

Supplementary data for **Polynuclear complexes of transition metals
with aminopolycarboxylate and polyoxometalates**

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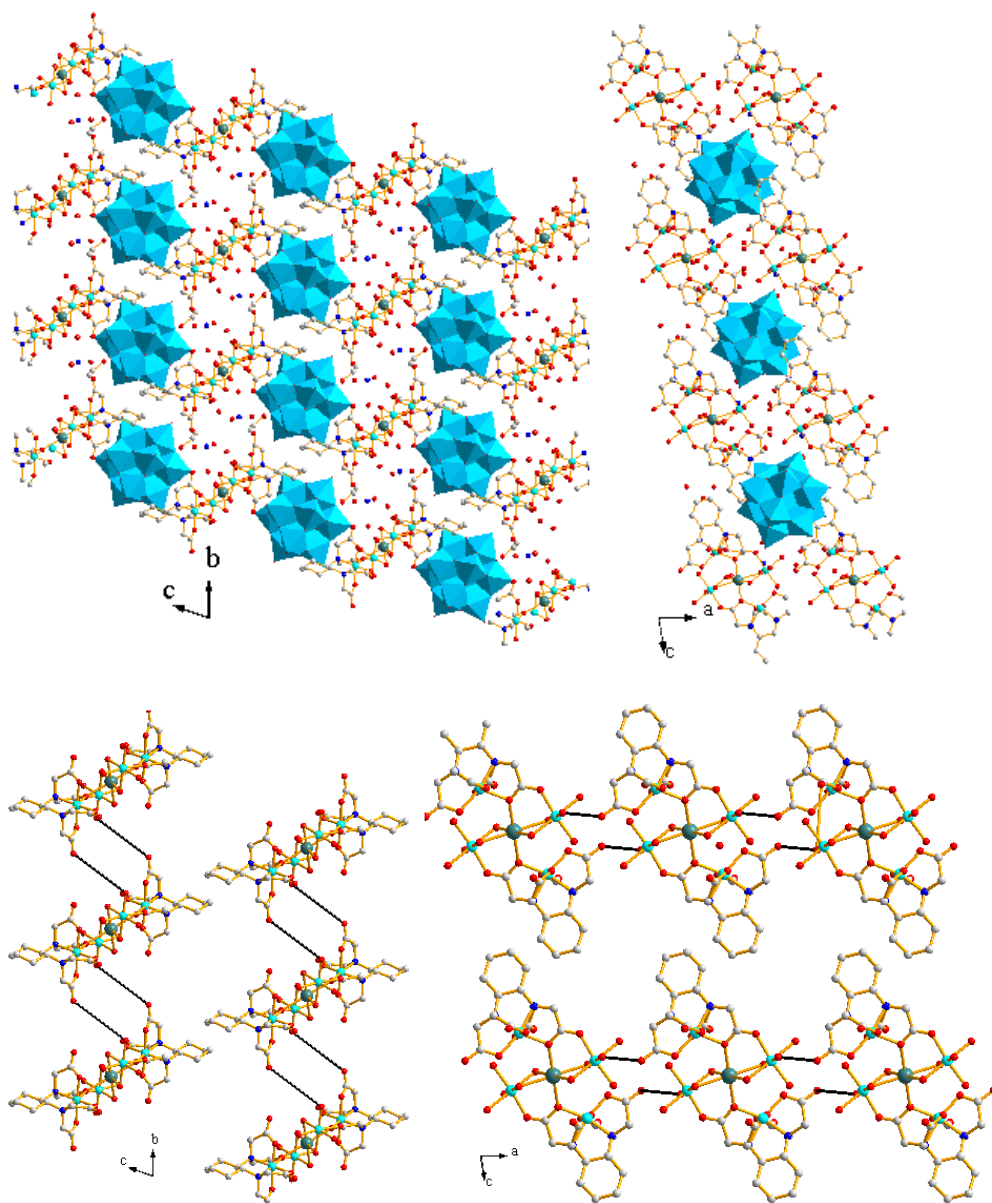


Fig. S1 Stacking drawing of 1 with SiW₁₂ (upper) and without SiW₁₂(low).

