Supporting Information

Structure and Electronic Spectra of Purine-Methyl Viologen Charge Transfer Complexes

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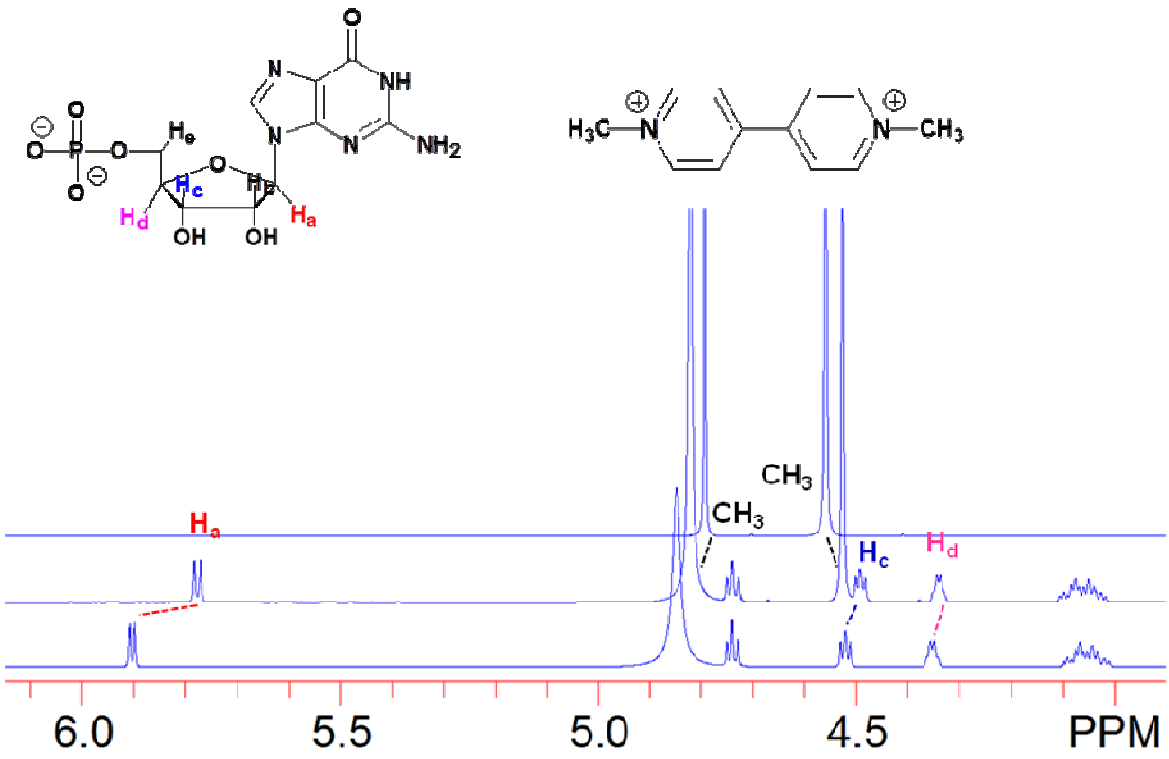


Figure S1. ^{1}H NMR spectra of **GMP^{2-}2Na+** and 1.0 equil (**MV^{2+}**2Cl^{-}) in D_2O, recorded at room temperature (at 500 MHz)

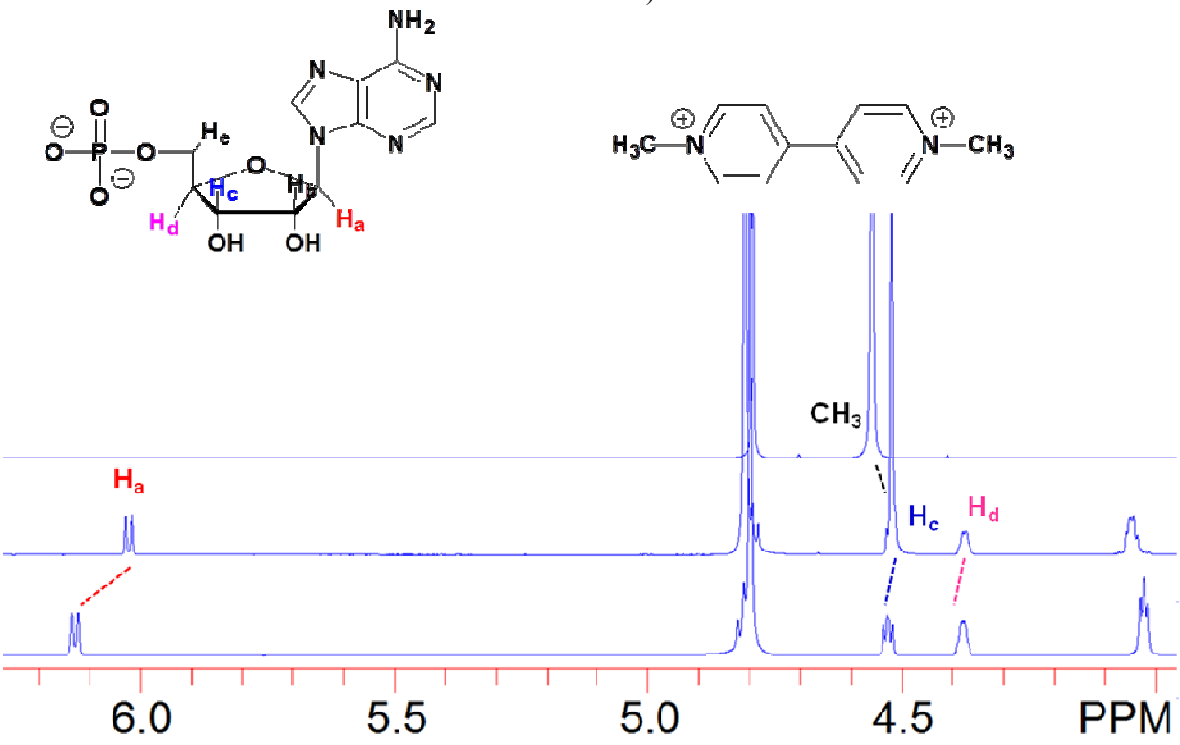


Figure S2. ^{1}H NMR spectra of **AMP^{2-}2Na+** and 1.0 equil (**MV^{2+}**2Cl^{-}) in D_2O, recorded at room temperature (at 500 MHz).

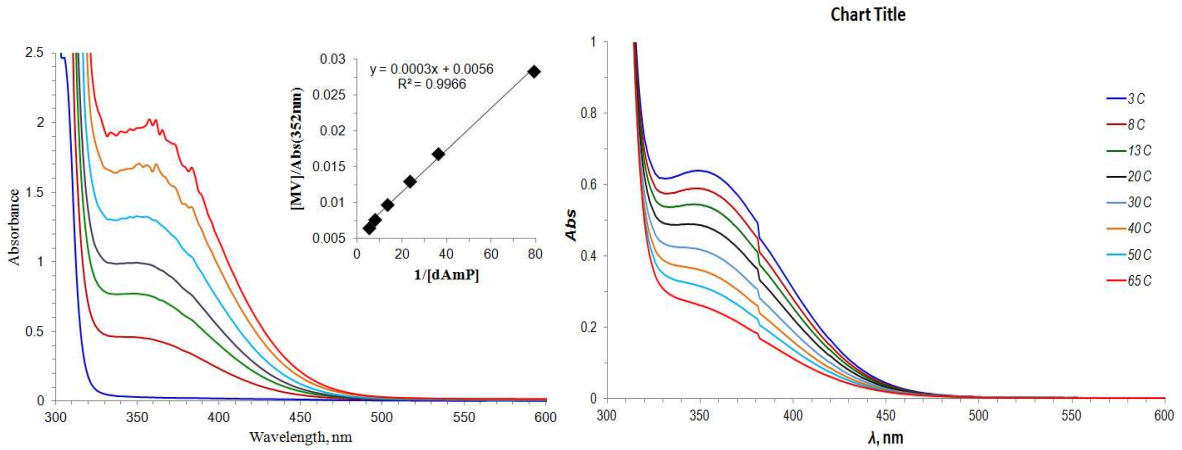


Figure S3. Absorption spectra of the **AMP**:**MV^{2+}** molecular complex as a function of the concentration of **AMP** and as a function of the temperature, Inset: Banesi-Hildebrand plot.

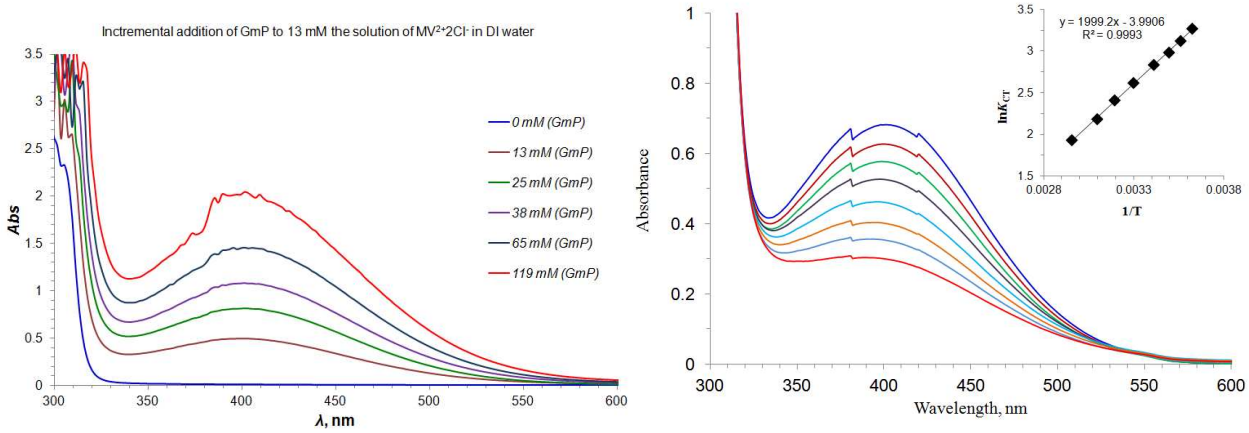


Figure S4. Absorption spectra of the **GMP**:**MV^{2+}** molecular complex as a function of the concentration of **GMP** and as a function of the temperature, Inset: Eyring plot.

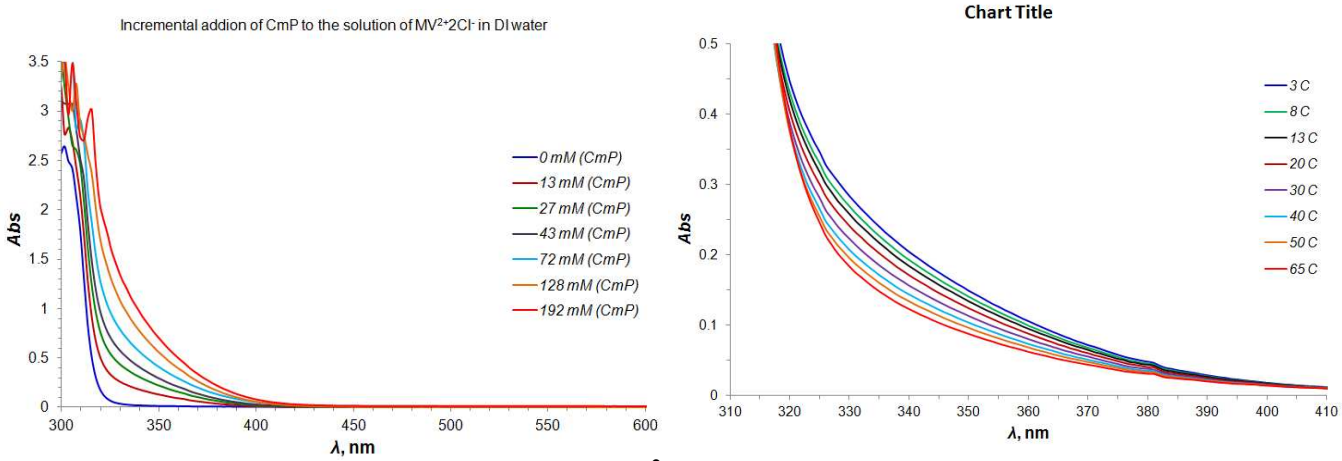


Figure S5. Absorption spectra of the **CMP**:**MV^{2+}** molecular complex as a function of the concentration of **CMP** and as a function of the temperature.

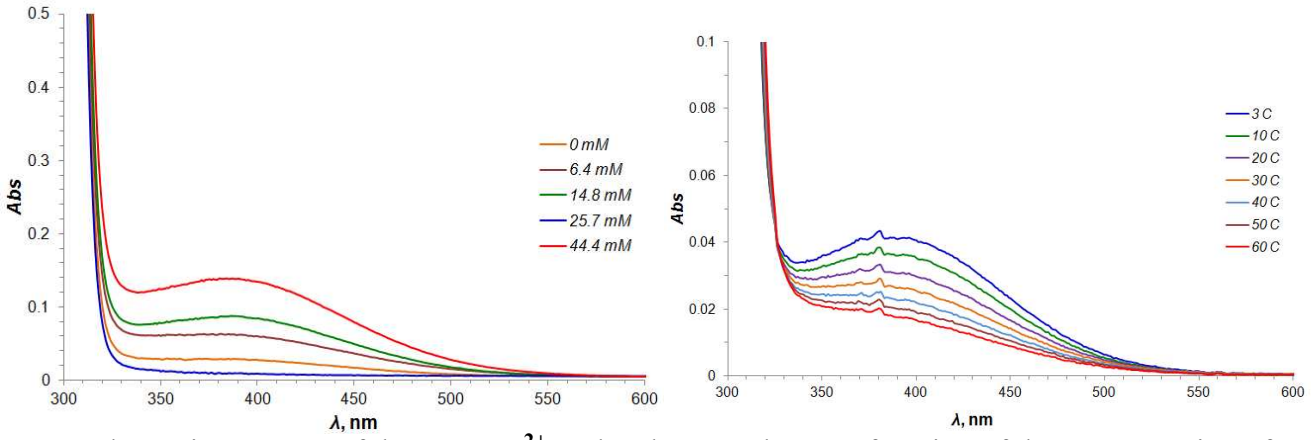


Figure S6. Absorption spectra of the **dG**:$\mathbf{MV^{2+}}$ molecular complex as a function of the concentration of **dG** and as a function of the temperature.

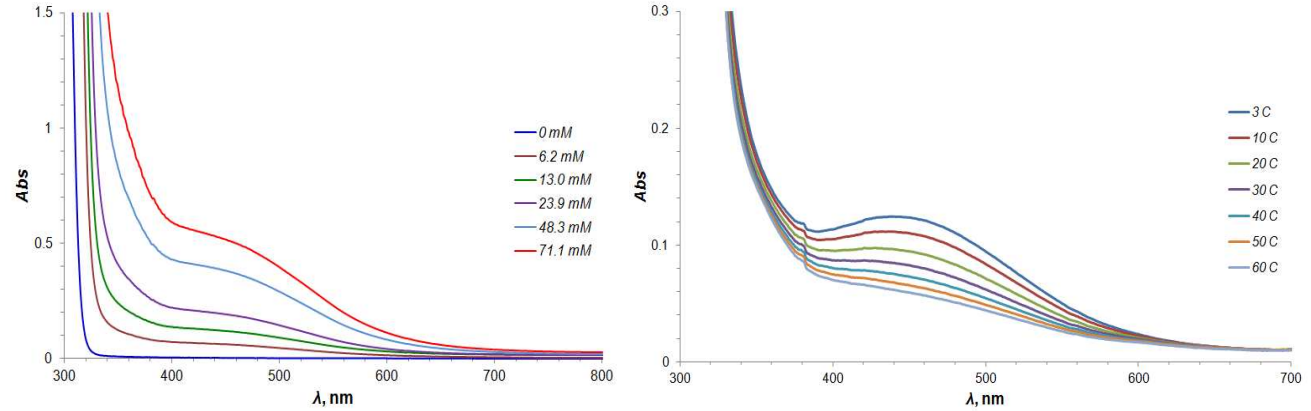


Figure S7. Absorption spectra of the **zG**:$\mathbf{MV^{2+}}$ molecular complex as a function of the concentration of **zG** and as a function of the temperature.

