Electronic Supplementary Material (ESI) for Dalton Transactions

A C_2-symmetric Antimonato Polyoxovanadate Cluster $[V_{16}Sb_4O_{42}(H_2O)]^{8-}$ derived from the $\{V_{18}O_{42}\}$ archetype

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Supplementary Information

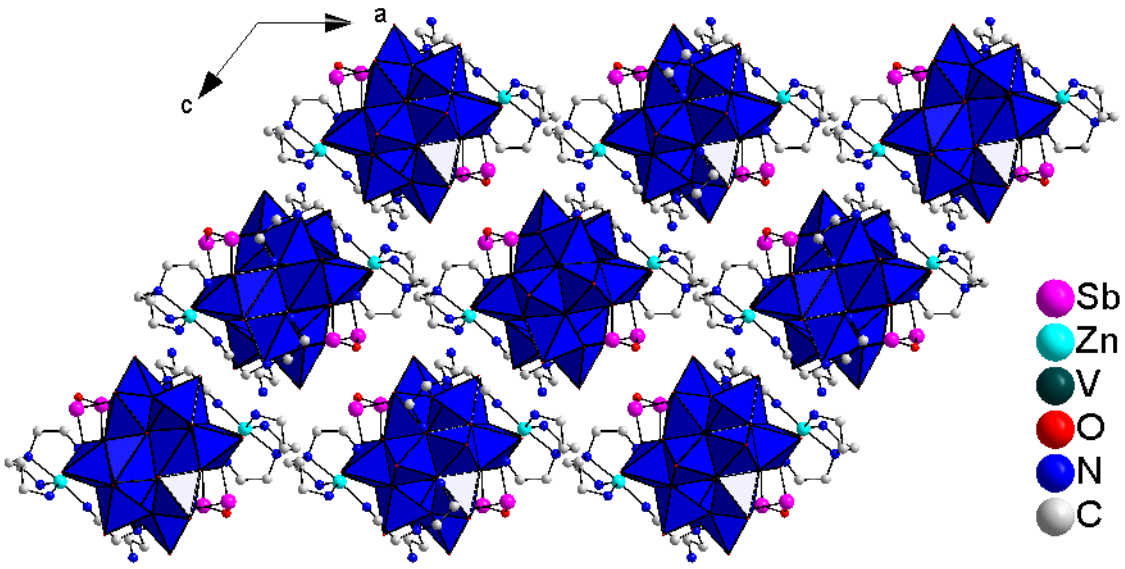

Fig. S1 Representation of the clusters in compound **1** in the *ac* plane. H atoms are not shown.

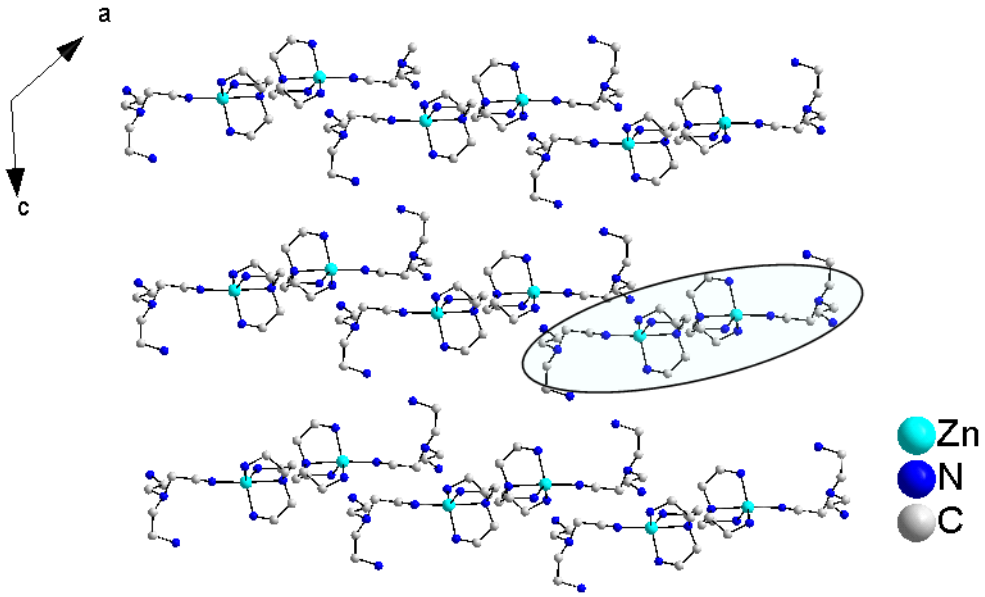

Fig. S2 The $Zn(tren)_2$ complexes in the structure of **1** in the (010) plane. A pair of *anti*-oriented neighboring complexes is encircled. H atoms omitted for clarity.

