Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information

Synthesis and Proton Conduction of a Crystalline 3-D Vanadoborate with $[V_6B_{20}]$ Architectures

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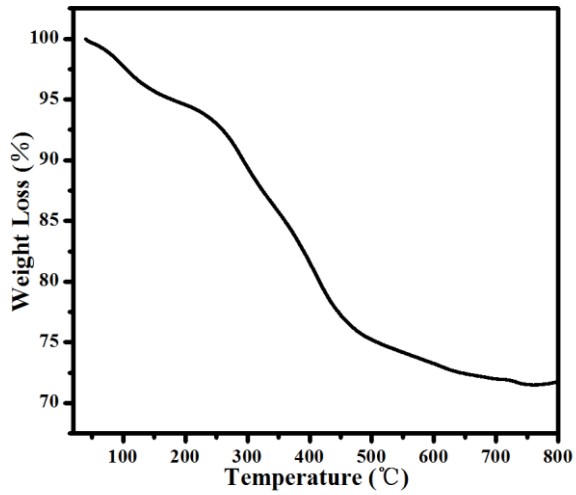

Fig. S1 TG curve of **1** in air

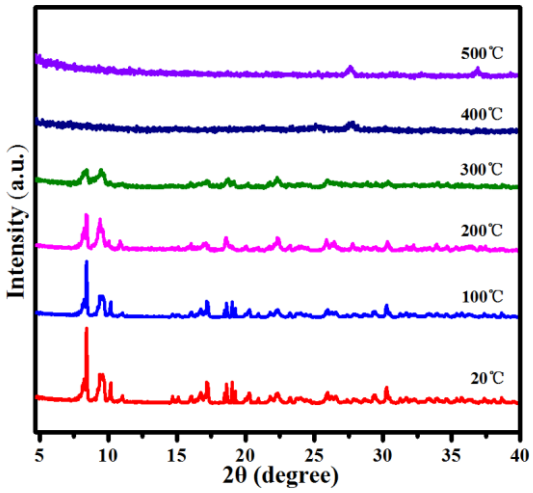

Fig. S2 Variable temperature PXRD patterns collected in air from 20 °C to 500 °C

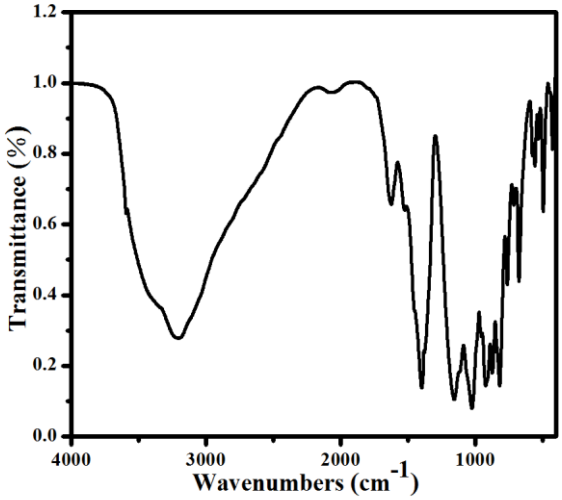

Fig. S3 The FT-IR spectrum of **1**

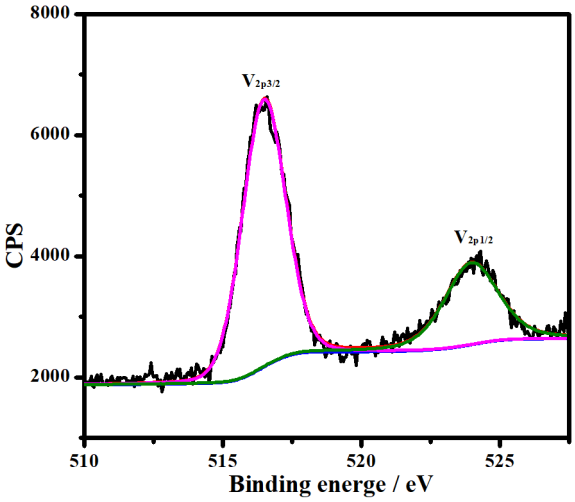

Fig. S4 The V2*p* XPS spectrum of **1**

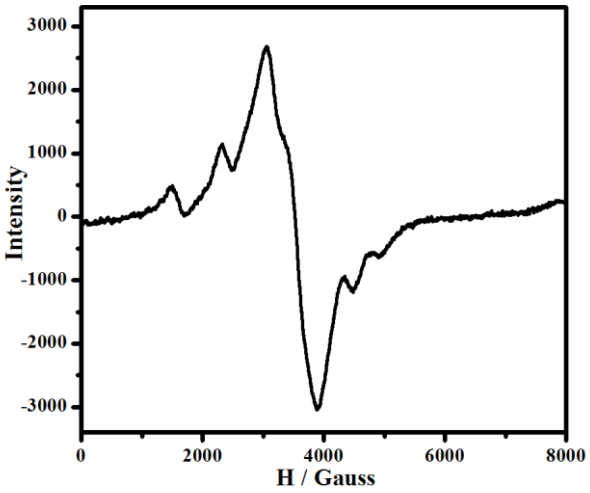

Fig. S5 EPR spectrum for compound **1**

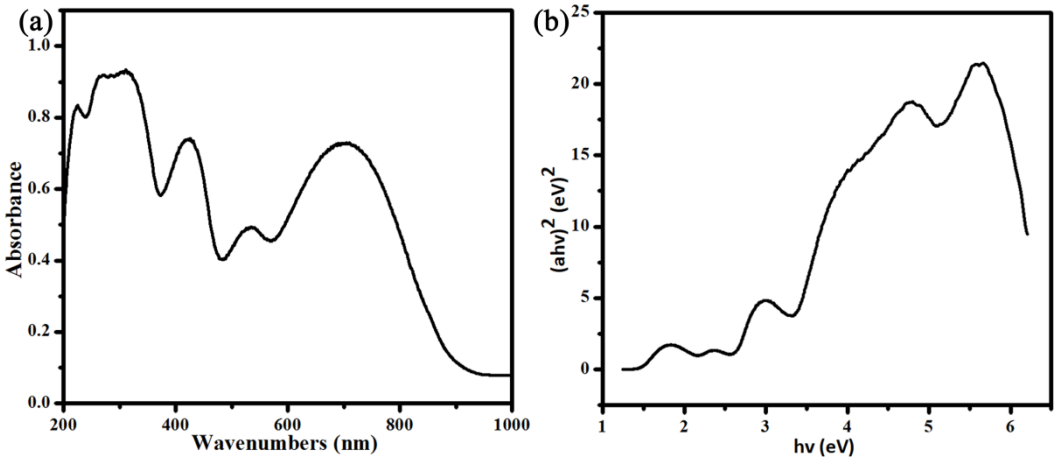

Fig. S6. UV-Vis diffuse reflectance spectrum of **1**

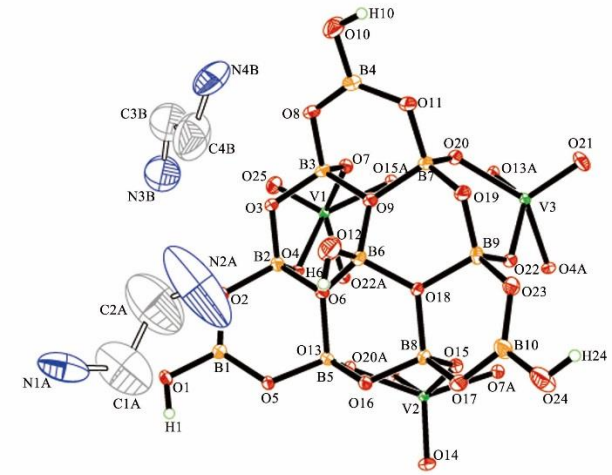

Fig. S7 The thermal ellipsoid plots (50% probability) and atomic labeling schemes of **1**

Comparison of three [V_6B_{20}]-containing compounds:

The vanadoborates in refs. 36 and 37 as well as in our work are all based on the [V_6B_{20}] clusters, but they differ greatly. For our compound $(H_2en)_4[(VO)_6(B_{10}O_{22}H_4)_2(H_2O)]\cdot 4H_2O$ (**1**), H_2en^{2+} cations and H_2O molecules are accommodated in the interclusters' space of the framework and interact with the [V_6B_{20}] polyanions via hydrogen bonds (N–H···O, O–H···O), through which the respective molecular species are integrated into 3-D architectures. For$\{V_6B_{20}O_{44}(OH)_8(H_2O)[K(H_2O)]_2\}\cdot 2(H_3dien)\cdot 6H_2O$ (**2**) reported in ref. 36, it is built up from [V_6B_{20}] clusters and dimeric [K_2O_{16}] units, which are interconnected to give a 3-D $\{B_{20}V_6O_{44}(OH)_8(H_2O)[K(H_2O)]_2\}_n$ architecture with 1-D tunnels filled with protonated H_3dien^{3+} ions. And for $(H_2NCH_2CH_2NH_3)_3\{(VO)_6[B_{10}O_{16}(OH)_6]_2\}\cdot 11H_2O$ (**3**) reported in ref. 37, its crystal structure is built up from the [V_6B_{20}] anions, enH^+ cations and H_2O molecules. Hydrogen bonds align the respective molecular species into a 3-D architecture. Compound **1** and compound **3** are similar in composition, but have obvious differences in structural aesthetics. In contradistinction to **3**, the obvious characteristic of **1** is that its [V_6B_{20}] cluster possesses a determined water molecule in the internal center. And the interclusters' space of **1** is filled with more ethylenediamine cations. Such different structural features may bring about great differences in their physic-chemical properties such as catalysis, magnetism, absorption, proton conduction and so on.

