Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary Information

Synthesis of modulator-driven highly stable zirconium-fumarate frameworks and their mechanistic investigations for the adsorption of arsenite and arsenate from aqueous solutions

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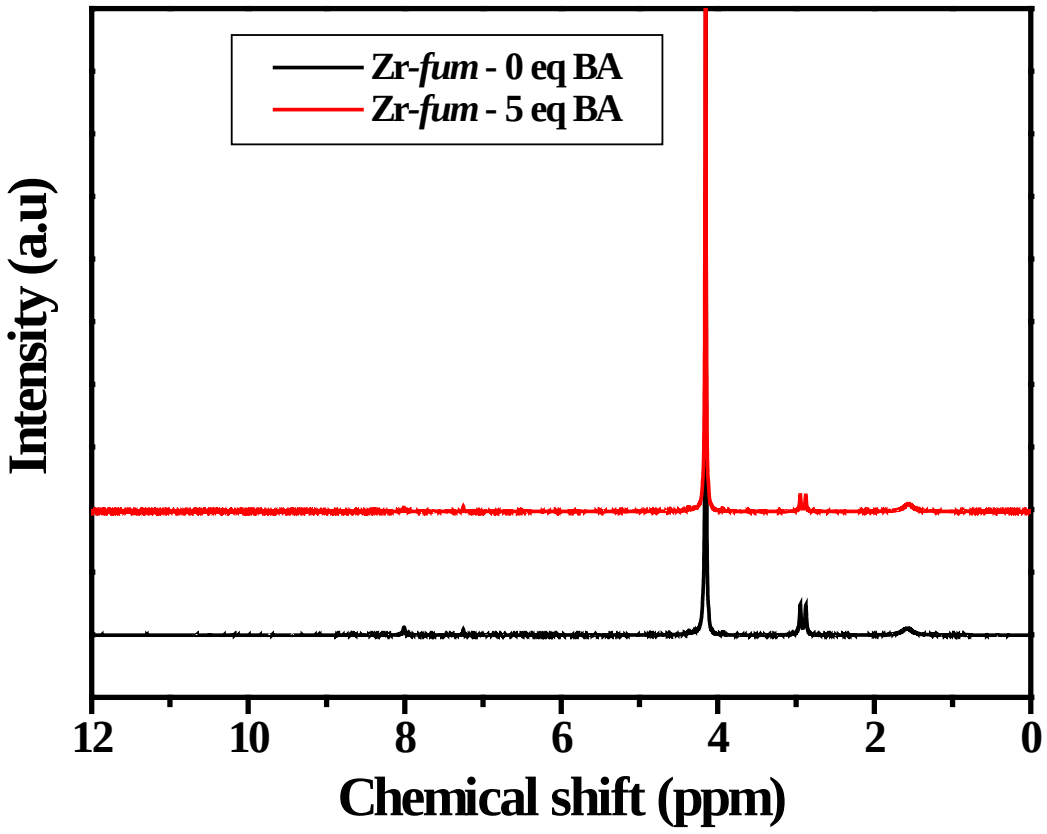

Figure S1. ^{1}H NMR spectra of Zr-*fum* MOF of 0 eq BA and 5 eq BA as ferrocene as reference.

