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

Electronic Supplementary Information

The origin of the electronic transitions of mixed valence polyoxovanadoborates [$V_{12}B_{18}O_{60}$]. From an experimental and theoretical understanding.

*Patricio Hermosilla-Ibáñez [a,b], Kerry Wrighton-Araneda [a,b], Laura Scarpetta-Pizo [a,b], Walter Cañón-Mancisidor [a,b], Marlen Gutierrez-Cutiño [a,b], Eric Le Fur [c], Verónica Paredes-García [b,d], and Diego Venegas-Yazigi [a,b]**

[a.] *Universidad de Santiago de Chile, Facultad de Química y Biología, Departamento de Química de los Materiales, Chile.*

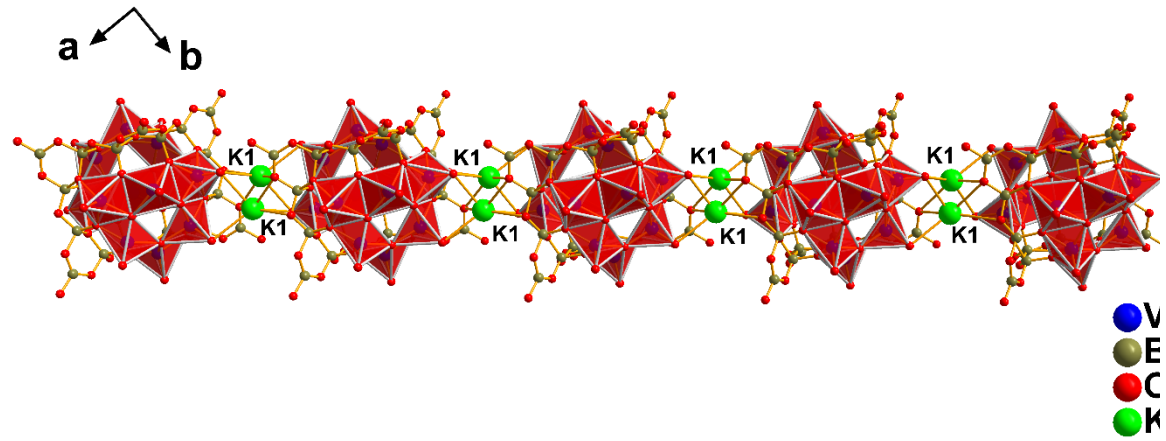
[b.] *Centro para el Desarrollo de la Nanociencia y la Nanotecnología, CEDENNA, Chile.*

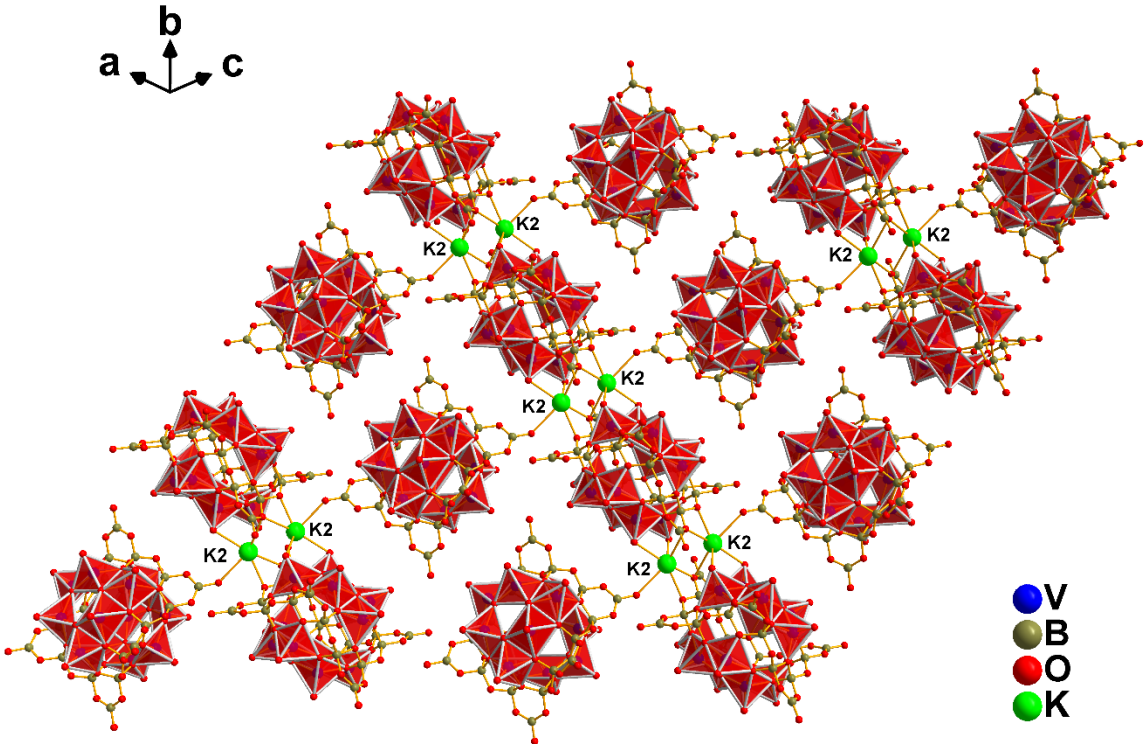
[c.] *Ecole Nationale Supérieure de Chimie de Rennes, CNRS, UMR 6226, "Institut des Sciences Chimiques de Rennes", 11 Allée de Beaulieu, CS 50837, 35708 Rennes cedex 7, France*

[d.] *Universidad Andres Bello, Facultad de Ciencias Exactas, Departamento de Ciencias Químicas, Chile.*

