Polymorphism in 1-Methylhydantoin: Investigation by Periodic DFT Calculations and Characterization of the Third Polymorph

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Supporting Information

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Table S1 – C_6 and R_{vdW} parameters used for the Grimme correction.[a]

Atom	C_6[28] (J nm^6 mol^{-1})	R_{vdW} (Å)
H	0.14	1.3013[31]
C	1.75	1.70[31,32]
N	1.23	1.55[31,32]
O	0.70	1.52[31,32]

[a] A cutoff distance of 25.0 Å was used to truncate direct lattice summation; Standard values of d = 20 and s_6 = 1.00 were used.[30]

Table S2 – Values of experimental (Exp.) and DFT-D(B3LYP)/6-31G(d,p) calculated (Calc) bond lengths, bond angles and torsion angles of polymorph **I** of 1-MH.

Bond length/ Å	Exp.	Calc	Calc.-Exp.	Bond angle/ º	Exp.	Calc	Calc-Exp.
N1-C2	1.33	1.35	0.02	C2-N1-C5	111.3	111.2	-0.1
N1-C5	1.45	1.45	0.00	C2-N1-C6	123.5	123.3	-0.2
N1-C6	1.44	1.45	0.01	C5-N1-C6	124.0	123.7	-0.3
C2=O7	1.23	1.24	0.01	C2-N3-C4	111.9	111.8	-0.1
C2-N3	1.39	1.4	0.01	O7=C2-N1	127.5	127.3	-0.2
N3-C4	1.36	1.37	0.01	O7=C2-N3	124.6	124.6	0.0
N3-H8	0.93	1.03	0.10	N1-C2-N3	107.9	108.1	0.2
C4=O9	1.21	1.22	0.01	C2-N3-H8	121.7	123.2	1.5
C4-C5	1.50	1.52	0.02	C4-N3-H8	126.3	124.9	-1.4
C5-H10	0.97	1.09	0.12	O9=C4-N3	126.3	126.2	-0.1
C5-H11	1.04	1.09	0.05	O9=C4-C5	127.7	127.8	0.1
C6-H12	0.96	1.09	0.13	N3-C4-C5	106.0	106.0	0.0
C6-H13	0.98	1.09	0.11	N1-C5-C4	102.8	102.7	-0.1
C6-H14	0.90	1.09	0.19	N1-C5-H10	110.6	113.3	2.7
				N1-C5-H11	113.1	111.8	-1.3
Torsion Angle/ º				C4-C5-H10	111.5	110.3	-1.2
				C4-C5-H11	112.0	110.8	-1.2
C5-N1-C2=O7	-177.7	-176.8	0.9	H10-C5-H11	107.0	108.0	1.0
C6-N1-C2=O7	-9.7	-11.3	-1.6	N1-C6-H12	110.0	111.0	1.0
C2-N1-C5-C4	-3.2	-2.6	0.6	N1-C6-H13	103.6	108.9	5.3
C4-N3-C2=O7	178.7	176.9	-1.8	N1-C6-H14	107.0	109.2	2.2
C2-N3-C4=O9	180.0	178.1	-1.9	H12-C6-H14	114.0	109.6	-4.4
O9=C4-C5-N1	-177.9	-179.5	-1.6	H12-C6-H13	105.2	108.2	3.0
C5-N1-C2-N3	3.6	4.0	0.4	H14-C6-H13	116.5	110.0	-6.5
C6-N1-C2-N3	171.6	169.4	-2.2				
C6-N1-C5-C4	-171.1	-168.0	3.1				
C4-N3-C2-N1	-2.5	-3.8	-1.3				
C2-N3-C4-C5	0.4	2.1	1.7				
N3-C4-C5-N1	1.6	0.3	-1.3				

Table S3 – Values of experimental (Exp.) and DFT-D(B3LYP)/6-31G(d,p) calculated (Calc) bond lengths, bond angles and torsion angles of polymorph **II** of 1-MH.

Bond length/ Å	Exp.	Calc.	Calc.-Exp.	Bond angle/ º	Exp.	Calc.	Calc.-Exp.
N1-C2	1.34	1.36	0.02	C2-N1-C5	111.8	111.1	-0.7
N1-C5	1.44	1.46	0.02	C2-N1-C6	123.6	124.9	1.3
N1-C6	1.45	1.45	0.00	C5-N1-C6	123.7	123.0	-0.7
C2=O7	1.22	1.23	0.01	C2-N3-C4	112.2	112.0	-0.2
C2-N3	1.39	1.40	0.01	O7=C2-N1	128.4	128.6	0.2
N3-C4	1.36	1.37	0.01	O7=C2-N3	124.3	123.7	-0.6
N3-H8	0.81	1.03	0.22	N1-C2-N3	107.2	107.7	0.5
C4=O9	1.21	1.23	0.02	C2-N3-H8	120.4	122.4	2.0
C4-C5	1.50	1.52	0.02	C4-N3-H8	126.7	125.4	-1.3
C5-H10	0.99	1.09	0.10	O9=C4-N3	127.1	126.8	-0.3
C5-H11	0.96	1.09	0.13	O9=C4-C5	126.9	126.9	0.0
C6-H12	1.01	1.09	0.08	N3-C4-C5	106.1	106.2	0.1
C6-H13	0.96	1.09	0.13	N1-C5-C4	102.7	102.9	0.2
C6-H14	0.95	1.09	0.14	N1-C5-H10	114.5	111.9	-2.6
				N1-C5-H11	114.2	113.1	-1.1
Torsion Angle/ º				C4-C5-H10	111.5	109.8	-1.7
				C4-C5-H11	110.1	111.6	1.5
C5-N1-C2=O7	-179.3	-179.5	-0.2	H10-C5-H11	105.6	107.1	1.5
C6-N1-C2=O7	-10.3	-11.5	-1.2	N1-C6-H12	109.6	109.7	0.1
C2-N1-C5-C4	-0.1	-0.8	-0.7	N1-C6-H13	111.0	110.0	-1.0
C4-N3-C2=O7	178.1	178.8	0.7	N1-C6-H14	114.5	110.9	-3.6
C2-N3-C4=O9	-177.4	-177.3	0.1	H12-C6-H14	105.0	108.4	3.4
O9=C4-C5-N1	178.5	177.9	-0.6	H12-C6-H13	105.0	108.9	3.9
C5-N1-C2-N3	1.7	0.8	-0.9	H14-C6-H13	111.0	108.9	-2.1
C6-N1-C2-N3	170.7	169.7	-1.0				
C6-N1-C5-C4	-169.1	-168.3	0.8				
C4-N3-C2-N1	-2.8	-2.3	0.5				
C2-N3-C4-C5	2.7	2.8	0.1				
N3-C4-C5-N1	-1.5	-2.1	-0.6				

