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Chirality Delivery from a Chiral Copper(II) Nucleotide Complex Molecule to Its Supramolecular Architecture.

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1) Materials and Instrumentation

All starting materials and solvents used in this work were of analytical grade and used as purchased from Alfa Aesar Chemical Company without further purification. FT-IR spectrum was measured as KBr pellets on a Nicolet Nexus FT- IR spectrometer in the 4000-400 cm^{-1} region. UV-vis spectrums were obtained from UV-5300PC spectropolarimeter. CD measurements were carried out at 25 °C under a constant flow of nitrogen on a JASCO model J-810 spectropolarimeter. X-ray structure study was carried out in Bruker-AXS CCD X-ray diffraction instrument.

2) Experimental procedure

5ml aqueous solution of Na2GMP·6H2O (20mg, 0.05mmol) mixed with 2ml methanol solution of CuCl2·2H2O (8mg, 0.05mmol) and green color precipitation formed. The acidity of the suspend solution was adjusted by 1M HCl and 1M NaOH untill the solution becomes clear just right (pH = 5~6). The reaction mixture was stirred for about 30 minutes and then filtered. The light green clavate single crystals suitable for x-ray diffraction were obtained by evaporation at room temperature after a few weeks. The yield is 68%. Anal.Calc. for C21 H55 Cu N10 Na O30 P2 :C, 23.62%; H, 5.04%; N,13.21%. Found: C, 23.42%; H, 5.11%; N, 13.01%. IR(KBr,cm-1): 1647 ν(C=O), 1482, 1413 ν(N7-C8), 1074 νa(PO3), 992 νs(PO3).

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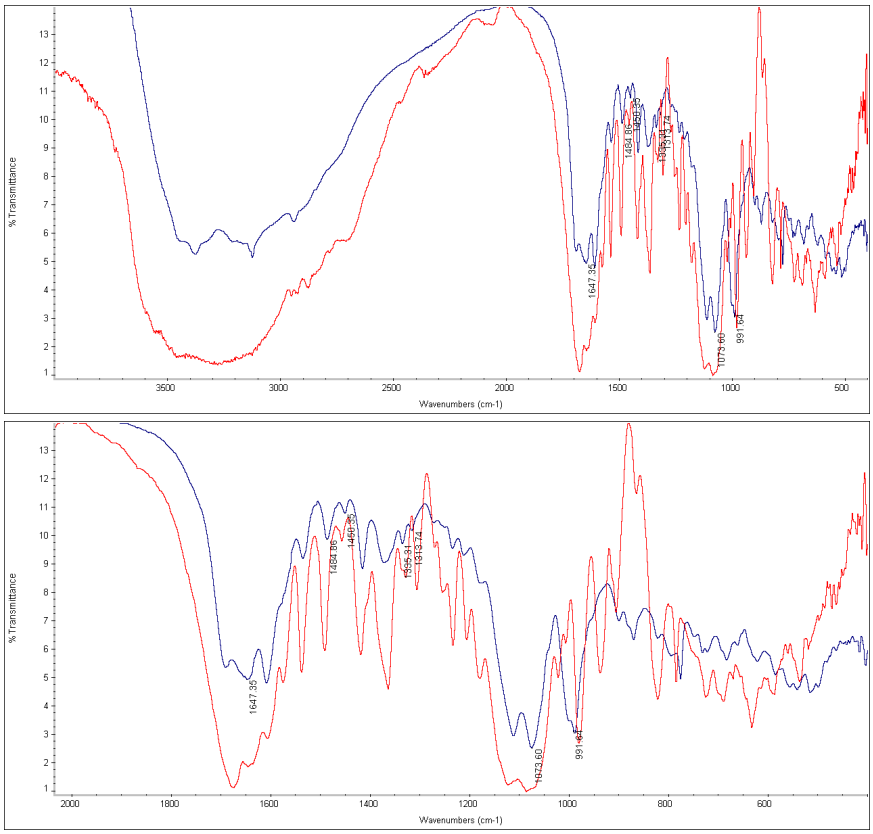

Figure 1S. The FT- IR spectrum of complex 1.(*above:* 4000-400cm^{-1}, *below*: 2000-400cm^{-1}).

3) Summary of Na-O Distances (Å) Used in the Analysis.

Table 1S. Summary of Na-O Distances (Å) Used in the Analysis[a]

CN	***no.***	***min***	***max***	***avg(sig)***	***val***
4	180	1.914	2.558	2.299(74)	0.230
5	310	2.129	2.679	2.368(75)	0.191
6	648	2.130	2.978	2.415(94)	0.168
7	266	2.250	2.915	2.485(111)	0.139
8	384	2.240	2.991	2.540(137)	0.120

CN is the coordination number; ***no.*** is the number of bonds found; ***min*** is the minimum Na-O distance; ***max*** is the maximum Na-O distance; ***avg*** is the average Na-O distance; ***sig*** is the standard deviation of the average value for the given ***CN*** and ***val*** is the valence calculated for the average distance[9].

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4) UV-vis Spectrum.

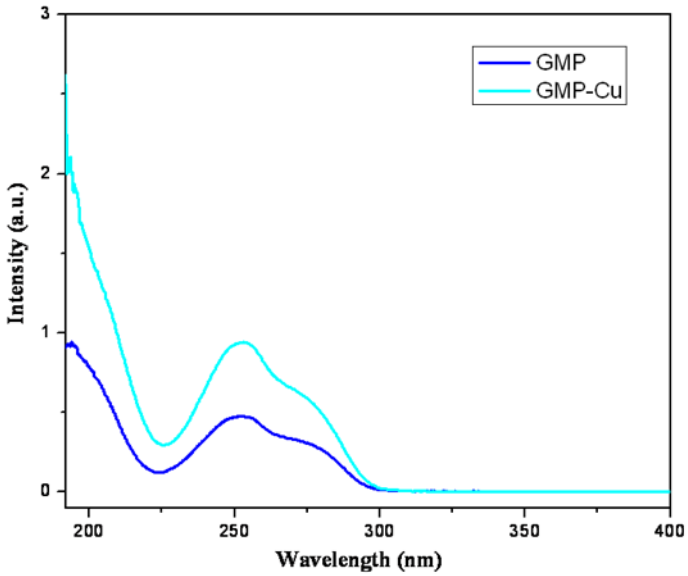

Figure 2S. The UV-vis spectra of complex 1 (0.1mg·ml^{-1} H_2O) and GMP(0.2mg·ml^{-1}) in aqueous solution with the sample cell of 1mm.

λmax of 5'-GMP is 254.4nm which is blue shifted to 254.2nm for 5'-GMP-Cu. The band at 190 ~ 224nm results due to the presence of the sugar moiety.

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5) Hydrogen Bonds of the Supramolecular Interaction.

