0.0920 (15)	0.0015 (10)	0.0589 (13)	0.0080 (10)
C8	0.0949 (15)	0.0510 (11)	0.1070 (18)	0.0048 (10)	0.0612 (15)	0.0002 (10)
C9	0.0766 (13)	0.0655 (13)	0.0842 (15)	0.0101 (10)	0.0441 (12)	−0.0066 (10)
C10	0.0562 (10)	0.0695 (12)	0.0600 (11)	0.0031 (8)	0.0334 (9)	−0.0026 (9)
C11	0.0557 (10)	0.0547 (10)	0.0615 (11)	0.0002 (7)	0.0319 (9)	−0.0001 (8)
N1	0.0563 (11)	0.0434 (10)	0.0603 (12)	0.000	0.0359 (10)	0.000
N2	0.0685 (9)	0.0526 (9)	0.0702 (10)	0.0018 (7)	0.0503 (9)	0.0019 (7)
N3	0.0634 (9)	0.0556 (9)	0.0663 (9)	0.0017 (7)	0.0434 (8)	−0.0011 (7)
N4	0.0780 (11)	0.0949 (14)	0.0733 (12)	0.0066 (10)	0.0469 (10)	−0.0077 (10)
O1	0.1125 (12)	0.0662 (9)	0.1074 (12)	−0.0021 (8)	0.0861 (11)	0.0069 (7)
O2	0.1550 (18)	0.0978 (14)	0.1371 (17)	−0.0115 (12)	0.1145 (15)	0.0072 (11)
O3	0.1362 (16)	0.1242 (15)	0.1246 (16)	0.0128 (12)	0.1007 (15)	−0.0147 (12)
O5	0.0975 (16)	0.0544 (12)	0.0868 (15)	0.000	0.0654 (13)	0.000
O6	0.1643 (19)	0.1363 (18)	0.1002 (14)	−0.0651 (14)	0.0939 (14)	−0.0337 (12)
C12	0.090 (2)	0.0651 (18)	0.080 (2)	−0.0044 (15)	0.0518 (17)	−0.0003 (14)
C13	0.114 (3)	0.124 (3)	0.128 (3)	0.012 (2)	0.080 (3)	−0.008 (2)

C14	0.152 (4)	0.118 (3)	0.138 (3)	−0.064 (3)	0.091 (3)	−0.016 (3)
O4	0.119 (3)	0.088 (2)	0.120 (6)	0.003 (3)	0.090 (4)	−0.002 (3)
N5	0.073 (3)	0.085 (3)	0.071 (6)	−0.0111 (18)	0.044 (4)	−0.0078 (18)
C12'	0.094 (6)	0.074 (6)	0.098 (7)	−0.016 (5)	0.063 (5)	−0.008 (5)
C13'	0.092 (7)	0.077 (7)	0.105 (8)	0.010 (6)	0.043 (6)	−0.016 (6)
C14'	0.104 (8)	0.175 (14)	0.133 (10)	−0.008 (8)	0.096 (8)	−0.035 (9)
O4'	0.103 (9)	0.126 (13)	0.088 (13)	0.006 (8)	0.063 (8)	0.002 (9)
N5'	0.064 (9)	0.083 (9)	0.043 (8)	−0.004 (6)	0.030 (7)	−0.001 (5)

Geometric parameters (Å, °)

C1—N1	1.333 (2)	N4—O2	1.202 (3)
C1—C2	1.380 (3)	O5—O6	6.641 (2)
C1—C4	1.500 (3)	O5—H5A	0.833 (16)
C2—C3	1.368 (3)	O6—H6A	0.799 (18)
C2—H2	0.9300	O6—H6B	0.843 (18)
C3—C2^{i}	1.368 (3)	C12—O4	1.272 (10)
C3—H3	0.9300	C12—N5	1.312 (5)
C4—O1	1.220 (2)	C12—H12A	0.9300
C4—N2	1.346 (2)	C13—N5	1.466 (6)
C5—N3	1.263 (2)	C13—H13A	0.9600
C5—C6	1.461 (3)	C13—H13B	0.9600
C5—H5	0.9300	C13—H13C	0.9600
C6—C11	1.397 (3)	C14—N5	1.408 (6)
C6—C7	1.385 (3)	C14—H14A	0.9600
C7—C8	1.369 (3)	C14—H14B	0.9600
C7—H7	0.9300	C14—H14C	0.9600
C8—C9	1.368 (3)	C12'—O4'	1.27 (2)
C8—H8	0.9300	C12'—N5'	1.394 (14)
C9—C10	1.375 (3)	C12'—H12B	0.9300
C9—H9	0.9300	C13'—N5'	1.414 (14)
C10—C11	1.384 (3)	C13'—H13D	0.9600
C10—N4	1.473 (3)	C13'—H13E	0.9600
C11—H11	0.9300	C13'—H13F	0.9600
N1—C1^{i}	1.333 (2)	C14'—N5'	1.440 (14)
N2—N3	1.376 (2)	C14'—H14D	0.9600
N2—O5	2.9082 (19)	C14'—H14E	0.9600
N2—H2A	0.90 (2)	C14'—H14F	0.9600
N4—O3	1.207 (2)		

