Supporting Information

Controllable Construction of Base Pairing and Chirality Study in Supramolecular Assemblies Based on Guanine Nucleotides

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Content

Section 1 Molecular Structure Diagram

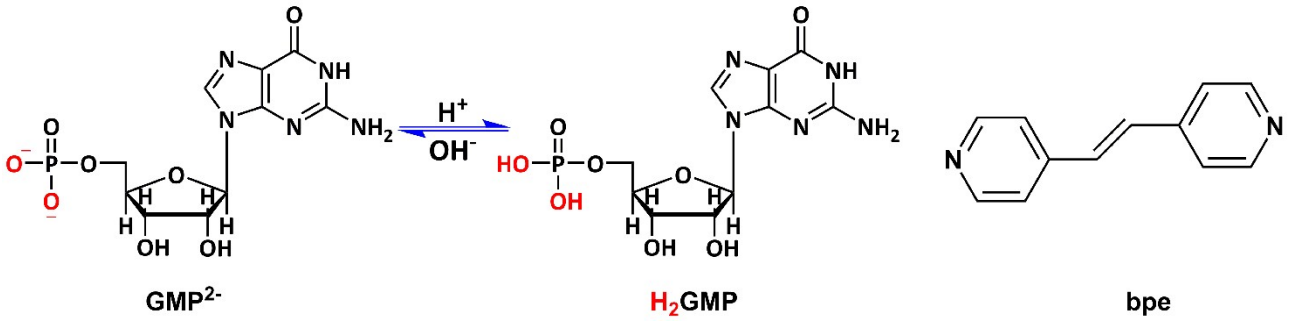

Fig. S1 Diagrams of different protonation states of **GMP** in aqueous solution and the structure of **bpe**.

Section 2 Materials

All chemical reagents used in this experiment are of analytical grade and require no further purification before use. The solvent water is deionized water. Guanosine 5'−monophosphate metal salt (GMP) was purchased from Adamas; 1,2−*bis*(4−pyridyl)ethylene (bpe) was purchased from Alfa Aesar. Metal salts ($Mn(CH_3COO)_2$, $Ni(CH_3COO)_2$) were purchased from Shanghai Bide Pharmaceutical Technology.

Section 3 Auxiliary ligand and GMP−M(II) binding

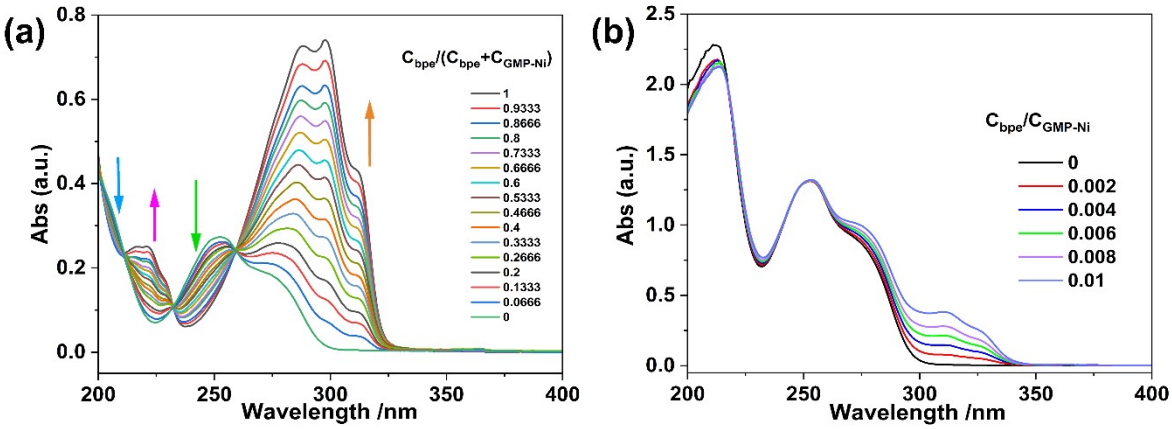

Fig. S2 (a) UV−*vis* absorption spectrums of GMP–M(II) / GMP (1:1) upon addition of bpe. The total

concentration of GMP−M(II) and bpe is held fixed (2.5×10^{-5} M), varying the ratio of the components $C_{bpe}/C_{bpe}+C_{GMP-Ni}$. **(b)** Electronic spectra of GMP−M(II)/GMP (1:1) upon addition of bpe.The total concentration of GMP−M and bpe is held fixed (2.5×10^{-5} M) varying the ratio of the components C_{bpe}/C_{GMP-Ni}.

Section 4 Crystalline Micrograph

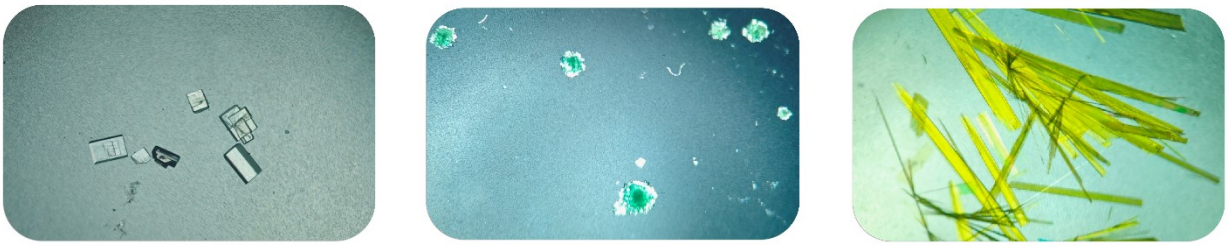

Fig. S3 (a) and **(c)** present the crystal images of **1** (transparent rod−like crystals) and **3** (yellow rod−like crystals), respectively. **(b)** present the crystal images of **2** (green block crystals).