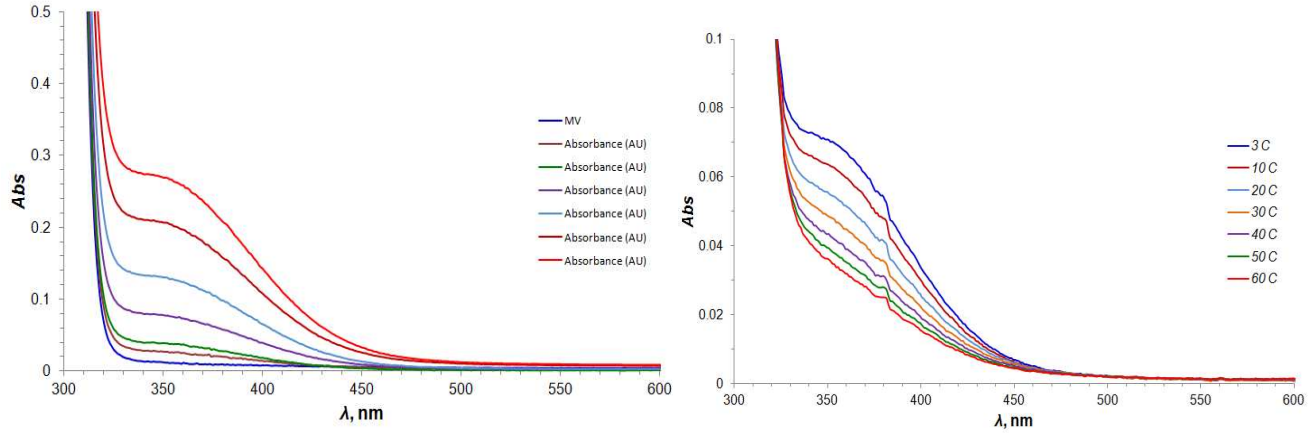


Figure S8. Absorption spectra of the **dA**:$\mathbf{MV^{2+}}$ molecular complex as a function of the concentration of **dA** and as a function of the temperature.

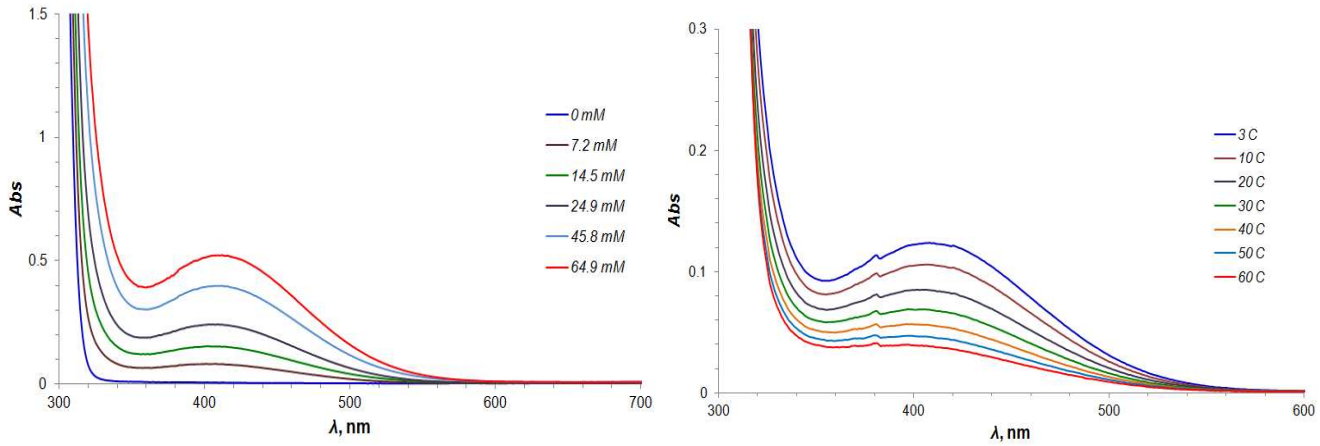


Figure S9. Absorption spectra of the **zA**:$\mathbf{MV^{2+}}$ molecular complex as a function of the concentration of **zA** and as a function of the temperature.

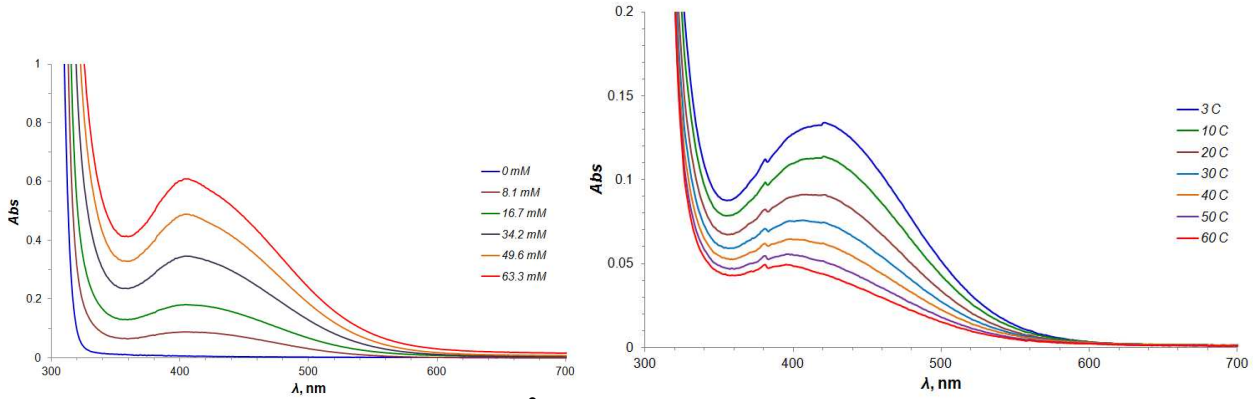


Figure S10. Absorption spectra of the **aA**:$\mathbf{MV^{2+}}$ molecular complex as a function of the concentration of **aA** and as a function of the temperature.

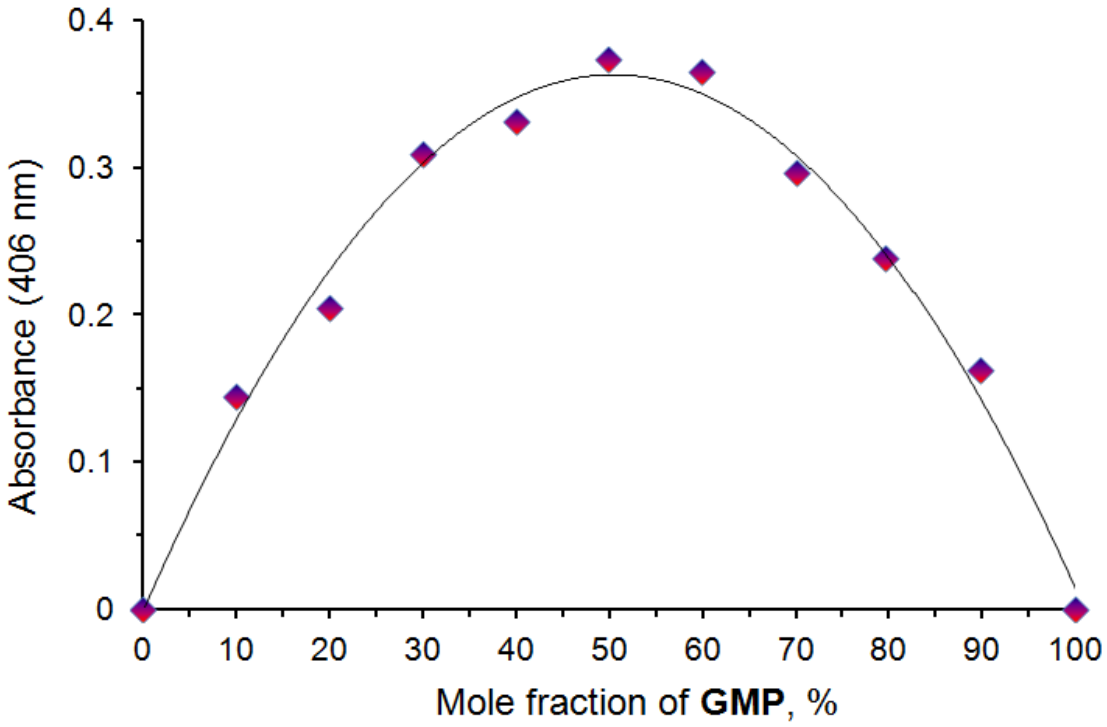


Figure S11. Jobs Plot of the **GMP:MV** complexation for the 1:1 dyad formation at total concetration of ~10 mM (c[**GMP**]+c[**MV**]).

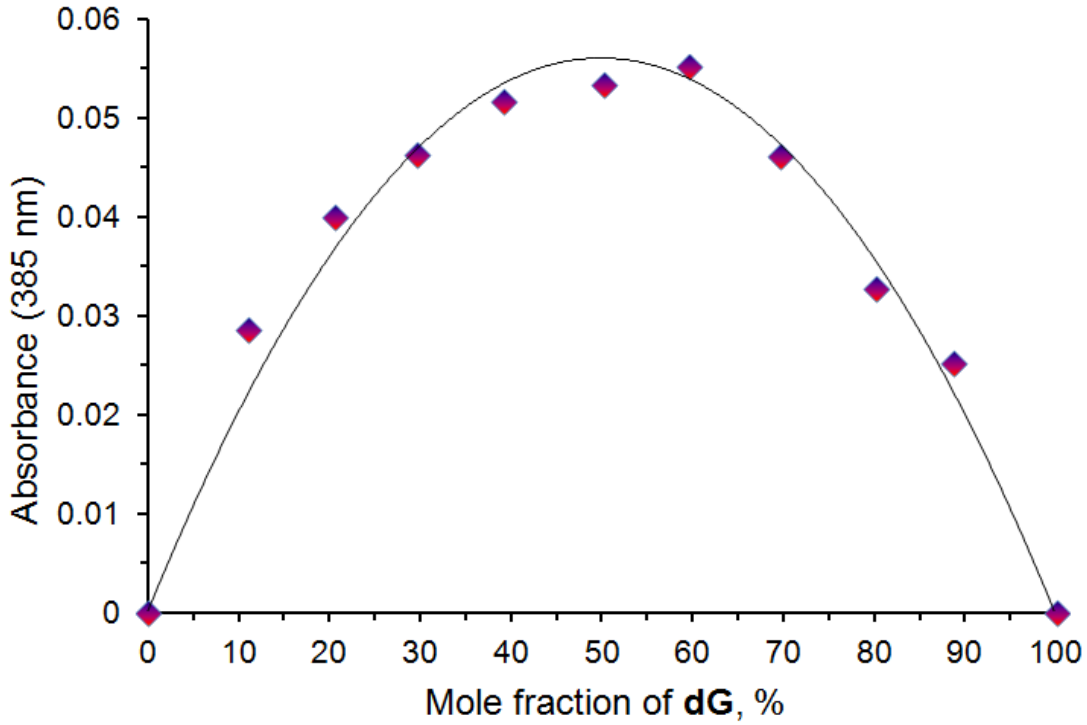


Figure S12. Jobs Plot of the **dG:MV** complexation for the 1:1 dyad formation at total concetration of ~10 mM (c[**dG**]+c[**MV**]).

Determination of extinction coeff ε_{CT} and equilibrium const K_{eq}

The nucleobase *[a]*, methyl viologen *[m]* and the adduct *[am]* coexist in solution. Therefore, the absorption spectrum in solution represents the sum of its components. Fortunately, the absorption band associated with the CT state of the adduct is distinct, and non-overlapping, with its constituent's absorption in the collective spectrum. Therefore, the CT band intensity can be used to obtain the equilibrium constant and molar extinction coefficients using the following analysis.

The thermodynamic equation for adduct formation can be written as

$$\underset{(a\text{-}x)}{nucleobase} + \underset{(m\text{-}x)}{methylviologen} \leftrightarrow \underset{x}{adduct} \qquad 1$$

Where, a and m are initial concentrations of the nucleobase and MV, respectively.

The equilibrium rate constant K_{eq} for this reaction can be written as

$$K_{eq} = \frac{x}{(a-x)(m-x)} \qquad 2$$

Now, since the charge transfer band of the adduct in UV-vis spectra is distinct from the absorption bands of both *nucleobase* and *methyl viologen*, the Beer-Lambert Law can be used to relate the concentration of *adduct* to the CT band absorbance.

$$A = \varepsilon.x.l \qquad 3$$

where A is absorbance at CT band maxima, ε is the corresponding molar extinction coefficient, and l is path length of the cell (***l*=1**). Equations 2 and 3 can be combined to give the following equation

$$A = \frac{\varepsilon}{2}\left\{\left(a+m+\frac{1}{K_{eq}}\right)-\sqrt{\left(a+m+\frac{1}{K_{eq}}\right)^2-4am}\right\} \qquad 4$$

The above equation for $A(a,m)$ was used to obtain the equilibrium constant K_{eq} and the extinction coefficient ε from the experimental data (Table S1). Once the molar extinction coefficient is known at CT-band maximum, the oscillator strength f for this band can be determined using the following relation.

$$f = 1.44 \times 10^{-19} \int \varepsilon_{CT}(\nu) d\nu, \qquad 5$$

where $\varepsilon_{CT}(\nu)$ is the molar extinction coefficient in the units of $Lmol^{-1}cm^{-1}$ and ν is the frequency in Hz. The calculated f values are provided in Table S1.

Table S1: Equilibrium constants K_{eq}, molar extinction coefficients ε_{CT} and oscillator strengths f of the charge-transfer bands for A:MV, G:MV, zA:MV, zG:MV and aA:MV, and nucleotides AmP:MV and GmP:MV.

Adduct	K_{eq} ($L.mol^{-1}$)	ε_{CT} ($Lmol^{-1}cm^{-1}$)	f
A:MV	5.29±0.64	103±8	0.003
G:MV	13.54±5.37	61±16	0.003
zA:MV	7.11±0.69	238±17	0.008
zG:MV	3.91±0.96	369±73	0.013
aA:MV	2.46±0	553±0	0.019
AmP:MV	17.07±1.91	199±8	0.007
GmP:MV	15.10±2.06	248±16	0.008

3a Structure of the complexes

The equilibrium structure of the four complexes is shown in Figure 3 of the manuscript. The key structural parameters, namely the effective stacking distance (between the pyridine group of MV^{2+} and the aromatic core of the purine base) and the dihedral angle (between the two pyridines of MV^{2+}) are provided in Table S2. It is seen that the purine bases have varied orientations with respect to the MV^{2+}. Except GMV, all purine bases are laterally shifted towards the center of MV^{2+}, imposing hindrance for mutual rotation of pyridines of MV^{2+}. As a result, in GMV, the stacking distance is smallest and dihedral angle is largest. On the contrary, for zGMV, the steric hindrance is maximum due to the presence of substituted methyl group followed by aAMV. For AMV and zAMV, the orientation of the purines with respect to MV^{2+} is similar, which results in similar stacking distance and dihedral angles. To compare the effect of water solvation on equilibrium geometry, the geometries were optimized without considering the effects of water solvation. The relative orientation of molecules is comparable to previous geometries, although the stacking distances and lateral shifts vary. No strong correlation was found between the two sets of geometries, although the importance of water solvation is realized.

