

## Electronic Supplementary Information (ESI)

### Halide encapsulation by dicarboxylate oxido-vanadium cage complexes

Margarita Gómez, Antonio Pastor, Eleuterio Álvarez, José Luis Olloqui-Sariego, and Agustín Galindo\*

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**Figure S1.** NMR spectra of  $[\text{NBu}_4]_2[\text{V}_8\text{O}_{16}(\text{oda})_4\text{C}2\text{Cl}]$  (**1**).

**Figure S2.** NMR spectra of  $[\text{NBu}_4]_2[\text{V}_8\text{O}_{16}(\text{glut})_4\text{C}2\text{Cl}]$  (**2**).

**Figure S3.** NMR spectra of  $[\text{NBu}_4][\text{V}_4\text{O}_8(\text{glut})_2\text{C}2\text{F}]$  (**3**).

**Figure S4.** Cyclic voltammograms normalised with respect to scan rate of polyoxovanadate complexes in 0.1M  $[\text{Bu}_4\text{N}]\text{PF}_6$  in acetonitrile at 25 °C. The scan rates are 0.02, 0.05, 0.1, 0.5, 1, 5, 10 and 50  $\text{Vs}^{-1}$ . The concentration of complexes **1** and **3** was 0.5mM, whereas that a saturated solution ( $< 0.1$  mM) was used for complex **2**.

**Figure S5.** Cyclic voltammograms for the polyoxovanadate complexes **1-3** recorded at 0.1  $\text{Vs}^{-1}$  in 0.1M  $[\text{Bu}_4\text{N}]\text{PF}_6$  in acetonitrile at 25 °C. The concentration of complexes **1** and **3** was 0.5mM, whereas that a saturated solution ( $< 0.1$  mM) was used for complex **2**.

**Table S1.** Crystallographic data for compounds  $[\text{NBu}_4]_2[\text{V}_8\text{O}_{16}(\text{oda})_4\text{C}2\text{Cl}]$  (**1**),  $[\text{NBu}_4]_2[\text{V}_8\text{O}_{16}(\text{glut})_4\text{C}2\text{Cl}]$  (**2**) and  $[\text{NBu}_4][\text{V}_4\text{O}_8(\text{glut})_2\text{C}2\text{F}]$  (**3**).

**Table S2.** Selected V-O bond distances for vanadium complexes **1-3**.

**Table S3** Comparison of selected computed and experimental structural parameters of **1** and **2**.

**Table S4** Comparison of selected computed and experimental structural parameters of **3**.

**Figure S6.** Optimised structure of **2ic**, an isomer of  $[\text{V}_8\text{O}_{16}(\text{glut})_4\text{C}2\text{Cl}]^{2-}$ , **2c**.

**Figure S7.** Optimised structures of  $[\text{V}_8\text{O}_{16}(\text{oda})_4]$ , **4c**, and  $[\text{V}_8\text{O}_{16}(\text{glut})_4]$ , **5c**.

**Figure S8.** Left: HOMO-6 of  $[\text{V}_8\text{O}_{16}(\text{oda})_4\text{C}2\text{Cl}]^{2-}$ , **1c**. Right: HOMO-5 of  $[\text{V}_8\text{O}_{16}(\text{glut})_4\text{C}2\text{Cl}]^{2-}$ , **2c**.

**Figure S9.** Optimised structures of  $[\text{V}_8\text{O}_{16}(\text{oda})_4\text{C}(\text{Cl}_2)]$ , **6c**, and  $[\text{V}_8\text{O}_{16}(\text{glut})_4\text{C}(\text{Cl}_2)]$ , **7c**.

**Figure S10.** Optimised structure of  $[\text{V}_8\text{O}_{16}(\text{glut})_4\text{C}2\text{F}]^{2-}$ , **8c**.

**Figure S11.** Thermogravimetric analyses for complexes **1-3**.

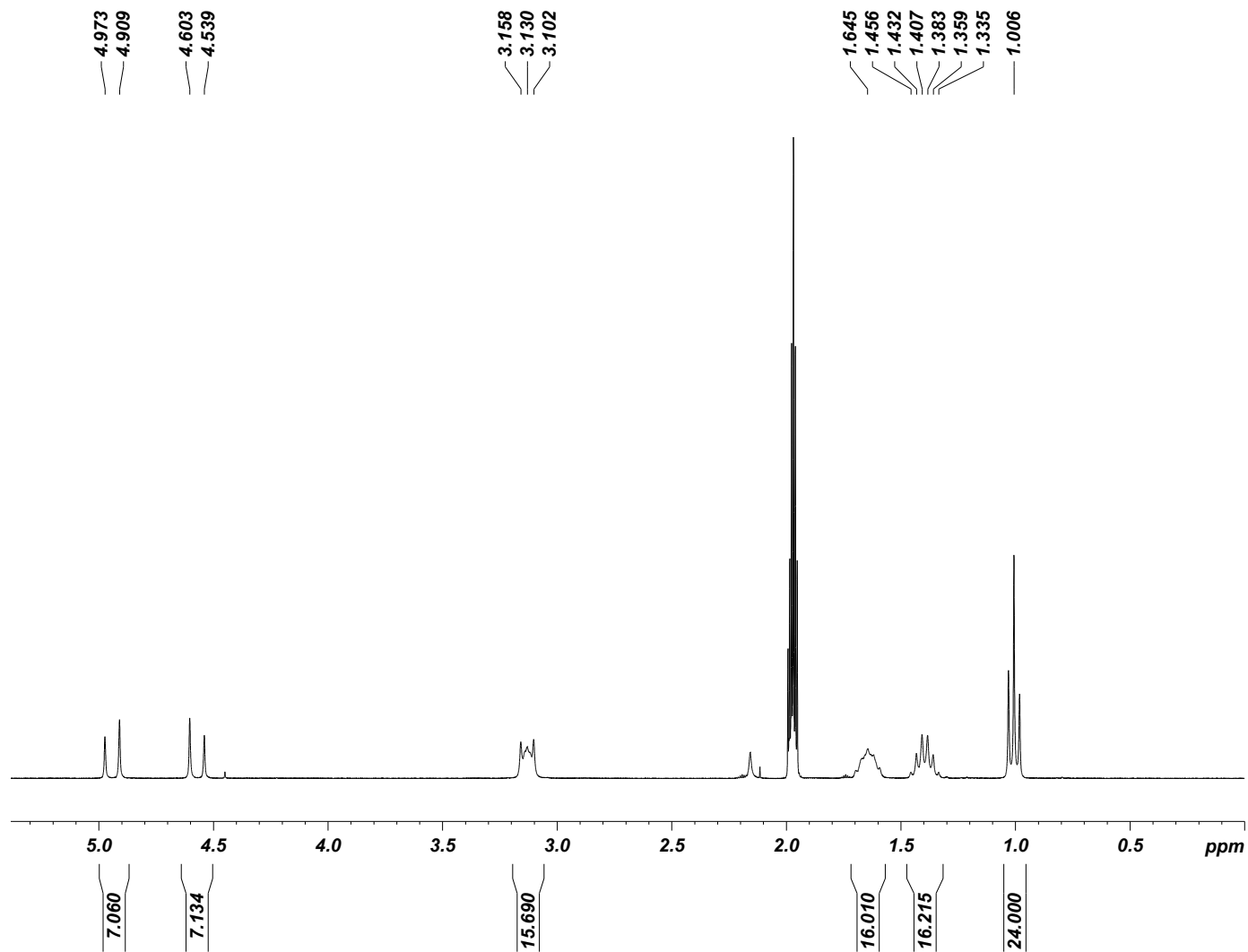
**Figure S12.** Comparison of the XRPDs for complexes **1-3**.

**Table S5.** Coordinates of the computed compounds.

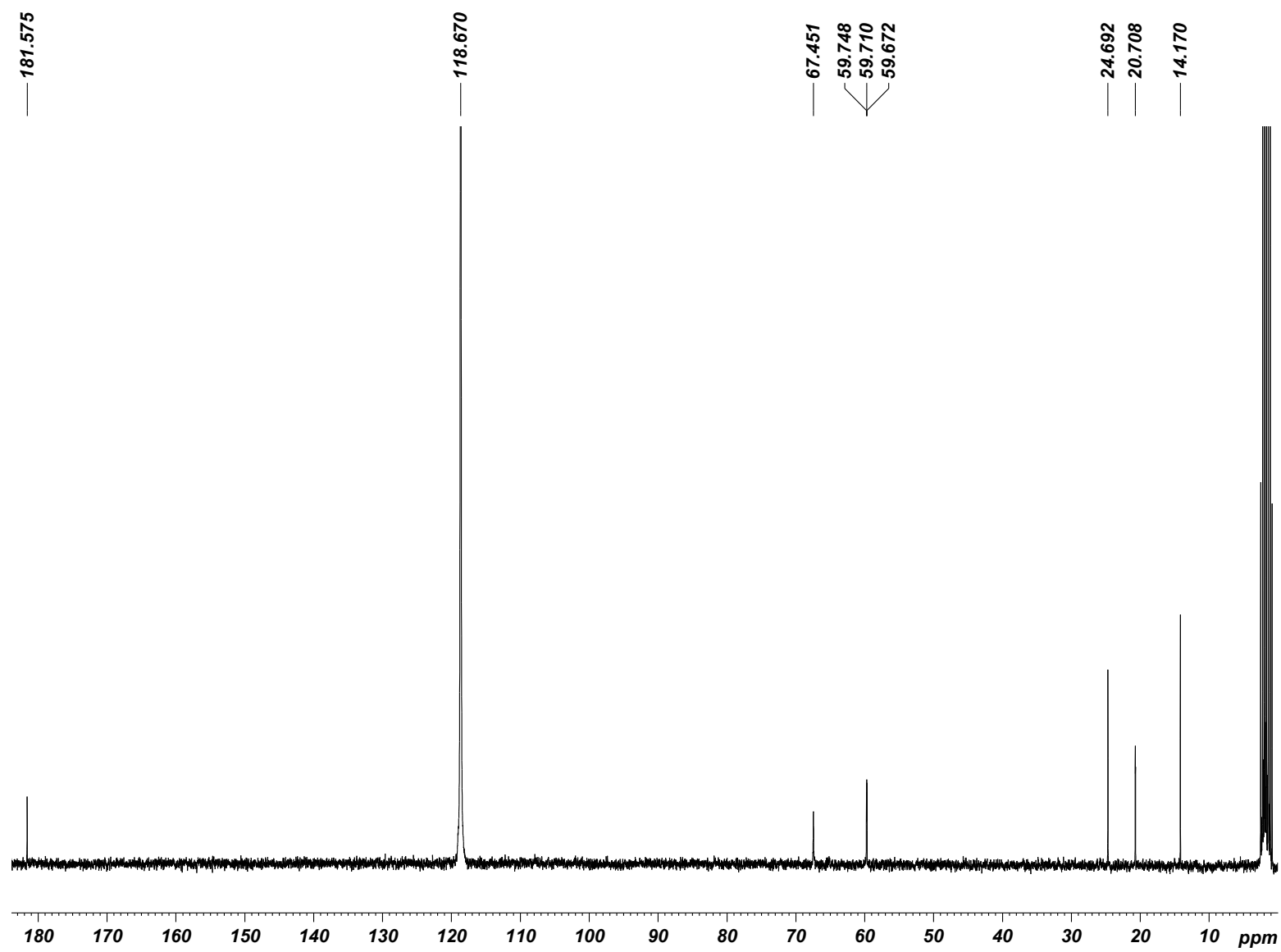
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**Figure S1.** NMR spectra of  $[\text{NBu}_4]_2[\text{V}_8\text{O}_{16}(\text{oda})_4 \cdot 2\text{Cl}]$  (**1**).

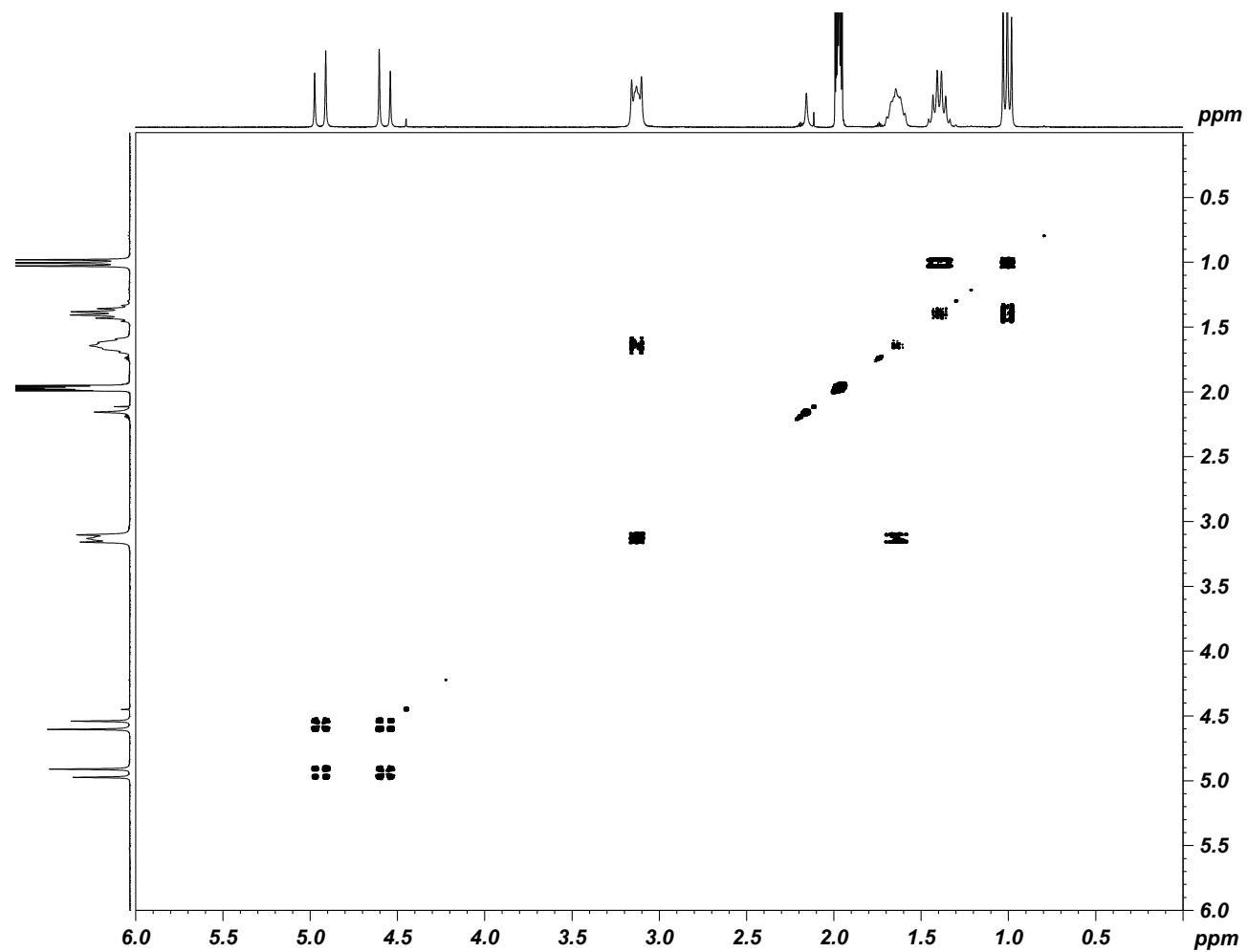
$^1\text{H}$  NMR ( $\text{CD}_3\text{CN}$ )