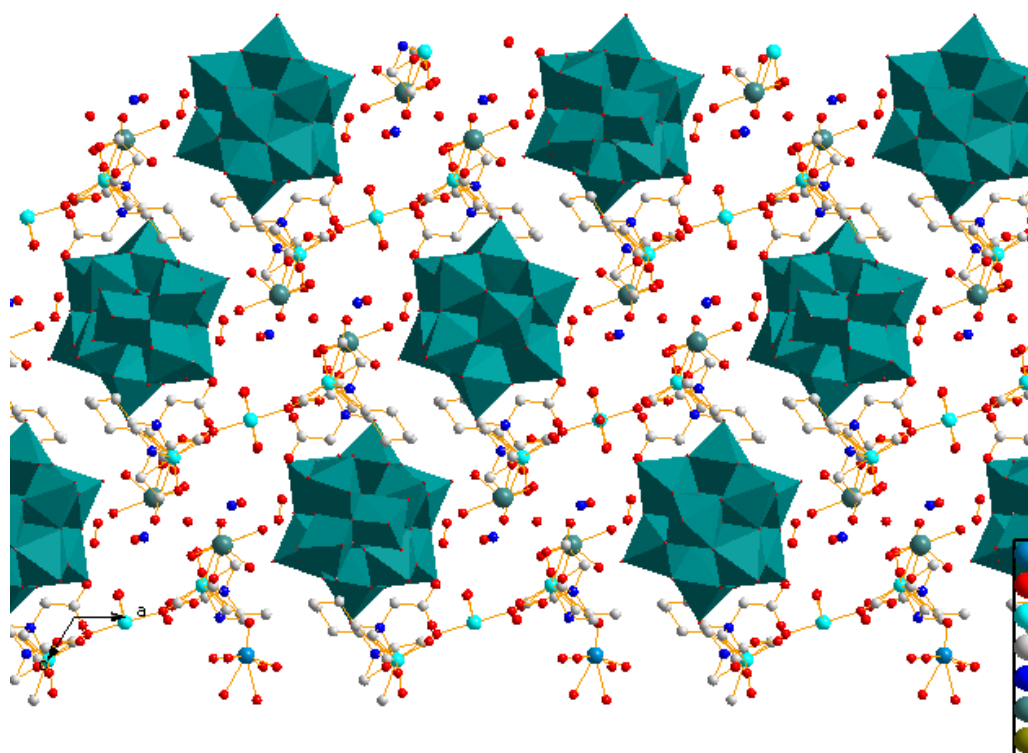


Fig. S2 Stacking drawing of **2**.