Table S4 – Values of experimental (Exp.) and DFT-D(B3LYP)/6-31G(d,p) calculated (Calc) bond lengths, bond angles and torsion angles of polymorph **III** of 1-MH.

MOLECULE **A**							
Bond length/ Å				Bond angle/ º			
	Exp.	Calc.	Calc.-Exp.		Exp.	Calc.	Calc.-Exp.
N1-C2	1.33	1.35	0.02	C2-N1-C5	111.7	111.1	-0.6
N1-C5	1.45	1.46	0.01	C2-N1-C6	125.2	125.8	0.6
N1-C6	1.45	1.45	0.00	C5-N1-C6	123.0	122.8	-0.2
C2=O7	1.22	1.24	0.02	C2-N3-C4	111.4	111.8	0.4
C2-N3	1.40	1.40	0.00	O7=C2-N1	128.8	128.4	-0.4
N3-C4	1.35	1.37	0.02	O7=C2-N3	123.4	123.7	0.3
N3-H8	0.86	1.03	0.17	N1-C2-N3	107.7	107.9	0.2
C4=O9	1.21	1.22	0.01	C2-N3-H8	124.3	122.9	-1.4
C4-C5	1.50	1.52	0.02	C4-N3-H8	124.3	124.5	0.2
C5-H10	0.97	1.10	0.13	O9=C4-N3	126.5	126.7	0.2
C5-H11	0.97	1.09	0.12	O9=C4-C5	126.9	127.3	0.4
C6-H12	0.96	1.09	0.13	N3-C4-C5	106.6	106.0	-0.6
C6-H13	0.96	1.09	0.13	N1-C5-C4	102.4	102.6	0.2
C6-H14	0.96	1.09	0.13	N1-C5-H10	111.3	111.2	-0.1
				N1-C5-H11	111.3	113.0	1.7
Torsion Angle/ º				C4-C5-H10	111.3	110.3	-1.0
				C4-C5-H11	111.3	111.8	0.5
C5-N1-C2=O7	-177.9	-177.2	0.7	H10-C5-H11	109.2	107.8	-1.4
C6-N1-C2=O7	-1.5	-3.2	-1.7	N1-C6-H12	109.5	110.2	0.7
C2-N1-C5-C4	-3.6	-6.1	-2.5	N1-C6-H13	109.5	109.5	0.0
C4-N3-C2=O7	-178.9	-177.5	1.4	N1-C6-H14	109.5	110.7	1.2
C2-N3-C4=O9	175.8	173.4	-2.4	H12-C6-H14	109.5	108.2	-1.3
O9=C4-C5-N1	-175.4	-172.6	2.8	H12-C6-H13	109.5	109.1	-0.4
C5-N1-C2-N3	1.4	2.5	1.1	H14-C6-H13	109.5	109.2	-0.3
C6-N1-C2-N3	177.8	176.5	-1.3				
C6-N1-C5-C4	179.9	179.6	-0.3				
C4-N3-C2-N1	1.8	2.8	1.0				
C2-N3-C4-C5	-4.0	-7.0	-3.0				
N3-C4-C5-N1	4.5	7.5	3.0				
MOLECULE **B**							
Bond length/ Å				Bond angle/ º			
N1-C2	1.33	1.35	0.02	C2-N1-C5	111.8	111.2	-0.6
N1-C5	1.45	1.46	0.01	C2-N1-C6	125.5	126.4	0.9
N1-C6	1.45	1.45	0.00	C5-N1-C6	122.7	122.4	-0.3
C2=O7	1.22	1.24	0.02	C2-N3-C4	112.6	112.1	-0.5
C2-N3	1.39	1.40	0.01	O7=C2-N1	128.4	128.6	0.2
N3-C4	1.36	1.37	0.01	O7=C2-N3	124.2	123.5	-0.7
N3-H8	0.86	1.03	0.17	N1-C2-N3	107.4	107.9	0.5
C4=O9	1.21	1.22	0.01	C2-N3-H8	123.7	122.1	-1.6
C4-C5	1.52	1.52	0.00	C4-N3-H8	123.7	125.8	2.1
C5-H10	0.97	1.09	0.12	O9=C4-N3	127.1	127.0	-0.1
C5-H11	0.97	1.09	0.12	O9=C4-C5	127.3	127.3	0.0
C6-H12	0.96	1.09	0.13	N3-C4-C5	105.6	105.7	0.1
C6-H13	0.96	1.09	0.13	N1-C5-C4	102.6	103.0	0.4
C6-H14	0.96	1.09	0.13	N1-C5-H10	111.3	112.2	0.9
				N1-C5-H11	111.3	111.4	0.1
				C4-C5-H10	111.2	110.8	-0.4