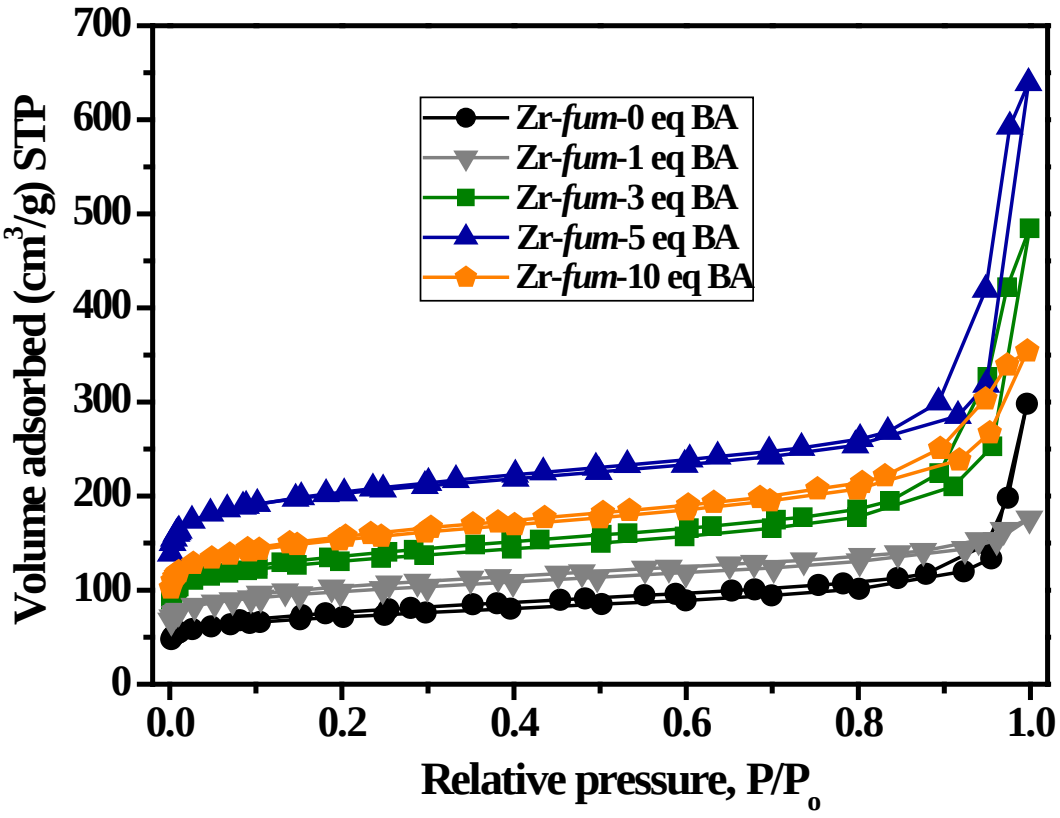

Figure S2. Nitrogen adsorption-desorption isotherms of the synthesized products under liquid nitrogen at 77 K.

Table S1. Physicochemical analysis of synthesized materials

Materials	BET SSA (m^2/g)	Pore volume (cm^3/g)	Avg. Pore size (nm)
Zr-*fum*-0 eq BA	260.4	0.357	3.358
Zr-*fum*-1 eq BA	363.2	0.120	3.354
Zr-*fum*-3 eq BA	483.9	0.569	3.058
Zr-*fum*-5 eq BA	760.1	0.700	3.352
Zr-*fum*-10 eq BA	566.1	0.334	3.288

