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Supplementary Information

A Ni-based MOF for selective detection and removal of Hg^{2+} in aqueous medium: a facile strategy

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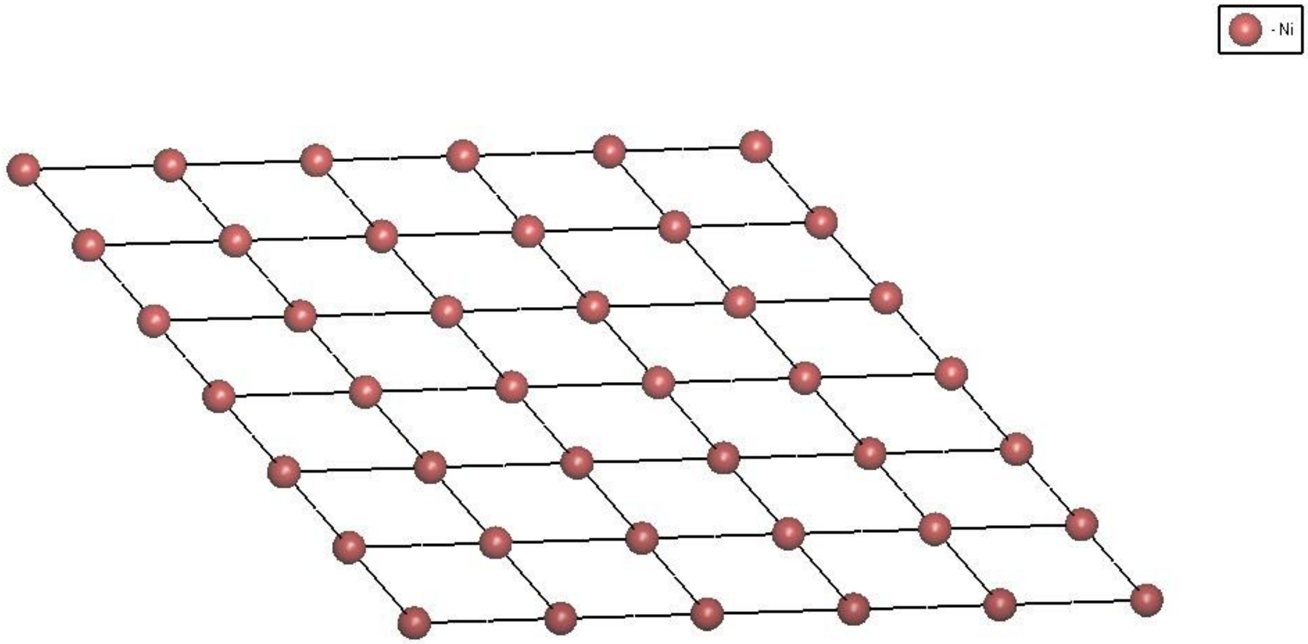

Fig. s1: A perspective view of the topology of complex **1** along 100 plane

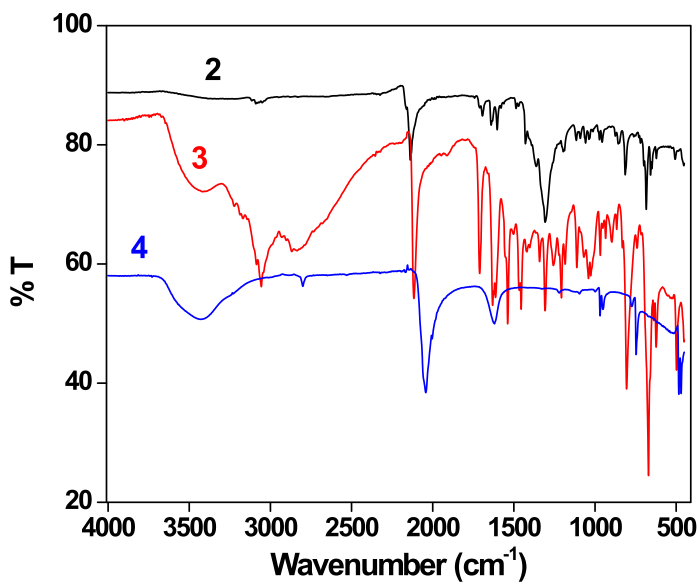

Fig. s2: FT-IR spectra of complex **2** (2, black), product from reaction of 3-bpd, SCN^- and Hg^{2+} (3, red) and mercuric thiocyanate (4, blue).

