Supplementary Material (ESI) for CrystEngComm

Supplementary information

Syntheses, structural aspects, luminescence and magnetism of four coordination polymers based on a new flexible polycarboxylate

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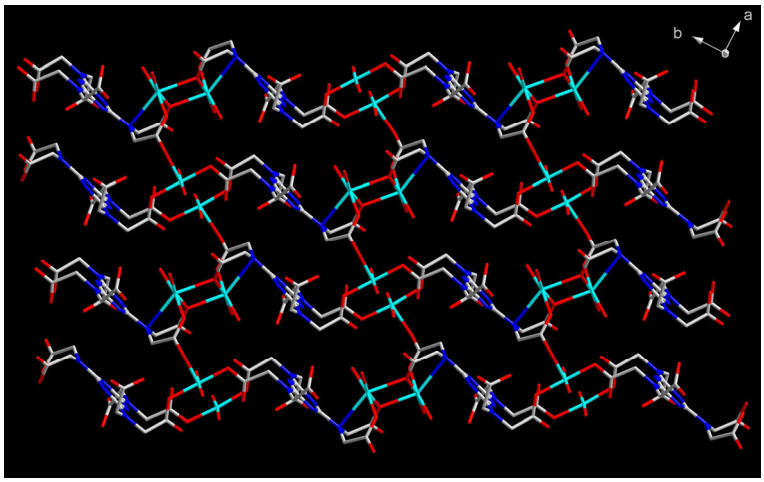

Fig. S1 View of 2D layers with the stick representation constructed from the tetranucleate units and flexible ligands in complex **2**.

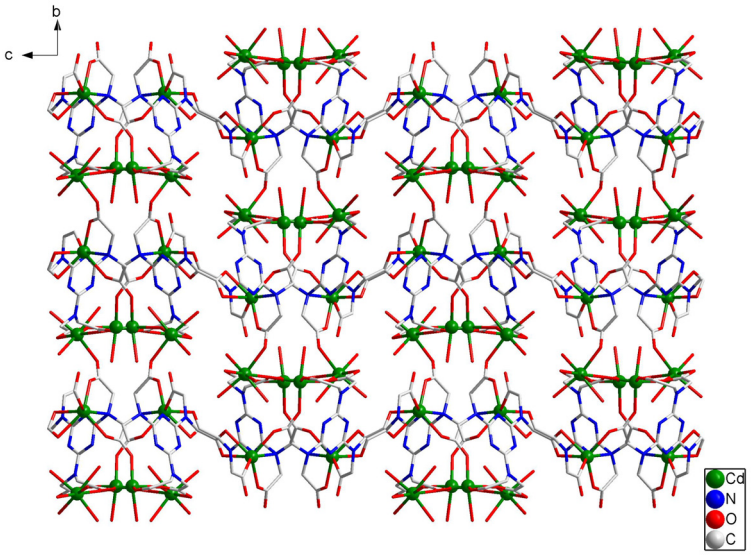

Fig. S2 View of the 3D network along a-axis in complex **3**. Hydrogen atoms are omitted for clarity.

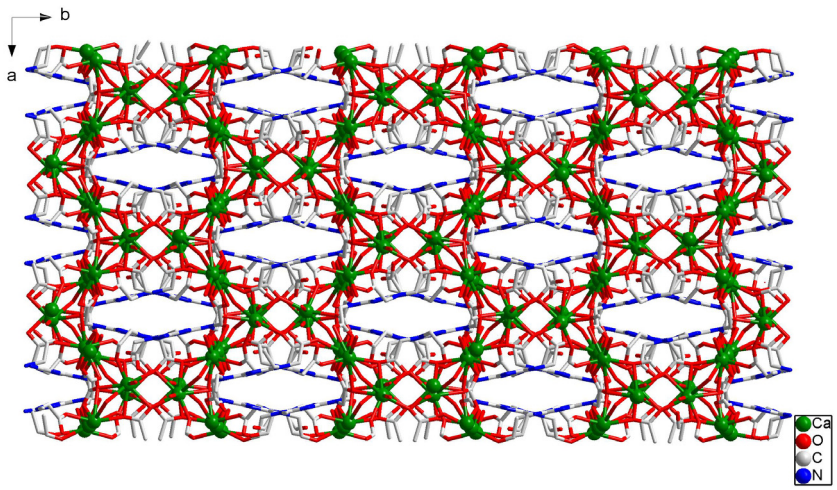

Fig. S3 View of rhombic channels packing along the *c*-axis with the ball-and-stick representation of complex **4**.