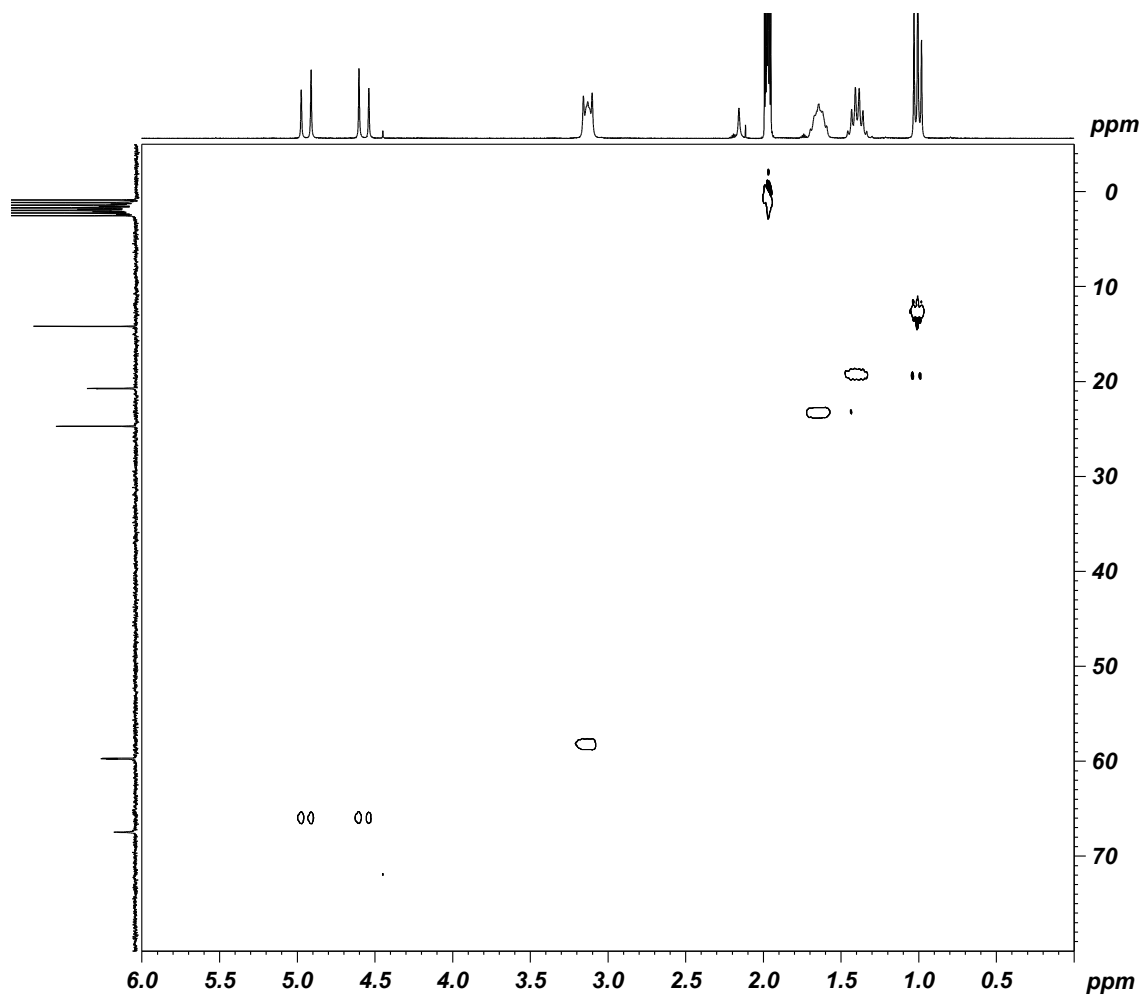
$^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CD}_3\text{CN}$ )



COSY (CD<sub>3</sub>CN)

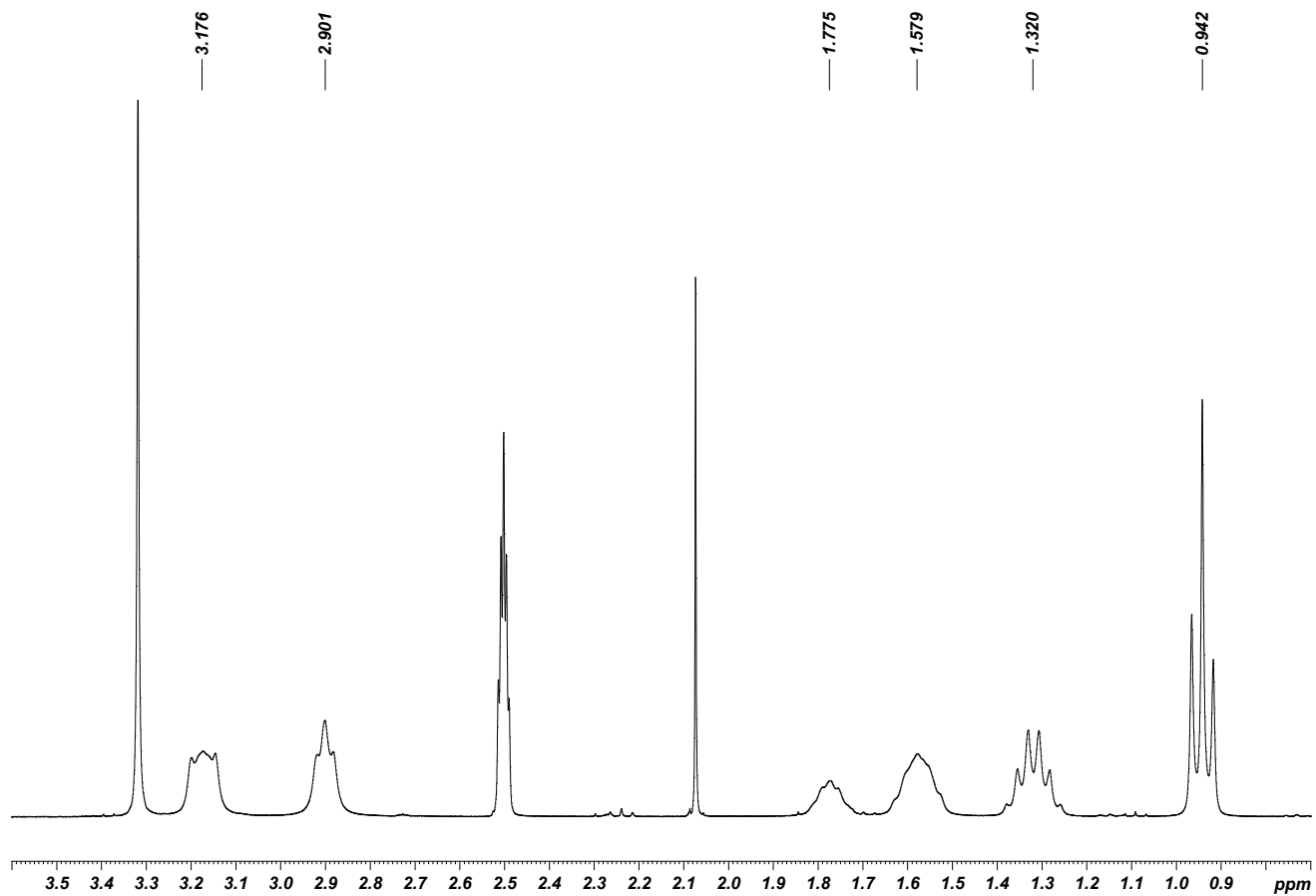


2D heteronuclear NMR (CD<sub>3</sub>CN)

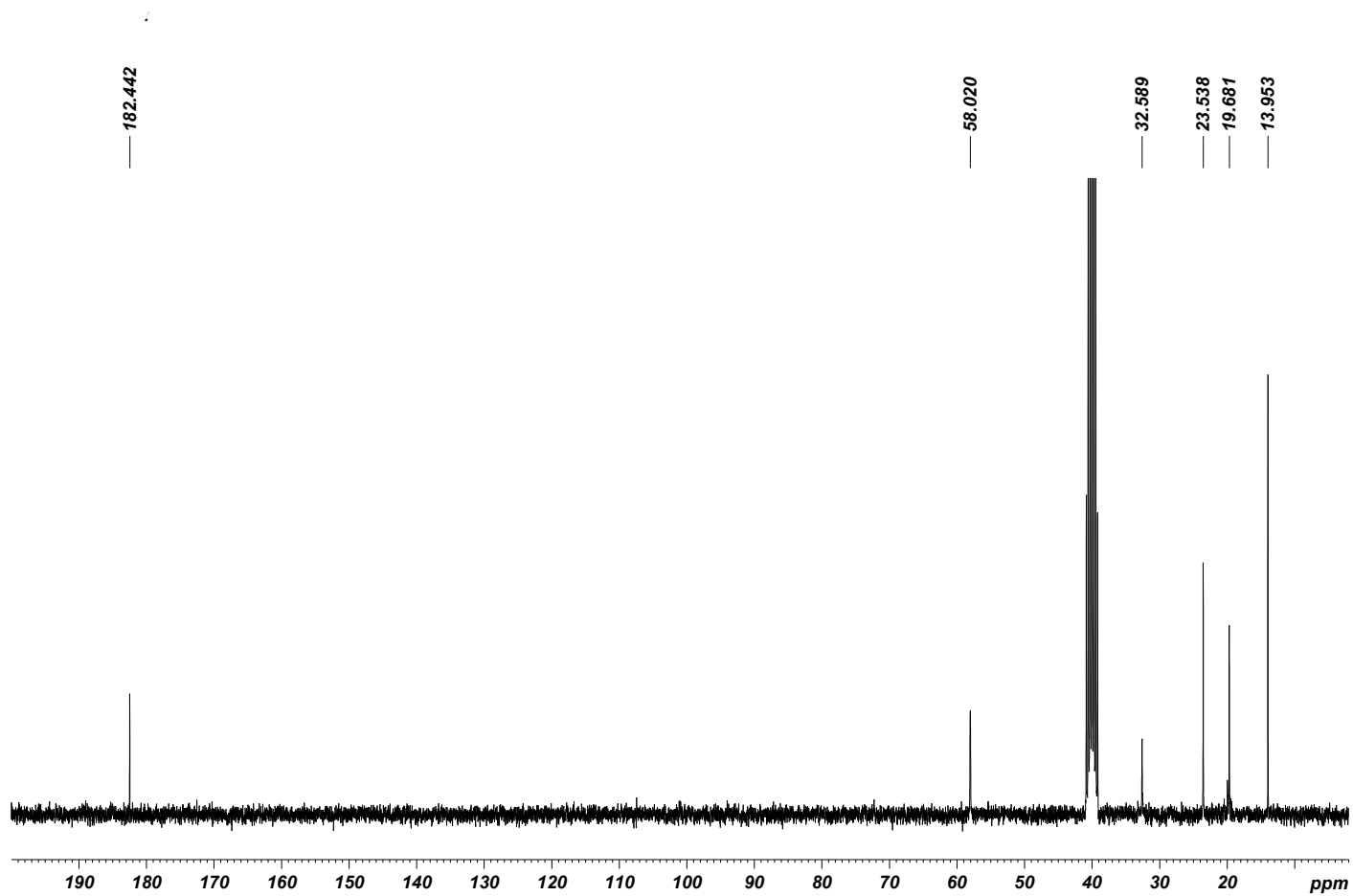


**Figure S2.** NMR spectra of  $[\text{NBu}_4]_2[\text{V}_8\text{O}_{16}(\text{glut})_4 \cdot 2\text{Cl}]$  (**2**).

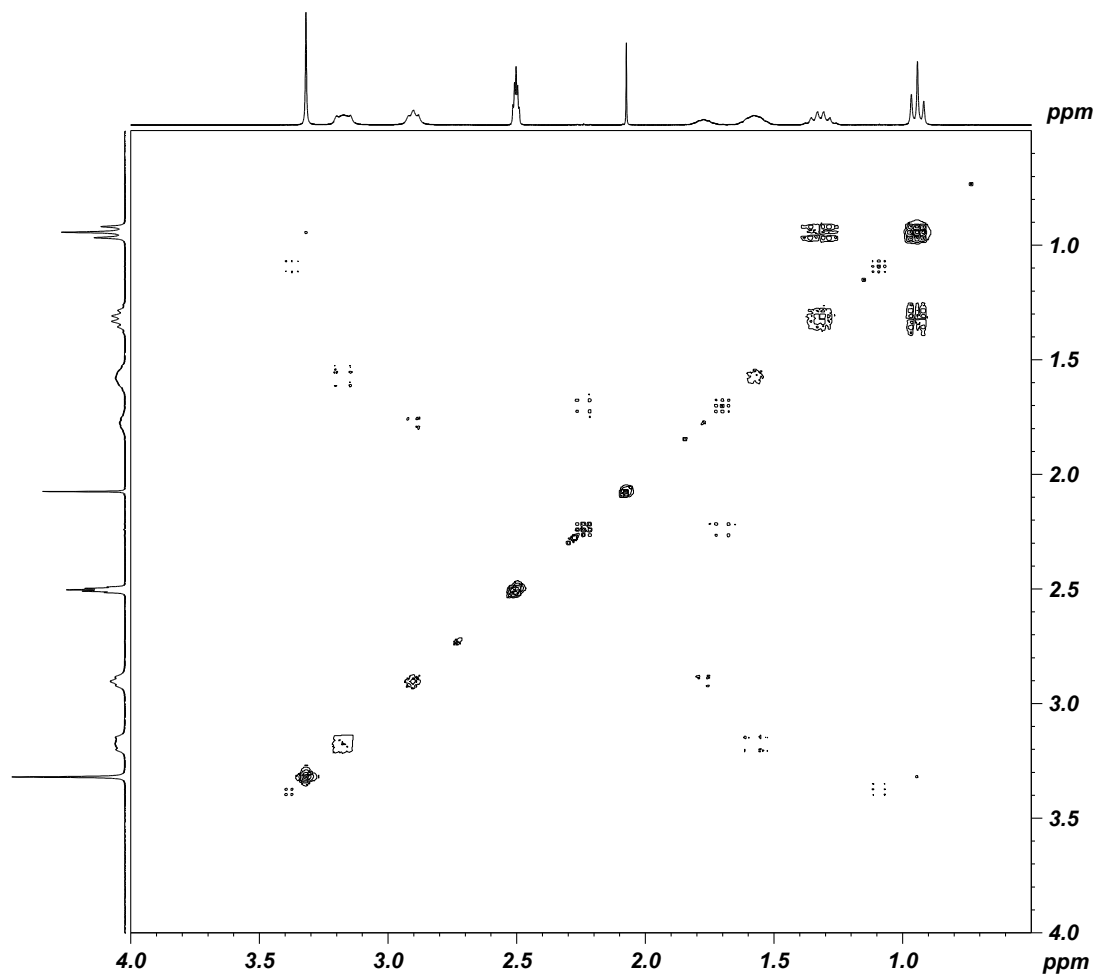
$^1\text{H}$  NMR (DMSO- $d_6$ )



$^{13}\text{C}\{^1\text{H}\}$  NMR (DMSO- $d_6$ )