E-mail: diego.venegas@usach.cl; Tel:(+)56-2-27181079

Figures





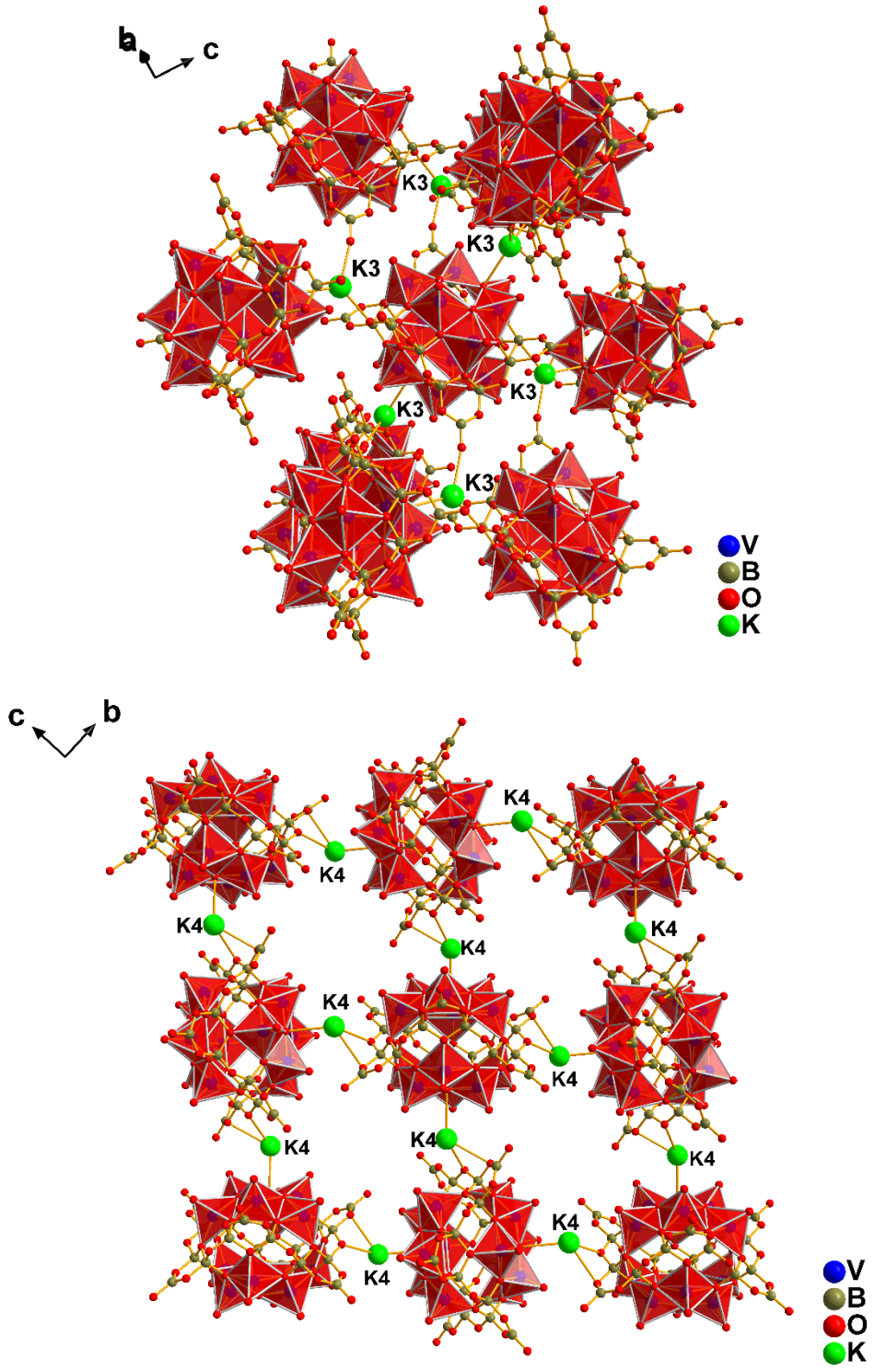
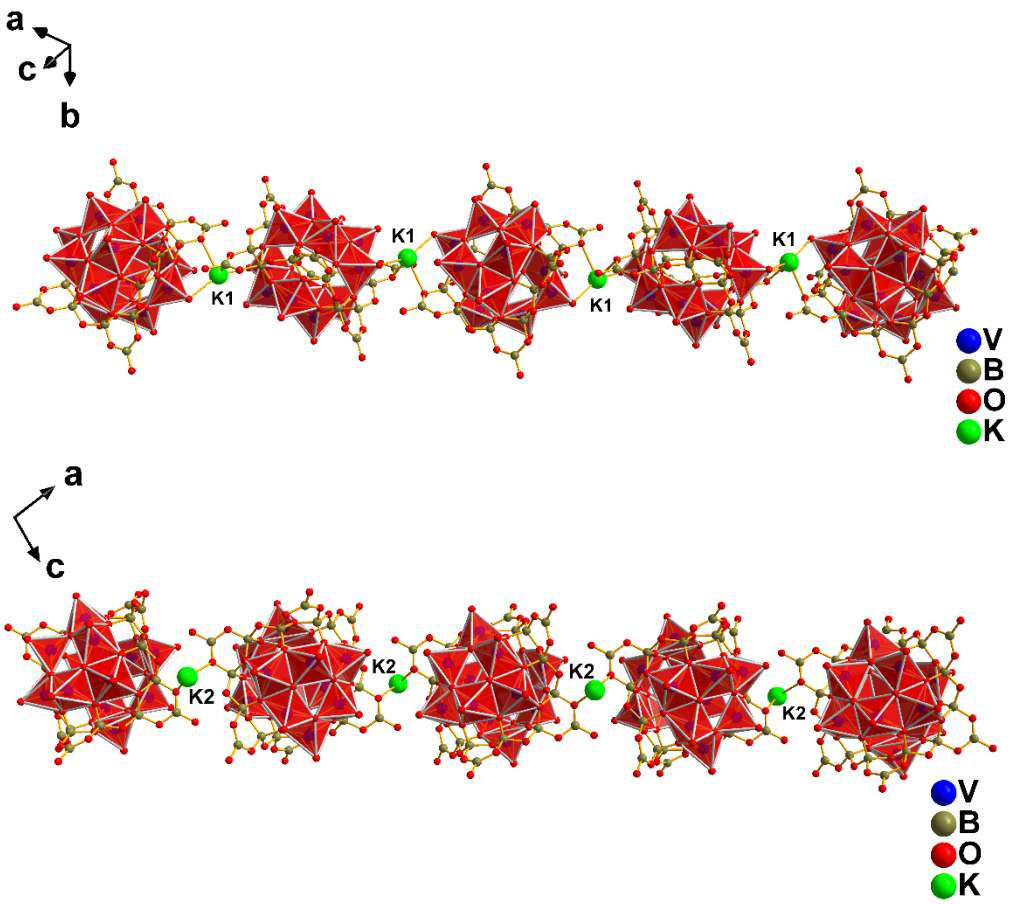


Figure S1. Connectivities of BVO polyanions through potassium cations K1, K2, K3 and K4 in compound **1.**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K