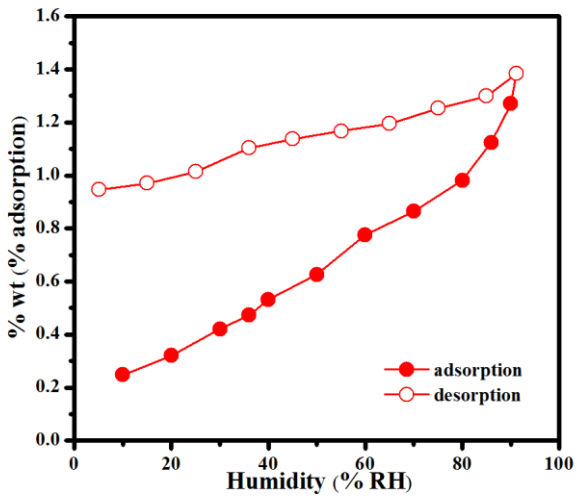

Fig. S8 Water adsorption (filled circles) and desorption (open circles) isotherms of **1** at 293 K

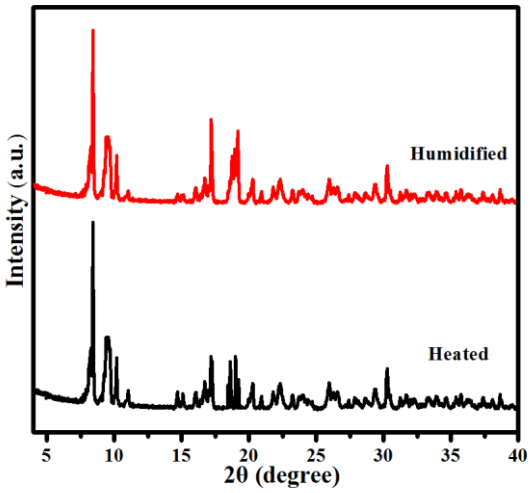

Fig. S9 XRD patterns of compound **1** treated after impedance measurement at 333 K (Heated) and at 98% RH (Humidified)

Table S1 Bond lengths [Å] for **1**

V(1)-O(25)	1.612(3)
V(1)-O(22)#1	1.947(3)
V(1)-O(4)	1.949(3)
V(1)-O(15)#1	1.959(3)
V(1)-O(7)	1.977(3)
V(1)-V(2)#1	3.0378(9)
V(1)-V(3)#1	3.0560(9)
V(2)-O(14)	1.615(3)
V(2)-O(15)	1.932(3)
V(2)-O(13)	1.949(3)
V(2)-O(7)#1	1.967(3)
V(2)-O(20)#1	1.976(3)
V(2)-V(3)#1	3.0592(9)
V(3)-O(21)	1.615(3)
V(3)-O(22)	1.947(3)
V(3)-O(13)#1	1.951(3)
V(3)-O(4)#1	1.969(3)
V(3)-O(20)	1.979(3)
O(1)-B(1)	1.366(5)
O(1)-H(1)	0.8400
O(2)-B(1)	1.370(5)
O(2)-B(2)	1.470(5)
O(3)-B(3)	1.429(5)
O(3)-B(2)	1.432(5)
O(4)-B(2)	1.467(5)

O(5)-B(1)	1.367(5)
O(5)-B(5)	1.462(5)
O(6)-B(6)	1.489(5)
O(6)-B(2)	1.522(5)
O(6)-B(5)	1.532(5)
O(7)-B(3)	1.474(5)
O(8)-B(4)	1.361(6)
O(8)-B(3)	1.470(5)
O(9)-B(6)	1.490(5)
O(9)-B(3)	1.529(5)
O(9)-B(7)	1.534(5)
O(10)-B(4)	1.381(6)
O(10)-H(10)	0.8400
O(11)-B(4)	1.359(6)
O(11)-B(7)	1.461(5)
O(12)-B(6)	1.439(6)
O(12)-H(12)	0.8400
O(13)-B(5)	1.466(6)
O(15)-B(8)	1.466(5)
O(16)-B(5)	1.425(5)
O(16)-B(8)	1.427(5)
O(17)-B(10)	1.356(6)
O(17)-B(8)	1.461(5)
O(18)-B(6)	1.479(5)
O(18)-B(9)	1.526(5)
O(18)-B(8)	1.526(5)
O(19)-B(7)	1.428(5)
O(19)-B(9)	1.435(5)
O(20)-B(7)	1.472(6)
O(22)-B(9)	1.459(5)
O(23)-B(10)	1.376(6)
O(23)-B(9)	1.474(5)
O(24)-B(10)	1.374(6)
O(24)-H(24)	0.8400
N(1A)-C(1B)	1.46(2)
N(1A)-C(1A)	1.537(18)
N(1A)-H(1AA)	0.9100
N(1A)-H(1AB)	0.9100
N(1A)-H(1AC)	0.9100
N(2A)-N(2B)	1.25(4)
N(2A)-C(2A)	1.505(19)
C(1A)-C(2B)	0.71(2)
C(1A)-C(1B)	1.23(3)
C(1A)-C(2A)	1.487(18)

