# Electronic Supplementary Information

## Neutral ligand TIPA-based two 2D metal-organic frameworks: ultrahigh selectivity of $C_2H_2/CH_4$ and efficient sensing and sorption of Cr(VI)

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**Materials and measurements**

All reagents and solvents employed were commercially available. Powder X-ray diffraction (PXRD) patterns were collected on a MiniFlex-II diffractometer diffractometer using Cu (λ = 1.54178 Å) radiation with a speed of 2 °/min. Thermogravimetric analysis (TG) was performed on a Netzsch STA449C equipped with a platinum pan and heated at a rate of 5 °C/min in air. $CO_2$ (99.99%), $N_2$ (99.99%), $CH_4$ (99.99%) and $C_2H_2$ (99.99%) gas adsorption measurements were performed using an ASAP 2020 system. Elemental analyses of C, N, and H were performed on a Vario EL III elemental analyzer. Fluorescence spectra for the compounds were collected on F-7000 FL Spectrophotometer equipped with a 150 W xenon lamp as the excitation source at room temperature. UV–visible absorption and emission spectra were recorded on a Lambda 750s UV−vis spectrophotometer.The infrared spectrum was measured with KBr pellets in the 4000–400 $cm^{-1}$ region on a Nicolet 170SX spectrometer.

## Powder X-ray Diffraction Studies

X-ray powder diffraction (XPD) patterns of **1** and **2** was collected on a MiniFlex-II diffractometer.

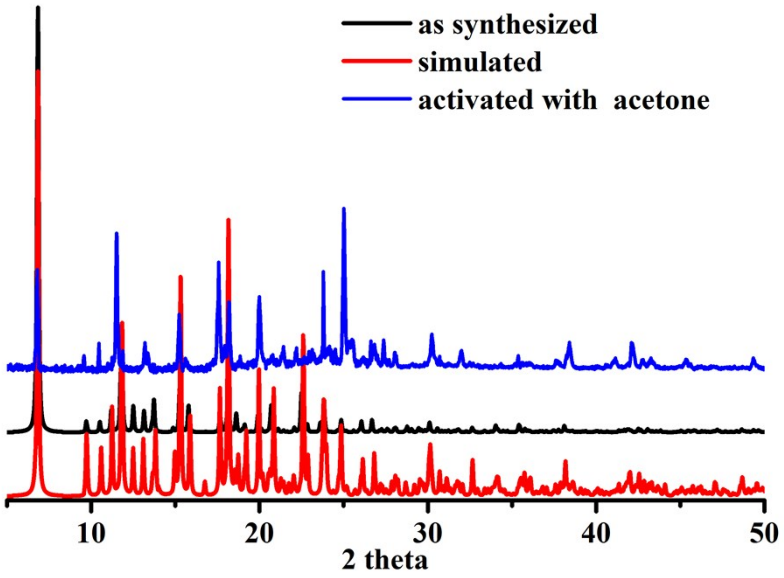


**Figure. S1** PXRD patterns of as-synthesized **1** as well as samples treated in the

acetone solution.