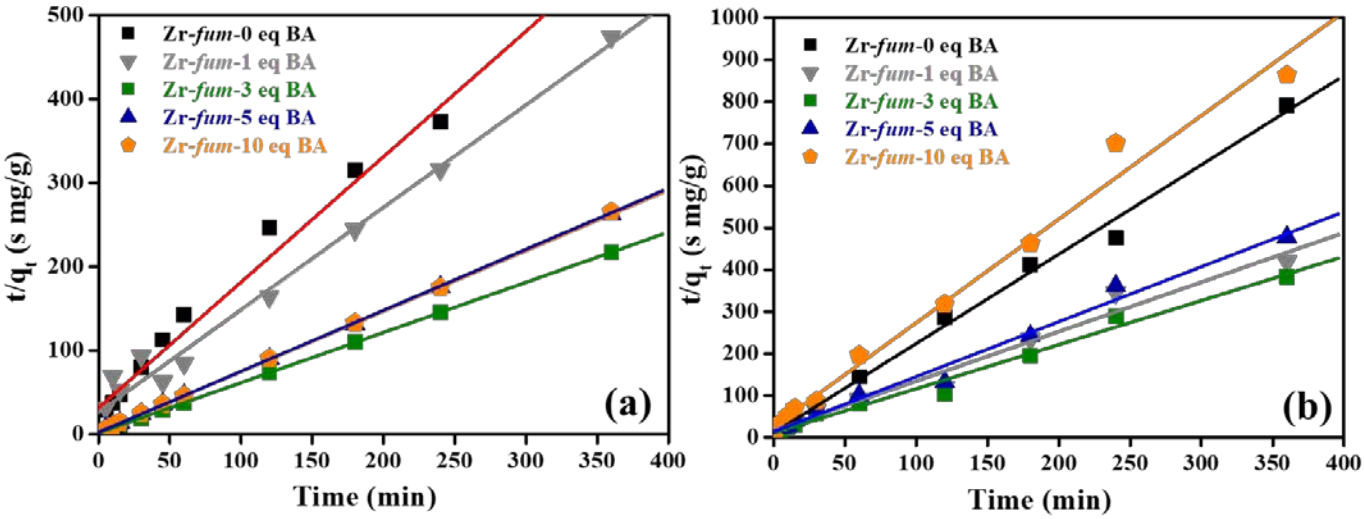

Figure S3. Pseudo-second-order kinetic models of **(a)** AsO_4^{3-} and **(b)** AsO_3^{3-} adsorption onto Zr-*fum*-0 eq BA, Zr-*fum*-1 eq BA, Zr-*fum*-3 eq BA, Zr-*fum*-5 eq BA and Zr-*fum*-10 eq BA. Experimental conditions: Initial conc. = 2 mM AsO_4^{3-} and 1.6 mM AsO_3^{3-}, dose ratio = 1 g/L, agitation = 100 rpm, temp = 25 °C.