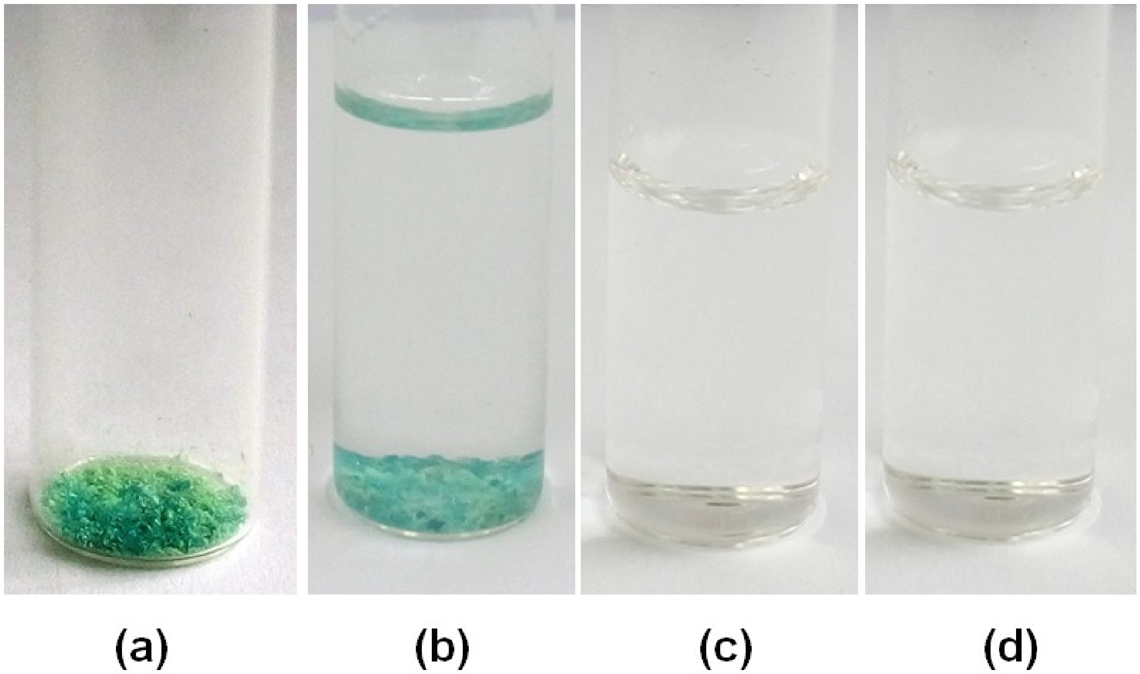

Fig. s3: Photographs of complex **1** in solid state (a), complex **1** in water (b), filtrate of solution containing complex **1** after its treatment with Hg^{2+} (c) and solution (c) after addition of dimethylglyoxime under ammoniacal condition (d).

