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Synthesis, characterization and dye adsorption property of a 2D nickel(II)-coordination polymer constructed from tetracarboxylic acid and 1,3-bis(imidazol-1-yl-methyl)benzene

Esengül Çiftçi[a], Tuğba Alp Arıcı[b], Mürsel Arıcı[a], Hakan Erer[a], and Okan Zafer Yeşilel[a,*]

[a]Department of Chemistry, Faculty of Science, Eskişehir Osmangazi University, 26040 Eskişehir, Türkiye

[b]Department of Chemical Technology, Emet Vocational School, Kütahya Dumlupınar University, 43700 Kütahya, Türkiye

Table S1. Selected bond distances and angles for complex **1** (Å, º)

Bond Lengths (Å)			
Ni1–O1	1.9690 (14)	Ni1–N4^{i}	2.0322 (17)
Ni1–O4^{iii}	2.1140 (14)	Ni1–N1	2.0117 (17)
Ni1–O3^{iii}	2.1058 (14)		
Bond Angles (°)			
O1–Ni1–O4^{iii}	98.43 (6)	N4^{i}–Ni1–O4^{iii}	105.63 (7)
O1–Ni1–O3^{iii}	160.22 (6)	N4^{i}–Ni1–O3^{iii}	97.24 (7)
O1–Ni1–N4^{i}	91.84 (6)	N1–Ni1–O4^{iii}	148.17 (6)
O1–Ni1–N1	103.11 (7)	N1–Ni1–O3^{iii}	93.24 (6)
O3^{iii}–Ni1–O4^{iii}	62.23 (5)	N1–Ni1–N4^{i}	96.89 (7)

Symmetry codes: (i) x, $-y+1/2$, $z-1/2$; (ii) $-x+2$, $-y+1$, $-z$; (iii) x, $-y+1/2$, $z+1/2$.

Table S2. Parameters of isotherm models for MB adsorption.

Langmuir model				**Freundlich model**		
K_L (L g^{-1})	q_{max} (mg g^{-1})	R_L	R^2	n	K_F (L g^{-1})	R^2
2.00×10^{-2}	194.67	9.10×10^{-2}	0.996	2.26	14.47	0.894

Table S3. Comparison of maximum adsorption capacities of MB for various CPs.

Adsorbent	q_m **(mg g^{-1})**	**Reference**
MoS_2-COOH@ UiO-66-NH_2	253.00	[1]
UiO-66-$(OH)_2$/GO	96.69	[2]
Co doped Fe-BDC MOF	23.92	[3]
UiO-66	107.00	[4]
Cu(I)-MOF	149.50	[5]
FMDC(1.0)	625.0	[6]
CP1 and CP2	45.15, 48.11	[7]
Co(II)-CP	473.57	[8]
Compound **1**	194.67	*This study*

