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2-Methyl-4-nitro-1-(4-nitrophenyl)-1*H*-imidazole

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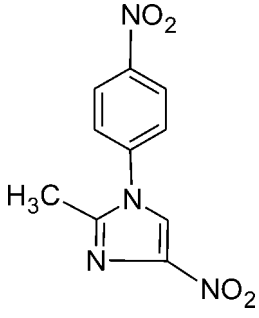
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.099; data-to-parameter ratio = 12.8.

In the title compound, $C_{10}H_8N_4O_4$, two planar fragments, *viz*. the imidazole and nitrophenyl rings, are tilted at a dihedral of 57.89 (7)°. The nitro groups are twisted with respect to the neighbouring ring planes; the dihedral angle is 7.0 (3)° for imidazole and 9.68 (8)° for benzene. The crystal structure consists of centrosymmetric dimers generated by C—H···O hydrogen bonds, which are connected by C—H···N hydrogen bonds into rows along the [001] direction. The neighbouring rows are connected *via* C—H···O interactions into a two-dimensional network in the *bc* plane.

Related literature

This is a part of our studies of intermolecular interactions on 4-nitroimidazole derivatives (Kubicki, 2004). The crystal structures of other 1-aryl-2-methyl-4-nitroimidazoles were described by Kowalski (1995, 1996), Kubicki (2004) and Kubicki & Wagner (2007). For related literature, see: Suwiński *et al.* (1993).



Experimental

Crystal data

$C_{10}H_8N_4O_4$
M_r = 248.20
Orthorhombic, *Pbca*
a = 8.1416 (9) Å
b = 12.7121 (10) Å
c = 20.7789 (13) Å
V = 2150.6 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 100 (1) K
0.4 × 0.15 × 0.05 mm

Data collection

Kuma KM-4-CCD four-circle diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.918, T_{max} = 1.000
11596 measured reflections
2092 independent reflections
1442 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.099
S = 1.01
2092 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···N3^{i}	0.94	2.40	3.338 (2)	177
C15—H15···O42^{ii}	0.91	2.55	3.333 (2)	145
C21—H21*A*···O141^{iii}	0.97	2.52	3.429 (2)	156
C5—H5···O141^{iv}	0.93	2.46	3.258 (2)	143

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *Stereochemical Workstation Operation Manual* (Siemens, 1989); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2111).

References

Kowalski, A. (1995). *Acta Cryst.* C**51**, 1670–1672.
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supplementary materials

Acta Cryst. (2007). E**63**, o3083 [**doi:10.1107/S1600536807026244**]

2-Methyl-4-nitro-1-(4-nitrophenyl)-1*H*-imidazole

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Comment

Simple 4-nitroimidzoles are convenient compounds for studying weak interactions in molecular crystals. The molecules are relatively simple, with few degrees of conformational freedom, and the appropriate choice of substituents can highlight certain kind of interaction. Here, in 1-(4-nitrophenyl)-2-methyl-4-nitroimidazole the available specific interactions range from π-π interactions, through weak hydrogen bonds to nitro-nitro interactions. It turned out that the crystal packing is determined by relatively short and directional C—H···N and C—H···O hydrogen bonds. The first level of organization is the centrosymmetric C—H···O bonded dimer. These dimers are connected by C—H···N hydrogen bonds along [001] direction producing the tapes which are connected into two-dimensional network in the *bc* plane. The plane of imidazole ring makes the angle of 57.89° with the benzene ring.

Experimental

The title compound has been synthesized by aromatic nucleophilic substitution by 4(5)-nitro-2-methylimidazole to 4-fluoronitrobenzene catalysed by sodium hydroxide [Suwiński *et al.*, (1993)].

Refinement

Hydrogen atoms were freely refined, and then, for the last cycles of refinement, both the refined geometry and displacement parameters were restrained to keep the refined values.

Figures

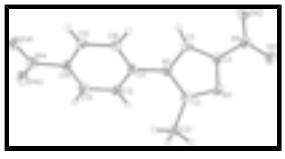

Fig. 1. Molecular structure of (I) with dispalcement parameters scalled at the 50% probability level (Siemens, 1989) and numbering scheme. The hydrogen atoms are drawn as spheres of arbitrary radii.

Fig. 2. The two-dimensional hydrogen-bonded network of (I) along *a* axis. Hydrogen bonds are drawn as dashed lines.