Section 5 UV−*vis* spectroscopy

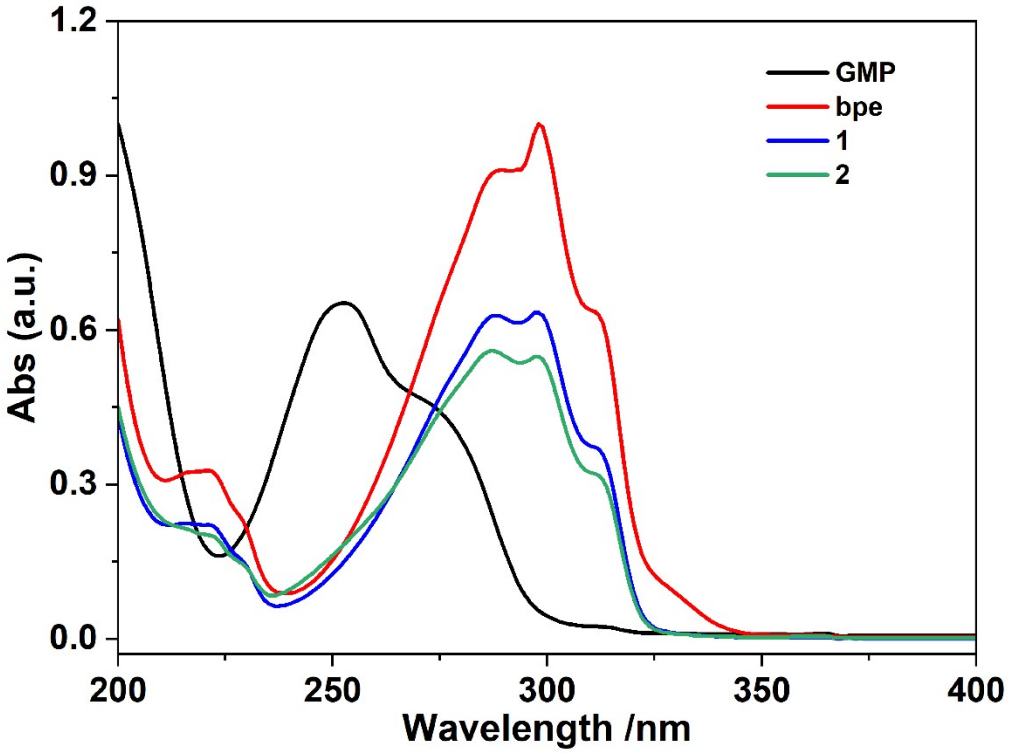

Fig S4 UV−*vis* spectra of GMP, bpe, **1**−**2**; The spectra were obtained by measuring 5.0×10^{-5} mol·L^{-1} solution in a 1 cm cell.

Section 6 X−ray Powder Diffraction

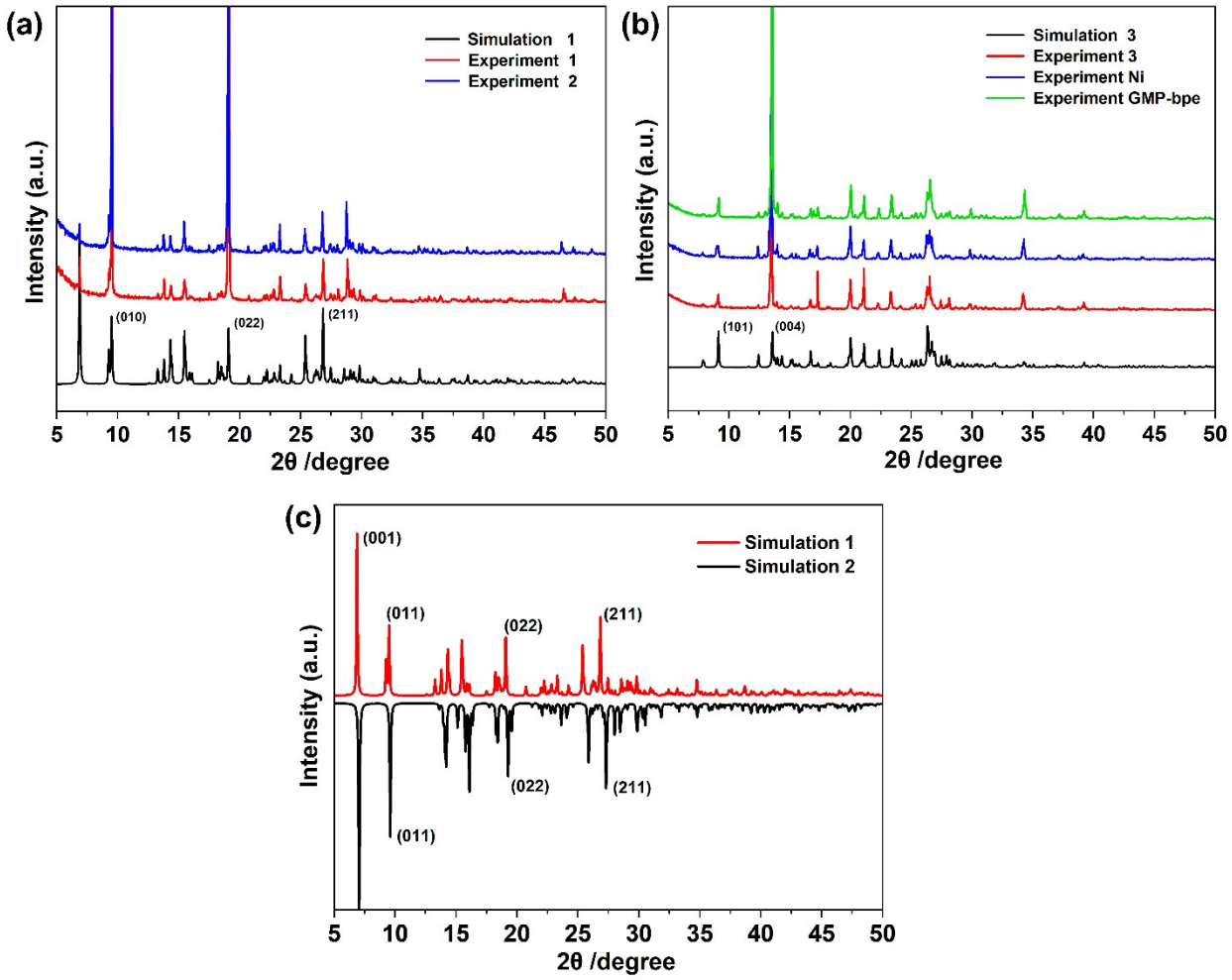

Fig. S5 PXRD patterns show the comparison between the experimental values and calculated ones for **(a) 1** and **2;(b) 3** and **GMP−bpe**. **(c)** PXRD patterns show the comparison between the calculated **1** and **2**.

