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3,5-Dinitro-*N*-(tri-2-pyridylmethyl)-benzamide

Katayoun Marjani, Hossein Abbastabar-Ahangar,* Leila Mohammadi, Mohsen Mousavi and Jafar Attar Gharamaleki

Faculty of Chemistry, Teacher Training University, 49 Mofateh Avenue 15614, Tehran, Iran
Correspondence e-mail: abbastabar@gmail.com

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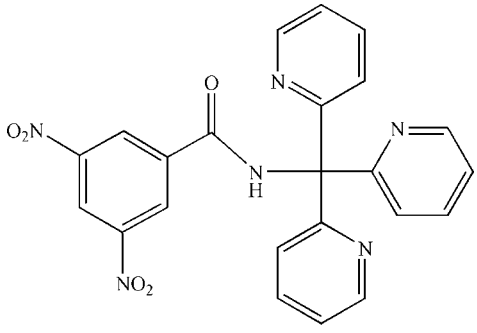
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.001 Å; R factor = 0.037; wR factor = 0.099; data-to-parameter ratio = 19.1.

The title compound, $C_{23}H_{16}N_6O_5$, was synthesized by reaction of tri-2-pyridylmethylamine and 3,5-dinitrobenzoyl chloride. There is an intramolecular N—H···N hydrogen bond [N···N = 2.5740 (12) Å] between the amide group and one of the three pyridine rings. The crystal packing is stabilized by weak intermolecular C—H···O hydrogen bonds.

Related literature

For reversible O_2 binding to Cu^I complexes with tripodal ligands, see: Lee *et al.* (1995), Jacobson *et al.* (1988); Tyekler *et al.* (1989). For fluoride as a terminal and a bridging ligand in Cu^{II}[tris(2-pyridylmethyl)amine] complexes, see: Jacobson *et al.* (1991). For the chemistry of $LCu^{II}Cl$ complexes with a quinolyl-containing tripodal tetradentate ligand L, see: Wei *et al.* (1994).



Experimental

Crystal data

$C_{23}H_{16}N_6O_5$
M_r = 456.42
Monoclinic, $P2_1/n$
a = 14.7680 (7) Å
b = 8.4109 (5) Å
c = 16.7738 (9) Å
β = 104.015 (5)°
V = 2021.49 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 100 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.970, T_{max} = 0.980
25445 measured reflections
5854 independent reflections
5015 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.099
S = 1.01
5854 reflections
307 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 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
N1—H1N···N4	0.88	2.07	2.5740 (12)	115
C16—H16A···O1^{i}	0.95	2.34	3.2796 (13)	169
C18—H18A···O4^{ii}	0.95	2.52	3.4414 (13)	164
C23—H23A···O3^{iii}	0.95	2.58	3.2522 (15)	128

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x-\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: CV2269).

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supplementary materials

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3,5-Dinitro-*N*-(tri-2-pyridylmethyl)benzamide

K. Marjani, H. Abbastabar-Ahangar, L. Mohammadi, M. Mousavi and J. Attar Gharamaleki

Comment

Tripodal ligands based on nitrogen heterocycles have secured an important place in inorganic chemistry. Ligands of this type reported to date can broadly be divided into two classes: those in which the arms of the tripod are connected *via* methylene linking groups to a teriary amine function, which is itself generally involved in coordination, and those in which the centeral linking atom does not coordinate to the metal for chemical or geometric reasons. An example of the first class is furnished by tris- (2-pyridyl-methyl) amine(tpm) and its derivatives, whose copper complexes have been extensively studied (Jacobson *et al.*,1988, 1991, Lee *et al.*, 1995, Tyekler *et al.*, 1989, Wei *et al.*,1994). The structure determnation of the title compound, $C_{23}H_{16}N_6O_5$, was undertaken as part of our studies on tpm derivaties. The crystal structure of free 3,5-dinitro-*N*-(tri-pyridin-2yl-methyl)-benzamide is shown in Fig.1. The only sp^3 carbon atom in the molecule, C8, has a distorted tetrahedral geometry with bond angles range from 105.82 (7) to 115.50 (8)°. The benzamide part of the molecule is nearly laying in a plane, but three pyridine rings make angles of 15.87 (5), 70.06 (5), and 75.70 (5)° with the plane of phenyl ring, giving a propeller-type geometry. From the two nitro groups, one is almost laying in the same plane with benzamide and the other is rotated out of this plane by angle of 29.25°, because of intermolecular van der Waals repulsion between two nitro groups in the packing of molecules (Fig. 2). The main point of interest in the structure is the intramolecular hydrogen bonding between the amido hydrogen atom and one of the pyridine rings (Fig. 3), N1—H1N···N4 [N1···N4 2.5740 (12) Å]. The packing of molecules in the solid state is stabilized by C—H···O intermolecular interactions with C···O distances range from 3.2522 (15) to 3.4414 (13) Å. There are also C—H···π intermolecular interactions, with H···π distances of 3.026 and 3.046 Å which take part in stabilization of molecular packing (Fig. 4).

