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1,1′-Methylenebis(2,3-dimethylimidazolium) dipicrate acetonitrile solvate

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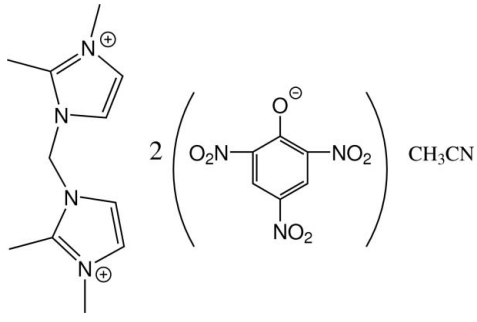
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.007 Å; R factor = 0.059; wR factor = 0.148; data-to-parameter ratio = 6.8.

In the title salt, $C_{11}H_{18}N_4^{2+}\cdot 2C_6H_2N_3O_7^-\cdot C_2H_3N$, the dihedral angle between the imidazolium rings in the dication is 74.4 (2)°, and the benzene rings of the two independent picrate anions are almost parallel, with a dihedral angle of 12.0 (1)° between them.

Related literature

For the synthesis of the title salt, see: Jin *et al.* (2005). For related heterocyclic organic salts used as energetic materials, see: Jin *et al.* (2006); Singh *et al.* (2006).



Experimental

Crystal data

$C_{11}H_{18}N_4^{2+}\cdot 2C_6H_2N_3O_7^-\cdot C_2H_3N$
M_r = 703.56
Orthorhombic, $P2_12_12_1$
a = 6.8715 (9) Å
b = 19.892 (3) Å
c = 22.594 (3) Å
V = 3088.2 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 292 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.963, T_{max} = 0.988
24762 measured reflections
3115 independent reflections
2528 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.148
S = 1.02
3115 reflections
455 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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: *SHELXTL* (Bruker, 2001); 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: BH2132).

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supplementary materials

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1,1'-Methylenebis(2,3-dimethylimidazolium) dipicrate acetonitrile solvate

J. Li

Comment

Polynitrogen heterocyclic organic salts with low melting points are a new class of energetic materials that has attracted considerable interest because of their "green chemistry" properties (Singh *et al.*, 2006). Imidazolium-based or triazolium-based dication picrate salts are good candidates for energetic ionic salts (Jin *et al.*, 2006). Based on this, the title organic salt (I, Fig. 1) was therefore prepared and its structure is reported here.

The asymmetric unit of the title compound contains one 1,1'-methylene-bis(2,3-dimethylimidazolium) dication, two picrate anions and one acetonitrile molecule. The dihedral angle between imidazolium rings in the dication moiety is 74.4°, and methyl groups at 2-positions in the imidazolium rings are arranged in the same direction. Benzene rings of two independent picrate anions are almost parallel, with a dihedral angle of 12.0°. In the crystal structure, π–π stacking occurs between benzene rings of two different picrate anions, with the shortest separation between ring centroids being 3.767 Å. Weak C—H···O hydrogen bonding occurs between dications and picrate anions.

Experimental

The salt $(C_{11}H_{18}N_4)^{2+}$ 2 $(C_6H_2N_3O_7)^-$ was synthesized using a slightly modified literature method (Jin *et al.*, 2005). The title solvate was crystallized by slow evaporation of an acetonitrile solution of the salt.

Refinement

H atoms were positioned geometrically with C—H bond lengths fixed to 0.93 (aromatic CH), 0.97 (methylene CH_2) or 0.96 Å (methyl CH_3). A riding model was used during the refinement process. The U_{iso} parameters for H atoms were constrained to be $1.2U_{eq}$ of the carrier C atom for aromatic and methylene groups, and $1.5U_{eq}$ of the carrier C atom for methyl groups. Measured Friedel pairs were merged before refinement.

Figures

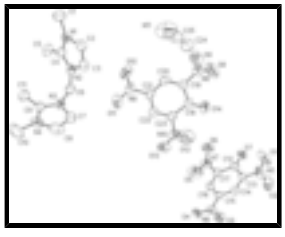


Fig. 1. The structure of (I) showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted.