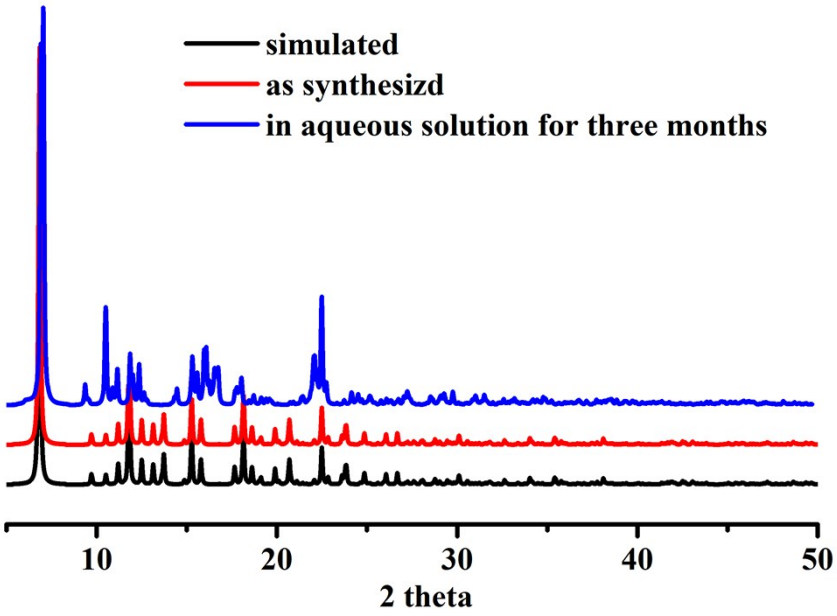


**Figure. S2** PXRD patterns of as-synthesized **2** as well as samples treated in water solution.

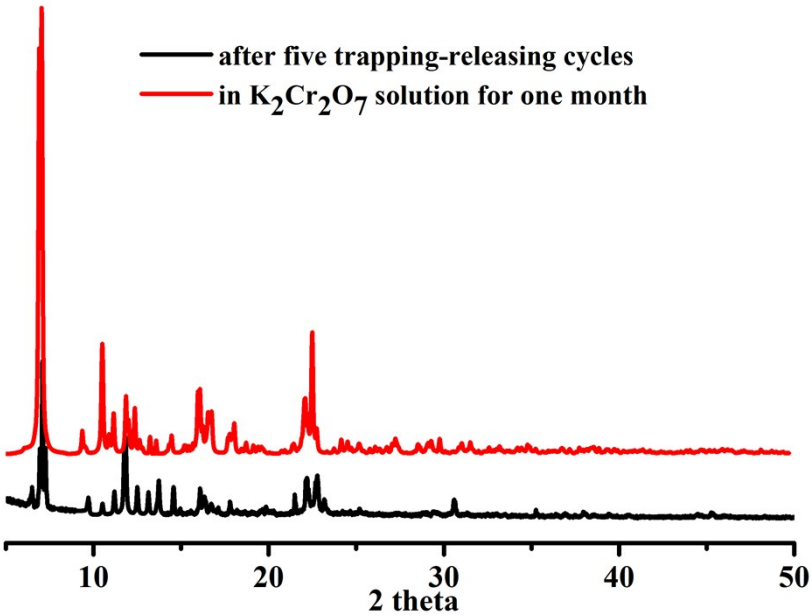


**Figure. S3** PXRD patterns of as-synthesized **2** as well as samples treated in corresponding solution.

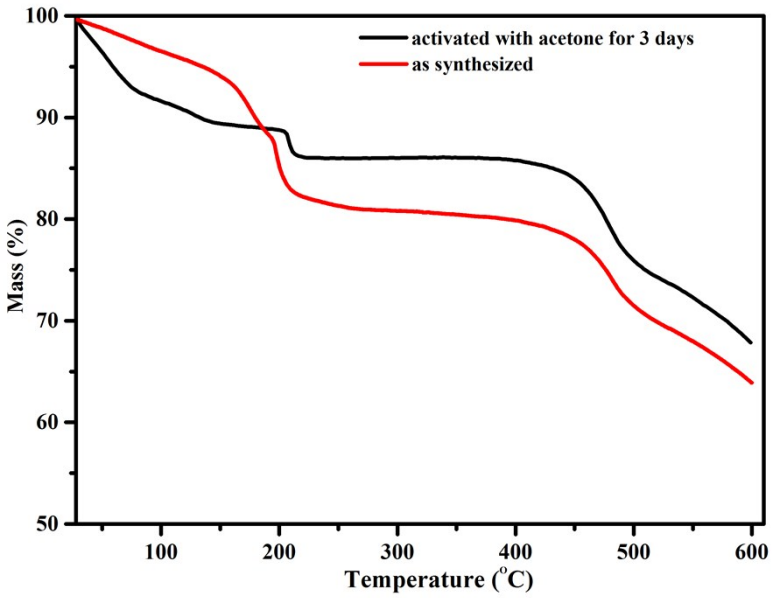