Section 7 IR Spectroscopy

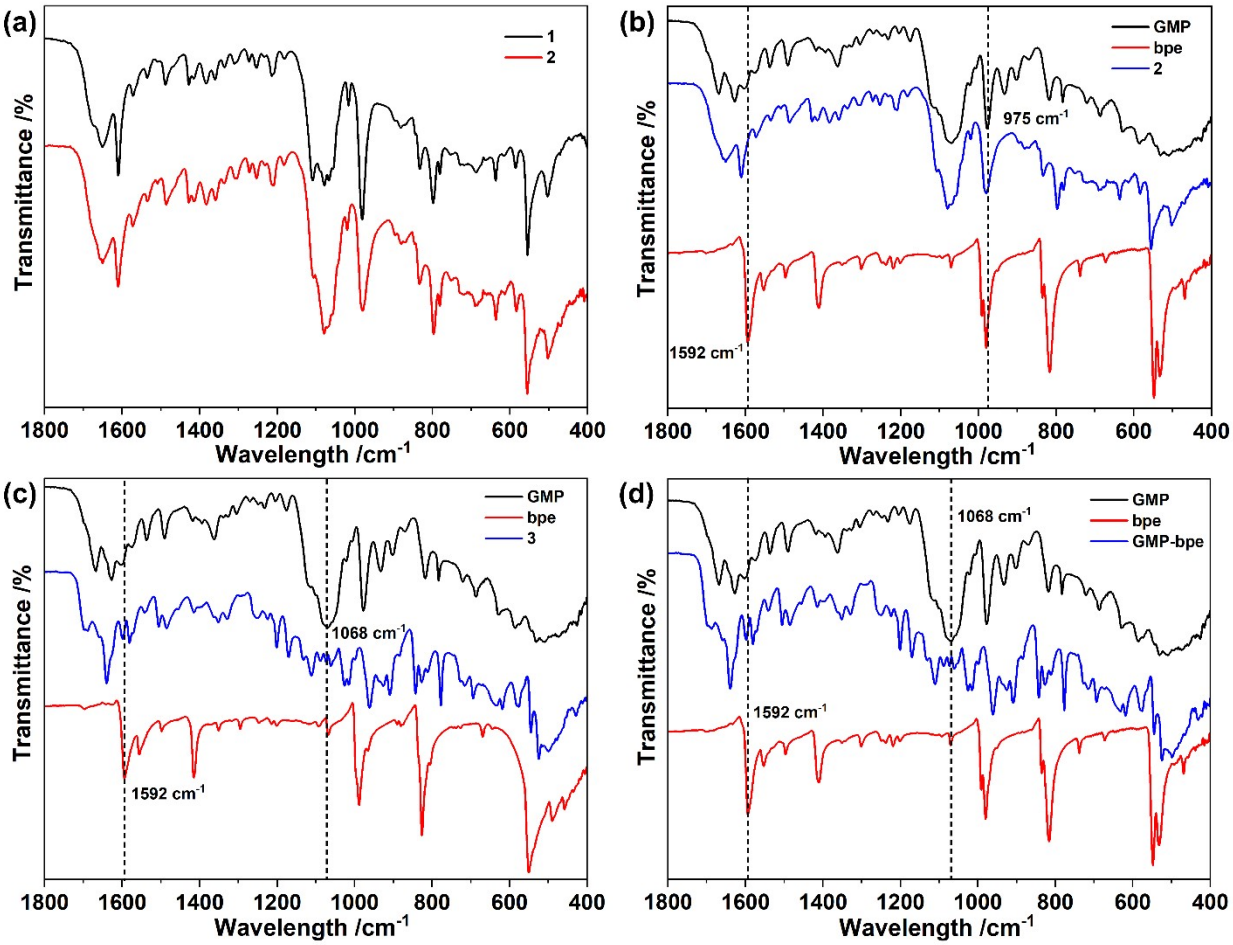

Fig. S6 IR spectra of **(a) 1** and **2**; **(b)** GMP, bpe and **2**; **(c)** GMP, bpe and **3**; **(d)** GMP, bpe and GMP−bpe.The 4000–1800 cm^{-1} wavenumber is not shown for clarity.

Section 8 Crystallographic structure diagram of 1

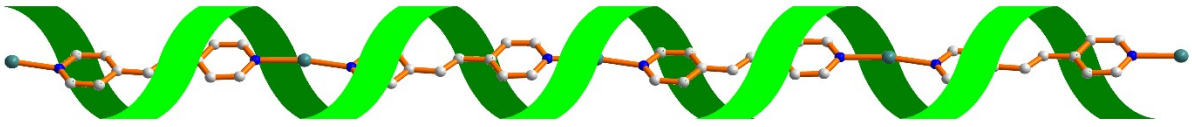

Fig. S7 Illustration of extended axial chirality based on coordination bonding.

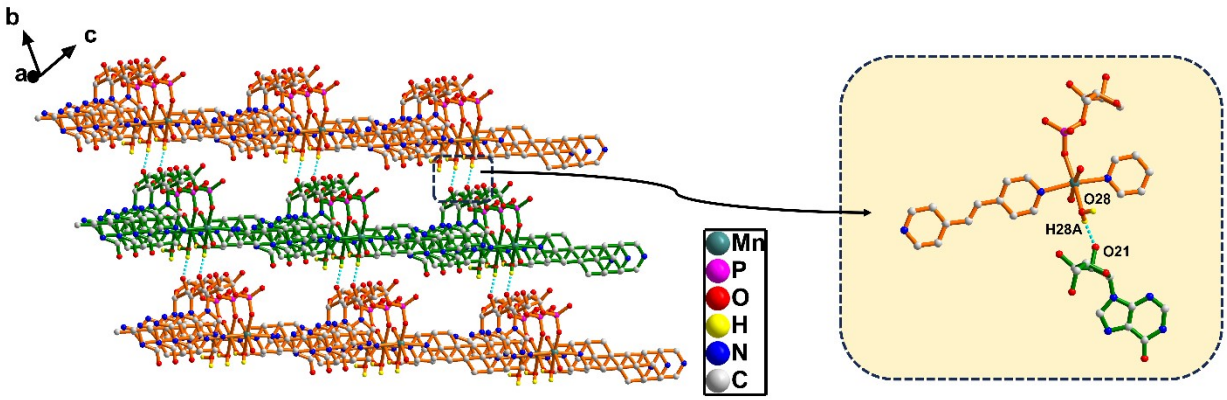

Fig. S8 The 3D structural diagram of **1**, with hydrogen bonding details on the right (Blue dotted line: O28−H28A···O21, 0.85 Å, 1.97 Å, 152.7°).

