Supplementary Information

Details make the difference: A family of heterometallic complexes with cube-like {$Cu_3Mn(\mu_3\text{-}O)_4$} and double open cube-like {$Cu_3Mn(\mu\text{-}O)_2(\mu_3\text{-}O)_2$} tetranuclear cores

O. Stetsiuk, O. V. Nesterova, V. N. Kokozay, K. V. Domasevitch, I. V. Omelchenko, O. V. Shishkin, B. Vranovičová, R. Boča, A. J. L. Pombeiro, S. R. Petrusenko

Table S1. Calculated magnetic parameters for **1–5**.[a]

Complex -fit	M_r	g_{Mn}	g_{Cu}	J_2/hc	J_4/hc	D_{Mn}/hc	$(zj)/hc$	χ_{TIM} [b]	$R(\chi)$ /%	$R(M)$ /%
1-a	1375.07	1.859	2.313	-54.8	-27.0	-13.6	-0.075	+0.2	4.0	3.4
1-b		1.850	2.087	-21.8	-39.5	-28.7	~ 0	+0.9	4.8	4.4
2-a	1088.49	1.869	2.349	-54.8	-27.0	-14.4	-0.013	+14.4	3.5	4.3
2-b		1.851	2.065	-21.7	-39.5	-28.7	0.028	+2.6	4.0	5.6
3-a	1064.25	1.988	2.009	-45.0	-37.5	-2.8	-0.079	+12.2	2.2	0.7
3-b		1.976	2.004	-35.0	-45.9	-0.3	-0.050	+14.1	1.5	0.8
4-a	1057.12	2.000	2.000	-52.5	-39.1	-2.5	~ 0	+15.0	1.9	1.0
4-b		2.000	2.004	-35.0	-46.9	-0.3	-0.047	+14.7	1.3	1.0
5-a	2340.09	1.851 [c]	2.178	-22.7	-11.6	-23.4	0.268	+40.0	2.5	3.3
5-b		1.889 [c]	2.336	-14.9	-28.3	-19.7	-0.063	+40.0	0.6	3.1

[a] Coupling constants conforming the definition $\hat{H}_{ij} = -J(\hat{S}_i \cdot \hat{S}_j)$ in cm^{-1}. J_2 – in two bases, J_4 – within four walls.

[b] Temperature independent magnetism χ_{TIM} in units of 10^{-9} m^3 mol^{-1} (SI).

[c] $g(Mn^{II})$ = 1.950 and 1.956.

Table S2. Data selected for the correlations for 6 new hits.

↓Complex	g_{Cu}	J_2	J_4	β_{M-O-M}	α_{M-O-M}	R_{M-M}	R_{M-M}	R_{M-O}	R_{M-O}	d_4-d_2	R_4-R_2
Abbrev.→	g	J2	J4	beta	alpha	d2	d4	R2	R4	d42	R42
1	2.313	–54.8	–27.0	102.53	97.47	3.510	3.144	2.239	1.959	-0.366	-0.280
2	2.349	–54.8	–27.0	101.96	97.81	3.501	3.177	2.253	1.957	-0.324	-0.296
3	2.009	–45.0	–37.5	102.81	97.82	3.496	3.136	2.226	1.950	-0.360	-0.276
4	2.000	–52.5	–39.1	99.55	98.61	3.407	3.158	2.220	1.961	-0.249	-0.259
5 unit A	2.178	–22.7	–11.6	100.64	99.27	3.542	3.210	2.292	1.953	-0.332	-0.339
5 unit B	2.178	–22.7	–11.6	98.32	99.88	3.509	3.235	2.307	1.854	-0.274	-0.453

Table S3. Pair correlation coefficients for 41 + 6 hits.

	g	J2	J4	beta	alpha	d2	d4	R2	R4	d42	R42
g		0.114	-0.287	-0.253	0.155	0.043	0.176	0.155	-0.026	0.029	-0.081
J2	0.114		-0.195	-0.210	0.754	0.223	0.344	0.307	-0.221	-0.050	-0.253
J4	-0.287	-0.195		0.385	-0.330	-0.169	-0.294	-0.323	0.117	0.026	0.205
beta	-0.253	-0.210	0.385		-0.501	0.275	-0.603	-0.097	-0.180	-0.421	-0.070
alpha	0.155	0.754	-0.330	-0.501		-0.009	0.677	0.177	-0.005	0.243	-0.071
d2	0.043	0.223	-0.169	0.275	-0.009		-0.545	0.929	-0.942	-0.956	-0.959
d4	0.176	0.344	-0.294	-0.603	0.677	-0.545		-0.337	0.642	0.767	0.534
R2	0.155	0.307	-0.323	-0.097	0.177	0.929	-0.337		-0.906	-0.830	-0.966
R4	-0.026	-0.221	0.117	-0.180	-0.005	-0.942	0.642	-0.906		0.945	0.984
d42	0.029	-0.050	0.026	-0.421	0.243	-0.956	0.767	-0.830	0.945		0.921
R42	-0.081	-0.253	0.205	-0.070	-0.071	-0.959	0.534	-0.966	0.984	0.921	

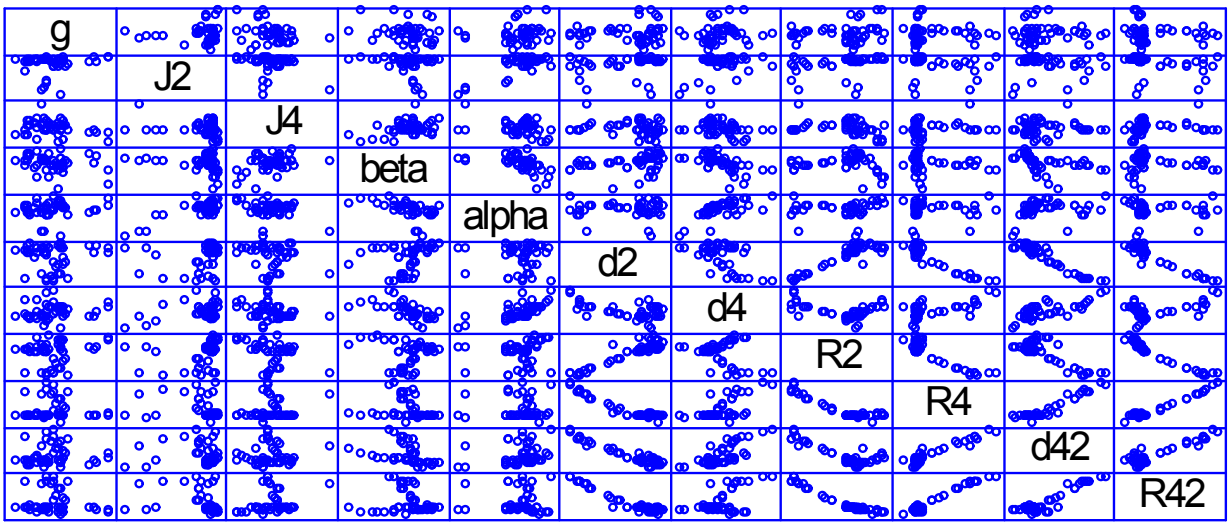

Figure S1. Brief view to the pair correlations for 41+6 hits.