Table S2: The stacking distance between pyridine group of methyl viologen and the nucleobase, and the dihedral angle between pyridines of methyl viologen, for complexes AMV, GMV, zAMV, zGMV, aAMV.

Complex	Stacking Distance (Å)	Dihedral Angle (°)
A:MV	3.19	36.4
G:MV*	3.15	43.5
zA:MV	3.19	36.3
zG:MV**	3.22	32.6
aA:MV**	3.24	25.1

*lateral shift of guanine away from methyl viologen reduces steric hinderance thereby increasing the dihedral angle and reducing the stacking distance; **steric hinderance of the substituents hinders effective stacking (larger stacking distances) as well as twist angle between the two pyridines moieties on methyl viologen (smaller dihedral angles)

3b Intermolecular interactions between purine donors and methyl viologen

Non-covalent interactions are weaker than covalent interactions, yet extremely important in stabilizing and proper functioning of biological systems. Since non-covalent interactions are so weak, highly accurate calculations are required to obtain accurate interaction energies. There are two available methods to calculate the intermolecular interaction energies, namely supermolecular approach and perturbative approach.[1,2] In the supermolecular approach, the interaction energies are calculated by subtracting the monomer energies of the components from the total energy. This approach suffers from basis set superposition error (BSSE), and doesn't provide any additional information about the nature of the interaction. To minimize BSSE errors and get accurate interaction energies, computationally demanding CCSD(T) calculations are required in complete basis set (CBS) limit. These calculations are only feasible for atomic and small molecular systems. On the other hand, symmetry adapted perturbation theory (SAPT) has evolved over the last decade as an alternate method to calculate interaction energies that are comparable to the CCSD(T)/CBS limit. In addition, this perturbative approach yields partitioning of the total interaction energies into physically defined energy components, such as electrostatic, induction, dispersion and exchange,[1] which provide information about the nature of the interaction. Towards this end, density functional theory-symmetry adapted perturbation theory with density fitting procedure (DF-DFT-SAPT)[3] has been developed in recent years that allows calculation of interaction energies for large molecular systems, such as the complexes that have been studied in this report. Note that we have shown in this manuscript that computationally less expensive DFT calculations can give reasonable total interaction energies (by supramolecular approach) that are comparable to SAPT energies, thus providing confidence that the DFT results are accurate in this application..

In the DF-DFT-SAPT method, the total interaction energies are divided into a first-order perturbation energy $E^{(1)}$, second-order perturbation energy $E_i^{(2)}$, and a higher order interaction energy $\delta(HF)$. The first-order energy contains electrostatic $E_{el}^{(1)}$ and exchange-repulsion $E_{Ex}^{(1)}$ contributions. The second-order energy is composed of induction $E_{i,0}^{(2)}$, exchange-induction $E_{i,Ex}^{(2)}$, dispersion $E_{D,0}^{(2)}$ and exchange-dispersion $E_{D,Ex}^{(2)}$ energies. The induction and dispersion energies are attractive, whereas the exchange energies are repulsive. The charge transfer energy is considered as a part of induction energy.

The DF-DFT-SAPT calculations were performed on the studied complexes to determine the total energy and various energy components. The PBE0AC exchange-correlation functional and aug-cc-pVDZ (avdz) basis set has been used in these calculations. Additional calculations were performed for these complexes by removing the two n-substituted methyl-groups in methyl viologen that results in the neutral bipyridine (BiPy) molecule. The results are summarized in Table S3-S5.

In DF-DFT-SAPT calculations, the monomer properties are calculated with DFT. To achieve accurate results with this approach (that are comparable to CCSD(T)), a correction factor is introduced to get the right asymptotic behavior of the xc-functional. The correction factor was varied by 10% to check its sensitivity to the SAPT interaction energies, and we found that the results remain qualitatively the same (Table S6). Next, the SAPT calculations were performed with a higher basis set, and we verified that the results remain qualitatively the same (Table S6).

Table S3: First-order DF-DFT-SAPT electrostatic $E_{el}^{(1)}$ and exchange-electrostatic $E_{Ex}^{(1)}$ perturbation energies (in kcal/mol), and the total energy $E^{(1)}$, for AMV, GMV, zAMV, zGMV and aAMV as well as for ABiPy, GBiPy, zABiPy, zGBiPy and aABiPy.

Complex	$E_{el}^{(1)}$	$E_{Ex}^{(1)}$	$E^{(1)}$
AMV	-18.69	21.80	03.11
GMV	-26.58	25.32	-01.26
zAMV	-19.00	22.60	03.59
zGMV	-19.67	26.24	06.57
aAMV	-23.88	27.08	3.19
ABiPy	-07.66	20.62	12.95
GBiPy	-10.51	24.77	14.26
zABiPy	-08.82	22.06	13.24
zGBiPy	-08.52	24.62	16.11
aABiPy	-9.29	26.41	17.11

Table S4: Second-order DF-DFT-SAPT perturbation energies (in kcal/mol) for AMV, GMV, zAMV, zGMV and aAMV as well as for ABiPy, GBiPy, zABiPy, zGBiPy and aABiPy: namely induction $E_{i,0}^{(2)}$, exchange-induction $E_{i,Ex}^{(2)}$, total induction $E_{i}^{(2)}$, dispersion $E_{D,0}^{(2)}$, exchange-dispersion $E_{D,Ex}^{(2)}$, total dispersion $E_{D}^{(2)}$, and total second-order $E^{(2)}$ energies.

Complex	$E_{i,0}^{(2)}$	$E_{i,Ex}^{(2)}$	$E_{i}^{(2)}$	$E_{D,0}^{(2)}$	$E_{D,Ex}^{(2)}$	$E_{D}^{(2)}$	$E^{(2)}$
AMV	-13.84	8.23	-5.61	-18.02	2.40	-15.62	-21.23
GMV	-16.36	9.30	-7.06	-20.34	2.75	-17.59	-24.65
zAMV	-15.26	9.52	-5.74	-18.77	2.59	-16.18	-21.91
zGMV	-16.50	10.06	-6.44	-21.17	2.88	-18.29	-24.73
aAMV	-17.82	11.64	-6.18	-22.16	3.17	-18.99	-25.17
ABiPy	-08.69	8.12	-0.57	-17.84	2.87	-14.97	-15.54
GBiPy	-11.59	10.05	-1.54	-19.98	3.33	-16.65	-18.19
zABiPy	-09.46	8.83	-0.62	-18.78	3.12	-15.66	-16.28
zGBiPy	-10.73	10.00	-0.73	-21.08	3.42	-17.66	-18.39
aABiPy	-11.96	11.27	-0.69	-22.23	3.77	-18.46	-19.15

Table S5: First- and second-order DF-DFT-SAPT perturbation energies (in kcal/mol) for AMV, GMV, zAMV, zGMV and aAMV as well as for ABiPy, GBiPy, zABiPy, zGBiPy and aABiPy: total electrostatic $E^{(1)}$, induction $E_i^{(2)}$ and dispersion $E_D^{(2)}$ energies; higher order contribution $\delta(HF)$, total interaction energy E.

Complex	$E^{(1)}$	$E_i^{(2)}$	$E_D^{(2)}$	$\delta(HF)$	E
AMV	03.11	-5.61	-15.62	-2.37	-20.49
GMV	-01.26	-7.06	-17.59	-2.98	-28.89
zAMV	03.59	-5.74	-16.18	-2.79	-21.11
zGMV	06.57	-6.44	-18.29	-3.31	-21.47
aAMV	03.19	-6.18	-18.99	-2.84	-24.82
ABiPy	12.95	-0.57	-14.97	-1.30	-03.89
GBiPy	14.26	-1.54	-16.65	-1.65	-05.58
zABiPy	13.24	-0.62	-15.66	-1.54	-04.58
zGBiPy	16.11	-0.73	-17.66	-1.67	-03.96
aABiPy	17.11	-0.69	-18.46	-1.50	-3.53

Table S6: The DF-DFT-SAPT perturbation energies (in kcal/mol) for AMV that have been calculated at avdz basis set and by varying the asymptotic shift parameter by 10%, and at higher basis set avtz. The total electrostatic $E^{(1)}$, induction $E_i^{(2)}$ and dispersion $E_D^{(2)}$ energies, higher order contribution $\delta(HF)$, and total interaction energy E are provided.

Complex	$E^{(1)}$	$E_i^{(2)}$	$E_D^{(2)}$	$\delta(HF)$	E
avdz	3.11	-5.61	-15.62	-2.37	-20.49
avdz (0.9)*	4.41	-5.64	-15.75	-2.37	-19.35
avdz (1.1)*	4.41	-5.64	-15.75	-2.37	-19.35
avtz	3.21	-5.61	-16.49	-2.39	-21.28

* The numbers turn out to be the same to two decimal places!

Table S7: Comparison of the interaction energies calculated by the perturbative approach (DF-DFT-SAPT) and the supramolecular approach (DFT, M06-2X/TZP) to demonstrate the reliability of the latter as an alternate method to obtain total interaction energies. Note that the energy decomposition analysis is not possible in the latter approach, and the former method is more accurate albeit time consuming.

Complex	E_{SAPT} (kcal/mol)	$E_{M06\text{-}2X}$ (kcal/mol)
A(Me):MV	-20.49	-22.74
G(Me):MV	-28.89	-31.71
zA(Me):MV	-21.11	-23.91
zG(Me):MV	-21.47	-24.64
aA(Me):MV	-24.82	-28.12

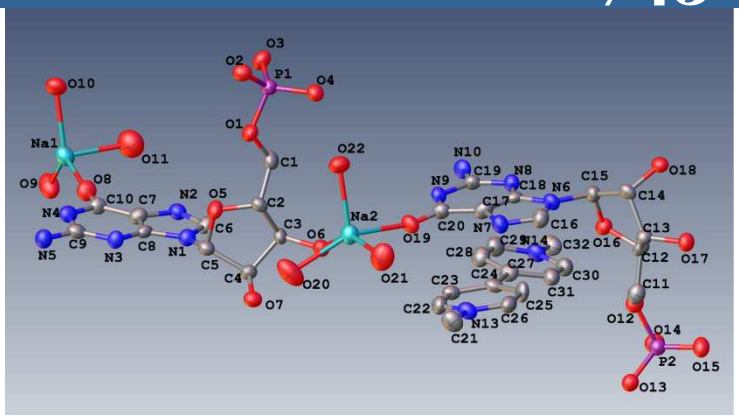
3c Effect of the solvent and effect of the redox properties on the excitation energies

Table S8: The excitation energies and oscillator strengths of the charge transfer states of AMV, GMV, zAMV, zGMV and aAMV, calculated by TDDFT calculations including and excluding the solvation effects of water. The difference of the ionization potential of the purine base and the electron affinity of methyl viologen (*IP-EA*) is also provided.

	λ_{water} (nm)	f_{water}	$\lambda_{nowater}$ (nm)	$f_{nowater}$	$\Delta E_{IP\text{-}EA}$ (eV)
AMV	380	0.006	526	0.004	4.43
GMV	415	0.003	550	0.003	4.04
zAMV	429	0.012	612	0.011	3.97
zGMV	493	0.016	736	0.016	3.63
aAMV	465	0.010	639	0.009	3.79

n1745a

Crystal Submitted by:
Almaz Jalilov
Crystal Submitted on:
03/30/2012
Data Collected on:
04/13/2012
Structure Solved by:
Amy Sarjeant



Experimental

Single crystals of $C_{32}H_{76}N_{12}Na_2O_{35}P_2$ **[n1745a]** were recrystallised from water/ethanol mounted in inert oil and transferred to the cold gas stream of a Bruker Kappa APEX CCD area detector equipped with a CU Kα microsource with MX optics. Twinabs (BRUKER)

Crystal structure determination of [n1745a] Crystal Data. **$C_{32}H_{76}N_{12}Na_2O_{35}P_2$, M =1296.97, monoclinic, a = 13.7459(6) Å, b = 9.9617(4) Å, c = 20.5301(10) Å, β = 96.623(3)°, U = 2792.5(2) Å^3, T = 100.02, space group $P2_1$ (no. 4), Z = 2, μ(CU Kα) = 1.839, 6009 reflections measured, 6009 unique (R_{int} = 0.0000) which were used in all calculations. The final $wR(F_2)$ was 0.1850 (all data).**

Refinement Details. 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 > 2sigma(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. 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 > 2sigma(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.

The crystal under investigation was found to be non-merohedrally twinned. The orientation matrices for the two components were identified using the program Cell_Now,[4] and the data were processed using both orientation matrices with SAINT, The exact twin matrix identified by the integration program was found to be -0.42406 0.00037 0.57450 -0.00048 -1.00000 -0.00004 1.42763 -0.00129 0.42406 The second domain is rotated from first domain by 179.8 \% about the real lattice (101) axis. The absorption correction was carried out using TWINABS V2008/4[4] to create an hklf5 file which was used in all refinements; the structure was solved using dual space methods with only the non-overlapping reflections of component 1. The twin fraction refined to a value of 0.278(3).

Most hydrogen atoms were found from residual electron density, however several hydrogen atoms on free water molecules and the hydrogen atoms on all nitrogen atoms were generated in calculated positions (SHELX "afix" commands for the N-riding hydrogen atoms, and Olex2[5] calculated positions for those on water molecules) despite being seen in the residual density map. All O-H and H-H distances on water molecules were refined with similar distance restraints (SADI). Hydrogen atoms on water molecules were refined with riding Uiso values of 1.5 times their parent atom.

The centroid-to-centroid distance between the purine and bipyridine rings is 4.0893(8)Ang. The interplanar angle is 8.99(2)deg.