Torsion Angle/ º			
C5-N1-C2=O7	179.6	178.7	-0.9
C6-N1-C2=O7	-2.8	-2.1	0.7
C2-N1-C5-C4	0.4	1.9	1.5
C4-N3-C2=O7	-179.1	-179.8	-0.7
C2-N3-C4=O9	179.3	180.0	0.7
O9=C4-C5-N1	179.4	179.2	-0.2
C5-N1-C2-N3	0.0	-1.5	-1.5
C6-N1-C2-N3	176.7	177.7	1.0
C6-N1-C5-C4	-176.4	-177.3	-0.9
C4-N3-C2-N1	0.5	0.5	0.0
C2-N3-C4-C5	0.7	0.7	0.0
N3-C4-C5-N1	-0.7	-1.5	-0.8

C4-C5-H11	111.2	111.0	-0.2
H10-C5-H11	109.2	108.4	-0.8
N1-C6-H12	109.5	110.9	1.4
N1-C6-H13	109.4	110.2	0.8
N1-C6-H14	109.5	109.9	0.4
H12-C6-H14	109.5	108.5	-1.0
H12-C6-H13	109.5	108.2	-1.3
H14-C6-H13	109.5	109.1	-0.4

MOLECULE **C**

Bond length/ Å			
N1-C2	1.34	1.35	0.01
N1-C5	1.48	1.46	-0.02
N1-C6	1.48	1.46	-0.02
C2=O7	1.22	1.24	0.02
C2-N3	1.39	1.40	0.01
N3-C4	1.35	1.37	0.02
N3-H8	0.86	1.03	0.17
C4=O9	1.20	1.22	0.02
C4-C5	1.52	1.52	0.00
C5-H10	0.97	1.10	0.13
C5-H11	0.97	1.10	0.13
C6-H12	0.96	1.09	0.13
C6-H13	0.96	1.09	0.13
C6-H14	0.96	1.09	0.13

Torsion Angle/ º			
C5-N1-C2=O7	175.8	176.9	1.1
C6-N1-C2=O7	1.9	1.6	-0.3
C2-N1-C5-C4	4.5	4.5	0.0
C4-N3-C2=O7	178.9	179.7	0.8
C2-N3-C4=O9	-177.6	-176.8	0.8
O9=C4-C5-N1	176.2	175.6	-0.6
C5-N1-C2-N3	-2.9	-2.6	0.3
C6-N1-C2-N3	-176.9	-177.9	-1.0
C6-N1-C5-C4	178.5	180.0	1.5
C4-N3-C2-N1	-0.1	-0.7	-0.6
C2-N3-C4-C5	2.9	3.5	0.6
N3-C4-C5-N1	-4.3	-4.7	-0.4

Bond angle/ º			
C2-N1-C5	111.4	111.1	-0.3
C2-N1-C6	124.9	125.5	0.6
C5-N1-C6	123.4	123.3	-0.1
C2-N3-C4	112.5	112.2	-0.3
O7=C2-N1	128.2	128.6	0.4
O7=C2-N3	124.3	123.7	-0.6
N1-C2-N3	107.6	107.8	0.2
C2-N3-H8	123.7	122.6	-1.1
C4-N3-H8	123.7	125.1	1.4
O9=C4-N3	127.5	128.8	1.3
O9=C4-C5	126.9	127.3	0.4
N3-C4-C5	105.6	105.9	0.3
N1-C5-C4	102.7	102.8	0.1
N1-C5-H10	111.2	112.0	0.8
N1-C5-H11	111.2	112.0	0.8
C4-C5-H10	111.2	111.2	0.0
C4-C5-H11	111.2	109.7	-1.5
H10-C5-H11	109.2	107.3	-1.9
N1-C6-H12	109.4	110.7	1.3
N1-C6-H13	109.5	109.7	0.2
N1-C6-H14	109.4	110.5	1.1
H12-C6-H14	109.5	108.9	-0.6
H12-C6-H13	109.5	108.8	-0.7
H14-C6-H13	109.5	108.1	-1.4

Single crystal X-Ray Crystallography

Data collection and structure refinement details

Data were collected at room temperature on an X-ray single crystal diffractometer equipped with a kappa-geometry goniometer, a 4K CCD detector (Bruker APEXII) and a sealed, fine focus, X-ray tube, emitting MoKα radiation (λ = 0.71073 Å). The *breamsstrahlung* radiation and the Kβ component were filtered by a graphite monochromator. Data collection and data reduction were performed using the Bruker APEXIII software package [1]. The measurements were performed on a small single crystal coated with perfluorinated ether oil mounted on top of a thin glass fibber. Initial lattice parameters were determined from a preliminary data collection consisting of set of 36 detector frames. A subsequent data collection was performed on a full sphere, using omega and phi scans of 0.5^{o} width. The data acquisition time was 10 s per frame. Reflections were merged and corrected for Lorentz and polarization effects, scan speed, and background using SAINT V8.38A [2] included in the APEXIII package. Absorption corrections, including odd and even spherical harmonics up to rank 3 and 6, respectively, were performed using SADABS-2016/2[3].