Experimental

To a solution of tris(2-pyridyl)methylamine (0.5 g, 1.9 mmol) and triethylamine (3.6 mmol) in THF(14 ml) was added 3,5-dinitrobenzoylchloride (0.58, 2.5 mmol). After stirring at 4–5°C for 2 h, the precipitate was filtered off, washed with water and recrystallized from ethanol as title compound(I), 3,5-dinitro-*N*-(tri-pyridin-2yl-methyl)-benzamide (0.87 g, 95%). mp: 220°C; IR: 3326, 1680, 1586, 1541, 1501, 1345 cm^{-1}.

Refinement

The hydrogen atom of NH-group was localized in difference Fourier synthesis and placed in idealized position (N—H 0.89 Å). The C-bound H atoms were placed in calculated positions (C—H 0.95 Å). All H atoms were refined in riding model approximation, with U_{iso}(H) = 1.2Ueq of the parent atom.

Figures

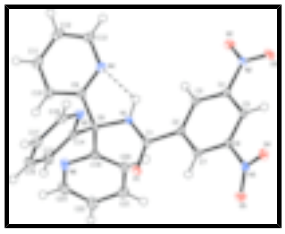

Fig.1.
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

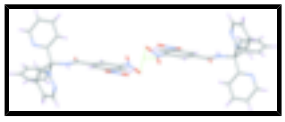

Fig. 2
Intermolecular van der Waals repulsion between two nitro groups.

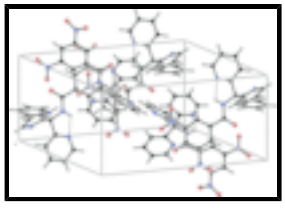

Fig. 3
The crystal packing of (I), hydrogen bond are shown as dashed lines.

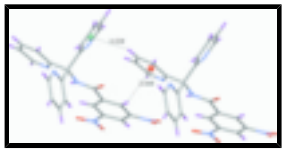

Fig. 4
C—H···π stacking interactions between two aromatic rings.

3,5-Dinitro-*N*-(tri-2-pyridylmethyl)benzamide

Crystal data

$C_{23}H_{16}N_6O_5$	F_{000} = 944
M_r = 456.42	D_x = 1.500 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 5259 reflections
a = 14.7680 (7) Å	θ = 2.7–30.0º
b = 8.4109 (5) Å	μ = 0.11 mm^{-1}
c = 16.7738 (9) Å	T = 100 (2) K
β = 104.015 (5)º	Prism, light-brown
V = 2021.49 (19) Å^3	0.30 × 0.20 × 0.20 mm
Z = 4	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	5854 independent reflections
Radiation source: fine-focus sealed tube	5015 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.025
T = 100(2) K	θ_{max} = 30.0º
φ and ω scans	θ_{min} = 1.7º

Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
T_{min} = 0.970, T_{max} = 0.980
25445 measured reflections