Table S9: Crystal data and structure refinement for n1745a

Identification code	n1745a
Empirical formula	$C_{32}H_{76}N_{12}Na_2O_{35}P_2$
Formula weight	1296.97
Temperature□/□K	100.02
Crystal system	monoclinic
Space group	$P2_1$
a□/□Å, b□/□Å, c□/□Å	13.7459(6), 9.9617(4), 20.5301(10)
α/°, β/°, γ/°	90.00, 96.623(3), 90.00
Volume□/□$Å^3$	2792.5(2)
Z	2
ρ_{calc}□/□mg mm^{-3}	1.542
μ□/□mm^{-1}	1.839
F(000)	1368
Crystal size□/□mm^3	0.636 × 0.17 × 0.051
2Θ range for data collection	6.48 to 117.94°
Index ranges	$-15 \leq h \leq 15$, $-11 \leq k \leq 11$, $-22 \leq l \leq 22$
Reflections collected	6009
Independent reflections	6009[R(int) = 0.0000]
Data/restraints/parameters	6009/875/691
Goodness-of-fit on F^2	1.045
Final R indexes [I>2σ (I)]	R_1 = 0.0703, wR_2 = 0.1722
Final R indexes [all data]	R_1 = 0.0857, wR_2 = 0.1850
Largest diff. peak/hole□/□e $Å^{-3}$	0.453/-0.404

Table S10 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for n1745a. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P1	880.2(13)	2355(2)	4182.7(10)	28.2(4)
P2	2790.2(14)	11096(2)	10327.5(10)	31.1(5)
Na1	-5214(2)	6899(3)	1642.0(16)	40.5(8)
Na2	3016(2)	6523(3)	5275.1(15)	38.6(8)
O1	856(4)	3849(6)	3891(3)	35.6(13)
O2	1386(4)	1581(5)	3682(3)	33.5(13)
O3	-176(4)	1900(6)	4183(3)	36.9(13)
O4	1430(4)	2402(6)	4864(2)	32.6(12)
O5	630(4)	6451(5)	3380(3)	34.1(13)
O6	1399(4)	7642(6)	5012(2)	32.0(12)
O7	1698(4)	9057(6)	3890(3)	32.2(13)
O8	-3617(4)	7401(6)	1811(3)	39.1(13)
O9	-6481(5)	8421(7)	1551(3)	57.5(18)
O10	-5280(4)	4576(6)	1485(3)	43.0(14)
O11	-5415(6)	6730(10)	2729(4)	79(2)
O12	2696(3)	9629(6)	9956(3)	33.3(13)
O13	3226(4)	12040(6)	9848(2)	32.6(12)
O14	1743(4)	11428(6)	10409(3)	36.8(13)
O15	3472(4)	10905(6)	10953(3)	37.1(13)
O16	2754(4)	6961(5)	9424(2)	31.2(12)
O17	4979(4)	6676(6)	10492(3)	32.8(12)
O18	3783(4)	4553(6)	10186(2)	32.2(12)
O19	2618(4)	6498(6)	6303(2)	33.8(13)
O20	3356(5)	7513(9)	4289(4)	69(2)
O21	4714(5)	6605(9)	5608(4)	62(2)
O22	2950(4)	4195(6)	5095(3)	43.2(14)
N1	-686(4)	7900(7)	3096(3)	30.6(15)
N2	-2317(4)	7736(7)	3134(3)	31.5(15)
N3	-601(4)	7772(7)	1928(3)	28.0(15)
N4	-2197(4)	7516(7)	1346(3)	32.8(15)
N5	-834(5)	7684(7)	790(3)	35.5(16)
C1	583(6)	4945(8)	4280(4)	33.0(19)
C2	1015(5)	6209(8)	4047(4)	28.5(17)
C3	740(5)	7436(8)	4432(3)	28.3(17)
C4	733(6)	8576(8)	3931(4)	31.2(18)

C5	362(6)	7824(8)	3282(4)	30.8(17)
C6	-1451(5)	7859(8)	3481(4)	31.2(18)
C7	-2110(5)	7704(8)	2470(4)	33.2(19)
C8	-1094(5)	7790(7)	2454(4)	26.3(17)
C9	-1199(5)	7668(8)	1367(4)	33.6(19)
C10	-2722(5)	7543(8)	1888(4)	30.0(17)
N13	3029(4)	9349(7)	7208(3)	34.6(16)
N14	-1166(5)	9426(7)	8818(3)	36.6(16)
C21	3921.7(9)	9272.4(13)	6858.6(7)	44(2)
C22	2150.1(10)	9491(2)	6858.6(7)	35.6(19)
C23	1293.0(9)	9475(2)	7151.5(7)	30.0(17)
C24	1363.2(8)	9295.3(14)	7832.8(6)	31.7(17)
C25	2301.3(8)	9163(2)	8178.2(6)	34.3(19)
C26	3105.0(8)	9195(2)	7865.2(6)	35.1(19)
C27	482.1(8)	9290.3(13)	8179.5(6)	34.2(18)
C28	-459.3(8)	9117(2)	7831.3(6)	40(2)
C29	-1267.3(8)	9167(2)	8165.0(6)	40(2)
C30	-283.7(9)	9572(2)	9169.8(7)	36.9(19)
C31	547.5(9)	9492(2)	8858.5(7)	36.1(19)
C32	-2055.3(8)	9603.1(14)	9155.1(6)	45(2)
N6	3212.7(8)	5810.9(16)	8510.2(6)	29.3(14)
N7	3929.4(8)	6116.3(15)	7597.7(6)	33.9(15)
N8	1504.7(8)	5841.8(13)	8066.1(6)	29.5(15)
N9	1344.6(8)	6153.7(15)	6910.7(6)	25.3(13)
N10	-14.4(8)	5936.0(15)	7452.0(6)	32.5(15)
C11	3575.8(9)	8926(2)	9873.4(6)	37(2)
C12	3446.6(8)	7466(2)	9950.2(6)	28.9(17)
C13	4384.7(8)	6678(2)	9880.2(6)	27.7(17)
C14	4011.9(8)	5289.0(18)	9644.2(5)	28.1(17)
C15	3058.5(8)	5702.8(17)	9197.3(5)	32.7(18)
C16	4076.5(8)	5951.0(17)	8236.9(6)	36.2(19)
C17	2940.0(8)	6053.5(13)	7448.1(6)	35.3(19)
C18	2479.6(8)	5889.5(14)	7996.3(6)	26.6(16)
C19	965.7(8)	5970.4(14)	7492.6(6)	30.6(18)
C20	2340.6(8)	6246.2(14)	6831.9(6)	31.4(18)
O1W	-2896.6(8)	4584.6(16)	7284.8(6)	77(2)
O2W	-1446.5(8)	5706.3(14)	8318.3(6)	104(3)
O3W	483.4(8)	6098.2(16)	9369.9(6)	59.2(18)

O4W	−1142.9(8)	2848.4(14)	9603.4(6)	45.9(15)
O5W	−2800.3(8)	8131(2)	6870.8(6)	70(2)
O6W	2762.0(8)	6044.6(19)	3010.5(6)	78(2)
O7W	−1505.4(8)	2205.1(14)	8084.9(6)	78(2)
O8W	2356.7(10)	10157(2)	5363.9(8)	40.9(14)
O9W	3998.9(8)	3068.3(13)	6242.5(6)	56.0(17)
O10W	4323.7(12)	10860.1(18)	5446.8(10)	72(2)
O11W	4257.5(8)	3943.8(17)	4153.9(6)	67(2)
O12W	−3609.3(8)	7688.7(18)	8020.2(5)	63(2)
O13W	5245.6(8)	5233.5(14)	6726.1(6)	61.4(19)

Table S11 Anisotropic Displacement Parameters ($Å^2×10^3$) for n1745a. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+...+2hka×b×U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	25.6(9)	28.1(11)	31(1)	−0.4(9)	4.1(8)	−1.2(8)
P2	32.1(10)	31.6(11)	29.7(10)	0.1(9)	4.2(8)	1.6(9)
Na1	35.4(16)	46(2)	41.0(18)	8.2(16)	6.8(13)	2.7(14)
Na2	35.4(16)	45(2)	35.8(17)	−1.1(15)	6.6(13)	1.7(14)
O1	44(3)	33(3)	29(3)	−4(2)	2(2)	−2(3)
O2	32(3)	31(3)	39(3)	0(2)	8(2)	−1(2)
O3	30(3)	43(3)	37(3)	−10(3)	3(2)	−6(3)
O4	35(3)	30(3)	32(3)	4(3)	2(2)	3(2)
O5	38(3)	35(3)	28(3)	−5(2)	1(2)	4(2)
O6	32(3)	36(3)	28(3)	4(2)	9(2)	−5(2)
O7	31(3)	26(4)	39(3)	3(3)	2(2)	1(2)
O8	30(3)	43(3)	43(3)	1(3)	1(2)	4(3)
O9	74(5)	58(5)	42(4)	4(3)	12(3)	23(4)
O10	38(3)	43(4)	48(4)	6(3)	8(3)	−10(3)
O11	75(5)	89(6)	77(5)	8(5)	21(4)	−3(5)
O12	26(3)	37(3)	36(3)	−2(3)	1(2)	4(2)
O13	30(3)	35(3)	32(3)	−2(3)	3(2)	−1(2)
O14	31(3)	36(3)	44(3)	−3(3)	8(2)	5(2)
O15	40(3)	41(3)	30(3)	0(3)	2(2)	7(3)
O16	33(3)	31(3)	30(3)	−3(2)	4(2)	−1(2)
O17	22(3)	42(3)	33(3)	0(3)	1(2)	2(2)
O18	34(3)	32(3)	30(3)	2(2)	5(2)	1(2)

O19	35(3)	38(3)	31(3)	7(3)	12(2)	1(2)
O20	48(4)	84(6)	76(5)	38(5)	18(4)	8(4)
O21	42(4)	89(6)	57(4)	−7(4)	19(3)	−7(4)
O22	44(3)	35(3)	49(4)	−2(3)	1(3)	−8(3)
N1	27(3)	32(4)	33(4)	−1(3)	3(3)	1(3)
N2	32(3)	30(4)	33(4)	2(3)	6(3)	0(3)
N3	20(3)	36(4)	28(4)	−3(3)	6(3)	1(3)
N4	28(3)	31(4)	38(4)	3(3)	−1(3)	3(3)
N5	32(3)	42(4)	33(4)	1(3)	3(3)	−2(3)
C1	35(4)	36(5)	26(4)	2(4)	−3(3)	6(4)
C2	29(4)	25(4)	32(4)	7(3)	5(3)	−1(3)
C3	35(4)	28(4)	21(4)	3(3)	−2(3)	4(4)
C4	34(4)	27(4)	32(4)	1(4)	1(3)	−6(3)
C5	36(4)	24(4)	32(4)	5(3)	5(3)	2(3)
C6	32(4)	32(5)	30(4)	−7(4)	5(3)	3(3)
C7	31(4)	31(5)	38(5)	−4(4)	6(3)	−1(3)
C8	26(4)	19(4)	33(4)	−2(3)	−2(3)	−3(3)
C9	33(4)	26(4)	41(5)	5(4)	2(4)	0(3)
C10	23(4)	31(4)	35(4)	1(4)	−1(3)	1(3)
N13	32(4)	35(4)	39(4)	6(3)	12(3)	1(3)
N14	35(4)	40(4)	37(4)	7(3)	12(3)	−5(3)
C21	30(4)	54(6)	51(5)	11(5)	13(4)	−1(4)
C22	44(5)	37(5)	25(4)	−2(4)	3(3)	−2(4)
C23	29(4)	23(4)	37(4)	2(4)	1(3)	−3(3)
C24	35(4)	23(4)	38(4)	6(4)	6(3)	2(3)
C25	35(4)	49(5)	19(4)	−2(4)	5(3)	−1(4)
C26	37(4)	32(5)	34(4)	−1(4)	−7(3)	1(4)
C27	32(4)	33(5)	39(5)	−4(4)	8(3)	4(4)
C28	43(5)	40(5)	38(5)	−5(4)	7(4)	4(4)
C29	35(4)	44(5)	39(5)	4(4)	1(4)	0(4)
C30	40(5)	40(5)	32(4)	0(4)	8(4)	−4(4)
C31	45(5)	32(5)	31(4)	3(4)	4(4)	5(4)
C32	46(5)	42(5)	51(5)	2(5)	20(4)	6(4)
N6	28(3)	32(4)	29(3)	4(3)	9(3)	−3(3)
N7	33(4)	39(4)	30(4)	3(3)	5(3)	−1(3)
N8	30(3)	33(4)	26(3)	0(3)	5(3)	1(3)
N9	23(3)	29(3)	24(3)	4(3)	3(2)	6(3)
N10	30(3)	40(4)	29(3)	0(3)	13(3)	2(3)

C11	28(4)	48(5)	35(4)	−5(4)	6(3)	0(4)
C12	22(4)	32(4)	32(4)	−5(4)	0(3)	−6(3)
C13	28(4)	26(4)	29(4)	−1(3)	3(3)	2(3)
C14	27(4)	28(4)	31(4)	8(3)	10(3)	0(3)
C15	40(4)	33(5)	25(4)	0(4)	4(3)	−5(4)
C16	37(4)	39(5)	31(4)	−3(4)	0(3)	2(4)
C17	27(4)	38(5)	42(5)	−7(4)	6(3)	−5(4)
C18	31(4)	16(4)	32(4)	0(3)	1(3)	0(3)
C19	31(4)	28(4)	33(4)	1(4)	5(3)	−7(3)
C20	29(4)	31(4)	34(4)	−1(4)	6(3)	−3(3)
O1W	78(5)	90(6)	65(5)	5(5)	16(4)	−4(5)
O2W	79(5)	152(10)	92(6)	−24(7)	63(5)	−5(6)
O3W	73(4)	49(4)	53(4)	7(3)	−7(3)	−6(4)
O4W	36(3)	52(4)	51(4)	6(3)	12(3)	6(3)
O5W	50(4)	97(6)	64(5)	−1(4)	15(3)	8(4)
O6W	62(5)	91(6)	81(5)	−12(5)	12(4)	1(4)
O7W	55(4)	95(7)	84(5)	33(5)	14(4)	7(4)
O8W	48(3)	31(3)	42(3)	−7(3)	−1(3)	0(3)
O9W	50(4)	70(5)	50(4)	4(4)	13(3)	5(3)
O10W	59(4)	88(6)	69(5)	14(5)	9(4)	5(4)
O11W	62(4)	83(6)	60(4)	−8(4)	24(4)	−13(4)
O12W	80(5)	70(5)	44(4)	16(4)	28(3)	37(4)
O13W	50(4)	78(5)	59(4)	0(4)	19(3)	9(4)

Table S12 Bond Lengths for n1745a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	O1	1.604(6)	N4	C10	1.394(10)
P1	O2	1.517(6)	N5	C9	1.338(10)
P1	O3	1.521(5)	C1	C2	1.494(11)
P1	O4	1.512(5)	C2	C3	1.526(11)
P2	O12	1.647(6)	C3	C4	1.530(11)
P2	O13	1.534(6)	C4	C5	1.563(11)
P2	O14	1.506(5)	C7	C8	1.404(10)
P2	O15	1.511(6)	C7	C10	1.389(11)
Na1	O8	2.239(6)	N13	C21	1.493(6)

Na1	O9	2.300(8)	N13	C22	1.339(7)
Na1	O10	2.336(7)	N13	C26	1.350(7)
Na1	O11	2.287(9)	N14	C29	1.356(7)
Na1	O17[1]	2.416(6)	N14	C30	1.346(7)
Na2	O6	2.490(6)	N14	C32	1.483(6)
Na2	O19	2.241(6)	C22	C23	1.3832
Na2	O20	2.347(7)	C23	C24	1.4023(12)
Na2	O21	2.357(7)	C24	C25	1.4043(11)
Na2	O22	2.349(7)	C24	C27	1.4739
O1	C1	1.429(10)	C25	C26	1.3410
O5	C2	1.432(9)	C27	C28	1.4149(11)
O5	C5	1.425(10)	C27	C31	1.4010
O6	C3	1.425(9)	C28	C29	1.3715
O7	C4	1.421(10)	C30	C31	1.3743
O8	C10	1.231(9)	N6	C15	1.4544
O12	C11	1.424(5)	N6	C16	1.3776
O16	C12	1.445(5)	N6	C18	1.3746
O16	C15	1.417(5)	N7	C16	1.3149
O17	Na1[2]	2.417(6)	N7	C17	1.3607
O17	C13	1.417(5)	N8	C18	1.3649
O18	C14	1.398(5)	N8	C19	1.3230
O19	C20	1.217(5)	N9	C19	1.3694
N1	C5	1.450(10)	N9	C20	1.4001
N1	C6	1.387(10)	N10	C19	1.3406
N1	C8	1.375(10)	C11	C12	1.4752
N2	C6	1.321(10)	C12	C13	1.5307
N2	C7	1.426(10)	C13	C14	1.5342
N3	C8	1.339(9)	C14	C15	1.5659
N3	C9	1.339(10)	C17	C18	1.3631
N4	C9	1.376(10)	C17	C20	1.4407