N1—C1—C2	122.48 (18)	O2—N4—C10	119.66 (18)
N1—C1—C4	118.58 (15)	N2—O5—H5A	115 (2)
C2—C1—C4	118.93 (17)	O6—O5—H5A	118 (2)
C3—C2—C1	119.4 (2)	O5—O6—H6B	146 (3)
C3—C2—H2	120.3	H6A—O6—H6B	114 (3)
C1—C2—H2	120.3	O4—C12—N5	123.7 (5)
C2^{i}—C3—C2	118.4 (3)	O4—C12—H12A	118.2
C2^{i}—C3—H3	120.8	N5—C12—H12A	118.2
C2—C3—H3	120.8	N5—C13—H13A	109.5

O1—C4—N2	124.07 (17)	N5—C13—H13B	109.5
O1—C4—C1	120.80 (16)	H13A—C13—H13B	109.5
N2—C4—C1	115.13 (15)	N5—C13—H13C	109.5
N3—C5—C6	122.41 (17)	H13A—C13—H13C	109.5
N3—C5—H5	118.8	H13B—C13—H13C	109.5
C6—C5—H5	118.8	N5—C14—H14A	109.5
C11—C6—C7	118.41 (17)	N5—C14—H14B	109.5
C11—C6—C5	122.13 (16)	H14A—C14—H14B	109.5
C7—C6—C5	119.46 (17)	N5—C14—H14C	109.5
C8—C7—C6	122.1 (2)	H14A—C14—H14C	109.5
C8—C7—H7	118.9	H14B—C14—H14C	109.5
C6—C7—H7	118.9	C12—N5—C14	121.2 (5)
C7—C8—C9	120.19 (19)	C12—N5—C13	119.8 (4)
C7—C8—H8	119.9	C14—N5—C13	117.6 (4)
C9—C8—H8	119.9	O4'—C12'—N5'	109 (2)
C10—C9—C8	118.04 (19)	O4'—C12'—H12B	125.7
C10—C9—H9	121.0	N5'—C12'—H12B	125.7
C8—C9—H9	121.0	N5'—C13'—H13D	109.5
C9—C10—C11	123.34 (19)	N5'—C13'—H13E	109.5
C9—C10—N4	118.96 (18)	H13D—C13'—H13E	109.5
C11—C10—N4	117.70 (18)	N5'—C13'—H13F	109.5
C6—C11—C10	117.86 (17)	H13D—C13'—H13F	109.5
C6—C11—H11	121.1	H13E—C13'—H13F	109.5
C10—C11—H11	121.1	N5'—C14'—H14D	109.5
C1^{i}—N1—C1	117.8 (2)	N5'—C14'—H14E	109.5
C4—N2—N3	118.92 (15)	H14D—C14'—H14E	109.5
C4—N2—O5	132.09 (12)	N5'—C14'—H14F	109.5
N3—N2—O5	108.77 (11)	H14D—C14'—H14F	109.5
C4—N2—H2A	124.1 (13)	H14E—C14'—H14F	109.5
N3—N2—H2A	117.0 (13)	C14'—N5'—C13'	119.0 (15)
C5—N3—N2	115.69 (15)	C14'—N5'—C12'	120.1 (16)
O3—N4—O2	122.6 (2)	C13'—N5'—C12'	114.2 (14)
O3—N4—C10	117.8 (2)		