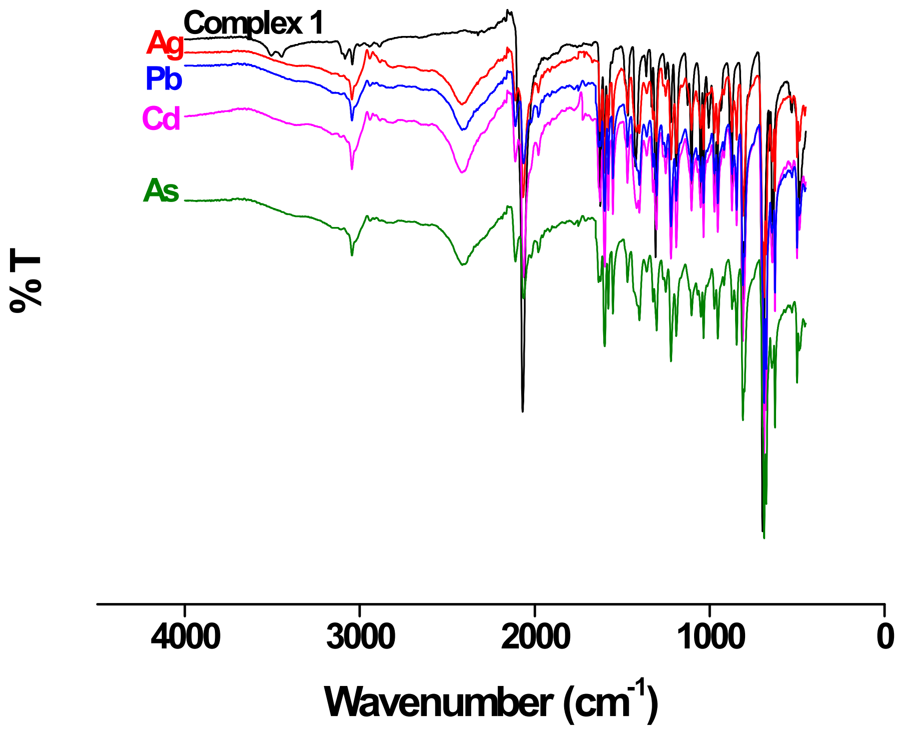

Fig. s4: FT-IR spectra of **1** (black) and **1** in the presence of Ag^{+} (red), Pb^{2+} (blue), Cd^{2+} (cyan) and As^{3+} (olive) ion.

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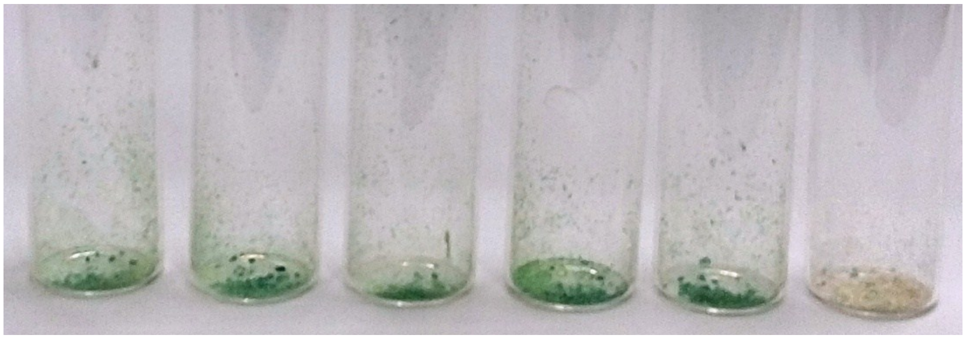

Fig. s5: Color of **1** in the presence of (from left) Mg^{2+}, Ca^{2+}, Al^{3+}, Zn^{2+}, Fe^{3+} and Hg^{2+} ions. Na^{+} or K^{+} ion cannot change color of **1**. This fact is evident from the method of synthesis of complex **1**. We used NaSCN or KSCN during synthesis. But complex **1** does not contain any sodium or potassium. Thus, color of **1** is unchanged in the presence of these metal ions.