h = −20→20
k = −11→11
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.099
S = 1.01
5854 reflections
307 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 0.7P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.01748 (5)	0.45777 (9)	0.20406 (4)	0.01672 (15)
O2	−0.14768 (5)	0.63598 (9)	0.50628 (5)	0.01808 (15)
O3	−0.15869 (6)	0.40284 (10)	0.55897 (5)	0.02180 (17)
O4	−0.06772 (5)	−0.06810 (9)	0.42580 (4)	0.01746 (15)
O5	0.04774 (6)	−0.02392 (9)	0.36962 (5)	0.02059 (16)
N1	−0.05234 (6)	0.67856 (9)	0.23889 (5)	0.01250 (15)
H1N	−0.0882	0.7203	0.2687	0.015*
N2	−0.13867 (6)	0.49091 (10)	0.50740 (5)	0.01297 (15)
N3	−0.01847 (6)	0.02066 (10)	0.39573 (5)	0.01351 (16)
N4	−0.14713 (6)	0.93786 (10)	0.22800 (5)	0.01410 (16)
N5	−0.17659 (6)	0.62099 (10)	0.09365 (5)	0.01511 (16)
N6	0.07998 (6)	0.89062 (12)	0.11185 (5)	0.01994 (18)
C1	−0.02372 (6)	0.52656 (11)	0.24925 (6)	0.01213 (17)
C2	−0.04297 (6)	0.44040 (11)	0.32212 (5)	0.01106 (16)
C3	−0.08127 (6)	0.51175 (11)	0.38158 (5)	0.01169 (17)

H3A	−0.0941	0.6225	0.3799	0.014*
C4	−0.10011 (6)	0.41669 (11)	0.44326 (5)	0.01135 (17)
C5	−0.08273 (6)	0.25483 (11)	0.44912 (5)	0.01207 (17)
H5A	−0.0985	0.1914	0.4906	0.014*
C6	−0.04106 (6)	0.19097 (11)	0.39097 (6)	0.01175 (17)
C7	−0.02000 (6)	0.27899 (11)	0.32824 (6)	0.01204 (17)
H7A	0.0095	0.2306	0.2900	0.014*
C8	−0.04345 (6)	0.77199 (11)	0.16808 (6)	0.01216 (17)
C9	−0.09891 (7)	0.92740 (11)	0.17038 (6)	0.01290 (17)
C10	−0.09967 (8)	1.04672 (12)	0.11226 (6)	0.01803 (19)
H10A	−0.0652	1.0353	0.0716	0.022*
C11	−0.15204 (8)	1.18218 (12)	0.11546 (7)	0.0207 (2)
H11A	−0.1532	1.2661	0.0773	0.025*
C12	−0.20278 (7)	1.19435 (12)	0.17478 (7)	0.0190 (2)
H12A	−0.2395	1.2859	0.1777	0.023*
C13	−0.19856 (7)	1.06983 (12)	0.22969 (6)	0.01668 (19)
H13A	−0.2334	1.0778	0.2703	0.020*
C14	−0.09476 (7)	0.68403 (11)	0.08846 (6)	0.01280 (17)
C15	−0.06228 (7)	0.67416 (13)	0.01756 (6)	0.0190 (2)
H15A	−0.0046	0.7217	0.0153	0.023*
C16	−0.11560 (8)	0.59356 (14)	−0.05022 (6)	0.0222 (2)
H16A	−0.0945	0.5844	−0.0992	0.027*
C17	−0.19969 (8)	0.52701 (13)	−0.04524 (6)	0.0197 (2)
H17A	−0.2376	0.4714	−0.0905	0.024*
C18	−0.22687 (7)	0.54382 (12)	0.02769 (6)	0.01676 (19)
H18A	−0.2846	0.4980	0.0312	0.020*
C19	0.06044 (7)	0.81051 (11)	0.17469 (6)	0.01321 (17)
C20	0.12964 (7)	0.76865 (12)	0.24395 (6)	0.01549 (18)
H20A	0.1139	0.7155	0.2887	0.019*
C21	0.22193 (7)	0.80587 (13)	0.24646 (6)	0.0189 (2)
H21A	0.2703	0.7764	0.2926	0.023*
C22	0.24271 (7)	0.88634 (14)	0.18117 (7)	0.0205 (2)
H22A	0.3053	0.9124	0.1811	0.025*
C23	0.16932 (8)	0.92757 (14)	0.11598 (7)	0.0225 (2)
H23A	0.1830	0.9853	0.0717	0.027*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0228 (4)	0.0149 (3)	0.0155 (3)	0.0031 (3)	0.0106 (3)	0.0018 (3)
O2	0.0229 (4)	0.0136 (3)	0.0192 (3)	0.0030 (3)	0.0080 (3)	−0.0013 (3)
O3	0.0298 (4)	0.0211 (4)	0.0198 (4)	0.0038 (3)	0.0164 (3)	0.0052 (3)
O4	0.0233 (4)	0.0122 (3)	0.0178 (3)	−0.0019 (3)	0.0068 (3)	0.0027 (3)
O5	0.0250 (4)	0.0162 (3)	0.0238 (4)	0.0062 (3)	0.0121 (3)	0.0019 (3)
N1	0.0159 (4)	0.0119 (4)	0.0115 (3)	0.0022 (3)	0.0068 (3)	0.0034 (3)
N2	0.0130 (3)	0.0148 (4)	0.0119 (3)	0.0014 (3)	0.0045 (3)	0.0005 (3)
N3	0.0185 (4)	0.0106 (3)	0.0113 (3)	0.0015 (3)	0.0033 (3)	0.0007 (3)
N4	0.0130 (4)	0.0143 (4)	0.0148 (4)	0.0011 (3)	0.0029 (3)	−0.0004 (3)