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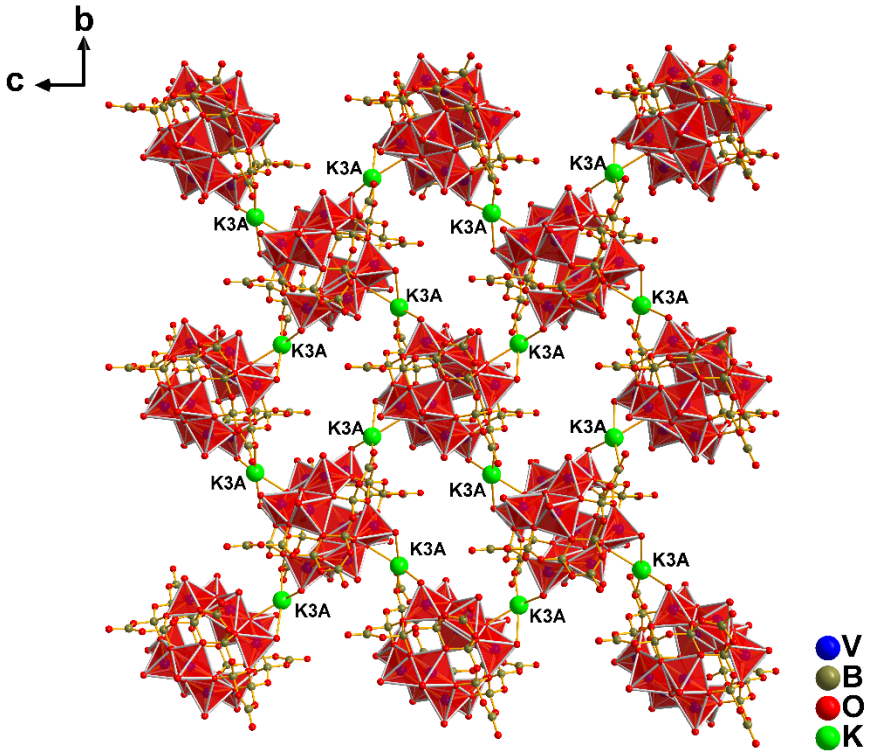
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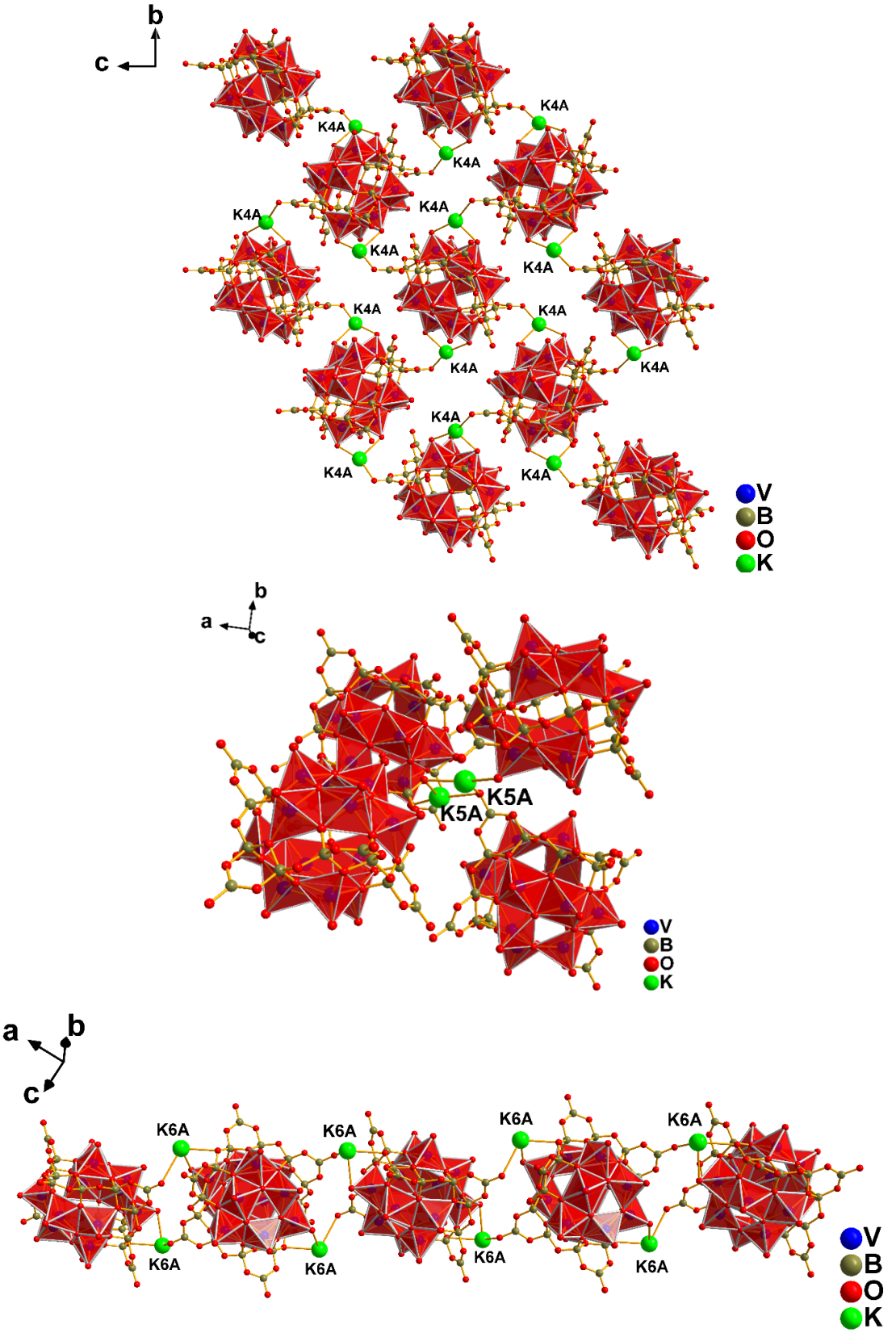

Figure S2. Connectivities of BVO polyanions through potassium cations K1, K2, K3A, K4A, K5A and K6A in compound **2.**