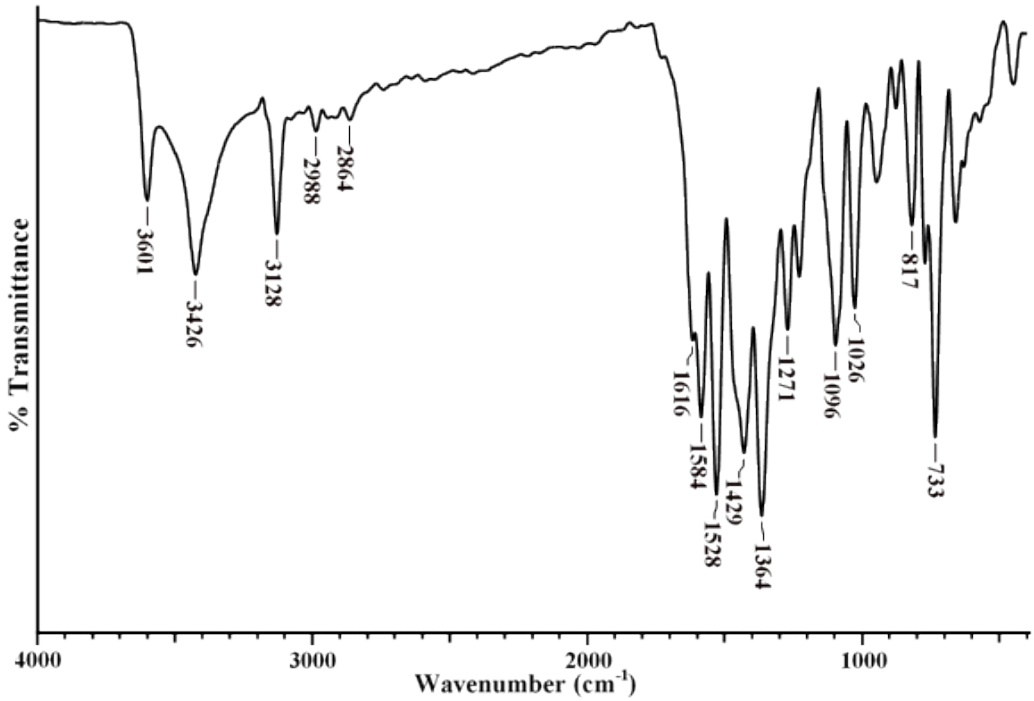

Fig. S1. IR spectrum of compound **1**

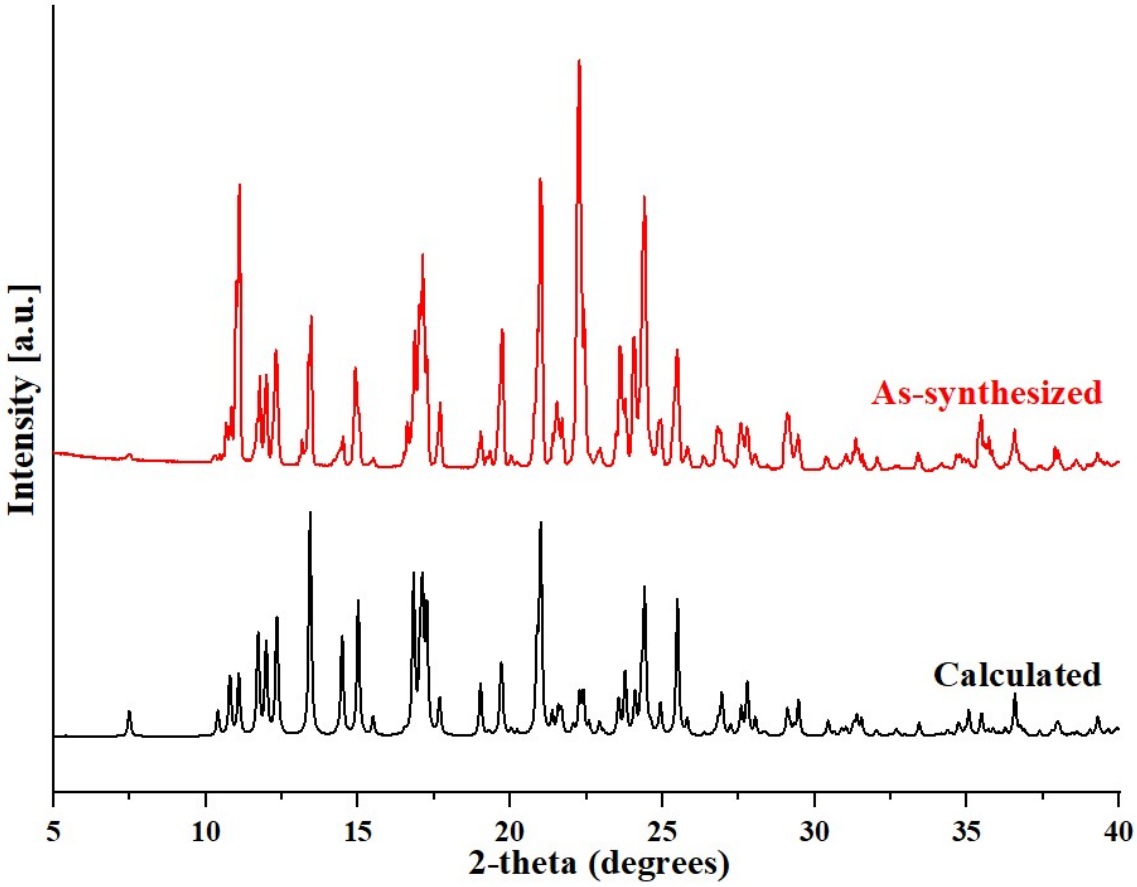

Fig S2. Simulated and experimental PXRD patterns of compound **1**

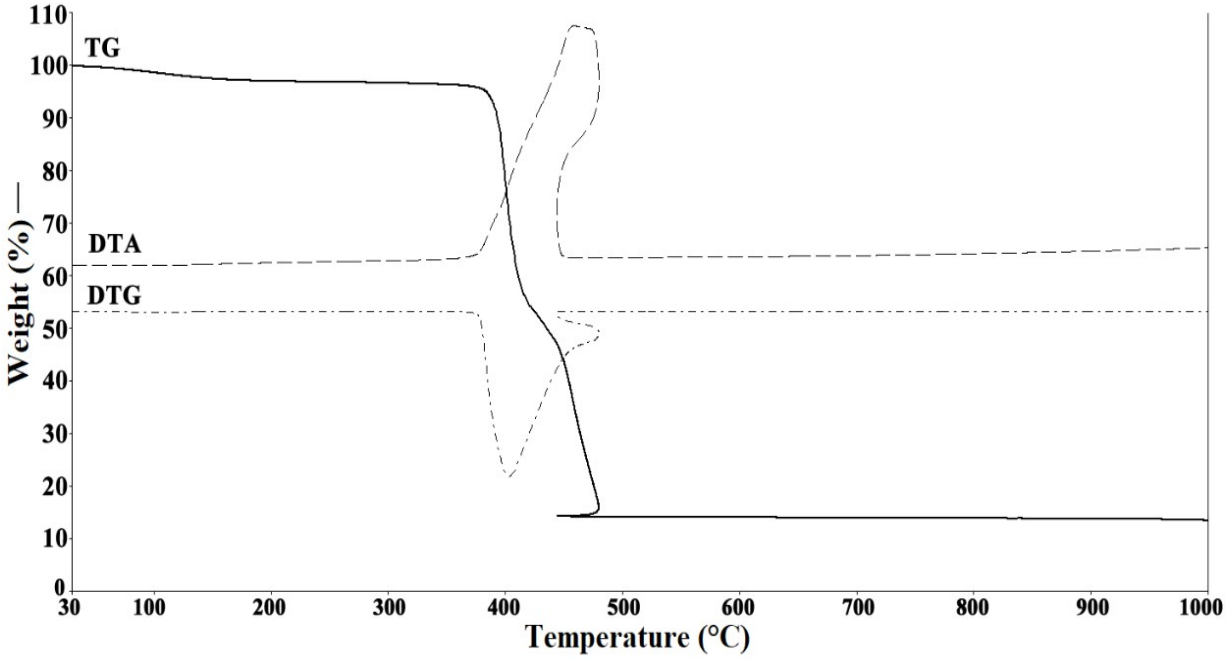

