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Table S1. Crystal data and structure refinement for 1.

Identification code	dave123a
Empirical formula	$H_{100}B_{32}O_{124}V_{12}$
Formula weight	3042.00
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Tetragonal
Space group	I4/m
Unit cell dimensions	a = 21.4932(6) Å alpha = 90° b = 21.4932(6) Å beta = 90° c = 16.6898(6) Å gamma = 90°
Volume, Z	7710.0(4) $Å^3$, 2
Density (calculated)	1.310 Mg/m^3
Absorption coefficient	0.796 mm^{-1}
F(000)	3056
Crystal size	0.14 x 0.12 x 0.12 mm
θ range for data collection	1.34 to 28.42°
Limiting indices	$-27 \le h \le 27$, $-14 \le k \le 26$, $-22 \le l \le 4$
Reflections collected	13850
Independent reflections	4073 (R_{int} = 0.0589)
Absorption correction	Psi
Max. and min. transmission	0.932 and 0.712
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4073 / 0 / 154
Goodness-of-fit on F^2	1.071
Final R indices [I>2σ(I)]	R1 = 0.0580, wR2 = 0.1420
R indices (all data)	R1 = 0.0824, wR2 = 0.1667
Largest diff. peak and hole	0.477 and -0.412 $eÅ^{-3}$

Table S2 . **Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.**

	x	y	z	U(eq)
V(1)	1355(1)	2278(1)	0	47(1)
V(2)	55(1)	2642(1)	0	50(1)
V(3)	2283(1)	1310(1)	0	47(1)
O(1)	1751(2)	2919(2)	0	63(1)
O(2)	9(2)	3370(2)	0	73(1)
O(3)	2956(2)	1630(2)	0	70(1)
O(4)	1750(1)	1707(1)	-746(2)	48(1)
O(5)	1919(1)	2125(1)	-2068(2)	51(1)
O(6)	952(1)	1626(1)	-1752(1)	50(1)
O(7)	1870(1)	3130(1)	-2667(2)	83(1)
O(8)	974(1)	2716(1)	-2072(2)	60(1)
O(9)	673(1)	2371(1)	-748(1)	49(1)
O(10)	14(1)	2183(1)	-1921(2)	56(1)
O(11)	-589(1)	2329(1)	-735(2)	50(1)
O(12)	-1034(1)	1882(1)	-1913(1)	51(1)
B(1)	1630(2)	1606(2)	-1616(3)	53(1)
B(2)	1594(2)	2641(2)	-2270(3)	55(1)
B(3)	653(2)	2211(2)	-1613(3)	49(1)
B(4)	-540(2)	2113(2)	-1521(3)	50(1)

Table S3. **Bond lengths [Å] and angles [°] for 1.**

V(1)-O(1)	1.620(4)	V(1)-O(9)	1.936(2)
V(1)-O(9)#1	1.936(2)	V(1)-O(4)#1	1.944(2)
V(1)-O(4)	1.944(2)	V(1)-V(3)	2.8803(12)
V(1)-V(2)	2.9021(12)	V(2)-O(2)	1.569(4)
V(2)-O(9)#1	1.913(2)	V(2)-O(9)	1.913(2)
V(2)-O(11)	1.967(2)	V(2)-O(11)#1	1.967(2)
V(2)-V(3)#2	3.0345(13)	V(3)-O(3)	1.602(4)
V(3)-O(4)	1.894(2)	V(3)-O(4)#1	1.894(2)
V(3)-O(11)#3	1.979(2)	V(3)-O(11)#4	1.979(2)
V(3)-V(2)#4	3.0345(13)	O(4)-B(1)	1.490(5)
O(5)-B(2)	1.353(5)	O(5)-B(1)	1.484(5)
O(6)-B(3)	1.432(5)	O(6)-B(1)	1.474(5)
O(7)-B(2)	1.376(5)	O(8)-B(2)	1.383(5)
O(8)-B(3)	1.497(5)	O(9)-B(3)	1.486(5)
O(10)-B(4)	1.372(5)	O(10)-B(3)	1.468(5)
O(11)-B(4)	1.396(5)	O(11)-V(3)#2	1.979(2)
O(12)-B(4)	1.343(5)	O(12)-B(1)#2	1.432(5)
B(1)-O(12)#3	1.432(5)		