Table 2S. Hydrogen Bonds of the Supramolecular Interaction

	D-H …A	d(H…A)	d(D…A)	<DHA
Intrastrand Hydrogen Bonds	O3A-H3OA…O6	1.897	2.693	164.0
	N9A-H9NA…O6	1.870	2.735	171.0
	N4B-H4NB…O14	1.850	2.715	169.1
	O11B-H11D…O14	2.061	2.841	160.0
	O21B-H21E…O15	1.910	2.724	170.9
Interstrand Hydrogen Bonds	O20B-H02E…O6	1.930	2.716	161.3
	O22A-H22D…O4	2.290	3.033	151.6
	O12A-H12OA…O16	1.830	2.631	167.0
	O20A-H20OA…O16	2.050	2.839	161.5
	O4A-H4OA…O8	1.825	2.650	174.0

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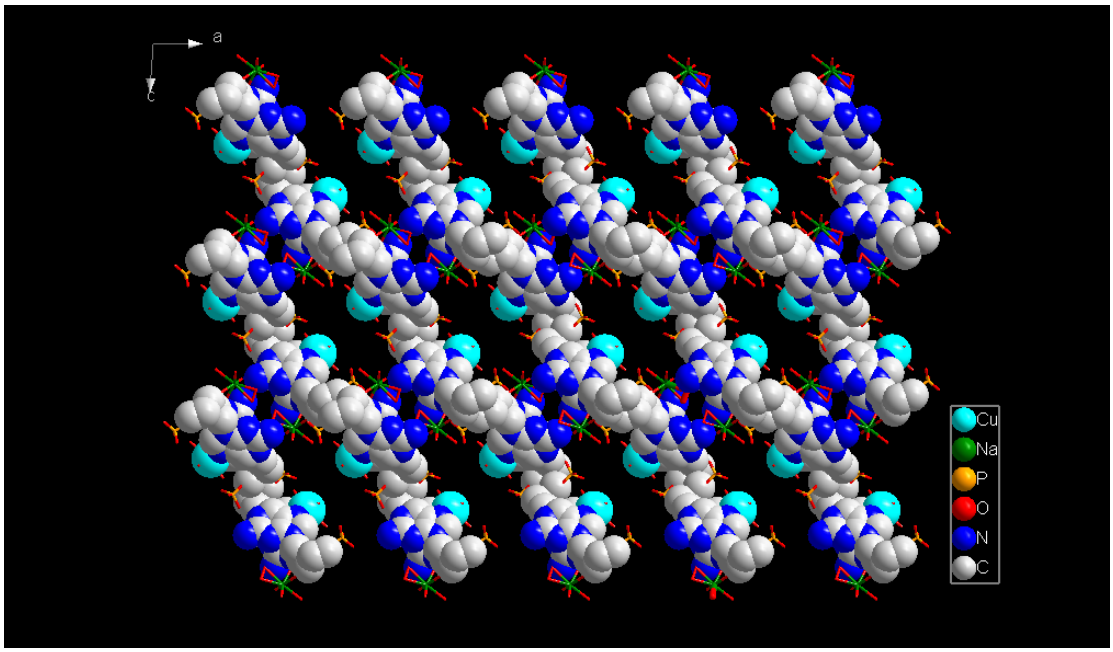

Figure 3S. The model of square grid 2D network architectures of complex **1**.

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6) The Intra- and Intermolecular Hydrogen Bonds of the Purdine Rings.

Table 3S. The Intra- and Intermolecular Hydrogen Bonds of the Purdine Rings

D-H …A	d(H…A)	d(D…A)	<DHA
N9-H9N…O6 [-x+2, y+1/2, -z+1]	1.870	2.735	171.0
N4-H4N…O14 [-x+1, y-1/2, -z]	1.850	2.716	169.1
N10-H0A…O20 [-x+2, y-1/2, -z]	2.220	3.002	165.0
N10-H0B…O28 [x+1, y+1, z]	2.200	2.956	154.6
O19-H19A…O10	1.890	2.687	161.3
O24-H24B…O2	1.870	2.717	175.8

7) The Description about Water Clusters.

Structural data of H-bonding in water clusters are very important for correctly describing the association of water molecules in different environments [1]. It possesses strongly polar hydrogen bonds which are responsible for a set of anomalous physical and chemical properties [2]. Novel motifs of water clusters as well as their main classification are reported substantially in resent years[3-7]. The formula of complex **1** clearly shows that each molecule contains six solvent water molecules. Two of them are disorder (O27, O29, O30). The occupation ratio of O30 and O30' is 0.5. All these water molecules connected to each other by hydrogen bonds forming water clusters $(H_2O)_6$ which include a coordinated water O17. Guest water molecule

O24 is an exception, because it bonded to the host molecule by intramolecular hydrogen bonds. The positions of O27 and O27' (O29 and O29') are practically the same with a tiny displacement and the position of O27 (O29) is more reasonable, which can be demonstrated by the date of hydrogen bonds (Table 4S.). O17 acted as a bridge which connected with guest water molecules O29 (O29') and O30 (O30') forming a catenulate water hexamers with a branch formed with O27. These discrete water hexamers are also extend end-to-head in the 1D chiral supramolecular channels and the aggregates are D6[4].

The phosphate oxygen atoms（O9，O15, O8A, O7B）and the coordinated water molecules (O21c) of the host molecule present in the inorganic-organic coordination complex can potentially act as hydrogen-bond acceptors, which would interacted with guest water clusters. The water-clusters connected with these O atoms of the host molecules present a ring appearance when viewed from b axis(fig.6S). The length and angle of the hydrogen bonds are listed in table 4S. The water hexamer is characterized by rather regular O-O bonds which is comparable to 2.758Å obtained from the ab initio calculations[8] and two lengthy ones. For the latter bonds, R(O30'…O26) = 3.190 and R(O30'…O18A)= 3.296 which implies that the H-bond pattern there is relatively weak. The confine of these values is larger than the range 2.77–2.84 Å [9] observed in the ice II phase. Bulk water also shows a short-range order in the O···O X-ray diffraction radial distribution curve of 2.85Å. The difference of O···O distance between the water molecule might arises from its different host environment. What's more, this catenulate water hexamer is higher-energy and less stable comparing with the cyclic water hexamers, but it can be stablized by the host framework of complex **1**.

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Table 4S. The Length and Angles of Hydrogen Bonds Related the Water-Clusters.

	D-H …A	d(D-H)	d(H…A)	<DHA	d(D…A)
(1)	O29-H29C…O25	0.850	1.890	175.4	2.739
	O29'-H29H…O25	0.850	2.010	166.3	2.841
	O30'-H30F…O26	0.850	2.350	169.7	3.190
	O17-H17A…O29	0.820	1.810	177.8	2.628
	O17-H17A…O29'	0.820	2.210	150.9	2.950
	O17-H17B…O30	0.850	1.950	160.7	2.763
	O17-H17B…O30'	0.850	1.970	159.7	2.785

	O25-H25C…O9	0.850	2.150	172.8	2.999
	O25-H25D…O15	0.850	1.830	172.3	2.680
	O26-H26C…O21C	0.850	1.960	177.2	2.808
	O26-H26D…O7 B	0.850	1.910	177.2	2.758
	O27-H27C…O8 A	0.850	1.970	170.0	2.811
(2)	O27-H27D…O15	0.850	2.000	171.1	2.847
	O27'-H27G…O15	0.850	1.880	167.7	2.716
	O27'-H27H…O8 A	0.850	2.000	167.5	2.835
	O29-H29B…O7A	0.850	1.860	147.0	2.613
	O29'-H29E…O7A	0.840	1.850	167.1	2.674
	O30'-H30E…O18	0.850	2.460	170.4	3.296

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8) Crystal Data of Complex **1**.