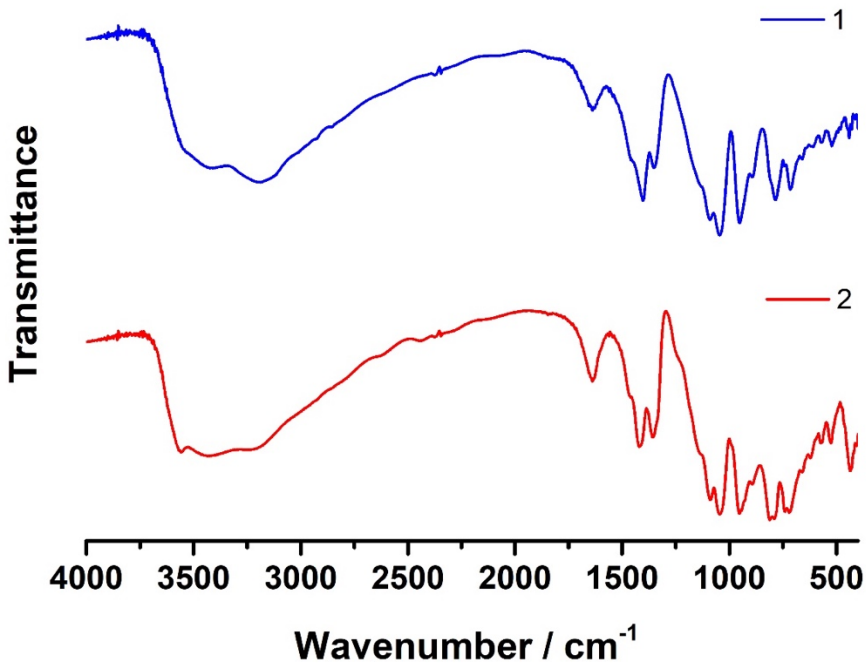

Figure S3. FTIR in KBr disk spectra in the 400 to 4000 cm^{-1} region for compound **1** and **2**.

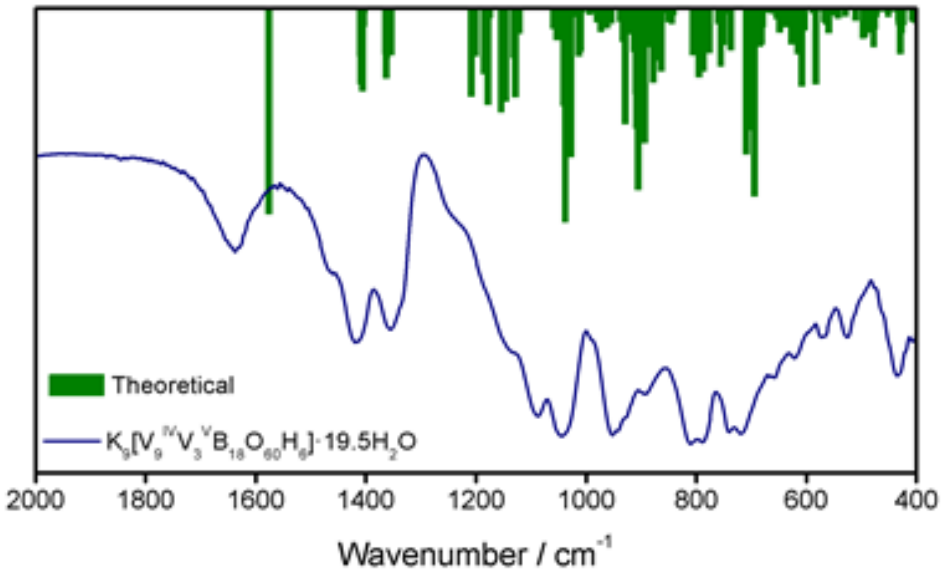

Figure S4. Overlapped spectrum between theoretical absorption and experimental FITR spectrum of **2**.

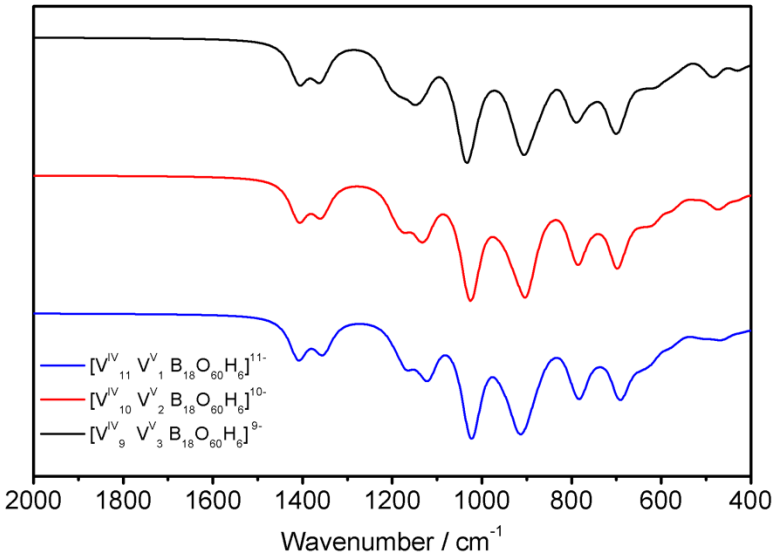

Figure S5. Simulated FTIR spectra of $[V^{IV}_9V^{V}_3B_{18}O_{60}H_6]^{9-}$, $[V^{IV}_{10}V^{V}_2B_{18}O_{60}H_6]^{10-}$ and $[V^{IV}_{11}V^{V}_1B_{18}O_{60}H_6]^{11-}$ clusters. The spectra were simulated considering a FWHM of 25 cm^{-1}.

Tables

Table S1. Selected bond distances (Å) for $[V_{12}B_{18}O_{60}]$ for compound **1**

V1	O1	2.003(5)	V3	O6	1.933(6)	V5	O12	1.926(5)
V1	O2	1.933(6)	V3	O7	1.948(6)	V5	O13	1.943(6)
V1	O3	1.957(5)	V3	O9	1.946(5)	V5	O15	2.006(6)
V1	O4	1.914(6)	V3	O10	1.621(7)	V5	O16	1.938(5)
V1	O5	1.623(6)	V3	O11	2.006(7)	V5	O17	1.612(5)
V2	O3	1.931(6)	V4	O7	1.935(5)	V6	O2	1.958(5)
V2	O4	1.960(6)	V4	O9	1.944(6)	V6	O3	1.945(6)
V2	O6	1.956(7)	V4	O12	1.944(5)	V6	O13	1.931(5)
V2	O7	1.934(6)	V4	O13	1.935(5)	V6	O16	1.932(6)
V2	O8	1.623(6)	V4	O14	1.622(6)	V6	O18	1.613(6)
B1	O6	1.465(12)	B2	$O2^{i}$	1.461(12)	B3	$O1^{i}$	1.530(11)
B1	$O15^{i}$	1.502(11)	B2	O11	1.505(13)	B3	O9	1.465(11)
B1	O22	1.500(11)	B2	O23	1.431(10)	B3	$O20^{i}$	1.479(9)
B1	$O26^{i}$	1.431(14)	B2	$O29^{i}$	1.484(10)	B3	O23	1.421(10)
B4	$O4^{i}$	1.466(11)	B5	$O11^{i}$	1.515(10)	B6	O27	1.350(17)
B4	O15	1.517(11)	B5	O16	1.473(12)	B6	O28	1.406(14)
B4	O24	1.428(12)	B5	O26	1.444(14)	B6	O29	1.347(15)
B4	O25	1.472(11)	B5	O27	1.488(12)			
B7	O19	1.373(14)	B8	O1	1.506(10)	B9	$O22^{i}$	1.351(17)
B7	O20	1.353(12)	B8	$O12^{i}$	1.478(9)	B9	O25	1.336(18)
B7	O21	1.376(11)	B8	O19	1.491(9)	B9	O30	1.372(16)
			B8	$O24^{i}$	1.423(10)			