C(1A)-N(2B)	1.82(3)
C(1A)-N(1B)	1.89(3)
C(1A)-H(1AD)	0.9900
C(1A)-H(1AE)	0.9900
C(2A)-C(2B)	1.11(3)
C(2A)-C(1B)	1.39(3)
C(2A)-N(2B)	1.66(3)
C(2A)-H(2AA)	0.9900
C(2A)-H(2AB)	0.9900
N(1B)-C(1B)	1.533(15)
N(1B)-H(1BA)	0.9100
N(1B)-H(1BB)	0.9100
N(1B)-H(1BC)	0.9100
N(2B)-C(2B)	1.474(15)
C(1B)-C(2B)	1.559(15)
C(1B)-H(1BD)	0.9900
C(1B)-H(1BE)	0.9900
C(2B)-H(2BA)	0.9900
C(2B)-H(2BB)	0.9900
N(3A)-C(3B)	1.213(19)
N(3A)-C(3A)	1.40(3)
N(3A)-H(3AA)	0.9100
N(3A)-H(3AB)	0.9100
N(3A)-H(3AC)	0.9100
N(4A)-C(4A)	1.16(4)
N(4A)-C(4B)	1.91(3)
C(3A)-C(3B)	1.03(3)
C(3A)-C(4B)	1.09(3)
C(3A)-C(4A)	1.593(19)
C(3A)-N(3B)	1.75(3)
C(3A)-H(3AD)	0.9900
C(3A)-H(3AE)	0.9900
C(4A)-C(4B)	0.77(3)
C(4A)-N(4B)	1.82(4)
C(4A)-H(4AA)	0.9900
C(4A)-H(4AB)	0.9900
N(3B)-C(3B)	1.439(16)
N(3B)-H(3BA)	0.9100
N(3B)-H(3BB)	0.9100
N(3B)-H(3BC)	0.9100
N(4B)-C(4B)	1.428(16)
C(3B)-C(4B)	1.556(16)
C(3B)-H(3BD)	0.9900
C(3B)-H(3BE)	0.9900

C(4B)-H(4BA)	0.9900
C(4B)-H(4BB)	0.9900

Table S2 Bond angles [°] for **1**

O(25)-V(1)-O(22)#1	110.50(14)
O(25)-V(1)-O(4)	108.44(14)
O(22)#1-V(1)-O(4)	76.98(12)
O(25)-V(1)-O(15)#1	111.43(14)
O(22)#1-V(1)-O(15)#1	88.85(12)
O(4)-V(1)-O(15)#1	140.12(12)
O(25)-V(1)-O(7)	107.67(14)
O(22)#1-V(1)-O(7)	141.83(11)
O(4)-V(1)-O(7)	91.21(12)
O(15)#1-V(1)-O(7)	77.20(12)
O(25)-V(1)-V(2)#1	120.84(11)
O(22)#1-V(1)-V(2)#1	115.18(8)
O(4)-V(1)-V(2)#1	116.67(9)
O(15)#1-V(1)-V(2)#1	38.35(8)
O(7)-V(1)-V(2)#1	39.51(8)
O(25)-V(1)-V(3)#1	118.81(11)
O(22)#1-V(1)-V(3)#1	38.30(8)
O(4)-V(1)-V(3)#1	38.96(8)
O(15)#1-V(1)-V(3)#1	115.76(8)
O(7)-V(1)-V(3)#1	118.73(8)
V(2)#1-V(1)-V(3)#1	120.34(3)
O(14)-V(2)-O(15)	106.79(14)
O(14)-V(2)-O(13)	110.66(14)
O(15)-V(2)-O(13)	90.00(12)
O(14)-V(2)-O(7)#1	106.12(13)
O(15)-V(2)-O(7)#1	78.09(12)
O(13)-V(2)-O(7)#1	143.19(12)
O(14)-V(2)-O(20)#1	110.26(14)
O(15)-V(2)-O(20)#1	142.96(12)
O(13)-V(2)-O(20)#1	77.01(12)
O(7)#1-V(2)-O(20)#1	91.73(12)
O(14)-V(2)-V(1)#1	116.96(11)
O(15)-V(2)-V(1)#1	39.00(8)
O(13)-V(2)-V(1)#1	116.94(9)
O(7)#1-V(2)-V(1)#1	39.76(8)
O(20)#1-V(2)-V(1)#1	118.55(8)
O(14)-V(2)-V(3)#1	122.32(11)
O(15)-V(2)-V(3)#1	116.36(8)
O(13)-V(2)-V(3)#1	38.37(9)
O(7)#1-V(2)-V(3)#1	118.37(8)