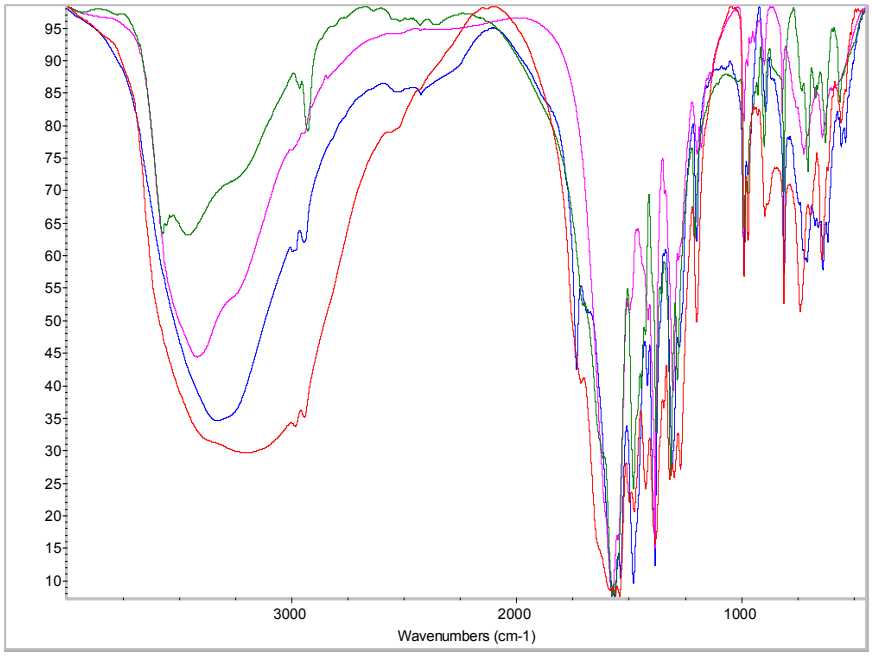

Figure S4. FT-IR spectra for complexes **1** (blue), **2** (red), **3** (purple) and **4** (green).

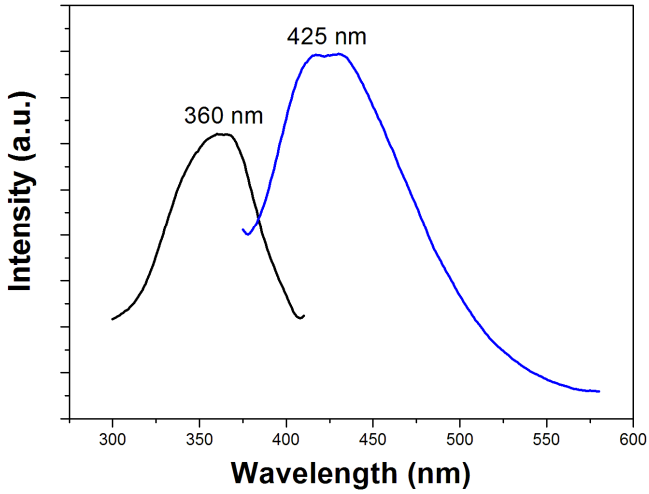

Figure S5. Solid-state excitation and emission spectra of H_6TTHA.

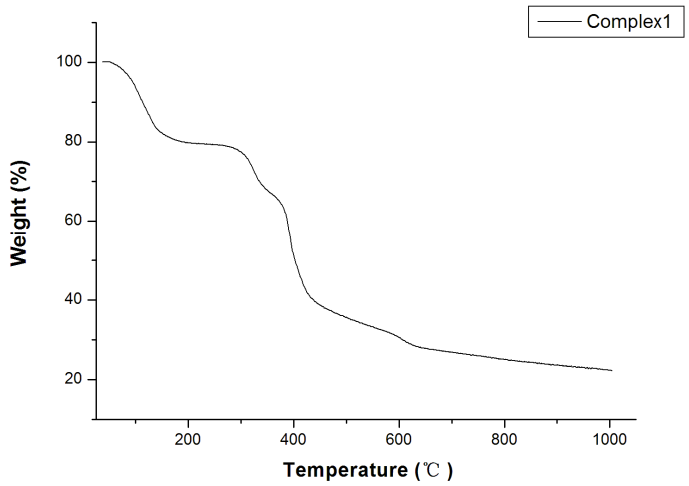

Figure S6. TGA curves for complex **1**.