Section 9 Crystallographic structure diagram of 3

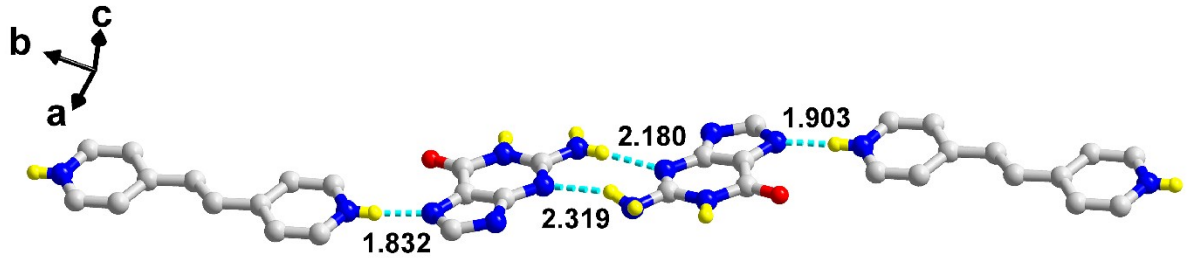

Fig S9 1D chains linked by hydrogen bonding in **3**.

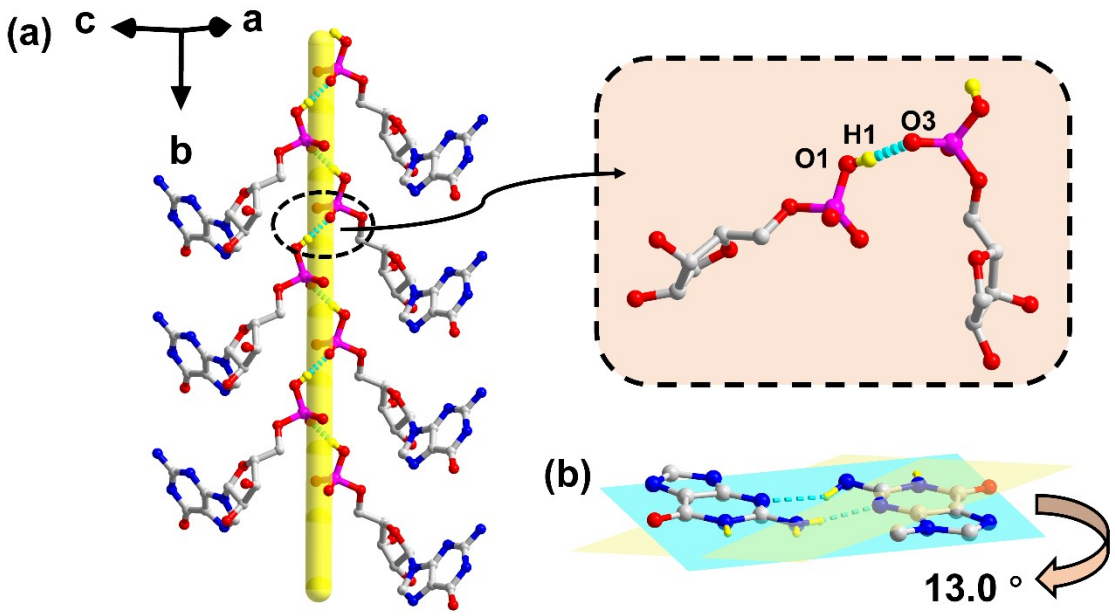

Fig. S10 (a) Schematic diagram of right−handed helix formed by interchain hydrogen bonding (blue dashed line, O1−H1···O3#1, 0.82 Å, 1.69 Å, 172.0°). **(b)** Dihedral angle between nucleobases in **3**.

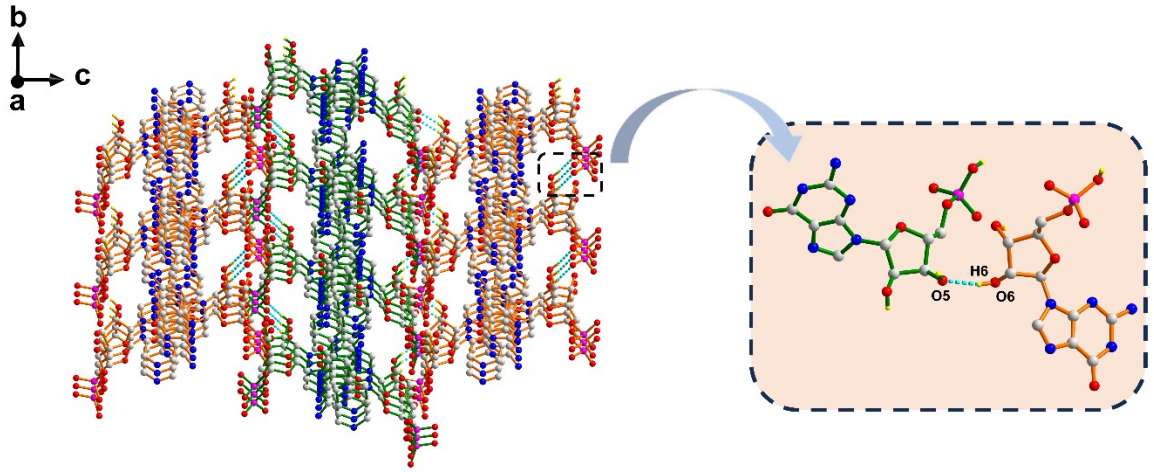

Fig. S11 The 3D structural diagram of **3**, with hydrogen bonding details on the right(Blue dotted line: O6−H6···O5, 0.82 Å, 1.96 Å,165.5°).

Section 10 Crystallographic structure diagram of GMP[1]

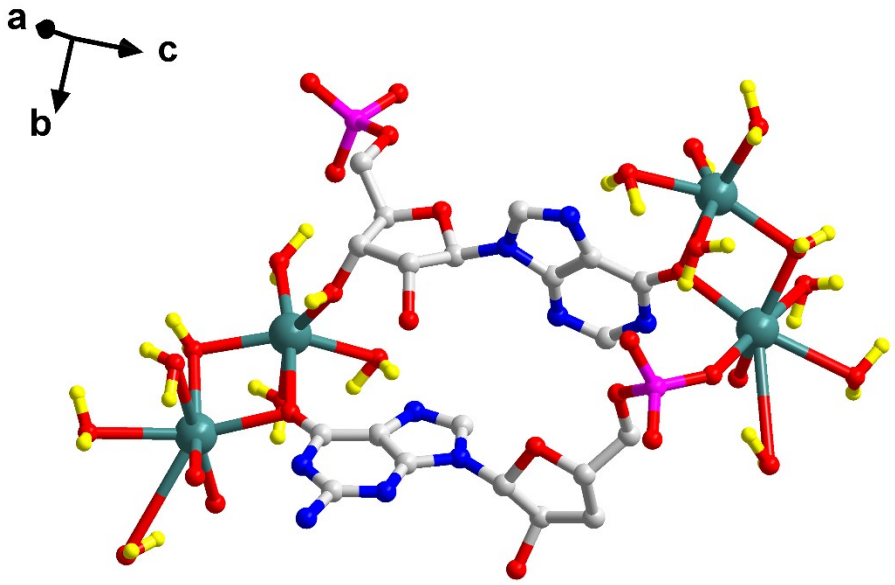

Fig. S12 Coordination environment diagram of GMP.