1,1'-Methylenebis(2,3-dimethylimidazolium) dipicrate acetonitrile solvate

Crystal data

$C_{11}H_{18}N_4^{2+}\cdot 2C_6H_2N_3O_7^-\cdot C_2H_3N$	$D_x = 1.513$ Mg m^{-3}
$M_r = 703.56$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Orthorhombic, $P2_12_12_1$	Cell parameters from 3413 reflections
$a = 6.8715$ (9) Å	$\theta = 2.2$–19.1°
$b = 19.892$ (3) Å	$\mu = 0.13$ mm^{-1}
$c = 22.594$ (3) Å	$T = 292$ (2) K
$V = 3088.2$ (7) Å^3	Block, yellow
$Z = 4$	0.30 × 0.20 × 0.10 mm
$F_{000} = 1456$	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	3115 independent reflections
Radiation source: fine-focus sealed tube	2528 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.061$
$T = 292(2)$ K	$\theta_{max} = 25.0$°
φ and ω scans	$\theta_{min} = 1.8$°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -7\rightarrow 8$
$T_{min} = 0.963$, $T_{max} = 0.988$	$k = -23\rightarrow 23$
24762 measured reflections	$l = -26\rightarrow 26$

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0737P)^2 + 1.7443P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.059$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.148$	$\Delta\rho_{max} = 0.23$ e Å^{-3}
$S = 1.02$	$\Delta\rho_{min} = -0.17$ e Å^{-3}
3115 reflections	Extinction correction: none
455 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.7131 (11)	0.6482 (3)	0.8910 (2)	0.0741 (19)
H1A	0.8431	0.6651	0.8955	0.111*
H1B	0.7147	0.6000	0.8931	0.111*
H1C	0.6323	0.6657	0.9221	0.111*
C2	0.4502 (9)	0.6533 (2)	0.8124 (2)	0.0524 (13)
H2A	0.3555	0.6293	0.8328	0.063*
C3	0.4341 (7)	0.6785 (2)	0.7583 (2)	0.0469 (12)
H3A	0.3264	0.6751	0.7335	0.056*
C4	0.7291 (7)	0.7041 (2)	0.7922 (2)	0.0442 (11)
C5	0.9315 (8)	0.7267 (3)	0.7962 (2)	0.0616 (15)
H5A	0.9834	0.7151	0.8343	0.092*
H5B	0.9367	0.7746	0.7911	0.092*
H5C	1.0071	0.7053	0.7658	0.092*
C6	0.6454 (8)	0.7456 (2)	0.68964 (18)	0.0450 (12)
H6A	0.7822	0.7572	0.6872	0.054*
H6B	0.6151	0.7158	0.6569	0.054*
C7	0.3515 (9)	0.8090 (3)	0.6568 (2)	0.0645 (16)
H7A	0.2891	0.7739	0.6374	0.077*
C8	0.2870 (10)	0.8710 (3)	0.6629 (3)	0.0751 (18)
H8A	0.1702	0.8877	0.6482	0.090*
C9	0.5714 (9)	0.8665 (2)	0.70769 (18)	0.0489 (13)
C10	0.4020 (16)	0.9780 (3)	0.7107 (3)	0.110 (3)
H10A	0.4724	0.9864	0.7467	0.164*
H10B	0.2671	0.9886	0.7165	0.164*
H10C	0.4540	1.0054	0.6796	0.164*
C11	0.7443 (12)	0.8842 (3)	0.7422 (2)	0.084 (2)
H11A	0.8574	0.8646	0.7242	0.126*
H11B	0.7306	0.8675	0.7818	0.126*
H11C	0.7584	0.9322	0.7431	0.126*
C12	0.4963 (7)	0.3526 (2)	0.1203 (2)	0.0406 (11)
C13	0.5179 (7)	0.3387 (2)	0.0577 (2)	0.0460 (12)
C14	0.5718 (7)	0.3846 (2)	0.0162 (2)	0.0460 (12)
H14A	0.5832	0.3718	−0.0233	0.055*
C15	0.6099 (7)	0.4507 (2)	0.03285 (19)	0.0397 (11)
C16	0.5968 (7)	0.4687 (2)	0.0917 (2)	0.0398 (11)
H16C	0.6232	0.5126	0.1032	0.048*
C17	0.5452 (7)	0.4220 (2)	0.13298 (19)	0.0386 (10)
C18	0.2943 (7)	0.4320 (2)	0.47497 (19)	0.0443 (12)
C19	0.2942 (8)	0.4199 (2)	0.53872 (19)	0.0441 (11)
C20	0.3446 (7)	0.4662 (2)	0.58034 (18)	0.0438 (12)
H20A	0.3457	0.4545	0.6202	0.053*
C21	0.3941 (7)	0.5308 (2)	0.56332 (19)	0.0399 (11)
C22	0.3897 (7)	0.5490 (2)	0.50438 (18)	0.0404 (11)
H22A	0.4177	0.5930	0.4934	0.048*
C23	0.3444 (7)	0.5024 (3)	0.46242 (19)	0.0452 (12)

