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Supporting Information for

Supramolecular Isomorphic Dodecanuclear Cobalt Clusters with Same Metal Shell but Different Core Ligands†

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Table S1 Selected bond lengths [Å] for **1** and **2**.

1		**2**	
Co1-O1	2.131(9)	Co1-O1	2.048(5)
Co1-O7	2.031(8)	Co1-O7	2.064(5)
Co1-O9	2.062(9)	Co1-O9	2.034(5)
Co1-O19	1.994(9)	Co1-O19	1.994(6)
Co1-N30	2.083(12)	Co1-N26	2.101(6)
Co2-O2	2.114(9)	Co2-O2	2.209(5)
Co2-O9	2.071(9)	Co2-O9	2.089(5)
Co2-O11	2.076(9)	Co2-O11	2.042(5)
Co2-N3	2.093(11)	Co2-N3	2.099(6)
Co2-N4	2.166(11)	Co2-N4	2.123(6)
Co2-N28	2.124(12)	Co2-N28	2.136(7)
Co3-O2	2.095(9)	Co3-O2	2.029(4)
Co3-O11	2.061(9)	Co3-O11	2.063(5)
Co3-O13	2.056(9)	Co3-O13	2.026(5)
Co3-N33	2.048(11)	Co3-O20	1.978(7)
Co3-N15	2.135(12)	Co3-N15	2.141(6)
Co3-N26	2.108(12)	Co4-O3	2.232(5)
Co4-O3	2.160(9)	Co4-O13	2.116(5)
Co4-O13	2.127(9)	Co4-O15	2.072(5)
Co4-O15	2.097(9)	Co4-N5	2.100(7)
Co4-N5	2.123(11)	Co4-N6	2.127(6)
Co4-N6	2.129(12)	Co4-N17	2.134(6)
Co4-N17	2.152(11)	Co5-O3	2.022(5)
Co5-O3	1.981(9)	Co5-O15	2.046(5)

Co5-O15	2.037(10)	Co5-O17	2.010(5)
Co5-O17	2.003(8)	Co5-N19	2.093(6)
Co5-N19	2.071(11)	Co5-N23	2.072(6)
Co5-N23	2.080(11)	Co6-O1	2.231(5)
Co6-O1	2.144(9)	Co6-O7	2.034(5)
Co6-O7	2.051(9)	Co6-O17	2.103(5)
Co6-O17	2.086(9)	Co6-N7	2.086(7)
Co6-N7	2.101(12)	Co6-N8	2.152(6)
Co6-N8	2.162(11)	Co6-N21	2.086(6)
Co6-N21	2.133(12)	Co7-O4	2.044(5)
Co7-O4	2.101(9)	Co7-O8	2.075(5)
Co7-O8	2.031(10)	Co7-O10	2.031(5)
Co7-O10	2.030(9)	Co7-O19	2.001(6)
Co7-O19	1.989(10)	Co7-N27	2.120(7)
Co7-N30	2.110(11)	Co8-O5	2.217(5)
Co8-O5	2.127(9)	Co8-O10	2.103(5)
Co8-O10	2.060(9)	Co8-O12	2.041(5)
Co8-O12	2.039(9)	Co8-N9	2.137(6)
Co8-N9	2.134(11)	Co8-N10	2.074(7)
Co8-N10	2.113(12)	Co8-N29	2.083(7)
Co8-N29	2.097(12)	Co9-O5	2.029(5)
Co9-O5	2.090(9)	Co9-O12	2.071(5)
Co9-O12	2.062(9)	Co9-O14	2.006(5)
Co9-O14	2.077(9)	Co9-O21	1.999(8)
Co9-N35	2.101(12)	Co9-N16	2.156(6)
Co9-N16	2.126(12)	Co10-O6	2.211(4)
Co9-N27	2.107(12)	Co10-O14	2.099(5)
Co10-O6	2.167(8)	Co10-O16	2.066(5)
Co10-O14	2.067(9)	Co10-N11	2.121(6)
Co10-O16	2.056(9)	Co10-N12	2.118(7)
Co10-N11	2.105(11)	Co10-N18	2.109(7)
Co10-N12	2.084(12)	Co11-O6	2.031(5)
Co10-N18	2.101(12)	Co11-O16	2.040(5)
Co11-O6	1.991(9)	Co11-O18	1.999(5)
Co11-O16	2.021(9)	Co11-N20	2.115(5)
Co11-O18	1.970(10)	Co11-N23	2.074(7)
Co11-N20	2.120(11)	Co12-O4	2.219(5)
Co11-N23	2.128(12)	Co12-O8	2.049(5)
Co12-O4	2.138(9)	Co12-O18	2.124(5)
Co12-O8	2.050(9)	Co12-N13	2.125(6)

Co12-O18	2.121(9)	Co12-N14	2.073(7)
Co12-N13	2.167(12)	Co12-N22	2.080(6)
Co12-N14	2.061(12)		
Co12-N22	2.059(11)		

Table S2 Selected bond angles [°] for **1** and **2**.

