

Supplementary Information

Table S1. Refined structural parameters for non-H atoms of [V₄O₄(OH)₂(O₂CC₆H₄CO₂)₄]·DMF with esds in parentheses.

ATOM	WYCKOFF POSITION	X	Y	Z	B _{iso} [Å ²]
V1	2 <i>m</i>	0.5000	1.0000	0.2820(6)	7.1(6)
V2	2 <i>n</i>	0.5000	0.5000	0.2769(6)	7.1(6)
V3	2 <i>m</i>	0.0000	0.0000	0.1990(5)	7.1(6)
V4	2 <i>n</i>	0.000	0.5000	0.1388(5)	7.1(6)
O1	4 <i>o</i>	0.452(1)	0.255(1)	0.295(2)	5.1(7)
O2	4 <i>o</i>	0.367(3)	0.205(4)	0.336(3)	5.1(7)
O3	4 <i>o</i>	0.147(2)	0.168(4)	-0.087(3)	5.1(7)
O4	4 <i>o</i>	0.072(1)	0.318(1)	-0.043(3)	5.1(7)
O5	4 <i>o</i>	0.5692(3)	0.753(1)	0.299(1)	5.1(7)
O6	4 <i>o</i>	0.682(2)	0.804(3)	0.294(3)	5.1(7)
O7	4 <i>o</i>	0.910(3)	0.845(2)	0.700(3)	5.1(7)
O8	4 <i>o</i>	0.801(4)	0.822(3)	0.696(3)	5.1(7)
O9	4 <i>o</i>	0.4657(8)	0.244(1)	0.2114(6)	5.1(7)
O10	4 <i>o</i>	-0.004(7)	0.242(5)	0.161(3)	5.1(7)
O11	2 <i>m</i>	-0.0799(8)	0.0000	0.213(1)	5.1(7)
O12	2 <i>n</i>	0.065(5)	0.5000	0.113(6)	5.1(7)
N1	2 <i>m</i>	0.2876(3)	0.0000	0.8607(3)	4.2(8)
C1	2 <i>m</i>	0.3535(3)	0.0000	0.9004(4)	2.6(7)
C2	2 <i>m</i>	0.233(1)	0.0000	0.872(2)	2.6(7)
C3	2 <i>m</i>	0.280(1)	0.0000	0.7836(4)	2.6(7)
O13	2 <i>m</i>	0.393(1)	0.0000	0.9944(4)	5.1(7)
C4	4 <i>o</i>	0.3191	0.2232	0.2007	2.6(7)
C5	4 <i>o</i>	0.3327	0.2366	0.1444	2.6(7)
C6	4 <i>o</i>	0.2483	0.2339	0.1831	2.6(7)
C7	4 <i>o</i>	0.2729	0.2364	0.0676	2.6(7)
C8	4 <i>o</i>	0.1908	0.2547	0.1079	2.6(7)
C9	4 <i>o</i>	0.2021	0.2539	0.0501	2.6(7)
C10	4 <i>o</i>	0.3785	0.2452	0.2776	2.6(7)
C11	4 <i>o</i>	0.1404	0.2466	-0.0259	2.6(7)
C12	4 <i>o</i>	0.6970	0.7478	0.4169	2.6(7)
C13	4 <i>o</i>	0.6653	0.7242	0.4587	2.6(7)
C14	4 <i>o</i>	0.7725	0.7550	0.4546	2.6(7)
C15	4 <i>o</i>	0.7116	0.7080	0.5384	2.6(7)
C16	4 <i>o</i>	0.8173	0.7522	0.5330	2.6(7)
C17	4 <i>o</i>	0.7864	0.7460	0.5748	2.6(7)
C18	4 <i>o</i>	0.6506	0.7729	0.3365	2.6(7)
C19	4 <i>o</i>	0.8316	0.7665	0.6548	2.6(7)

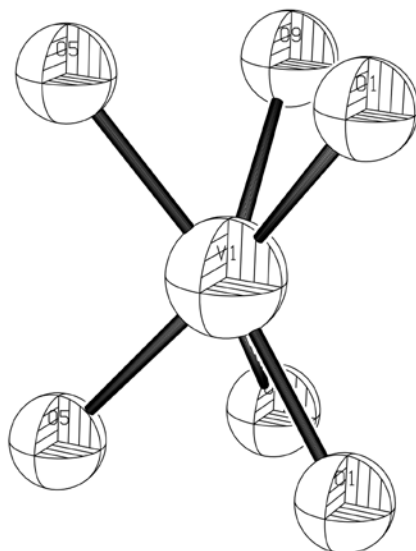


Fig. S1 Trigonal-prismatic geometry of $[\text{V}_4\text{O}_4(\text{OH})_2(\text{O}_2\text{CC}_6\text{H}_4\text{CO}_2)_4]\cdot\text{DMF}$ in detail.

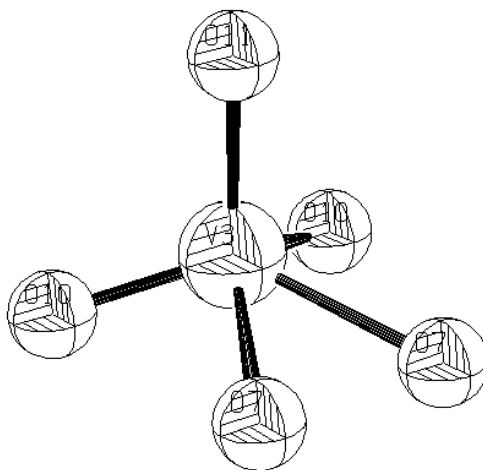


Fig. S2 Square-pyramidal geometry of $[\text{V}_4\text{O}_4(\text{OH})_2(\text{O}_2\text{CC}_6\text{H}_4\text{CO}_2)_4]\cdot\text{DMF}$ in detail.