N1	0.6344 (7)	0.66949 (19)	0.83277 (16)	0.0471 (10)
N2	0.6081 (6)	0.71095 (18)	0.74543 (15)	0.0404 (9)
N3	0.5287 (6)	0.80642 (18)	0.68472 (15)	0.0428 (10)
N4	0.4213 (8)	0.9066 (2)	0.69458 (18)	0.0594 (13)
N5	0.4805 (8)	0.2704 (2)	0.0365 (3)	0.0695 (14)
N6	0.6621 (6)	0.5002 (2)	−0.01062 (18)	0.0478 (10)
N7	0.5364 (7)	0.4458 (2)	0.19413 (17)	0.0557 (11)
N8	0.2372 (9)	0.3548 (2)	0.5608 (2)	0.0697 (14)
N9	0.4476 (6)	0.5793 (2)	0.60762 (19)	0.0507 (11)
N10	0.3432 (8)	0.5242 (3)	0.40170 (19)	0.0655 (13)
O1	0.5078 (10)	0.2236 (2)	0.0698 (2)	0.113 (2)
O2	0.4290 (11)	0.2639 (3)	−0.0144 (3)	0.131 (3)
O3	0.6682 (7)	0.4835 (2)	−0.06244 (15)	0.0756 (13)
O4	0.7010 (6)	0.55727 (18)	0.00612 (15)	0.0638 (11)
O5	0.4936 (9)	0.5039 (2)	0.20295 (17)	0.0990 (18)
O6	0.5771 (9)	0.4075 (2)	0.23366 (16)	0.0894 (16)
O7	0.4331 (5)	0.31289 (16)	0.15760 (15)	0.0548 (9)
O8	0.2527 (13)	0.3065 (2)	0.5306 (2)	0.134 (3)
O9	0.1711 (11)	0.3505 (3)	0.6100 (2)	0.135 (3)
O10	0.4597 (7)	0.5618 (2)	0.65896 (16)	0.0778 (13)
O11	0.4817 (7)	0.6368 (2)	0.59179 (19)	0.0726 (12)
O12	0.3750 (12)	0.4856 (3)	0.36221 (18)	0.133 (3)
O13	0.3162 (10)	0.5829 (2)	0.39161 (17)	0.0992 (19)
O14	0.2484 (7)	0.39015 (19)	0.43756 (15)	0.0724 (12)
N11	0.6450 (16)	0.3457 (5)	0.6714 (3)	0.164 (4)
C24	0.7279 (13)	0.2882 (4)	0.5744 (3)	0.087 (2)
H24A	0.8665	0.2833	0.5714	0.130*
H24B	0.6812	0.3147	0.5419	0.130*
H24C	0.6678	0.2446	0.5733	0.130*
C25	0.6803 (11)	0.3209 (4)	0.6291 (3)	0.085 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.099 (5)	0.070 (4)	0.053 (3)	0.017 (4)	−0.012 (3)	0.011 (3)
C2	0.057 (4)	0.044 (3)	0.056 (3)	−0.001 (3)	0.005 (3)	0.000 (2)
C3	0.039 (3)	0.042 (3)	0.060 (3)	0.000 (2)	0.000 (2)	−0.005 (2)
C4	0.046 (3)	0.042 (3)	0.044 (3)	0.009 (2)	0.000 (2)	−0.011 (2)
C5	0.053 (3)	0.071 (4)	0.060 (3)	−0.002 (3)	−0.006 (3)	−0.017 (3)
C6	0.049 (3)	0.049 (3)	0.036 (2)	−0.002 (2)	0.007 (2)	−0.009 (2)
C7	0.067 (4)	0.055 (3)	0.071 (3)	−0.024 (3)	−0.027 (3)	0.014 (3)
C8	0.055 (4)	0.079 (5)	0.091 (4)	−0.004 (4)	−0.004 (4)	0.039 (4)
C9	0.074 (4)	0.045 (3)	0.028 (2)	−0.019 (3)	0.007 (2)	−0.001 (2)
C10	0.199 (10)	0.048 (3)	0.082 (4)	0.023 (5)	0.029 (6)	−0.002 (3)
C11	0.130 (6)	0.072 (4)	0.050 (3)	−0.048 (4)	−0.023 (4)	0.008 (3)
C12	0.032 (3)	0.037 (2)	0.052 (3)	0.006 (2)	0.002 (2)	0.008 (2)
C13	0.041 (3)	0.035 (2)	0.062 (3)	−0.001 (2)	0.002 (2)	0.002 (2)
C14	0.039 (3)	0.051 (3)	0.048 (3)	0.000 (2)	0.006 (2)	−0.005 (2)