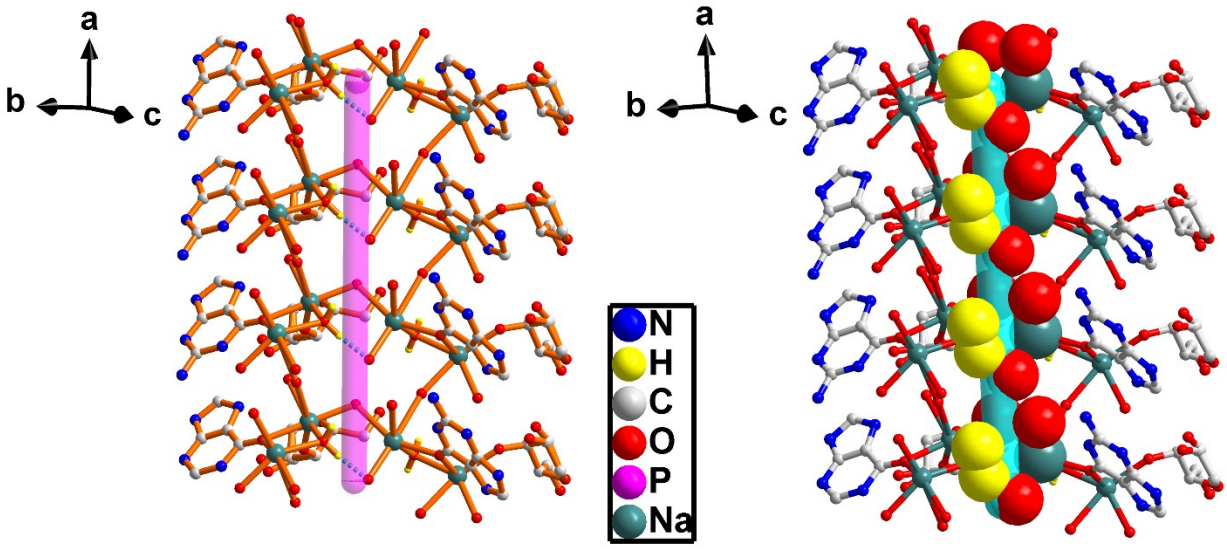

Fig. S13 Helical structure diagram of GMP.

Section 11 Solid−state UV−*vis* absorption spectroscopy

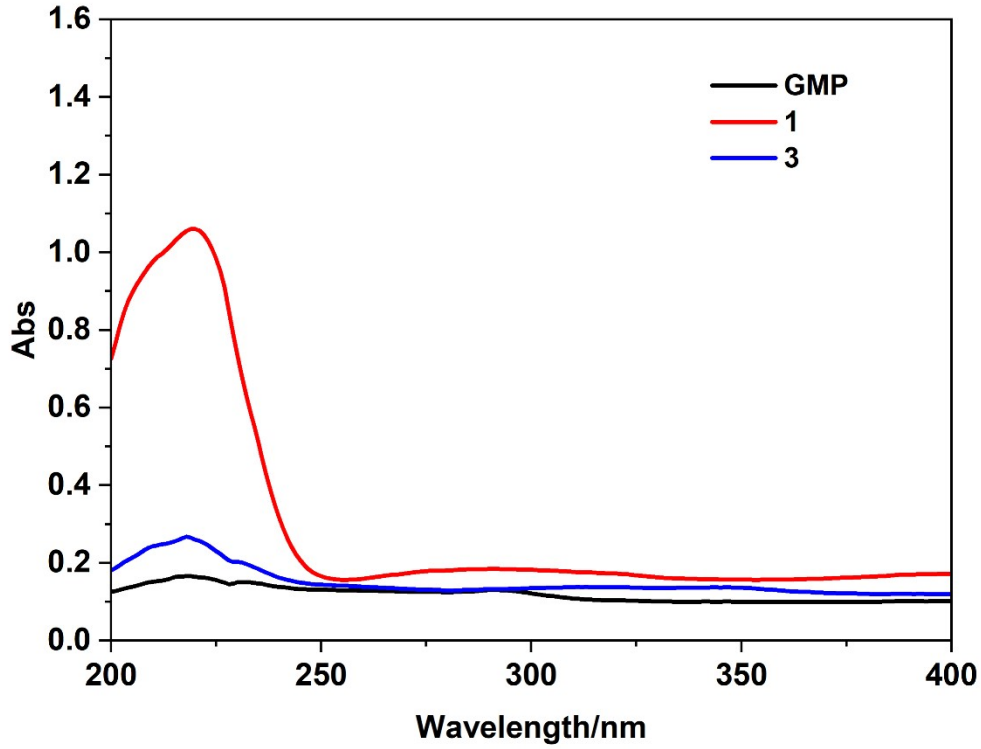

Fig. S14 UV−*vis* spectra of **GMP**, **1** and **3** in solid state at room temperature (Sample : KBr = 1 : 200).

Section 12 Selected Bond lengths (Å), angles (°) and Torsion angles(°) of 1−3.

Table S1 Selected Bond lengths (Å) and angles (°) for **1**.

Bond lengths (Å)		Bond angles (°)	
Mn(2)−O(28)	2.228(6)	O(28)−Mn(2)−N(2)#1	86.0(3)
Mn(2)−O(26)	2.111(6)	O(28)−Mn(2)−N(3)	90.2(3)
Mn(2)−O(27)	2.187(6)	O(26)−Mn(2)−O(28)	170.1(2)
Mn(2)−O(29)	2.193(6)	O(26)−Mn(2)−O(27)	99.4(2)
Mn(2)−N(2)#1	2.332(7)	O(26)−Mn(2)−O(29)	86.9(2)
Mn(2)−N(3)	2.279(7)	O(26)−Mn(2)−N(2)#1	88.8(3)
		O(26)−Mn(2)−N(3)	96.1(2)
		O(27)−Mn(2)−O(28)	88.4(2)
		O(27)−Mn(2)−O(29)	173.2(3)
		O(27)−Mn(2)−N(2)#1	84.6(3)
		O(27)−Mn(2)−N(3)	86.9(2)
		O(29)−Mn(2)−O(28)	85.6(2)