Symmetry code: i 0.5-x, 0.5-y,1-z

Table S2. Selected angles (º) for $[V_{12}B_{18}O_{60}]$ for compound **1**

O2	V1	O1	90.3(2)	O3	V2	O4	77.5(2)	O6	V3	O7	78.9(3)
O2	V1	O3	79.1(2)	O3	V2	O6	144.8(2)	O6	V3	O9	138.1(2)
O3	V1	O1	147.2(2)	O3	V2	O7	95.0(2)	O6	V3	O11	89.9(3)
O4	V1	O1	90.8(2)	O6	V2	O4	87.8(2)	O7	V3	O11	145.5(2)
O4	V1	O2	138.7(2)	O7	V2	O4	144.5(2)	O9	V3	O7	77.8(2)
O4	V1	O3	78.0(2)	O7	V2	O6	78.7(2)	O9	V3	O11	90.0(2)
O5	V1	O1	105.3(3)	O8	V2	O3	106.3(4)	O10	V3	O6	108.8(4)
O5	V1	O2	110.9(4)	O8	V2	O4	109.8(3)	O10	V3	O7	107.0(4)
O5	V1	O3	107.5(3)	O8	V2	O6	108.8(4)	O10	V3	O9	111.1(3)
O5	V1	O4	108.5(4)	O8	V2	O7	105.6(3)	O10	V3	O11	107.5(4)
O7	V4	O9	78.1(2)	O12	V5	O13	78.7(2)	O3	V6	O2	78.7(2)
O7	V4	O12	144.8(2)	O12	V5	O15	90.3(2)	O13	V6	O2	143.9(2)
O7	V4	O13	93.2(2)	O12	V5	O16	139.2(2)	O13	V6	O3	92.9(2)
O12	V4	O9	88.7(2)	O13	V5	O15	145.8(2)	O13	V6	O16	78.9(2)
O13	V4	O9	144.1(2)	O16	V5	O13	78.5(2)	O16	V6	O2	87.6(2)
O13	V4	O12	78.5(2)	O16	V5	O15	89.9(2)	O16	V6	O3	144.4(2)
O14	V4	O7	106.7(3)	O17	V5	O12	109.6(3)	O18	V6	O2	108.8(3)
O14	V4	O9	109.1(3)	O17	V5	O13	107.7(3)	O18	V6	O3	108.8(4)
O14	V4	O12	108.4(3)	O17	V5	O15	106.5(3)	O18	V6	O13	107.2(3)
O14	V4	O13	106.7(3)	O17	V5	O16	109.5(3)	O18	V6	O16	106.7(4)
O6	B1	$O15^i$	108.8(7)	$O2^i$	B2	O11	107.9(6)	O9	B3	$O1^i$	107.5(6)
O6	B1	O22	109.7(9)	$O2^i$	B2	$O29^i$	109.9(8)	O9	B3	$O20^i$	110.1(7)
O22	B1	$O15^i$	108.7(7)	O23	B2	$O2^i$	111.0(7)	$O20^i$	B3	$O1^i$	108.2(6)
$O26^i$	B1	O6	110.0(8)	O23	B2	O11	113.0(8)	O23	B3	$O1^i$	112.2(7)
$O26^i$	B1	$O15^i$	113.2(9)	O23	B2	$O29^i$	106.1(6)	O23	B3	O9	110.8(7)
$O26^i$	B1	O22	106.5(8)	$O29^i$	B2	O11	108.8(7)	O23	B3	$O20^i$	108.1(6)
$O4^i$	B4	O15	108.3(6)	O16	B5	$O11^i$	107.4(6)	O27	B6	O28	118.7(11)
$O4^i$	B4	O25	109.1(7)	O16	B5	O27	108.9(9)	O29	B6	O27	125.2(10)
O24	B4	$O4^i$	111.0(8)	O26	B5	$O11^i$	113.2(9)	O29	B6	O28	116.1(12)
O24	B4	O15	112.3(7)	O26	B5	O16	110.9(7)				
O24	B4	O25	106.1(7)	O26	B5	O27	107.3(7)				
O25	B4	O15	109.9(8)	O27	B5	$O11^i$	109.1(7)				

O19	B7	O21	119.7(9)	$O12^{i}$	B8	O1	107.8(5)	$O24^{i}$	B8	O19	107.1(6)
O20	B7	O19	122.6(8)	$O12^{i}$	B8	O19	108.4(6)				
O20	B7	O21	117.7(10)	O19	B8	O1	109.3(6)	$O22^{i}$	B9	O30	116.5(14)
				$O24^{i}$	B8	O1	113.5(6)	O25	B9	$O22^{i}$	124.1(10)
				$O24^{i}$	B8	$O12^{i}$	110.5(6)	O25	B9	O30	119.4(12)

Symmetry code: i 0.5-x, 0.5-y,1-z

Table S3. Selected bond distances (Å) for $[V_{12}B_{18}O_{60}]$ for compound **2**