C15	0.037 (3)	0.041 (2)	0.041 (2)	0.003 (2)	0.002 (2)	0.004 (2)
C16	0.033 (3)	0.032 (2)	0.054 (3)	0.005 (2)	−0.002 (2)	−0.002 (2)
C17	0.029 (2)	0.041 (2)	0.046 (2)	0.005 (2)	0.000 (2)	0.004 (2)
C18	0.039 (3)	0.055 (3)	0.039 (2)	−0.003 (2)	−0.004 (2)	−0.007 (2)
C19	0.047 (3)	0.041 (3)	0.044 (2)	−0.007 (2)	−0.003 (2)	0.000 (2)
C20	0.038 (3)	0.062 (3)	0.032 (2)	0.003 (2)	0.001 (2)	0.006 (2)
C21	0.032 (3)	0.046 (3)	0.042 (2)	−0.002 (2)	−0.001 (2)	−0.009 (2)
C22	0.031 (3)	0.050 (3)	0.041 (2)	−0.003 (2)	0.006 (2)	−0.001 (2)
C23	0.041 (3)	0.058 (3)	0.036 (2)	−0.003 (2)	0.000 (2)	0.004 (2)
N1	0.065 (3)	0.035 (2)	0.041 (2)	0.012 (2)	0.000 (2)	0.0040 (17)
N2	0.038 (2)	0.041 (2)	0.042 (2)	0.0032 (18)	0.0031 (18)	−0.0053 (16)
N3	0.050 (3)	0.042 (2)	0.0368 (19)	−0.010 (2)	−0.0022 (18)	0.0012 (17)
N4	0.085 (4)	0.045 (2)	0.049 (2)	0.012 (3)	0.017 (3)	0.0088 (19)
N5	0.070 (4)	0.045 (3)	0.093 (4)	−0.006 (3)	0.015 (3)	−0.013 (3)
N6	0.042 (2)	0.054 (3)	0.047 (2)	0.004 (2)	0.004 (2)	0.008 (2)
N7	0.065 (3)	0.055 (3)	0.047 (2)	0.009 (2)	0.002 (2)	0.006 (2)
N8	0.090 (4)	0.062 (3)	0.057 (3)	−0.016 (3)	−0.013 (3)	0.004 (2)
N9	0.038 (2)	0.063 (3)	0.051 (2)	−0.003 (2)	0.001 (2)	−0.020 (2)
N10	0.084 (4)	0.075 (3)	0.038 (2)	−0.008 (3)	−0.005 (2)	0.005 (2)
O1	0.173 (6)	0.043 (2)	0.124 (4)	−0.007 (3)	0.060 (4)	0.000 (3)
O2	0.188 (7)	0.077 (3)	0.127 (5)	−0.027 (4)	−0.055 (5)	−0.032 (3)
O3	0.108 (4)	0.076 (3)	0.043 (2)	−0.006 (3)	0.010 (2)	0.0103 (19)
O4	0.085 (3)	0.042 (2)	0.064 (2)	−0.010 (2)	0.002 (2)	0.0109 (17)
O5	0.161 (5)	0.070 (3)	0.066 (2)	0.049 (3)	0.004 (3)	−0.013 (2)
O6	0.156 (5)	0.065 (2)	0.047 (2)	0.006 (3)	−0.013 (3)	0.0113 (19)
O7	0.051 (2)	0.050 (2)	0.063 (2)	−0.0072 (18)	0.0027 (18)	0.0188 (17)
O8	0.240 (8)	0.055 (3)	0.106 (4)	−0.033 (4)	0.013 (5)	−0.006 (3)
O9	0.224 (8)	0.120 (4)	0.060 (3)	−0.100 (5)	0.000 (4)	0.027 (3)
O10	0.090 (3)	0.100 (3)	0.044 (2)	−0.009 (3)	−0.008 (2)	−0.019 (2)
O11	0.079 (3)	0.054 (2)	0.085 (3)	−0.013 (2)	0.003 (2)	−0.022 (2)
O12	0.234 (8)	0.122 (4)	0.043 (2)	0.001 (5)	0.016 (4)	−0.010 (3)
O13	0.157 (6)	0.078 (3)	0.063 (2)	−0.018 (3)	−0.031 (3)	0.024 (2)
O14	0.100 (3)	0.064 (2)	0.053 (2)	−0.013 (3)	−0.013 (2)	−0.0145 (18)
N11	0.223 (11)	0.178 (8)	0.091 (5)	0.074 (8)	0.045 (6)	−0.015 (5)
C24	0.086 (5)	0.095 (5)	0.079 (4)	0.002 (4)	0.009 (4)	−0.002 (4)
C25	0.090 (5)	0.090 (5)	0.076 (4)	0.028 (4)	0.013 (4)	0.012 (4)