Table 5S. Crystal data and structure refinement for complex **1**

Empirical formula	C_{21} $H_{53.5}$ Cu N_{10} Na O_{30} P_2
Formula weight	1074.71
Temperature	103(2) K
Wavelength	0.71073 Å

Crystal system, space group	monoclinic, $P2_1$
Unit cell dimensions	a = 14.842(3) Å alpha = 90°
	b = 8.6829(15) Å beta = 93.973(3)°
	c = 16.272(3) Å gamma = 90°
Volume	2091.9(7) $Å^3$
Z, Calculated density	2, 1.706 $mg \cdot m^{-3}$
Absorption coefficient	0.723 mm^{-1}
F(000)	1119
Crystal size	0.40 x0.13 x0.04 mm^3
Theta range for data collection	3.03° to 27.48°.
Limiting indices	$-19 \le h \le 13$, $-11 \le k \le 11$, $-21 \le l \le 21$
Reflections collected / unique	16717 / 9366
R_{int}	0.0275
Completeness to theta = 27.48	99.7 %
Absorption correction	Empirical
Max. and min. transmission	0.9717 and 0.7608
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9366 / 7 / 635

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Goodness-of-fit on F^2	0.995
Final R indices [I>2σ(I)]	R1 = 0.0466, wR2 = 0.1159
R indices (all data)	R1 = 0.0578, wR2 = 0.1228
Absolute structure parameter	-0.008(11)
Largest diff. peak and hole	1.836 and -0.697e. $Å^{-3}$

Table 6S. Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters (A^2 x 10^3) for Complex **1**. U(eq) is defined as One Third of the Trace of the Orthogonalized Uij tensor.

	x	y	z	U(eq)
Cu(1)	6547(1)	4055(1)	3355(1)	15(1)
Na(1)	7835(1)	7581(2)	-1423(1)	22(1)
P(1)	8263(1)	364(1)	5652(1)	13(1)
P(2)	3932(1)	7824(1)	1592(1)	12(1)
C(1)	7974(3)	1745(4)	3167(2)	16(1)
C(2)	7482(3)	2390(4)	1943(2)	13(1)
C(3)	6987(3)	2891(4)	1213(2)	14(1)
C(4)	8191(3)	1628(4)	504(2)	16(1)
C(5)	8259(3)	1550(4)	1856(2)	12(1)
C(6)	9398(3)	293(4)	2871(2)	14(1)
C(7)	10070(3)	1212(4)	3427(2)	15(1)
C(8)	10556(3)	-75(5)	3926(2)	16(1)
C(9)	9824(3)	-1251(4)	4018(2)	14(1)
C(10)	9351(3)	-1214(4)	4810(2)	17(1)
C(11)	6759(3)	6483(4)	2143(2)	15(1)
C(12)	8200(3)	6746(4)	1933(2)	13(1)
C(13)	9698(3)	6624(4)	2013(2)	14(1)
C(14)	8897(3)	5338(4)	3081(2)	14(1)
C(15)	8097(2)	5843(4)	2624(2)	11(1)

C(16)	7133(2)	8023(4)	896(2)	12(1)
C(17)	6611(2)	7109(4)	217(2)	13(1)
C(18)	6142(3)	8403(4)	-276(2)	14(1)
C(19)	5896(2)	9526(4)	398(2)	12(1)
C(20)	4953(2)	9409(4)	695(2)	16(1)
C(23)	592(5)	10006(10)	-86(5)	74(2)

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N(1)	7313(2)	2497(4)	2774(2)	14(1)
N(2)	8570(2)	1138(4)	2646(2)	14(1)
N(3)	8647(2)	1150(4)	1164(2)	16(1)
N(4)	7416(2)	2489(4)	510(2)	15(1)
N(5)	8472(2)	1315(4)	-251(2)	20(1)
N(6)	7182(2)	5691(4)	2739(2)	14(1)
N(7)	7346(2)	7157(4)	1643(2)	13(1)
N(8)	8963(2)	7161(4)	1589(2)	14(1)
N(9)	9671(2)	5736(4)	2713(2)	12(1)
N(10)	10507(2)	6987(4)	1764(2)	19(1)
O(1)	9165(2)	-1022(3)	3326(1)	15(1)
O(2)	6255(2)	3600(3)	1129(2)	21(1)
O(3)	10625(2)	2106(3)	2941(2)	20(1)
O(4)	11263(2)	-647(3)	3455(2)	21(1)

O(5)	8982(2)	277(3)	4944(2)	17(1)
O(6)	8755(2)	-177(3)	6455(2)	15(1)
O(7)	7493(2)	-716(3)	5395(2)	22(1)
O(8)	8000(2)	2042(3)	5673(2)	18(1)
O(9)	6564(2)	9279(3)	1082(2)	14(1)
O(10)	8964(2)	4634(3)	3745(2)	19(1)
O(11)	7234(2)	6232(3)	-214(2)	16(1)
O(12)	6790(2)	9064(4)	-760(2)	17(1)
O(13)	4807(2)	7921(3)	1048(2)	14(1)
O(14)	3131(2)	8397(3)	1043(2)	14(1)
O(15)	4127(2)	8864(3)	2330(2)	17(1)
O(16)	3879(2)	6143(3)	1809(2)	17(1)
O(17)	5767(2)	5652(4)	3791(2)	26(1)
O(18)	5891(3)	2385(4)	3862(2)	37(1)
O(19)	7469(2)	4308(3)	4570(2)	22(1)
O(20)	7853(2)	10024(4)	-2153(2)	20(1)
O(21)	6469(2)	6832(3)	-2326(2)	26(1)
O(22)	8288(2)	5035(4)	-1701(2)	31(1)
O(23)	9367(4)	8048(7)	-1039(4)	40(1)
O(24)	5054(2)	3804(4)	2310(2)	28(1)
O(25)	5816(2)	9839(4)	2721(2)	37(1)
O(26)	7246(3)	6495(5)	6160(3)	53(1)

O(27)	3770(10)	7440(20)	3849(9)	49(2)
O(28)	136(4)	9411(6)	510(4)	81(2)
O(29)	6371(4)	8424(6)	4173(3)	39(2)
O(30)	4994(12)	8807(19)	5059(7)	129(7)
O(23')	9157(6)	7631(12)	-322(7)	40(1)

O(27')	3627(5)	8433(10)	3888(4)	49(2)
O(29')	7025(13)	8287(16)	3870(9)	40(6)
O(30')	4531(9)	9807(17)	4599(7)	90(4)

Table 7S. Bond Lengths [A] and Angles [deg] for Complex 1.

Cu(1)-O(18)	1.960(3)
Cu(1)-O(17)	1.969(3)
Cu(1)-N(6)	2.010(3)
Cu(1)-N(1)	2.041(3)
Cu(1)-O(19)	2.335(3)
Na(1)-O(12)	2.338(3)
Na(1)-O(23)	2.351(6)

Na(1)-O(22)	2.363(4)
Na(1)-O(20)	2.432(3)
Na(1)-O(21)	2.506(3)
Na(1)-O(11)	2.506(3)
Na(1)-O(23')	2.564(10)
P(1)-O(8)	1.510(3)
P(1)-O(7)	1.515(3)
P(1)-O(6)	1.525(3)
P(1)-O(5)	1.625(3)
P(2)-O(16)	1.505(3)
P(2)-O(15)	1.515(3)
P(2)-O(14)	1.520(3)
P(2)-O(13)	1.625(3)
C(1)-N(1)	1.308(5)
C(1)-N(2)	1.372(5)
C(1)-H(1)	0.9500
C(2)-C(5)	1.379(5)
C(2)-N(1)	1.396(5)
C(2)-C(3)	1.421(5)
C(3)-O(2)	1.249(5)
C(3)-N(4)	1.391(5)
C(4)-N(3)	1.297(5)

C(4)-N(5)	1.353(5)
C(4)-N(4)	1.373(5)
C(5)-N(3)	1.346(5)

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C(5)-N(2)	1.381(5)
C(6)-O(1)	1.417(5)
C(6)-N(2)	1.457(5)
C(6)-C(7)	1.524(5)
C(6)-H(6)	1.0000
C(7)-O(3)	1.413(5)
C(7)-C(8)	1.533(5)
C(7)-H(7)	1.0000
C(8)-O(4)	1.431(5)
C(8)-C(9)	1.505(5)
C(8)-H(8)	1.0000
C(9)-O(1)	1.453(4)
C(9)-C(10)	1.511(5)
C(9)-H(9)	1.0000
C(10)-O(5)	1.429(4)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900