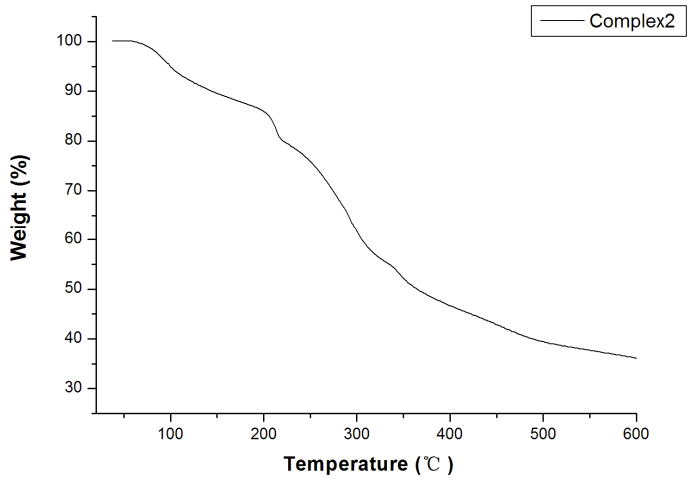

Figure S7. TGA curves for complex **2**.

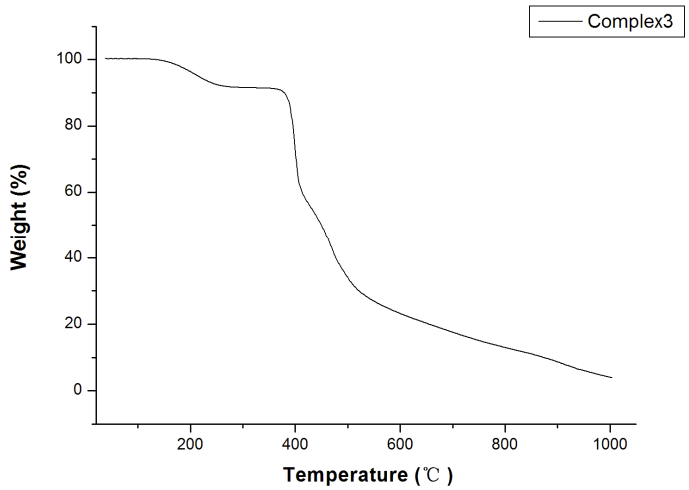

Figure S8. TGA curves for complex **3**.

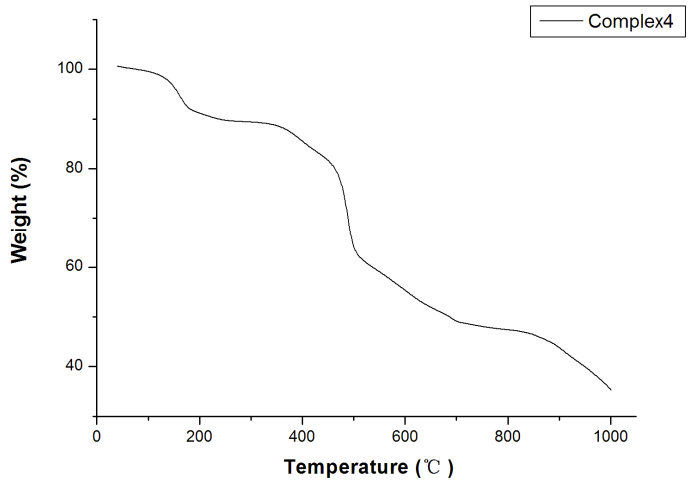

Figure S9. TGA curves for complex **4**.