[1]-1+X,+Y,-1+Z; [2]1+X,+Y,1+Z

Table S13 Bond Angles for n1745a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	P1	O1	102.1(3)	C10	C7	C8	119.5(7)
O2	P1	O3	111.2(3)	N1	C8	C7	106.2(7)

O3	P1	O1	107.3(3)	N3	C8	N1	125.9(6)
O4	P1	O1	107.7(3)	N3	C8	C7	127.9(7)
O4	P1	O2	115.1(3)	N3	C9	N4	123.1(7)
O4	P1	O3	112.6(3)	N5	C9	N3	120.3(7)
O13	P2	O12	105.2(3)	N5	C9	N4	116.6(7)
O14	P2	O12	102.8(3)	O8	C10	N4	119.8(7)
O14	P2	O13	112.7(3)	O8	C10	C7	128.4(7)
O14	P2	O15	116.1(3)	C7	C10	N4	111.8(6)
O15	P2	O12	106.9(3)	C22	N13	C21	119.2(5)
O15	P2	O13	111.9(3)	C22	N13	C26	120.6(5)
O8	Na1	O9	125.8(3)	C26	N13	C21	120.1(5)
O8	Na1	O10	105.3(2)	C29	N14	C32	119.2(5)
O8	Na1	O11	95.3(3)	C30	N14	C29	122.3(5)
O8	Na1	O17[1]	87.4(2)	C30	N14	C32	118.4(5)
O9	Na1	O10	128.7(3)	N13	C22	C23	121.8(3)
O9	Na1	O17[1]	98.6(2)	C22	C23	C24	118.1
O10	Na1	O17[1]	77.4(2)	C23	C24	C25	118.0
O11	Na1	O9	87.3(3)	C23	C24	C27	121.1
O11	Na1	O10	93.1(3)	C25	C24	C27	120.9
O11	Na1	O17[1]	170.5(3)	C26	C25	C24	121.0
O19	Na2	O6	84.3(2)	C25	C26	N13	120.6(3)
O19	Na2	O20	155.8(3)	C28	C27	C24	120.7
O19	Na2	O21	93.9(2)	C31	C27	C24	121.2
O19	Na2	O22	97.4(2)	C31	C27	C28	118.0
O20	Na2	O6	83.5(2)	C29	C28	C27	119.3
O20	Na2	O21	86.9(3)	N14	C29	C28	120.3(3)
O20	Na2	O22	106.7(3)	N14	C30	C31	119.3(3)
O21	Na2	O6	151.3(3)	C30	C31	C27	120.6
O22	Na2	O6	113.0(2)	C16	N6	C15	129.2
O22	Na2	O21	95.7(3)	C18	N6	C15	124.9
C1	O1	P1	119.7(5)	C18	N6	C16	105.8
C5	O5	C2	110.9(6)	C16	N7	C17	104.7
C3	O6	Na2	125.6(4)	C19	N8	C18	111.0
C10	O8	Na1	173.4(6)	C19	N9	C20	125.8
C11	O12	P2	118.0(3)	O12	C11	C12	111.0(2)
C15	O16	C12	111.1(3)	O16	C12	C11	109.9(2)
C13	O17	Na1[2]	138.5(3)	O16	C12	C13	103.9(2)
C20	O19	Na2	167.9(4)	C11	C12	C13	112.5

C6	N1	C5	130.1(7)	O17	C13	C12	108.9(2)
C8	N1	C5	122.0(6)	O17	C13	C14	114.6(3)
C8	N1	C6	107.0(6)	C12	C13	C14	103.8
C6	N2	C7	104.5(6)	O18	C14	C13	108.7(2)
C8	N3	C9	112.2(6)	O18	C14	C15	110.7(2)
C9	N4	C10	125.3(7)	C13	C14	C15	100.0
O1	C1	C2	109.0(6)	O16	C15	N6	109.6(2)
O5	C2	C1	109.4(6)	O16	C15	C14	107.4(2)
O5	C2	C3	105.9(6)	N6	C15	C14	112.5
C1	C2	C3	112.2(6)	N7	C16	N6	112.2
O6	C3	C2	112.1(6)	N7	C17	C18	111.5
O6	C3	C4	114.1(6)	N7	C17	C20	130.4
C2	C3	C4	103.3(6)	C18	C17	C20	117.9
O7	C4	C3	110.9(6)	N8	C18	N6	124.0
O7	C4	C5	109.0(6)	C17	C18	N6	105.8
C3	C4	C5	101.1(6)	C17	C18	N8	130.2
O5	C5	N1	108.6(6)	N8	C19	N9	124.0
O5	C5	C4	106.6(6)	N8	C19	N10	120.6
N1	C5	C4	114.6(6)	N10	C19	N9	115.5
N2	C6	N1	113.0(7)	O19	C20	N9	121.9(2)
C8	C7	N2	109.3(6)	O19	C20	C17	127.1(2)
C10	C7	N2	131.1(7)	N9	C20	C17	111.0

[1]-1+X,+Y,-1+Z; [2]1+X,+Y,1+Z

Table S14 Hydrogen Bonds for n1745a.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O7	H7	O2[1]	0.80(9)	1.78(9)	2.578(8)	172(8)
O9	H9A	O1W[2]	0.902(14)	2.23(9)	2.874(7)	128(9)
O11	H11B	O6W[3]	0.908(14)	2.07(7)	2.723(8)	128(8)
O20	H20B	O7	0.899(14)	1.97(7)	2.793(9)	152(12)
O21	H21A	O10W[4]	0.899(14)	2.15(10)	2.766(7)	125(9)
O21	H21B	O11W[5]	0.898(14)	2.07(10)	2.740(8)	131(11)
O22	H22A	O9W	0.897(14)	1.98(3)	2.848(6)	162(8)
O22	H22B	O4	0.896(14)	1.86(2)	2.747(8)	169(9)
N4	H4	O13[6]	0.88	1.85	2.726(8)	177.1
N5	H5A	O4W[7]	0.88	2.09	2.928(6)	159.5

N5	H5B	O14[6]	0.88	2.13	2.912(9)	147.7
O18	H18	O13[8]	0.78	1.91	2.684(8)	176.2
N9	H9	O3[7]	0.88	1.86	2.710(5)	162.3
N10	H10C	O2W	0.88	1.99	2.810	155.0
N10	H10D	O2[7]	0.88	2.04	2.894(5)	164.5
O1W	H1WA	O9[9]	0.90	1.99	2.874(7)	166.4
O1W	H1WB	O13W[3]	0.90	1.86	2.753	170.2
O2W	H2WA	O14[10]	0.89	2.05	2.784(6)	139.1
O5W	H5WA	O2[7]	0.89	2.02	2.821(5)	148.1
O6W	H6WA	O11[11]	0.90	1.97	2.723(8)	139.6
O6W	H6WB	O7W[7]	0.90	2.14	2.912(2)	143.3
O7W	H7WB	N3[6]	0.89	2.31	2.954(6)	129.2
O9W	H9WB	O10W[8]	0.90	2.24	2.806	120.6
O10W	H10E	O8W	0.90	2.04	2.779	138.9
O11W	H11F	O22	0.90	2.19	2.797(6)	124.2
O12W	H12A	O15[10]	0.90	1.90	2.747(6)	155.9
O12W	H12B	O5W	0.90	1.94	2.758	150.2
O13W	H13A	O1W[11]	0.90	2.11	2.753	128.2
O13W	H13B	N7	0.90	1.97	2.828	159.2
O8W	H8WB	O6	0.89	2.07	2.884(6)	151.7

[1]+X,1+Y,+Z; [2]-1-X,1/2+Y,1-Z; [3]-1+X,+Y,+Z; [4]1-X,-1/2+Y,1-Z; [5]1-X,1/2+Y,1-Z; [6]-X,-1/2+Y,1-Z; [7]-X,1/2+Y,1-Z; [8]+X,-1+Y,+Z; [9]-1-X,-1/2+Y,1-Z; [10]-X,-1/2+Y,2-Z; [11]1+X,+Y,+Z

Table S15 Torsion Angles for n1745a.

A	B	C	D	Angle/°
P1	O1	C1	C2	155.8(5)
P2	O12	C11	C12	143.3(3)
Na1	O8	C10	N4	70(5)
Na1	O8	C10	C7	-108(5)
Na1[1]	O17	C13	C12	24.8(6)
Na1[1]	O17	C13	C14	-90.9(5)
Na2	O6	C3	C2	13.2(8)
Na2	O6	C3	C4	-103.7(7)
Na2	O19	C20	N9	-70.7(19)
Na2	O19	C20	C17	111.6(17)
O1	C1	C2	O5	61.7(7)

O1	C1	C2	C3	178.9(6)
O2	P1	O1	C1	-169.3(5)
O3	P1	O1	C1	73.7(6)
O4	P1	O1	C1	-47.7(6)
O5	C2	C3	O6	-154.2(6)
O5	C2	C3	C4	-30.9(7)
O6	Na2	O19	C20	95.0(18)
O6	C3	C4	O7	40.2(9)
O6	C3	C4	C5	155.7(6)
O7	C4	C5	O5	90.7(7)
O7	C4	C5	N1	-149.0(6)
O9	Na1	O8	C10	-168(5)
O10	Na1	O8	C10	7(5)
O11	Na1	O8	C10	102(5)
O12	C11	C12	O16	66.0(3)
O12	C11	C12	C13	-178.7(2)
O13	P2	O12	C11	69.6(4)
O14	P2	O12	C11	-172.2(4)
O15	P2	O12	C11	-49.5(5)
O16	C12	C13	O17	-157.2(4)
O16	C12	C13	C14	-34.8(2)
$O17^2$	Na1	O8	C10	-69(5)
O17	C13	C14	O18	38.0(3)
O17	C13	C14	C15	154.1(2)
O18	C14	C15	O16	89.7(3)
O18	C14	C15	N6	-149.7(3)
O19	Na2	O6	C3	-142.6(5)
O20	Na2	O6	C3	58.4(6)
O20	Na2	O19	C20	155.1(16)
O21	Na2	O6	C3	129.6(6)
O21	Na2	O19	C20	-113.7(18)
O22	Na2	O6	C3	-47.0(6)
O22	Na2	O19	C20	-17.5(19)
N2	C7	C8	N1	-1.1(9)
N2	C7	C8	N3	178.9(7)
N2	C7	C10	O8	1.0(16)
N2	C7	C10	N4	-177.4(8)
C1	C2	C3	O6	86.6(8)

C1	C2	C3	C4	-150.1(6)
C2	O5	C5	N1	-116.3(6)
C2	O5	C5	C4	7.7(8)
C2	C3	C4	O7	-81.7(7)
C2	C3	C4	C5	33.8(7)
C3	C4	C5	O5	-26.2(7)
C3	C4	C5	N1	94.1(7)
C5	O5	C2	C1	135.7(6)
C5	O5	C2	C3	14.5(8)
C5	N1	C6	N2	-169.6(7)
C5	N1	C8	N3	-8.8(11)
C5	N1	C8	C7	171.3(7)
C6	N1	C5	O5	80.9(9)
C6	N1	C5	C4	-38.2(11)
C6	N1	C8	N3	-179.2(7)
C6	N1	C8	C7	0.8(8)
C6	N2	C7	C8	1.0(9)
C6	N2	C7	C10	177.5(9)
C7	N2	C6	N1	-0.4(9)
C8	N1	C5	O5	-87.1(8)
C8	N1	C5	C4	153.8(7)
C8	N1	C6	N2	-0.3(9)
C8	N3	C9	N4	-3.7(11)
C8	N3	C9	N5	177.6(7)
C8	C7	C10	O8	177.1(8)
C8	C7	C10	N4	-1.2(11)
C9	N3	C8	N1	-179.4(7)
C9	N3	C8	C7	0.6(11)
C9	N4	C10	O8	179.7(8)
C9	N4	C10	C7	-1.8(12)
C10	N4	C9	N3	4.7(13)
C10	N4	C9	N5	-176.6(7)
C10	C7	C8	N1	-178.1(7)
C10	C7	C8	N3	1.9(13)
N13	C22	C23	C24	-0.4(4)
N14	C30	C31	C27	1.4(4)
C21	N13	C22	C23	175.5(3)
C21	N13	C26	C25	-175.1(3)

C22	N13	C26	C25	1.0(7)
C22	C23	C24	C25	0.9
C22	C23	C24	C27	179.0
C23	C24	C25	C26	-0.6
C23	C24	C27	C28	16.5
C23	C24	C27	C31	-161.8
C24	C25	C26	N13	-0.4(4)
C24	C27	C28	C29	-177.6
C24	C27	C31	C30	175.8
C25	C24	C27	C28	-165.6
C25	C24	C27	C31	16.2
C26	N13	C22	C23	-0.6(7)
C27	C24	C25	C26	-178.6
C27	C28	C29	N14	2.3(4)
C28	C27	C31	C30	-2.5
C29	N14	C30	C31	1.8(7)
C30	N14	C29	C28	-3.6(7)
C31	C27	C28	C29	0.7
C32	N14	C29	C28	174.2(3)
C32	N14	C30	C31	-176.1(3)
N7	C17	C18	N6	-1.6
N7	C17	C18	N8	176.7
N7	C17	C20	O19	1.0(3)
N7	C17	C20	N9	-177.0
C11	C12	C13	O17	84.0(3)
C11	C12	C13	C14	-153.6
C12	O16	C15	N6	-118.6(3)
C12	O16	C15	C14	3.8(4)
C12	C13	C14	O18	-80.5(2)
C12	C13	C14	C15	35.5
C13	C14	C15	O16	-24.8(2)
C13	C14	C15	N6	95.8
C15	O16	C12	C11	139.8(3)
C15	O16	C12	C13	19.2(4)
C15	N6	C16	N7	-175.3
C15	N6	C18	N8	-1.7
C15	N6	C18	C17	176.7
C16	N6	C15	O16	100.5(2)

C16	N6	C15	C14	−18.8
C16	N6	C18	N8	−177.6
C16	N6	C18	C17	0.7
C16	N7	C17	C18	1.8
C16	N7	C17	C20	175.8
C17	N7	C16	N6	−1.3
C18	N6	C15	O16	−74.4(2)
C18	N6	C15	C14	166.3
C18	N6	C16	N7	0.4
C18	N8	C19	N9	−1.2
C18	N8	C19	N10	179.3
C18	C17	C20	O19	174.6(3)
C18	C17	C20	N9	−3.3
C19	N8	C18	N6	178.6
C19	N8	C18	C17	0.6
C19	N9	C20	O19	−175.1(3)
C19	N9	C20	C17	3.0
C20	N9	C19	N8	−0.7
C20	N9	C19	N10	178.8
C20	C17	C18	N6	−176.4
C20	C17	C18	N8	1.8

[1]1+X,+Y,1+Z; [2]-1+X,+Y,-1+Z

Table S16 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for n1745a.