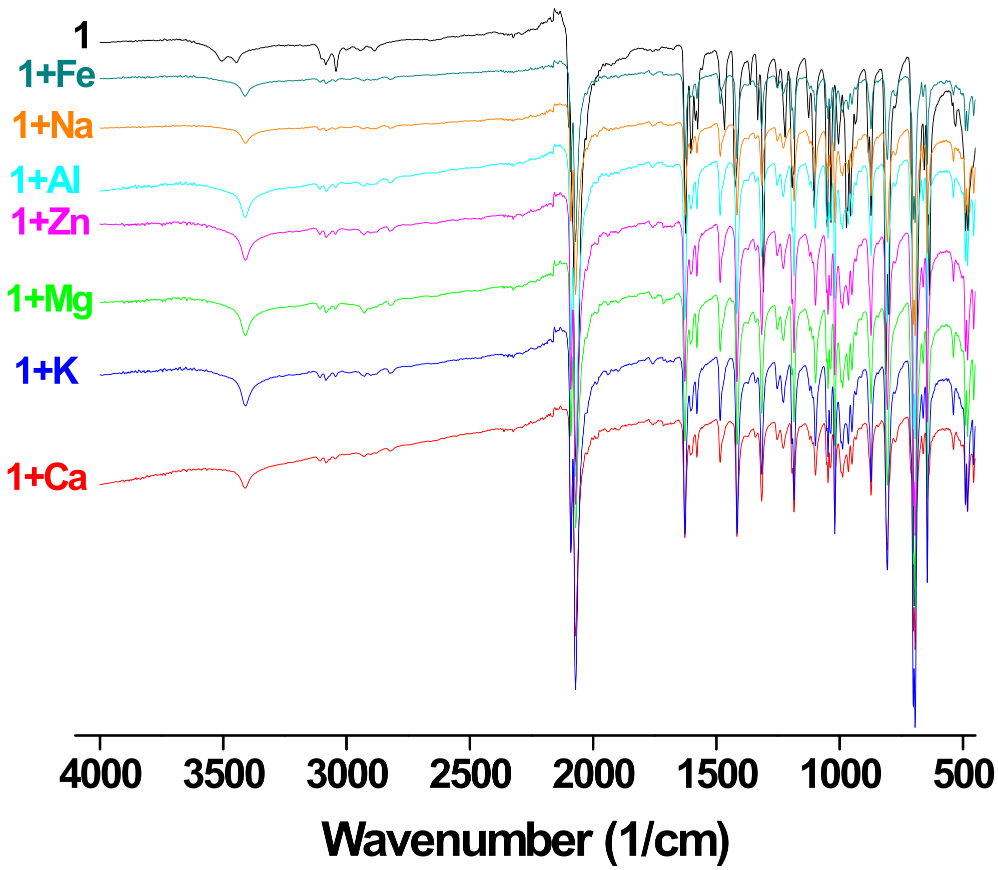

Fig. s6: FT-IR spectra of **1** (black) and **1** in the presence of Na^{+}, K^{+}, Mg^{2+}, Ca^{2+}, Al^{3+}, Zn^{2+}, Fe^{3+} and Hg^{2+} ions

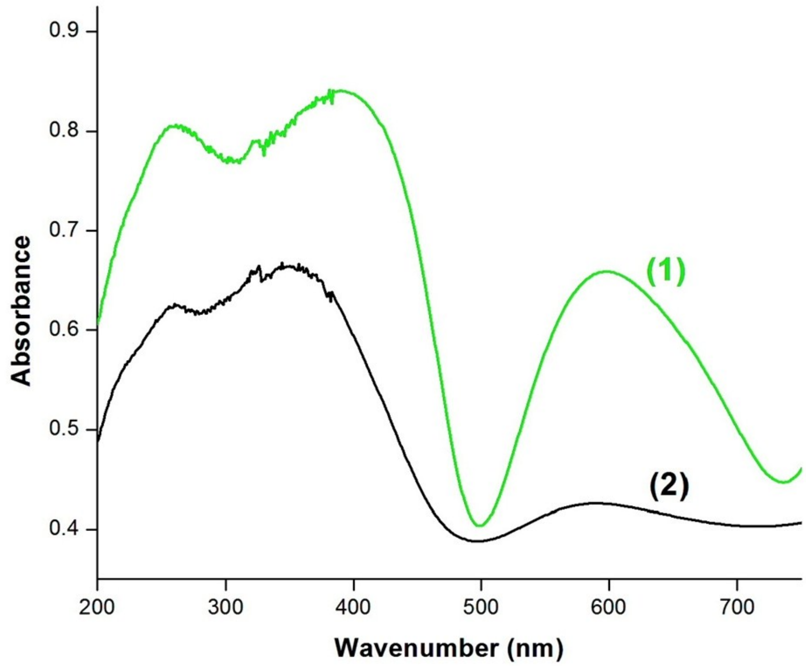

Fig. s7: UV-vis spectra of complex **1** and complex **1** in the presence of Hg^{2+} in solid state.

