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Data Article

Data on the fluoride adsorption from aqueous solutions by metal-organic frameworks (ZIF-8 and Uio-66)

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ABSTRACT

The variables examined were initial fluoride concentration, ZIF-8 and Uio-66 dosage, pH, and contact time. The residual concentration of fluoride was measured by a spectrophotometer. According to BET, the specific surface area of the ZIF-8 and Uio-66 was 1050 m^2/g and 800 m^2/g, respectively. Total pore volume and average pore diameter of the ZIF-8 and Uio-66 were 0.57 cm^3/g, 0.45 cm^3/g and 4.5 nm, 3.2 nm, respectively. The best pH for fluoride adsorption was neutral conditions. By increasing the ZIF-8 and Uio-66 dose, the fluoride uptake increased at first, but then decreased. Also, the maximum adsorption for ZIF-8 and Uio-66 was observed in adsorbent dose 0.2 and 0.6 g/L, respectively. The best model for describing kinetic and isotherms of fluoride adsorption were the pseudo-second-order model and Langmuir isotherm model, respectively. Based on the Langmuir model, the adsorption capacity of fluoride by ZIF-8 and Uio-66 was reported to be 25 mg/g and 20 mg/g, respectively.

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Specifications table

Subject area	*Water treatment*
More specific subject area	*Adsorption*
Type of data	*Figures and tables*
How data was acquired	*Spectrophotometer (UV-UVIS, 570 nm)*
Data format	*Analyzed*
Experimental factors	*The main variables examined were initial concentration of fluoride, ZIF-8 and Uio-66 dosage, pH, and contact time. At first, a stock solution of fluoride (NaF, 1000 mg/l) was made and stored under standard conditions. At the end of the experiments, the remaining adsorbents were separated using a centrifuge (3000 rpm, 5 min). After separation, the residual fluoride was measured by a spectrophotometer DR-5000.*
Experimental features	*ZIF-8 was first synthesized. In the second step, the absorbent of Uio-66 was synthesized. After synthesizing adsorbents, the general characterization of the adsorbent was determined based on XRD, SEM, and BET.*
Data source location	*Khorramabad, Lorestan University of Medical Sciences, Iran*
Data accessibility	*Data are included in this article*
Related research article	*A.A. Mohammadi, A. Alinejad, B. Kamarehie, S. Javan, A. Ghaderpoury, M. Ahmadpour, M. Ghaderpoori. Metal organic framework Uio-66 for adsorption of methylene blue dye from aqueous solutions. Int J Environ Sci Te. 14 (2017) 1959–1968.*

Value of the data

- The dataset will be useful for the application of the metal-organic framework in the fluoride adsorption from aqueous solutions.
- The data of this project can be used to improve drinking water quality by the authorities.
- Information from this data, including, kinetic and isotherm constants, will be informative for predicting and modelling the adsorption capacity and mechanism of fluoride uptake by ZIF-8 and Uio-66.
- The characterization data of the ZIF-8 and Uio-66 are useful for the scientific community to complete the studies for emerging absorbers.

1. Data

The XRD and SEM results of synthesized ZIF-8 and Uio-66 are shown in Fig. 1. All adsorption experiments were performed in triplicate. Results of BET present in Table 1. The effects of an adsorbent dose of ZIF-8 and Uio-66 on fluoride adsorption are presented in Fig. 2. The effects of solution pH of ZIF-8 and Uio-66 on fluoride adsorption are depicted in Fig. 3. The effects of the initial concentration of ZIF-8 and Uio-66 on fluoride adsorption are shown in Fig. 4. Calculated parameters of kinetic models for the fluoride adsorption onto ZIF-8 and Uio-66 are summarized in Table 2. As illustrated in Table 2, the pseudo-second-order model for ZIF-8 and Uio-66 has the highest R^2 (coefficient of determination). As a result, the model was the most suitable model to express the kinetics of the fluoride adsorption onto ZIF-8 and Uio-66. Calculated parameters of isotherm models for the fluoride adsorption onto ZIF-8 and Uio-66 are given in Table 3. As illustrated in Table 3, the Langmuir isotherm model for ZIF-8 and Uio-66 has the highest R^2. As a result, the model was the most suitable model to express the isotherm of the fluoride adsorption onto ZIF-8 and Uio-66.