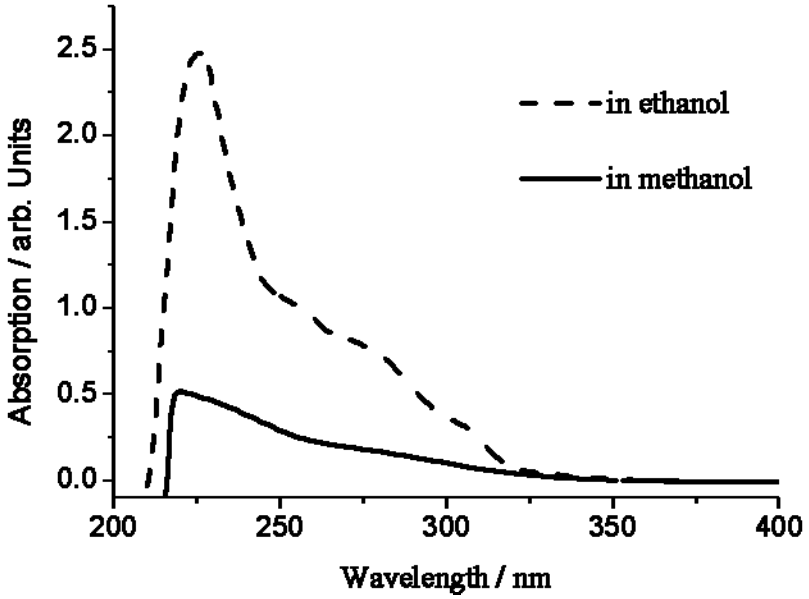

Fig. S3 UV spectra of compound **1** in ethanol and methanol.

Table S1 Bond lengths [Å] for $\{(trenH_2)Zn(tren)\}_2[V_{16}Sb_4O_{42}(H_2O)]\cdot xH_2O$ (x = 6–10).

Sb(1)-O(18)	1.952(4)	N(6)-C(11)	1.463(7)
Sb(1)-O(10)	1.960(4)	N(6)-C(10)	1.468(8)
Sb(1)-O(19)	1.966(4)	N(6)-C(8)	1.478(8)
Sb(2)-O(10)	1.947(4)	N(4)-C(4)	1.473(9)
Sb(2)-O(4)	1.948(4)	N(4)-C(2)	1.476(9)
Sb(2)-O(5)	1.952(4)	N(4)-C(6)	1.484(9)
V(1)-V(7)	2.9458(13)	N(8)-C(12)	1.483(8)
V(1)-V(6)	2.9472(13)	C(2)-C(1)	1.533(11)
V(2)-V(8)	2.9927(13)	C(6)-C(3)	1.520(9)
V(2)-V(6)	3.0417(13)	N(3)-C(3)	1.481(8)
V(3)-V(4)	2.9631(13)	N(2)-C(5)	1.490(8)
V(3)-V(6)	3.0064(12)	N(5)-C(7)	1.483(8)
V(4)-V(4)#1	2.729(2)	N(1)-C(1)	1.470(10)
V(4)-V(5)	3.1013(13)	C(10)-C(9)	1.511(10)
V(5)-V(7)	3.0704(13)	N(7)-C(9)	1.500(9)
V(7)-V(8)#1	2.9293(13)	C(12)-C(11)	1.531(8)
V(8)-V(7)#1	2.9293(13)	C(8)-C(7)	1.513(8)
V(8)-V(8)#1	2.9668(19)	C(5)-C(4)	1.530(11)

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

Table S2 Angles [°] for $\{(trenH_2)Zn(tren)\}_2[V_{16}Sb_4O_{42}(H_2O)]\cdot xH_2O$ (x = 6–10).