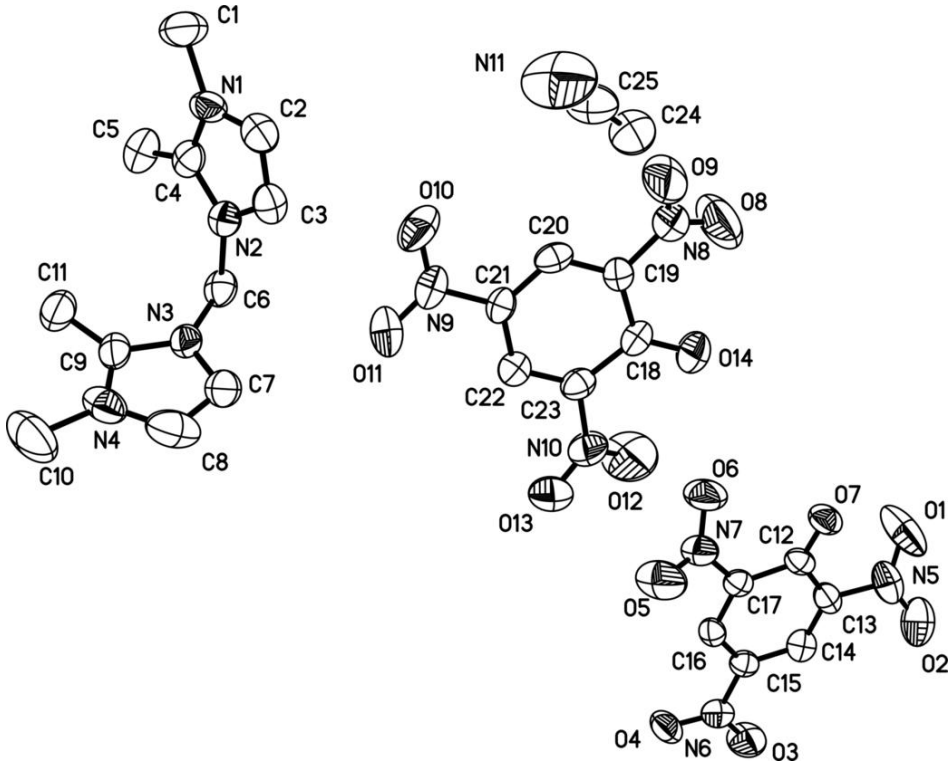
Geometric parameters (Å, °)