N5	0.0156 (4)	0.0138 (4)	0.0169 (4)	0.0004 (3)	0.0058 (3)	0.0006 (3)
N6	0.0169 (4)	0.0253 (5)	0.0179 (4)	−0.0031 (3)	0.0048 (3)	0.0076 (3)
C1	0.0137 (4)	0.0122 (4)	0.0109 (4)	−0.0008 (3)	0.0037 (3)	0.0016 (3)
C2	0.0117 (4)	0.0113 (4)	0.0103 (4)	−0.0003 (3)	0.0029 (3)	0.0014 (3)
C3	0.0116 (4)	0.0114 (4)	0.0119 (4)	0.0002 (3)	0.0025 (3)	0.0007 (3)
C4	0.0112 (4)	0.0128 (4)	0.0106 (4)	0.0006 (3)	0.0036 (3)	−0.0004 (3)
C5	0.0126 (4)	0.0124 (4)	0.0113 (4)	−0.0004 (3)	0.0032 (3)	0.0014 (3)
C6	0.0139 (4)	0.0087 (4)	0.0124 (4)	0.0006 (3)	0.0028 (3)	0.0008 (3)
C7	0.0132 (4)	0.0119 (4)	0.0111 (4)	−0.0002 (3)	0.0031 (3)	0.0000 (3)
C8	0.0141 (4)	0.0117 (4)	0.0117 (4)	0.0011 (3)	0.0050 (3)	0.0034 (3)
C9	0.0138 (4)	0.0120 (4)	0.0125 (4)	0.0004 (3)	0.0024 (3)	0.0009 (3)
C10	0.0229 (5)	0.0154 (4)	0.0163 (4)	0.0017 (4)	0.0057 (4)	0.0040 (4)
C11	0.0247 (5)	0.0141 (4)	0.0217 (5)	0.0027 (4)	0.0023 (4)	0.0049 (4)
C12	0.0171 (4)	0.0130 (4)	0.0241 (5)	0.0030 (3)	−0.0005 (4)	−0.0022 (4)
C13	0.0136 (4)	0.0172 (4)	0.0183 (4)	0.0013 (3)	0.0019 (3)	−0.0032 (4)
C14	0.0146 (4)	0.0116 (4)	0.0124 (4)	0.0025 (3)	0.0038 (3)	0.0025 (3)
C15	0.0176 (4)	0.0260 (5)	0.0151 (4)	−0.0003 (4)	0.0071 (4)	0.0013 (4)
C16	0.0236 (5)	0.0305 (6)	0.0134 (4)	0.0025 (4)	0.0061 (4)	−0.0009 (4)
C17	0.0208 (5)	0.0199 (5)	0.0163 (4)	0.0034 (4)	0.0005 (4)	−0.0021 (4)
C18	0.0149 (4)	0.0144 (4)	0.0202 (5)	0.0014 (3)	0.0028 (4)	0.0004 (3)
C19	0.0144 (4)	0.0126 (4)	0.0135 (4)	−0.0003 (3)	0.0051 (3)	0.0011 (3)
C20	0.0174 (4)	0.0159 (4)	0.0135 (4)	−0.0003 (3)	0.0044 (3)	0.0017 (3)
C21	0.0163 (4)	0.0206 (5)	0.0180 (5)	−0.0016 (4)	0.0008 (4)	0.0001 (4)
C22	0.0162 (4)	0.0241 (5)	0.0218 (5)	−0.0051 (4)	0.0057 (4)	−0.0002 (4)
C23	0.0194 (5)	0.0297 (6)	0.0195 (5)	−0.0068 (4)	0.0070 (4)	0.0056 (4)