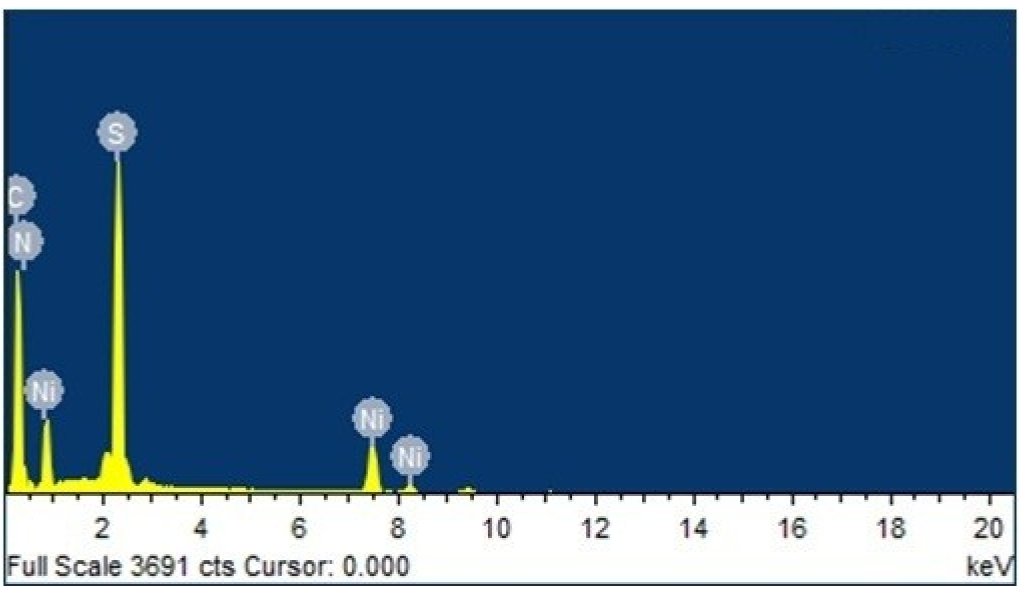

Fig. s8: EDX spectrum of complex **1**

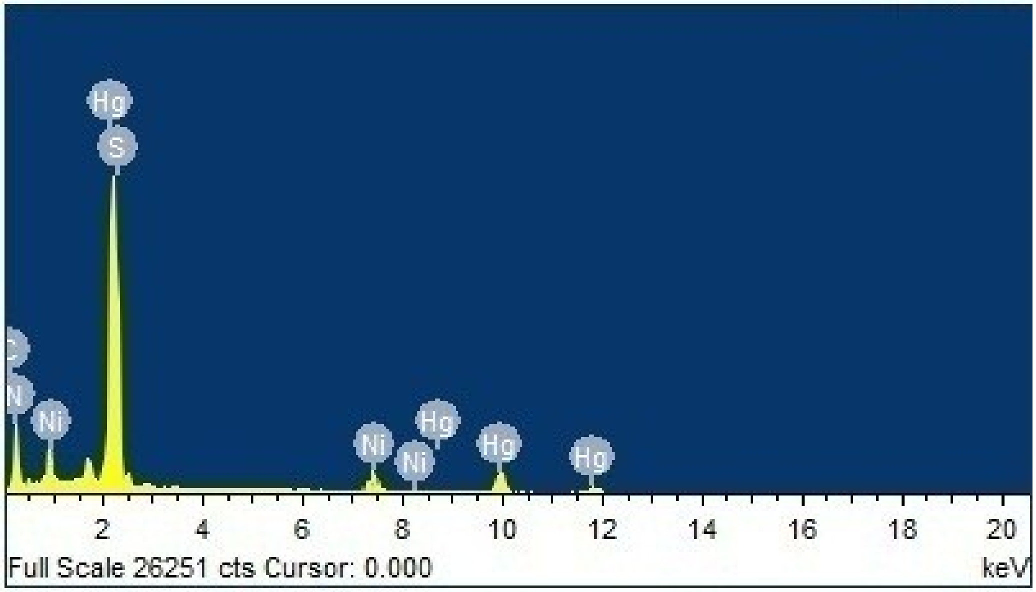

Fig. s9: EDX spectrum of complex **2**

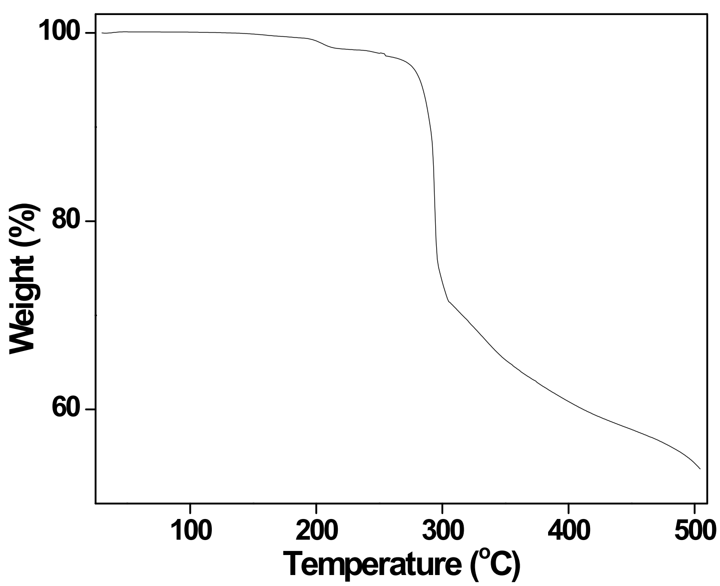

Fig. s10: TGA of complex **1**. It confirms stability of the framework upto at least 195°C.