C(11)-N(6)	1.313(5)
C(11)-N(7)	1.364(5)
C(11)-H(11)	0.9500
C(12)-N(8)	1.347(5)
C(12)-N(7)	1.370(5)
C(12)-C(15)	1.388(5)
C(13)-N(10)	1.333(5)
C(13)-N(8)	1.334(5)
C(13)-N(9)	1.378(5)
C(14)-O(10)	1.240(5)
C(14)-N(9)	1.376(5)
C(14)-C(15)	1.426(5)
C(15)-N(6)	1.390(5)
C(16)-O(9)	1.425(4)
C(16)-N(7)	1.445(4)
C(16)-C(17)	1.527(5)
C(16)-H(16)	1.0000
C(17)-O(11)	1.420(4)
C(17)-C(18)	1.521(5)
C(17)-H(17)	1.0000
C(18)-O(12)	1.407(4)
C(18)-C(19)	1.531(5)

C(18)-H(18)	1.0000
C(19)-O(9)	1.454(4)

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C(19)-C(20)	1.514(5)
C(19)-H(19)	1.0000
C(20)-O(13)	1.437(4)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(23)-O(28)	1.325(8)
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
N(4)-H(4N)	0.8800
N(5)-H(5A)	0.8095
N(5)-H(5B)	0.8095
N(9)-H(9N)	0.870(19)
N(10)-H(0A)	0.8055
N(10)-H(0B)	0.8102
O(3)-H(3O)	0.819(10)
O(4)-H(4O)	0.828(10)
O(11)-H(11O)	0.814(10)

O(12)-H(12O)	0.81(2)
O(17)-H(17A)	0.8197
O(17)-H(17B)	0.8490
O(18)-H(18A)	0.8238
O(18)-H(18B)	0.8030
O(19)-H(19A)	0.8259
O(19)-H(19B)	0.8219
O(20)-H(02A)	0.8215
O(20)-H(02B)	0.8191
O(21)-H(21A)	0.8201
O(21)-H(21B)	0.8484
O(22)-H(22A)	0.8147
O(22)-H(22B)	0.8171
O(23)-H(23F)	0.8477
O(23)-H(23G)	0.8418
O(24)-H(24A)	0.8389
O(24)-H(24B)	0.8437
O(25)-H(25C)	0.8499
O(25)-H(25D)	0.8501
O(26)-H(26C)	0.8505
O(26)-H(26D)	0.8500
O(27)-H(27C)	0.8503

O(27)-H(27D)	0.8500

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O(28)-H(28O)	0.8400
O(29)-H(29B)	0.8501
O(29)-H(29C)	0.8496
O(30)-H(30C)	0.8499
O(30)-H(30D)	0.8500
O(23')-H(23E)	0.8501
O(27')-H(27G)	0.8502
O(27')-H(27H)	0.8497
O(29')-H(29E)	0.8438
O(29')-H(29H)	0.8500
O(30')-H(30E)	0.8499
O(30')-H(30F)	0.8501

O(18)-Cu(1)-O(17)	92.75(14)
O(18)-Cu(1)-N(6)	174.97(14)
O(17)-Cu(1)-N(6)	89.40(14)
O(18)-Cu(1)-N(1)	90.78(15)
O(17)-Cu(1)-N(1)	173.48(14)
N(6)-Cu(1)-N(1)	86.66(12)

O(18)-Cu(1)-O(19)	89.56(13)
O(17)-Cu(1)-O(19)	87.35(12)
N(6)-Cu(1)-O(19)	95.08(12)
N(1)-Cu(1)-O(19)	98.16(12)
O(18)-Cu(1)-O(24)	78.22(13)
O(17)-Cu(1)-O(24)	78.85(12)
N(6)-Cu(1)-O(24)	97.76(11)
N(1)-Cu(1)-O(24)	96.53(12)
O(19)-Cu(1)-O(24)	160.99(9)
O(12)-Na(1)-O(23)	116.29(17)
O(12)-Na(1)-O(22)	144.13(13)
O(23)-Na(1)-O(22)	85.97(18)
O(12)-Na(1)-O(20)	76.99(11)
O(23)-Na(1)-O(20)	86.35(18)
O(22)-Na(1)-O(20)	135.21(13)
O(12)-Na(1)-O(21)	82.95(11)
O(23)-Na(1)-O(21)	158.30(17)
O(22)-Na(1)-O(21)	82.77(12)
O(20)-Na(1)-O(21)	88.64(11)
O(12)-Na(1)-O(11)	67.12(10)
O(23)-Na(1)-O(11)	105.18(17)
O(22)-Na(1)-O(11)	80.47(11)

O(20)-Na(1)-O(11)	143.84(11)
O(21)-Na(1)-O(11)	91.21(11)
O(12)-Na(1)-O(23')	99.7(2)
O(23)-Na(1)-O(23')	29.8(3)
O(22)-Na(1)-O(23')	86.3(3)
O(20)-Na(1)-O(23')	107.0(3)
O(21)-Na(1)-O(23')	164.3(3)
O(11)-Na(1)-O(23')	75.9(2)
O(12)-Na(1)-H(23G)	107.8
O(23)-Na(1)-H(23G)	19.6
O(22)-Na(1)-H(23G)	101.2
O(20)-Na(1)-H(23G)	66.8
O(21)-Na(1)-H(23G)	149.1
O(11)-Na(1)-H(23G)	119.7
O(23')-Na(1)-H(23G)	44.6
O(8)-P(1)-O(7)	114.34(17)
O(8)-P(1)-O(6)	112.79(16)
O(7)-P(1)-O(6)	110.71(16)
O(8)-P(1)-O(5)	104.11(15)
O(7)-P(1)-O(5)	107.22(16)
O(6)-P(1)-O(5)	107.04(15)
O(16)-P(2)-O(15)	113.73(16)

O(16)-P(2)-O(14)	113.85(16)
O(15)-P(2)-O(14)	111.73(15)
O(16)-P(2)-O(13)	103.59(15)
O(15)-P(2)-O(13)	106.54(15)
O(14)-P(2)-O(13)	106.52(15)
N(1)-C(1)-N(2)	112.5(3)
N(1)-C(1)-H(1)	123.7
N(2)-C(1)-H(1)	123.7
C(5)-C(2)-N(1)	110.0(3)
C(5)-C(2)-C(3)	117.6(3)
N(1)-C(2)-C(3)	132.2(3)
O(2)-C(3)-N(4)	118.5(3)
O(2)-C(3)-C(2)	129.7(4)
N(4)-C(3)-C(2)	111.8(3)
N(3)-C(4)-N(5)	120.8(4)
N(3)-C(4)-N(4)	124.0(3)
N(5)-C(4)-N(4)	115.3(3)
N(3)-C(5)-C(2)	129.1(3)
N(3)-C(5)-N(2)	125.2(3)
C(2)-C(5)-N(2)	105.6(3)
O(1)-C(6)-N(2)	107.8(3)
O(1)-C(6)-C(7)	106.6(3)