Geometric parameters (Å, °)

O1—C1	1.2260 (11)	C8—C9	1.5480 (13)
O2—N2	1.2271 (11)	C8—C14	1.5540 (13)
O3—N2	1.2281 (11)	C9—C10	1.3973 (13)
O4—N3	1.2323 (11)	C10—C11	1.3854 (15)
O5—N3	1.2230 (11)	C10—H10A	0.9500
N1—C1	1.3445 (12)	C11—C12	1.3867 (16)
N1—C8	1.4564 (11)	C11—H11A	0.9500
N1—H1N	0.8853	C12—C13	1.3860 (15)
N2—C4	1.4723 (12)	C12—H12A	0.9500
N3—C6	1.4686 (12)	C13—H13A	0.9500
N4—C9	1.3352 (12)	C14—C15	1.3885 (13)
N4—C13	1.3491 (13)	C15—C16	1.3924 (15)
N5—C18	1.3412 (13)	C15—H15A	0.9500
N5—C14	1.3417 (12)	C16—C17	1.3829 (16)
N6—C19	1.3401 (12)	C16—H16A	0.9500
N6—C23	1.3407 (13)	C17—C18	1.3840 (15)
C1—C2	1.5061 (12)	C17—H17A	0.9500
C2—C3	1.3957 (12)	C18—H18A	0.9500
C2—C7	1.3971 (13)	C19—C20	1.3939 (13)
C3—C4	1.3880 (12)	C20—C21	1.3891 (14)
C3—H3A	0.9500	C20—H20A	0.9500

C4—C5	1.3845 (13)	C21—C22	1.3836 (15)
C5—C6	1.3818 (13)	C21—H21A	0.9500
C5—H5A	0.9500	C22—C23	1.3844 (15)
C6—C7	1.3821 (12)	C22—H22A	0.9500
C7—H7A	0.9500	C23—H23A	0.9500
C8—C19	1.5454 (13)		
C1—N1—C8	122.07 (8)	C11—C10—C9	118.28 (10)
C1—N1—H1N	121.1	C11—C10—H10A	120.9
C8—N1—H1N	115.6	C9—C10—H10A	120.9
O2—N2—O3	124.52 (8)	C10—C11—C12	119.49 (10)
O2—N2—C4	118.04 (8)	C10—C11—H11A	120.3
O3—N2—C4	117.43 (8)	C12—C11—H11A	120.3
O5—N3—O4	124.28 (8)	C13—C12—C11	118.41 (9)
O5—N3—C6	118.05 (8)	C13—C12—H12A	120.8
O4—N3—C6	117.67 (8)	C11—C12—H12A	120.8
C9—N4—C13	118.10 (9)	N4—C13—C12	122.87 (10)
C18—N5—C14	117.72 (9)	N4—C13—H13A	118.6
C19—N6—C23	118.20 (9)	C12—C13—H13A	118.6
O1—C1—N1	123.80 (8)	N5—C14—C15	122.37 (9)
O1—C1—C2	119.62 (8)	N5—C14—C8	113.07 (8)
N1—C1—C2	116.57 (8)	C15—C14—C8	124.53 (9)
C3—C2—C7	119.90 (8)	C14—C15—C16	118.95 (10)
C3—C2—C1	124.19 (8)	C14—C15—H15A	120.5
C7—C2—C1	115.91 (8)	C16—C15—H15A	120.5
C4—C3—C2	118.30 (8)	C17—C16—C15	119.10 (10)
C4—C3—H3A	120.9	C17—C16—H16A	120.4
C2—C3—H3A	120.9	C15—C16—H16A	120.5
C5—C4—C3	123.51 (8)	C16—C17—C18	117.96 (10)
C5—C4—N2	117.57 (8)	C16—C17—H17A	121.0
C3—C4—N2	118.90 (8)	C18—C17—H17A	121.0
C6—C5—C4	116.02 (8)	N5—C18—C17	123.88 (10)
C6—C5—H5A	122.0	N5—C18—H18A	118.1
C4—C5—H5A	122.0	C17—C18—H18A	118.1
C7—C6—C5	123.36 (8)	N6—C19—C20	121.90 (9)
C7—C6—N3	118.28 (8)	N6—C19—C8	116.62 (8)
C5—C6—N3	118.35 (8)	C20—C19—C8	121.44 (8)
C6—C7—C2	118.75 (8)	C21—C20—C19	118.97 (9)
C6—C7—H7A	120.6	C21—C20—H20A	120.5
C2—C7—H7A	120.6	C19—C20—H20A	120.5
N1—C8—C19	109.79 (7)	C22—C21—C20	119.36 (10)
N1—C8—C9	106.41 (7)	C22—C21—H21A	120.3
C19—C8—C9	110.08 (8)	C20—C21—H21A	120.3
N1—C8—C14	108.81 (7)	C21—C22—C23	117.80 (9)
C19—C8—C14	115.50 (8)	C21—C22—H22A	121.1
C9—C8—C14	105.82 (7)	C23—C22—H22A	121.1
N4—C9—C10	122.83 (9)	N6—C23—C22	123.72 (10)
N4—C9—C8	116.87 (8)	N6—C23—H23A	118.1
C10—C9—C8	120.26 (8)	C22—C23—H23A	118.1