Space group assignment was based upon systematic absences, *E* statistics, and successful refinement of the structure in space group $P2_12_12_1$. The structure was solved by a dual-space method using SHELXT 2014/5 [4] and refined by full matrix least-squares (minimizing $\Sigma w(F_o^2-F_c^2)^2$) using SHELXL-2018/3 [5]. The weighting scheme was $w=1/[s^2(F_o^2)+(0.0437P)^2+0.1746P]$

where $P=(F_o^2+2F_c^2)/3$'where $P=(F_o^2+2F_c^2)/3$, as suggested by SHELXL-2018/3. The final quality factors of the refinement were $R_1(I>2\sigma) = 0.0371$, $wR_{all} = 0.0928$ and GOF = 1.045 for 3888 independent reflections and 229 refined parameters. Default SHELXL-2018/3 values for atomic scattering factors for all atoms and anomalous dispersion corrections for the non-hydrogen atoms were used. All atoms were refined anisotropically with exception for the H atoms. The H atoms attached to the C atoms were initially placed idealized positions and refined as riding using SHELXL defaults. Those attached to the N atoms had their positions freely refined with an isotopic displacement parameter constrained to 1.2X Uiso of the parent atom. The ORTEP plot of the molecule was generated by PLATON [6] and the drawing of the crystal structure by Mercury [7].

CCDC 2010673 contains additional crystallographic data for this paper. These data are provided free of charge by The Cambridge Crystallographic Data Centre. Standard crystallographic tables generated from the CIF by the Supplementary Material option of PLATON [6] are given below.

[1]Bruker (2016). *APEX3*, Bruker AXS Inc., Madison, Wisconsin, USA.

[2]Bruker (2016). *SAINT V8.38A*, Bruker AXS Inc., Madison, Wisconsin, USA.

[3] Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.

[4] Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8

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[6] Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

[7] C. F. Macrae, I. Sovago, S. J. Cottrell, P. T. A. Galek, P. McCabe, E. Pidcock, M. Platings, G. P. Shields, J. S. Stevens, M. Towler and P. A. Wood, J. Appl. Cryst., **53**, 226-235, 2020

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C r y s t a l l o g h r a p h i c T a b l e s
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B E L O N G I N G TO T H E P A P E R

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C o n t e n t s
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Table S4 - Crystal Data and Details of the Structure Determination

Formula			C4 H6 N2 O2
Formula Weight			114.11
Crystal System			orthorhombic
Space group		P212121	(No. 19)
a, b, c [Angstrom]	7.8466(2)	9.8257(3)	20.3107(7)
V [Ang**3]			1565.92(8)
Z			12
D(calc) [g/cm**3]			1.452
Mu(MoKa) [/mm]			0.118
F(000)			720
Crystal Size [mm]		0.18 x 0.18 x 0.60	
Data Collection			
Temperature (K)			293
Radiation [Angstrom]		MoKa	0.71073
Theta Min-Max [Deg]			2.3, 28.3
Dataset		-10: 10 ; -13: 13 ; -27: 27	
Tot., Uniq. Data, R(int)		45996, 3888, 0.040	
Observed Data [I > 2.0 sigma(I)]			2898
Refinement			
Nref, Npar			3888, 229
R, wR2, S		0.0371, 0.0928, 1.04	
w = ^2^(FO^2^)+(0.0437P)^2^+0.1746P] WHERE P=(FO^2^+2FC^2^)/3'			
Max. and Av. Shift/Error			0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]			-0.23, 0.16

Table S5 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms

Atom	x	y	z	U(eq) [Ang^2]
O7A	0.5256(2)	0.26703(18)	0.49530(10)	0.0520(6)
O9A	0.1379(2)	0.60983(18)	0.47874(11)	0.0630(7)
N1A	0.5594(2)	0.4987(2)	0.48573(11)	0.0435(7)
N3A	0.2989(2)	0.4161(2)	0.48715(10)	0.0397(6)
C2A	0.4711(3)	0.3828(2)	0.49033(11)	0.0359(7)
C4A	0.2724(3)	0.5512(2)	0.48073(13)	0.0410(7)
C5A	0.4481(3)	0.6142(2)	0.47587(14)	0.0439(8)
C6A	0.7434(3)	0.5077(3)	0.48384(15)	0.0516(9)
O7B	-0.0562(2)	0.50869(17)	0.31127(11)	0.0545(6)
O9B	0.3592(2)	0.82506(19)	0.34004(11)	0.0648(7)
N1B	-0.0698(2)	0.7385(2)	0.33139(10)	0.0419(6)
N3B	0.1830(2)	0.64396(19)	0.32064(10)	0.0389(6)
C2B	0.0072(3)	0.6205(2)	0.32061(11)	0.0377(7)
C4B	0.2190(3)	0.7759(2)	0.33337(12)	0.0397(7)
C5B	0.0514(3)	0.8487(2)	0.33773(13)	0.0416(7)
C6B	-0.2528(3)	0.7590(3)	0.33289(14)	0.0524(9)
O7C	0.4539(2)	0.45993(17)	0.31755(11)	0.0564(7)
O9C	0.8466(2)	0.12548(18)	0.34908(11)	0.0650(7)
N1C	0.4233(2)	0.2309(2)	0.33671(10)	0.0428(6)
N3C	0.6824(2)	0.31467(19)	0.33074(10)	0.0402(6)
C2C	0.5097(3)	0.3463(2)	0.32720(12)	0.0376(7)
C4C	0.7107(3)	0.1812(2)	0.34296(12)	0.0424(8)
C5C	0.5358(3)	0.1165(2)	0.34718(15)	0.0467(8)
C6C	0.2396(3)	0.2195(3)	0.34020(15)	0.0552(9)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S6 - Hydrogen Atom Positions and Isotropic Displacement Parameters