N(2)-C(6)-C(7)	113.1(3)
O(1)-C(6)-H(6)	109.8
N(2)-C(6)-H(6)	109.8
C(7)-C(6)-H(6)	109.8
O(3)-C(7)-C(6)	109.8(3)
O(3)-C(7)-C(8)	115.2(3)
C(6)-C(7)-C(8)	101.4(3)
O(3)-C(7)-H(7)	110.1
C(6)-C(7)-H(7)	110.1
C(8)-C(7)-H(7)	110.1
O(4)-C(8)-C(9)	112.3(3)
O(4)-C(8)-C(7)	107.8(3)
C(9)-C(8)-C(7)	103.3(3)
O(4)-C(8)-H(8)	111.1
C(9)-C(8)-H(8)	111.1
C(7)-C(8)-H(8)	111.1
O(1)-C(9)-C(8)	106.4(3)
O(1)-C(9)-C(10)	109.3(3)
C(8)-C(9)-C(10)	116.9(3)
O(1)-C(9)-H(9)	108.0
C(8)-C(9)-H(9)	108.0
C(10)-C(9)-H(9)	108.0

O(5)-C(10)-C(9)	110.8(3)
O(5)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10A)	109.5
O(5)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	108.1
N(6)-C(11)-N(7)	112.0(3)
N(6)-C(11)-H(11)	124.0
N(7)-C(11)-H(11)	124.0
N(8)-C(12)-N(7)	124.9(3)
N(8)-C(12)-C(15)	129.1(3)
N(7)-C(12)-C(15)	106.0(3)
N(10)-C(13)-N(8)	118.8(3)
N(10)-C(13)-N(9)	117.5(3)
N(8)-C(13)-N(9)	123.7(3)
O(10)-C(14)-N(9)	119.0(3)
O(10)-C(14)-C(15)	128.3(4)
N(9)-C(14)-C(15)	112.8(3)
C(12)-C(15)-N(6)	109.0(3)
C(12)-C(15)-C(14)	117.5(3)
N(6)-C(15)-C(14)	133.4(3)
O(9)-C(16)-N(7)	108.5(3)

O(9)-C(16)-C(17)	105.8(3)
N(7)-C(16)-C(17)	114.1(3)
O(9)-C(16)-H(16)	109.4
N(7)-C(16)-H(16)	109.4
C(17)-C(16)-H(16)	109.4
O(11)-C(17)-C(18)	115.2(3)
O(11)-C(17)-C(16)	108.7(3)
C(18)-C(17)-C(16)	100.9(3)
O(11)-C(17)-H(17)	110.6
C(18)-C(17)-H(17)	110.6
C(16)-C(17)-H(17)	110.6
O(12)-C(18)-C(17)	106.9(3)
O(12)-C(18)-C(19)	110.3(3)
C(17)-C(18)-C(19)	102.5(3)
O(12)-C(18)-H(18)	112.2
C(17)-C(18)-H(18)	112.2
C(19)-C(18)-H(18)	112.2
O(9)-C(19)-C(20)	110.0(3)
O(9)-C(19)-C(18)	105.7(3)
C(20)-C(19)-C(18)	117.2(3)
O(9)-C(19)-H(19)	107.9
C(20)-C(19)-H(19)	107.9

C(18)-C(19)-H(19)	107.9
O(13)-C(20)-C(19)	110.9(3)
O(13)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20A)	109.5
O(13)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	108.1
O(28)-C(23)-H(23A)	109.5
O(28)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
O(28)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(1)-N(1)-C(2)	105.1(3)
C(1)-N(1)-Cu(1)	121.8(3)
C(2)-N(1)-Cu(1)	129.6(3)
C(1)-N(2)-C(5)	106.7(3)
C(1)-N(2)-C(6)	127.3(3)
C(5)-N(2)-C(6)	125.9(3)
C(4)-N(3)-C(5)	112.4(3)
C(4)-N(4)-C(3)	125.0(3)
C(4)-N(4)-H(4N)	117.5

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C(3)-N(4)-H(4N)	117.5
C(4)-N(5)-H(5A)	120.0
C(4)-N(5)-H(5B)	120.0
H(5A)-N(5)-H(5B)	120.0
C(11)-N(6)-C(15)	105.8(3)
C(11)-N(6)-Cu(1)	121.5(3)
C(15)-N(6)-Cu(1)	129.1(3)
C(11)-N(7)-C(12)	107.2(3)
C(11)-N(7)-C(16)	127.8(3)
C(12)-N(7)-C(16)	124.7(3)
C(13)-N(8)-C(12)	111.9(3)
C(14)-N(9)-C(13)	124.9(3)
C(14)-N(9)-H(9N)	109(3)
C(13)-N(9)-H(9N)	126(3)
C(13)-N(10)-H(0A)	119.7
C(13)-N(10)-H(0B)	123.1
H(0A)-N(10)-H(0B)	117.2
C(6)-O(1)-C(9)	109.8(3)
C(7)-O(3)-H(3O)	108(4)
C(8)-O(4)-H(4O)	107(4)

C(10)-O(5)-P(1)	115.3(2)
C(16)-O(9)-C(19)	109.5(3)
C(17)-O(11)-Na(1)	114.6(2)
C(17)-O(11)-H(11O)	115(3)
Na(1)-O(11)-H(11O)	94(3)
C(18)-O(12)-Na(1)	122.3(3)
C(18)-O(12)-H(12O)	120(5)
Na(1)-O(12)-H(12O)	107(5)
C(20)-O(13)-P(2)	114.4(2)
Cu(1)-O(17)-H(17A)	121.2
Cu(1)-O(17)-H(17B)	104.1
H(17A)-O(17)-H(17B)	109.5
Cu(1)-O(18)-H(18A)	111.0
Cu(1)-O(18)-H(18B)	117.3
H(18A)-O(18)-H(18B)	109.4
Cu(1)-O(19)-H(19A)	103.6
Cu(1)-O(19)-H(19B)	118.4
H(19A)-O(19)-H(19B)	107.8
Na(1)-O(20)-H(02A)	113.7
Na(1)-O(20)-H(02B)	111.4
H(02A)-O(20)-H(02B)	110.4

Na(1)-O(21)-H(21A)	114.9
Na(1)-O(21)-H(21B)	121.0
H(21A)-O(21)-H(21B)	108.3
Na(1)-O(22)-H(22A)	116.5
Na(1)-O(22)-H(22B)	124.7
H(22A)-O(22)-H(22B)	111.0
Na(1)-O(23)-H(23F)	124.9
Na(1)-O(23)-H(23G)	50.1
H(23F)-O(23)-H(23G)	109.6
Cu(1)-O(24)-H(24A)	125.4
Cu(1)-O(24)-H(24B)	84.2
H(24A)-O(24)-H(24B)	107.3
H(25C)-O(25)-H(25D)	108.2
H(26C)-O(26)-H(26D)	108.5
H(27C)-O(27)-H(27D)	108.6
C(23)-O(28)-H(28O)	109.5
H(29B)-O(29)-H(29C)	111.0
H(30C)-O(30)-H(30D)	97.8
Na(1)-O(23')-H(23E)	143.7
H(23F)-O(23')-H(23E)	81.9
H(27G)-O(27')-H(27H)	108.7

H(29E)-O(29')-H(29H)	111.1
H(30E)-O(30')-H(30F)	108.0

Symmetry transformations used to generate equivalent atoms.