O(18)-Sb(1)-O(10)	96.36(17)	O(12)-V(2)-O(18)	78.02(16)
O(18)-Sb(1)-O(19)	93.74(17)	O(2)-V(2)-O(18)	148.24(17)
O(10)-Sb(1)-O(19)	97.20(17)	O(8)-V(2)-O(18)	88.69(17)
O(10)-Sb(2)-O(4)	94.32(17)	O(13)-V(2)-V(8)	112.27(16)
O(10)-Sb(2)-O(5)	98.22(17)	O(12)-V(2)-V(8)	122.48(12)
O(4)-Sb(2)-O(5)	96.59(18)	O(2)-V(2)-V(8)	39.55(12)
O(14)-V(1)-O(17)	104.6(2)	O(8)-V(2)-V(8)	41.10(11)
O(14)-V(1)-O(3)	109.3(2)	O(18)-V(2)-V(8)	123.90(13)
O(17)-V(1)-O(3)	146.05(19)	O(13)-V(2)-V(6)	111.42(16)
O(14)-V(1)-O(11)	110.3(2)	O(12)-V(2)-V(6)	38.42(11)
O(17)-V(1)-O(11)	90.11(17)	O(2)-V(2)-V(6)	125.16(13)
O(3)-V(1)-O(11)	80.09(16)	O(8)-V(2)-V(6)	120.83(12)
O(14)-V(1)-O(12)	104.72(19)	O(18)-V(2)-V(6)	39.65(12)
O(17)-V(1)-O(12)	80.10(16)	V(8)-V(2)-V(6)	136.29(4)
O(3)-V(1)-O(12)	89.49(16)	O(9)-V(3)-O(17)	108.2(2)
O(11)-V(1)-O(12)	144.99(18)	O(9)-V(3)-O(6)	107.8(2)
O(14)-V(1)-V(7)	112.62(16)	O(17)-V(3)-O(6)	93.28(17)
O(17)-V(1)-V(7)	125.23(13)	O(9)-V(3)-O(1)	110.6(2)
O(3)-V(1)-V(7)	40.08(11)	O(17)-V(3)-O(1)	140.85(18)
O(11)-V(1)-V(7)	40.27(12)	O(6)-V(3)-O(1)	79.93(17)
O(12)-V(1)-V(7)	124.18(12)	O(9)-V(3)-O(4)	107.9(2)
O(14)-V(1)-V(6)	104.00(16)	O(17)-V(3)-O(4)	78.36(16)
O(17)-V(1)-V(6)	39.88(11)	O(6)-V(3)-O(4)	144.19(19)
O(3)-V(1)-V(6)	126.07(12)	O(1)-V(3)-O(4)	84.98(17)
O(11)-V(1)-V(6)	125.47(13)	O(9)-V(3)-V(4)	111.37(16)
O(12)-V(1)-V(6)	40.80(11)	O(17)-V(3)-V(4)	125.60(13)
V(7)-V(1)-V(6)	143.38(4)	O(6)-V(3)-V(4)	39.72(12)
O(13)-V(2)-O(12)	110.1(2)	O(1)-V(3)-V(4)	40.55(11)
O(13)-V(2)-O(2)	106.6(2)	O(4)-V(3)-V(4)	120.91(13)
O(12)-V(2)-O(2)	92.01(17)	O(9)-V(3)-V(6)	110.07(16)
O(13)-V(2)-O(8)	108.1(2)	O(17)-V(3)-V(6)	38.40(12)
O(12)-V(2)-O(8)	141.67(17)	O(6)-V(3)-V(6)	125.74(12)
O(2)-V(2)-O(8)	80.64(17)	O(1)-V(3)-V(6)	119.25(12)
O(13)-V(2)-O(18)	105.17(19)	O(4)-V(3)-V(6)	40.22(11)
O(17)-V(6)-O(4)	79.17(17)	V(4)-V(3)-V(6)	138.49(4)
O(12)-V(6)-O(4)	140.18(18)	O(21)-V(4)-O(1)#1	107.4(2)
O(7)-V(6)-O(18)	109.6(2)	O(21)-V(4)-O(6)	116.7(2)