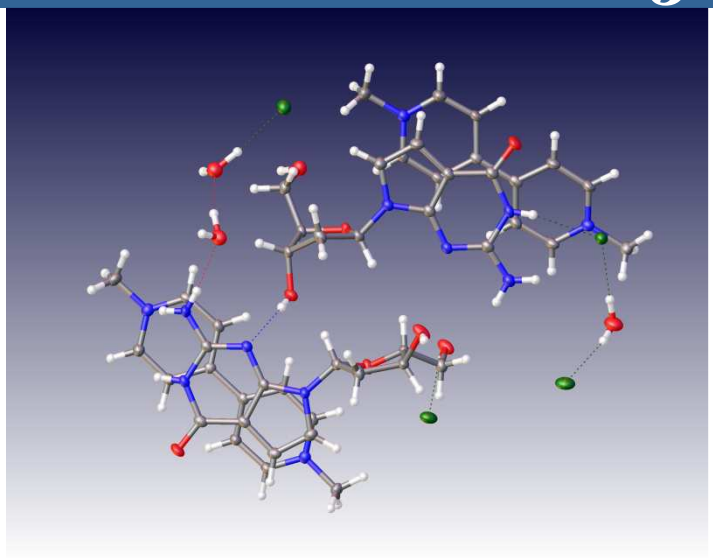
Atom	*x*	*y*	*z*	U(eq)
H11A	−4900(50)	7260(90)	2880(40)	61
H7	1620(50)	9850(90)	3860(40)	20(20)
H9A	−6630(80)	8210(110)	1960(20)	86
H9B	−6060(70)	9120(80)	1610(50)	86
H10A	−5130(60)	3820(50)	1280(50)	65
H10B	−5820(40)	4400(80)	1680(40)	65
H11B	−5820(70)	6760(150)	3050(40)	119
H20A	3500(90)	7190(120)	3900(30)	103
H20B	2970(80)	8230(80)	4190(50)	103
H21A	5120(70)	5970(70)	5490(60)	93
H21B	4890(80)	7380(50)	5430(60)	93

H22A	3380(50)	3940(80)	5430(30)	65
H22B	2510(50)	3530(60)	5030(40)	65
H4	−2532	7392	958	39
H5A	−199	7762	779	43
H5B	−1230	7615	423	43
H1A	827	4789	4747	40
H1B	−139	5023	4241	40
H2	1744	6124	4081	34
H3	63	7314	4555	34
H4A	279	9316	4027	37
H5	705	8196	2918	37
H6A	−1361	7913	3946	37
H21C	4176	8352	6881	66
H21D	4422	9885	7067	66
H21E	3753	9530	6399	66
H22	2115	9606	6397	43
H23	674	9582	6898	36
H25	2367	9048	8641	41
H26	3733	9109	8108	42
H28	−531	8969	7371	48
H29	−1900	9019	7938	48
H30	−236	9729	9629	44
H31	1172	9575	9106	43
H32A	−2240	10554	9147	67
H32B	−1920	9300	9611	67
H32C	−2593	9073	8930	67
H18	3640	3826	10076	67
H9	925	6219	6555	30
H10C	−304	5827	7809	39
H10D	−368	6022	7069	39
H11C	4109	9245	10202	44
H11D	3766	9114	9432	44
H12	3212	7269	10383	35
H13	4746	7106	9539	33
H14	4489	4809	9394	34
H15	2536	5021	9243	39
H16	4706	5930	8482	43
H1WA	−3042	4098	7630	115

H1WB	−3473	4823	7060	115
H2WA	−1721	6228	8600	155
H2WB	−917	5366	8555	155
H3WA	794	5313	9411	89
H3WB	100	6079	8986	89
H4WA	−1327	2836	10005	69
H4WB	−1186	3693	9459	69
H5WA	−2262	7630	6860	104
H5WB	−3316	7596	6761	104
H6WA	3219	6125	2731	117
H6WB	2183	6205	2775	117
H7WA	−1674	2826	8365	117
H7WB	−908	1912	8239	117
H9WA	4009	2757	6655	84
H9WB	4516	2691	6081	84
H10E	3698	11049	5502	108
H10F	4296	10029	5247	108
H11E	4564	3373	3903	101
H11F	3862	3432	4368	101
H12A	−3383	7113	8338	94
H12B	−3168	7680	7729	94
H13A	5600	4579	6938	92
H13B	4945	5667	7030	92
H6	1049	7372	5304	40(20)
H17	5479	6744	10454	20(20)
H8WA	1863	10382	5584	27
H8WB	2222	9381	5163	27

n2056

Crystal Submitted by:
Almaz Jalilov
Crystal Submitted on:
07/09/2012
Data Collected on:
07/20/2012
Structure Solved by:
Amy Sarjeant



Experimental

Single crystals of $C_{23}H_{31}Cl_2N_6O_{5.5}$ **[n2056]** were recrystallised from **[solvents]** mounted in inert oil and transferred to the cold gas stream of a Bruker Kappa APEX CCD area detector equipped with a CuKα microsource with MX optics. SADABS-2008/1 (Bruker,2008) was used for absorption correction. wR2(int) was 0.0564 before and 0.0414 after correction. The Ratio of minimum to maximum transmission is 0.9085. The λ/2 correction factor is 0.0015.

Crystal structure determination of [n2056]

Crystal Data. $C_{23}H_{31}Cl_2N_6O_{5.5}$, M =550.44, monoclinic, a = 6.74980(10) Å, b = 22.7723(3) Å, c = 16.6038(2) Å, β = 90.2810(10)°, U = 2552.11(6) Å^3, T = 100.0, space group P2$_1$ (no. 4), Z = 4, μ(CuKα) = 2.708, 28299 reflections measured, 9063 unique (R_{int} = 0.0293) which were used in all calculations. The final $wR(F_2)$ was 0.0737 (all data).

Refinement Details. 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.

Table S17: Crystal data and structure refinement for n2056

Identification code	n2056
Empirical formula	$C_{23}H_{31}Cl_2N_6O_{5.5}$
Formula weight	550.44
Temperature□/□K	100.0
Crystal system	monoclinic
Space group	$P2_1$
a□/□Å, b□/□Å, c□/□Å	6.74980(10), 22.7723(3), 16.6038(2)
α/°, β/°, γ/°	90.00, 90.2810(10), 90.00
Volume□/□$Å^3$	2552.11(6)
Z	4
ρ_{calc}□/□mg mm^{-3}	1.433
μ□/□mm^{-1}	2.708
F(000)	1156
Crystal size□/□mm^3	0.111 × 0.049 × 0.021
2Θ range for data collection	5.32 to 136.08°
Index ranges	$-8 \leq h \leq 5$, $-27 \leq k \leq 27$, $-19 \leq l \leq 19$
Reflections collected	28299
Independent reflections	9063[R(int) = 0.0293]
Data/restraints/parameters	9063/1/726
Goodness-of-fit on F^2	1.024
Final R indexes [I>2σ (I)]	R_1 = 0.0287, wR_2 = 0.0727
Final R indexes [all data]	R_1 = 0.0301, wR_2 = 0.0737
Largest diff. peak/hole□/□e $Å^{-3}$	0.279/-0.174

Table S18 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for n2056. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cl2	-7036.2(8)	-2755.5(2)	-4559.2(3)	22.04(11)
Cl3	-7449.5(8)	1750.6(2)	-7318.8(3)	26.40(12)
Cl1	-5695.5(8)	-3101.2(2)	-9695.4(3)	27.35(12)
Cl4	-9890.8(9)	-3840.0(2)	-6848.2(3)	31.90(13)
O3A	-7527(2)	-353.8(7)	-9827.8(9)	21.7(3)
O2A	-5078(2)	-293.4(6)	-8342.6(8)	17.7(3)
O2	-10045(2)	-1746.9(6)	-9479.7(8)	20.8(3)
O1W	-10756(3)	1124.1(8)	-9785.5(10)	27.2(3)
N3	-10888(2)	-321.1(7)	-10883(1)	16.3(3)
O4	-7521(2)	-2409.9(7)	-8294.1(10)	27.1(4)
O4A	-2463(2)	689.4(7)	-8396.2(10)	25.7(3)
O1	-11378(2)	-752.9(7)	-13287.8(8)	25.9(3)
N5A	-1984(3)	-2731.5(8)	-5037.7(10)	18.8(3)
O1A	-6630(3)	-909.7(7)	-4532.3(8)	26.9(3)
C5	-10696(3)	58.3(9)	-11478.0(12)	16.3(4)
O2W	-7917(3)	1758.5(8)	-9159.0(11)	29.4(4)
N2	-10888(3)	-97.7(8)	-12276.5(10)	17.1(3)
N2A	-6900(3)	-1581.4(8)	-5542.1(11)	18.2(4)
C15	-6298(3)	-1079.8(9)	-12082.0(12)	15.0(4)
O3	-13504(3)	-1721.2(8)	-7901.5(9)	28.7(4)
N5	-6992(2)	-2273.8(7)	-11933.7(10)	17.3(3)
N6A	-2008(3)	233.8(8)	-6194.8(11)	21.6(4)
C3	-11406(3)	-1085.3(9)	-11923.3(12)	16.8(4)
O3W	-6266(3)	-3841.0(9)	-5644.8(11)	37.5(4)
N6	-5410(3)	761.1(8)	-12314.7(11)	19.4(4)
N1A	-7115(3)	-332.0(8)	-7198.9(10)	18.3(4)
C1A	-6986(3)	184.2(10)	-6740.9(13)	22.2(4)
N4A	-7024(3)	-2322.7(8)	-6494.2(13)	23.6(4)
N3A	-7100(3)	-1366.4(8)	-6937(1)	17.7(3)
N1	-11497(3)	-1350.0(7)	-10630.3(10)	16.8(3)
C4A	-6811(3)	-1004.6(9)	-5261.9(12)	18.7(4)
N4	-10292(3)	620.9(8)	-11334.9(13)	21.6(4)
C16	-6645(3)	-1339.3(9)	-11327.0(12)	16.6(4)
C3A	-6914(3)	-586.2(9)	-5900.8(12)	18.7(4)
C15A	-1956(3)	-1563.7(9)	-5482.5(12)	17.1(4)
C13	-6650(3)	-2040.8(9)	-12667.9(12)	18.7(4)
C6	-11249(3)	-880.8(9)	-11133.2(12)	14.9(4)

C13A	−1892(3)	−2586.3(10)	−5817.7(13)	23.1(5)
C14	−6309(3)	−1450.5(9)	−12757.7(12)	18.0(4)
C2	−11719(3)	−1704.3(9)	−11891.7(12)	17.8(4)
C21A	−1955(3)	−934.9(9)	−5727.1(12)	16.4(4)
C14A	−1884(3)	−2009.5(10)	−6054.0(12)	22.3(4)
C23A	−2200(3)	−189.9(9)	−6752.2(12)	19.3(4)
C19	−5319(3)	508.1(9)	−11578.1(12)	19.6(4)
C5A	−7015(3)	−1748.0(9)	−6335.7(12)	18.4(4)
C12A	−1970(4)	−3356.4(10)	−4802.8(14)	24.5(5)
C10A	−5106(3)	122.1(9)	−9002.2(12)	17.7(4)
C4	−11237(3)	−667.3(9)	−12560.4(12)	18.0(4)
C22A	−2180(3)	−771.7(10)	−6536.5(12)	19.7(4)
C1	−11777(3)	−1852.7(9)	−11099.9(13)	19.5(4)
C6A	−7047(3)	−800.2(9)	−6684.3(12)	17.3(4)
C12	−7421(3)	−2909.3(9)	−11876.1(13)	21.5(4)
C7A	−7046(3)	−388.3(9)	−8065.9(12)	19.1(4)
C23	−5754(3)	429.1(9)	−12974.8(13)	20.4(4)
C2A	−6868(3)	37.7(9)	−5946.2(13)	22.2(4)
C20A	−1747(3)	−482.9(10)	−5164.1(13)	22.3(5)
C22	−6023(3)	−164.4(9)	−12917.1(12)	19.3(4)
C8	−13477(3)	−1552.9(10)	−9386.3(13)	22.5(4)
C20	−5566(3)	−85.8(9)	−11491.8(12)	18.0(4)
C17	−6988(3)	−1931.6(9)	−11277.1(12)	17.7(4)
C9	−12837(3)	−1924.7(9)	−8663.3(12)	18.0(4)
C18A	−2044(4)	854.1(10)	−6445.9(14)	30.7(5)
C19A	−1791(4)	91.4(10)	−5411.4(13)	27.0(5)
C11	−9612(3)	−2464.3(10)	−8424.9(13)	23.1(4)
C16A	−2035(3)	−1730.5(10)	−4672.1(12)	21.2(4)
C10	−10581(3)	−1893.9(9)	−8668.4(12)	17.3(4)
C18	−5163(4)	1403.7(9)	−12392.2(14)	26.8(5)
C9A	−7242(3)	132.9(9)	−9296.7(12)	18.7(4)
C21	−5955(3)	−439.2(9)	−12166.2(12)	15.2(4)
C7	−11533(3)	−1343.5(9)	−9758.5(12)	18.7(4)
C8A	−8370(3)	44.3(10)	−8514.5(13)	21.1(4)
C17A	−2064(3)	−2311.8(10)	−4467.1(13)	22.7(5)
C11A	−4419(3)	716.8(9)	−8706.4(13)	21.8(4)

Table S19 Anisotropic Displacement Parameters ($Å^2×10^3$) for n2056. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+...+2hka×b×U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl2	29.1(3)	20.1(2)	16.9(2)	-0.17(18)	-1.23(19)	-1.4(2)
Cl3	32.9(3)	25.2(2)	21.1(2)	-0.33(19)	2.3(2)	2.6(2)
Cl1	30.6(3)	30.8(3)	20.7(2)	-9.3(2)	0.7(2)	-3.6(2)
Cl4	33.8(3)	32.1(3)	29.8(3)	-15.0(2)	0.7(2)	2.4(2)
O3A	26.1(9)	23.7(8)	15.2(7)	-1.9(6)	-4.8(6)	1.4(6)
O2A	19.3(7)	19.1(7)	14.7(7)	4.6(5)	-1.4(5)	4.0(6)
O2	21.5(8)	25.5(8)	15.5(7)	5.6(6)	-0.5(6)	3.4(6)
O1W	26.6(9)	28.7(8)	26.2(8)	-1.2(7)	-1.6(7)	4.2(8)
N3	19.0(9)	16.8(8)	13.1(8)	0.3(6)	-1.2(6)	-0.2(7)
O4	26.4(8)	36.1(9)	18.8(8)	-4.6(7)	-5.1(7)	11.0(7)
O4A	25.2(8)	27.1(8)	24.9(8)	2.5(7)	-4.0(7)	-2.1(7)
O1	37.9(9)	29.2(8)	10.6(7)	-2.4(6)	-2.1(6)	2.3(7)
N5A	19.1(9)	19.9(8)	17.5(8)	-2.1(7)	-2.4(7)	2.1(7)
O1A	41.8(10)	28.6(8)	10.4(7)	-1.0(6)	0.7(6)	-0.9(7)
C5	14.2(9)	20.9(10)	13.8(9)	-1.2(8)	-0.7(7)	1.2(8)
O2W	32.3(9)	30.2(9)	25.7(9)	-1.4(7)	1.0(8)	0.4(7)
N2	19.3(9)	20.1(9)	11.9(8)	2.6(7)	-0.9(6)	-1.1(7)
N2A	21.7(9)	20.6(9)	12.2(8)	3.3(7)	-1.8(7)	-0.1(7)
C15	11.7(9)	17.4(9)	15.9(10)	0.4(7)	-1.1(7)	2.0(7)
O3	23.3(9)	47.3(10)	15.3(7)	-3.8(7)	1.5(6)	3.2(7)
N5	15.9(8)	18.0(8)	18.0(9)	1.1(7)	-1.6(7)	-0.3(7)
N6A	26.1(10)	21.6(9)	17.0(9)	-0.3(7)	-0.6(7)	-2.0(7)
C3	14.2(10)	22.6(10)	13.6(9)	-1.7(8)	-1.7(8)	2.2(8)
O3W	49.9(12)	36.8(10)	25.7(9)	-10.3(8)	-2.3(8)	3.0(9)
N6	19.8(9)	17.7(9)	20.7(9)	0.2(7)	1.2(7)	0.7(7)
N1A	21.6(9)	19.3(8)	13.9(8)	-0.8(7)	-1.5(7)	0.0(7)
C1A	28.3(12)	19.5(10)	18.8(11)	-1.1(8)	2.6(9)	0.1(9)
N4A	31.8(11)	22.7(9)	16.1(10)	0.2(8)	-2.0(8)	-1.0(8)
N3A	20.8(9)	19.3(8)	13.0(8)	0.3(7)	-2.4(7)	-0.1(7)
N1	22.4(9)	14.7(8)	13.3(8)	0.6(6)	-0.9(7)	0.4(7)
C4A	18.3(10)	23(1)	14.9(10)	-1.2(8)	1.0(8)	0.2(8)
N4	34.9(11)	18.0(9)	12.1(10)	3.2(8)	-0.8(8)	-4.8(8)
C16	14.9(9)	22(1)	13.0(9)	-0.7(8)	-1.4(7)	1.7(8)
C3A	18.9(10)	23.1(10)	14(1)	-0.5(8)	1.3(8)	1.1(8)
C15A	11.4(9)	24.9(10)	15.1(9)	-3.1(8)	-1.3(7)	1.8(8)
C13	22.2(11)	21.2(10)	12.6(9)	-1.8(8)	-1.2(8)	2.1(8)
C6	12.8(9)	17.6(9)	14.3(9)	1.0(7)	-1.7(7)	1.8(8)