Table 8S. Anisotropic Displacement Parameters (A^2 x 10^3) for Complex **1**.
The Anisotropic Displacement Factor Exponent Takes the Form:
$-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
Cu(1)	18(1)	13(1)	15(1)	2(1)	3(1)	-1(1)
Na(1)	22(1)	20(1)	25(1)	-1(1)	6(1)	1(1)
P(1)	17(1)	14(1)	9(1)	0(1)	-1(1)	-3(1)
P(2)	13(1)	13(1)	10(1)	-2(1)	1(1)	-2(1)
C(1)	21(2)	12(2)	15(2)	0(2)	0(2)	-2(2)
C(2)	16(2)	10(2)	14(2)	1(1)	2(1)	-2(1)
C(3)	14(2)	10(2)	17(2)	1(2)	0(1)	-2(2)
C(4)	17(2)	13(2)	17(2)	2(2)	3(2)	-3(2)
C(5)	16(2)	9(2)	11(2)	1(1)	-3(2)	0(1)
C(6)	22(2)	11(2)	10(2)	-1(2)	0(1)	4(2)
C(7)	20(2)	12(2)	14(2)	2(2)	-2(2)	2(2)
C(8)	14(2)	20(2)	12(2)	-3(2)	-3(1)	3(2)
C(9)	23(2)	11(2)	8(2)	-1(1)	-3(1)	4(1)
C(10)	27(2)	10(2)	14(2)	0(1)	2(2)	4(2)
C(11)	17(2)	10(2)	18(2)	1(2)	1(2)	1(2)

C(12)	14(2)	12(2)	14(2)	0(2)	-3(2)	0(2)
C(13)	15(2)	14(2)	13(2)	-2(2)	-1(1)	-1(2)
C(14)	20(2)	9(2)	15(2)	-4(1)	1(2)	2(2)
C(15)	14(2)	9(2)	11(2)	0(1)	-1(1)	-1(1)
C(16)	11(2)	11(2)	13(2)	3(1)	-1(1)	-1(1)
C(17)	11(2)	15(2)	11(2)	-1(1)	-1(1)	-1(1)
C(18)	14(2)	16(2)	11(2)	2(2)	-1(1)	-4(2)
C(19)	9(2)	14(2)	12(2)	3(1)	0(1)	0(1)
C(20)	14(2)	18(2)	15(2)	2(2)	3(1)	1(1)
C(23)	60(5)	71(5)	92(6)	-11(5)	11(4)	-24(4)
N(1)	18(2)	11(2)	13(2)	0(1)	2(1)	-1(1)
N(2)	17(2)	15(2)	10(1)	1(1)	-2(1)	1(1)
N(3)	16(2)	17(2)	15(2)	-1(1)	-1(1)	1(1)
N(4)	15(2)	18(2)	11(1)	4(1)	-2(1)	0(1)
N(5)	24(2)	24(2)	12(2)	5(1)	2(1)	3(2)
N(6)	18(2)	10(2)	13(2)	4(1)	-3(1)	-4(1)
N(7)	12(1)	13(2)	13(2)	2(1)	-2(1)	-2(1)

N(8)	16(2)	14(2)	13(2)	2(1)	0(1)	1(1)
N(9)	12(1)	11(2)	12(2)	2(1)	-5(1)	2(1)
N(10)	11(2)	23(2)	23(2)	8(2)	2(1)	2(1)

O(1)	22(1)	11(1)	12(1)	1(1)	-5(1)	0(1)
O(2)	16(1)	27(2)	20(1)	2(1)	-2(1)	5(1)
O(3)	25(2)	13(1)	23(2)	-2(1)	5(1)	-3(1)
O(4)	25(2)	19(2)	18(1)	3(1)	4(1)	9(1)
O(5)	28(2)	10(1)	13(1)	1(1)	4(1)	2(1)
O(6)	16(1)	18(1)	10(1)	1(1)	-1(1)	1(1)
O(7)	25(1)	24(2)	17(1)	2(1)	-6(1)	-9(1)
O(8)	21(1)	18(1)	16(1)	1(1)	0(1)	2(1)
O(9)	16(1)	11(1)	13(1)	-1(1)	-5(1)	3(1)
O(10)	20(1)	21(1)	17(1)	9(1)	-5(1)	1(1)
O(11)	14(1)	14(1)	18(1)	-3(1)	3(1)	1(1)
O(12)	17(1)	19(1)	15(1)	8(1)	5(1)	4(1)
O(13)	15(1)	12(1)	15(1)	4(1)	4(1)	0(1)
O(14)	13(1)	19(1)	10(1)	-2(1)	0(1)	0(1)
O(15)	20(1)	17(1)	12(1)	0(1)	-2(1)	-1(1)
O(16)	22(1)	13(1)	16(1)	0(1)	3(1)	-2(1)
O(17)	24(2)	24(2)	30(2)	3(1)	9(1)	0(1)
O(18)	56(2)	30(2)	26(2)	3(2)	10(2)	-14(2)
O(19)	23(1)	25(2)	18(1)	3(1)	2(1)	-3(1)
O(20)	17(1)	30(2)	15(1)	-1(1)	8(1)	2(1)
O(21)	26(2)	17(2)	35(2)	1(1)	3(1)	-2(1)
O(22)	27(2)	21(2)	46(2)	-6(2)	23(2)	-3(1)

O(23)	25(2)	49(3)	44(3)	-7(3)	0(2)	3(2)
O(24)	36(2)	25(2)	24(2)	3(1)	6(1)	6(1)
O(25)	36(2)	41(2)	32(2)	-4(2)	-6(2)	-13(2)
O(26)	68(3)	42(2)	53(2)	8(2)	25(2)	-2(2)
O(27)	46(3)	65(4)	39(3)	-14(4)	19(2)	-16(4)
O(28)	83(4)	69(4)	94(4)	3(3)	29(3)	12(3)
O(29)	49(4)	37(3)	27(3)	10(2)	-16(3)	-18(3)
O(30)	201(14)	151(13)	46(5)	46(7)	86(8)	109(12)
O(23')	25(2)	49(3)	44(3)	-7(3)	0(2)	3(2)
O(27')	46(3)	65(4)	39(3)	-14(4)	19(2)	-16(4)
O(29')	60(13)	34(8)	24(7)	-19(6)	-15(8)	4(7)
O(30')	93(9)	118(10)	66(7)	1(7)	47(7)	5(8)

Table 9S. Hydrogen Coordinates (x 10^4) and Isotropic Displacement Parameters (A^2 x 10^3) for Complex **1**.

	x	y	z	U(eq)

H(1)	8035	1632	3749	19
H(6)	9688	-33	2363	17
H(7)	9740	1894	3800	18
H(8)	10802	310	4476	19
H(9)	10096	-2297	3963	17
H(10A)	8860	-1988	4784	20
H(10B)	9785	-1485	5277	20
H(11)	6121	6577	2068	18
H(16)	7703	8428	684	14
H(17)	6157	6420	456	15
H(18)	5598	8033	-617	17
H(19)	5976	10596	188	14
H(20A)	4870	10217	1113	19
H(20B)	4503	9585	227	19
H(23A)	896	9179	-369	89
H(23B)	1042	10735	150	89
H(23C)	173	10544	-481	89
H(9N)	10140(20)	5400(50)	3010(20)	9(10)
H(3O)	10730(40)	2920(30)	3190(30)	31(14)
H(4O)	11470(30)	-1420(40)	3700(30)	36(16)
H(11O)	7020(30)	5530(40)	-490(20)	21(13)

H(12O)	6650(50)	9790(60)	-1060(40)	80(20)
H(4N)	7171	2812	33	18
H(5A)	8930(19)	820(20)	-295(3)	24
H(5B)	8182(12)	1619(13)	-659(17)	24
H(0A)	10949	6538	1954	23
H(0B)	10580	7616	1407	23
H(17A)	5959	6519	3898	31
H(17B)	5579	5249	4222	31
H(18A)	5768	1691	3528	44
H(18B)	5447	2614	4089	44
H(19A)	7968	4529	4407	26
H(19B)	7536	3556	4875	26
H(02A)	8009	9949	-2626	24
H(02B)	7366	10466	-2150	24

H(21A)	6349	5910	-2326	31
H(21B)	5980	7333	-2315	31
H(22A)	7938	4352	-1593	37
H(22B)	8586	4785	-2083	37
H(23F)	9563	8497	-599	47
H(23G)	8983	8612	-1297	47

H(24A)	4685	4515	2192	34
H(24B)	5427	3790	1942	34
H(25C)	6073	9709	2275	44
H(25D)	5270	9549	2642	44
H(26C)	7013	6631	6617	64
H(26D)	7317	7370	5939	64
H(27C)	3213	7362	3936	59
H(27D)	3814	7865	3383	59
H(28O)	-10	10116	828	97
H(29B)	6838	8843	4408	46
H(29C)	6227	8851	3712	46
H(30C)	5423	9429	4989	155
H(30D)	5168	8078	4759	155
H(23E)	9360	8077	118	47
H(27G)	3710	8503	3378	59
H(27H)	3121	7999	3941	59
H(29E)	7130	8728	4329	48
H(29H)	6729	8871	3530	48
H(30E)	4935	10404	4436	108
H(30F)	4019	10156	4420	108

Electronic Supplementary Information for Dalton Transactions

Table 10S. Torsion Angles [deg] for Complex **1**.