C1—N1	1.485 (6)	C13—N5	1.462 (6)
C1—H1A	0.9600	C14—C15	1.394 (6)
C1—H1B	0.9600	C14—H14A	0.9300
C1—H1C	0.9600	C15—C16	1.380 (6)
C2—C3	1.326 (7)	C15—N6	1.436 (6)
C2—N1	1.385 (7)	C16—C17	1.363 (6)
C2—H2A	0.9300	C16—H16C	0.9300
C3—N2	1.389 (6)	C17—N7	1.462 (6)
C3—H3A	0.9300	C18—O14	1.227 (5)
C4—N1	1.318 (6)	C18—C19	1.460 (6)

C4—N2	1.352 (6)	C18—C23	1.471 (7)
C4—C5	1.465 (8)	C19—C20	1.361 (6)
C5—H5A	0.9600	C19—N8	1.443 (6)
C5—H5B	0.9600	C20—C21	1.382 (6)
C5—H5C	0.9600	C20—H20A	0.9300
C6—N3	1.456 (6)	C21—C22	1.381 (6)
C6—N2	1.459 (5)	C21—N9	1.438 (6)
C6—H6A	0.9700	C22—C23	1.361 (6)
C6—H6B	0.9700	C22—H22A	0.9300
C7—C8	1.317 (8)	C23—N10	1.439 (6)
C7—N3	1.372 (7)	N5—O2	1.211 (7)
C7—H7A	0.9300	N5—O1	1.213 (7)
C8—N4	1.365 (8)	N6—O3	1.218 (5)
C8—H8A	0.9300	N6—O4	1.226 (5)
C9—N3	1.335 (6)	N7—O6	1.207 (5)
C9—N4	1.337 (7)	N7—O5	1.209 (5)
C9—C11	1.464 (8)	N8—O8	1.182 (6)
C10—N4	1.471 (7)	N8—O9	1.205 (6)
C10—H10A	0.9600	N9—O10	1.214 (5)
C10—H10B	0.9600	N9—O11	1.222 (6)
C10—H10C	0.9600	N10—O12	1.197 (6)
C11—H11A	0.9600	N10—O13	1.204 (6)
C11—H11B	0.9600	N11—C25	1.103 (8)
C11—H11C	0.9600	C24—C25	1.435 (9)
C12—O7	1.234 (5)	C24—H24A	0.9600
C12—C17	1.448 (6)	C24—H24B	0.9600
C12—C13	1.451 (7)	C24—H24C	0.9600
C13—C14	1.360 (6)		
N1—C1—H1A	109.5	C17—C16—H16C	120.0
N1—C1—H1B	109.5	C15—C16—H16C	120.0
H1A—C1—H1B	109.5	C16—C17—C12	125.1 (4)
N1—C1—H1C	109.5	C16—C17—N7	115.9 (4)
H1A—C1—H1C	109.5	C12—C17—N7	119.0 (4)
H1B—C1—H1C	109.5	O14—C18—C19	124.6 (5)
C3—C2—N1	107.2 (5)	O14—C18—C23	125.0 (4)
C3—C2—H2A	126.4	C19—C18—C23	110.3 (4)
N1—C2—H2A	126.4	C20—C19—N8	116.0 (4)
C2—C3—N2	107.2 (5)	C20—C19—C18	124.8 (4)
C2—C3—H3A	126.4	N8—C19—C18	119.3 (4)
N2—C3—H3A	126.4	C19—C20—C21	119.9 (4)
N1—C4—N2	107.0 (4)	C19—C20—H20A	120.0
N1—C4—C5	126.0 (5)	C21—C20—H20A	120.0
N2—C4—C5	126.9 (5)	C22—C21—C20	120.4 (4)
C4—C5—H5A	109.5	C22—C21—N9	120.0 (4)
C4—C5—H5B	109.5	C20—C21—N9	119.5 (4)
H5A—C5—H5B	109.5	C23—C22—C21	119.9 (4)
C4—C5—H5C	109.5	C23—C22—H22A	120.1
H5A—C5—H5C	109.5	C21—C22—H22A	120.1
H5B—C5—H5C	109.5	C22—C23—N10	117.5 (4)