	O(29)−Mn(2)−N(2)#1	98.2(3)
	O(29)−Mn(2)−N(3)	89.9(2)
	N(3)−Mn(2)−N(2)#1	170.7(3)
	P(1)−O(26)−Mn(2)	138.6(4)
	C(20)−N(2)−Mn(2)#2	123.0(7)
	C(24)−N(2)−Mn(2)#2	119.9(6)
	C(30)−N(3)−Mn(2)	124.1(6)
	C(29)−N(3)−Mn(2)	118.7(6)

Symmetry transformations used to generate equivalent atoms: #1:+x,−1+y,1+z; #2:+x,1+y,−1+z

Tables S2 Selected H–bonding distances (Å) and angles (°) for **1.**

D−H	**A**	**d(H···A)/Å**	**d(D···A)/Å**	**∠DHA /°**	**Symmetry**
O(28)−H(28A)	O21	1,97	2.755(8)	152.7	[1+x,−1+y,+z]
O(22)−H(22)	O24	1.92	2.690(9)	157.0	[−1+x,+y,+z]

Table S3 Selected Torsion angles for **1.**

Torsion angles /°		**Torsion angles /°**	
Mn(2)#1−N(2)−C(20)−C(21)	−175.5(8)	C(35)−N(7)−C(36)−N(6)	−179.7(8)
Mn(2)#1−N(2)−C(24)−C(23)	174.9(9)	C(35)−N(7)−C(36)−N(5)	−1.7(13)
Mn(2)−N(3)−C(30)−C(31)	−172.2(8)	C(32)−N(5)−C(36)−N(7)	−0.9(15)
Mn(2)−N(3)−C(29)−C(28)	171.7(8)	C(32)−N(5)−C(36)−N(6)	177.2(9)
P(1)−O(23)−C(42)−C(39)	−153.8(6)	C(37)−N(8)−C(35)−N(7)	−178.3(8)
O(26)−P(1)−O(23)−C(42)	177.1(7)	C(37)−N(8)−C(35)−C(34)	0.2(10)
O(22)−C(40)−C(39)−O(20)	−158.7(6)	C(37)−N(8)−C(38)−O(20)	73.5(11)
O(22)−C(40)−C(39)−C(42)	81.5(9)	C(37)−N(8)−C(38)−C(41)	−46.9(12)
O(22)−C(40)−C(41)−O(21)	39.0(10)	C(37)−N(9)−C(34)−C(35)	1.4(11)
O(22)−C(40)−C(41)−C(38)	155.4(7)	C(37)−N(9)−C(34)−C(32)	178.8(10)
O(19)−C(32)−C(34)−N(9)	1.5(18)	C(38)−O(20)−C(39)−C(40)	21.2(8)
O(19)−C(32)−C(34)−C(35)	178.6(11)	C(38)−O(20)−C(39)−C(42)	146.1(7)
O(23)−P(1)−O(26)−Mn(2)	103.6(6)	C(38)−N(8)−C(35)−N(7)	1.2(14)
O(20)−C(38)−C(41)−O(21)	92.6(8)	C(38)−N(8)−C(35)−C(34)	179.6(8)
O(20)−C(38)−C(41)−C40)	−23.0(8)	C(38)−N(8)−C(37)−N(9)	−178.7(8)
O(20)−C(39)−C(42)−O(23)	−66.6(8)	C(22)−C(23)−C(24)−N(2)	0.9(19)
N(8)−C(35)−C(34)−N(9)	−1.0(10)	C(20)−N(2)−C(24)−C(23)	−0.7(17)
N(8)−C(35)−C(34)−C(32)	−178.6(8)	C(39)−O(20)−C(38)−N(8)	−124.0(7)
N(8)−C(38)−C(41)−O(21)	−146.1(7)	C(39)−O(20)−C(38)−C(41)	1.2(9)
N(8)−C(38)−C(41)−C(40)	98.4(8)	C(39)−C(40)−C(41)−O(21)	−81.7(8)
N(7)−C(35)−C(34)−N(9)	177.4(8)	C(29)−N(3)−C(30)−C(31)	0.4(15)
N(7)−C(35)−C(34)−C(32)	−0.2(15)	C(34)−N(9)−C(37)N(8)	−1.3(11)
O(25)−P(1)−O(26)−Mn(2)	−140.1(6)	C(41)−C(40)−C(39)−O(20)	−34.9(8)

O(25)−P(1)−O(23)−C(42)	57.5(8)	C(24)−N(2)−C(20)−C(21)	−0.1(16)
N(2)−C(20)−C(21)−C(22)	0.7(16)	C(36)−N(7)−C(35)−C(34)	2.2(14)
O(24)−P(1)−O(26)−Mn(2)	−11.4(7)	C(36)−N(5)−C(32)−O(19)	−177.9(9)
O(24)−P(1)−O(23)−C(42)	−65.3(7)	C(36)−N(5)−C(32)−C(34)	2.7(13)
N(3)−C(30)−C(31)−C(27)	1.4(17)	C(30)−N(3)−C(29)−C(28)	−1.4(15)
N(3)−C(29)−C(28)−C(27)	0.5(16)	C(40)−C(39)−C(42)−O(23)	51.3(9)
N(5)−C(32)−C(34)−N(9)	−179.3(9)	C(35)−N(8)−C(37)−N(9)	0.8(11)
N(5)−C(32)−C(34)−C(35)	−2.1(13)	C(35)−N(8)−C(38)−O(20)	−105.8(9)
C(36)−N(7)−C(35)−N(8)	−179.7(8)	C(35)−N(8)−C(38)−C(41)	133.8(9)

Symmetry transformations used to generate equivalent atoms: #1:+x,−1+y,1+z

Table S4 Selected Bond lengths (Å) and angles (°) for **2**.

Bond lengths (Å)		**Bond angles (°)**	
Ni(1)−O(1)	2.082(6)	O(1)−Ni(1)−N(1)	87.2(2)
Ni(1)−O(2)	2.063(5)	O(1)−Ni(1)−N(2)#1	91.2(3)
Ni(1)−O(3)	2.060(5)	O(2)−Ni(1)−O(1)	87.3(2)
Ni(1)−O(4)	2.073(6)	O(2)−Ni(1)−O(4)	95.5(2)
Ni(1)−N(1)	2.133(6)	O(2)−Ni(1)−N(1)	87.2(2)
Ni(1)−N(2)[1]	2.112(7)	O(2)−Ni(1)−N(2)#1	88.3(2)
P(1)−O(5)	1.509(6)	O(3)−Ni(1)−O(1)	87.5(2)
P(1)−O(4)	1.526(6)	O(3)−Ni(1)−O(2)	174.2(2)
P(1)−O(7)	1.598(7)	O(3)−Ni(1)−O(4)	89.9(2)
P(1)−O(6)	1.525(8)	O(3)−Ni(1)−N(1)	95.1(2)
		O(3)−Ni(1)−N(2)#1	89.3(2)
		O(4)−Ni(1)−O(1)	174.9(3)
		O(4)−Ni(1)−N(1)	88.7(3)
		O(4)−Ni(1)−N(2)#1	93.1(3)
		N(2)#1−Ni(1)−N(1)	175.3(3)
		P(1)−O(4)−Ni(1)	135.5(3)
		C(4)−N(1)−Ni(1)	121.4(5)
		C(8)−N(1)−Ni(1)	121.3(5)
		C(15)−N(2)−Ni(1)#2	124.5(6)
		C(24)−N(2)−Ni(1)#2	119.7(6)