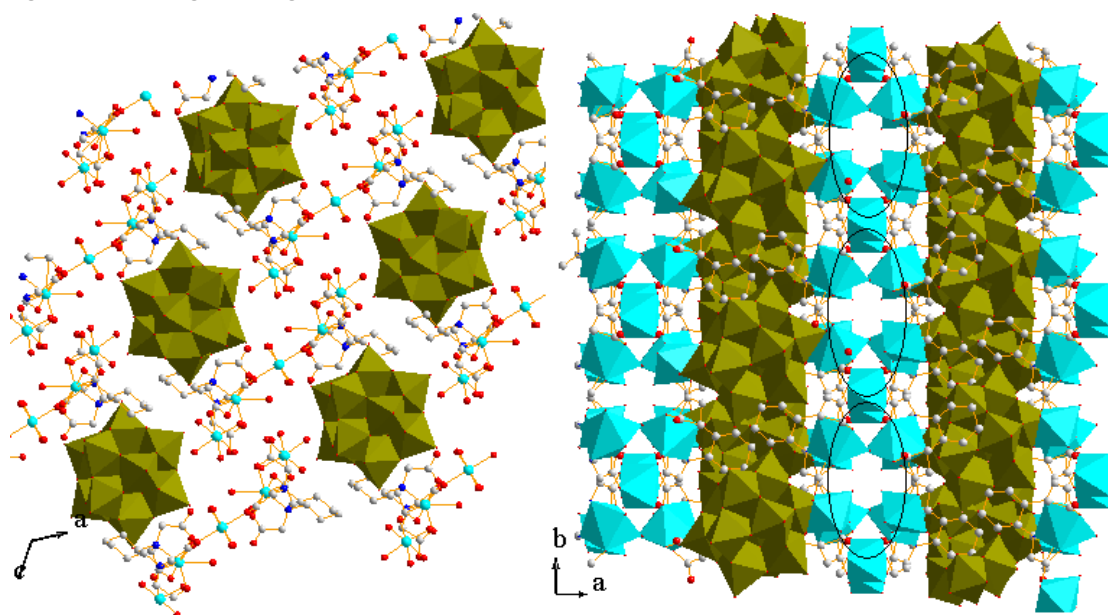


Fig. S3 Stacking drawing of **3** viewed from different directions.

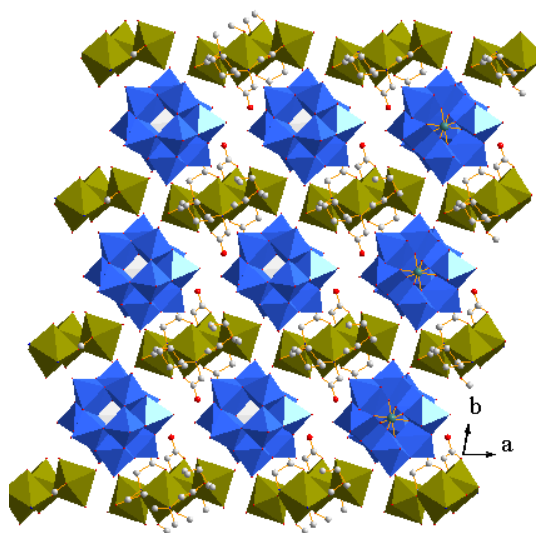


Fig. S4 Stacking drawing of **4** viewed from c-axis direction

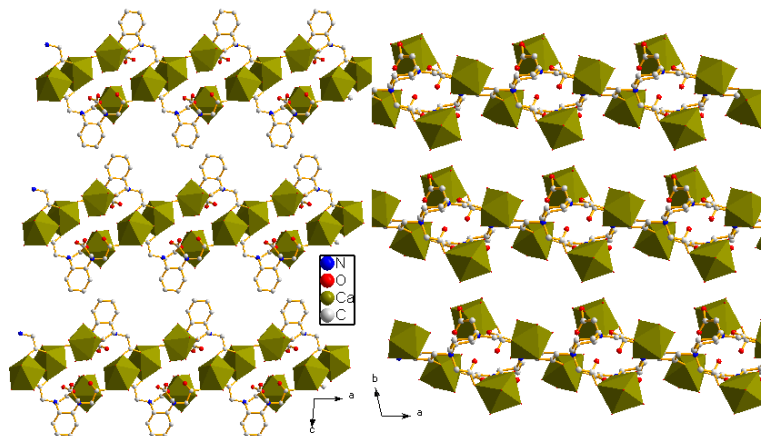


Fig. S5 Stacking drawing of **5** viewed from different directions

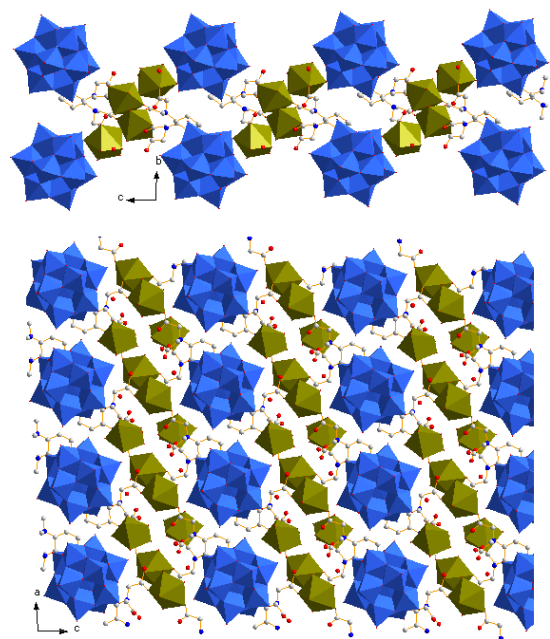


Fig. S6 Stacking drawing of **6** viewed from different directions

Table S1 Hydrogen bonds with H...A < r(A) + 2.000 Å and <DHA > 110 deg of **1-4**.