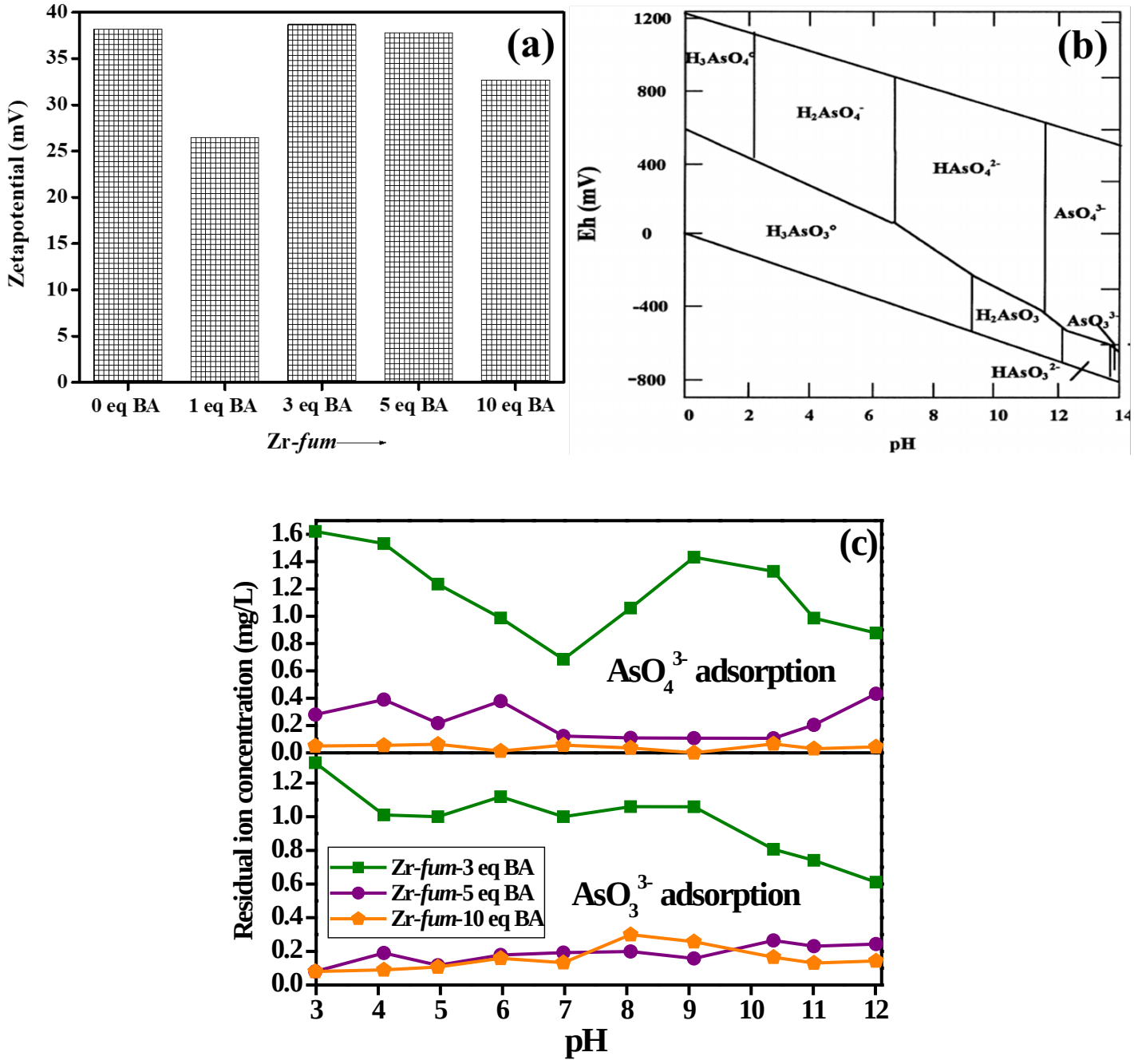

Figure S4. (a) Zeta potential at pH 6.8 and (b) Eh-pH diagram of the arsenic species and (c) residual ion concentration of Zr-*fum*-3 eq BA, Zr-*fum*-5 eq BA and Zr-*fum*-10 eq BA.

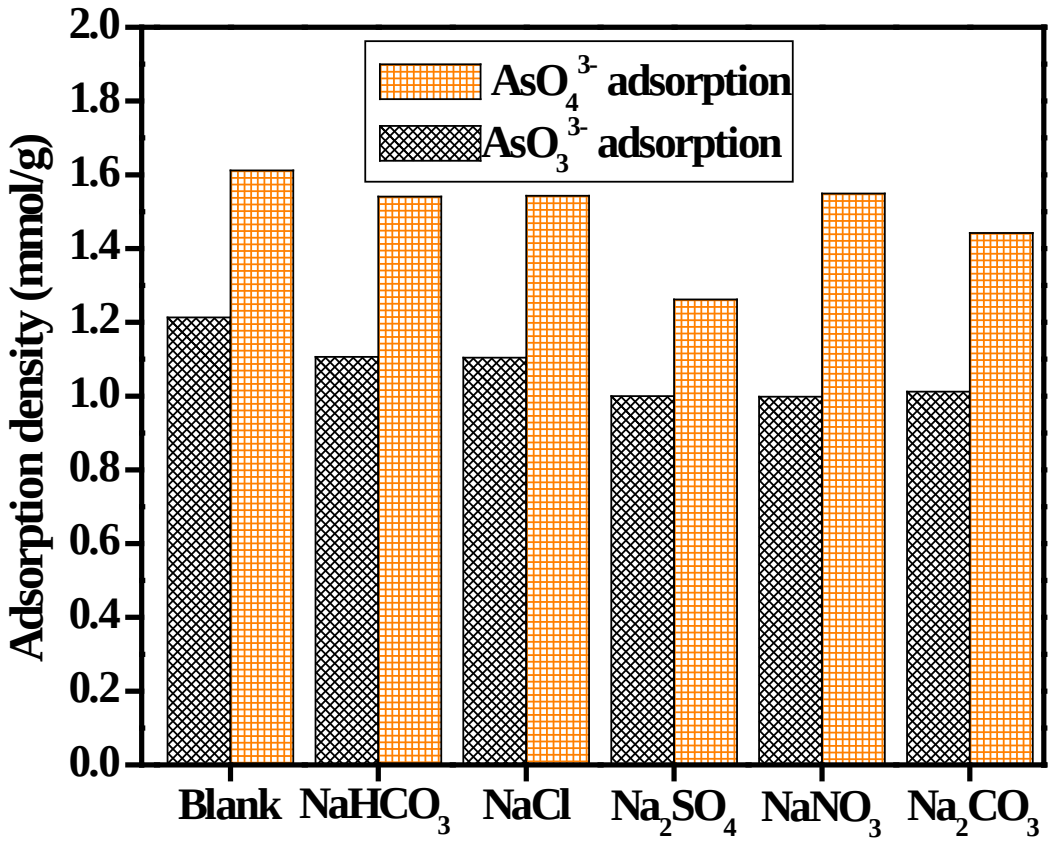

Figure S5. Effect of coexisting anions on synthesized Zr-*fum*-5 eq BA MOFs.