Symmetry transformations used to generate equivalent atoms: #1:+x,1+y,−1+z; #2:+x,−1+y,1+z

Table S5 Selected Torsion angles for **2.**

Torsion angles /°		**Torsion angles /°**	
Ni(1)−N(1)−C(4)−C(12)	−179.1(7)	C(6)−N(3)−C(2)−N(4)	0.9(12)
Ni(1)−N(1)−C(8)−C(21)	−179.4(8)	C(7)−C(3)−C(10)−O(9)	83.7(8)

Ni(1)#1−N(2)−C(15)−C(14)	−176.1(11)	C(8)−N(1)−C(4)−C(12)	−0.3(13)
Ni(1)#1−N(2)−C(24)−C(13)	176.6(9)	C(10)−C(1)−C(5)−O(8)	−24.2(8)
P(1)−O(7)−C(7)−C(3)	−159.5(6)	C(10)−C(1)−C(5)−N(4)	95.9(7)
O(5)−P(1)−O(4)−Ni(1)	−2.7(7)	C(10)−C(3)−C(7)−O(7)	48.4(9)
O(5)−P(1)−O(7)−C(7)	−56.5(8)	C(15)−N(2)−C(24)−C(13)	0.2(16)
O(4)−P(1)−O(7)−C(7)	−176.0(7)	C(16)−N(6)−C(18)−N(5)	−2(3)
O(8)−C(3)−C(7)−O(7)	−68.2(9)	C(16)−N(6)−C(18)−N(7)	177.3(15)
O(8)−C(3)−C(10)−O(9)	−157.4(6)	C(16)−C(6)−C(23)−N(5)	−2(2)
O(8)−C(3)−C(10)−C(1)	−33.5(7)	C(16)−C(6)−C(23)−N(4)	178.3(12)
O(10)−C(1)−C(5)−O(8)	91.9(7)	C(18)−N(5)−C(23)−N(4)	−179.2(12)
O(10)−C(1)−C(5)−N(4)	−147.9(6)	C(18)−N(5)−C(23)−C(6)	2(2)
O(10)−C(1)−C(10)−O(9)	38.7(9)	C(18)−N(6)−C(16)−O(11)	−178.0(16)
O(10)−C(1)−C(10)−C(3)	−82.4(7)	C(18)−N(6)−C(16)−C(6)	2(2)
O(7)−P(1)−O(4)−Ni(1)	113.1(6)	C(22)−C(13)−C(24)−N(2)	−1.2(18)
O(6)−P(1)−O(4)−Ni(1)	−130.8(6)	C(22)−C(14)−C(15)−N(2)	1(2)
O(6)−P(1)−O(7)−C(7)	65.0(8)	C(23)−N(5)−C(18)−N(7)	−179.1(13)
N(3)−C(6)−C(16)−O(11)	−3(3)	C(23)−N(5)−C(18)−N(6)	1(2)
N(3)−C(6)−C(16)−N(6)	177.2(13)	C(23)−N(4)−C(2)−N(3)	−0.3(12)
N(3)−C(6)−C(23)−N(5)	−179.6(12)	C(23)−N(4)−C(5)−O(8)	−115.1(10)
N(3)−C(6)−C(23)−N(4)	1.2(15)	C(23)−N(4)−C(5)−C(1)	125.8(10)
N(1)−C(4)−C(12)−C(9)	0.9(15)	C(23)−C(6)−C(16)−O(11)	−179.8(16)
N(1)−C(8)−C(21)−C(9)	−3.9(18)	C(23)−C(6)−C(16)−N(6)	1(2)
C(2)−N(3)−C(6)−C(16)	−178.1(14)	C(24)−N(2)−C(15)−C(14)	0.1(18)
C(2)−N(3)−C(6)−C(23)	−1.3(14)	C(4)−N(1)−C(8)−C(21)	1.8(14)
C(2)−N(4)−C(5)−O(8)	68.6(11)	C(5)−O(8)−C(3)−C(7)	142.4(7)
C(2)−N(4)−C(5)−C(1)	−50.5(12)	C(5)−O(8)−C(3)−C(10)	18.8(9)
C(2)−N(4)−C(23)−N(5)	−179.8(12)	C(5)−N(4)−C(2)−N(3)	176.6(9)
C(2)−N(4)−C(23)−C(6)	−0.5(13)	C(5)−N(4)−C(23)−N(5)	3.3(18)
C(3)−O(8)−C(5)−N(4)	−119.8(7)	C(5)−N(4)−C(23)−C(6)	−177.5(10)
C(3)−O(8)−C(5)−C(1)	3.6(9)	C(5)−C(1)−C(10)−O(9)	155.9(6)

Symmetry transformations used to generate equivalent atoms: #1:+x,1+y,−1+z

Table S6 Selected Bond lengths (Å) and angles (°)for **3**.

Bond lengths (Å)		**Bond angles (°)**	
P(1)−O(1)	1.550(5)	O(1)−P(1)−O(4)	97.8(2)
P(1)−O(2)	1.483(4)	O(2)−P(1)−O(1)	114.4(3)
P(1)−O(3)	1.506(5)	O(2)−P(1)−O(3)	114.6(3)
P(1)−O(4)	1.602(4)	O(2)−P(1)−O(4)	109.7(2)
O(4)−C(1)	1.434(7)	O(3)−P(1)−O(1)	110.7(3)
O(5)−C(3)	1.406(6)	O(3)−P(1)−O(4)	108.2(3)
O(6)−C(4)	1.404(7)	O(8)−C(9)−N(4)	121.7(6)
O(7)−C(2)	1.445(7)	O(8)−C(9)−C(8)	127.8(7)