2-Methyl-4-nitro-1-(4-nitrophenyl)-1*H*-imidazole

Crystal data

$C_{10}H_8N_4O_4$	F_{000} = 1024
M_r = 248.20	D_x = 1.533 Mg m^{-3}

Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 3523 reflections
a = 8.1416 (9) Å	θ = 4–22º
b = 12.7121 (10) Å	μ = 0.12 mm^{-1}
c = 20.7789 (13) Å	*T* = 100 (1) K
V = 2150.6 (3) Å^3	Needle, colourless
Z = 8	0.4 × 0.15 × 0.05 mm

Data collection

Kuma KM-4-CCD four-circle diffractometer	2092 independent reflections
Radiation source: fine-focus sealed tube	1442 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.054
T = 100(1) K	θ_{max} = 26.0º
ω scan	θ_{min} = 3.2º
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	*h* = −9→10
T_{min} = 0.918, T_{max} = 1.000	*k* = −15→14
11596 measured reflections	*l* = −25→25

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.038	H-atom parameters constrained
$wR(F^2)$ = 0.099	$w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 0.1988P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.001
2092 reflections	$\Delta\rho_{max}$ = 0.23 e Å^{-3}
163 parameters	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Primary atom site location: structure-invariant direct methods	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}
N1	0.88142 (17)	0.07302 (11)	0.63572 (7)	0.0169 (4)
C11	0.7321 (2)	0.09541 (14)	0.60164 (8)	0.0157 (4)
C12	0.5883 (2)	0.11064 (14)	0.63618 (9)	0.0179 (4)
H12	0.5884	0.1074	0.6814	0.022*
C13	0.4431 (2)	0.13081 (13)	0.60316 (9)	0.0190 (4)
H13	0.3489	0.1428	0.6262	0.013*
C14	0.4484 (2)	0.13426 (13)	0.53655 (9)	0.0166 (4)
N14	0.29294 (19)	0.14829 (11)	0.50133 (8)	0.0205 (4)
O141	0.29927 (17)	0.16023 (10)	0.44276 (6)	0.0265 (3)
O142	0.16320 (16)	0.14491 (10)	0.53195 (7)	0.0287 (4)
C15	0.5904 (2)	0.12051 (13)	0.50162 (9)	0.0171 (4)
H15	0.5864	0.1234	0.4579	0.018*
C16	0.7355 (2)	0.10102 (14)	0.53454 (8)	0.0176 (4)
H16	0.8411	0.0954	0.5120	0.025*
C2	0.9542 (2)	0.13460 (13)	0.68233 (9)	0.0172 (4)
C21	0.8855 (2)	0.23579 (14)	0.70574 (9)	0.0204 (4)
H21A	0.8362	0.2761	0.6711	0.051*
H21B	0.9711	0.2734	0.7232	0.036*
H21C	0.8029	0.2243	0.7389	0.028*
N3	1.09046 (17)	0.09022 (12)	0.70367 (7)	0.0174 (3)
C4	1.1017 (2)	−0.00159 (14)	0.66976 (8)	0.0160 (4)
N4	1.23301 (18)	−0.07395 (12)	0.68067 (7)	0.0200 (4)
O41	1.32853 (17)	−0.05715 (11)	0.72537 (6)	0.0293 (4)
O42	1.24362 (16)	−0.15076 (10)	0.64383 (6)	0.0258 (3)
C5	0.9775 (2)	−0.01455 (14)	0.62716 (8)	0.0184 (4)
H5	0.9442	−0.0686	0.5998	0.019*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0150 (8)	0.0190 (8)	0.0167 (8)	−0.0009 (6)	0.0001 (6)	0.0012 (6)
C11	0.0159 (9)	0.0134 (9)	0.0177 (9)	−0.0014 (7)	−0.0023 (8)	0.0006 (8)
C12	0.0179 (9)	0.0220 (10)	0.0138 (9)	−0.0015 (8)	−0.0004 (8)	0.0009 (8)
C13	0.0169 (10)	0.0185 (10)	0.0216 (10)	−0.0025 (7)	0.0054 (8)	−0.0007 (8)
C14	0.0145 (9)	0.0134 (9)	0.0219 (10)	−0.0012 (7)	−0.0063 (8)	0.0000 (8)
N14	0.0214 (9)	0.0147 (8)	0.0255 (9)	−0.0013 (6)	−0.0036 (7)	0.0008 (7)
O141	0.0332 (9)	0.0256 (8)	0.0207 (7)	−0.0006 (6)	−0.0100 (6)	0.0030 (6)
O142	0.0209 (7)	0.0293 (8)	0.0360 (9)	−0.0005 (6)	−0.0024 (7)	0.0065 (7)
C15	0.0224 (10)	0.0146 (9)	0.0143 (9)	−0.0033 (8)	−0.0016 (8)	0.0010 (7)
C16	0.0187 (9)	0.0158 (10)	0.0181 (10)	−0.0018 (7)	0.0020 (8)	0.0000 (8)
C2	0.0191 (10)	0.0174 (9)	0.0151 (9)	−0.0046 (7)	0.0016 (8)	0.0006 (8)
C21	0.0188 (10)	0.0218 (10)	0.0206 (10)	−0.0026 (8)	−0.0009 (8)	−0.0025 (8)
N3	0.0190 (8)	0.0193 (8)	0.0141 (8)	−0.0037 (7)	−0.0001 (6)	0.0007 (6)
C4	0.0144 (9)	0.0171 (9)	0.0165 (10)	−0.0007 (7)	0.0015 (8)	0.0017 (7)