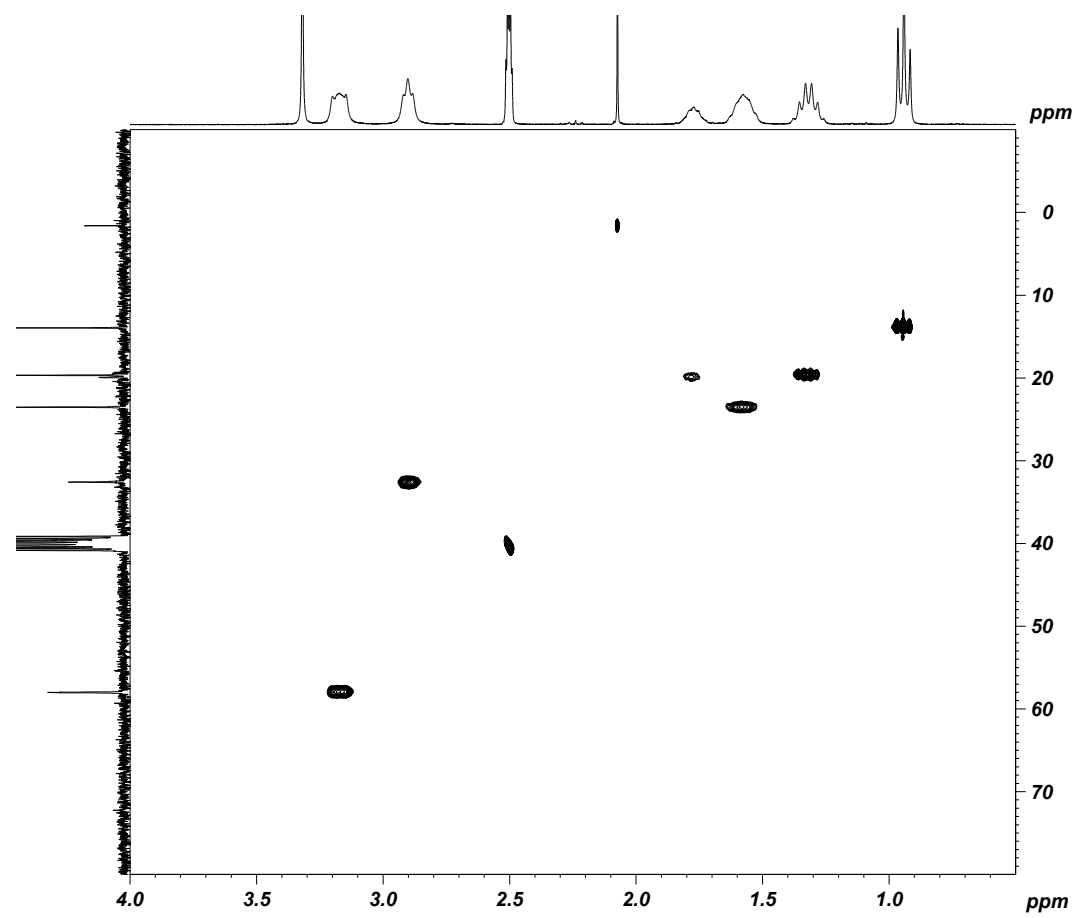


COSY (DMSO-d<sub>6</sub>)



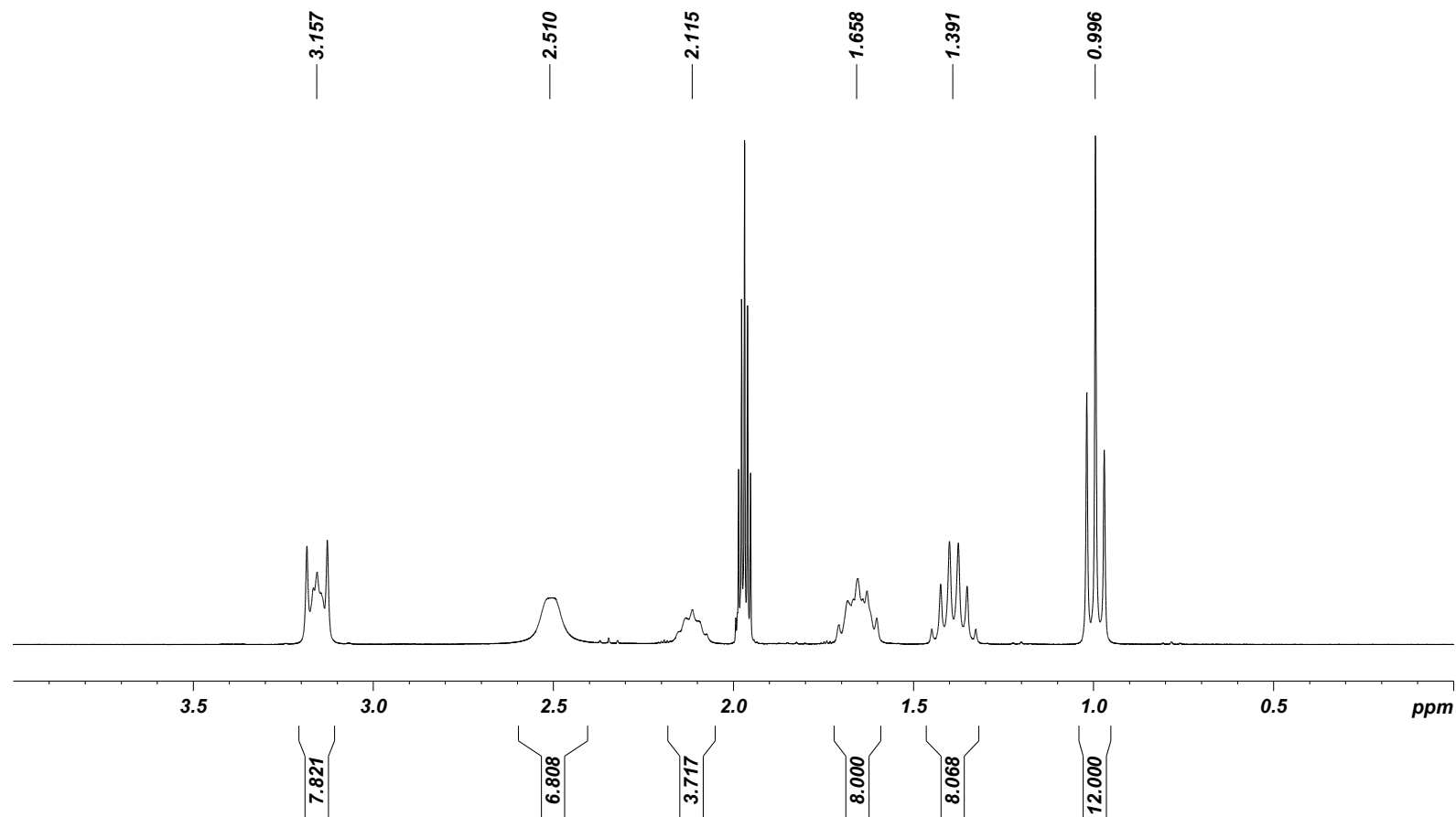


2D heteronuclear NMR (DMSO-d<sub>6</sub>)

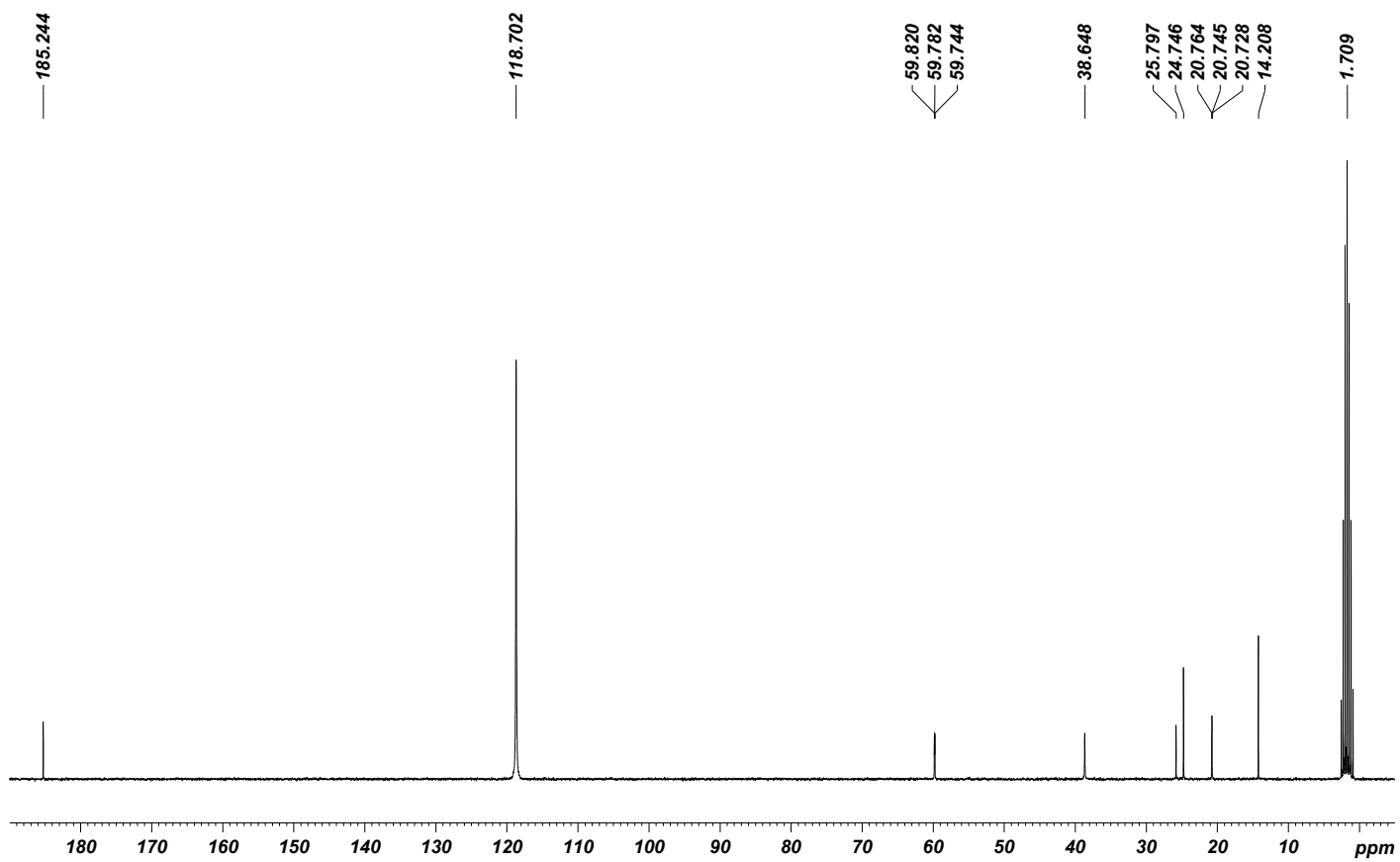


**Figure S3.** NMR spectra of  $[\text{NBu}_4][\text{V}_4\text{O}_8(\text{glut})_2\text{CF}]$  (**3**).

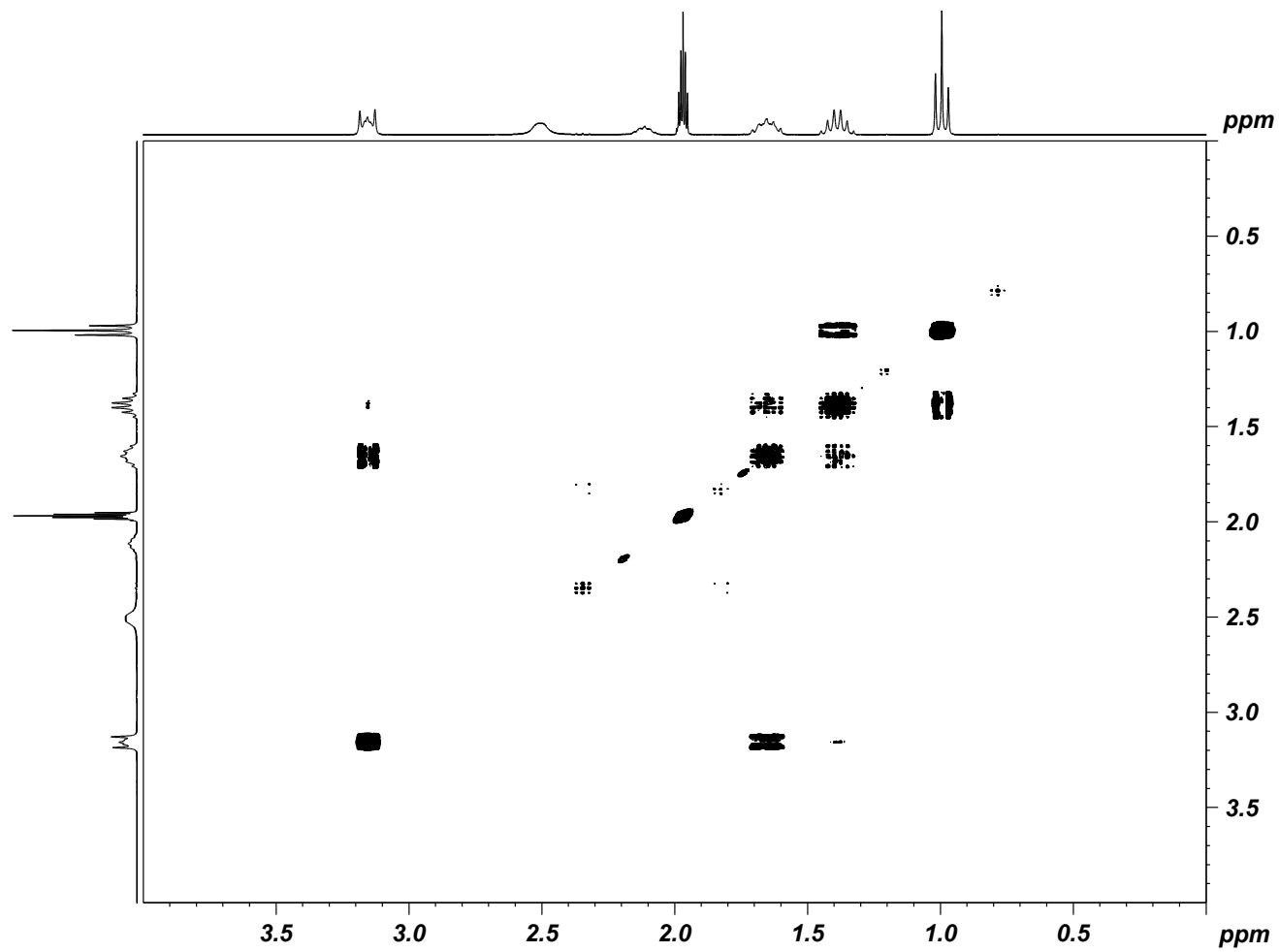
$^1\text{H}$  NMR ( $\text{CD}_3\text{CN}$ )



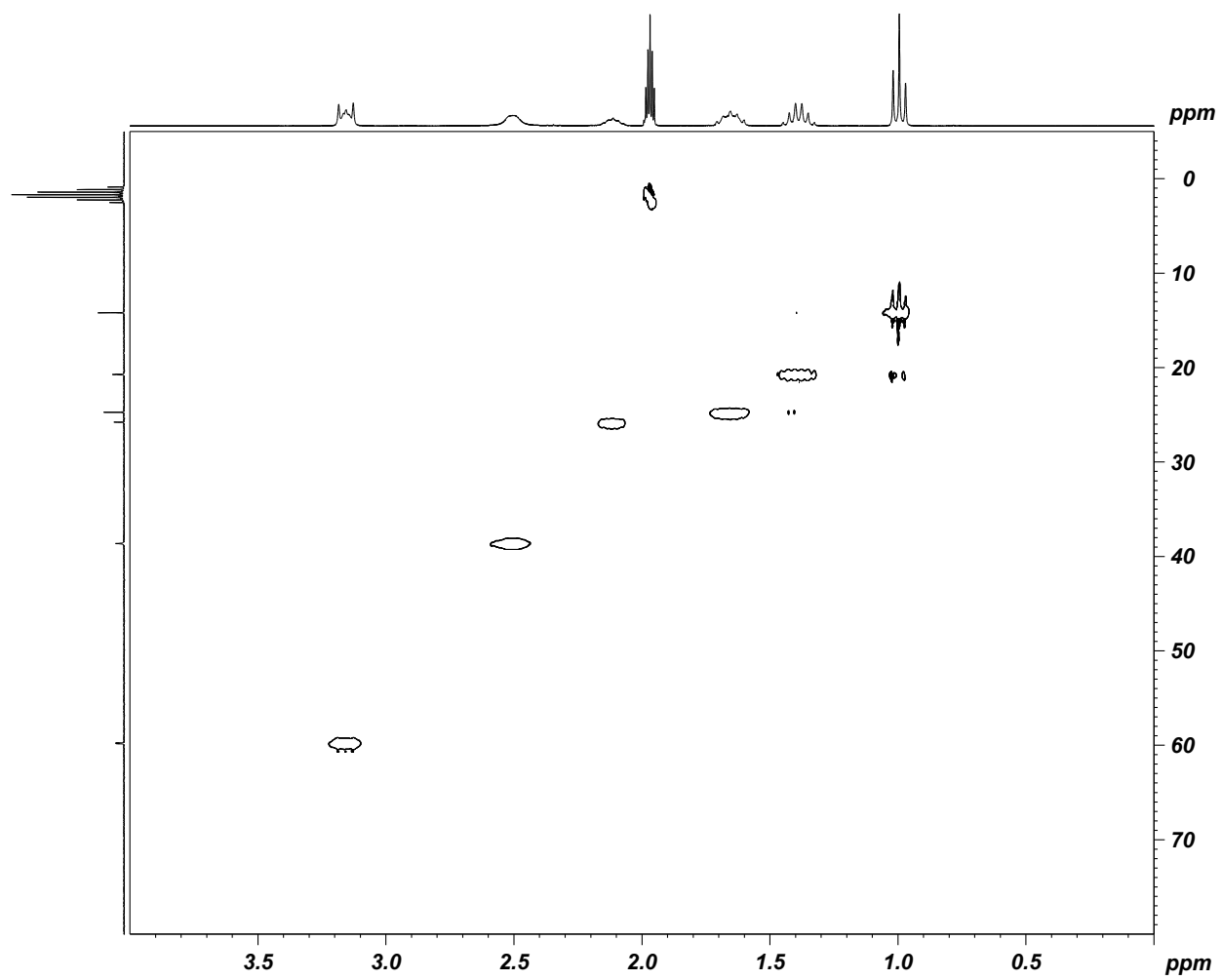
$^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CD}_3\text{CN}$ )