V1 O1 1.622(4)	V2 O2 1.640(4)	V3 O3 1.622(4)
V1 O7 2.007(4)	V2 O9 1.937(4)	V3 O11 1.938(4)
V1 O8 1.935(4)	V2 O10 1.932(4)	V3 O12 1.954(4)
V1 O9 1.938(4)	V2 O11 1.971(4)	V3 O13 2.012(4)
V1 O10 1.940(4)	V2 O12 1.924(4)	V3 O14 1.935(4)
V4 O4 1.616(4)	V5 O5 1.622(4)	V6 O6 1.622(4)
V4 O12 1.924(4)	V5 O15 1.916(4)	V6 O8 1.965(4)
V4 O14 1.944(4)	V5 O16 1.947(4)	V6 O10 1.923(4)
V4 O15 1.944(4)	V5 O17 2.000(4)	V6 O16 1.936(4)
V4 O16 1.936(4)	V5 O18 1.932(4)	V6 O18 1.954(4)
	B2 O13 1.492(7)	B3 $O8^{i}$ 1.467(7)
B1 O21 1.369(7)	B2 $O18^{i}$ 1.459(7)	B3 O13 1.523(7)
B1 O22 1.358(7)	B2 O20 1.457(7)	B3 O19 1.433(7)
B1 O23 1.377(8)	B2 O21 1.481(7)	B3 O22 1.488(7)
B4 O7 1.512(7)	B5 O9 1.483(7)	B6 O26 1.364(7)
B4 $O15^{i}$ 1.461(7)	B5 $O17^{i}$ 1.516(7)	B6 O27 1.378(7)
B4 O24 1.433(7)	B5 O24 1.422(7)	B6 O28 1.339(7)
B4 O25 1.491(7)	B5 O28 1.487(7)	
B7 O11 1.461(7)	B8 $O7^{i}$ 1.511(7)	B9 O25 1.349(7)
B7 $O17^{i}$ 1.511(7)	B8 O14 1.482(6)	B9 $O29^{i}$ 1.360(7)
B7 O20 1.469(7)	B8 O19 1.434(7)	B9 O30 1.373(7)
B7 O26 1.472(7)	B8 O29 1.470(7)	

Symmetry code: i 1.5-x, 0.5-y, 2-z

Table S4. Selected angles (º) for $[V_{12}B_{18}O_{60}]$ for compound **2**

O1	V1	O7	106.43(18)	O2	V2	O9	107.55(18)	O3	V3	O11	109.03(18)
O1	V1	O8	109.40(19)	O2	V2	O10	106.40(18)	O3	V3	O12	105.93(18)
O1	V1	O9	108.05(18)	O2	V2	O11	109.60(18)	O3	V3	O13	107.52(18)
O1	V1	O10	107.55(19)	O2	V2	O12	107.96(18)	O3	V3	O14	111.21(19)
O8	V1	O7	91.21(15)	O9	V2	O11	88.35(16)	O11	V3	O12	77.32(16)
O8	V1	O9	140.42(16)	O10	V2	O9	78.20(16)	O11	V3	O13	91.41(16)
O8	V1	O10	79.04(16)	O10	V2	O11	143.90(17)	O12	V3	O13	146.55(16)
O9	V1	O7	90.18(16)	O12	V2	O9	144.38(16)	O14	V3	O11	137.36(17)
O9	V1	O10	77.97(16)	O12	V2	O10	94.48(16)	O14	V3	O12	78.71(16)
O10	V1	O7	145.98(16)	O12	V2	O11	77.22(15)	O14	V3	O13	89.59(16)
O4	V4	O12	107.03(19)	O5	V5	O15	109.69(19)	O6	V6	O8	108.04(19)
O4	V4	O14	107.56(19)	O5	V5	O16	106.84(19)	O6	V6	O10	109.02(19)
O4	V4	O15	108.77(19)	O5	V5	O17	104.62(18)	O6	V6	O16	107.07(19)
O4	V4	O16	106.01(19)	O5	V5	O18	110.07(18)	O6	V6	O18	108.70(19)
O12	V4	O14	79.24(16)	O15	V5	O16	79.12(16)	O10	V6	O8	78.74(16)
O12	V4	O15	144.09(17)	O15	V5	O17	89.68(16)	O10	V6	O16	92.20(16)
O12	V4	O16	94.20(16)	O15	V5	O18	138.72(17)	O10	V6	O18	142.20(17)
O14	V4	O15	87.43(16)	O16	V5	O17	148.53(16)	O16	V6	O8	144.80(16)
O16	V4	O14	146.26(17)	O18	V5	O16	79.29(16)	O16	V6	O18	79.02(16)
O16	V4	O15	78.70(16)	O18	V5	O17	90.76(16)	O18	V6	O8	87.55(16)
				$O18^{i}$	B2	O13	109.9(4)	$O8^{i}$	B3	O13	108.0(4)
O21	B1	O23	120.1(5)	$O18^{i}$	B2	O21	109.6(5)	$O8^{i}$	B3	O22	110.3(4)
O22	B1	O21	122.5(5)	O20	B2	O13	113.3(5)	O19	B3	$O8^{i}$	110.8(4)
O22	B1	O23	117.3(5)	O20	B2	$O18^{i}$	108.4(4)	O19	B3	O13	113.0(4)
				O20	B2	O21	106.3(4)	O19	B3	O22	106.8(4)
				O21	B2	O13	109.4(4)	O22	B3	O13	107.8(4)
$O15^{i}$	B4	O7	108.0(4)	O25	B4	O7	108.8(4)	O24	B5	O28	108.1(4)
$O15^{i}$	B4	O25	108.5(4)					O28	B5	$O17^{i}$	107.6(4)
O24	B4	O7	112.8(5)	O9	B5	$O17^{i}$	108.8(4)				
O24	B4	$O15^{i}$	111.4(5)	O9	B5	O28	108.8(4)	O26	B6	O27	116.9(5)
O24	B4	O25	107.1(4)	O24	B5	O9	109.9(5)	O28	B6	O26	123.2(5)
				O24	B5	$O17^{i}$	113.5(5)	O28	B6	O27	119.9(5)

O11	B7	O17^{i}	108.1(4)	O14	B8	O7^{i}	107.3(4)	O29	B8	O14	110.5(4)
O11	B7	O20	109.9(4)	O19	B8	O7^{i}	112.5(4)	O25	B9	O29^{i}	122.4(5)
O11	B7	O26	110.7(4)	O19	B8	O14	110.3(4)	O25	B9	O30	120.6(5)
O20	B7	O17^{i}	111.3(4)	O19	B8	O29	107.7(4)	O29^{i}	B9	O30	117.0(5)
O20	B7	O26	106.2(4)	O29	B8	O7^{i}	108.7(4)				
O26	B7	O17^{i}	110.7(4)								

Symmetry code: i 1.5-x, 0.5-y, 2-z

Table S5. Bond Valence Sum (BVS) calculations based on X-ray crystallographic data.