N3—C6—N2	111.2 (4)	C22—C23—C18	124.6 (4)
N3—C6—H6A	109.4	N10—C23—C18	118.0 (4)
N2—C6—H6A	109.4	C4—N1—C2	109.9 (4)
N3—C6—H6B	109.4	C4—N1—C1	125.8 (5)
N2—C6—H6B	109.4	C2—N1—C1	124.2 (5)
H6A—C6—H6B	108.0	C4—N2—C3	108.6 (4)
C8—C7—N3	106.6 (5)	C4—N2—C6	128.0 (4)
C8—C7—H7A	126.7	C3—N2—C6	123.4 (4)
N3—C7—H7A	126.7	C9—N3—C7	109.9 (5)
C7—C8—N4	108.2 (6)	C9—N3—C6	126.4 (4)
C7—C8—H8A	125.9	C7—N3—C6	123.7 (4)
N4—C8—H8A	125.9	C9—N4—C8	109.1 (4)
N3—C9—N4	106.2 (5)	C9—N4—C10	126.2 (6)
N3—C9—C11	126.9 (6)	C8—N4—C10	124.7 (7)
N4—C9—C11	126.9 (5)	O2—N5—O1	123.5 (5)
N4—C10—H10A	109.5	O2—N5—C13	117.5 (5)
N4—C10—H10B	109.5	O1—N5—C13	118.9 (5)
H10A—C10—H10B	109.5	O3—N6—O4	122.8 (4)
N4—C10—H10C	109.5	O3—N6—C15	118.6 (4)
H10A—C10—H10C	109.5	O4—N6—C15	118.6 (4)
H10B—C10—H10C	109.5	O6—N7—O5	122.6 (4)
C9—C11—H11A	109.5	O6—N7—C17	119.0 (4)
C9—C11—H11B	109.5	O5—N7—C17	118.4 (4)
H11A—C11—H11B	109.5	O8—N8—O9	120.6 (5)
C9—C11—H11C	109.5	O8—N8—C19	120.4 (5)
H11A—C11—H11C	109.5	O9—N8—C19	119.0 (5)
H11B—C11—H11C	109.5	O10—N9—O11	122.3 (4)
O7—C12—C17	123.9 (4)	O10—N9—C21	119.4 (5)
O7—C12—C13	125.4 (4)	O11—N9—C21	118.3 (4)
C17—C12—C13	110.6 (4)	O12—N10—O13	120.6 (5)
C14—C13—C12	124.9 (4)	O12—N10—C23	121.1 (5)
C14—C13—N5	116.5 (5)	O13—N10—C23	118.2 (5)
C12—C13—N5	118.6 (4)	C25—C24—H24A	109.5
C13—C14—C15	119.9 (4)	C25—C24—H24B	109.5
C13—C14—H14A	120.0	H24A—C24—H24B	109.5
C15—C14—H14A	120.0	C25—C24—H24C	109.5
C16—C15—C14	119.5 (4)	H24A—C24—H24C	109.5
C16—C15—N6	119.9 (4)	H24B—C24—H24C	109.5
C14—C15—N6	120.6 (4)	N11—C25—C24	179.3 (9)
C17—C16—C15	120.0 (4)		

Fig. 1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