N4	0.0186 (8)	0.0223 (9)	0.0192 (8)	−0.0031 (7)	0.0000 (7)	0.0019 (7)
O41	0.0266 (8)	0.0300 (8)	0.0312 (8)	0.0016 (6)	−0.0140 (7)	−0.0031 (6)
O42	0.0278 (8)	0.0229 (7)	0.0266 (8)	0.0022 (6)	0.0009 (6)	−0.0056 (6)
C5	0.0232 (10)	0.0157 (9)	0.0162 (9)	−0.0005 (8)	0.0018 (8)	−0.0008 (8)

Geometric parameters (Å, °)

N1—C5	1.372 (2)	C15—H15	0.9093
N1—C2	1.379 (2)	C16—H16	0.9824
N1—C11	1.436 (2)	C2—N3	1.321 (2)
C11—C12	1.387 (2)	C2—C21	1.485 (2)
C11—C16	1.396 (2)	C21—H21A	0.9710
C12—C13	1.390 (2)	C21—H21B	0.9201
C12—H12	0.9414	C21—H21C	0.9739
C13—C14	1.386 (2)	N3—C4	1.366 (2)
C13—H13	0.9168	C4—C5	1.354 (2)
C14—C15	1.376 (2)	C4—N4	1.428 (2)
C14—N14	1.473 (2)	N4—O41	1.2301 (19)
N14—O141	1.2274 (19)	N4—O42	1.2436 (19)
N14—O142	1.2339 (19)	C5—H5	0.9323
C15—C16	1.387 (2)		
C5—N1—C2	107.85 (15)	C15—C16—H16	121.6
C5—N1—C11	125.42 (15)	C11—C16—H16	119.3
C2—N1—C11	126.72 (15)	N3—C2—N1	110.74 (15)
C12—C11—C16	121.75 (16)	N3—C2—C21	125.22 (16)
C12—C11—N1	119.16 (15)	N1—C2—C21	124.02 (16)
C16—C11—N1	119.08 (15)	C2—C21—H21A	111.8
C11—C12—C13	119.20 (17)	C2—C21—H21B	107.1
C11—C12—H12	120.7	H21A—C21—H21B	109.3
C13—C12—H12	120.1	C2—C21—H21C	111.3
C14—C13—C12	118.21 (16)	H21A—C21—H21C	108.6
C14—C13—H13	122.8	H21B—C21—H21C	108.7
C12—C13—H13	119.0	C2—N3—C4	104.37 (15)
C15—C14—C13	123.28 (16)	C5—C4—N3	113.01 (16)
C15—C14—N14	118.37 (16)	C5—C4—N4	125.75 (16)
C13—C14—N14	118.28 (16)	N3—C4—N4	121.24 (15)
O141—N14—O142	123.47 (16)	O41—N4—O42	123.86 (16)
O141—N14—C14	118.14 (15)	O41—N4—C4	118.76 (15)
O142—N14—C14	118.37 (16)	O42—N4—C4	117.38 (15)
C14—C15—C16	118.56 (17)	C4—C5—N1	104.02 (15)
C14—C15—H15	119.4	C4—C5—H5	134.9
C16—C15—H15	122.0	N1—C5—H5	120.8
C15—C16—C11	118.99 (16)		
C5—N1—C11—C12	122.19 (19)	N1—C11—C16—C15	178.68 (15)
C2—N1—C11—C12	−58.0 (2)	C5—N1—C2—N3	−0.3 (2)
C5—N1—C11—C16	−57.6 (2)	C11—N1—C2—N3	179.90 (15)
C2—N1—C11—C16	122.18 (19)	C5—N1—C2—C21	−179.11 (16)
C16—C11—C12—C13	0.8 (3)	C11—N1—C2—C21	1.0 (3)
N1—C11—C12—C13	−179.07 (15)	N1—C2—N3—C4	−0.44 (19)