Fig S3. TG, DTA and DTG curves of compound **1**

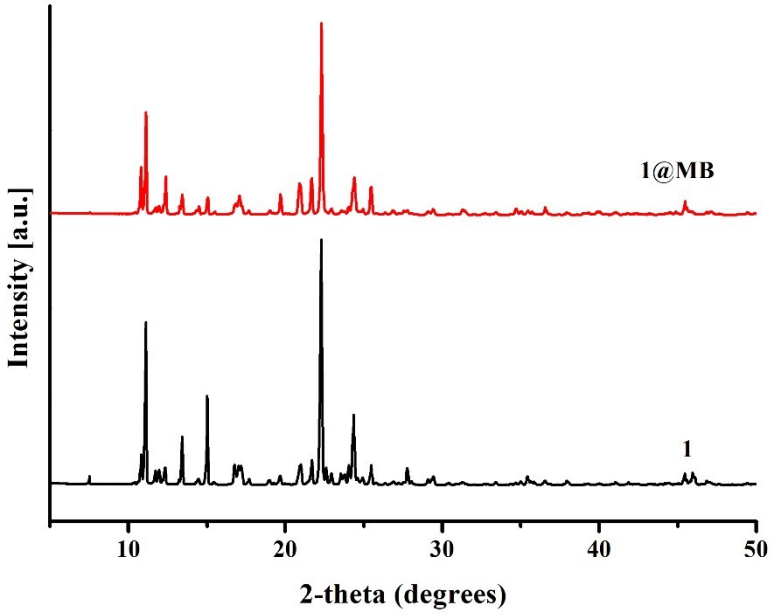

Fig. S4. PXRD patterns of as-synthesized compound and dye loaded compound **1**

References

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