Electronic Supplementary Information (ESI)

3D heterometallic Ni(II)/K(I) MOF with a rare rna topology: synthesis, structural features, and photocatalytic dye degradation modeling†

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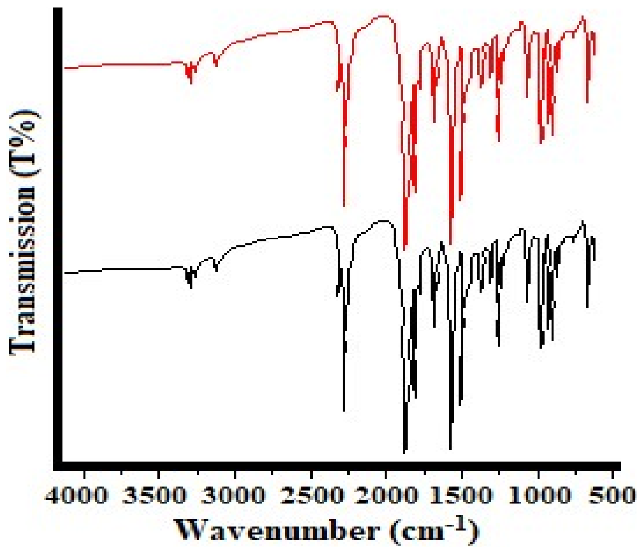

Figure S1. IR spectra of **1** (top: as synthesized microcrystals) and **1s** (bottom: sonochemically prepared sample).

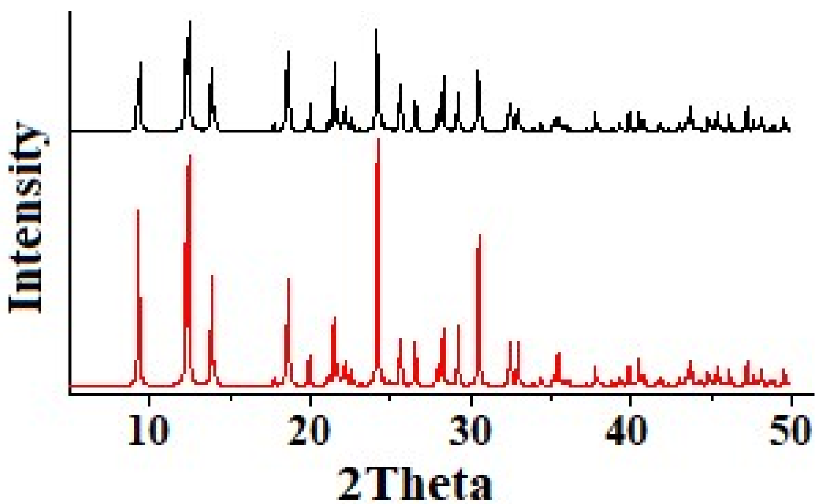

Figure S2. PXRD patterns: compound **1s** (top: sonochemical synthesis), simulated from single crystal X-ray data of **1** (bottom).

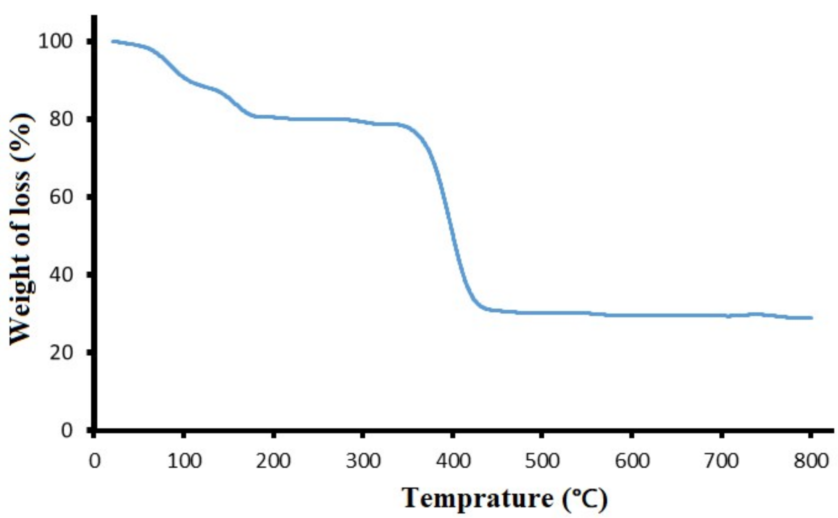

Figure S3. TGA of **1s** (sample of entry 5, Table 3).