**Figure. S4** TGA curves of compound **1** under nitrogen gas atmosphere.

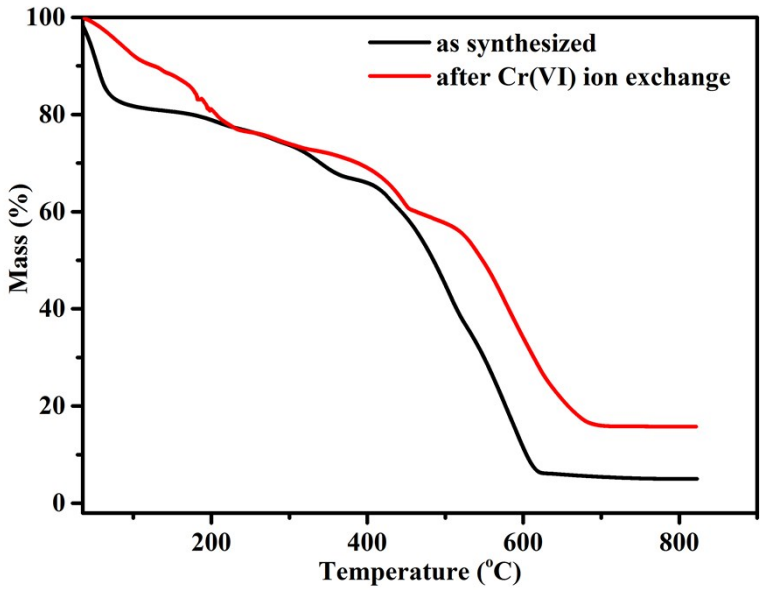


**Figure. S5** TGA curves of compound **2** under air atmosphere.

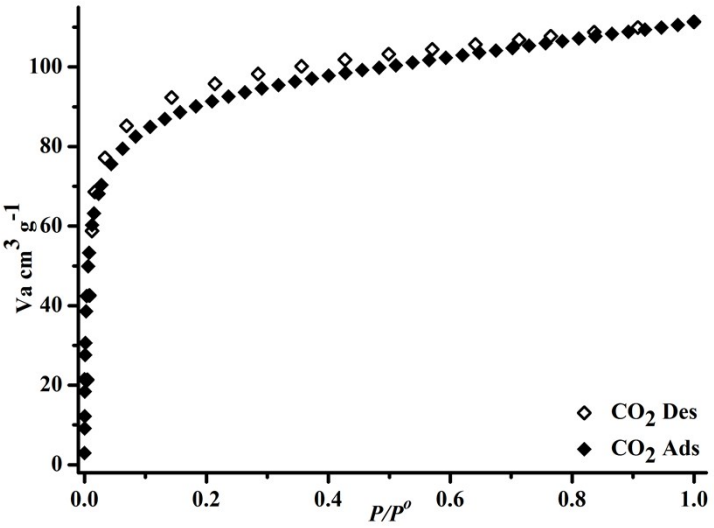


**Figure. S6** $CO_2$ sorption isotherms of compound **1** at 195 K.

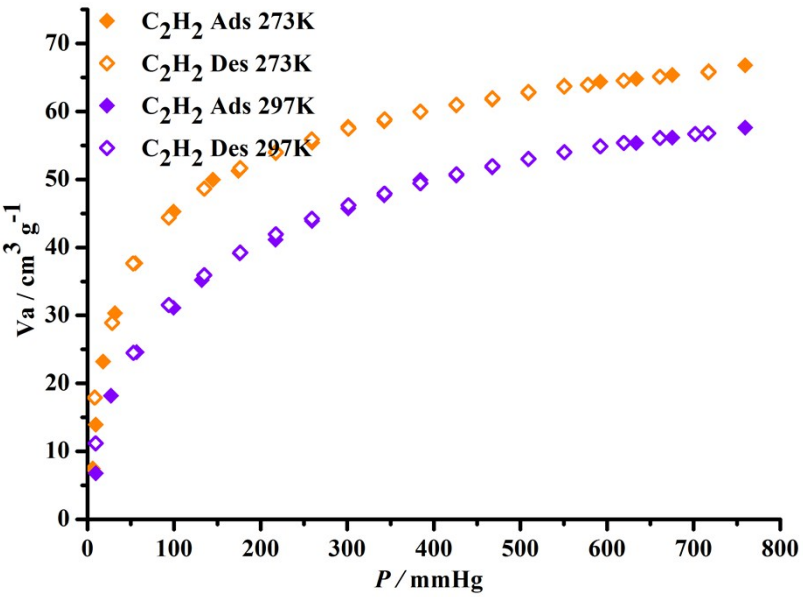