C8—N1—C1—O1	5.21 (15)	C14—C8—C9—C10	−67.74 (11)
C8—N1—C1—C2	−175.97 (8)	N4—C9—C10—C11	0.72 (15)
O1—C1—C2—C3	173.68 (9)	C8—C9—C10—C11	178.49 (9)
N1—C1—C2—C3	−5.20 (13)	C9—C10—C11—C12	−0.96 (16)
O1—C1—C2—C7	−6.32 (13)	C10—C11—C12—C13	0.53 (16)
N1—C1—C2—C7	174.81 (8)	C9—N4—C13—C12	−0.44 (14)
C7—C2—C3—C4	−3.42 (13)	C11—C12—C13—N4	0.19 (15)
C1—C2—C3—C4	176.58 (8)	C18—N5—C14—C15	1.19 (14)
C2—C3—C4—C5	0.17 (14)	C18—N5—C14—C8	179.32 (8)
C2—C3—C4—N2	178.72 (8)	N1—C8—C14—N5	41.43 (10)
O2—N2—C4—C5	174.58 (8)	C19—C8—C14—N5	165.39 (8)
O3—N2—C4—C5	−4.67 (12)	C9—C8—C14—N5	−72.57 (9)
O2—N2—C4—C3	−4.06 (13)	N1—C8—C14—C15	−140.49 (9)
O3—N2—C4—C3	176.70 (8)	C19—C8—C14—C15	−16.52 (13)
C3—C4—C5—C6	2.56 (14)	C9—C8—C14—C15	105.51 (10)
N2—C4—C5—C6	−176.01 (8)	N5—C14—C15—C16	−1.18 (15)
C4—C5—C6—C7	−2.16 (14)	C8—C14—C15—C16	−179.09 (9)
C4—C5—C6—N3	178.22 (8)	C14—C15—C16—C17	0.59 (16)
O5—N3—C6—C7	29.26 (13)	C15—C16—C17—C18	−0.09 (16)
O4—N3—C6—C7	−150.69 (9)	C14—N5—C18—C17	−0.66 (15)
O5—N3—C6—C5	−151.10 (9)	C16—C17—C18—N5	0.12 (16)
O4—N3—C6—C5	28.96 (12)	C23—N6—C19—C20	1.46 (16)
C5—C6—C7—C2	−0.95 (14)	C23—N6—C19—C8	179.27 (10)
N3—C6—C7—C2	178.68 (8)	N1—C8—C19—N6	177.27 (8)
C3—C2—C7—C6	3.80 (13)	C9—C8—C19—N6	−65.91 (11)
C1—C2—C7—C6	−176.20 (8)	C14—C8—C19—N6	53.81 (12)
C1—N1—C8—C19	−70.57 (11)	N1—C8—C19—C20	−4.91 (12)
C1—N1—C8—C9	170.33 (8)	C9—C8—C19—C20	111.91 (10)
C1—N1—C8—C14	56.72 (11)	C14—C8—C19—C20	−128.36 (9)
C13—N4—C9—C10	−0.02 (14)	N6—C19—C20—C21	−2.46 (15)
C13—N4—C9—C8	−177.86 (8)	C8—C19—C20—C21	179.83 (9)
N1—C8—C9—N4	−5.49 (11)	C19—C20—C21—C22	1.36 (15)
C19—C8—C9—N4	−124.40 (9)	C20—C21—C22—C23	0.58 (16)
C14—C8—C9—N4	110.16 (9)	C19—N6—C23—C22	0.65 (18)
N1—C8—C9—C10	176.62 (9)	C21—C22—C23—N6	−1.66 (18)
C19—C8—C9—C10	57.71 (11)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···N4	0.88	2.07	2.574 (1)	115
C16—H16A···O1^{i}	0.95	2.34	3.2796 (13)	169
C18—H18A···O4^{ii}	0.95	2.52	3.4414 (13)	164
C23—H23A···O3^{iii}	0.95	2.58	3.2522 (15)	128