O(20)#1-V(2)-V(3)#1	39.37(8)
V(1)#1-V(2)-V(3)#1	120.71(3)
O(21)-V(3)-O(22)	111.23(14)
O(21)-V(3)-O(13)#1	110.68(14)
O(22)-V(3)-O(13)#1	138.09(12)
O(21)-V(3)-O(4)#1	109.56(14)
O(22)-V(3)-O(4)#1	76.52(11)
O(13)#1-V(3)-O(4)#1	89.19(12)
O(21)-V(3)-O(20)	108.50(14)
O(22)-V(3)-O(20)	90.43(12)
O(13)#1-V(3)-O(20)	76.90(12)
O(4)#1-V(3)-O(20)	141.94(11)
O(21)-V(3)-V(1)#1	119.92(11)
O(22)-V(3)-V(1)#1	38.30(8)
O(13)#1-V(3)-V(1)#1	115.16(9)
O(4)#1-V(3)-V(1)#1	38.49(8)
O(20)-V(3)-V(1)#1	117.87(8)
O(21)-V(3)-V(2)#1	121.13(11)
O(22)-V(3)-V(2)#1	114.68(8)
O(13)#1-V(3)-V(2)#1	38.32(8)
O(4)#1-V(3)-V(2)#1	115.26(8)
O(20)-V(3)-V(2)#1	39.31(8)
V(1)#1-V(3)-V(2)#1	118.95(3)
B(1)-O(1)-H(1)	109.5
B(1)-O(2)-B(2)	121.3(3)
B(3)-O(3)-B(2)	117.2(3)
B(2)-O(4)-V(1)	125.1(2)
B(2)-O(4)-V(3)#1	129.0(2)
V(1)-O(4)-V(3)#1	102.54(13)
B(1)-O(5)-B(5)	123.2(3)
B(6)-O(6)-B(2)	122.2(3)
B(6)-O(6)-B(5)	122.5(3)
B(2)-O(6)-B(5)	115.3(3)
B(3)-O(7)-V(2)#1	128.2(2)
B(3)-O(7)-V(1)	124.6(2)
V(2)#1-O(7)-V(1)	100.73(13)
B(4)-O(8)-B(3)	121.7(3)
B(6)-O(9)-B(3)	121.3(3)
B(6)-O(9)-B(7)	121.2(3)
B(3)-O(9)-B(7)	116.4(3)
B(4)-O(10)-H(10)	109.5
B(4)-O(11)-B(7)	121.5(3)
B(6)-O(12)-H(12)	109.5
B(5)-O(13)-V(2)	124.9(2)

B(5)-O(13)-V(3)#1	128.8(2)
V(2)-O(13)-V(3)#1	103.31(13)
B(8)-O(15)-V(2)	125.2(2)
B(8)-O(15)-V(1)#1	129.7(2)
V(2)-O(15)-V(1)#1	102.65(13)
B(5)-O(16)-B(8)	116.2(3)
B(10)-O(17)-B(8)	120.9(3)
B(6)-O(18)-B(9)	122.2(3)
B(6)-O(18)-B(8)	122.9(3)
B(9)-O(18)-B(8)	114.9(3)
B(7)-O(19)-B(9)	117.4(3)
B(7)-O(20)-V(2)#1	128.6(2)
B(7)-O(20)-V(3)	123.5(2)
V(2)#1-O(20)-V(3)	101.32(13)
B(9)-O(22)-V(3)	126.6(2)
B(9)-O(22)-V(1)#1	127.9(2)
V(3)-O(22)-V(1)#1	103.39(13)
B(10)-O(23)-B(9)	122.5(3)
B(10)-O(24)-H(24)	109.5
O(1)-B(1)-O(5)	119.3(4)
O(1)-B(1)-O(2)	118.3(4)
O(5)-B(1)-O(2)	122.5(4)
O(3)-B(2)-O(4)	112.9(3)
O(3)-B(2)-O(2)	110.1(3)
O(4)-B(2)-O(2)	109.0(3)
O(3)-B(2)-O(6)	108.4(3)
O(4)-B(2)-O(6)	107.8(3)
O(2)-B(2)-O(6)	108.5(3)
O(3)-B(3)-O(8)	110.6(3)
O(3)-B(3)-O(7)	111.8(3)
O(8)-B(3)-O(7)	110.1(3)
O(3)-B(3)-O(9)	109.2(3)
O(8)-B(3)-O(9)	108.1(3)
O(7)-B(3)-O(9)	106.9(3)
O(11)-B(4)-O(8)	124.4(4)
O(11)-B(4)-O(10)	118.5(4)
O(8)-B(4)-O(10)	117.1(4)
O(16)-B(5)-O(5)	110.3(3)
O(16)-B(5)-O(13)	112.5(3)
O(5)-B(5)-O(13)	110.4(3)
O(16)-B(5)-O(6)	108.7(3)
O(5)-B(5)-O(6)	106.9(3)
O(13)-B(5)-O(6)	107.9(3)
O(12)-B(6)-O(18)	112.5(3)