**Figure. S7** $C_2H_2$ sorption isotherms of compound **1** at 273 and 297 K, respectively.

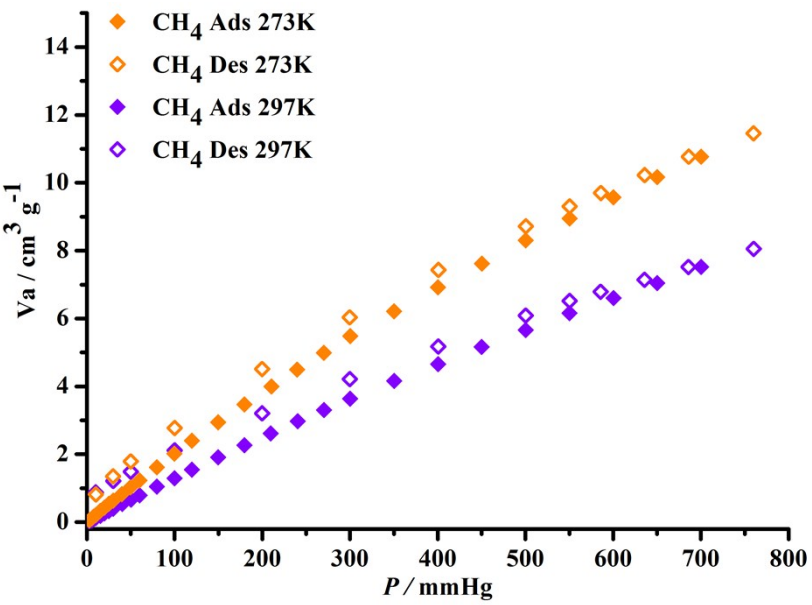


**Figure. S8** $CH_4$ sorption isotherms of compound **1** at 273 and 297 K, respectively.

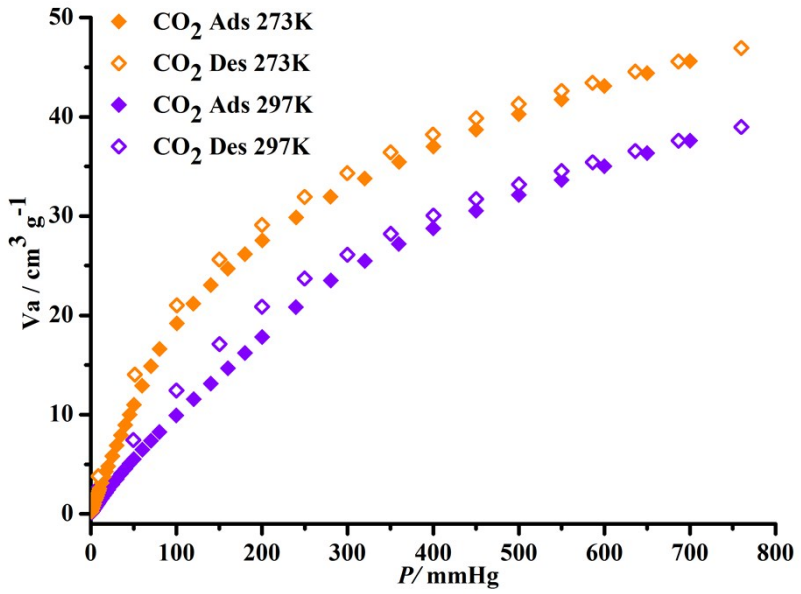


**Figure. S9** $CO_2$ sorption isotherms of compound **1** at 273 and 297 K, respectively.

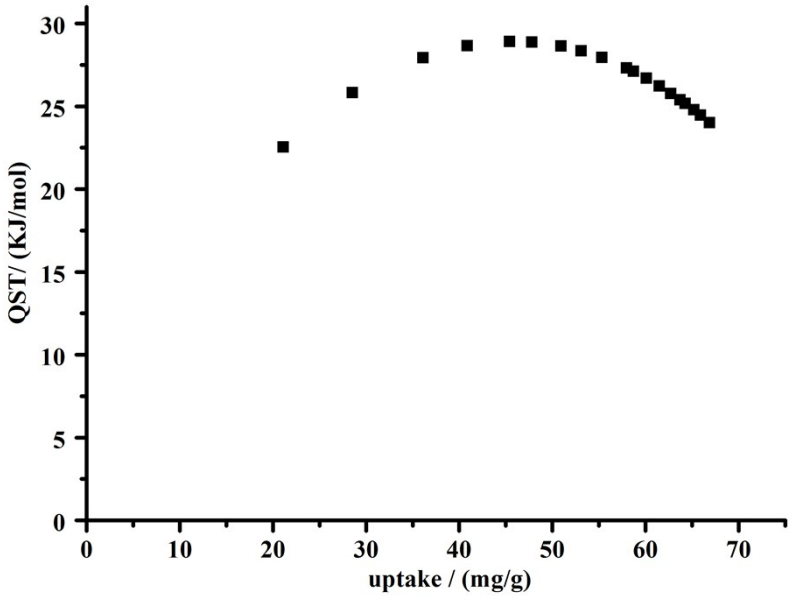