	D-H	d(D-H)	d(H...A)	<DHA	d(D...A)	A
1	O5W-H25B	0.960	2.610	167.18	3.553	O15 [-x+1, -y+1, -z]
	O5W-H25C	0.960	1.728	171.92	2.682	O4W
	O6W-H26A	0.960	2.244	120.81	2.857	O15W [-x+2, -y+1, -z]
	O6W-H26A	0.960	2.274	135.95	3.038	O5W [-x+2, -y+1, -z]
	O6W-H26A	0.960	2.427	115.40	2.968	O27 [-x+2, -y+1, -z]
	O6W-H26B	0.960	1.836	175.59	2.794	O24
	O7W-H27B	0.960	2.071	150.62	2.945	O1W [-x+2, -y, -z]
	O7W-H27C	0.960	1.945	142.22	2.766	O13W
	O11W-H21A	0.960	2.254	134.18	3.003	O7W [-x+2, -y+1, -z]
	O11W-H21A	0.960	2.282	121.25	2.898	O15W [-x+2, -y+1, -z]
	O11W-H21A	0.960	2.532	118.01	3.101	O27 [-x+2, -y+1, -z]
	O11W-H21B	0.960	1.748	168.70	2.696	O2W [-x+2, -y+1, -z]
	O15W-H22A	0.960	1.993	132.65	2.736	O4W [-x+1, -y+1, -z]
	O15W-H22C	0.960	2.114	113.97	2.653	O26 [-x+2, -y+1, -z]
	N12-H99H	0.960	1.491	147.60	2.358	O2W
	N12-H99E	0.960	1.747	117.01	2.344	O1W
	N12-H99G	0.960	1.780	114.25	2.344	O1W [-x+2, -y, -z]
	O40-H40	0.820		143	3.029	O12 [x, y, z+1]
	O1W-H17A	1.420	1.998	154.75	3.338	O40
2	O1W-H21B	0.960	2.151	145.67	2.993	O11W [-x+1/2, -y+3/2, -z]
	O1W-H21C	0.960	2.188	165.99	3.128	O5 [-x+1/2, -y+3/2, -z]
	O1W-H21C	0.960	2.593	113.02	3.097	O6W' [-x+1/2, -y+3/2, -z]
	O2W-H22A	0.960	2.254	177.93	3.214	O5W [x, y-1, z]
	O2W-H22B	0.960	2.138	158.95	3.053	O16 [-x+1/2, -y+3/2, -z]
	O4W-H24A	0.960	1.220	122.38	1.914	O6W [-x+1/2, y-1/2, -z+1/2]
	O4W-H24A	0.960	1.923	157.49	2.833	O6W' [-x+1/2, y-1/2, -z+1/2]
	O4W-H24C	0.960	2.321	136.45	3.089	N3 [-x+1/2, y-3/2, -z+1/2]
	O8W-H28B	0.960	2.338	117.18	2.904	O6 [-x+1/2, -y+5/2, -z]
	O8W-H28C	0.960		163	2.878	O6W [-x+1/2, y-1/2, -z+1/2]
	O9W-H29A	0.960	1.908	171.10	2.861	O45 [-x+1, -y+1, -z+1]
	O9W-H29B	0.960	2.023	115.80	2.589	N3 [-x+1/2, y-3/2, -z+1/2]
	O10W-H30A	0.960	2.458	136.52	3.223	O42 [-x+1, -y+1, -z+1]
	O10W-H30B	0.960	2.271	161.96	3.198	N3 [x+1/2, -y+5/2, z+1/2]
	O11W-H23A	0.960	1.875	170.57	2.826	O42 [-x+1/2, y+3/2, -z+1/2]
	O11W-H23B	0.960	2.320	126.60	2.993	O1W [-x+1/2, -y+3/2, -z]
3	O1W-H21A	0.961	1.905	159.01	2.823	O16 [-x+1/2, y-1/2, -z+1/2]
	O1W-H21B	0.960		147	3.009	O2W
	O2W-H22B	0.959	1.940	154.29	2.835	OW1 [x, -y, z+1/2]
	O2W-H22B	0.959	2.416	113.20	2.930	OW5 [x, y-1, z]
	O2W-H22C	0.960		142	2.693	O11 [-x+1, -y, -z+1]
	O3W-H23A	0.960	2.437	148.87	3.297	OW3 [-x+1, -y, -z+1]
	O3W-H23B	0.960		156	3.026	O1W