O(7)−C(5)	1.407(7)	O(4)−C(1)−C(2)	111.1(5)
O(8)−C(9)	1.214(8)	N(3)−C(10)−N(4)	123.3(6)
N(1)−C(6)	1.299(8)	N(5)−C(10)−N(3)	119.7(6)
N(1)−C(8)	1.377(8)	N(5)−C(10)−N(4)	117.0(6)
N(2)−C(5)	1.457(7)	N(2)−C(5)−C(4)	112.5(5)
N(2)−C(6)	1.381(8)	N(1)−C(6)−N(2)	112.6(6)
N(2)−C(7)	1.374(7)	N(3)−C(7)−N(2)	125.1(5)
N(3)−C(7)	1.351(7)	N(3)−C(7)−C(8)	129.2(5)
N(3)−C(10)	1.324(7)	N(12)−C(30)−C(29)	120.2(7)
N(4)−C(9)	1.394(9)	N(1)−C(8)−C(9)	129.7(6)
N(4)−C(10)	1.371(8)	N(4)−C(9)−C(8)	110.6(6)
N(5)−C(10)	1.317(8)	N(11)−C(21)−C(22)	119.9(7)
N(11)−C(21)	1.341(9)	N(12)−C(31)−C(32)	120.0(7)
N(11)−C(25)	1.333(9)	N(11)−C(25)−C(24)	119.9(7)
N(12)−C(30)	1.334(9)	C(25)−N(11)−C(21)	121.7(6)
N(12)−C(31)	1.326(9)	C(31)−N(12)−C(30)	122.2(7)
P(2)−O(9)	1.554(5)	C(6)−N(1)−C(8)	104.7(5)
P(2)−O(10)	1.494(5)	C(6)−N(2)−C(5)	127.8(5)
P(2)−O(11)	1.489(5)	C(7)−N(2)−C(5)	125.8(5)
		C(7)−N(2)−C(6)	105.9(5)
		C(7)−C(8)−N(1)	111.1(5)
		C(1)−O(4)−P(1)	115.8(4)
		C(10)−N(3)−C(7)	111.7(5)
		C(10)−N(4)−C(9)	125.9(5)

Tables S7 Selected H–bonding distances (Å) and angles (°) for **3.**

D−H	**A**	**d(H···A)/Å**	**d(D···A)/Å**	**∠DHA /°**	**Symmetry**
O(1)−H(1)	O3	1.69	2.505(6)	172.0	[1−x,−1/2+y,1−z]
O(6)−H(6)	O5	1.96	2.759(6)	165.5	[−x,1/2+y,1−z]
N(11)−H(11)	N1	1.83	2.690(8)	175.3	[+x,−1+y,+z]
N(12)−H(12A)	N7	1.90	2.763(8)	177.2	[2−x,3/2+y,1−z]

Table S8 Selected Torsion angles for **3.**

Torsion angles /°		**Torsion angles /°**	
O(4)−C(1)−C(2)−O(7)	70.2	C(8)−N(1)−C(6)−N(2)	0.4
O(4)−C(1)−C(2)−C(3)	−172.4	C(9)−N(4)−C(10)−N(3)	−4.3
O(5)−C(3)−C(4)−O(6)	−13.6	C(9)−N(4)−C(10)−N(5)	177.6
O(5)−C(3)−C(4)−C(5)	105.4	C(10)−N(3)−C(7)−N(2)	−179.4
O(6)−C(4)−C(5)−O(7)	159.2	C(10)−N(3)−C(7)−C(8)	1.6
O(6)−C(4)−C(5)−N(2)	−81.7	C(10)−N(4)−C(9)−O(8)	−179.5
O(7)−C(2)−C(3)−O(5)	−129.6	C(10)−N(4)−C(9)−C(8)	1.4

O(7)−C(2)−C(3)−C(4)	−3.7	C(11)−C(12)−C(13)−O(14)	131.4
O(12)−C(11)−C(12)−O(13)	−62.5	C(11)−C(12)−C(13)−C(14)	−107.4
O(12)−C(11)−C(12)−C(13)	58.3	C(12)−O(13)−C(15)−N(6)	−140.6
O(13)−C(12)−C(13)−O(14)	−107.9	C(12)−O(13)−C(15)−C(14)	−18.7
O(13)−C(12)−C(13)−C14)	13.3	C(12)−C(13)−C(14)−O(15)	−142.2
O(14)−C(13)−C(14)−O15)	−23.9	C(12)−C(13)−C(14)−C(15)	−23.6
O(14)−C(13)−C(14)−C15)	94.7	C(13)−C(14)−C(15)−O(13)	26.5
O(15)−C(14)−C(15)−O(13)	150.2	C(13)−C(14)−C(15)−N(6)	143.3
O(15)−C(14)−C(15)−N(6)	−92.9	C(15)−O(13)−C(12)−C(11)	128.2
N(1)−C(8)−C(9)−O(8)	0.1	C(15)−O(13)−C(12)−C(13)	3.2
N(2)−C(7)−C(8)−N(1)	−0.7	C(15)−N(6)−C(16)−N(7)	−173.2
N(7)−C(17)−C(18)−N(6)	−0.1	C(15)−N(6)−C(18)−C(17)	173.0
C(1)−C(2)−C(3)−O(5)	111.7	C(16)−N(6)−C(15)−O(13)	46.3
C(1)−C(2)−C(3)−C(4)	−122.4	C(16)−N(6)−C(15)−C(14)	−70.9
C(2)−O(7)−C(5)−N(2)	−160.9	C(16)−N(6)−C(18)−C(17)	0.2
C(2)−O(7)−C(5)−C(4)	−39.5	C(16)−N(7)−C(17)−C(18)	0.0
C(2)−C(3)−C(4)−O(6)	−137.3	C(17)−N(7)−C(16)−N(6)	0.2
C(2)−C(3)−C(4)−C(5)	−18.4	C(18)−N(6)−C(15)−O(13)	−125.1
C(3)−C(4)−C(5)−O(7)	35.8	C(18)−N(6)−C(15)−C(14)	117.6
C(3)−C(4)−C(5)−N(2)	154.9	C(18)−N(6)−C(16)−N(7)	−0.2
C(5)−O(7)−C(2)−C(1)	146.6	C(7)−N(2)−C(5)−O(7)	−85.8
C(5)−O(7)−C(2)−C(3)	26.5	C(7)−N(2)−C(5)−C(4)	156.6
C(5)−N(2)−C(6)−N(1)	171.3	C(7)−N(2)−C(6)−N(1)	−0.8
C(5)−N(2)−C(7)−C(8)	−171.4	C(6)−N(2)−C(5)−O(7)	103.6
C(6)−N(1)−C(8)−C(7)	0.2	C(6)−N(2)−C(5)−C(4)	−14.0
		C(6)−N(2)−C(7)−C(8)	0.8

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