O(1)-V(1)-O(9)	108.01(12)	O(1)-V(1)-O(9)#1	108.01(12)
O(9)-V(1)-O(9)#1	80.28(14)	O(1)-V(1)-O(4)#1	107.96(12)
O(9)-V(1)-O(4)#1	144.03(11)	O(9)#1-V(1)-O(4)#1	89.03(10)
O(1)-V(1)-O(4)	107.96(12)	O(9)-V(1)-O(4)	89.03(10)
O(9)#1-V(1)-O(4)	144.03(11)	O(4)#1-V(1)-O(4)	79.72(14)
O(2)-V(2)-O(9)#1	110.34(14)	O(2)-V(2)-O(9)	110.35(14)
O(9)#1-V(2)-O(9)	81.42(14)	O(2)-V(2)-O(11)	107.22(14)
O(9)#1-V(2)-O(11)	142.29(11)	O(9)-V(2)-O(11)	88.75(10)
O(2)-V(2)-O(11)#1	107.22(14)	O(9)#1-V(2)-O(11)#1	88.75(10)
O(9)-V(2)-O(11)#1	142.29(11)	O(11)-V(2)-O(11)#1	77.1(2)
O(3)-V(3)-O(4)	110.66(13)	O(3)-V(3)-O(4)#1	110.66(13)
O(4)-V(3)-O(4)#1	82.2(2)	O(3)-V(3)-O(11)#3	106.91(14)
O(4)-V(3)-O(11)#3	88.58(10)	O(4)#1-V(3)-O(11)#3	142.20(11)
O(3)-V(3)-O(11)#4	106.91(14)	O(4)-V(3)-O(11)#4	142.20(11)
O(4)#1-V(3)-O(11)#4	88.58(10)	O(11)#3-V(3)-O(11)#4	76.6(2)
B(1)-O(4)-V(3)	132.9(2)	B(1)-O(4)-V(1)	129.8(2)
V(3)-O(4)-V(1)	97.26(12)	B(2)-O(5)-B(1)	121.9(3)
B(3)-O(6)-B(1)	116.4(3)	B(2)-O(8)-B(3)	118.8(3)
B(3)-O(9)-V(2)	133.2(2)	B(3)-O(9)-V(1)	128.7(2)
V(2)-O(9)-V(1)	97.87(11)	B(4)-O(10)-B(3)	130.2(3)
B(4)-O(11)-V(2)	130.2(2)	B(4)-O(11)-V(3)#2	128.7(2)
V(2)-O(11)-V(3)#2	100.51(12)	B(4)-O(12)-B(1)#2	130.6(3)
O(12)#3-B(1)-O(6)	110.3(3)	O(12)#3-B(1)-O(5)	108.1(3)
O(6)-B(1)-O(5)	108.3(3)	O(12)#3-B(1)-O(4)	113.3(3)
O(6)-B(1)-O(4)	108.6(3)	O(5)-B(1)-O(4)	108.2(3)
O(5)-B(2)-O(7)	121.6(4)	O(5)-B(2)-O(8)	122.2(3)
O(7)-B(2)-O(8)	116.2(4)	O(6)-B(3)-O(10)	109.1(3)
O(6)-B(3)-O(9)	110.3(3)	O(10)-B(3)-O(9)	112.1(3)
O(6)-B(3)-O(8)	110.4(3)	O(10)-B(3)-O(8)	106.4(3)
O(9)-B(3)-O(8)	108.4(3)	O(12)-B(4)-O(10)	119.3(4)
O(12)-B(4)-O(11)	121.4(4)	O(10)-B(4)-O(11)	119.1(4)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,-z #2 -y,x,z #3 y,-x,z #4 y,-x,-z

Table S4. **Anisotropic displacement parameters [$Å^2$ x 10^3] for 1.**

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
V(1)	33(1)	33(1)	74(1)	0	0	-1(1)
V(2)	36(1)	38(1)	77(1)	0	0	0(1)
V(3)	35(1)	33(1)	73(1)	0	0	-2(1)
O(1)	41(2)	37(2)	112(3)	0	0	-2(2)
O(2)	60(3)	49(3)	111(3)	0	0	8(2)
O(3)	43(2)	62(3)	105(3)	0	0	-4(2)
O(4)	39(2)	32(1)	72(2)	2(1)	3(1)	6(1)
O(5)	37(1)	37(2)	79(2)	14(1)	12(1)	4(1)
O(6)	42(2)	39(2)	67(2)	5(1)	3(1)	-8(1)
O(7)	49(2)	60(2)	139(3)	36(2)	17(2)	2(2)
O(8)	38(2)	44(2)	99(2)	21(1)	5(1)	4(1)
O(9)	32(1)	45(2)	69(2)	2(1)	4(1)	2(1)
O(10)	35(2)	64(2)	68(2)	9(1)	-2(1)	-2(1)
O(11)	27(1)	41(2)	80(2)	2(1)	1(1)	-4(1)
O(12)	38(2)	48(2)	67(2)	10(1)	-7(1)	-5(1)
B(1)	44(3)	43(3)	70(3)	9(2)	8(2)	-6(2)
B(2)	41(3)	39(3)	84(3)	13(2)	6(2)	-1(2)
B(3)	37(2)	42(3)	69(3)	1(2)	7(2)	0(2)
B(4)	37(2)	47(3)	67(3)	9(2)	0(2)	-1(2)

Table S5. **Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.**

	x	y	z	U(eq)
H(5A)	2335(1)	2095(1)	-2217(2)	61
H(6A)	731(1)	1277(1)	-1919(1)	60
H(7A)	2237(1)	3050(1)	-2748(2)	65
H(8A)	760(1)	3074(1)	-2220(2)	72