C13A	28.3(12)	25.1(11)	15.9(10)	−6.1(8)	−3.4(8)	4.8(9)
C14	21.9(11)	19.1(10)	13.0(9)	−0.5(8)	−1.5(8)	−0.4(8)
C2	15.7(10)	18.3(10)	19.5(10)	−4.5(8)	−1.1(8)	2.5(8)
C21A	12.3(9)	22.5(10)	14.5(9)	−2.0(8)	0.9(7)	0.9(8)
C14A	27.1(12)	26.6(11)	13.1(9)	−0.2(8)	0.4(8)	2.7(9)
C23A	18.4(10)	25.7(11)	13.7(10)	1.2(8)	−1.2(8)	−0.3(8)
C19	17.8(10)	25.2(11)	15.6(10)	−5.8(8)	0.6(8)	0.6(8)
C5A	15.8(10)	23.2(10)	16.3(10)	−0.9(8)	−1.7(8)	−0.4(8)
C12A	29.4(12)	21.3(10)	22.8(11)	−0.9(8)	−1.9(9)	4.0(9)
C10A	21.2(10)	19.1(10)	12.8(9)	3.2(8)	−1.6(8)	2.3(8)
C4	15(1)	22.9(10)	16(1)	−3.1(8)	−0.7(8)	2.7(8)
C22A	19(1)	27.7(11)	12.3(9)	−4.3(8)	−0.3(8)	−0.8(9)
C1	18(1)	16.4(9)	24.0(11)	−1.8(8)	−1.6(8)	−0.8(8)
C6A	15(1)	21.3(10)	15.6(10)	0.0(8)	−1.0(8)	0.2(8)
C12	26.8(12)	16.1(10)	21.4(10)	2.0(8)	−1.6(9)	−3.0(8)
C7A	22.5(11)	22.9(10)	12(1)	0.7(8)	−1.9(8)	−1.1(9)
C23	25.3(11)	18.3(10)	17.6(10)	0.9(8)	−0.9(8)	0.1(8)
C2A	26.3(11)	21.4(11)	18.9(10)	−5.0(8)	1.4(8)	0.2(9)
C20A	30.9(12)	24.3(11)	11.7(10)	−2.0(8)	−3.2(8)	−3.1(9)
C22	22.2(11)	20.1(10)	15.4(10)	−1.2(8)	−3.3(8)	1.2(8)
C8	20.7(11)	27.0(11)	19.6(10)	4.6(8)	−1.3(8)	4.9(9)
C20	18.7(10)	22(1)	13.3(9)	0.7(8)	0.4(8)	0.5(8)
C17	18.2(10)	22.7(10)	12.0(9)	3.4(8)	−1.8(7)	1.5(8)
C9	24.7(11)	16.6(9)	12.5(9)	0.2(8)	−1.2(8)	−0.9(8)
C18A	48.4(16)	21.8(11)	22.0(11)	1.6(9)	−4.5(10)	−6.1(10)
C19A	39.2(13)	24.4(11)	17.4(11)	−3.2(9)	−2.6(9)	−3.4(10)
C11	27.9(12)	23.6(11)	17.9(10)	3.1(8)	−1.1(9)	3.2(9)
C16A	25.2(11)	24.0(11)	14.3(10)	−5.3(8)	−1.0(8)	1.4(8)
C10	24.8(11)	16.0(9)	11.2(9)	0.8(7)	−1.6(8)	−0.9(8)
C18	34.8(13)	18(1)	27.6(12)	−1.1(9)	−1(1)	−4.1(9)
C9A	25.1(11)	17.1(9)	13.8(10)	1.7(8)	−5.3(8)	2.6(8)
C21	12.1(9)	16.9(9)	16.7(9)	−1.3(8)	0.3(7)	1.6(7)
C7	25.4(11)	16.2(9)	14.6(10)	0.7(8)	−3.2(8)	3.9(8)
C8A	18.6(10)	26.4(11)	18.2(10)	−0.2(8)	−2.3(8)	2.8(9)
C17A	30.5(12)	24.8(11)	12.6(10)	−2.9(8)	−0.7(8)	1.4(9)
C11A	23.0(11)	20.5(10)	21.9(11)	4.6(8)	−2.2(8)	0.3(9)

Table S20 Bond Lengths for n2056.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O3A	C9A	1.429(3)	C15A	C21A	1.488(3)
O3A	H3A	0.79(4)	C15A	C14A	1.391(3)
O2A	C10A	1.447(2)	C15A	C16A	1.399(3)
O2A	C7A	1.425(3)	C13	H13	0.9500
O2	C10	1.436(2)	C13	C14	1.372(3)
O2	C7	1.436(2)	C13A	H13A	0.9500
O1W	H1WA	0.96(3)	C13A	C14A	1.371(3)
O1W	H1WB	0.81(3)	C14	H14	0.9500
N3	C5	1.319(3)	C2	H2B	0.9500
N3	C6	1.362(3)	C2	C1	1.358(3)
O4	C11	1.432(3)	C21A	C22A	1.402(3)
O4	H4	0.86(4)	C21A	C20A	1.397(3)
O4A	C11A	1.416(3)	C14A	H14A	0.9500
O4A	H4A	0.87(4)	C23A	H23A	0.9500
O1	C4	1.227(3)	C23A	C22A	1.372(3)
N5A	C13A	1.338(3)	C19	H19	0.9500
N5A	C12A	1.475(3)	C19	C20	1.370(3)
N5A	C17A	1.347(3)	C12A	H12A	0.9800
O1A	C4A	1.236(3)	C12A	H12B	0.9800
C5	N2	1.378(3)	C12A	H12C	0.9800
C5	N4	1.331(3)	C10A	H10A	1.0000
O2W	H2WA	0.84(3)	C10A	C9A	1.520(3)
O2W	H2WB	0.94(4)	C10A	C11A	1.513(3)
N2	C4	1.400(3)	C22A	H22A	0.9500
N2	H2	0.87(3)	C1	H1	0.9500
N2A	C4A	1.395(3)	C12	H12D	0.9800
N2A	C5A	1.373(3)	C12	H12E	0.9800
N2A	H2A	0.78(3)	C12	H12F	0.9800
C15	C16	1.407(3)	C7A	H7A	1.0000
C15	C14	1.404(3)	C7A	C8A	1.522(3)
C15	C21	1.484(3)	C23	H23	0.9500
O3	C9	1.422(3)	C23	C22	1.367(3)
O3	H3	0.83(4)	C2A	H2AA	0.9500
N5	C13	1.350(3)	C20A	H20A	0.9500
N5	C12	1.479(3)	C20A	C19A	1.371(3)
N5	C17	1.340(3)	C22	H22	0.9500
N6A	C23A	1.343(3)	C22	C21	1.396(3)
N6A	C18A	1.473(3)	C8	H8A	0.9900

N6A	C19A	1.348(3)	C8	H8B	0.9900
C3	C6	1.396(3)	C8	C9	1.529(3)
C3	C2	1.426(3)	C8	C7	1.529(3)
C3	C4	1.428(3)	C20	H20	0.9500
O3W	H3WA	0.85(4)	C20	C21	1.403(3)
O3W	H3WB	0.87(4)	C17	H17	0.9500
N6	C19	1.353(3)	C9	H9	1.0000
N6	C23	1.351(3)	C9	C10	1.524(3)
N6	C18	1.478(3)	C18A	H18A	0.9800
N1A	C1A	1.403(3)	C18A	H18B	0.9800
N1A	C6A	1.367(3)	C18A	H18C	0.9800
N1A	C7A	1.446(3)	C19A	H19A	0.9500
C1A	H1A	0.9500	C11	H11C	0.9900
C1A	C2A	1.363(3)	C11	H11D	0.9900
N4A	C5A	1.335(3)	C11	C10	1.509(3)
N4A	H4AA	0.87(3)	C16A	H16A	0.9500
N4A	H4AB	0.83(3)	C16A	C17A	1.367(3)
N3A	C5A	1.325(3)	C10	H10	1.0000
N3A	C6A	1.356(3)	C18	H18D	0.9800
N1	C6	1.367(3)	C18	H18E	0.9800
N1	C1	1.397(3)	C18	H18F	0.9800
N1	C7	1.448(3)	C9A	H9A	1.0000
C4A	C3A	1.427(3)	C9A	C8A	1.522(3)
N4	H4B	0.78(3)	C7	H7	1.0000
N4	H4C	0.74(3)	C8A	H8AA	0.9900
C16	H16	0.9500	C8A	H8AB	0.9900
C16	C17	1.371(3)	C17A	H17A	0.9500
C3A	C6A	1.392(3)	C11A	H11A	0.9900
C3A	C2A	1.423(3)	C11A	H11B	0.9900

Table S21 Bond Angles for n2056.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C9A	O3A	H3A	111(3)	C23A	C22A	C21A	120.46(19)
C7A	O2A	C10A	109.52(15)	C23A	C22A	H22A	119.8
C7	O2	C10	105.83(15)	N1	C1	H1	125.3
H1WA	O1W	H1WB	100(3)	C2	C1	N1	109.38(18)
C5	N3	C6	113.73(17)	C2	C1	H1	125.3
C11	O4	H4	110(2)	N1A	C6A	C3A	108.25(18)
C11A	O4A	H4A	108(2)	N3A	C6A	N1A	123.18(18)

C13A	N5A	C12A	119.60(18)	N3A	C6A	C3A	128.57(19)
C13A	N5A	C17A	120.50(19)	N5	C12	H12D	109.5
C17A	N5A	C12A	119.90(18)	N5	C12	H12E	109.5
N3	C5	N2	122.86(18)	N5	C12	H12F	109.5
N3	C5	N4	121.17(19)	H12D	C12	H12E	109.5
N4	C5	N2	115.97(19)	H12D	C12	H12F	109.5
H2WA	O2W	H2WB	112(3)	H12E	C12	H12F	109.5
C5	N2	C4	125.28(18)	O2A	C7A	N1A	110.00(16)
C5	N2	H2	114.4(17)	O2A	C7A	H7A	108.6
C4	N2	H2	120.3(16)	O2A	C7A	C8A	106.86(17)
C4A	N2A	H2A	121(2)	N1A	C7A	H7A	108.6
C5A	N2A	C4A	125.62(19)	N1A	C7A	C8A	114.10(17)
C5A	N2A	H2A	113(2)	C8A	C7A	H7A	108.6
C16	C15	C21	121.59(18)	N6	C23	H23	119.4
C14	C15	C16	117.34(18)	N6	C23	C22	121.26(19)
C14	C15	C21	121.07(18)	C22	C23	H23	119.4
C9	O3	H3	110(2)	C1A	C2A	C3A	107.13(19)
C13	N5	C12	118.50(17)	C1A	C2A	H2AA	126.4
C17	N5	C13	120.42(18)	C3A	C2A	H2AA	126.4
C17	N5	C12	121.06(17)	C21A	C20A	H20A	120.0
C23A	N6A	C18A	119.52(18)	C19A	C20A	C21A	120.03(19)
C23A	N6A	C19A	120.14(18)	C19A	C20A	H20A	120.0
C19A	N6A	C18A	120.35(18)	C23	C22	H22	119.9
C6	C3	C2	107.81(18)	C23	C22	C21	120.13(19)
C6	C3	C4	117.89(18)	C21	C22	H22	119.9
C2	C3	C4	134.30(19)	H8A	C8	H8B	108.9
H3WA	O3W	H3WB	106(3)	C9	C8	H8A	110.9
C19	N6	C18	119.71(18)	C9	C8	H8B	110.9
C23	N6	C19	120.13(18)	C7	C8	H8A	110.9
C23	N6	C18	120.15(18)	C7	C8	H8B	110.9
C1A	N1A	C7A	127.72(17)	C7	C8	C9	104.50(17)
C6A	N1A	C1A	108.23(17)	C19	C20	H20	119.8
C6A	N1A	C7A	123.51(17)	C19	C20	C21	120.34(19)
N1A	C1A	H1A	125.6	C21	C20	H20	119.8
C2A	C1A	N1A	108.84(18)	N5	C17	C16	121.50(18)
C2A	C1A	H1A	125.6	N5	C17	H17	119.2
C5A	N4A	H4AA	118(2)	C16	C17	H17	119.2
C5A	N4A	H4AB	118.8(19)	O3	C9	C8	115.36(18)
H4AA	N4A	H4AB	122(3)	O3	C9	H9	109.6
C5A	N3A	C6A	112.93(17)	O3	C9	C10	108.10(16)
C6	N1	C1	108.43(16)	C8	C9	H9	109.6
C6	N1	C7	127.25(17)	C10	C9	C8	104.38(16)