O(17)-V(6)-O(18)	137.95(18)	O(1)#1-V(4)-O(6)	135.90(18)
O(12)-V(6)-O(18)	78.64(16)	O(21)-V(4)-O(1)	104.5(2)
O(4)-V(6)-O(18)	93.96(17)	O(1)#1-V(4)-O(1)	89.36(17)
O(7)-V(6)-V(1)	113.37(17)	O(6)-V(4)-O(1)	80.90(17)
O(17)-V(6)-V(1)	39.92(12)	O(21)-V(4)-O(5)#1	109.4(2)
O(12)-V(6)-V(1)	41.51(11)	O(1)#1-V(4)-O(5)#1	88.47(17)
O(4)-V(6)-V(1)	114.93(12)	O(6)-V(4)-O(5)#1	76.68(16)
O(18)-V(6)-V(1)	114.97(11)	O(1)-V(4)-O(5)#1	145.10(17)
O(7)-V(6)-V(3)	113.14(17)	O(21)-V(4)-V(4)#1	105.73(17)
O(17)-V(6)-V(3)	38.17(12)	O(1)#1-V(4)-V(4)#1	45.47(12)
O(12)-V(6)-V(3)	114.13(12)	O(6)-V(4)-V(4)#1	117.93(13)
O(4)-V(6)-V(3)	41.26(12)	O(1)-V(4)-V(4)#1	44.73(12)
O(18)-V(6)-V(3)	125.47(13)	O(5)#1-V(4)-V(4)#1	128.80(13)
V(1)-V(6)-V(3)	76.61(3)	O(21)-V(4)-V(3)	113.43(17)
O(7)-V(6)-V(2)	115.08(17)	O(1)#1-V(4)-V(3)	121.32(12)
O(17)-V(6)-V(2)	112.20(13)	O(6)-V(4)-V(3)	39.88(12)
O(12)-V(6)-V(2)	38.14(12)	O(1)-V(4)-V(3)	41.37(12)
O(4)-V(6)-V(2)	124.70(14)	O(5)#1-V(4)-V(3)	114.06(12)
O(18)-V(6)-V(2)	40.55(11)	V(4)#1-V(4)-V(3)	83.17(4)
V(1)-V(6)-V(2)	77.18(3)	O(21)-V(4)-V(5)	119.70(17)
V(3)-V(6)-V(2)	131.02(4)	O(1)#1-V(4)-V(5)	117.46(12)
O(16)-V(7)-O(3)	108.5(2)	O(6)-V(4)-V(5)	36.79(12)
O(16)-V(7)-O(11)	113.2(2)	O(1)-V(4)-V(5)	113.79(12)
O(3)-V(7)-O(11)	81.31(16)	O(5)#1-V(4)-V(5)	39.90(12)
O(16)-V(7)-O(8)#1	109.4(2)	V(4)#1-V(4)-V(5)	134.33(2)
O(3)-V(7)-O(8)#1	82.32(17)	V(3)-V(4)-V(5)	75.31(3)
O(11)-V(7)-O(8)#1	137.28(18)	O(20)-V(5)-O(6)	108.7(2)
O(16)-V(7)-O(19)#1	108.9(2)	O(20)-V(5)-O(11)	109.3(2)
O(3)-V(7)-O(19)#1	142.09(18)	O(6)-V(5)-O(11)	91.40(17)
O(11)-V(7)-O(19)#1	78.31(16)	O(20)-V(5)-V(7)	111.83(17)
O(8)#1-V(7)-O(19)#1	91.43(16)	O(6)-V(5)-V(7)	122.56(12)
O(16)-V(7)-V(8)#1	110.52(17)	O(11)-V(5)-V(7)	37.42(12)
O(3)-V(7)-V(8)#1	40.31(12)	O(19)#1-V(5)-V(7)	40.40(11)
O(11)-V(7)-V(8)#1	115.32(12)	O(5)#1-V(5)-V(7)	125.97(13)
O(8)#1-V(7)-V(8)#1	42.51(12)	O(20)-V(5)-V(4)	112.13(17)
O(19)#1-V(7)-V(8)#1	127.04(13)	O(6)-V(5)-V(4)	36.48(12)
O(16)-V(7)-V(1)	114.22(16)	O(11)-V(5)-V(4)	121.14(12)
O(3)-V(7)-V(1)	40.53(12)	O(19)#1-V(5)-V(4)	123.60(13)
O(11)-V(7)-V(1)	41.05(12)	O(5)#1-V(5)-V(4)	39.86(11)