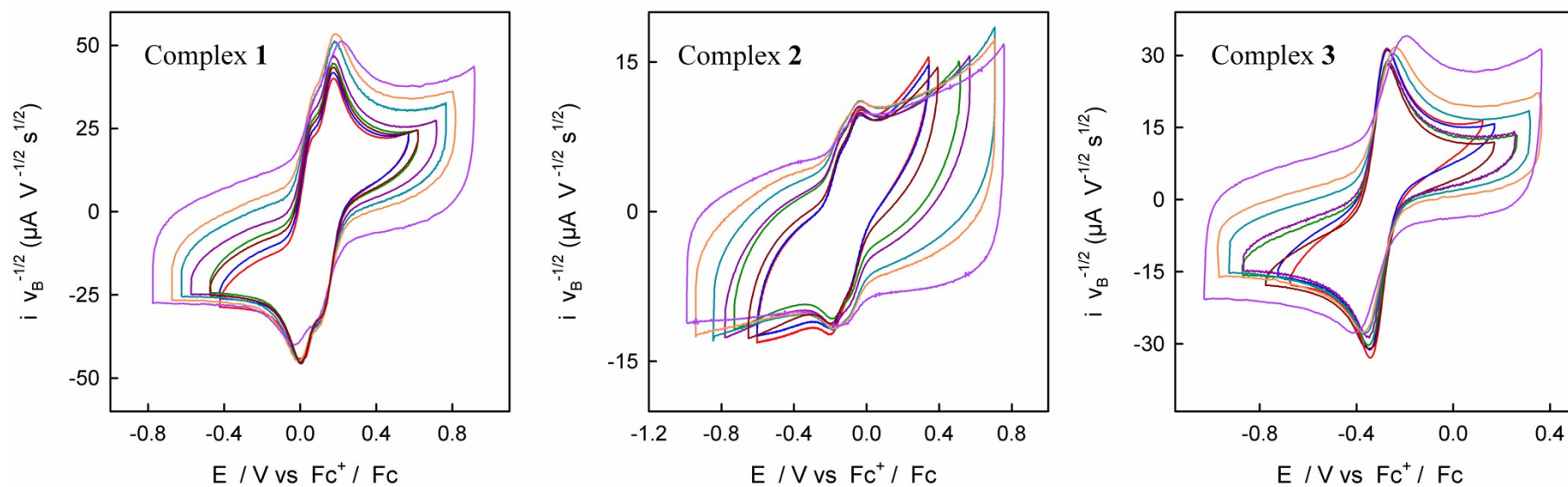
COSY (CD<sub>3</sub>CN)



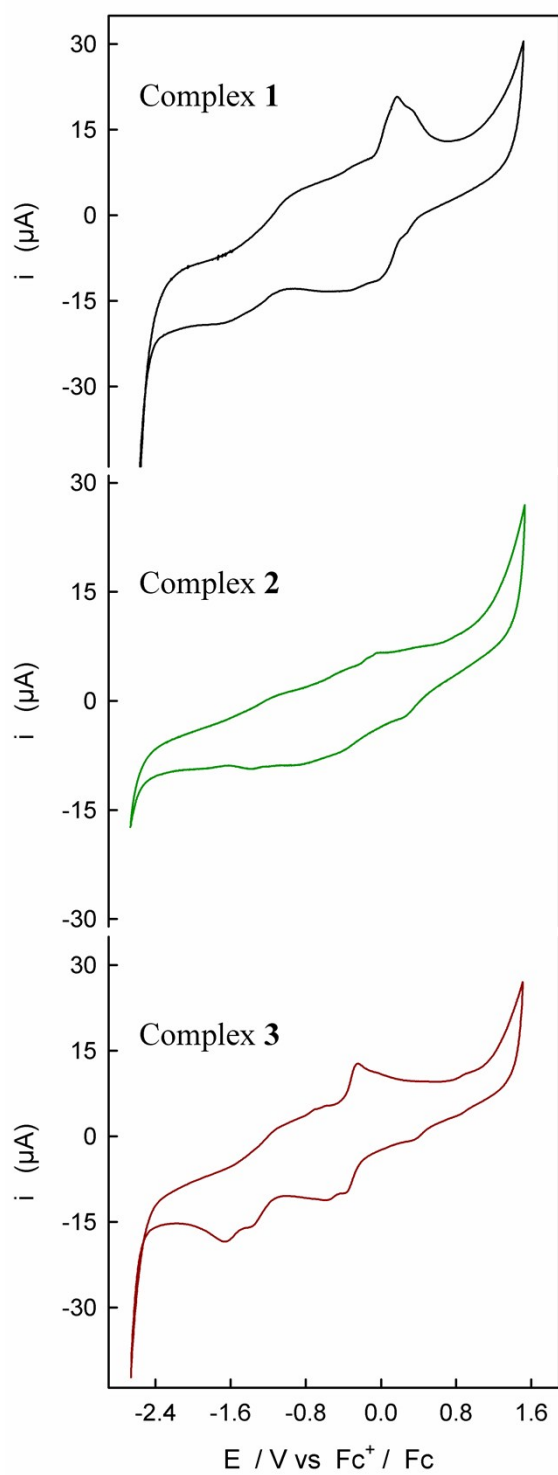
2D heteronuclear NMR (CD<sub>3</sub>CN)



**Figure S4.** Cyclic voltammograms normalised with respect to scan rate of polyoxovanadate complexes in 0.1M [Bu<sub>4</sub>N]PF<sub>6</sub> in acetonitrile at 25 °C. The scan rates are 0.02, 0.05, 0.1, 0.5, 1, 5, 10 and 50 Vs<sup>-1</sup>. The concentration of complexes **1** and **3** was 0.5mM, whereas that a saturated solution (< 0.1 mM) was used for complex **2**.



**Figure S5.** Cyclic voltammograms for the indicated polyoxovanadate complexes **1-3** recorded at  $0.1 \text{ Vs}^{-1}$  in  $0.1 \text{ M } [\text{Bu}_4\text{N}]\text{PF}_6$  in acetonitrile at  $25 \text{ }^\circ\text{C}$ . The concentration of complexes **1** and **3** was  $0.5 \text{ mM}$ , whereas that a saturated solution ( $< 0.1 \text{ mM}$ ) was used for complex **2**.



**Table S1.** Crystallographic data for compounds [Bu<sub>4</sub>N]<sub>2</sub>[V<sub>8</sub>O<sub>16</sub>(oda)<sub>4</sub>·2Cl] (**1**), [Bu<sub>4</sub>N]<sub>2</sub>[V<sub>8</sub>O<sub>16</sub>(glut)<sub>4</sub>·2Cl] (**2**) and [Bu<sub>4</sub>N][V<sub>4</sub>O<sub>8</sub>(glut)<sub>2</sub>·F] (**3**).

	<b>1</b>	<b>2</b>	<b>3</b>
Empirical formula	C <sub>54</sub> H <sub>97</sub> Cl <sub>2</sub> N <sub>5</sub> O <sub>36</sub> V <sub>8</sub>	C <sub>52</sub> H <sub>96</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>32</sub> V <sub>8</sub>	C <sub>26</sub> H <sub>48</sub> FNO <sub>16</sub> V <sub>4</sub>
Formula weight	1870.78	1739.72	853.41
Temperature (K)	193(2)	193(2)	193(2)
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	P $\bar{1}$	P $\bar{1}$	P2 <sub>1</sub> /c
a (Å)	16.3158(6)	14.8986(4)	23.418(12)
b (Å)	16.3786(6)	16.7125(5)	13.297(8)
c (Å)	16.7821(6)	17.4333(5)	23.133(13)
$\alpha$ (°)	90.9530(10)	64.2850(10)	90
$\beta$ (°)	117.9780(10)	85.7850(10)	90.199(13)
$\gamma$ (°)	93.3520(10)	86.1320(10)	90
Volume (Å <sup>3</sup> )	3948.8(2)	3897.24(19)	7203(7)
Z	2	2	8
Density (calculated, Mg·m <sup>-3</sup> )	1.573	1.483	1.574
Absorption coefficient (mm <sup>-1</sup> )	1.059	1.062	1.079
F(000)	1924	1792	3520
Crystal size (mm <sup>3</sup> )	0.40 x 0.30 x 0.15	0.30 x 0.20 x 0.20	0.45 x 0.40 x 0.30
Reflections collected	71065	49714	69352
Independent reflections	14200	14080	13007
Final R indices [I>2 $\sigma$ (I)], R <sub>I</sub> [a]	0.0450	0.0586	0.0556
R indices (all data), wR(F <sup>2</sup> ) [b]	0.1375	0.1739	0.1759
S(F <sup>2</sup> ) [c]	1.089	1.030	1.076
CCDC	1573268	1573269	1573270

[a]  $R_I = \Sigma||F_o| - |F_c| / \Sigma|F_o|$ ; [b]  $wR(F^2) = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$ . [c] Goodness-of-fit,  $S(F^2) = \{\Sigma[w(F_o^2 - F_c^2)^2] / (n-p)\}^{1/2}$  where n is the reflections number and p is the parameters number.



**Table S2.** Selected V-O bond distances for vanadium complexes **1-3**.

Distances (Å)	<b>1</b>		<b>2</b>		<b>3</b>
V=O	V(1)-O(21) 1.585(2)	V(5)-O(29) 1.588(2)	V(1)-O(1) 1.590(3)		V(1)-O(21) 1.585(2)
	V(2)-O(22) 1.584(2)	V(6)-O(30) 1.585(2)	V(2)-O(3) 1.593(3)		V(2)-O(22) 1.584(2)
	V(3)-O(23) 1.591(2)	V(7)-O(31) 1.586(2)	V(3)-O(9) 1.587(3)		V(3)-O(23) 1.591(2)
	V(4)-O(24) 1.592(2)	V(8)-O(32) 1.588(2)	V(4)-O(11) 1.596(3)		V(4)-O(24) 1.592(2)
V-O	V(1)-O(25) 1.729(2)	V(5)-O(33) 1.739(2)	V(1)-O(2) 1.785(3)		V(1)-O(25) 1.729(2)
	V(1)-O(28) 1.907(2)	V(5)-O(36) 1.896(2)	V(1)-O(4) 1.839(3)		V(1)-O(28) 1.907(2)
	V(2)-O(26) 1.735(2)	V(6)-O(34) 1.734(2)	V(2)-O(12)#1 1.784(3)		V(2)-O(26) 1.735(2)
	V(2)-O(25) 1.903(2)	V(6)-O(33) 1.890(2)	V(2)-O(2) 1.834(3)		V(2)-O(25) 1.903(2)
	V(3)-O(27) 1.729(2)	V(7)-O(35) 1.737(2)	V(3)-O(4)#1 1.789(3)		V(3)-O(27) 1.729(2)
	V(3)-O(26) 1.887(2)	V(7)-O(34) 1.901(2)	V(3)-O(10) 1.844(3)		V(3)-O(26) 1.887(2)
	V(4)-O(28) 1.735(2)	V(8)-O(36) 1.743(2)	V(4)-O(10) 1.792(3)		V(4)-O(28) 1.735(2)
	V(4)-O(27) 1.901(2)	V(8)-O(35) 1.895(2)	V(4)-O(12) 1.846(3)		V(4)-O(27) 1.901(2)
V-O (carboxylate)	V(1)-O(11) 1.991(2)	V(5)-O(19) 1.986(2)	V(1)-O(7) 1.994(3)		V(1)-O(11) 1.991(2)
	V(1)-O(6) 2.049(2)	V(5)-O(4) 2.047(2)	V(1)-O(5) 2.009(3)		V(1)-O(6) 2.049(2)
	V(2)-O(16) 1.983(2)	V(6)-O(14) 1.981(2)	V(2)-O(16)#1 2.000(3)		V(2)-O(16) 1.983(2)
	V(2)-O(12) 2.045(2)	V(6)-O(20) 2.052(2)	V(2)-O(8) 2.023(3)		V(2)-O(12) 2.045(2)
	V(3)-O(1) 1.983(2)	V(7)-O(9) 1.976(2)	V(3)-O(6)#1 2.001(3)		V(3)-O(1) 1.983(2)
	V(3)-O(17) 2.061(2)	V(7)-O(15) 2.059(2)	V(3)-O(13) 2.012(3)		V(3)-O(17) 2.061(2)
	V(4)-O(7) 1.978(2)	V(8)-O(5) 1.998(2)	V(4)-O(14) 1.990(3)		V(4)-O(7) 1.978(2)
	V(4)-O(2) 2.056(2)	V(8)-O(10) 2.053(2)	V(4)-O(15) 2.023(3)		V(4)-O(2) 2.056(2)

Symmetry transformations used to generate equivalent atoms of complex **2**: #1 -x,-y+1,-z; #2 -x+1,-y+1,-z+1.

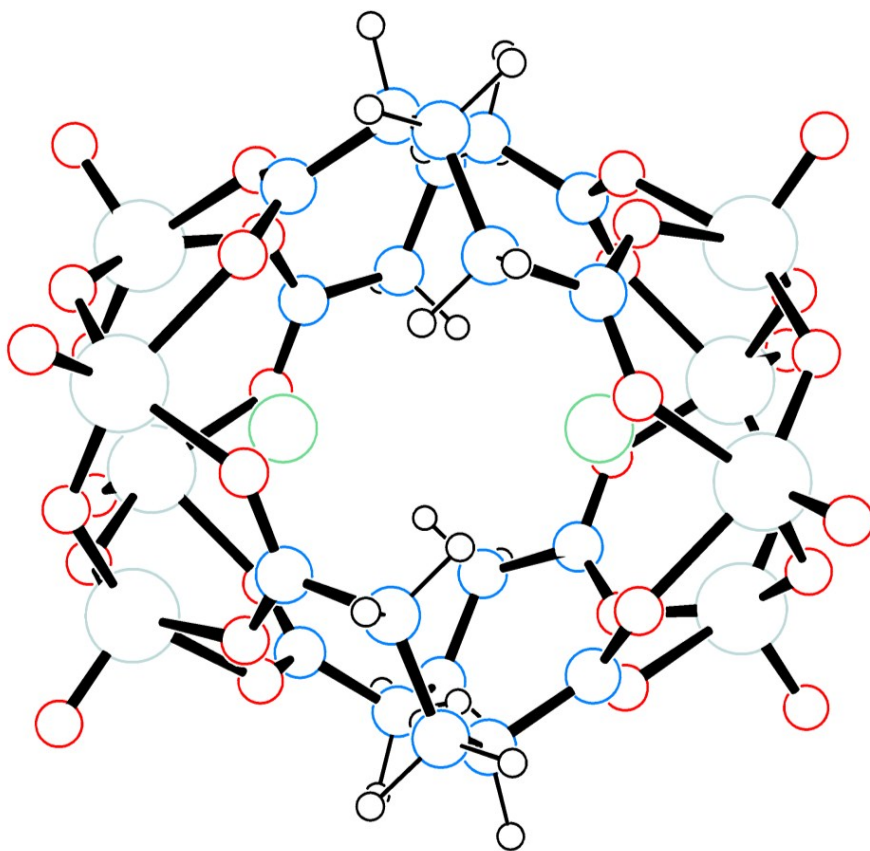
**Table S3.** Comparison of selected computed and experimental structural parameters of **1** and **2**.

