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 m²/g and 800 m²/g, respectively. Total pore volume and average pore diameter of the ZIF-8 and Uio-66 were 0.57 cm³/g, 0.45 cm³/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. 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. |  
| 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.
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.

Table 1

| 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                     |

Fig. 1. Results of XRD and SEM of synthesized ZIF-8 and Uio-66.
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            | $k_1$    | 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            | $k_2$    | 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              |
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 H2SO4 [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 (qe, mg/g) and the removal efficiency (%) on the ZIF-8 and Uio-66 was computed based on Eqs. (1) and (2), respectively [9,10]:

\[
q_e, \text{mg/g} = \frac{(C_0(mg/l) - C_t(mg/l))V(L)}{m(g)} \tag{1}
\]

\[
R_\% = \frac{(C_0(mg/l) - C_t(mg/l))}{C_0(mg/l)} \tag{2}
\]

where, \(C_0\) 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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