C1	N1	C7	124.29(17)	C10	C9	H9	109.6
O1A	C4A	N2A	119.71(19)	N6A	C18A	H18A	109.5
O1A	C4A	C3A	128.0(2)	N6A	C18A	H18B	109.5
N2A	C4A	C3A	112.27(18)	N6A	C18A	H18C	109.5
C5	N4	H4B	119.1(17)	H18A	C18A	H18B	109.5
C5	N4	H4C	122(2)	H18A	C18A	H18C	109.5
H4B	N4	H4C	118(3)	H18B	C18A	H18C	109.5
C15	C16	H16	120.1	N6A	C19A	C20A	121.4(2)
C17	C16	C15	119.74(18)	N6A	C19A	H19A	119.3
C17	C16	H16	120.1	C20A	C19A	H19A	119.3
C6A	C3A	C4A	117.63(19)	O4	C11	H11C	109.0
C6A	C3A	C2A	107.53(18)	O4	C11	H11D	109.0
C2A	C3A	C4A	134.8(2)	O4	C11	C10	113.08(18)
C14A	C15A	C21A	121.06(19)	H11C	C11	H11D	107.8
C14A	C15A	C16A	117.4(2)	C10	C11	H11C	109.0
C16A	C15A	C21A	121.58(18)	C10	C11	H11D	109.0
N5	C13	H13	119.6	C15A	C16A	H16A	119.9
N5	C13	C14	120.83(19)	C17A	C16A	C15A	120.20(19)
C14	C13	H13	119.6	C17A	C16A	H16A	119.9
N3	C6	C3	127.71(18)	O2	C10	C9	105.79(15)
N3	C6	N1	124.57(18)	O2	C10	C11	109.95(17)
N1	C6	C3	107.72(17)	O2	C10	H10	109.3
N5A	C13A	H13A	119.5	C9	C10	H10	109.3
N5A	C13A	C14A	120.9(2)	C11	C10	C9	113.01(17)
C14A	C13A	H13A	119.5	C11	C10	H10	109.3
C15	C14	H14	119.9	N6	C18	H18D	109.5
C13	C14	C15	120.16(19)	N6	C18	H18E	109.5
C13	C14	H14	119.9	N6	C18	H18F	109.5
C3	C2	H2B	126.7	H18D	C18	H18E	109.5
C1	C2	C3	106.64(18)	H18D	C18	H18F	109.5
C1	C2	H2B	126.7	H18E	C18	H18F	109.5
C22A	C21A	C15A	121.09(18)	O3A	C9A	C10A	108.08(17)
C20A	C21A	C15A	121.76(18)	O3A	C9A	H9A	111.9
C20A	C21A	C22A	117.14(19)	O3A	C9A	C8A	110.95(17)
C15A	C14A	H14A	119.9	C10A	C9A	H9A	111.9
C13A	C14A	C15A	120.3(2)	C10A	C9A	C8A	101.58(16)
C13A	C14A	H14A	119.9	C8A	C9A	H9A	111.9
N6A	C23A	H23A	119.6	C22	C21	C15	121.36(18)
N6A	C23A	C22A	120.86(19)	C22	C21	C20	117.47(18)
C22A	C23A	H23A	119.6	C20	C21	C15	121.16(18)
N6	C19	H19	119.7	O2	C7	N1	107.51(16)
N6	C19	C20	120.65(18)	O2	C7	C8	105.67(16)

C20	C19	H19	119.7	O2	C7	H7	109.6
N4A	C5A	N2A	117.4(2)	N1	C7	C8	114.78(17)
N3A	C5A	N2A	122.96(19)	N1	C7	H7	109.6
N3A	C5A	N4A	119.63(19)	C8	C7	H7	109.6
N5A	C12A	H12A	109.5	C7A	C8A	C9A	102.05(17)
N5A	C12A	H12B	109.5	C7A	C8A	H8AA	111.4
N5A	C12A	H12C	109.5	C7A	C8A	H8AB	111.4
H12A	C12A	H12B	109.5	C9A	C8A	H8AA	111.4
H12A	C12A	H12C	109.5	C9A	C8A	H8AB	111.4
H12B	C12A	H12C	109.5	H8AA	C8A	H8AB	109.2
O2A	C10A	H10A	109.8	N5A	C17A	C16A	120.75(19)
O2A	C10A	C9A	105.26(16)	N5A	C17A	H17A	119.6
O2A	C10A	C11A	109.67(16)	C16A	C17A	H17A	119.6
C9A	C10A	H10A	109.8	O4A	C11A	C10A	111.27(17)
C11A	C10A	H10A	109.8	O4A	C11A	H11A	109.4
C11A	C10A	C9A	112.26(17)	O4A	C11A	H11B	109.4
O1	C4	N2	119.40(19)	C10A	C11A	H11A	109.4
O1	C4	C3	128.1(2)	C10A	C11A	H11B	109.4
N2	C4	C3	112.48(17)	H11A	C11A	H11B	108.0
C21A	C22A	H22A	119.8				

Table S22 Hydrogen Bonds for n2056.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N4	H4B	O1W	0.78(3)	2.06(3)	2.835(3)	171(2)
O2W	H2WA	Cl1[1]	0.84(3)	2.28(3)	3.116(2)	175(3)
N2A	H2A	Cl2	0.78(3)	2.37(3)	3.1339(19)	169(3)
O1W	H1WA	O2W	0.96(3)	1.67(3)	2.612(2)	168(3)
O2W	H2WB	Cl3	0.94(4)	2.14(4)	3.0702(18)	167(3)
O3W	H3WA	Cl4	0.85(4)	2.31(4)	3.152(2)	170(3)
O4A	H4A	O1W[2]	0.87(4)	1.94(4)	2.767(2)	159(4)
N4A	H4AB	O4	0.83(3)	2.22(3)	3.012(3)	161(3)
O1W	H1WB	Cl1[3]	0.81(3)	2.29(3)	3.0937(18)	169(3)
O3W	H3WB	Cl2	0.87(4)	2.23(4)	3.105(2)	179(3)
O4	H4	Cl1	0.86(4)	2.23(4)	3.0723(18)	167(3)
O3A	H3A	N3	0.79(4)	2.09(4)	2.861(2)	163(4)
O3	H3	O4[4]	0.83(4)	2.49(3)	3.197(2)	144(3)
O3	H3	N3A[4]	0.83(4)	2.42(3)	3.025(3)	131(3)

[1]-1-X,1/2+Y,-2-Z; [2]1+X,+Y,+Z; [3]-2-X,1/2+Y,-2-Z; [4]-1+X,+Y,+Z

Table S23 Torsion Angles for n2056.

A	B	C	D	Angle/°
O3A	C9A	C8A	C7A	77.49(19)
O2A	C10A	C9A	O3A	-82.45(19)
O2A	C10A	C9A	C8A	34.34(19)
O2A	C10A	C11A	O4A	60.3(2)
O2A	C7A	C8A	C9A	27.9(2)
N3	C5	N2	C4	-2.3(3)
O4	C11	C10	O2	72.2(2)
O4	C11	C10	C9	-169.84(16)
N5A	C13A	C14A	C15A	0.5(3)
O1A	C4A	C3A	C6A	177.7(2)
O1A	C4A	C3A	C2A	-0.5(4)
C5	N3	C6	C3	0.7(3)
C5	N3	C6	N1	179.83(18)
C5	N2	C4	O1	-179.90(19)
C5	N2	C4	C3	0.8(3)
N2A	C4A	C3A	C6A	-1.1(3)
N2A	C4A	C3A	C2A	-179.3(2)
C15	C16	C17	N5	0.3(3)
O3	C9	C10	O2	-145.75(16)
O3	C9	C10	C11	93.9(2)
N5	C13	C14	C15	0.4(3)
N6A	C23A	C22A	C21A	-0.1(3)
C3	C2	C1	N1	-0.4(2)
N6	C19	C20	C21	-1.2(3)
N6	C23	C22	C21	0.3(3)
N1A	C1A	C2A	C3A	0.3(2)
N1A	C7A	C8A	C9A	149.72(17)
C1A	N1A	C6A	N3A	-178.69(19)
C1A	N1A	C6A	C3A	1.1(2)
C1A	N1A	C7A	O2A	73.0(3)
C1A	N1A	C7A	C8A	-47.0(3)
C4A	N2A	C5A	N4A	177.9(2)
C4A	N2A	C5A	N3A	-1.6(3)
C4A	C3A	C6A	N1A	-179.58(18)
C4A	C3A	C6A	N3A	0.2(3)
C4A	C3A	C2A	C1A	178.7(2)
N4	C5	N2	C4	177.5(2)
C16	C15	C14	C13	0.0(3)
C16	C15	C21	C22	-166.42(19)

C16	C15	C21	C20	13.0(3)
C15A	C21A	C22A	C23A	179.20(19)
C15A	C21A	C20A	C19A	-178.7(2)
C15A	C16A	C17A	N5A	1.1(3)
C13	N5	C17	C16	0.1(3)
C6	N3	C5	N2	1.4(3)
C6	N3	C5	N4	-178.37(19)
C6	C3	C2	C1	1.1(2)
C6	C3	C4	O1	-178.1(2)
C6	C3	C4	N2	1.2(3)
C6	N1	C1	C2	-0.4(2)
C6	N1	C7	O2	-124.2(2)
C6	N1	C7	C8	118.5(2)
C13A	N5A	C17A	C16A	-0.6(3)
C14	C15	C16	C17	-0.4(3)
C14	C15	C21	C22	12.9(3)
C14	C15	C21	C20	-167.69(19)
C2	C3	C6	N3	177.93(19)
C2	C3	C6	N1	-1.3(2)
C2	C3	C4	O1	1.9(4)
C2	C3	C4	N2	-178.8(2)
C21A	C15A	C14A	C13A	-179.8(2)
C21A	C15A	C16A	C17A	179.1(2)
C21A	C20A	C19A	N6A	-0.8(4)
C14A	C15A	C21A	C22A	9.7(3)
C14A	C15A	C21A	C20A	-170.9(2)
C14A	C15A	C16A	C17A	-0.8(3)
C23A	N6A	C19A	C20A	0.4(3)
C19	N6	C23	C22	0.2(3)
C19	C20	C21	C15	-177.81(19)
C19	C20	C21	C22	1.6(3)
C5A	N2A	C4A	O1A	-177.0(2)
C5A	N2A	C4A	C3A	1.9(3)
C5A	N3A	C6A	N1A	179.92(19)
C5A	N3A	C6A	C3A	0.1(3)
C12A	N5A	C13A	C14A	-179.4(2)
C12A	N5A	C17A	C16A	178.6(2)
C10A	O2A	C7A	N1A	-130.97(17)
C10A	O2A	C7A	C8A	-6.6(2)
C10A	C9A	C8A	C7A	-37.2(2)
C4	C3	C6	N3	-2.1(3)
C4	C3	C6	N1	178.69(18)

C4	C3	C2	C1	-178.9(2)
C22A	C21A	C20A	C19A	0.7(3)
C1	N1	C6	N3	-178.23(18)
C1	N1	C6	C3	1.0(2)
C1	N1	C7	O2	57.7(2)
C1	N1	C7	C8	-59.6(3)
C6A	N1A	C1A	C2A	-0.9(2)
C6A	N1A	C7A	O2A	-97.5(2)
C6A	N1A	C7A	C8A	142.40(19)
C6A	N3A	C5A	N2A	0.5(3)
C6A	N3A	C5A	N4A	-179.04(19)
C6A	C3A	C2A	C1A	0.4(2)
C12	N5	C13	C14	177.87(19)
C12	N5	C17	C16	-178.22(19)
C7A	O2A	C10A	C9A	-17.7(2)
C7A	O2A	C10A	C11A	103.28(18)
C7A	N1A	C1A	C2A	-172.59(19)
C7A	N1A	C6A	N3A	-6.5(3)
C7A	N1A	C6A	C3A	173.27(18)
C23	N6	C19	C20	0.2(3)
C23	C22	C21	C15	178.3(2)
C23	C22	C21	C20	-1.2(3)
C2A	C3A	C6A	N1A	-1.0(2)
C2A	C3A	C6A	N3A	178.8(2)
C20A	C21A	C22A	C23A	-0.3(3)
C8	C9	C10	O2	-22.5(2)
C8	C9	C10	C11	-142.81(18)
C17	N5	C13	C14	-0.5(3)
C9	C8	C7	O2	21.2(2)
C9	C8	C7	N1	139.47(17)
C18A	N6A	C23A	C22A	-179.8(2)
C18A	N6A	C19A	C20A	-179.8(2)
C19A	N6A	C23A	C22A	0.1(3)
C16A	C15A	C21A	C22A	-170.15(19)
C16A	C15A	C21A	C20A	9.3(3)
C16A	C15A	C14A	C13A	0.0(3)
C10	O2	C7	N1	-159.38(16)
C10	O2	C7	C8	-36.36(19)
C18	N6	C19	C20	179.2(2)
C18	N6	C23	C22	-178.8(2)
C9A	C10A	C11A	O4A	176.92(17)
C21	C15	C16	C17	178.92(18)

C21	C15	C14	C13	−179.29(19)
C7	O2	C10	C9	36.95(19)
C7	O2	C10	C11	159.28(17)
C7	N1	C6	N3	3.4(3)
C7	N1	C6	C3	−177.31(19)
C7	N1	C1	C2	178.04(18)
C7	C8	C9	O3	119.2(2)
C7	C8	C9	C10	0.7(2)
C17A	N5A	C13A	C14A	−0.2(3)
C11A	C10A	C9A	O3A	158.29(17)
C11A	C10A	C9A	C8A	−84.9(2)

Table S24 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for n2056.

Atom	*x*	*y*	*z*	U(eq)
H1A	−6981	572	−6950	27
H16	−6642	−1105	−10854	20
H13	−6646	−2289	−13128	22
H13A	−1833	−2887	−6213	28
H14	−6080	−1292	−13278	22
H2B	−11859	−1963	−12338	21
H14A	−1829	−1914	−6610	27
H23A	−2351	−86	−7303	23
H19	−5081	745	−11116	23
H12A	−2818	−3580	−5172	37
H12B	−2471	−3396	−4252	37
H12C	−613	−3508	−4828	37
H10A	−4220	−18	−9443	21
H22A	−2321	−1066	−6938	24
H1	−11977	−2238	−10897	23
H12D	−8728	−2990	−12110	32
H12E	−7407	−3029	−11309	32
H12F	−6411	−3130	−12171	32
H7A	−7457	−796	−8215	23
H23	−5810	612	−13489	24
H2AA	−6772	302	−5505	27
H20A	−1575	−574	−4610	27
H22	−6258	−390	−13389	23
H8A	−14248	−1791	−9776	27
H8B	−14293	−1215	−9212	27

H20	−5474	−259	−10972	22
H17	−7228	−2103	−10765	21
H9	−13272	−2340	−8745	22
H18A	−721	971	−6626	46
H18B	−2439	1100	−5990	46
H18C	−2994	904	−6889	46
H19A	−1666	395	−5023	32
H11C	−10237	−2609	−7924	28
H11D	−9852	−2760	−8851	28
H16A	−2069	−1439	−4263	25
H10	−10130	−1574	−8297	21
H18D	−5402	1590	−11870	40
H18E	−6112	1555	−12790	40
H18F	−3812	1491	−12569	40
H9A	−7586	514	−9561	22
H7	−11218	−939	−9560	22
H8AA	−8505	417	−8214	25
H8AB	−9702	−123	−8615	25
H17A	−2140	−2421	−3916	27
H11A	−4469	1001	−9157	26
H11B	−5324	857	−8280	26
H4B	−10320(30)	736(10)	−10894(16)	7(5)
H2WA	−6900(50)	1800(14)	−9442(19)	36(8)
H4C	−10180(40)	838(12)	−11666(17)	18(7)
H2A	−6920(40)	−1844(14)	−5245(19)	34(8)
H1WA	−9700(50)	1382(13)	−9622(18)	37(8)
H4AA	−7090(50)	−2566(14)	−6090(20)	41(8)
H2WB	−7600(50)	1721(16)	−8610(20)	57(10)
H2	−10720(40)	192(12)	−12615(16)	20(6)
H3WA	−7300(50)	−3876(17)	−5930(20)	56(10)
H4A	−1660(60)	798(17)	−8770(20)	60(11)
H4AB	−7120(40)	−2431(12)	−6968(18)	25(7)
H1WB	−11600(50)	1366(13)	−9897(18)	32(8)
H3WB	−6470(50)	−3532(15)	−5340(20)	43(9)
H4	−6880(50)	−2554(16)	−8700(20)	52(10)
H3A	−8590(50)	−343(16)	−10040(20)	53(10)
H3	−14710(50)	−1772(14)	−7863(19)	43(9)

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