Distances (Å)	<b>1</b>				<b>1c</b>	<b>2</b>		<b>2c</b>
V=O	V(1)-O(21)	1.585(2)	V(5)-O(29)	1.588(2)	1.569	V(1)-O(1)	1.590(3)	1.571
	V(2)-O(22)	1.584(2)	V(6)-O(30)	1.585(2)		V(2)-O(3)	1.593(3)	
	V(3)-O(23)	1.591(2)	V(7)-O(31)	1.586(2)		V(3)-O(9)	1.587(3)	
	V(4)-O(24)	1.592(2)	V(8)-O(32)	1.588(2)		V(4)-O(11)	1.596(3)	
V-O	V(1)-O(25)	1.729(2)	V(5)-O(33)	1.739(2)	1.722	V(1)-O(2)	1.785(3)	1.726
	V(1)-O(28)	1.907(2)	V(5)-O(36)	1.896(2)	1.865	V(1)-O(4)	1.839(3)	1.861
	V(2)-O(26)	1.735(2)	V(6)-O(34)	1.734(2)		V(2)-O(12)#1	1.784(3)	1.728
	V(2)-O(25)	1.903(2)	V(6)-O(33)	1.890(2)		V(2)-O(2)	1.834(3)	1.858
	V(3)-O(27)	1.729(2)	V(7)-O(35)	1.737(2)		V(3)-O(4)#1	1.789(3)	1.726
	V(3)-O(26)	1.887(2)	V(7)-O(34)	1.901(2)		V(3)-O(10)	1.844(3)	1.857
	V(4)-O(28)	1.735(2)	V(8)-O(36)	1.743(2)		V(4)-O(10)	1.792(3)	1.725
	V(4)-O(27)	1.901(2)	V(8)-O(35)	1.895(2)		V(4)-O(12)	1.846(3)	1.856
V-O (carboxylate)	V(1)-O(11)	1.991(2)	V(5)-O(19)	1.986(2)	2.006	V(1)-O(7)	1.994(3)	2.011
	V(1)-O(6)	2.049(2)	V(5)-O(4)	2.047(2)	2.079	V(1)-O(5)	2.009(3)	2.064
	V(2)-O(16)	1.983(2)	V(6)-O(14)	1.981(2)		V(2)-O(16)#1	2.000(3)	1.999
	V(2)-O(12)	2.045(2)	V(6)-O(20)	2.052(2)		V(2)-O(8)	2.023(3)	2.058
	V(3)-O(1)	1.983(2)	V(7)-O(9)	1.976(2)		V(3)-O(6)#1	2.001(3)	2.002
	V(3)-O(17)	2.061(2)	V(7)-O(15)	2.059(3)		V(3)-O(13)	2.012(3)	2.052
	V(4)-O(7)	1.978(2)	V(8)-O(5)	1.998(2)		V(4)-O(14)	1.990(3)	
	V(4)-O(2)	2.056(2)	V(8)-O(10)	2.053(2)		V(4)-O(15)	2.023(3)	
Cl...Cl	4.049(1)				3.868	4.728(1)		4.613

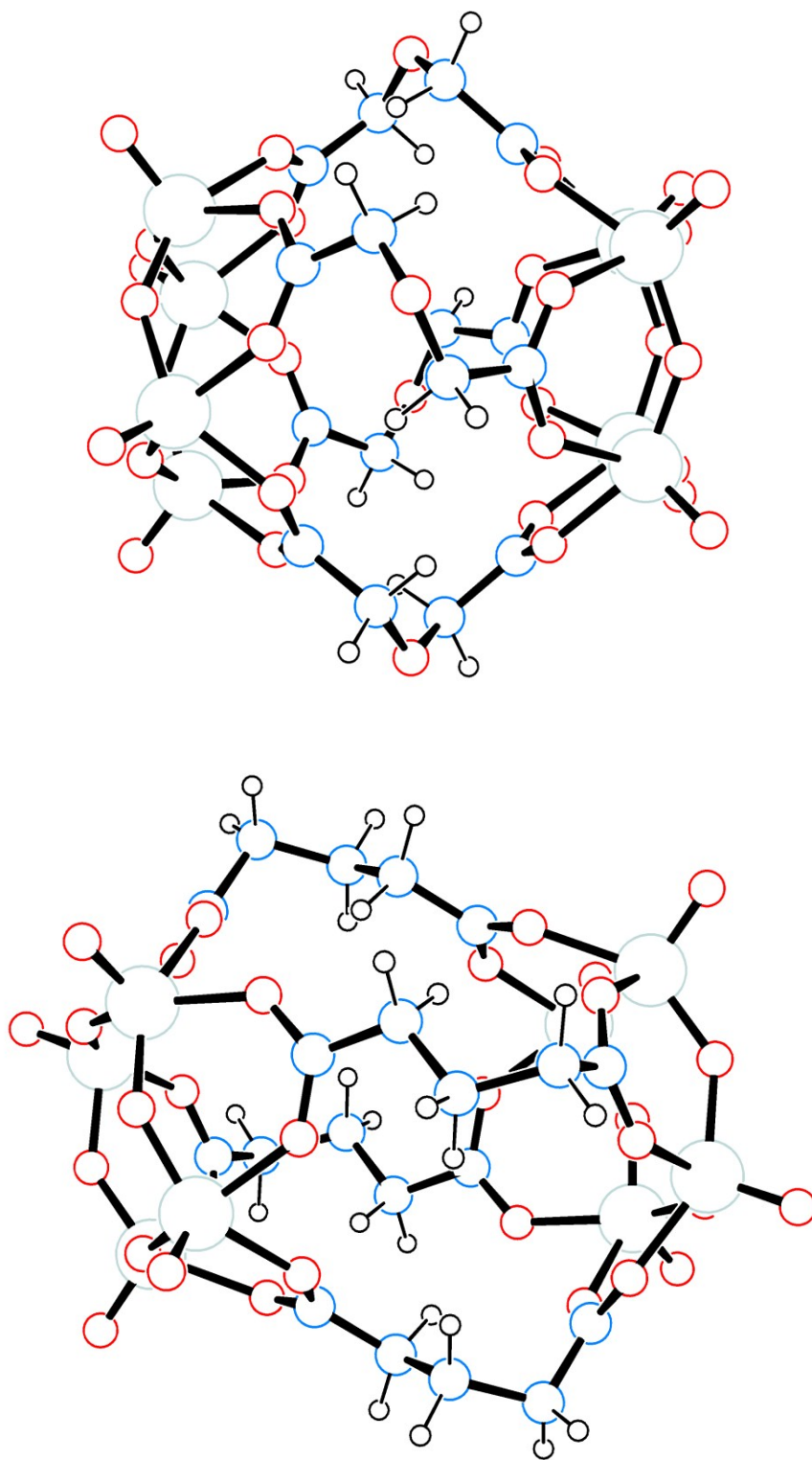
**Table S4.** Comparison of selected computed and experimental structural parameters of **3**.

Distances (Å)	<b>3</b>	<b>3c</b>	
V=O	V(1)-O(1)	1.589(3)	1.573
	V(2)-O(8)	1.588(3)	
	V(3)-O(12)	1.590(3)	
	V(4)-O(16)	1.586(3)	
V-O	V(1)-O(2)	1.788(3)	1.707
	V(1)-O(3)	1.926(3)	1.963
	V(2)-O(2)	1.921(3)	1.708
	V(2)-O(9)	1.788(3)	1.962
	V(3)-O(13)	1.788(3)	1.708
	V(3)-O(9)	1.930(3)	1.964
	V(4)-O(3)	1.784(3)	1.707
	V(4)-O(13)	1.935(3)	1.964
V-O (carboxylate)	V(1)-O(6)	1.994(3)	2.020
	V(1)-O(4)	1.999(3)	2.023
	V(2)-O(10)	1.995(3)	2.017
	V(2)-O(5)	2.005(3)	2.027
	V(3)-O(11)	1.993(3)	2.018
	V(3)-O(14)	2.001(3)	2.026
	V(4)-O(7)	1.993(3)	2.019
	V(4)-O(15)	2.015(3)	2.024
V-F	V(1)-F(1)	2.229(2)	2.241
	V(2)-F(1)	2.228(2)	2.245
	V(3)-F(1)	2.243(2)	2.246
	V(4)-F(1)	2.216(2)	2.246

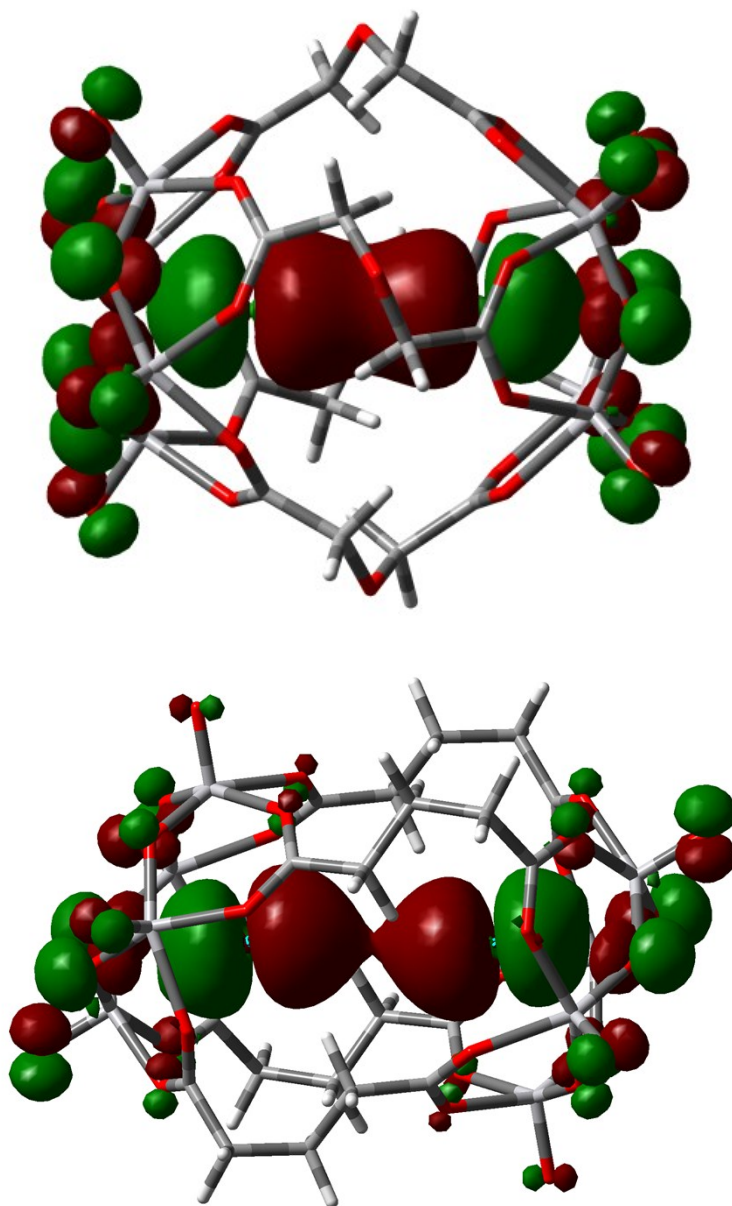
**Figure S6.** Optimised structure of **2ic**, an isomer of  $[\text{V}_8\text{O}_{16}(\text{glut})_4\text{C}2\text{Cl}]^{2-}$ , **2ic**.



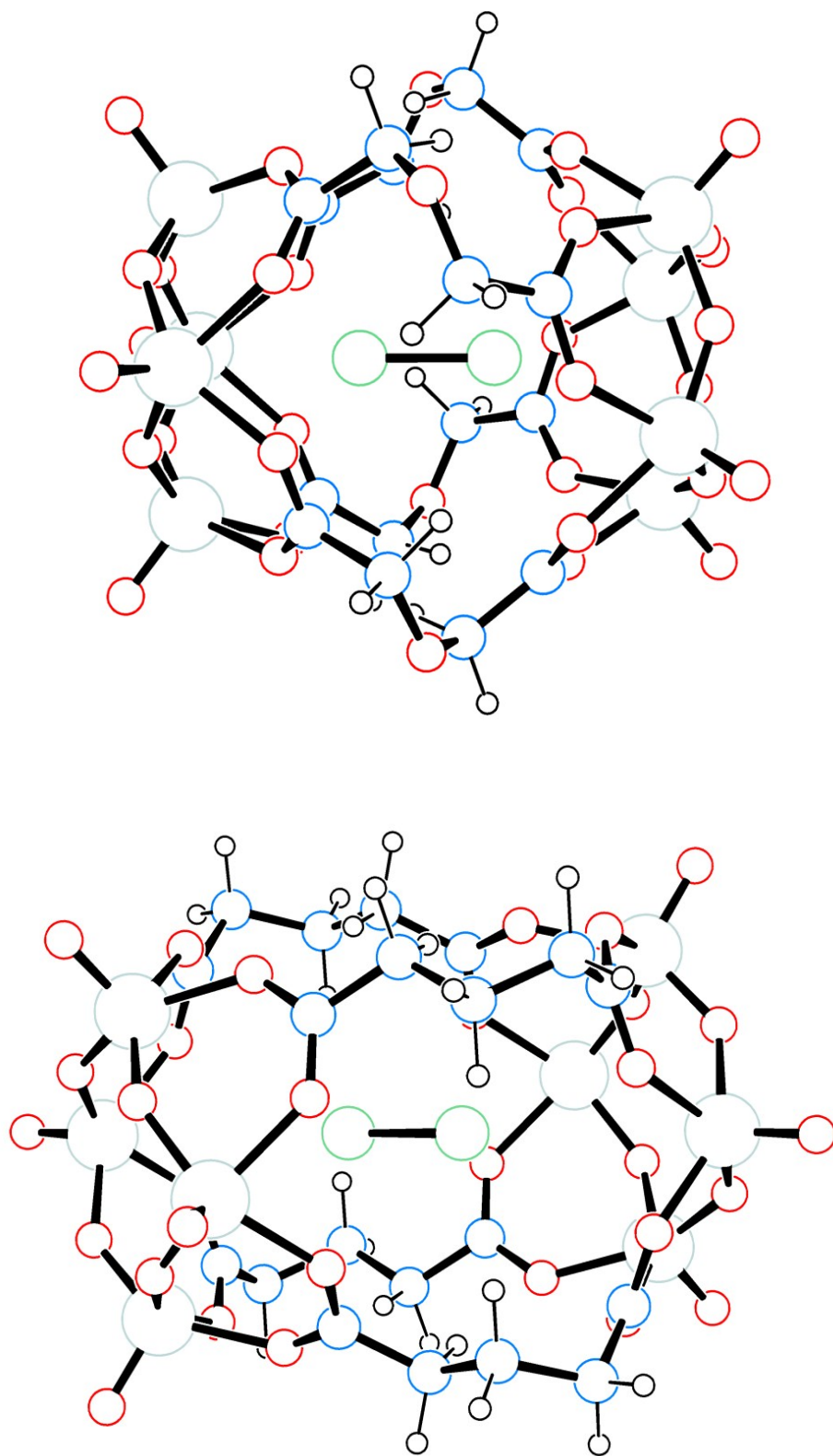
**Figure S7.** Optimised structures of  $[V_8O_{16}(oda)_4]$ , **4c**, and  $[V_8O_{16}(glut)_4]$ , **5c**.