**Figure. S10** The enthalpies ($Q_{st,n=0}$/kJ mol$^{-1}$) of $C_2H_2$ on complex **1** at 273 and 297 K obtained from the virial equation.

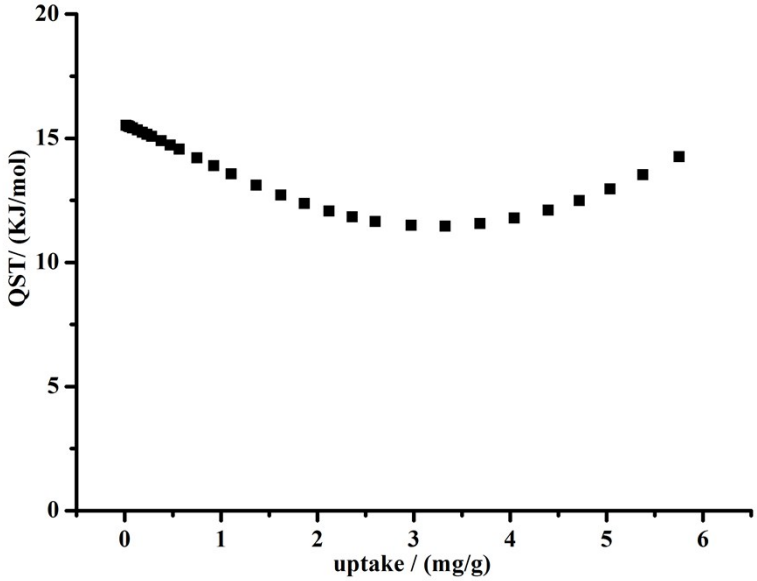


**Figure. S11** The enthalpies ($Q_{st,n=0}$/kJ mol$^{-1}$) of $CH_4$ on complex **1** at 273 and 297 K obtained from the virial equation.