O(12)-B(6)-O(6)	113.1(3)
O(18)-B(6)-O(6)	107.0(3)
O(12)-B(6)-O(9)	110.2(3)
O(18)-B(6)-O(9)	107.2(3)
O(6)-B(6)-O(9)	106.4(3)
O(19)-B(7)-O(11)	109.8(3)
O(19)-B(7)-O(20)	113.1(3)
O(11)-B(7)-O(20)	110.0(3)
O(19)-B(7)-O(9)	108.5(3)
O(11)-B(7)-O(9)	108.4(3)
O(20)-B(7)-O(9)	106.9(3)
O(16)-B(8)-O(17)	109.4(3)
O(16)-B(8)-O(15)	112.9(3)
O(17)-B(8)-O(15)	110.0(3)
O(16)-B(8)-O(18)	108.7(3)
O(17)-B(8)-O(18)	108.5(3)
O(15)-B(8)-O(18)	107.1(3)
O(19)-B(9)-O(22)	111.6(3)
O(19)-B(9)-O(23)	111.9(3)
O(22)-B(9)-O(23)	110.0(3)
O(19)-B(9)-O(18)	107.8(3)
O(22)-B(9)-O(18)	108.5(3)
O(23)-B(9)-O(18)	106.9(3)
O(17)-B(10)-O(24)	117.3(4)
O(17)-B(10)-O(23)	123.0(4)
O(24)-B(10)-O(23)	119.8(4)
C(1B)-N(1A)-C(1A)	48.5(13)
C(1B)-N(1A)-H(1AA)	102.8
C(1A)-N(1A)-H(1AA)	109.5
C(1B)-N(1A)-H(1AB)	146.3
C(1A)-N(1A)-H(1AB)	109.5
H(1AA)-N(1A)-H(1AB)	109.5
C(1B)-N(1A)-H(1AC)	67
C(1A)-N(1A)-H(1AC)	109.5
H(1AA)-N(1A)-H(1AC)	109.5
H(1AB)-N(1A)-H(1AC)	109.5
N(2B)-N(2A)-C(2A)	73.6(17)
C(2B)-C(1A)-C(1B)	104(3)
C(2B)-C(1A)-C(2A)	45(3)
C(1B)-C(1A)-C(2A)	60.7(16)
C(2B)-C(1A)-N(1A)	153(3)
C(1B)-C(1A)-N(1A)	62.5(15)
C(2A)-C(1A)-N(1A)	111.7(17)
C(2B)-C(1A)-N(2B)	50(2)

C(1B)-C(1A)-N(2B)	107.7(14)
C(2A)-C(1A)-N(2B)	59.2(13)
N(1A)-C(1A)-N(2B)	109.2(18)
C(2B)-C(1A)-N(1B)	149(3)
C(1B)-C(1A)-N(1B)	53.9(11)
C(2A)-C(1A)-N(1B)	105.4(19)
N(1A)-C(1A)-N(1B)	8.7(15)
N(2B)-C(1A)-N(1B)	111.7(15)
C(2B)-C(1A)-H(1AD)	74.4
C(1B)-C(1A)-H(1AD)	158.1
C(2A)-C(1A)-H(1AD)	109.3
N(1A)-C(1A)-H(1AD)	109.3
N(2B)-C(1A)-H(1AD)	53.9
N(1B)-C(1A)-H(1AD)	117.7
C(2B)-C(1A)-H(1AE)	94.1
C(1B)-C(1A)-H(1AE)	93.9
C(2A)-C(1A)-H(1AE)	109.3
N(1A)-C(1A)-H(1AE)	109.3
N(2B)-C(1A)-H(1AE)	141.2
N(1B)-C(1A)-H(1AE)	107.1
H(1AD)-C(1A)-H(1AE)	107.9
C(2B)-C(2A)-C(1B)	76.2(13)
C(2B)-C(2A)-C(1A)	26.9(12)
C(1B)-C(2A)-C(1A)	50.6(13)
C(2B)-C(2A)-N(2A)	106(3)
C(1B)-C(2A)-N(2A)	122(2)
C(1A)-C(2A)-N(2A)	111.0(17)
C(2B)-C(2A)-N(2B)	60.4(17)
C(1B)-C(2A)-N(2B)	109.1(14)
C(1A)-C(2A)-N(2B)	70.5(15)
N(2A)-C(2A)-N(2B)	46.0(16)
C(2B)-C(2A)-H(2AA)	132.9
C(1B)-C(2A)-H(2AA)	59.1
C(1A)-C(2A)-H(2AA)	109.4
N(2A)-C(2A)-H(2AA)	109.4
N(2B)-C(2A)-H(2AA)	145.4
C(2B)-C(2A)-H(2AB)	87.2
C(1B)-C(2A)-H(2AB)	128.1
C(1A)-C(2A)-H(2AB)	109.4
N(2A)-C(2A)-H(2AB)	109.4
N(2B)-C(2A)-H(2AB)	104
H(2AA)-C(2A)-H(2AB)	108
C(1B)-N(1B)-C(1A)	40.5(9)
C(1B)-N(1B)-H(1BA)	109.5