C(5)-C(2)-C(3)-O(2)	176.7(4)
N(1)-C(2)-C(3)-O(2)	1.1(7)
C(5)-C(2)-C(3)-N(4)	-2.9(5)
N(1)-C(2)-C(3)-N(4)	-178.4(4)
N(1)-C(2)-C(5)-N(3)	178.3(4)
C(3)-C(2)-C(5)-N(3)	1.9(6)
N(1)-C(2)-C(5)-N(2)	0.0(4)
C(3)-C(2)-C(5)-N(2)	-176.5(3)
O(1)-C(6)-C(7)-O(3)	154.1(3)
N(2)-C(6)-C(7)-O(3)	-87.7(4)
O(1)-C(6)-C(7)-C(8)	31.8(4)
N(2)-C(6)-C(7)-C(8)	150.1(3)
O(3)-C(7)-C(8)-O(4)	-33.7(4)
C(6)-C(7)-C(8)-O(4)	84.7(4)
O(3)-C(7)-C(8)-C(9)	-152.7(3)
C(6)-C(7)-C(8)-C(9)	-34.3(4)
O(4)-C(8)-C(9)-O(1)	-90.3(3)
C(7)-C(8)-C(9)-O(1)	25.5(4)

O(4)-C(8)-C(9)-C(10)	147.4(3)
C(7)-C(8)-C(9)-C(10)	-96.8(4)
O(1)-C(9)-C(10)-O(5)	-65.4(4)
C(8)-C(9)-C(10)-O(5)	55.4(4)
N(8)-C(12)-C(15)-N(6)	-178.5(4)
N(7)-C(12)-C(15)-N(6)	1.1(4)
N(8)-C(12)-C(15)-C(14)	4.3(6)
N(7)-C(12)-C(15)-C(14)	-176.1(3)
O(10)-C(14)-C(15)-C(12)	173.8(4)
N(9)-C(14)-C(15)-C(12)	-5.1(5)
O(10)-C(14)-C(15)-N(6)	-2.5(7)
N(9)-C(14)-C(15)-N(6)	178.6(4)
O(9)-C(16)-C(17)-O(11)	157.8(3)
N(7)-C(16)-C(17)-O(11)	-82.9(4)
O(9)-C(16)-C(17)-C(18)	36.3(3)
N(7)-C(16)-C(17)-C(18)	155.6(3)
O(11)-C(17)-C(18)-O(12)	-38.7(4)
C(16)-C(17)-C(18)-O(12)	78.1(3)
O(11)-C(17)-C(18)-C(19)	-154.8(3)
C(16)-C(17)-C(18)-C(19)	-38.0(3)

O(12)-C(18)-C(19)-O(9)	-86.1(3)
C(17)-C(18)-C(19)-O(9)	27.5(4)
O(12)-C(18)-C(19)-C(20)	151.0(3)
C(17)-C(18)-C(19)-C(20)	-95.5(4)
O(9)-C(19)-C(20)-O(13)	-59.5(4)
C(18)-C(19)-C(20)-O(13)	61.3(4)
N(2)-C(1)-N(1)-C(2)	-0.3(4)
N(2)-C(1)-N(1)-Cu(1)	-161.1(3)
C(5)-C(2)-N(1)-C(1)	0.2(4)
C(3)-C(2)-N(1)-C(1)	176.0(4)
C(5)-C(2)-N(1)-Cu(1)	158.9(3)
C(3)-C(2)-N(1)-Cu(1)	-25.3(6)
O(18)-Cu(1)-N(1)-C(1)	-76.1(3)
O(17)-Cu(1)-N(1)-C(1)	161.2(11)
N(6)-Cu(1)-N(1)-C(1)	108.3(3)
O(19)-Cu(1)-N(1)-C(1)	13.6(3)
O(24)-Cu(1)-N(1)-C(1)	-154.3(3)
O(18)-Cu(1)-N(1)-C(2)	128.3(3)
O(17)-Cu(1)-N(1)-C(2)	5.5(15)
N(6)-Cu(1)-N(1)-C(2)	-47.4(3)
O(19)-Cu(1)-N(1)-C(2)	-142.1(3)
O(24)-Cu(1)-N(1)-C(2)	50.0(3)

N(1)-C(1)-N(2)-C(5)	0.3(4)
N(1)-C(1)-N(2)-C(6)	177.2(3)
N(3)-C(5)-N(2)-C(1)	-178.6(4)
C(2)-C(5)-N(2)-C(1)	-0.2(4)
N(3)-C(5)-N(2)-C(6)	4.4(6)
C(2)-C(5)-N(2)-C(6)	-177.2(3)
O(1)-C(6)-N(2)-C(1)	59.1(5)
C(7)-C(6)-N(2)-C(1)	-58.5(5)
O(1)-C(6)-N(2)-C(5)	-124.6(4)
C(7)-C(6)-N(2)-C(5)	117.9(4)
N(5)-C(4)-N(3)-C(5)	-179.2(4)
N(4)-C(4)-N(3)-C(5)	2.1(5)
C(2)-C(5)-N(3)-C(4)	-1.2(6)
N(2)-C(5)-N(3)-C(4)	176.8(4)
N(3)-C(4)-N(4)-C(3)	-3.9(6)
N(5)-C(4)-N(4)-C(3)	177.3(3)
O(2)-C(3)-N(4)-C(4)	-175.6(3)
C(2)-C(3)-N(4)-C(4)	4.0(5)
N(7)-C(11)-N(6)-C(15)	-0.3(4)

N(7)-C(11)-N(6)-Cu(1)	-160.6(3)

C(12)-C(15)-N(6)-C(11)	-0.5(4)
C(14)-C(15)-N(6)-C(11)	176.0(4)
C(12)-C(15)-N(6)-Cu(1)	157.8(3)
C(14)-C(15)-N(6)-Cu(1)	-25.7(6)
O(18)-Cu(1)-N(6)-C(11)	50(2)
O(17)-Cu(1)-N(6)-C(11)	-65.0(3)
N(1)-Cu(1)-N(6)-C(11)	109.8(3)
O(19)-Cu(1)-N(6)-C(11)	-152.3(3)
O(24)-Cu(1)-N(6)-C(11)	13.7(3)
O(18)-Cu(1)-N(6)-C(15)	-105.0(18)
O(17)-Cu(1)-N(6)-C(15)	139.7(3)
N(1)-Cu(1)-N(6)-C(15)	-45.5(3)
O(19)-Cu(1)-N(6)-C(15)	52.4(3)
O(24)-Cu(1)-N(6)-C(15)	-141.7(3)
N(6)-C(11)-N(7)-C(12)	1.0(4)
N(6)-C(11)-N(7)-C(16)	175.3(3)
N(8)-C(12)-N(7)-C(11)	178.4(4)
C(15)-C(12)-N(7)-C(11)	-1.2(4)
N(8)-C(12)-N(7)-C(16)	3.8(6)
C(15)-C(12)-N(7)-C(16)	-175.8(3)
O(9)-C(16)-N(7)-C(11)	57.3(5)
C(17)-C(16)-N(7)-C(11)	-60.5(5)