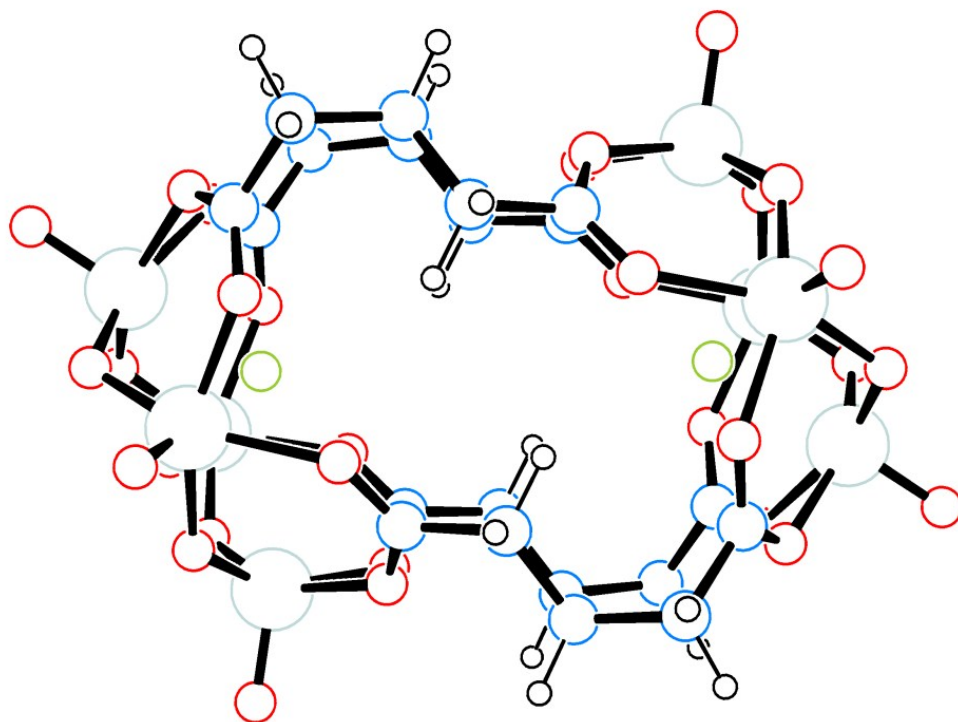
**Figure S8.** Left: HOMO-6 of  $[\text{V}_8\text{O}_{16}(\text{oda})_4\text{Cl}_2]^{2-}$ , **1c**. Right: HOMO-5 of  $[\text{V}_8\text{O}_{16}(\text{glut})_4\text{Cl}_2]^{2-}$ , **2c**.



**Figure S9.** Optimised structures of  $[V_8O_{16}(oda)_4\subset(Cl_2)]$ , **6c**, and  $[V_8O_{16}(glut)_4\subset(Cl_2)]$ , **7c**.

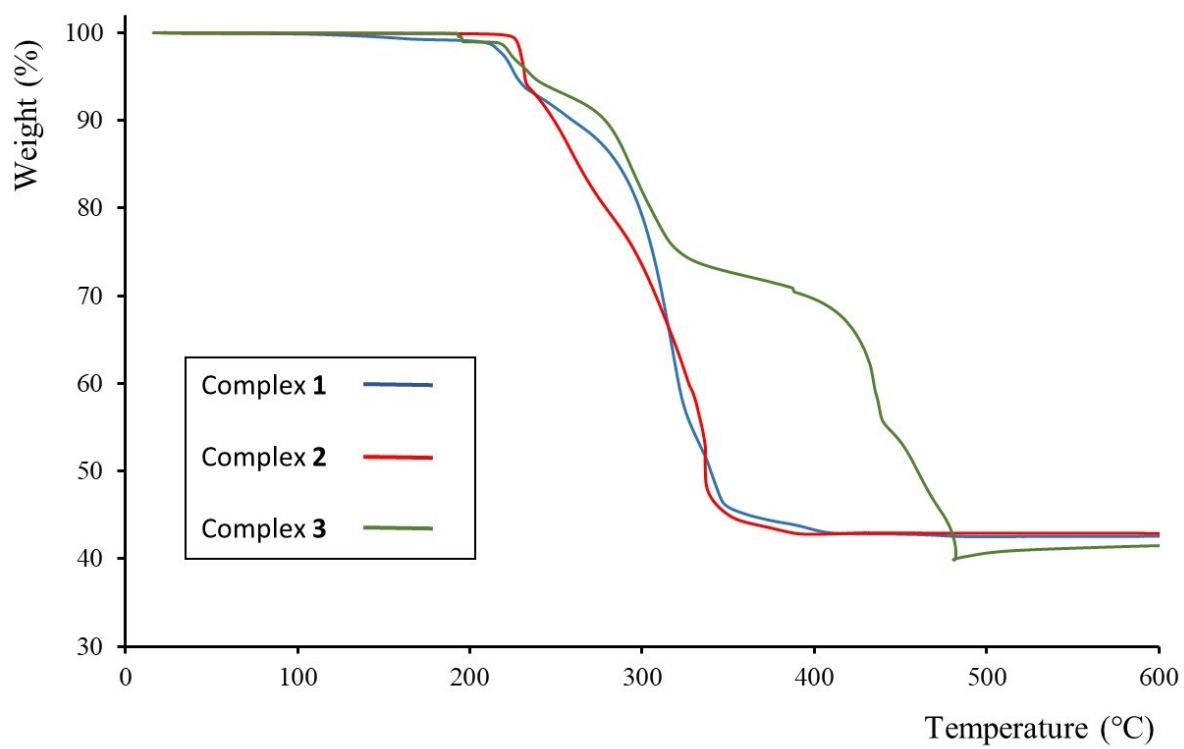


**Figure S10.** Optimised structure of  $[\text{V}_8\text{O}_{16}(\text{glut})_4\subset 2\text{F}]^{2-}$ , **8c**.

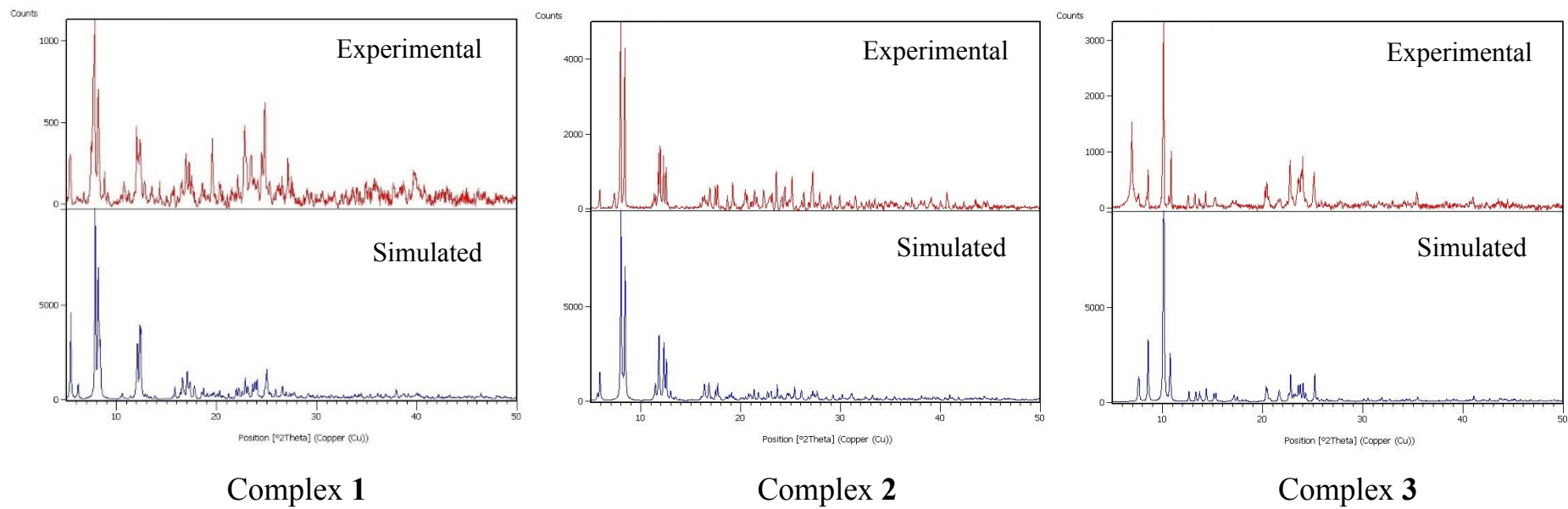




**Figure S11.** Thermogravimetric analyses for complexes **1-3**.

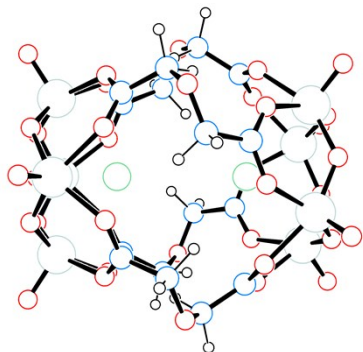


**Figure S12.** Comparison of the XRPDs for complexes **1-3**.



**Table S5.** Fractional coordinates of the computed compounds.

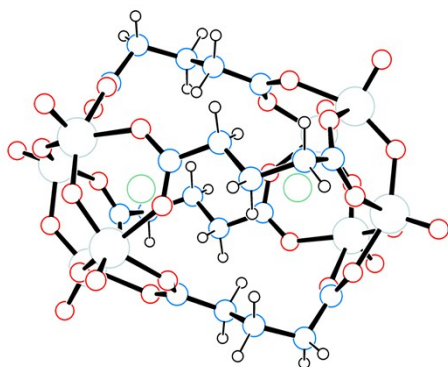
**Anion of complex 1,  $[V_8O_{16}(oda)_4\subset 2Cl]^{2-}$**



V	3.72893500	2.22653800	0.64268800
V	3.72870400	0.64227800	-2.22650000
V	3.72852700	-2.22689100	-0.64266400
V	3.72832900	-0.64288500	2.22659200
V	-3.72956400	-2.28547900	0.37916800
V	-3.72908600	-0.37889700	-2.28561900
V	-3.72879800	2.28611200	-0.37924000
V	-3.72875300	0.37938300	2.28556400
O	2.23419200	-3.14269100	0.33302400
O	2.27719100	-2.12409600	2.35802100
O	0.00024000	-3.52739000	3.13995900
O	-2.27863800	-2.59002700	1.83823400
O	-2.23327000	-0.69414800	3.08124100
O	2.27816800	2.35830400	2.12426600
O	2.23397000	0.33303100	3.14216500
O	0.00113200	3.14093000	3.52656700
O	-2.23305200	3.08175300	0.69400200
O	-2.27699900	1.83782200	2.58930000
O	2.23490400	3.14253700	-0.33301700
O	2.27774400	2.12387700	-2.35800300
O	0.00081000	3.52695900	-3.13968800
O	-2.23329200	0.69426300	-3.08160300
O	-2.27736600	2.58964800	-1.83780400
O	2.23467900	-0.33341300	-3.14271200
O	2.27783300	-2.35852000	-2.12437100
O	0.00024700	-3.13999100	-3.52648700
O	-2.23406900	-3.08160800	-0.69401400
O	-2.27789400	-1.83770700	-2.58936300
O	4.57697000	3.47626200	1.06934000
O	4.57633600	1.06917200	-3.47643000
O	4.57617300	-3.47692800	-1.06916700
O	4.57579400	-1.06962100	3.47667700
O	4.39848500	1.72032700	-0.86117000
O	4.39845200	-0.86166900	-1.72075900
O	4.39804100	-1.72094200	0.86134200
O	4.39813000	0.86097100	1.72079600
O	-4.57656800	-3.57692400	0.65793800
O	-4.57560600	-0.65769000	-3.57736500
O	-4.57534200	3.57784000	-0.65806600
O	-4.57511100	0.65848700	3.57737600
O	-4.39973900	-1.60994500	-1.05607700
O	-4.39921300	1.05659100	-1.61046900
O	-4.39901600	1.61080900	1.05611300
O	-4.39955000	-1.05569400	1.61043500
C	1.79322800	-2.91139900	1.50774500

C	0.51858600	-3.69036200	1.83688200
H	-0.22138800	-3.43485300	1.06955300
H	0.74721200	-4.75471200	1.72619400
C	-1.79291900	-1.83471500	2.71588900
C	-0.51787300	-2.25153200	3.45186600
H	0.22231900	-1.46011400	3.28714400
H	-0.74702000	-2.26447500	4.52176700
C	1.79376900	1.50807100	2.91136700
C	0.51985200	1.83813400	3.69126100
H	-0.22030700	1.07019600	3.43815500
H	0.74996000	1.72949400	4.75552400
C	-1.79195000	2.71592400	1.83408100
C	-0.51650600	3.45149000	2.25019300
H	0.22371300	3.28502100	1.45917600
H	-0.74473800	4.52159500	2.26142900
C	1.79387300	2.91122300	-1.50769900
C	0.51935200	3.69037500	-1.83670000
H	-0.22052100	3.43527400	-1.06913500
H	0.74825900	4.75470600	-1.72639100
C	-1.79227900	1.83442300	-2.71587100
C	-0.51700900	2.25094800	-3.45149200
H	0.22314900	1.45960600	-3.28616300
H	-0.74565400	2.26342500	-4.52149600
C	1.79369800	-1.50812100	-2.91143900
C	0.51900500	-1.83716900	-3.69031100
H	-0.22072800	-1.06942600	-3.43530900
H	0.74778400	-1.72721000	-4.75471500
C	-1.79286900	-2.71576100	-1.83413200
C	-0.51734700	-3.45114800	-2.25024600
H	0.22279900	-3.28481700	-1.45911500
H	-0.74545800	-4.52128300	-2.26181900
Cl	1.93107700	-0.00029100	-0.00080900
Cl	-1.93660300	-0.00047300	-0.00005700

**Anion of complex 2,  $[V_8O_{16}(\text{glut})_4\text{C}2\text{Cl}]^{2-}$**

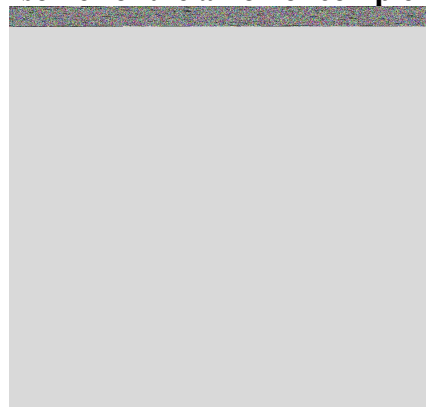


V	-3.12158300	2.79317100	-0.14217300
V	-4.00215400	0.52178100	-2.33994300
V	3.97910400	-0.76326300	-2.29072900
V	4.87907500	1.49282000	-0.08984100
O	-3.42355500	4.33394100	-0.16422200
O	-4.08687600	2.12473800	-1.40693300
O	-4.77021000	0.84088300	-3.67227100
O	-4.10972900	2.17144900	1.30307800
O	-1.58257100	2.80241100	1.21472000
O	-2.13875300	1.32900100	2.83974700
O	-1.53343600	2.73121400	-1.35420400
O	-2.13567600	1.18698800	-2.89481100