C(1A)-N(1B)-H(1BA)	102.6
C(1B)-N(1B)-H(1BB)	109.5
C(1A)-N(1B)-H(1BB)	75
H(1BA)-N(1B)-H(1BB)	109.5
C(1B)-N(1B)-H(1BC)	109.5
C(1A)-N(1B)-H(1BC)	143.2
H(1BA)-N(1B)-H(1BC)	109.5
H(1BB)-N(1B)-H(1BC)	109.5
N(2A)-N(2B)-C(2B)	101.3(18)
N(2A)-N(2B)-C(2A)	60.3(14)
C(2B)-N(2B)-C(2A)	40.9(11)
N(2A)-N(2B)-C(1A)	105.3(19)
C(2B)-N(2B)-C(1A)	21.6(8)
C(2A)-N(2B)-C(1A)	50.2(9)
C(1A)-C(1B)-C(2A)	68.7(14)
C(1A)-C(1B)-N(1A)	69.0(12)
C(2A)-C(1B)-N(1A)	122.7(17)
C(1A)-C(1B)-N(1B)	85.6(13)
C(2A)-C(1B)-N(1B)	134.5(16)
N(1A)-C(1B)-N(1B)	16.6(14)
C(1A)-C(1B)-C(2B)	26.1(9)
C(2A)-C(1B)-C(2B)	43.8(14)
N(1A)-C(1B)-C(2B)	92.9(11)
N(1B)-C(1B)-C(2B)	109.4(10)
C(1A)-C(1B)-H(1BD)	130.2
C(2A)-C(1B)-H(1BD)	67.3
N(1A)-C(1B)-H(1BD)	119.1
N(1B)-C(1B)-H(1BD)	109.8
C(2B)-C(1B)-H(1BD)	109.8
C(1A)-C(1B)-H(1BE)	110.1
C(2A)-C(1B)-H(1BE)	114
N(1A)-C(1B)-H(1BE)	115.8
N(1B)-C(1B)-H(1BE)	109.8
C(2B)-C(1B)-H(1BE)	109.8
H(1BD)-C(1B)-H(1BE)	108.2
C(1A)-C(2B)-C(2A)	108(3)
C(1A)-C(2B)-N(2B)	108(3)
C(2A)-C(2B)-N(2B)	78.6(18)
C(1A)-C(2B)-C(1B)	50(3)
C(2A)-C(2B)-C(1B)	60.1(17)
N(2B)-C(2B)-C(1B)	110.4(12)
C(1A)-C(2B)-H(2BA)	63.4
C(2A)-C(2B)-H(2BA)	169.1
N(2B)-C(2B)-H(2BA)	109.6