Atom	x	y	z	U(iso) [Ang^2]
H8A	0.228(3)	0.358(3)	0.4916(12)	0.0480
H10A	0.46624	0.65527	0.43301	0.0530
H11A	0.46510	0.68254	0.50971	0.0530
H12A	0.79147	0.41860	0.48936	0.0770
H13A	0.78214	0.56599	0.51869	0.0770
H14A	0.77853	0.54452	0.44223	0.0770
H8B	0.259(3)	0.582(3)	0.3174(12)	0.0470
H10B	0.03897	0.89496	0.37964	0.0500
H11B	0.03860	0.91420	0.30234	0.0500
H12B	-0.28425	0.82471	0.30009	0.0790
H13B	-0.28594	0.79154	0.37558	0.0790
H14B	-0.30938	0.67434	0.32400	0.0790
H8C	0.758(4)	0.375(3)	0.3261(12)	0.0480
H10C	0.52071	0.04783	0.31335	0.0560
H11C	0.51704	0.07548	0.39002	0.0560
H12C	0.18909	0.30679	0.33190	0.0830
H13C	0.20717	0.18854	0.38324	0.0830
H14C	0.20078	0.15553	0.30777	0.0830

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S7 - (An)isotropic Displacement Parameters

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
O7A	0.0369(9)	0.0333(10)	0.0858(14)	0.0034(8)	-0.0030(8)	0.0054(8)
O9A	0.0352(9)	0.0464(12)	0.1075(15)	-0.0007(11)	0.0014(10)	0.0116(8)
N1A	0.0272(9)	0.0335(11)	0.0698(14)	0.0069(10)	-0.0062(9)	-0.0014(8)
N3A	0.0260(9)	0.0312(11)	0.0620(12)	0.0014(9)	-0.0003(9)	-0.0041(8)
C2A	0.0263(10)	0.0310(12)	0.0504(13)	0.0006(10)	-0.0017(9)	0.0002(9)
C4A	0.0318(11)	0.0349(13)	0.0562(14)	-0.0013(11)	0.0003(11)	0.0046(9)
C5A	0.0333(11)	0.0300(13)	0.0685(16)	0.0036(11)	-0.0057(11)	-0.0015(9)
C6A	0.0266(11)	0.0523(16)	0.0759(17)	0.0056(14)	-0.0052(11)	-0.0049(11)
O7B	0.0409(9)	0.0386(10)	0.0841(13)	-0.0083(9)	0.0052(8)	-0.0137(8)
O9B	0.0335(9)	0.0469(11)	0.1139(17)	0.0003(11)	-0.0083(10)	-0.0124(8)
N1B	0.0267(8)	0.0336(11)	0.0655(13)	0.0020(10)	-0.0005(8)	0.0004(7)
N3B	0.0247(9)	0.0291(10)	0.0629(12)	-0.0006(9)	0.0010(8)	0.0003(7)
C2B	0.0276(10)	0.0355(13)	0.0499(13)	0.0021(10)	0.0021(9)	-0.0040(9)
C4B	0.0305(10)	0.0320(12)	0.0565(14)	0.0057(10)	-0.0006(10)	-0.0026(9)
C5B	0.0366(11)	0.0280(12)	0.0602(15)	0.0014(11)	0.0001(10)	-0.0001(9)
C6B	0.0271(11)	0.0584(16)	0.0718(17)	-0.0002(14)	0.0013(10)	0.0060(11)
O7C	0.0392(9)	0.0329(9)	0.0971(15)	0.0054(9)	0.0057(9)	0.0069(7)
O9C	0.0388(10)	0.0479(11)	0.1084(16)	0.0021(11)	-0.0013(10)	0.0123(8)
N1C	0.0277(9)	0.0350(11)	0.0658(13)	0.0019(10)	-0.0025(9)	-0.0050(8)
N3C	0.0262(9)	0.0279(10)	0.0666(13)	-0.0015(9)	0.0023(8)	-0.0021(8)
C2C	0.0295(10)	0.0312(12)	0.0520(14)	-0.0034(10)	0.0017(9)	-0.0011(9)
C4C	0.0344(11)	0.0342(13)	0.0587(15)	-0.0044(10)	-0.0008(11)	0.0002(9)
C5C	0.0394(12)	0.0300(12)	0.0706(17)	-0.0002(12)	0.0000(11)	-0.0035(10)
C6C	0.0293(12)	0.0636(17)	0.0727(18)	-0.0004(14)	0.0006(11)	-0.0119(11)

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Table S8 - Bond Distances (Angstrom)

O7A	-C2A	1.219(3)	N3B	-H8B	0.86(3)
O9A	-C4A	1.203(3)	C4B	-C5B	1.500(3)
N1A	-C2A	1.336(3)	O7C	-C2C	1.215(3)
N1A	-C5A	1.446(3)	O9C	-C4C	1.205(3)
N1A	-C6A	1.447(3)	N1C	-C5C	1.445(3)
N3A	-C2A	1.392(3)	N1C	-C2C	1.335(3)
N3A	-C4A	1.350(3)	N1C	-C6C	1.448(3)
N3A	-H8A	0.80(3)	N3C	-C4C	1.353(3)
C4A	-C5A	1.515(3)	N3C	-C2C	1.392(3)
O7B	-C2B	1.221(3)	C5B	-H10B	0.9700
O9B	-C4B	1.209(3)	C5B	-H11B	0.9700
N1B	-C5B	1.447(3)	C6B	-H12B	0.9600
N1B	-C2B	1.326(3)	C6B	-H13B	0.9600
N1B	-C6B	1.450(3)	C6B	-H14B	0.9600
N3B	-C4B	1.352(3)	N3C	-H8C	0.84(3)
N3B	-C2B	1.399(3)	C4C	-C5C	1.515(3)
C5A	-H10A	0.9700	C5C	-H10C	0.9700
C5A	-H11A	0.9700	C5C	-H11C	0.9700
C6A	-H12A	0.9600	C6C	-H12C	0.9600
C6A	-H13A	0.9600	C6C	-H13C	0.9600
C6A	-H14A	0.9600	C6C	-H14C	0.9600