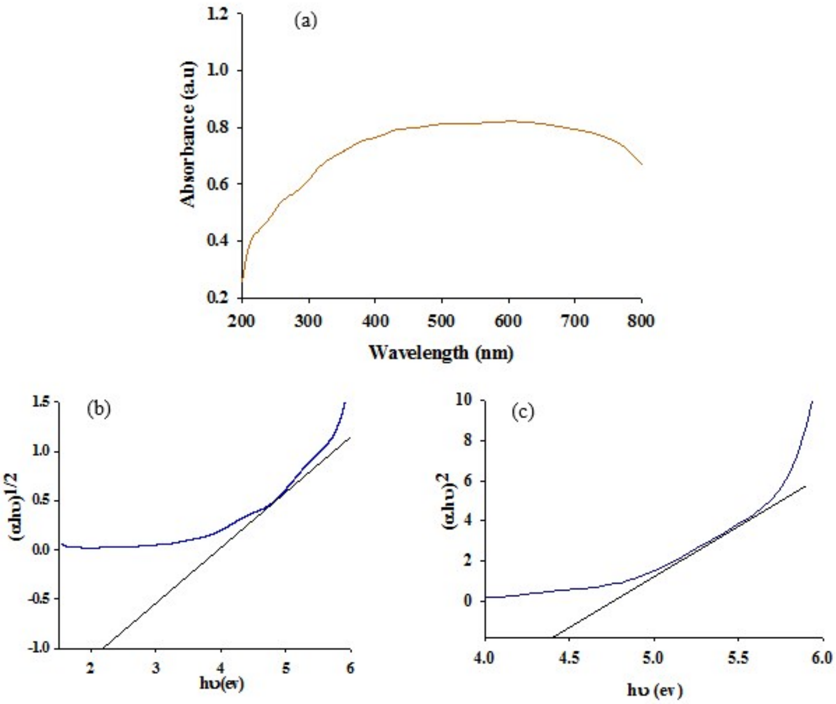

Figure S4. (a) UV–Vis DRS of **1s**. (b,c) Typical Tauc plots for allowed direct (b) and indirect (c) transitions in **1s**.

Table S1. Central composite design with predictive values and their experimental results in photocatalytic experiments.

Trial no.	Factor level				Response: Deg. (%)	
	X_1	X_2	X_3	X_4	Observed	Predicted
1	0	0	0	+2	87.8	85.7
2	-1	+1	+1	-1	70.3	69.6
3	0	0	0	0	94.5	93.5
4	-1	+1	-1	-1	70.3	71.5
5	-1	+1	+1	+1	71.1	70.3
6	+1	-1	-1	-1	79.6	79.2
7	+1	-1	-1	+1	84.0	82.8
8	+1	+1	+1	-1	79.3	79.6
9	+1	+1	-1	+1	88.4	87.2
10	+2	0	0	0	94.3	92.8
11	0	0	-1	0	95.6	93.5
12	0	0	+1	-2	80.6	80.7
13	0	0	-1	0	91.0	93.4
14	-1	+1	-1	+1	70.7	72.9
15	-1	-1	+1	-1	64.7	65.8
16	+1	-1	0	-1	75.9	76.6
17	0	0	+1	0	94.9	93.5
18	-1	+1	+1	-1	85.5	84.0

19	0	0	0	0	80.9	80.0
20	+1	0	-1	-1	97.9	98.6
21	0	+1	0	0	81.0	80.0
22	0	0	-2	0	92.2	93.5
23	+1	+1	0	+1	100.0	97.8
24	0	-2	0	0	70.6	70.3
25	-1	-1	0	+1	83.0	82.3
26	+1	-1	0	+1	78.5	81.0
27	-1	-1	0	+1	61.7	63.3
28	-2	0	+2	0	65.4	65.1
29	0	0	0	0	92.5	93.4
30	0	+2	0	0	80.0	80.4

Table S2. Comparison of different photocatalysts for BCG degradation.

Catalyst	Initial Concentration (BCG)	Irradiation Time (min)	% Degradation Efficiency (%)	Ref.
Ni(II)/K(I) MOF	6.0 mg/L	46	94	This work
Ti/SnO_2-RuO_2	100 mg/L	150	91	[50]
Fe(III)/H_2O_2	6×10^{-5} M	70	74	[51]
PTA/ZR13	1×10^{-5} M	20	73	[52]
ZnO	1×10^{-5} M	75	64	[53]
WO_3/ZnO	1×10^{-5} M	75	60	[53]
CuS-Cp	10.0 mg/L	480	60	[54]
ZnO-Cp	10.0 mg/L	480	56	[54]