C(1B)-C(2B)-H(2BA)	109.6
C(1A)-C(2B)-H(2BB)	141.7
C(2A)-C(2B)-H(2BB)	74.6
N(2B)-C(2B)-H(2BB)	109.6
C(1B)-C(2B)-H(2BB)	109.6
H(2BA)-C(2B)-H(2BB)	108.1
C(3B)-N(3A)-C(3A)	45.6(14)
C(3B)-N(3A)-H(3AA)	111.1
C(3A)-N(3A)-H(3AA)	109.5
C(3B)-N(3A)-H(3AB)	66.3
C(3A)-N(3A)-H(3AB)	109.5
H(3AA)-N(3A)-H(3AB)	109.5
C(3B)-N(3A)-H(3AC)	137.9
C(3A)-N(3A)-H(3AC)	109.5
H(3AA)-N(3A)-H(3AC)	109.5
H(3AB)-N(3A)-H(3AC)	109.5
C(4A)-N(4A)-C(4B)	7(2)
C(3B)-C(3A)-C(4B)	95(3)
C(3B)-C(3A)-N(3A)	57.4(17)
C(4B)-C(3A)-N(3A)	124(3)
C(3B)-C(3A)-C(4A)	114(3)
C(4B)-C(3A)-C(4A)	25.7(19)
N(3A)-C(3A)-C(4A)	118(2)
C(3B)-C(3A)-N(3B)	55.3(16)
C(4B)-C(3A)-N(3B)	123(3)
N(3A)-C(3A)-N(3B)	2.0(9)
C(4A)-C(3A)-N(3B)	119(2)
C(3B)-C(3A)-H(3AD)	137.8
C(4B)-C(3A)-H(3AD)	122.1
N(3A)-C(3A)-H(3AD)	107.7
C(4A)-C(3A)-H(3AD)	107.7
N(3B)-C(3A)-H(3AD)	109.1
C(3B)-C(3A)-H(3AE)	54.1
C(4B)-C(3A)-H(3AE)	82.7
N(3A)-C(3A)-H(3AE)	107.7
C(4A)-C(3A)-H(3AE)	107.7
N(3B)-C(3A)-H(3AE)	105.8
H(3AD)-C(3A)-H(3AE)	107.1
C(4B)-C(4A)-N(4A)	162(5)
C(4B)-C(4A)-C(3A)	37(3)
N(4A)-C(4A)-C(3A)	126(3)
C(4B)-C(4A)-N(4B)	48(3)
N(4A)-C(4A)-N(4B)	143(3)
C(3A)-C(4A)-N(4B)	84.1(18)

C(4B)-C(4A)-H(4AA)	87.9
N(4A)-C(4A)-H(4AA)	105.9
C(3A)-C(4A)-H(4AA)	105.9
N(4B)-C(4A)-H(4AA)	81.9
C(4B)-C(4A)-H(4AB)	80.1
N(4A)-C(4A)-H(4AB)	105.9
C(3A)-C(4A)-H(4AB)	105.9
N(4B)-C(4A)-H(4AB)	39.1
H(4AA)-C(4A)-H(4AB)	106.2
C(3B)-N(3B)-C(3A)	36.0(12)
C(3B)-N(3B)-H(3BA)	109.5
C(3A)-N(3B)-H(3BA)	119.4
C(3B)-N(3B)-H(3BB)	109.5
C(3A)-N(3B)-H(3BB)	126.8
H(3BA)-N(3B)-H(3BB)	109.5
C(3B)-N(3B)-H(3BC)	109.5
C(3A)-N(3B)-H(3BC)	73.7
H(3BA)-N(3B)-H(3BC)	109.5
H(3BB)-N(3B)-H(3BC)	109.5
C(4B)-N(4B)-C(4A)	23.9(10)
C(3A)-C(3B)-N(3A)	77(2)
C(3A)-C(3B)-N(3B)	89(2)
N(3A)-C(3B)-N(3B)	11.6(10)
C(3A)-C(3B)-C(4B)	44.1(18)
N(3A)-C(3B)-C(4B)	104.5(14)
N(3B)-C(3B)-C(4B)	113.9(13)
C(3A)-C(3B)-H(3BD)	85
N(3A)-C(3B)-H(3BD)	107.3
N(3B)-C(3B)-H(3BD)	108.8
C(4B)-C(3B)-H(3BD)	108.8
C(3A)-C(3B)-H(3BE)	152.8
N(3A)-C(3B)-H(3BE)	119.5
N(3B)-C(3B)-H(3BE)	108.8
C(4B)-C(3B)-H(3BE)	108.8
H(3BD)-C(3B)-H(3BE)	107.7
C(4A)-C(4B)-C(3A)	117(4)
C(4A)-C(4B)-N(4B)	108(3)
C(3A)-C(4B)-N(4B)	131(2)
C(4A)-C(4B)-C(3B)	142(4)
C(3A)-C(4B)-C(3B)	41.2(17)
N(4B)-C(4B)-C(3B)	107.3(14)
C(4A)-C(4B)-N(4A)	11(3)
C(3A)-C(4B)-N(4A)	107(2)
N(4B)-C(4B)-N(4A)	115.5(14)

C(3B)-C(4B)-N(4A)	136.8(15)
C(4A)-C(4B)-H(4BA)	69.6
C(3A)-C(4B)-H(4BA)	70.1
N(4B)-C(4B)-H(4BA)	110.3
C(3B)-C(4B)-H(4BA)	110.3
N(4A)-C(4B)-H(4BA)	60.7
C(4A)-C(4B)-H(4BB)	43
C(3A)-C(4B)-H(4BB)	115.8
N(4B)-C(4B)-H(4BB)	110.3
C(3B)-C(4B)-H(4BB)	110.3
N(4A)-C(4B)-H(4BB)	49.3
H(4BA)-C(4B)-H(4BB)	108.5

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z+1