C11—C12—C13—C14	0.4 (2)	C21—C2—N3—C4	178.40 (17)
C12—C13—C14—C15	−1.1 (3)	C2—N3—C4—C5	1.0 (2)
C12—C13—C14—N14	175.83 (15)	C2—N3—C4—N4	−178.39 (15)
C15—C14—N14—O141	−8.9 (2)	C5—C4—N4—O41	−172.79 (17)
C13—C14—N14—O141	173.95 (15)	N3—C4—N4—O41	6.5 (2)
C15—C14—N14—O142	169.37 (15)	C5—C4—N4—O42	7.3 (3)
C13—C14—N14—O142	−7.8 (2)	N3—C4—N4—O42	−173.35 (15)
C13—C14—C15—C16	0.8 (3)	N3—C4—C5—N1	−1.2 (2)
N14—C14—C15—C16	−176.21 (15)	N4—C4—C5—N1	178.22 (15)
C14—C15—C16—C11	0.4 (2)	C2—N1—C5—C4	0.84 (18)
C12—C11—C16—C15	−1.1 (3)	C11—N1—C5—C4	−179.31 (15)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···N3^{i}	0.94	2.40	3.338 (2)	177
C15—H15···O42^{ii}	0.91	2.55	3.333 (2)	145
C21—H21A···O141^{iii}	0.97	2.52	3.429 (2)	156
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Symmetry codes: (i) *x*−1/2, *y*, −*z*+3/2; (ii) −*x*+2, −*y*, −*z*+1; (iii) *x*+1/2, −*y*+1/2, −*z*+1; (iv) −*x*+1, −*y*, −*z*+1.

Fig. 1

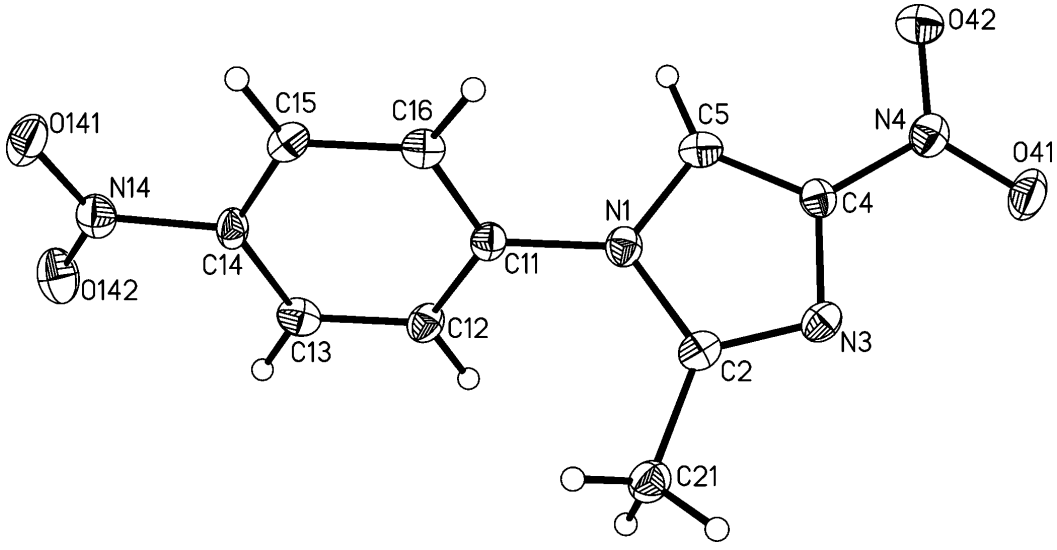
O42
C15
C16
C5
N4
O41
O141
N14
N1
C4
C14
C11
O142
C12
N3
C13
C2
C21

Fig. 2