O(8)#1-V(7)-V(1)	115.65(12)	V(7)-V(5)-V(4)	135.96(4)
O(19)#1-V(7)-V(1)	115.00(12)	O(7)-V(6)-O(17)	112.0(2)
V(8)#1-V(7)-V(1)	78.32(3)	O(7)-V(6)-O(12)	111.0(2)
O(16)-V(7)-V(5)	114.94(17)	O(17)-V(6)-O(12)	80.84(16)
O(3)-V(7)-V(5)	114.93(12)	O(7)-V(6)-O(4)	108.4(2)
O(11)-V(7)-V(5)	38.18(12)	V(7)-O(3)-V(1)	99.39(17)
O(8)#1-V(7)-V(5)	122.05(12)	Sb(2)-O(4)-V(6)	139.6(2)
O(19)#1-V(7)-V(5)	40.29(11)	Sb(2)-O(4)-V(3)	121.87(19)
V(8)#1-V(7)-V(5)	134.03(4)	V(6)-O(4)-V(3)	98.52(17)
V(1)-V(7)-V(5)	77.47(3)	Sb(2)-O(5)-V(4)#1	117.3(2)
O(15)-V(8)-O(3)#1	113.9(2)	Sb(2)-O(5)-V(5)#1	141.0(2)
O(15)-V(8)-O(2)	107.7(2)	V(4)#1-O(5)-V(5)#1	100.24(17)
O(3)#1-V(8)-O(2)	138.34(17)	V(4)-O(6)-V(3)	100.40(19)
O(15)-V(8)-O(2)#1	105.1(2)	V(4)-O(6)-V(5)	106.74(19)
O(3)#1-V(8)-O(2)#1	91.96(17)	V(3)-O(6)-V(5)	146.5(2)
O(2)-V(8)-O(2)#1	80.16(18)	V(2)-O(8)-V(7)#1	147.7(2)
O(15)-V(8)-O(8)	112.2(2)	V(2)-O(8)-V(8)	98.47(17)
O(3)#1-V(8)-O(8)	81.69(16)	V(7)#1-O(8)-V(8)	95.68(17)
O(2)-V(8)-O(8)	79.95(16)	Sb(2)-O(10)-Sb(1)	131.2(2)
O(2)#1-V(8)-O(8)	141.56(17)	V(7)-O(11)-V(1)	98.67(18)
O(15)-V(8)-V(7)#1	116.24(16)	V(7)-O(11)-V(5)	104.40(18)
O(3)#1-V(8)-V(7)#1	40.36(11)	V(1)-O(11)-V(5)	148.1(2)
O(2)-V(8)-V(7)#1	115.94(12)	V(2)-O(12)-V(6)	103.44(18)
O(2)#1-V(8)-V(7)#1	125.72(12)	V(2)-O(12)-V(1)	146.4(2)
O(8)-V(8)-V(7)#1	41.81(12)	Sb(1)-O(18)-V(6)	136.7(2)
O(15)-V(8)-V(8)#1	108.73(16)	Sb(1)-O(18)-V(2)	123.5(2)
O(3)#1-V(8)-V(8)#1	122.87(12)	V(6)-O(18)-V(2)	99.80(18)
O(2)-V(8)-V(8)#1	40.17(12)	Sb(1)-O(19)-V(5)#1	141.9(2)
O(2)#1-V(8)-V(8)#1	40.16(12)	Sb(1)-O(19)-V(7)#1	118.65(19)
O(8)-V(8)-V(8)#1	115.10(12)	V(6)-O(17)-V(1)	100.20(18)
V(7)#1-V(8)-V(8)#1	134.69(3)	V(5)#1-O(19)-V(7)#1	99.32(17)
O(15)-V(8)-V(2)	115.65(17)	C(11)-N(6)-C(10)	112.3(5)
O(3)#1-V(8)-V(2)	113.94(12)	C(11)-N(6)-C(8)	111.2(5)
O(2)-V(8)-V(2)	39.53(12)	C(10)-N(6)-C(8)	111.7(5)
O(2)#1-V(8)-V(2)	113.59(13)	C(4)-N(4)-C(2)	112.0(6)
O(8)-V(8)-V(2)	40.43(12)	C(4)-N(4)-C(6)	112.1(5)
V(7)#1-V(8)-V(2)	79.07(3)	C(2)-N(4)-C(6)	112.9(5)
V(8)#1-V(8)-V(2)	76.98(4)	C(4)-N(4)-Zn(1)	106.9(4)
V(4)#1-O(1)-V(4)	89.80(17)	C(2)-N(4)-Zn(1)	106.1(4)