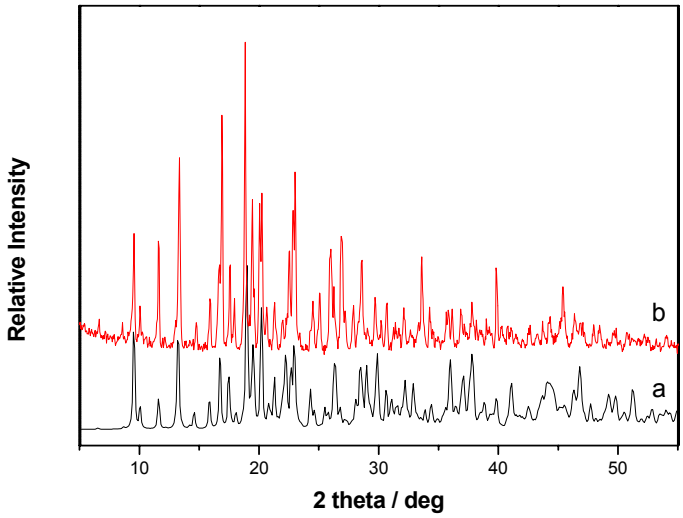

Figure S10. X-ray powder diffraction of complex **1** (a) simulated from single crystal data, (b) polycrystalline as newly synthesized.

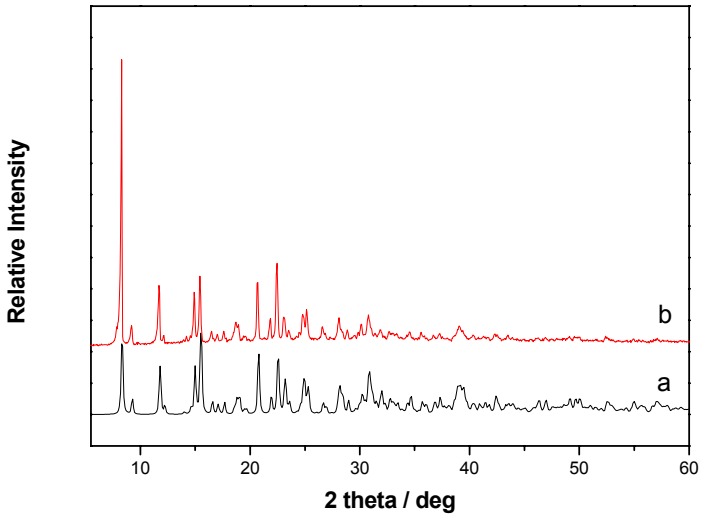

Figure S11. X-ray powder diffraction of complex **2** (a) simulated from single crystal data, (b) polycrystalline as newly synthesized.

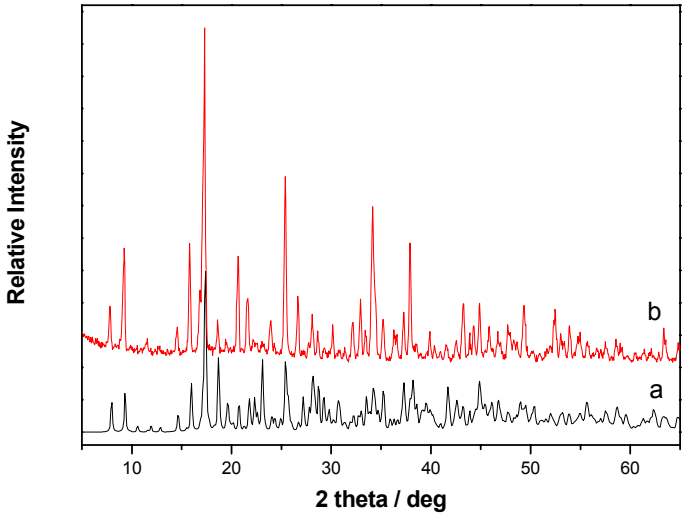

Figure S12. X-ray powder diffraction of complex **3** (a) simulated from single crystal data, (b) polycrystalline as newly synthesized.

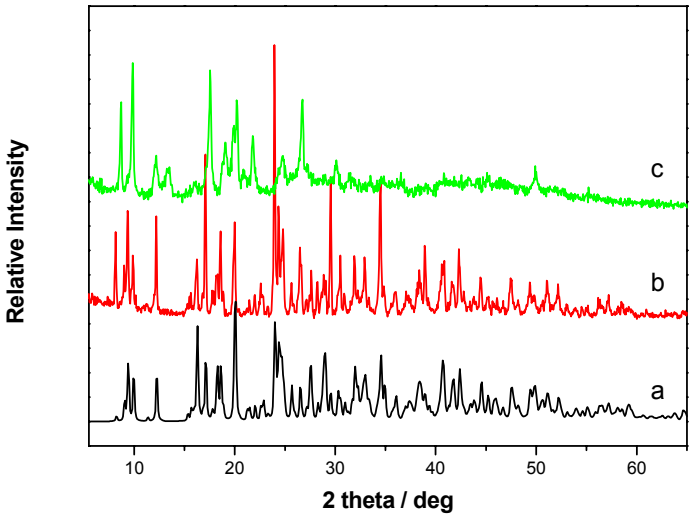

Figure S13. X-ray powder diffraction of complex **4** (a) simulated from single crystal data, (b) polycrystalline as newly synthesized, (c) heated at 250°C for 6h.