O(9)-C(16)-N(7)-C(12)	-129.3(4)
C(17)-C(16)-N(7)-C(12)	113.0(4)
N(10)-C(13)-N(8)-C(12)	-177.6(4)
N(9)-C(13)-N(8)-C(12)	0.7(5)
N(7)-C(12)-N(8)-C(13)	178.6(4)
C(15)-C(12)-N(8)-C(13)	-1.8(6)
O(10)-C(14)-N(9)-C(13)	-174.4(3)
C(15)-C(14)-N(9)-C(13)	4.6(5)
N(10)-C(13)-N(9)-C(14)	175.9(4)
N(8)-C(13)-N(9)-C(14)	-2.6(6)
N(2)-C(6)-O(1)-C(9)	-138.6(3)
C(7)-C(6)-O(1)-C(9)	-16.9(4)
C(8)-C(9)-O(1)-C(6)	-5.7(4)
C(10)-C(9)-O(1)-C(6)	121.3(3)
C(9)-C(10)-O(5)-P(1)	166.3(2)
O(8)-P(1)-O(5)-C(10)	179.1(3)
O(7)-P(1)-O(5)-C(10)	-59.4(3)
O(6)-P(1)-O(5)-C(10)	59.5(3)

N(7)-C(16)-O(9)-C(19)	-142.8(3)
C(17)-C(16)-O(9)-C(19)	-19.9(4)

C(20)-C(19)-O(9)-C(16)	122.5(3)
C(18)-C(19)-O(9)-C(16)	-4.9(4)
C(18)-C(17)-O(11)-Na(1)	22.2(4)
C(16)-C(17)-O(11)-Na(1)	-90.1(3)
O(12)-Na(1)-O(11)-C(17)	-1.3(2)
O(23)-Na(1)-O(11)-C(17)	111.3(3)
O(22)-Na(1)-O(11)-C(17)	-165.6(2)
O(20)-Na(1)-O(11)-C(17)	6.2(3)
O(21)-Na(1)-O(11)-C(17)	-83.1(2)
O(23')-Na(1)-O(11)-C(17)	105.8(3)
C(17)-C(18)-O(12)-Na(1)	40.6(4)
C(19)-C(18)-O(12)-Na(1)	151.3(2)
O(23)-Na(1)-O(12)-C(18)	-119.3(3)
O(22)-Na(1)-O(12)-C(18)	4.0(4)
O(20)-Na(1)-O(12)-C(18)	161.5(3)
O(21)-Na(1)-O(12)-C(18)	71.3(3)
O(11)-Na(1)-O(12)-C(18)	-23.0(2)
O(23')-Na(1)-O(12)-C(18)	-93.1(3)
C(19)-C(20)-O(13)-P(2)	164.9(2)
O(16)-P(2)-O(13)-C(20)	174.3(2)
O(15)-P(2)-O(13)-C(20)	-65.4(3)
O(14)-P(2)-O(13)-C(20)	54.0(3)

Symmetry transformations used to generate equivalent atoms.

Table 11S. Hydrogen bonds for Complex 1 [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(19)-H(19A)...O(10)	0.83	1.89	2.687(4)	161.3
O(19)-H(19B)...O(8)	0.82	1.94	2.741(4)	164.7
O(23)-H(23G)...O(20)	0.84	2.44	3.273(7)	173.9
O(24)-H(24A)...O(16)	0.84	1.93	2.762(4)	174.2
O(24)-H(24B)...O(2)	0.84	1.87	2.717(4)	175.8
O(25)-H(25C)...O(9)	0.85	2.15	2.999(4)	172.8
O(25)-H(25D)...O(15)	0.85	1.83	2.680(4)	172.3
O(27)-H(27D)...O(15)	0.85	2.00	2.847(15)	171.1
O(29)-H(29C)...O(25)	0.85	1.89	2.739(6)	175.4

O(17)-H(17A)...O(29)	0.82	1.81	2.628(6)	177.8
O(17)-H(17A)...O(29')	0.82	2.21	2.950(17)	150.9
O(27')-H(27G)...O(15)	0.85	1.88	2.716(7)	167.7
O(29')-H(29H)...O(25)	0.85	2.01	2.841(15)	166.3

N(9)-H(9N)...O(6)#1	0.870(19)	1.87(2)	2.735(4)	171(4)
O(3)-H(3O)...O(6)#1	0.819(10)	1.897(18)	2.693(4)	164(5)
O(11)-H(11O)...O(14)#2	0.814(10)	2.061(19)	2.841(4)	160(5)
N(4)-H(4N)...O(14)#2	0.88	1.85	2.716(4)	169.1
O(21)-H(21A)...O(15)#2	0.82	1.91	2.724(4)	170.9
O(22)-H(22A)...O(14)#2	0.81	2.05	2.814(4)	155.8
O(12)-H(12O)...O(16)#3	0.81(2)	1.83(3)	2.631(4)	167(8)
O(20)-H(02B)...O(16)#3	0.82	2.05	2.839(4)	161.5
O(21)-H(21B)...O(24)#3	0.85	2.00	2.838(4)	171.1
O(4)-H(4O)...O(8)#4	0.828(10)	1.825(12)	2.650(4)	174(6)
N(10)-H(0B)...O(28)#5	0.81	2.20	2.956(7)	154.6
O(23)-H(23F)...O(28)#5	0.85	2.10	2.942(9)	174.1
O(17)-H(17B)...O(30)#6	0.85	1.95	2.763(11)	160.7
O(17)-H(17B)...O(30')#6	0.85	1.97	2.785(11)	159.7
O(18)-H(18A)...O(25)#7	0.82	2.08	2.885(5)	165.1
O(20)-H(02A)...O(6)#8	0.82	1.93	2.716(4)	161.3
O(22)-H(22B)...O(4)#9	0.82	2.29	3.033(4)	151.6
O(26)-H(26C)...O(21)#10	0.85	1.96	2.808(5)	177.2
O(26)-H(26D)...O(7)#11	0.85	1.91	2.758(5)	177.2
O(29)-H(29B)...O(7)#11	0.85	1.86	2.613(5)	147.0
O(29')-H(29E)...O(7)#11	0.84	1.85	2.674(13)	167.1
O(30')-H(30E)...O(18)#11	0.85	2.46	3.296(13)	170.4

O(27)-H(27C)...O(8)#12	0.85	1.97	2.811(14)	170.0
O(27')-H(27H)...O(8)#12	0.85	2.00	2.835(7)	167.5
O(30')-H(30F)...O(26)#12	0.85	2.35	3.190(14)	169.7
N(10)-H(0A)...O(20)#13	0.81	2.22	3.002(4)	165.0

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y+1/2,-z+1 #2 -x+1,y-1/2,-z #3 -x+1,y+1/2,-z

#4 -x+2,y-1/2,-z+1 #5 x+1,y,z #6 -x+1,y-1/2,-z+1

#7 x,y-1,z #8 x,y+1,z-1 #9 -x+2,y+1/2,-z

#10 x,y,z+1 #11 x,y+1,z #12 -x+1,y+1/2,-z+1

#13 -x+2,y-1/2,-z