1		**2**	
Co1-O1-Co6	97.2(3)	Co1-O1-Co6	99.00(18)
Co3-O2-Co2	98.8(4)	Co3-O2-Co2	98.84(19)
Co5-O3-Co4	104.5(4)	Co5-O3-Co4	101.67(18)
Co7-O4-Co12	99.0(3)	Co7-O4-Co12	100.00(18)
Co9-O5-Co8	98.4(4)	Co9-O5-Co8	99.14(19)
Co11-O6-Co10	104.2(4)	Co11-O6-Co10	101.85(19)
Co1-O7-Co6	103.5(4)	Co6-O7-Co1	105.2(2)
Co7-O8-Co12	104.4(4)	Co12-O8-Co7	104.8(2)
Co1-O9-Co2	109.2(4)	Co1-O9-Co2	108.6(2)
Co7-O10-Co8	111.5(4)	Co7-O10-Co8	108.6(2)
Co3-O11-Co2	101.2(4)	Co2-O11-Co3	103.4(2)
Co8-O12-Co9	102.2(4)	Co8-O12-Co9	103.7(2)
Co3-O13-Co4	106.4(4)	Co3-O13-Co4	106.9(2)
Co9-O14-Co10	106.9(4)	Co9-O14-Co10	106.7(2)
Co5-O15-Co4	104.8(4)	Co5-O15-Co4	106.6(2)
Co11-O16-Co10	107.2(4)	Co11-O16-Co10	106.7(2)
Co5-O17-Co6	109.6(4)	Co5-O17-Co6	109.1(2)
Co11-O18-Co12	108.5(4)	Co11-O18-Co12	108.5(2)
Co1-O19-Co7	114.7(5)	Co1-O19-Co7	123.5(3)
Co5-N23-Co11	123.3(5)	Co11-N23-Co5	124.5(3)
Co1-N30-Co7	106.2(5)		

Table S3 Bond valence calculations for **1** and **2** with $S = \exp[(r_0 - r) / B]$, $r_0 = 1.680$ Å for Co-O and 1.790 Å for Co-N, B = 0.37 and r is the Co-O/N ond lengths[1].

	Co1	Co2	Co3	Co4	Co5	Co6	Co7	Co8	Co9	Co10	Co11	Co12
1	1.96	2.24	2.4	2.11	2.19	2.20	2.10	2.34	2.34	2.28	2.11	2.31
2	1.99	2.18	1.97	2.10	2.10	2.19	2.01	2.21	1.95	2.16	2.07	2.22

1. *(a)* W. Liu and H. H. Thorp, *Inorg. Chem.*, 1993, **32**, 4102-4105. *(b)* N. E. Brese and M. O'Keeffe, *Acta Cryst.*, 1991, **B47**, 192-197. *(c)* G. J. Palenik, *Inorg. Chem.*, 1997, **36**, 122.

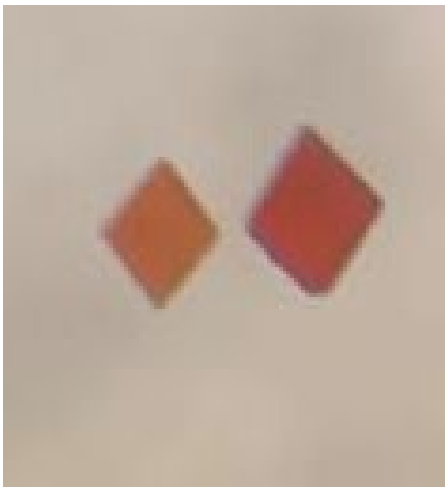

Fig. S1 The morphology of crystal of **1** (left) and **2** (right) under the microscope.

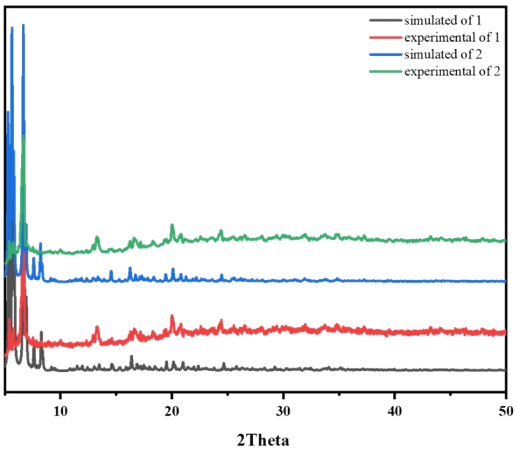

Fig. S2 Powder X-ray diffraction pattern of **1** and **2**.

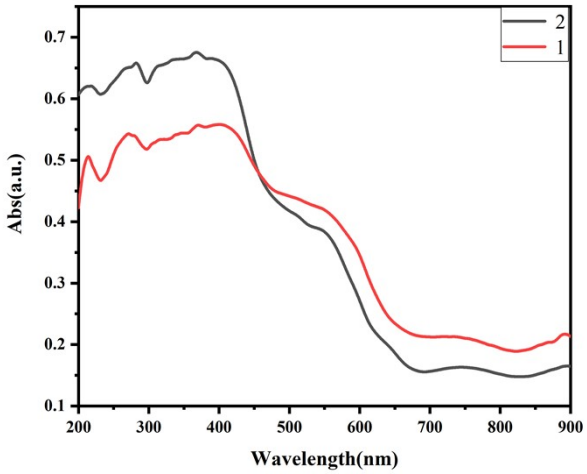

Fig. S3 The UV-vis spectra of **1** and **2**.