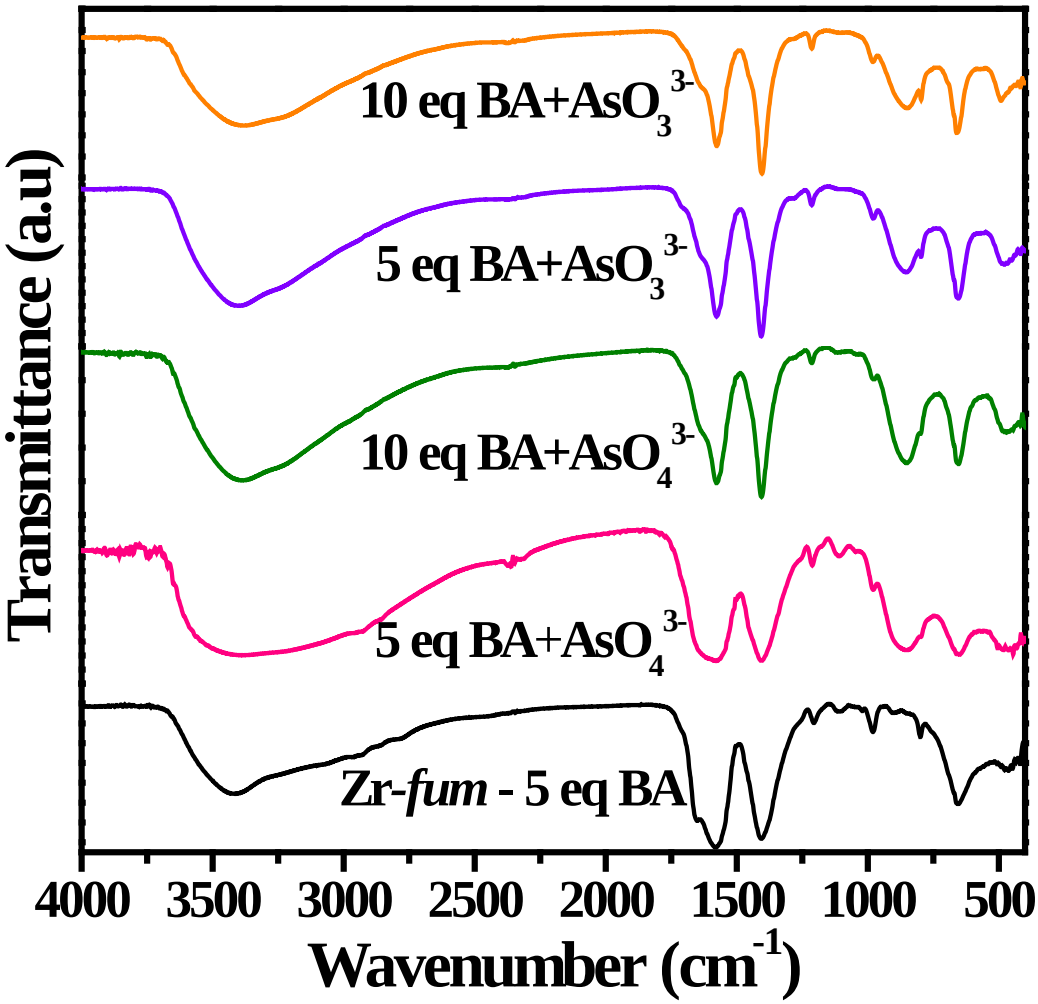

Figure S6. FTIR spectra of after adsorption of AsO_4^{3-} and AsO_3^{3-} using Zr-*fum*-5 eq BA and Zr-*fum*-10eq BA.