Symmetry codes: (i) −*x*, −*y*+1, −*z*; (ii) −*x*−1/2, *y*+1/2, −*z*+1/2; (iii) *x*+1/2, −*y*+3/2, *z*−1/2.

Fig. 1

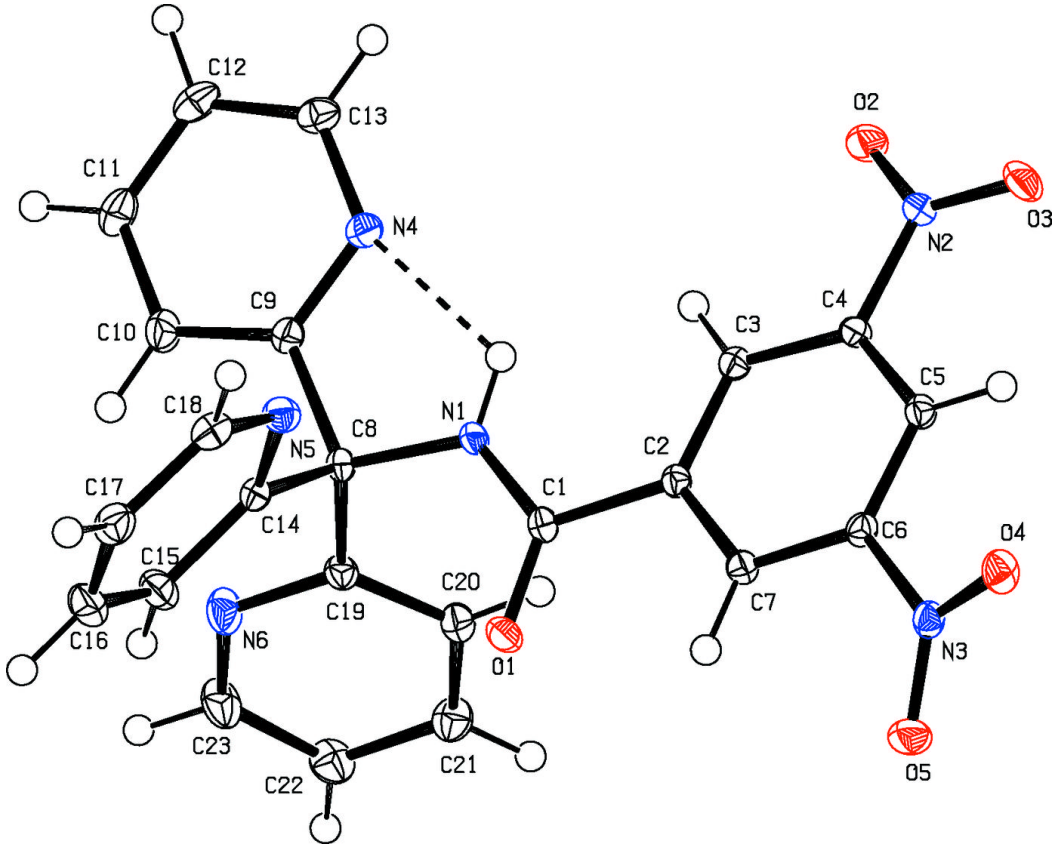
C12
C13
C11
N4
C9
C10
C18
N5
C8
N1
C17
C14
C15
C16
N6
C19
C20
O1
C23
C22
C21
C1
C2
C3
C4
C5
C6
C7
O2
N2
O3
O4
N3
O5