O	4.77849100	-1.10934700	-3.59769500
O	5.14433900	0.33314000	-1.34064600
O	6.17398600	2.38271700	-0.08299400
O	5.11942600	0.38071500	1.37903600
O	3.18872700	1.03451700	-2.92667700
O	3.75589300	2.57223400	-1.36121200
O	3.76848900	2.62302800	1.23473000
O	3.13048200	1.20607300	2.88495500
C	-1.33501400	2.12648900	2.24994200
C	0.05454700	2.22191800	2.85160700
H	0.56378100	1.29140300	2.57177300
H	-0.04544800	2.19132400	3.94188000
C	0.86967500	3.43160000	2.38797800
H	0.37631100	4.35499400	2.71347100
H	0.89035800	3.45981800	1.29528700
C	2.31786600	3.43838300	2.92946500
H	2.78837100	4.39561600	2.68945600
H	2.31921600	3.30141900	4.01566400
C	3.15436400	2.33712700	2.29921500
C	-1.31432600	1.98981000	-2.36468800
C	0.07638600	2.04056400	-2.97090300
H	-0.02402200	1.92222800	-4.05496500
H	0.58643900	1.13610100	-2.61622700
C	0.89123900	3.28467000	-2.60699200
H	0.90905600	3.40390800	-1.52067000
H	0.39950600	4.17801400	-3.00999400
C	2.34085000	3.24622700	-3.14272200
H	2.34599700	3.02377200	-4.21449300
H	2.81184900	4.21913800	-2.97750800
C	3.17330500	2.19438200	-2.42812000
V	3.12153600	-2.79300700	0.14212200
V	4.00212600	-0.52184500	2.33987900
V	-3.97918000	0.76333900	2.29075000
V	-4.87874000	-1.49271000	0.08991600
O	3.42342800	-4.33379000	0.16418900
O	4.08694700	-2.12471000	1.40696500
O	4.77019800	-0.84078900	3.67222900
O	4.10976900	-2.17139300	-1.30304500
O	1.58257800	-2.80253500	-1.21484600
O	2.13877600	-1.32909700	-2.83982700
O	1.53343000	-2.73105900	1.35423800
O	2.13581800	-1.18715500	2.89509700
O	-4.77853300	1.10951100	3.59771600
O	-5.14441500	-0.33316500	1.34076000
O	-6.17351900	-2.38279100	0.08294100
O	-5.11945900	-0.38057400	-1.37905200
O	-3.18886300	-1.03450400	2.92687000
O	-3.75575700	-2.57224200	1.36132600
O	-3.76850600	-2.62311300	-1.23493900
O	-3.13062000	-1.20610500	-2.88515500
C	1.33499100	-2.12653500	-2.25000700
C	-0.05456500	-2.22192300	-2.85167800
H	-0.56377900	-1.29140800	-2.57180700
H	0.04542700	-2.19128300	-3.94195200
C	-0.86971300	-3.43161300	-2.38811200
H	-0.37632300	-4.35500100	-2.71358000
H	-0.89047800	-3.45984200	-1.29542200
C	-2.31786500	-3.43837500	-2.92970100
H	-2.78838100	-4.39562700	-2.68978500
H	-2.31914000	-3.30134000	-4.01589000
C	-3.15440400	-2.33717500	-2.29941000

C	1.31437200	-1.98978900	2.36482100
C	-0.07632200	-2.04054700	2.97106700
H	0.02409300	-1.92223900	4.05513100
H	-0.58635600	-1.13606500	2.61641500
C	-0.89120900	-3.28462400	2.60713100
H	-0.90908000	-3.40381000	1.52080300
H	-0.39947600	-4.17799400	3.01007400
C	-2.34079600	-3.24615600	3.14292000
H	-2.34589800	-3.02365400	4.21468100
H	-2.81180500	-4.21907300	2.97776700
C	-3.17326900	-2.19434500	2.42828800
Cl	2.30425800	0.09142700	0.00171800
Cl	-2.30470000	-0.09196100	-0.00176800

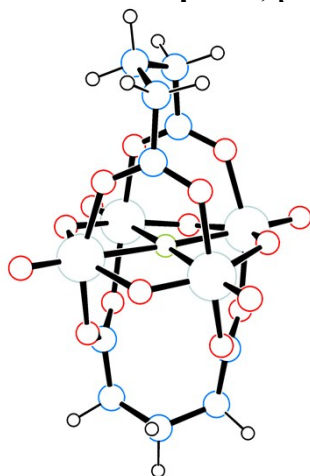
**Isomer of the anion of complex 2,  $[V_8O_{16}(\text{glut})_4\subset 2\text{Cl}]^{2-}$**



V	3.71508300	2.25563000	0.52051100
V	3.71505500	0.52044900	-2.25553300
V	3.71504900	-2.25557000	-0.52044500
V	3.71505100	-0.52049700	2.25566100
V	-3.71520700	-2.23095700	0.61761400
V	-3.71516500	-0.61763600	-2.23099900
V	-3.71522400	2.23102500	-0.61768200
V	-3.71524500	0.61765100	2.23097700
O	2.22649700	-3.11791100	0.50061800
O	2.27722300	-1.99798900	2.46501600
O	-2.27689900	-2.37595400	2.10319700
O	-2.22629300	-0.36438500	3.13605000
O	2.27722000	2.46496200	1.99799700
O	2.22644600	0.50054700	3.11788800
O	-2.22622700	3.13600500	0.36436300
O	-2.27687200	2.10316000	2.37593200
O	2.22657400	3.11798900	-0.50054400
O	2.27730700	1.99809400	-2.46496100
O	-2.22615500	0.36441300	-3.13598600
O	-2.27682400	2.37597500	-2.10312900
O	2.22658000	-0.50062400	-3.11797300
O	2.27731400	-2.46503600	-1.99806700
O	-2.22625600	-3.13605900	-0.36442300
O	-2.27684700	-2.10318400	-2.37597900
O	4.56158200	3.52952900	0.88168800
O	4.56150600	0.88164500	-3.52946000
O	4.56149600	-3.52952500	-0.88154700
O	4.56151800	-0.88159900	3.52960100
O	4.39164700	1.67106900	-0.95104200
O	4.39168500	-0.95112900	-1.67104800
O	4.39159100	-1.67105600	0.95116900

O	4.39154900	0.95110300	1.67111700
O	-4.56143900	-3.48811300	1.03398600
O	-4.56137000	-1.03397600	-3.48818200
O	-4.56147800	3.48817200	-1.03403100
O	-4.56150300	1.03404500	3.48810700
O	-4.39191300	-1.71100100	-0.87777200
O	-4.39185600	0.87776000	-1.71104800
O	-4.39188900	1.71102000	0.87769100
O	-4.39194500	-0.87771600	1.71100100
C	1.78620200	-2.84147200	1.66808400
C	0.55506300	-3.62621900	2.08918700
H	-0.21439700	-3.44016900	1.33309600
H	0.81474600	-4.68768000	1.99300000
C	-1.78588200	-1.54286500	2.91086800
C	-0.55443100	-1.92837200	3.71312600
H	0.21475500	-1.18110200	3.49331900
H	-0.81378600	-1.78482600	4.76930900
C	1.78618400	1.66803300	2.84146800
C	0.55505700	2.08915000	3.62622700
H	-0.21441700	1.33307300	3.44018500
H	0.81474900	1.99296000	4.68768600
C	-1.78584400	2.91083300	1.54285300
C	-0.55441200	3.71310800	1.92838500
H	0.21478600	3.49333500	1.18111600
H	-0.81379400	4.76928700	1.78485700
C	1.78628100	2.84155900	-1.66802300
C	0.55513500	3.62630400	-2.08910800
H	-0.21432000	3.44024300	-1.33301400
H	0.81480900	4.68776800	-1.99291700
C	-1.78577800	1.54289900	-2.91080000
C	-0.55433200	1.92844300	-3.71304800
H	0.21487000	1.18118900	-3.49324200
H	-0.81368300	1.78489400	-4.76923200
C	1.78628200	-1.66809600	-2.84153400
C	0.55512800	-2.08918500	-3.62626500
H	-0.21432000	-1.33308500	-3.44019900
H	0.81479000	-1.99300200	-4.68773200
C	-1.78583000	-2.91086000	-1.54289100
C	-0.55436600	-3.71309900	-1.92839400
H	0.21481900	-3.49326200	-1.18113000
H	-0.81369900	-4.76928300	-1.78482300
C	0.00072400	3.34119100	-3.49085500
C	0.00072000	-3.49093100	-3.34113400
C	0.00066100	-3.34110700	3.49093900
C	0.00067800	3.49091200	3.34111800
H	-0.78828800	3.69016800	4.07523300
H	0.79060000	4.23244200	3.50621100
H	-0.78831400	-4.07521800	3.69017500
H	0.79056500	-3.50621000	4.23248500
H	-0.78825600	-3.69018000	-4.07524100
H	0.79062500	-4.23247900	-3.50622500
H	-0.78827500	4.07528200	-3.69007600
H	0.79061400	3.50632100	-4.23241000
Cl	1.92551400	-0.00010900	-0.00037800
Cl	-1.92907500	-0.00023700	0.00003200

Anion of complex 3,  $[V_4O_8(\text{glut})_2CF]^-$



V	-0.04476300	-2.20971700	0.12795100
V	-0.11477400	-0.09564300	-2.23770000
V	-0.06546900	2.26842200	-0.11909200
V	0.22475200	0.15250500	2.23136600
F	0.00132900	0.02707100	0.00050300
O	-0.07639200	-3.77234200	0.30397300
O	-0.39257000	-1.89899300	-1.51555200
O	0.42251700	-1.51191300	1.90312000
O	1.92655900	-1.97481700	-0.22762800
O	1.84475800	-0.55608100	-1.99506700
O	-1.93560000	-1.81389500	0.73008500
O	-1.78245200	-0.04302400	2.13782300
O	-0.18981300	-0.26812600	-3.79911800
O	0.13097500	1.56791300	-1.94243900
O	-2.08483200	0.11130800	-1.85277400
O	-2.02890200	1.88224000	-0.43696700
O	-0.11526300	3.83118400	-0.28667300
O	-0.16114400	1.95587800	1.55657900
O	1.93871600	2.02222000	-0.07369000
O	2.11929600	0.61329900	1.69369200
O	0.38181000	0.32353200	3.78675800
C	2.45039700	-1.22016500	-1.10435400
C	3.96549200	-1.08285500	-1.05048400
H	4.29235200	-0.51950800	-1.92833500
H	4.38846500	-2.09203300	-1.10580500
C	4.46415700	-0.41579100	0.24988200
H	4.10001400	-0.98488000	1.10978900
H	5.55872200	-0.47724600	0.25749100
C	4.06646600	1.06499900	0.42014300
H	4.61136500	1.47492800	1.27892400
H	4.32821900	1.65371800	-0.46269600
C	2.58213700	1.25529000	0.70412400
C	-2.42150400	-0.86415600	1.41320000
C	-3.93271100	-0.69200200	1.33715000
H	-4.21487000	0.16886500	1.94855500
H	-4.37891100	-1.58907100	1.78286500
C	-4.45287400	-0.55389100	-0.10851800
H	-5.54512500	-0.64550900	-0.08775100
H	-4.06727200	-1.38355100	-0.70750800
C	-4.10656700	0.78000000	-0.80557100
H	-4.60861900	0.80202600	-1.77911000
H	-4.45428500	1.63109500	-0.21435000
C	-2.61457100	0.94730900	-1.05751200



**[V<sub>8</sub>O<sub>16</sub>(oda)<sub>4</sub>], 4c**

V	-3.61675300	-2.22150400	-0.85210800
V	-3.61678700	0.85224800	-2.22139100
V	-3.61663200	2.22128600	0.85216400
V	-3.61680300	-0.85240700	2.22137600
V	3.61639300	1.64720500	1.71766300
V	3.61664600	1.71865700	-1.64512800
V	3.61704900	-1.64690200	-1.71773000
V	3.61723400	-1.71853800	1.64517600
O	-2.04595100	2.22667600	2.08728600
O	-2.15321900	0.23477300	3.15820300
O	0.00080300	0.96345400	4.78285000
O	2.15279700	1.00612500	3.00109900
O	2.04655100	-1.24540000	2.78614000
O	-2.15275300	-3.15809500	0.23472800
O	-2.04537400	-2.08678800	2.22643000
O	0.00034600	-4.78363800	0.96420100
O	2.04555100	-2.78656200	-1.24474700
O	2.15367600	-3.00335500	1.00652300
O	-2.04590300	-2.22683100	-2.08712400
O	-2.15318800	-0.23495500	-3.15813500
O	0.00068800	-0.96369700	-4.78283100
O	2.04520100	1.24459600	-2.78438000
O	2.15382800	-1.00652500	-3.00238900
O	-2.04557100	2.08686100	-2.22672100
O	-2.15257700	3.15761700	-0.23470800
O	-0.00017800	4.78393500	-0.96439700
O	2.04549400	2.78760700	1.24479100
O	2.15344100	3.00401700	-1.00649700
O	-4.51650300	-3.40829100	-1.30403900
O	-4.51653800	1.30375200	-3.40834300
O	-4.51631800	3.40816900	1.30397200
O	-4.51638600	-1.30395800	3.40844300
O	-4.17300100	-0.81580400	-1.69366400
O	-4.17308600	1.69453400	-0.81614600
O	-4.17309600	0.81560500	1.69369600
O	-4.17318100	-1.69492100	0.81627300
O	4.51640600	2.52061600	2.63931700
O	4.51681000	2.63662000	-2.52226500
O	4.51706600	-2.52050200	-2.63920400
O	4.51806900	-2.63616200	2.52197300
O	4.17400100	1.88129800	0.09722300
O	4.17196200	0.09670800	-1.87375500
O	4.17442100	-1.88133900	-0.09730300
O	4.17180400	-0.09637000	1.87332000
C	-1.68550500	1.38972800	2.98397200
C	-0.54121100	1.88412400	3.86552200
H	0.22110700	2.30301400	3.19959300
H	-0.93982700	2.70954700	4.46471600
C	1.68552700	-0.12638500	3.28796200
C	0.54005600	-0.24063000	4.29079800
H	-0.22381300	-0.88091000	3.83628700
H	0.93613500	-0.77343300	5.16166500
C	-1.68520700	-2.98384400	1.38975900
C	-0.54129000	-3.86570800	1.88449400
H	0.22133600	-3.19996100	2.30314300
H	-0.94017000	-4.46437800	2.71016900
C	1.68544700	-3.28936000	-0.12580600
C	0.53999900	-4.29221900	-0.23996000
H	-0.22364200	-3.83803400	-0.88072100

H	0.93629900	-5.16337200	-0.77215800
C	-1.68547200	-1.38990600	-2.98383900
C	-0.54112700	-1.88430300	-3.86533700
H	0.22129200	-2.30293700	-3.19934400
H	-0.93960500	-2.70993100	-4.46433600
C	1.68539200	0.12579900	-3.28777800
C	0.54006300	0.24032100	-4.29075100
H	-0.22375100	0.88075800	-3.83639900
H	0.93643800	0.77299300	-5.16157700
C	-1.68524500	2.98368800	-1.38988600
C	-0.54149400	3.86575100	-1.88461700
H	0.22131600	3.20009000	-2.30305500
H	-0.94040000	4.46420800	-2.71043200
C	1.68522800	3.29016200	0.12578000
C	0.53962000	4.29283500	0.23982200
H	-0.22389800	3.83863200	0.88071500

### [V<sub>8</sub>O<sub>16</sub>(glut)<sub>4</sub>], 5c

V	-2.97158100	0.15439400	-2.86024500
V	-3.92835200	-2.34011700	-0.81096700
V	3.91876100	-2.41711900	0.55965700
V	4.86345400	0.07597200	-1.48864300
O	-3.29023500	0.25997800	-4.38267100
O	-3.88556000	-1.17081900	-2.22970800
O	-4.74967600	-3.57623100	-1.28576000
O	-3.91132600	1.48082300	-2.02090500
O	-1.41604400	1.43728100	-2.59027600
O	-2.03299300	2.91966100	-1.00023200
O	-1.37457100	-1.05742200	-2.78312400
O	-2.01593100	-2.70849500	-1.38019300
O	4.75673300	-3.69967900	0.84329400
O	4.97597900	-1.26993100	-0.40066200
O	6.19970600	0.14289500	-2.28637400
O	4.95744500	1.37661400	-0.19183200
O	3.10463800	-2.78653000	-1.26085400
O	3.68363900	-1.07473500	-2.62027200
O	3.65729400	1.42261700	-2.40007900
O	3.06909700	2.98739500	-0.87769200
C	-1.23517400	2.47595700	-1.89157600
C	0.06484100	3.23937600	-2.04962600
H	0.60997700	3.10074500	-1.10696900
H	-0.18497700	4.30544200	-2.07745200
C	0.92301600	2.82444200	-3.25053600
H	0.49668400	3.23847600	-4.16959200
H	0.90294300	1.73728900	-3.36714400
C	2.39317200	3.29686000	-3.13930400
H	2.90325200	3.11814300	-4.08830900
H	2.44240800	4.36251800	-2.89945300
C	3.11998200	2.52019300	-2.06178200
C	-1.20922300	-2.17629800	-2.20401700
C	0.09039900	-2.91941100	-2.44469000
H	-0.16062600	-3.97645000	-2.58322200
H	0.63795300	-2.88062600	-1.49405600
C	0.94734700	-2.38223200	-3.59732100
H	0.92906800	-1.28897300	-3.59945500
H	0.51896800	-2.69767200	-4.55376700
C	2.41736100	-2.86456300	-3.53969600
H	2.46671400	-3.94948400	-3.41260500
H	2.92496700	-2.58774800	-4.46620100
C	3.14725500	-2.20613600	-2.38795500