$[V_9^{IV}V_3^{V}B_{18}O_{60}]$	Compound **1**		Compound **2**	
	V(IV)	V(V)	V(IV)	V(V)
V1	4.10	4.32	4.07	4.29
V2	4.13	4.35	4.09	4.31
V3	4.05	4.27	4.05	4.26
V4	4.18	4.40	4.22	4.45
V5	4.13	4.35	4.12	4.34
V6	4.20	4.43	4.15	4.37
mean calculated value	**4.24**		**4.23**	

Table S6. Bond Valence Sum calculations for vanadium atoms of the relaxed structures of $[V^{IV}_{9}V^{V}_{3}\ B_{18}O_{60}H_6]^{9-}$, $[V^{IV}_{10}V^{V}_{2}B_{18}O_{60}H_6]^{10-}$ and $[V^{IV}_{11}V^{V}_{1}B_{18}O_{60}H_6]^{11-}$ clusters.

cluster		$[V^{IV}_{9}V^{V}_{3}\ B_{18}O_{60}H_6]^{9-}$		$[V^{IV}_{10}V^{V}_{2}B_{18}O_{60}H_6]^{10-}$		$[V^{IV}_{11}V^{V}_{1}B_{18}O_{60}H_6]^{11-}$	
	Atoms	V^{IV}	V^{V}	V^{IV}	V^{V}	V^{IV}	V^{V}
Bond -Valence Sum	V (1)	3.88	4.08	3.89	4.09	3.89	4.09
	V (2)	4.74	**4.99**	4.75	**5.00**	4.75	**5.01**
	V (3)	4.00	4.21	3.89	4.09	3.89	4.10
	V (4)	4.73	**4.98**	3.99	4.21	4.00	4.21
	V (5)	3.90	4.11	3.90	4.10	3.90	4.10
	V (6)	3.90	4.11	3.99	4.20	3.99	4.20
	V (7)	4.74	**4.99**	3.89	4.09	3.90	4.11
	V (8)	3.90	4.10	4.75	**5.00**	3.98	4.19
	V (9)	3.89	4.09	3.89	4.09	3.90	4.11
	V (10)	3.98	4.19	3.99	4.21	3.98	4.19
	V (11)	3.99	4.20	3.90	4.10	3.90	4.11
	V (12)	3.90	4.11	3.99	4.20	3.98	4.19

Table S7. Distribution of Spin density for each mixed valence degree of the vanadium centres for $[V^{IV}_{9}V^{V}_{3}\ B_{18}O_{60}H_6]^{9-}$, $[V^{IV}_{10}V^{V}_{2}B_{18}O_{60}H_6]^{10-}$, $[V^{IV}_{11}V^{V}_{1}B_{18}O_{60}H_6]^{11-}$ clusters.

Atoms	$[V^{IV}_{9}V^{V}_{3}\ B_{18}O_{60}H_6]^{9-}$	$[V^{IV}_{10}V^{V}_{2}B_{18}O_{60}H_6]^{10-}$	$[V^{IV}_{11}V^{V}_{1}B_{18}O_{60}H_6]^{11-}$
V (1)	1.17	1.17	1.17
V (2)	**0.02**	**0.03**	**0.03**
V (3)	1.15	1.17	1.17
V (4)	**0.03**	1.15	1.15
V (5)	1.17	1.18	1.18
V (6)	1.17	1.15	1.15
V (7)	**0.03**	1.17	1.17
V (8)	1.17	**0.03**	1.16
V (9)	1.17	1.17	1.17
V (10)	1.16	1.15	1.16
V (11)	1.15	1.18	1.17
V (12)	1.18	1.15	1.16

Table S8. Summary of the principal vibration for **2** and their assignment according to DFT calculations ($[V^{IV}_{9}V^{V}_{3}\ B_{18}O_{60}H_{6}]^{9-}$).

$\bar{\nu}_{exp}$ (cm^{-1})	$\bar{\nu}_{theo}$ (cm^{-1})	Assignment
1630–1640	1576	H–O–H Water scissoring
1407–1424	1408	B_{tri}–O–H scissoring; O–B_{tri} symmetric stretching
1349–1365	1363	O–B_{tri}–OH asymmetric stretching
1146–1147	1154	*B_{tetra}–O–B_{tetra} scissoring; B_{tri}–O–H scissoring
1082–1095	1128	* B_{tetra} –O– B_{tetra} asymmetric stretching; B_{tri}–O–H scissoring
1043–1053	1038	* O–B_{tetra}–O asymmetric stretching; B_{tri}–O–H scissoring
949–958	928	V_B–O_t symmetric stretching; O–B_{tetra}–O asymmetric stretching; O–V_B–O symmetric stretching
889-899	894	O–B_{tetra}–O symmetric stretching; O–B_{tri}–OH symmetric stretching
816-799	805	O–B_{tetra}–O asymmetric stretching, B_{tri}–O–H scissoring
784–791	794	B_{tetra} –O– B_{tetra} asymmetric stretching; B_{tri}–O–H scissoring
714-726	709	*V–O–V asymmetric stretching; O–B_{tetra}–O symmetric stretching

*: indicate the major contribution

Table S9. Summary of the principal vibration for **3** and their assignment according to DFT calculations ($[V^{IV}_{10}V^{V}_{2}B_{18}O_{60}H_{6}]^{10-}$).

$\bar{\nu}_{exp}$ (cm^{-1})	$\bar{\nu}_{theo}$ (cm^{-1})	Assignment
1630–1640	1576	H–O–H Water scissoring
1420–1425	1408	B_{tri}–O–H scissoring; O–B_{tri} symmetric stretching
1352–1358	1363	O–B_{tri}–OH asymmetric stretching
1145–1147	1173	*B_{tetra}–O–B_{tetra} scissoring; B_{tri}–O–H scissoring
1088–1092	1139	* O–B_{tetra}–O asymmetric stretching; B_{tri}–O–H scissoring
1042–1046	1023	*B_{tri} –O– H scissoring; O–B_{tetra}–O symmetric stretching
949–951	901	V(big triangle)–O_t symmetric stretching; O–B_{tetra}–O asymmetric stretching; O–V(big triangle)–O symmetric stretching
784–788	784	O–B_{tetra}– O asymmetric stretching
713–717	698	*V–O–V asymmetric stretching; O–B_{tetra}–O symmetric stretching

*: indicate the major contribution

Table S10. Summary of the principal vibration for **4** and their assignment according to DFT calculations ($[V^{IV}_{11}V^{V}_{1}B_{18}O_{60}H_6]^{11-}$).