Table s1: Selected bond lengths (in Å) and selected bond angles (in degree) of complex **1**

Ni1−N8	2.021(3)
Ni1−N1	2.147(3)
Ni1−N5	2.190(3)
Ni2−N7	2.055(3)
Ni2−N6	2.173(3)
Ni2−N2	2.181(3)
N8^{vi} −Ni1−N8	180.0
N8^{vi}−Ni1−N1^{i}	90.81(10)
N8−Ni1−N1^{i}	89.19(10)
N8^{vi}−Ni1−N1	89.19(10)
N8−Ni1−N1	90.81(10)
N1^{i}−Ni1−N1	180.0
N8^{vi}−Ni1−N5	88.99(10)
N8−Ni1−N5	91.01(10)
N1^{i}−Ni1−N5	91.71(10)
N1−Ni1−N5	88.28(10)
N8^{vi}−Ni1−N5^{iii}	91.01(10)
N8−Ni1−N5^{iii}	88.99(10)
N1^{i}−Ni1−N5^{iii}	88.29(10)
N1−Ni1−N5^{iii}	91.72(10)
N5−Ni1−N5^{iii}	180.00(13)
N7^{v}−Ni2−N7	179.999(1)
N7^{v}−Ni2−N6	90.69(10)
N7−Ni2−N6	89.31(10)
N7^{v}−Ni2−N6^{iv}	89.31(10)
N7−Ni2−N6^{iv}	90.69(10)
N6−Ni2−N6^{iv}	180.00(11)

N7^{v}−Ni2−N2^{ii}	91.66(11)
N7−Ni2−N2^{ii}	88.34(11)
N6−Ni2−N2^{ii}	96.44(10)
N6^{iv}−Ni2−N2^{ii}	83.56(10)
N7^{v}−Ni2−N2	88.34(11)
N7−Ni2−N2	91.66(11)
N6−Ni2−N2	83.56(10)
N6^{iv}−Ni2−N2	96.44(10)
N2^{ii}−Ni2−N2	179.998(1)
C17−N5−Ni1	118.6(2)
C23−N6−Ni2	121.9(2)
C19−N6−Ni2	120.3(2)
C1−N1−Ni1	123.1(2)
C5−N1−Ni1	120.5(2)
C11−N2−Ni2	117.4(2)
C7−N2−Ni2	124.5(2)
C26−N8−Ni1	169.5(3)
C25−N7−Ni2	175.8(3)

Table s2: Comparison of some of recently published results on Hg uptake studies

Sl No.	Compounds	Hg uptake Capacity (mg g^{-1})	Type of adsorption	Post synthetic modification	Theoretical Studies	Ref.
1	Fe_3O_4@SiO_2@HKUST-1	264	Not mentioned	Yes	No	s1
2	Zn(hip)(L).(DMF)(H_2O) (H_2hip = 5-hydroxyisophthalic acid, L = N^4,$N^{4'}$-di(pyridine-4-yl)biphenyl-4,4′-dicarboxamide)	278	Both physisorption and chemisorption with different contributions	No	No	s2
3	Thiol-functionalized $[Cu_3(BTC)_2(H_2O)_3]_n$ (BTC = benzene-1,3,5-tricarboxylate)	714.29	Chemisorption	Yes	No	s3
4	ZnS Nano Crystals Sorbent	720	Not mentioned	No	No	s4
5	Gold Nanoparticle-Aluminum Oxide Adsorbent	676	Not mentioned	No	No	s5
6	Thiol-Functionalized Zn-Doped Biomagnetite Particles (MPTMS)	416	Not mentioned	Yes	No	s6
7	Manganese dioxide nanowhiskers (MDN)	199.53	Physisorption	Yes	No	s7
8	Diatom silica microparticles modified with self-assembled monolayers of 3-mercaptopropyl-trimethoxysilane MPTMS-DE	185.2	Not mentioned	Modified with self-assembled monolayers of 3-mercaptopropyl-	No	s8

				trimethoxysilane (MPTMS)		
9	Diatom silica microparticles modified with self-assembled monolayers of 3-aminopropyl-trimethoxysilane APTES-DE	131.7	Not mentioned	Modified with self-assembled monolayers of 3-aminopropyl-trimethoxysilane (APTES)	No	s8
10	Diatom silica microparticles modified with self-assembled monolayers of n-(2-aminoethyl)-3-aminopropyl-trimethoxysilane AEAPTMS-DE	169.5	Not mentioned	Modified with self-assembled monolayers of n-(2-aminoethyl)-3-aminopropyl-trimethoxysilane (AEAPTMS)	No	s8
11	Fe_3O_4 Magnetic Nanoparticles	97.7	Not mentioned	No	No	s9
12	$[Ni(3\text{-bpd})_2(NCS)_2]_n$	713	Chemisorption	No	Yes	Present Work

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