Table S1 Photoluminescent data for complexes **3** and **4** at different temperature.

complex		Emission band (nm)	Emission integrated area ($\times 10^6$)	Lifetime (ns)		
				τ_1	τ_2	τ_3
3	R.T.	371	2.25589	0.403 (96.12%)	10.120 (3.88%)	
	10 K	372	11.8584			
4	R.T.	379	2.75676	67.944 (55.79%)	0.704 (36.55%)	10.032 (7.66%)
	10 K	380	6.62479			

Table S2 Selected bond lengths (Å) and angles (°) for complexes **1-4**.

1							
Co1-O8	2.060(3)	Co2-O15	2.072(3)	Co2-O16	2.129(3)	O12A-Co1-O12	180
Co1-O12	2.116(3)	Co2-O2	2.093(3)	Co2-O14	2.109(3)	O2-Co2-O11B	176.46(11)
Co1-O17	2.138(3)	Co2-O11B	2.097(3)	Co2-O13	2.138(3)		
2							
Cu1-O2	1.926(12)	Cu2-O28	2.016(10)	Cu4-O15	1.957(10)	O20B-Cu2-O13	88.2(4)
Cu1-O3	1.936(12)	Cu2-O13	2.261(10)	Cu4-O32	1.991(11)	O12C-Cu3-O24D	174.4(4)
Cu1-O25	1.950(12)	Cu3-O12C	1.925(10)	Cu4-O2	2.423(12)	O12C-Cu3-O4	97.9(4)
Cu1-O26	1.982(12)	Cu3-O29	1.970(10)	Cu4-N10	2.694(14)	O24D-Cu3-O4	87.2(4)
Cu1-O15	2.342(11)	Cu3-O30	1.984(10)	O2-Cu1-O3	93.6(5)	O14-Cu4-O15	93.1(5)
Cu1-N4	2.749(14)	Cu3-O24D	1.987(10)	O2-Cu1-O15	79.8(4)	O14-Cu4-O2	91.3(5)
Cu2-O7A	1.937(9)	Cu3-O4	2.267(10)	O3-Cu1-O15	93.3(5)	O15-Cu4-O2	77.2(4)
Cu2-O27	1.968(10)	Cu4-O14	1.901(11)	O7A-Cu2-O20B	175.4(4)		
Cu2-O20B	1.970(11)	Cu4-O31	1.947(12)	O7A-Cu2-O13	90.0(4)		
3							
Cd1-O13	2.289(7)	Cd2-N6	2.608(7)	O7-Cd2-O6	127.4(2)	O10D-Cd2-N6	92.8(2)
Cd1-O8A	2.295(6)	Cd3-O2	2.213(7)	O11C-Cd2-O10D	120.7(3)	O9D-Cd2-N6	114.7(2)
Cd1-O16	2.301(8)	Cd3-O1E	2.273(6)	O7-Cd2-O10D	87.4(3)	O2-Cd3-O1E	114.4(2)
Cd1-O14	2.311(6)	Cd3-O5E	2.276(6)	O6-Cd2-O10D	127.6(2)	O2-Cd3-O5E	124.4(3)
Cd1-O3	2.347(6)	Cd3-O4	2.286(7)	O11C-Cd2-O9D	91.6(3)	O1E-Cd3-O5E	86.8(2)
Cd1-O1B	2.453(6)	Cd3-O15	2.329(8)	O7-Cd2-O9D	141.9(2)	O2-Cd3-O4	118.8(3)
Cd2-O11C	2.162(9)	O8A-Cd1-O3	91.5(3)	O6-Cd2-O9D	86.2(2)	O1E-Cd3-O4	124.4(2)

