

Dynamic Magnetic Materials Based on the Cationic Coordination Polymer [Cu(btix)₂]²ⁿ⁺ (btix = 1,4-bis(triazol-1-ylmethyl)benzene): Tuning the Structural and Magnetic Properties through Anion Exchange

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Supporting Information

Table S1. Elemental analysis for compounds **1–6**.

Compound		C [%]	H [%]	N [%]
1	exptl	38.59	3.32	22.92
	calcd	40.17	3.37	23.42
2	exptl	37.59	3.43	21.88
	calcd	38.30	3.26	22.62
3	exptl	36.91	3.18	21.54
	calcd	34.56	2.90	20.15
4	exptl	41.39	3.55	27.27
	calcd	43.15	3.62	29.35
5	exptl	46.21	3.90	26.94
	calcd	46.87	3.93	27.33
6	exptl	37.53	3.19	42.17
	calcd	37.16	3.12	43.34

Table S2. Unit cell parameters from Pawley refinements for compounds **1–5** and those of analogous compounds from single crystal diffraction data.

	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
1	24.2369	9.5970	15.5184	90	124.50	90
Cu(btix) ₂ (BF ₄) ^a	23.820	9.5063	15.544	90	123.97	90
2	24.2443	9.5894	15.5118	90	124.46	90
Cu(btix) ₂ (BF ₄) ^a	23.820	9.5063	15.544	90	123.97	90
3	24.2372	9.5946	15.5158	90	124.45	
Cu(btix) ₂ (BF ₄) ^a	23.820	9.5063	15.544	90	123.97	90
4	8.0338	21.0590	8.3511	90	100.46	90
Co(btix) ₂ (NO ₃) ₂ ^b	8.2019	20.7198	8.4751	90	105.60	90
5	7.6511	21.3942	8.5296	90	106.65	90
Cu(btix) ₂ Cl ₂ ^c	7.6671	21.327	8.5287	90	106.559	90

a: this work

b: Coronado, E.; Giménez-Marqués, M.; Mínguez Espallargas, G. *Inorg. Chem.* **2012**, *51*, 4403

c: Ding, B.; Liu, Y.-Y.; Huang, Y.-Q.; Shi, W.; Cheng, P.; Liao, D.-Z.; Yan, S.-P. *Cryst. Growth Des.* **2009**, *9*, 593

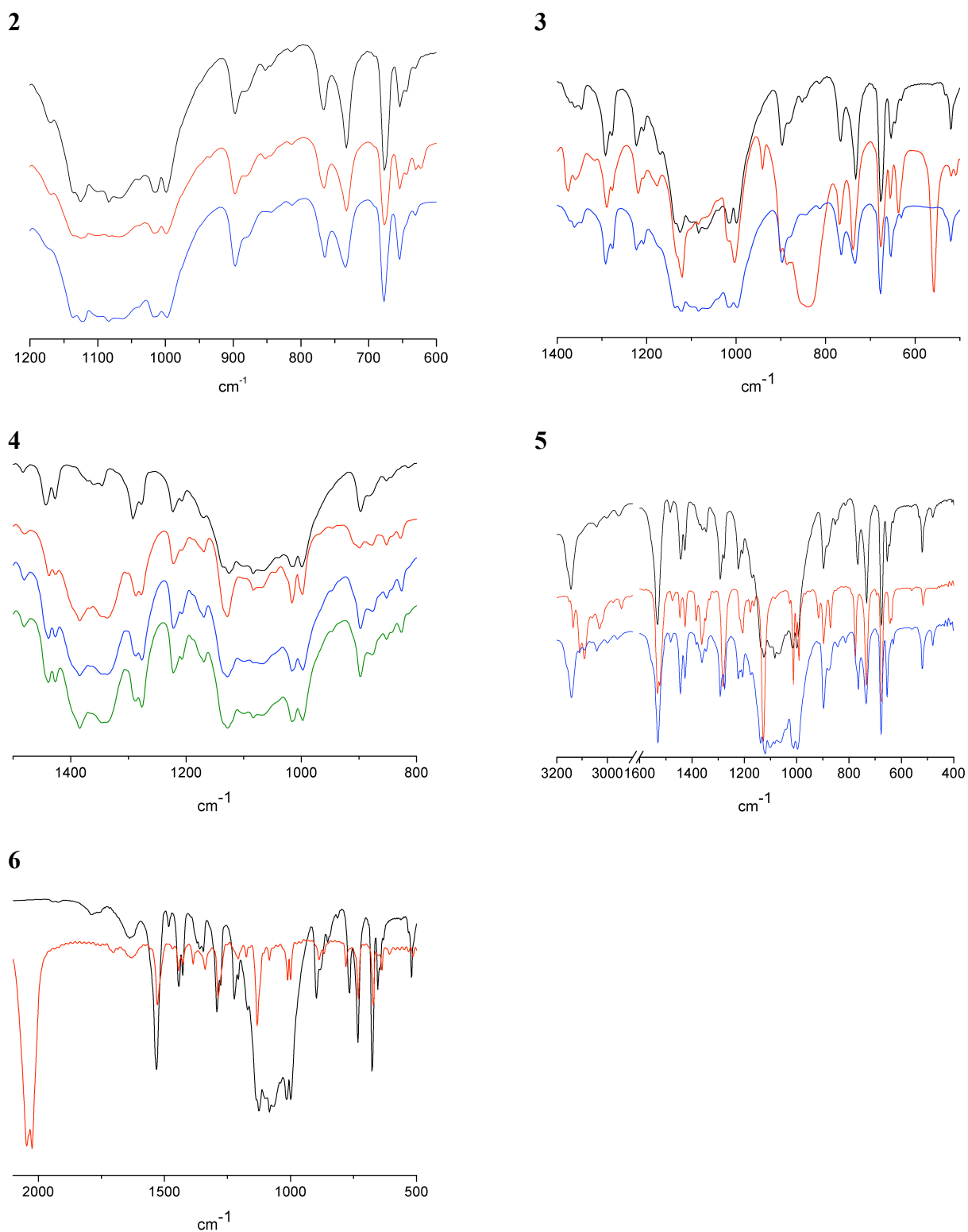


Figure S1. Infra-red spectra of the pristine materials (with BF_4^-), shown in black, after anion exchange, shown in red, and recovered materials (shown in blue and green after immersion for 1 day and 3 days, respectively): a) ClO_4^- (2), b) PF_6^- (3), c) NO_3^- (4), d) Cl^- (5) and e) N_3^- (6).