V(4)#1-O(1)-V(3)	151.9(2)	C(6)-N(4)-Zn(1)	106.3(4)
V(4)-O(1)-V(3)	98.08(18)	C(3)-N(3)-Zn(1)	108.9(4)
V(2)-O(2)-V(8)	100.92(18)	C(5)-N(2)-Zn(1)	109.5(4)
V(2)-O(2)-V(8)#1	145.8(2)	C(7)-N(5)-Zn(1)	117.5(4)
V(8)-O(2)-V(8)#1	99.67(18)	C(1)-N(1)-Zn(1)	112.7(4)
V(8)#1-O(3)-V(7)	99.33(18)	N(6)-C(10)-C(9)	111.4(5)
V(8)#1-O(3)-V(1)	147.9(2)	N(8)-C(12)-C(11)	110.9(5)
O(20)-V(5)-O(19)#1	108.3(2)	N(6)-C(8)-C(7)	113.3(5)
O(6)-V(5)-O(19)#1	142.98(18)	N(6)-C(11)-C(12)	108.0(5)
O(11)-V(5)-O(19)#1	77.67(16)	N(7)-C(9)-C(10)	109.4(5)
O(20)-V(5)-O(5)#1	106.2(2)	N(5)-C(7)-C(8)	113.3(5)
O(6)-V(5)-O(5)#1	76.34(16)	N(2)-C(5)-C(4)	108.2(6)
O(11)-V(5)-O(5)#1	144.41(18)	N(4)-C(6)-C(3)	109.4(5)
O(19)#1-V(5)-O(5)#1	92.15(16)	N(4)-C(2)-C(1)	109.8(6)
V(6)-O(12)-V(1)	97.68(17)	N(4)-C(4)-C(5)	109.7(5)
V(3)-O(17)-V(6)	103.43(19)	N(3)-C(3)-C(6)	109.4(5)
V(3)-O(17)-V(1)	148.8(2)	N(1)-C(1)-C(2)	109.9(5)

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

Table S3 Bond valence sum data for the V atoms.

Atom	Σ s	Atom	Σ s
V1	4.06	V5	3.96
V2	4.04	V6	4.08
V3	4.13	V7	3.99
V4	4.04	V8	4.03

Table S4 Selected bond lengths (Å) and the angles (°) around the Zn^{2+} cation.

distance / Å	angle / °	angle / °
Zn(1)-N(3) 2.066(6)	N(1)-Zn(1)-N(4) 80.0(2)	N(2)-Zn(1)-N(1) 125.9(2)
Zn(1)-N(2) 2.091(5)	N(2)-Zn(1)-N(5) 99.2(2)	N(5)-Zn(1)-N(1) 96.8(2)
Zn(1)-N(5) 2.102(5)	N(3)-Zn(1)-N(2) 118.7(2)	N(3)-Zn(1)-N(4) 81.1(2)
Zn(1)-N(1) 2.103(5)	N(3)-Zn(1)-N(5) 102.9(2)	N(2)-Zn(1)-N(4) 80.3(2)
Zn(1)-N(4) 2.269(5)	N(3)-Zn(1)-N(1) 107.2(2)	N(5)-Zn(1)-N(4) 175.6(2)

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