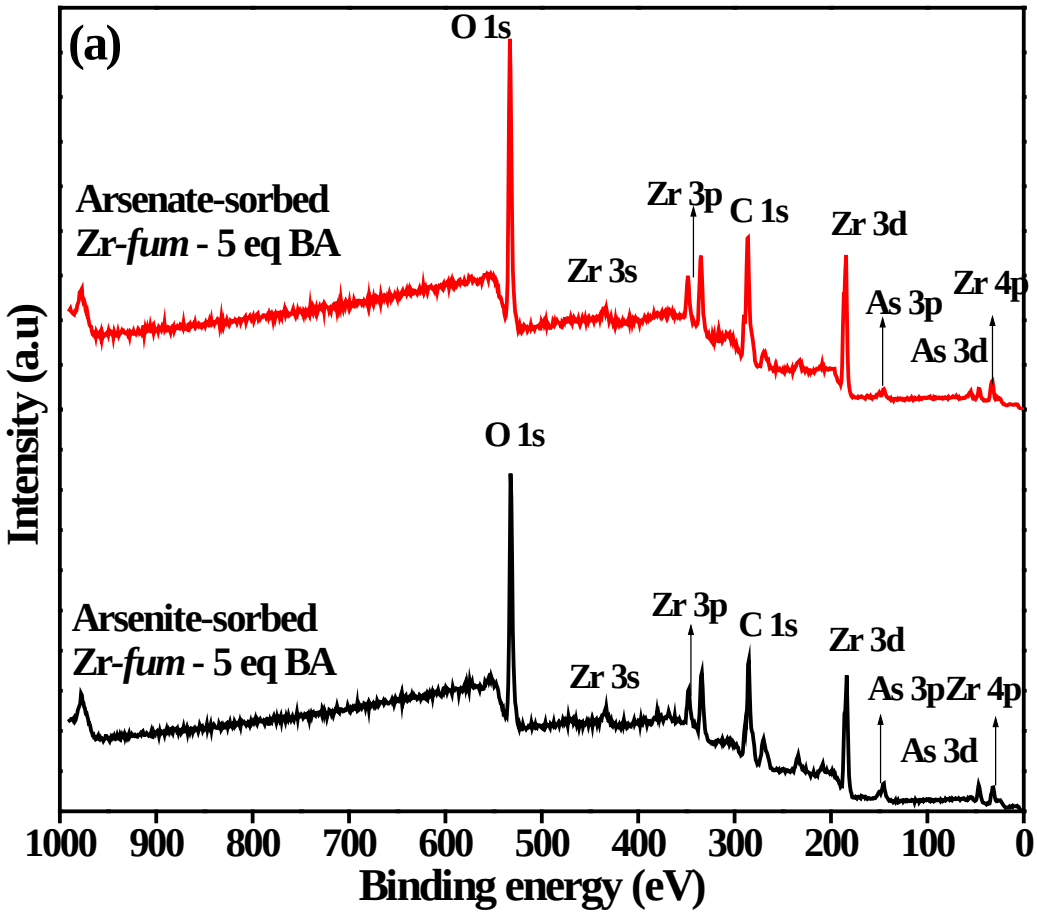

Figure S7. XPS spectra of after adsorption of AsO_4^{3-} and AsO_3^{3-} on Zr-*fum*-5 eq BA

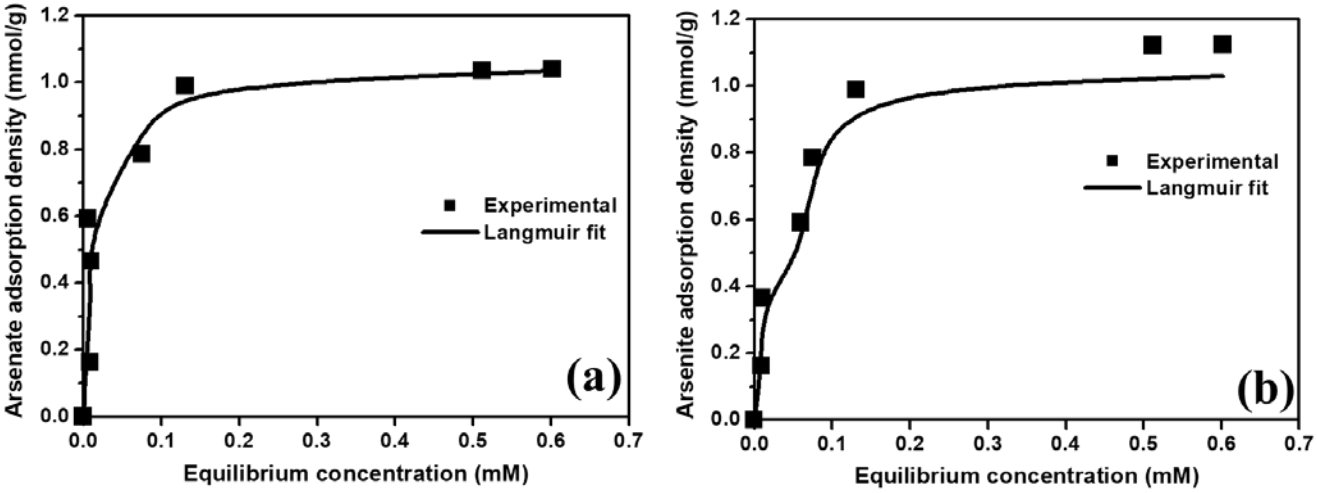

Figure S8. Langmuir adsorption isotherm for Zr-*fum*-5 eq BA MOF (a) AsO_4^{3-} and (b) AsO_3^{3-} adsorption.