Fig. 2

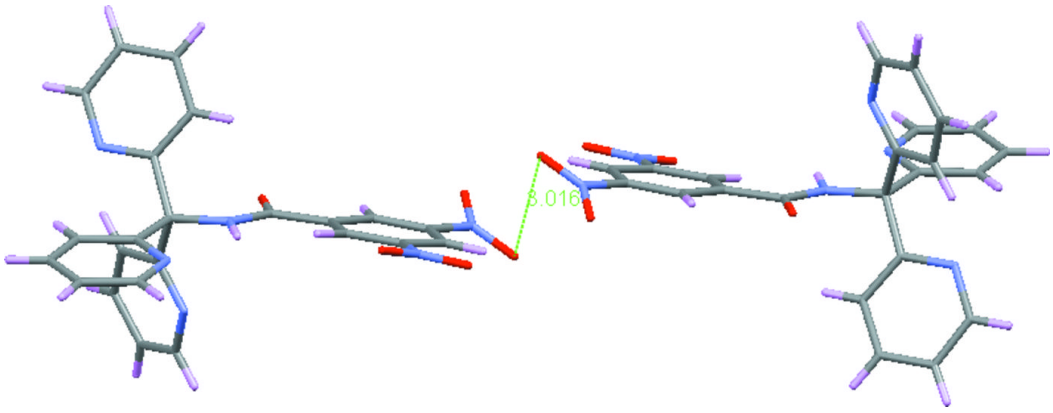

Fig. 3

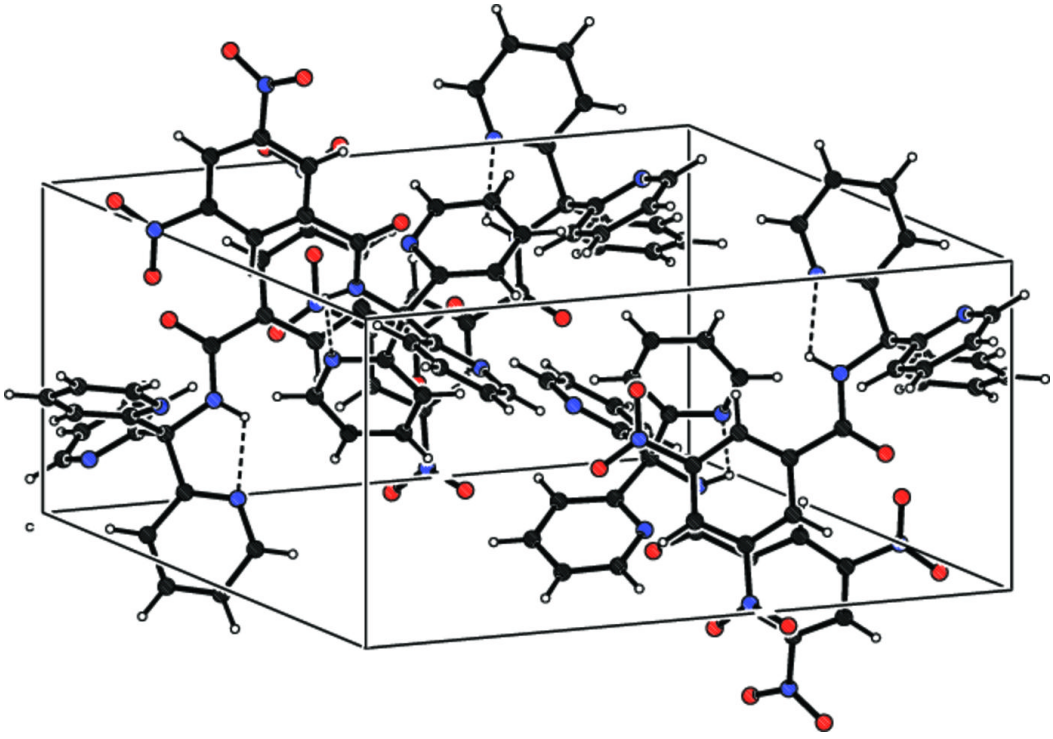

Fig. 4