N1—C1—C2—C3	0.1 (3)	C2—C1—N1—C1^{i}	−0.07 (15)
C4—C1—C2—C3	179.59 (17)	C4—C1—N1—C1^{i}	−179.52 (19)
C1—C2—C3—C2^{i}	−0.07 (14)	O1—C4—N2—N3	0.8 (3)
N1—C1—C4—O1	175.80 (17)	C1—C4—N2—N3	−179.30 (15)
C2—C1—C4—O1	−3.7 (3)	O1—C4—N2—O5	−173.09 (14)
N1—C1—C4—N2	−4.1 (2)	C1—C4—N2—O5	6.8 (3)
C2—C1—C4—N2	176.45 (18)	C6—C5—N3—N2	−179.94 (16)
N3—C5—C6—C11	0.1 (3)	C4—N2—N3—C5	−179.27 (17)
N3—C5—C6—C7	−179.70 (17)	O5—N2—N3—C5	−4.04 (19)
C11—C6—C7—C8	0.1 (3)	C9—C10—N4—O3	2.0 (3)
C5—C6—C7—C8	179.9 (2)	C11—C10—N4—O3	−177.54 (19)
C6—C7—C8—C9	0.8 (4)	C9—C10—N4—O2	−177.7 (2)
C7—C8—C9—C10	−0.4 (4)	C11—C10—N4—O2	2.7 (3)
C8—C9—C10—C11	−1.0 (3)	C4—N2—O5—O6	132.8 (3)
C8—C9—C10—N4	179.4 (2)	N3—N2—O5—O6	−41.54 (13)

C7—C6—C11—C10	−1.4 (3)	O4—C12—N5—C14	−12.8 (15)
C5—C6—C11—C10	178.74 (17)	O4—C12—N5—C13	−179.1 (8)
C9—C10—C11—C6	1.9 (3)	O4'—C12'—N5'—C14'	170 (3)
N4—C10—C11—C6	−178.49 (16)	O4'—C12'—N5'—C13'	−39 (4)

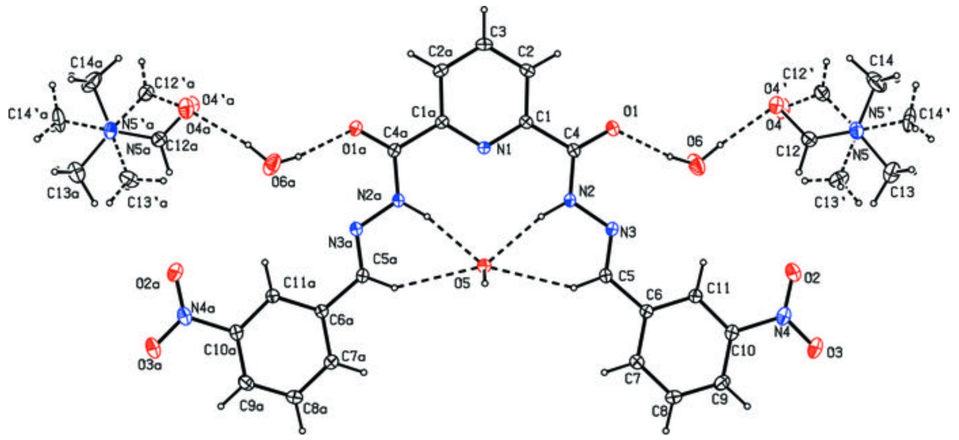
Symmetry codes: (i) −*x*, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5A···O6^{ii}	0.833 (16)	1.864 (17)	2.692 (2)	173 (3)
C9—H9···O4^{iii}	0.93	2.60	3.438 (10)	150
N2—H2A···O5	0.90 (2)	2.03 (2)	2.9082 (19)	166.4 (19)
O6—H6A···O1	0.799 (18)	2.05 (2)	2.834 (2)	167 (4)
O6—H6B···O4	0.843 (18)	1.89 (2)	2.728 (7)	175 (4)
C5—H5···O5	0.93	2.48	3.2860 (18)	145

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

Fig. 1


C3
C2a
C2
C14a
C12'a
O4'a
O4a
C14'a
N5'a
N5a
C12a
C13a
C13'a
O6a
O1a
C4a
C1a
C1
N1
C4
O1
O6
C12'
O4'
O4
C12
C14
N5'
N5
C14'
C13'
C13
N2a
N2
N3a
N3
C5a
O5
C5
O2a
N4a
C11a
C6a
C6
C11
O2
N4
O3a
C10a
C7a
C10
O3
C7
C9a
C8a
C8
C9