Table S9 - Bond Angles (Degrees)

C2A	-N1A	-C5A	111.43(17)	O7B	-C2B	-N1B	128.8(2)
C2A	-N1A	-C6A	124.8(2)	O7B	-C2B	-N3B	123.4(2)
C5A	-N1A	-C6A	123.4(2)	N1B	-C2B	-N3B	107.78(18)
C2A	-N3A	-C4A	112.66(18)	C2B	-N3B	-H8B	124.8(18)
O7A	-C2A	-N1A	128.2(2)	C4B	-N3B	-H8B	123.5(18)
O7A	-C2A	-N3A	124.3(2)	O9B	-C4B	-N3B	126.5(2)
N1A	-C2A	-N3A	107.45(18)	O9B	-C4B	-C5B	126.92(19)
C2A	-N3A	-H8A	120.1(19)	N3B	-C4B	-C5B	106.59(18)
C4A	-N3A	-H8A	127(2)	N1B	-C5B	-C4B	102.37(16)
O9A	-C4A	-N3A	127.5(2)	C5C	-N1C	-C6C	122.8(2)
O9A	-C4A	-C5A	126.92(19)	C2C	-N1C	-C5C	111.82(17)
N3A	-C4A	-C5A	105.55(18)	C2C	-N1C	-C6C	125.3(2)
N1A	-C5A	-C4A	102.71(16)	C2C	-N3C	-C4C	112.68(18)
C5B	-N1B	-C6B	123.0(2)	N1B	-C5B	-H11B	111.00
C2B	-N1B	-C5B	111.70(17)	C4B	-C5B	-H10B	111.00
C2B	-N1B	-C6B	125.2(2)	C4B	-C5B	-H11B	111.00
C2B	-N3B	-C4B	111.36(18)	N1B	-C5B	-H10B	111.00
N1A	-C5A	-H11A	111.00	H10B	-C5B	-H11B	109.00
C4A	-C5A	-H10A	111.00	H12B	-C6B	-H14B	109.00
C4A	-C5A	-H11A	111.00	H13B	-C6B	-H14B	109.00
N1A	-C5A	-H10A	111.00	H12B	-C6B	-H13B	109.00
H10A	-C5A	-H11A	109.00	N1B	-C6B	-H12B	109.00
H12A	-C6A	-H14A	110.00	N1B	-C6B	-H13B	109.00
H13A	-C6A	-H14A	109.00	N1B	-C6B	-H14B	109.00
H12A	-C6A	-H13A	109.00	O7C	-C2C	-N1C	128.4(2)
N1A	-C6A	-H12A	109.00	O7C	-C2C	-N3C	124.3(2)
N1A	-C6A	-H13A	109.00	N1C	-C2C	-N3C	107.29(17)
N1A	-C6A	-H14A	109.00	C2C	-N3C	-H8C	121(2)

Table S9 - Bond Angles (Degrees) (continued)

C4C	-N3C	-H8C	126(2)	C4C	-C5C	-H11C	111.00
O9C	-C4C	-N3C	127.2(2)	H10C	-C5C	-H11C	109.00
O9C	-C4C	-C5C	127.24(19)	N1C	-C6C	-H12C	109.00
N3C	-C4C	-C5C	105.57(18)	N1C	-C6C	-H13C	109.00
N1C	-C5C	-C4C	102.63(16)	N1C	-C6C	-H14C	109.00
N1C	-C5C	-H10C	111.00	H12C	-C6C	-H13C	109.00
N1C	-C5C	-H11C	111.00	H12C	-C6C	-H14C	109.00
C4C	-C5C	-H10C	111.00	H13C	-C6C	-H14C	109.00

Table S10 - Torsion Angles (Degrees)

C5A	-N1A	-C2A	-O7A	175.9(2)
C5A	-N1A	-C2A	-N3A	-2.9(3)
C6A	-N1A	-C2A	-O7A	2.0(4)
C6A	-N1A	-C2A	-N3A	-176.9(2)
C2A	-N1A	-C5A	-C4A	4.5(3)
C6A	-N1A	-C5A	-C4A	178.5(2)
C4A	-N3A	-C2A	-O7A	-179.0(2)
C4A	-N3A	-C2A	-N1A	-0.2(3)
C2A	-N3A	-C4A	-O9A	-177.6(3)
C2A	-N3A	-C4A	-C5A	2.9(3)
O9A	-C4A	-C5A	-N1A	176.2(3)
N3A	-C4A	-C5A	-N1A	-4.3(3)
C5B	-N1B	-C2B	-O7B	-177.9(3)
C5B	-N1B	-C2B	-N3B	1.4(3)
C6B	-N1B	-C2B	-O7B	-1.4(4)
C6B	-N1B	-C2B	-N3B	177.8(2)
C2B	-N1B	-C5B	-C4B	-3.6(3)
C6B	-N1B	-C5B	-C4B	179.8(2)
C4B	-N3B	-C2B	-O7B	-178.9(2)
C4B	-N3B	-C2B	-N1B	1.9(3)
C2B	-N3B	-C4B	-O9B	175.8(2)
C2B	-N3B	-C4B	-C5B	-4.1(3)
O9B	-C4B	-C5B	-N1B	-175.3(3)
N3B	-C4B	-C5B	-N1B	4.5(3)
C5C	-N1C	-C2C	-O7C	-179.5(3)
C5C	-N1C	-C2C	-N3C	0.1(3)
C6C	-N1C	-C2C	-O7C	-2.8(4)
C6C	-N1C	-C2C	-N3C	176.7(2)

Table S10 - Torsion Angles (Degrees) (continued)