$\bar{\nu}_{exp}$ (cm^{-1})	$\bar{\nu}_{theo}$ (cm^{-1})	Assignment
1640-1610	1660	H-N-H scissoring.
	1576	H–O–H Water scissoring
1524-1500	1568	H-N-H Wagging.
1410–1390	1410	B_{tri}–O–H scissoring; O–B_{tri} asymmetric stretching.
	1387	Twisting H–C–H and wagging H-N-H.
1367–1350	1350	O–B_{tri}–OH asymmetric stretching.
1153–1141	1169	*B_{tetra}–O–B_{tetra} symmetric stretching; O–B_{tetra}–O symmetric stretching; B_{tri}–O–H scissoring.
1064–1034	1022	*B_{tri}–O–H scissoring; O–B_{tetra}–O symmetric stretching
	1064	H–C–H Twisting; H-N-H T Wagging.
963–934	904	B_{tetra}–O–B_{tetra} symmetric stretching; O–B_{tri} symmetric stretching; V(big triangle)–O_t symmetric stretching; B_{tri}–O–H scissoring.
800–780	780	B_{tetra}–O–B_{tetra} asymmetric stretching
727–710	694	*V–O–V asymmetric stretching; O–B_{tetra}–O symmetric stretching.

Table S11. Electronic parameters of the most intense excitation for Band I, II and III of mixed valence cluster $[V^{IV}_9V^{V}_3B_{18}O_{60}H_6]^{9-}$, $[V^{IV}_{10}V^{V}_2B_{18}O_{60}H_6]^{10-}$ and $[V^{IV}_{11}V^{V}_1B_{18}O_{60}H_6]^{11-}$. H = Homo and L = Lumo.

	Band	λ / nm	Assignments	*f*	Orbital Contribution
$V^{IV}_9V^{V}_3$	I	787	d-d V^{IV} (d_{xy}) → V^{IV} (d_{xz-yz})	0.0006	H-(α) → L+17(α) (14%); H-2(α) → L+2 (α) (6%); H-2(α) → L+16(α) (7%)
		723	IVCT V^{IV}(d_{xy}) → V^{V} (d_{xy})	0.0012	H-3 (α) → L + 1 (α) (11%); H-3(α) → L+19(α) (16%); H-3(α) → L+4 (α) (4%)
	II	593	d-d V^{IV} (d_{xy}) → V^{IV} ($d_{x^2-y^2}$) IVCT V^{IV} (d_{xy}) → V^{V} (d_{xy})	0.0023	H-2(α) → L+2 (α) (26%); H-1(α) → L+2 (α) (22%); H-(α) → L+29(A) (8%)
		536	IVCT V^{IV} (d_{xy}) → V^{V} (d_{xy})	0.0085	H-3(α) → L+1 (α) (55%); H-1(α) → L (α) (15%); H-2 (α) → L(α) (4%)
	III	353	LMCT O($p_{x,y}$) → V^{IV} (d_{xy})	0.0059	H-10(α) → L (α) (13%); H-1(β) → L (β) (26%); H-3 (β) → L (β) (5%)
		328	IVCT V^{IV} (d_{xy}) → V^{IV} (d_{xz-yz}) LMCT O($p_{x,y}$) → V^{IV} (d_{xz-yz})	0.0074	H-10(α) → L+2(α) (16%); H-1(β) → L+2(β) (13%); H-15(α) → L+2(α) (6%)
$V^{IV}_{10}V^{V}_2$	I	812	d-d V^{IV} (d_{xy}) → V^{IV} (d_{xz-yz})	0.0005	H-1(α) → L+11(α) (11%); H-1(α) → L (α) (8%); H (α) →L+1 (α) (8%)
		785	IVCT V^{IV} (d_{xy}) → V^{V} (d_{xy})	0.0012	H-4(α) → L+ 1 (α) (5%); H-4(α) → L+15(α) (6%); H-1(α)→ L+13(α) (8%)
	II	589	d-d V^{IV} (d_{xy}) → V^{IV} ($d_{x^2-y^2}$)	0.0048	H-4(α) → L+1(α) (23%); H-2(α) → L(α) (21%); H-5(α)→ (α) (6%)
		476	IVCT V^{IV} (d_{xy}) → V^{V} (d_{xy})	0.0056	H-2(α) → L(α) (31%); H-4(α) → L+1(α) (6%); H-1(α)→ L+55(α) (6%)
	III	332	LMCT O($p_{x,y}$) → V^{IV} (d_{xy})	0.0139	H-12(β)→L(β) (13%); H-4(β)→L(β) (11%); H-(β)→L(β) (11%)
		331	IVCT V^{IV} (d_{xy}) → V^{IV} (d_{xz-yz}) LMCT O($p_{x,y}$) → V^{IV} (d_{xz-yz})	0.0144	H-12(α)→L(α) (13%); H-6(α)→L+3(α) (15%); H-1(α)→L+3(α) (14%)
$V^{IV}_{11}V^{V}_1$	I	819	d-d V^{IV} (d_{xy}) → V^{IV} ($d_{xz,yz}$)	0.0003	H-3(α)→L(α) (12%); H-3(α)→L+5(α) (13%); H-3(α)→L+7(α) (10%)
		792	IVCT V^{IV} (d_{xy}) → V^{V} (d_{xy})	0.0006	H-3(α)→L+6(α) (11%); H-8(α)→L+6(α) (4%); H-3(α)→ L+3(α) (5%)
	II	590	d-d V^{IV} (d_{xy}) → V^{IV} ($d_{x^2-y^2}$)	0.0026	H-8(α)→L(α) (17%); H-7(α)→L(α) (18%); H-6(α)→L(A) (10%)
		486	IVCT V^{IV} (d_{xy}) → V^{V} (d_{xy})	0.0018	H-3(α)→L(α) (21%); H-8(α)→L+53(α) (5%); H-7(α)→ L+53(α) (5%)
	III	335	IVCT V^{IV} (d_{xy}) → V^{IV} (d_{xy}) LMCT O($p_{x,y}$) → V^{IV} (d_{xy})	0.0057	H-15(α) → L(α) (9%); H-11(α) → L(α) (5%); H-10(α) → L+2(α) (9%)
		320	IVCT V^{IV} (d_{xy}) → V^{IV} (d_{xz-yz}) LMCT O($p_{x,y}$) → V^{IV} (d_{xz-yz})	0.0051	H-(α)→L+10(α) (21%); H(α)→L+12(A) (15%); H(α)→L+16(A) (17%)