Cd2-O7	2.231(6)	O8A-Cd1-O1B	84.4(2)	O10D-Cd2-O9D	55.1(2)	O5E-Cd3-O4	76.6(2)
Cd2-O6	2.265(6)	O3-Cd1-O1B	174.6(2)	O11C-Cd2-N6	146.0(3)	Cd3F-O1-Cd1C	109.2(2)
Cd2-O10D	2.342(7)	O11C-Cd2-O7	104.0(3)	O7-Cd2-N6	69.0(2)		
Cd2-O9D	2.414(7)	O11C-Cd2-O6	90.5(3)	O6-Cd2-N6	71.2(2)		
4							
Ca1-O7A	2.307(4)	Ca3-O2	2.323(4)	O2W-Ca1-O10C	65.50(14)	O5-Ca2-O2W	62.48(13)
Ca1-O5	2.352(3)	O7A-Ca1-O5	154.79(16)	O11B-Ca1-O10C	112.40(11)	O11C-Ca3-O11B	180
Ca1-O3W	2.408(5)	O7A-Ca1-O2W	88.0(2)	O9C-Ca1-O10C	49.30(10)	O11C-Ca3-O9C	97.12(12)
Ca1-O2W	2.489(5)	O5-Ca1-O2W	69.2(2)	O12B-Ca1-O10C	148.30(14)	O11B-Ca3-O9C	82.88(12)
Ca1-O11B	2.512(3)	O7A-Ca1-O11B	120.22(16)	O8D-Ca2-O6D	88.56(13)	O9C-Ca3-O9B	180
Ca1-O9C	2.589(4)	O5-Ca1-O11B	83.15(12)	O8D-Ca2-O10C	82.16(14)	O11C-Ca3-O2	88.45(12)
Ca1-O12B	2.644(4)	O2W-Ca1-O11B	151.72(19)	O6D-Ca2-O10C	151.31(14)	O11B-Ca3-O2	91.55(12)
Ca1-O10C	2.675(4)	O7A-Ca1-O9C	83.46(14)	O8D-Ca2-O6	153.05(15)	O9C-Ca3-O2	84.01(12)
Ca2-O8D	2.276(4)	O5-Ca1-O9C	95.91(12)	O6D-Ca2-O6	71.13(13)	O9B-Ca3-O2	95.99(12)
Ca2-O6D	2.360(3)	O2W-Ca1-O9C	114.29(14)	O10C-Ca2-O6	123.99(12)	O2E-Ca3-O2	180
Ca2-O10C	2.404(3)	O11B-Ca1-O9C	73.04(11)	O8D-Ca2-O5	148.76(13)	Ca2D-O6-Ca2	108.40(13)
Ca2-O4W	2.416(4)	O7A-Ca1-O12B	82.58(16)	O6D-Ca2-O5	121.59(11)	Ca1-O5-Ca2	103.55(13)
Ca2-O6	2.525(4)	O5-Ca1-O12B	122.16(13)	O10C-Ca2-O5	74.46(11)	Ca1-O2W-Ca2	93.90(18)
Ca2-O5	2.532(4)	O2W-Ca1-O12B	143.80(17)	O6-Ca2-O5	51.25(10)	Ca3B-O11-Ca1B	103.11(13)
Ca2-O1W	2.623(9)	O11B-Ca1-O12B	50.01(11)	O8D-Ca2-O2W	89.11(15)	Ca3B-O9-Ca1F	100.77(12)
Ca2-O2W	2.757(7)	O9C-Ca1-O12B	99.31(14)	O6D-Ca2-O2W	142.04(16)	Ca2F-O10-Ca1F	98.03(11)
Ca3-O11B	2.293(3)	O7A-Ca1-O10C	88.48(13)	O10C-Ca2-O2W	65.23(15)		
Ca3-O9B	2.294(3)	O5-Ca1-O10C	72.64(11)	O6-Ca2-O2W	96.15(15)		

[a]Symmetry codes for **1**: (A) -x,-y+1,-z+1; (B) x+1,y,z; for **2**: (A) x-1/2,y+1/2,z; (B) x,y-1,z; (C) x,y+1,z; (D) x+1/2,y-1/2,z; for **3**: (A) -x-1/2,y-1/2,z; (B) x+1,y,z; (C) x-1,y,z; (D) x-1/2,-y+1/2,-z+1; (E) x+1/2,y,-z+1/2; (F) x-1/2,y,-z+1/2; for **4**: (A) -x,y-1/2,-z+1/2; (B) -x-1/2,-y+1/2,z; (C) x+1/2,y-1/2,-z; (D) -x+1/2,-y+1/2,z; (E) -x,-y,-z; (F) x-1/2,y+1/2,-z.