C2C	-N1C	-C5C	-C4C	0.4(3)
C6C	-N1C	-C5C	-C4C	-176.4(2)
C4C	-N3C	-C2C	-O7C	179.0(2)
C4C	-N3C	-C2C	-N1C	-0.6(3)
C2C	-N3C	-C4C	-O9C	-179.4(3)
C2C	-N3C	-C4C	-C5C	0.8(3)
O9C	-C4C	-C5C	-N1C	179.5(3)
N3C	-C4C	-C5C	-N1C	-0.7(3)

Table S11 – Contact Distances(Angstrom)

O7A	.C5C	3.353(3)	N3C	.C4B_u	3.443(3)
O7A	.C6A	2.927(3)	N3C	.O7B_j	2.828(2)
O7A	.N3A_a	2.822(2)	O7A	.H12A_b	2.6100
O7B	.C5B_l	3.410(3)	O7A	.H11C	2.8500
O7B	.N3C_k	2.828(2)	O7A	.H8A	2.50(2)
O7B	.C6B	2.936(3)	O7A	.H12A	2.5700
O7C	.C6C	2.936(3)	O7A	.H8A_a	2.03(3)
O7C	.N3B	2.791(2)	O7A	.H13C_c	2.8800
O9A	.N3B	3.248(3)	O7B	.H8C_k	1.99(3)
O9A	.C5A_e	3.228(3)	O7B	.H12C	2.8000
O9A	.C6A_d	3.256(3)	O7B	.H14B	2.5800
O9A	.C2B	3.373(3)	O7B	.H8B	2.58(2)
O9B	.C6B_j	3.116(3)	O7B	.H11B_l	2.4900
O9B	.C5C_m	3.185(3)	O7C	.H14B_j	2.8100
O9C	.C2A_a	3.406(3)	O7C	.H8B	1.94(3)
O9C	.C6C_t	3.224(3)	O7C	.H8C	2.53(3)
O9C	.C5B_s	3.167(3)	O7C	.H12C	2.5800
N1A	.C4A	2.313(3)	O7C	.H10C_n	2.8000
N1B	.C4B	2.296(3)	O9A	.H11A_e	2.4600
N1C	.C4C	2.311(3)	O9A	.H10A	2.7700
N3A	.C5A	2.283(3)	O9A	.H8A	2.59(3)
N3A	.O7A_b	2.822(2)	O9A	.H11A	2.7400
N3B	.C4A	3.449(3)	O9B	.H8B	2.56(3)
N3B	.O9A	3.248(3)	O9B	.H12B_j	2.9100
N3B	.O7C	2.791(2)	O9B	.H13B_j	2.9000
N3B	.C5B	2.288(3)	O9B	.H10A	2.6600
N3B	.C4C_n	3.445(3)	O9B	.H11B	2.7700
N3C	.C5C	2.286(3)	O9B	.H10B	2.7300

Table S11 - Contact Distances(Angstrom) (continued)

O9B	.H10C_m	2.5900	C5B	.N3B	2.288(3)
O9C	.H11B_s	2.7400	C5B	.O9C_p	3.167(3)
O9C	.H14C_t	2.9200	C5B	.O7B_q	3.410(3)
O9C	.H10C	2.7700	C5C	.N3C	2.286(3)
O9C	.H8C	2.59(3)	C5C	.O7A	3.353(3)
O9C	.H10B_s	2.7900	C5C	.O9B_v	3.185(3)
O9C	.H11C	2.7600	C6A	.O9A_i	3.256(3)
N1A	.H10B_f	2.9300	C6A	.O7A	2.927(3)
N1A	.H8A	2.95(2)	C6B	.O7B	2.936(3)
C2A	.C2C	3.346(3)	C6B	.O9B_r	3.116(3)
C2A	.O9C_g	3.406(3)	C6B	.C6C_o	3.539(4)
C2A	.C4A	2.282(3)	C6C	.O7C	2.936(3)
C2B	.O9A	3.373(3)	C6C	.O9C_k	3.224(3)
C2B	.C4B	2.272(3)	C6C	.C6B_l	3.539(4)
C2C	.C4C	2.285(3)	C2A	.H10A	2.9200
C2C	.C2A	3.346(3)	C2A	.H11A	2.9700
N3A	.H10A	2.9100	C2A	.H14A	3.0500
N3B	.H11B	2.9100	C2A	.H13A	3.0900
N3C	.H10C	2.9300	C2A	.H12A	2.5400
N3C	.H11C	2.9400	C2B	.H10B	2.9600
C4A	.N1A	2.313(3)	C2B	.H13B	3.0600
C4A	.N3B	3.449(3)	C2B	.H14C_o	3.1000
C4B	.N1B	2.296(3)	C2B	.H12B	3.0700
C4B	.N3C_n	3.443(3)	C2B	.H14B	2.5400
C4C	.N3B_u	3.445(3)	C2B	.H11B	2.9200
C4C	.N1C	2.311(3)	C2C	.H13C	3.0600
C5A	.N3A	2.283(3)	C2C	.H10C	2.9500
C5A	.O9A_h	3.228(3)	C2C	.H11C	2.9500

Table S11 - Contact Distances(Angstrom) (continued)