	O4W-H24A	0.960	2.115	134.10	2.867	O4W [-x+1, -y, -z+1]
	O4W-H24A	0.960	2.436	131.18	3.151	O26
	O4W-H24B	0.960	1.852	145.56	2.699	OW3
	O5W-H25A	0.960	2.342	122.18	2.966	O30 [-x+1, y, -z+1/2]
	O5W-H25A	0.960	2.544	128.93	3.234	O9W [-x+1, y, -z+1/2]
	O5W-H25B	0.960	2.292	121.88	2.916	O30
	O5W-H25B	0.960	2.510	136.01	3.269	O38
	O6W-H26A	0.960	2.611	151.27	3.483	OW4 [-x+1, y+1, -z+1/2]
	O6W-H26B	0.960	2.505	122.60	3.129	OW5 [x, -y+1, z-1/2]
	O7W-H27A	0.960		145	2.815	O2W
	O7W-H27B	0.960	2.439	127.71	3.120	O29
	O9W-H29A	0.960	2.290	114.09	2.821	O30
	O9W-H29A	0.960	2.370	149.58	3.234	O5W [-x+1, y, -z+1/2]
	O9W-H29B	0.960	1.990	173.39	2.946	O2W [-x+1, -y, -z+1]
4	O1W-H16A	0.960	1.858	146.33	2.709	O6 [-x+2, -y+2, -z+1]
	O1W-H16B	0.960	2.437	157.20	3.343	O27
	O1W-H16B	0.960	2.638	122.32	3.254	O18
	O2W-H17B	0.960	2.153	114.64	2.698	O34 [-x+2, -y+2, -z+2]
	OW3-H18A	0.960	1.725	169.01	2.674	O7W
	OW3-H18C	0.960	2.020	159.60	2.939	O3W
	O5W-H15A	0.960	2.325	133.48	3.065	O32 [-x+1, -y+2, -z+1]
	O5W-H15C	0.960	1.969	167.79	2.915	OW3
	O8W-H8A	0.960	2.633	159.87	3.549	N4 [x+1, y, z]
	O9W-H9A	0.960	1.869	153.01	2.759	O9W [-x+1, -y+3, -z+1]
	O9W-H9B	0.960	2.057	125.38	2.728	O5 [x, y+1, z]
	O9W-H9B	0.960	2.595	170.50	3.546	O30 [x, y+1, z]
	N3-H99A	0.960	1.796	139.14	2.599	O3W
	N3-H99B	0.960	2.467	173.42	3.422	O9W
	N3-H99C	0.960	1.795	145.28	2.641	O21
	N3-H99D	0.960	2.503	126.21	3.166	O12 [x-1, y+1, z]
	N3-H99D	0.960	2.619	125.90	3.276	O14 [x-1, y+1, z]
	N4-H98A	0.960	1.837	145.06	2.680	O5W
	N4-H98C	0.960	2.004	155.15	2.903	O1W [-x+1, -y+2, -z+1]
5	O1W-H20A	0.960	2.500	140.12	3.295	O6 [-x-1, -y-3, -z-1]
	O1W-H20B	0.960	2.094	126.73	2.776	N4 [x-1, y, z]
	O2W-H21A	0.960	2.406	144.85	3.238	N4 [x-1, y, z]
	O2W-H21B	0.960	2.408	121.87	3.027	N3' [x-1, y, z]
	O2W-H21B	0.960	2.623	121.20	3.227	O6
	O3W-H22A	0.960	2.422	161.44	3.346	O1 [-x, -y-3, -z-1]
	O3W-H22B	0.960	2.432	154.18	3.323	O20 [x-1, y-1, z]
	O3W-H22B	0.960	2.590	133.18	3.321	O30 [x-1, y-1, z]
	O5W-H24B	0.960		156	2.700	O3 [-x, -y-3, -z-1]
	O5W-H24C	0.960	2.252	119.53	2.850	N4 [-x, -y-3, -z-1]
	O6W-H26A	0.960	2.181	140.08	2.981	O4W [-x, -y-2, -z-1]