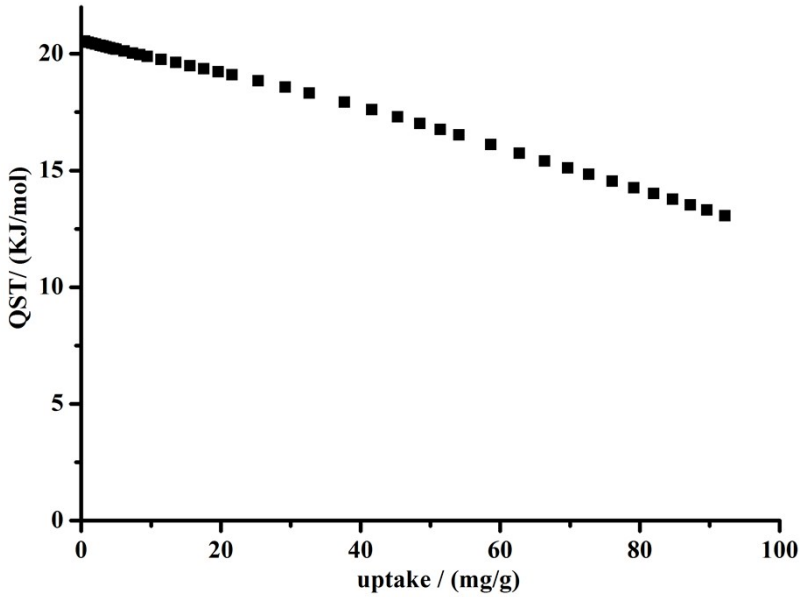


**Figure. S12** The enthalpies ($Q_{st,n=0}$/kJ $mol^{-1}$) of $CO_2$ on complex **1** at 273 and 297 K obtained from the virial equation.

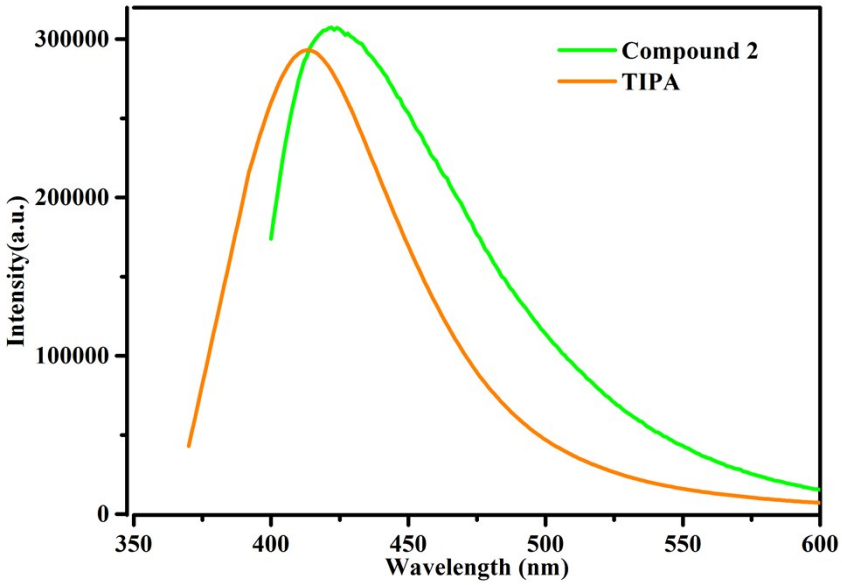


**Figure. S13** The fluorescence spectra for **2** and TIPA.

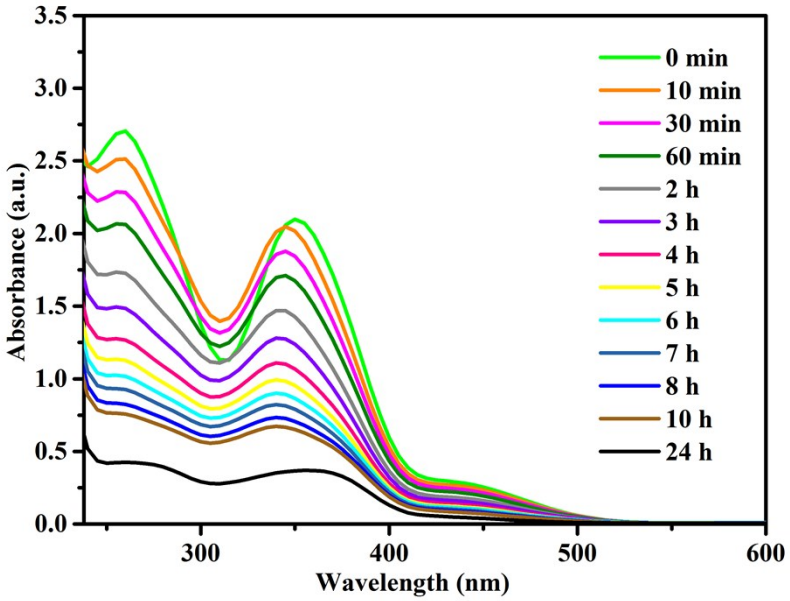


**Figure. S14** UV-vis adsorption spectra of chromate exchange solution on **2**, the exchange process carried out at $2\times10^{-3}$ mol $L^{-1}$, the Cr(VI) was thoroughly adsorbed after 24 h.