C2C	.H8B	3.05(3)	H8B	.O9B	2.56(3)
C2C	.H14C	3.0900	H8B	.O7B	2.58(2)
C2C	.H12C	2.5500	H8C	.O7B_j	1.99(3)
C4B	.H10A	3.0400	H8C	.O9C	2.59(3)
C5A	.H13A	2.8000	H8C	.O7C	2.53(3)
C5A	.H8A	3.07(3)	H10A	.O9B	2.6600
C5A	.H10B_f	3.0200	H10A	.O9A	2.7700
C5A	.H14A	2.7700	H10A	.C4B	3.0400
C5B	.H13B	2.8100	H10A	.N3A	2.9100
C5B	.H12B	2.7500	H10A	.C6A	2.8100
C5C	.H14C	2.7700	H10A	.C2A	2.9200
C5C	.H13C	2.7700	H10B	.C2B	2.9600
C6A	.H10A	2.8100	H10B	.H11A_e	2.4400
C6A	.H11A	2.8300	H10B	.C5A_e	3.0200
C6B	.H14A_d	3.0700	H10B	.O9C_p	2.7900
C6B	.H10B	2.8200	H10B	.O9B	2.7300
C6B	.H14C_o	3.0600	H10B	.N1A_e	2.9300
C6B	.H11B	2.8200	H10B	.C6B	2.8200
C6C	.H11C	2.7900	H10C	.C2C	2.9500
C6C	.H10C	2.8300	H10C	.C6C	2.8300
C6C	.H12B_l	3.0500	H10C	.N3C	2.9300
H8A	.O9A	2.59(3)	H10C	.O9B_v	2.5900
H8A	.O7A	2.50(2)	H10C	.O9C	2.7700
H8A	.N1A	2.95(2)	H10C	.O7C_w	2.8000
H8A	.C5A	3.07(3)	H11A	.H10B_f	2.4400
H8A	.O7A_b	2.03(3)	H11A	.C6A	2.8300
H8B	.C2C	3.05(3)	H11A	.O9A	2.7400
H8B	.O7C	1.94(3)	H11A	.C2A	2.9700

Table S11 - Contact Distances(Angstrom) (continued)

H11A	.O9A_h	2.4600	H12C	.O7C	2.5800
H11B	.C6B	2.8200	H13A	.C2A	3.0900
H11B	.O9B	2.7700	H13A	.C5A	2.8000
H11B	.C2B	2.9200	H13B	.C5B	2.8100
H11B	.O9C_p	2.7400	H13B	.C2B	3.0600
H11B	.N3B	2.9100	H13B	.O9B_r	2.9000
H11B	.O7B_q	2.4900	H13C	.O7A_b	2.8800
H11C	.N3C	2.9400	H13C	.C5C	2.7700
H11C	.O7A	2.8500	H13C	.C2C	3.0600
H11C	.O9C	2.7600	H14A	.C2A	3.0500
H11C	.C2C	2.9500	H14A	.C5A	2.7700
H11C	.C6C	2.7900	H14A	.C6B_j	3.0700
H12A	.O7A	2.5700	H14B	.O7B	2.5800
H12A	.O7A_a	2.6100	H14B	.O7C_k	2.8100
H12A	.C2A	2.5400	H14B	.C2B	2.5400
H12B	.C5B	2.7500	H14C	.O9C_k	2.9200
H12B	.C2B	3.0700	H14C	.C2C	3.0900
H12B	.C6C_o	3.0500	H14C	.C5C	2.7700
H12B	.O9B_r	2.9100	H14C	.C2B_l	3.1000
H12C	.C2C	2.5500	H14C	.C6B_l	3.0600
H12C	.O7B	2.8000			

Table S12 - Hydrogen Bonds (Angstrom, Deg)

N3A -- H8A .. O7A	0.80(3)	2.03(3)	2.822(2)	172(3)	3_456
N3B -- H8B .. O7C	0.86(3)	1.94(3)	2.791(2)	171(2)	.
N3C -- H8C .. O7B	0.84(3)	1.99(3)	2.828(2)	176(3)	1_655
C5C -- H10C .. O9B	0.9700	2.5900	3.185(3)	120.00	1_545
C5A -- H11A .. O9A	0.9700	2.4600	3.228(3)	136.00	3_566
C5B -- H11B .. O7B	0.9700	2.4900	3.410(3)	158.00	4_555
C6A -- H12A .. O7A	0.9600	2.5700	2.927(3)	102.00	.
C6C -- H12C .. O7C	0.9600	2.5800	2.936(3)	102.00	.
C6B -- H14B .. O7B	0.9600	2.5800	2.936(3)	102.00	.

Translation of Symmetry Code to Equiv. Pos

a =[3556.00] = [4_556] = 1/2+x,1/2-y,1-z
b =[3456.00] = [4_456] = -1/2+x,1/2-y,1-z
c =[3556.00] = [4_556] = 1/2+x,1/2-y,1-z
d =[1455.00] = [1_455] = -1+x,y,z
e =[3466.00] = [4_466] = -1/2+x,3/2-y,1-z
f =[3566.00] = [4_566] = 1/2+x,3/2-y,1-z
h =[3566.00] = [4_566] = 1/2+x,3/2-y,1-z
i =[1655.00] = [1_655] = 1+x,y,z
j =[1655.00] = [1_655] = 1+x,y,z
k =[1455.00] = [1_455] = -1+x,y,z
l =[4545.00] = [3_545] = -x,-1/2+y,1/2-z
m =[1565.00] = [1_565] = x,1+y,z
n =[4655.00] = [3_655] = 1-x,1/2+y,1/2-z
o =[4555.00] = [3_555] = -x,1/2+y,1/2-z
p =[1465.00] = [1_465] = -1+x,1+y,z
q =[4555.00] = [3_555] = -x,1/2+y,1/2-z
r =[1455.00] = [1_455] = -1+x,y,z
s =[1645.00] = [1_645] = 1+x,-1+y,z
u =[4645.00] = [3_645] = 1-x,-1/2+y,1/2-z
v =[1545.00] = [1_545] = x,-1+y,z
w =[4645.00] = [3_645] = 1-x,-1/2+y,1/2-z