	O6W-H26A	0.960	2.330	111.81	2.831	O8W
	O6W-H26A	0.960	2.573	127.66	3.250	O8 [-x, -y-2, -z-1]
	O4W-H30A	0.960	2.153	145.86	2.996	O26 [x-1, y-1, z]
	O4W-H30A	0.960	2.432	124.45	3.078	O16 [-x+1, -y-1, -z]
	O4W-H30B	0.960	2.309	129.95	3.016	O2W
	O7W-H31A	0.960	1.768	171.84	2.722	N3 [-x, -y-2, -z-1]
	O7W-H31A	0.960	2.605	121.05	3.207	N3' [x-1, y, z]
6	O3W-H24A	0.960	2.305	127.65	2.990	O38 [-x+2, -y-1, -z+1]
	O3W-H24A	0.960	2.385	159.08	3.299	O8W [-x+2, -y-1, -z+1]
	O3W-H24C	0.960	2.116	161.54	3.041	O40 [-x+2, -y-1, -z+1]
	O9W-H38A	0.960	2.011	167.82	2.957	OW3 [-x+1, -y-1, -z+1]
	O9W-H38B	0.960	1.999	139.47	2.799	O6 [-x+2, -y-1, -z+1]
	O1W-H31B	0.960	2.500	158.70	3.413	O29
	O1W-H31C	0.960		142	3.085	O2W
	O2W-H32B	0.960		133	3.085	O1W
	O2W-H32C	0.960	2.549	169.17	3.496	O19 [x-1, y, z]
	O2W-H32C	0.960	2.581	111.98	3.072	O28 [x-1, y, z]
	O4W-H33A	0.960	2.052	152.49	2.937	O17
	O4W-H33B	0.960		156	3.098	O2W
	O5W-H34A	0.960	2.313	130.93	3.030	O6 [x-1, y, z]
	O5W-H34A	0.960	2.636	150.66	3.505	O3W [x-1, y, z]
	O5W-H34B	0.960	2.392	171.95	3.345	O19 [x-1, y, z]
	O6W-H35A	0.960	2.609	156.17	3.509	O8W [-x+2, -y-1, -z+1]
	O6W-H35B	0.960	2.323	145.06	3.158	OW1 [-x+2, -y-1, -z+1]
	O7W-H36A	0.960	2.498	141.61	3.305	O14 [x, y-1, z]
	O7W-H36B	0.960	2.299	110.28	2.781	OW2 [x, y-1, z]
	O8W-H37A	0.960	1.917	139.35	2.718	O45 [-x+2, -y-1, -z+1]
	O8W-H37B	0.960	2.017	135.21	2.782	O3W [x-1, y, z]
	O10W-H39B	0.960		151	3.108	O8W
	O10W-H39C	0.960	2.382	129.83	3.086	O27 [x, y+1, z]
	O11W-H40A	0.960	2.170	121.01	2.789	O27 [-x+1, -y-1, -z+1]
	O11W-H40B	0.960	2.441	150.78	3.312	OW4 [-x+1, -y, -z+1]