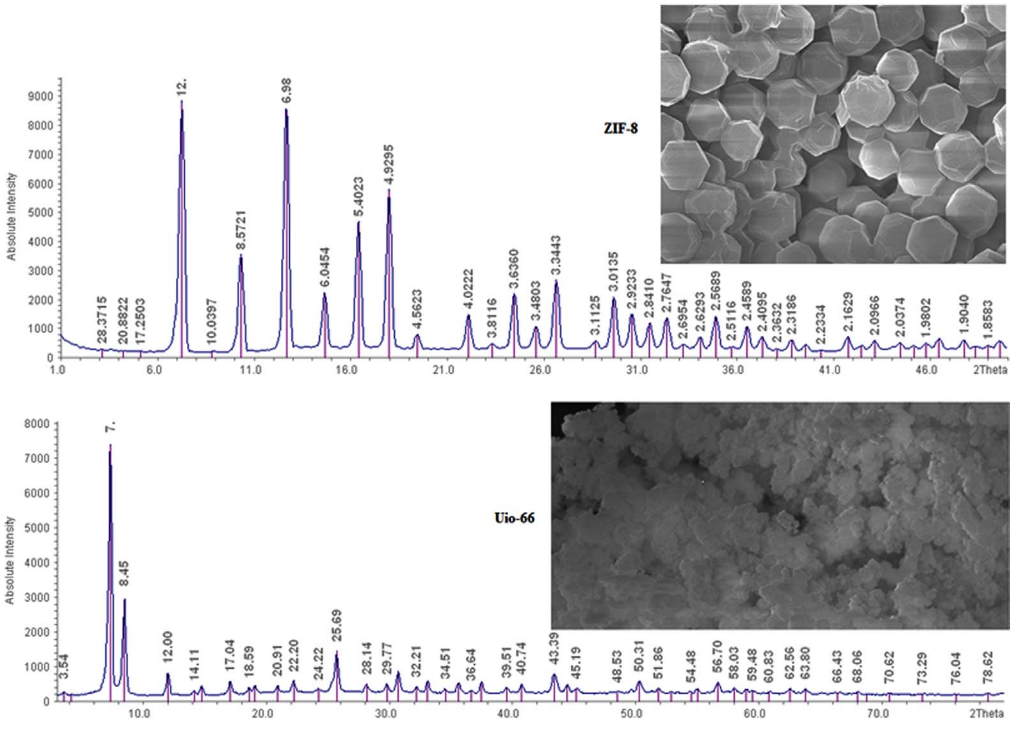

Fig. 1. Results of XRD and SEM of synthesized ZIF-8 and Uio-66.

Table 1
Results of BET for synthesized ZIF-8 and Uio-66.

Adsorbent	SA_{BET} ($m^2\ g^{-1}$)	$SA_{Langmuir}$ ($m^2\ g^{-1}$)	Total pore volume ($m^3\ g^{-1}$)	Mean pore diameter (nm)
ZIF-8	1050	1150	0.57	4.5
Uio-66	800	970	0.45	3.2

2. Experimental design, materials, and methods

2.1. Materials

Chemicals used were zinc nitrate hexahydrate, methanol, N, N-dimethylformamide, zirconium chloride, 2-methylimidazole, and terephthalic acid. All the above-mentioned materials are prepared with high purity. The Materials were purchased from MERK and Sigma-Aldrich companies.

2.2. Synthesis of ZIF-8 and Uio-66

ZIF-8 was first synthesized. This adsorbent was synthesized based on the procedure presented by two previous works [1,2]. In the second step, the absorbent of Uio-66 was synthesized. For the synthesis of this absorbent, previous studies were used [3,4]. After synthesizing adsorbents, the general characterization of the adsorbent was determined based on XRD, SEM, and BET.

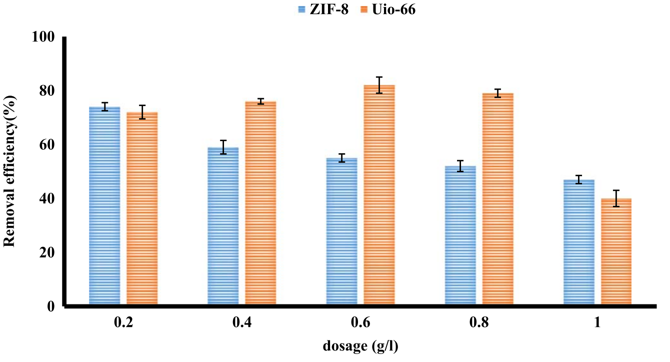

Fig. 2. The effect of adsorbent dose of ZIF-8 and Uio-66 on fluoride adsorption.