V	2.97160000	-0.15440000	2.86025000
V	3.92835400	2.34011700	0.81096100
V	-3.91876100	2.41711700	-0.55965900
V	-4.86346700	-0.07596600	1.48863600
O	3.29026800	-0.25997800	4.38267300
O	3.88557400	1.17081000	2.22969400
O	4.74967200	3.57623200	1.28575700
O	3.91133500	-1.48083500	2.02091100
O	1.41605800	-1.43728300	2.59029000
O	2.03299500	-2.91965900	1.00024000
O	1.37459300	1.05742400	2.78315100
O	2.01593400	2.70848500	1.38019900
O	-4.75672700	3.69967800	-0.84330800
O	-4.97599400	1.26994100	0.40066200
O	-6.19972400	-0.14290400	2.28635900
O	-4.95744000	-1.37660100	0.19181400
O	-3.10464200	2.78652400	1.26085400
O	-3.68366700	1.07474200	2.62027700
O	-3.65730700	-1.42261100	2.40007100
O	-3.06910900	-2.98739500	0.87769100
C	1.23518400	-2.47596100	1.89159500
C	-0.06484300	-3.23936200	2.04963000
H	-0.60997000	-3.10072800	1.10696800
H	0.18496700	-4.30543000	2.07745900
C	-0.92302500	-2.82442000	3.25053400
H	-0.49669300	-3.23844800	4.16959300
H	-0.90295600	-1.73726800	3.36713500
C	-2.39317900	-3.29684800	3.13930300
H	-2.90326000	-3.11813100	4.08830800
H	-2.44240900	-4.36250700	2.89945600
C	-3.12000100	-2.52019200	2.06178100
C	1.20924000	2.17630000	2.20404400
C	-0.09039500	2.91939600	2.44469600
H	0.16062200	3.97643700	2.58323300
H	-0.63793700	2.88061100	1.49405500
C	-0.94735600	2.38221300	3.59731700
H	-0.92908400	1.28895300	3.59944400
H	-0.51897700	2.69764100	4.55376700
C	-2.41736700	2.86455800	3.53969600
H	-2.46670900	3.94948000	3.41260400
H	-2.92497200	2.58774900	4.46620200
C	-3.14727800	2.20614000	2.38796000

**[V<sub>8</sub>O<sub>16</sub>(oda)<sub>4</sub>Cl<sub>2</sub>], 6c**

V	3.64945900	-1.43128600	1.92118800
V	3.65266400	1.91933000	1.43107600
V	3.65944700	1.42850300	-1.91395900
V	3.65648100	-1.92337800	-1.42355200
V	-3.64865800	0.49498100	-2.34504100
V	-3.65022400	2.34488300	0.48832100
V	-3.65826300	-0.48861700	2.33919400
V	-3.65790000	-2.33883500	-0.49549400
O	2.12915300	0.77778300	-3.02442400
O	2.18869100	-1.47828800	-2.79356400
O	0.00744500	-1.72402400	-4.54263600
O	-2.17991600	-0.74550000	-3.07856100
O	-2.12349500	-2.58598600	-1.75284400
O	2.17735600	-2.79797600	1.47846900
O	2.12148300	-3.02887400	-0.77755900
O	-0.00645100	-4.54639000	1.71947700

O	-2.12931400	-1.75218500	2.58598500
O	-2.19147300	-3.07708900	0.74495300
O	2.11474700	-0.77947200	3.02387400
O	2.17827700	1.47650700	2.79523600
O	-0.00123200	1.72334500	4.54791500
O	-2.11930000	2.58632800	1.74947400
O	-2.18638600	0.74694600	3.07627100
O	2.12099700	3.02517300	0.77917800
O	2.18729900	2.79642400	-1.47669000
O	0.00721300	4.54893700	-1.72541100
O	-2.11317400	1.75115300	-2.58614300
O	-2.17647900	3.07799000	-0.74683300
O	4.57020500	-2.18987600	2.92071000
O	4.57436300	2.91025400	2.19974100
O	4.58641100	2.18477300	-2.90951300
O	4.58120800	-2.91448400	-2.18830000
O	4.19041100	0.20448400	1.85782200
O	4.20074700	1.86672400	-0.20285700
O	4.19681100	-0.20811700	-1.84625700
O	4.19770500	-1.87051500	0.21265800
O	-4.56973000	0.73673900	-3.57603300
O	-4.57250300	3.57567700	0.72665600
O	-4.58539300	-0.72660100	3.56639100
O	-4.58452100	-3.56592800	-0.73588500
O	-4.19145400	1.53488900	-1.08193300
O	-4.19587500	1.08143800	1.52629500
O	-4.19976600	-1.52556200	1.07315600
O	-4.19580100	-1.07345200	-1.53498700
C	1.73662400	-0.41046400	-3.28611600
C	0.55608700	-0.45958700	-4.25669200
H	-0.19717000	0.24119800	-3.87832200
H	0.91524600	-0.06250500	-5.21151000
C	-1.72834800	-1.87062700	-2.73633000
C	-0.54476500	-2.47831000	-3.49004000
H	0.20514100	-2.74888100	-2.73777200
H	-0.90123400	-3.41042600	-3.93990700
C	1.72604700	-3.28972300	0.41007100
C	0.54311000	-4.25745900	0.45621100
H	-0.20906700	-3.87486400	-0.24353500
H	0.89994700	-5.21175800	0.05583400
C	-1.73823300	-2.73685900	1.87008200
C	-0.55712500	-3.49513100	2.47678600
H	0.19418500	-2.74550200	2.75069700
H	-0.91546300	-3.94747500	3.40700700
C	1.72476100	0.40923800	3.28735800
C	0.54671900	0.45895500	4.26082300
H	-0.20768600	-0.24190200	3.88503900
H	0.90885100	0.06235100	5.21474400
C	-1.73102400	1.87114700	2.73570900
C	-0.55156300	2.47908300	3.49548800
H	0.20035300	2.75348000	2.74669100
H	-0.91214200	3.40899600	3.94671500
C	1.73272900	3.28916300	-0.40997700
C	0.55551800	4.26348700	-0.46083000
H	-0.19863400	3.88921900	0.24114700
H	0.91852700	5.21779100	-0.06587900
C	-1.72269700	2.73689400	-1.87138900
C	-0.54289700	3.49551800	-2.48003300
H	0.20914200	2.74639600	-2.75317400
H	-0.90305000	3.94556500	-3.41067100
C1	1.00893600	-0.00523200	-0.01129500

C1	-1.01904000	-0.01264800	0.00633300
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**[V<sub>8</sub>O<sub>16</sub>(glut)<sub>4</sub>(Cl<sub>2</sub>)]<sub>7c</sub>**

V	3.16414900	-0.26911800	2.76483600
V	4.03775900	-2.44482000	0.35199400
V	-4.00312600	-2.34420200	-0.79468700
V	-4.63708000	-0.17826800	1.66232700
O	3.56134300	-0.37077200	4.26862500
O	4.05761400	-1.48608900	1.92260300
O	4.95828700	-3.67874400	0.59142200
O	4.06858300	1.15634800	2.05709000
O	1.60927400	1.06232900	2.79456700
O	2.18359000	2.79181400	1.45373400
O	1.57020300	-1.48777500	2.58678800
O	2.19797400	-2.95718600	0.98522200
O	-4.90687500	-3.53202400	-1.24076700
O	-4.94686700	-1.36944100	0.44430700
O	-5.82863900	-0.20847100	2.66708600
O	-4.91723500	1.29014800	0.58809700
O	-3.08371500	-3.07576100	0.87647600
O	-3.33834700	-1.47593300	2.45011000
O	-3.23305300	1.00954000	2.50454500
O	-3.10256700	2.95605000	1.37008600
C	1.41605800	2.20457000	2.28820600
C	0.13696600	2.95676800	2.60335000
H	-0.40048000	3.02073000	1.64838600
H	0.42101600	3.98905600	2.83495100
C	-0.75545800	2.35638900	3.69422100
H	-0.36308600	2.61830300	4.68141300
H	-0.74513300	1.26530700	3.63531600
C	-2.21535200	2.85871400	3.59265300
H	-2.76300100	2.55592700	4.48953900
H	-2.25435900	3.94716900	3.50346500
C	-2.92343200	2.24280300	2.40235500
C	1.40473400	-2.53303500	1.88284500
C	0.12085200	-3.32567700	2.03723700
H	0.39520200	-4.38585200	2.03115600
H	-0.42767800	-3.17035000	1.09875000
C	-0.75543100	-2.97416800	3.24382700
H	-0.75737100	-1.89387500	3.40934300
H	-0.33807000	-3.42634200	4.14877300
C	-2.21233200	-3.46783000	3.07197500
H	-2.23866800	-4.51315800	2.75423100
H	-2.73950800	-3.37102400	4.02463200
C	-2.95378600	-2.62597400	2.05239000
V	-3.16413300	0.26911300	-2.76483600
V	-4.03776300	2.44481700	-0.35199700
V	4.00315100	2.34420100	0.79469400
V	4.63707000	0.17826500	-1.66232800
O	-3.56133000	0.37076200	-4.26862400
O	-4.05760200	1.48608300	-1.92260700
O	-4.95829100	3.67873900	-0.59144000
O	-4.06856200	-1.15634900	-2.05708100
O	-1.60925800	-1.06233700	-2.79457300
O	-2.18356600	-2.79181200	-1.45372600
O	-1.57019100	1.48777600	-2.58678800
O	-2.19796800	2.95718500	-0.98522200
O	4.90690600	3.53201700	1.24077300
O	4.94687800	1.36943100	-0.44430500
O	5.82861900	0.20845200	-2.66710000

O	4.91722300	-1.29015300	-0.58810500
O	3.08374200	3.07577300	-0.87646900
O	3.33834900	1.47594300	-2.45010100
O	3.23300700	-1.00951400	-2.50452000
O	3.10253100	-2.95603900	-1.37006800
C	-1.41604200	-2.20457700	-2.28821100
C	-0.13696000	-2.95678800	-2.60336900
H	0.40048900	-3.02077600	-1.64840700
H	-0.42102700	-3.98906800	-2.83498900
C	0.75546800	-2.35640500	-3.69423800
H	0.36312200	-2.61832300	-4.68144000
H	0.74513600	-1.26532300	-3.63533100
C	2.21536200	-2.85869900	-3.59264700
H	2.76303100	-2.55588900	-4.48951600
H	2.25439500	-3.94715300	-3.50346400
C	2.92334700	-2.24276600	-2.40231000
C	-1.40472500	2.53303500	-1.88284400
C	-0.12084900	3.32568700	-2.03724100
H	-0.39521200	4.38585900	-2.03118000
H	0.42767900	3.17038600	-1.09874900
C	0.75544400	2.97416800	-3.24382000
H	0.75739000	1.89387300	-3.40932600
H	0.33808400	3.42633100	-4.14877300
C	2.21234200	3.46784400	-3.07196300
H	2.23866900	4.51317100	-2.75421500
H	2.73951700	3.37104700	-4.02462000
C	2.95381400	2.62599400	-2.05238500
Cl	-0.81586500	0.00867600	0.62062600
Cl	0.81578800	-0.00867400	-0.62065400

**[V<sub>8</sub>O<sub>16</sub>(glut)<sub>4</sub>C<sub>2</sub>F]<sup>2-</sup>, 8c**

V	3.16119800	-2.84061500	0.01897800
V	3.97740400	-0.60052400	-2.19396000
V	-3.98243100	0.53874100	-2.20963100
V	-4.87576200	-1.41624500	-0.01731500
O	3.49069700	-4.37622000	0.01515000
O	4.10904700	-2.13995400	-1.35918300
O	4.62777900	-0.92876000	-3.58692700
O	4.05727300	-2.16946800	1.33697000
O	1.53088500	-2.76914100	1.21143000
O	2.06864700	-1.14594000	2.68784100
O	1.58376100	-2.75584500	-1.25785000
O	2.05536900	-1.06807300	-2.67986600
O	-4.57719500	0.97510300	-3.59801700
O	-5.28789200	-0.35931400	-1.48404600
O	-6.12668100	-2.36937500	0.00216000
O	-5.19037900	-0.36242000	1.35527400
O	-3.13625200	-1.15239200	-2.90784000
O	-3.82112500	-2.62307600	-1.33894600
O	-3.69681500	-2.56479300	1.19096500
O	-3.18912500	-1.13271800	2.86321200
C	1.29158400	-2.02283500	2.20777200
C	-0.07239200	-2.14670200	2.86670700
H	-0.61512500	-1.22323400	2.63031600
H	0.08160600	-2.11866800	3.95128300
C	-0.88500600	-3.37310900	2.44297700
H	-0.39342900	-4.28331200	2.80536500
H	-0.89933100	-3.44614000	1.35226000
C	-2.33732000	-3.35226200	2.96986500
H	-2.81277800	-4.31294600	2.75424900

H	-2.35179500	-3.18009300	4.05067100
C	-3.15441100	-2.26274900	2.29252700
C	1.30292500	-1.97613700	-2.21549700
C	-0.06690500	-2.10524100	-2.85956900
H	0.07710200	-2.06894200	-3.94552300
H	-0.61737700	-1.18946900	-2.61284900
C	-0.86025600	-3.34548700	-2.43969200
H	-0.90072500	-3.40446700	-1.34831700
H	-0.33600000	-4.24770200	-2.77519000
C	-2.29849000	-3.37428100	-3.00559200
H	-2.28424300	-3.21466100	-4.08870000
H	-2.75148500	-4.34635000	-2.79383600
C	-3.16601300	-2.30249500	-2.36594600
V	-3.16100100	2.84351000	-0.03584900
V	-4.01504900	0.65170300	2.30040400
V	4.01939200	-0.60811300	2.31441000
V	4.87231000	1.42559600	-0.07041600
O	-3.50328700	4.37608100	0.00778600
O	-4.07958700	2.11919400	1.37964000
O	-4.75682500	0.99586100	3.64088900
O	-4.09753400	2.17771400	-1.30751100
O	-1.55073200	2.82059500	-1.21509000
O	-2.01898800	1.11712200	-2.61860800
O	-1.56971200	2.71933600	1.25961400
O	-2.09361900	1.09291600	2.73803700
O	4.74673400	-1.00901200	3.64760400
O	5.15773800	0.30452100	1.40994100
O	6.11854100	2.37372600	0.07944500
O	5.32165400	0.40792700	-1.41256100
O	3.14199700	1.08805300	2.92221500
O	3.66846100	2.51649900	1.25266300
O	3.82849600	2.65754000	-1.27842200
O	3.19484000	1.19679900	-2.87779700
C	-1.27037300	2.02483500	-2.17131600
C	0.10146500	2.15802600	-2.81170700
H	0.65055300	1.24074900	-2.56816600
H	-0.04296000	2.12451700	-3.89777900
C	0.89948000	3.39493400	-2.39177000
H	0.37844600	4.29990500	-2.72470100
H	0.94504000	3.45246500	-1.30055600
C	2.33586400	3.41569600	-2.96313400
H	2.79631500	4.38410400	-2.75007100
H	2.31702800	3.25892900	-4.04643900
C	3.19603800	2.33291500	-2.33201600
C	-1.32104400	1.97988000	2.24987900
C	0.04047300	2.10170100	2.91245600
H	-0.11465100	2.06729600	3.99666600
H	0.58533400	1.18056300	2.67155300
C	0.85049300	3.33195500	2.49595400
H	0.86644900	3.40980800	1.40549700
H	0.35592800	4.23919800	2.86173100
C	2.30141400	3.31045200	3.02602500
H	2.31313000	3.13518200	4.10640800
H	2.77721700	4.27183400	2.81445500
C	3.12051200	2.22529100	2.34386200
F	3.08438600	0.14696100	-0.29330200
F	-3.08785300	-0.15562500	-0.27744200