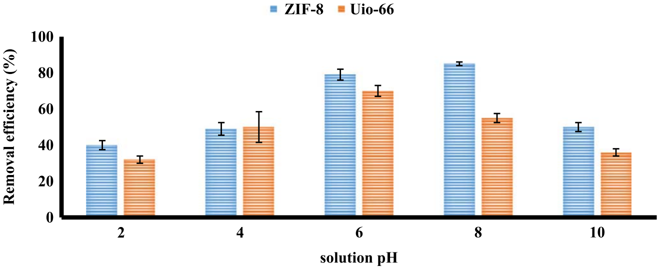

Fig. 3. The effect of solution pH of ZIF-8 and Uio-66 on fluoride adsorption.

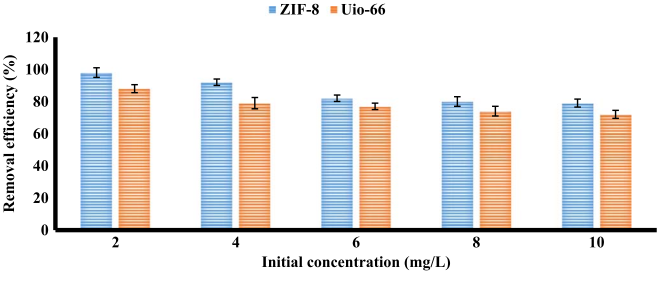

Fig. 4. The effect of initial concentration of ZIF-8 and Uio-66 on fluoride adsorption.

Table 2
Calculated parameters of kinetic models for the fluoride adsorption onto ZIF-8 and Uio-66.

Kinetics (ZIF-8)	Constants	F concentration ($mg\,l^{-1}$)		kinetics (Uio-66)	Constants	F concentration ($mg\,l^{-1}$)	
		2	4			2	4
Pseudo-First-Order	k_1	0.0156	0.0167	Pseudo-First-Order	k_1	0.0187	0.0196
	R^2	0.745	0.667		R^2	0.765	0.798
	q_{cal}	5.678	12.674		q_{cal}	6.576	14.243
Pseudo-Second-Order	k_2	0.0443	0.0465	Pseudo-Second-Order	k_2	0.0456	0.0645
	R^2	0.895	0.834		R^2	0.886	0.978
	$q_{e\ (cal)}$	12.6	17.5		$q_{e\ (cal)}$	13	15.7

Table 3
Calculated parameters of isotherm models for the fluoride adsorption onto ZIF-8 and Uio-66.

Isotherm (ZIF-8)	Constants	F concentration (mg l^{-1})		Isotherm (Uio-66)	Constants	F concentration (mg l^{-1})	
		2	**4**			**2**	**4**
Freundlich	n	3.5	5.3	**Freundlich**	n	2.7	3.6
	R^2	0.775	0.845		R^2	0.675	0.778
	K_F	18.5	18.9		K_F	19	19.8
Langmuir	K_L	1.5	1.8	**Langmuir**	K_L	0.576	0.657
	R^2	0.897	0.898		R^2	0.879	0.898
	q_m	25	29		q_m	20	28

2.3. *The adsorption experiments*

Fluoride adsorption was investigated by the metal-organic frameworks of ZIF-8 and Uio-66. The experiments were performed in batch conditions. The main variables examined were initial concentration of fluoride, ZIF-8 and Uio-66 dosage, solution pH, and contact time. At first, a stock solution of fluoride (NaF, 1000 mg/l) was made and stored under standard conditions. An adsorbent of ZIF-8 and Uio-66 was added to 50 ml of fluoride solution. The solution pH was adjusted using NaOH [0.1 N] and H_2SO_4 [0.1 N]. At the end, the used adsorbents were separated using a centrifuge (3000 rpm, 5 min). After separation, the final concentration of fluoride was measured by a spectrophotometer DR-5000 (UV-UVIS, 570 nm) [5–8]. Finally, fluoride adsorbed (q_e, mg/g) and the removal efficiency (%) on the ZIF-8 and Uio-66 was computed based on Eqs. (1) and (2), respectively [9,10]:

$$q_e, \mathrm{mg/g} = \frac{(C_o(\mathrm{mg/l}) - C_e(\mathrm{mg/l})V(\mathrm{L})}{\mathrm{m(g)}} \tag{1}$$

$$R, \% = \frac{(C_0(\mathrm{mg/l}) - C_t(\mathrm{mg/l}))}{C_0(\mathrm{mg/l})} \tag{2}$$

where, C_o *and* C_e, *and* C_t are an initial, equilibrium, and final concentration, respectively. V and m are the volume of solution and the adsorbent weight, respectively [11–23].

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Transparency document. Supplementary material

Transparency document associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.08.159.

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