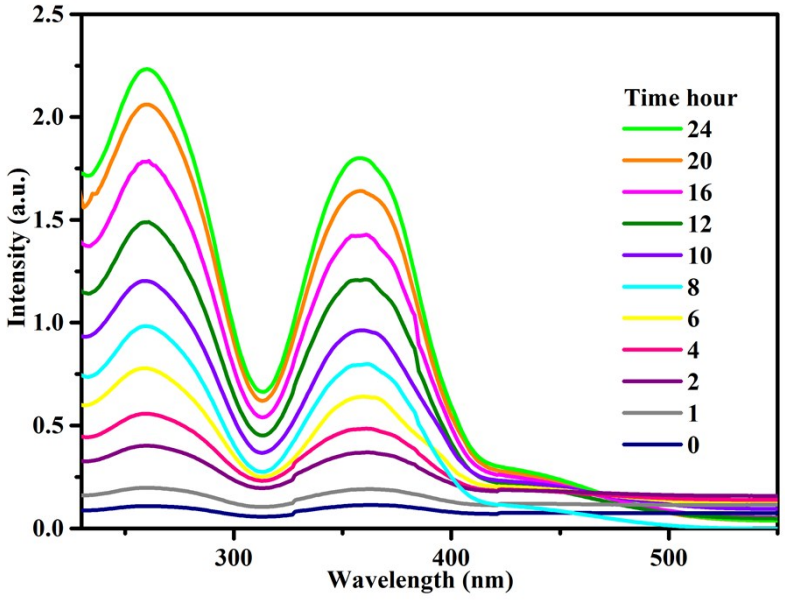


**Figure. S15** UV-vis adsorption spectra of chromate exchange solution on **2**, the exchange process carried out at $2\times10^{-3}$ mol $L^{-1}$, the Cr(VI) was thoroughly desorbed after 24 h.

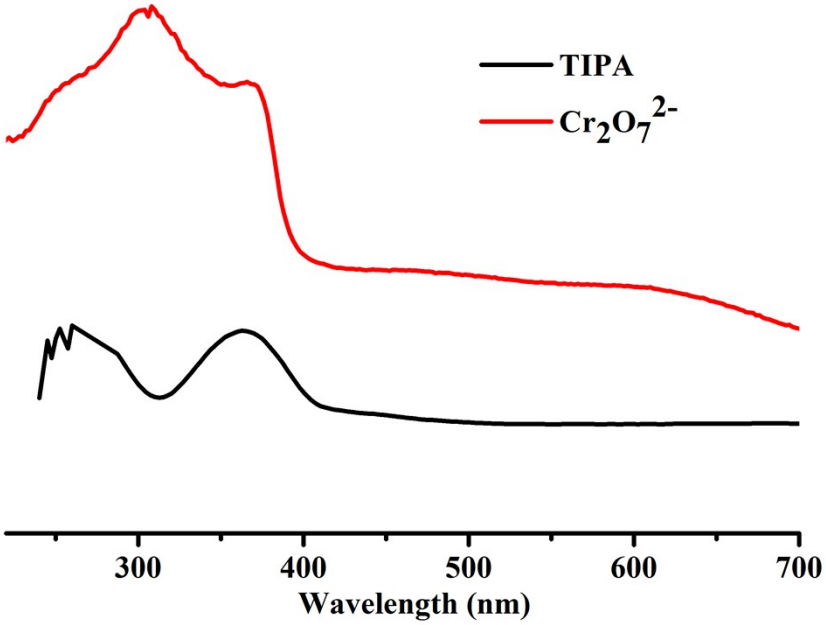


**Figure. S16** UV-vis absorption spectrum of TIPA and $Cr_2O_7^{2-}$ in aqueous solution.

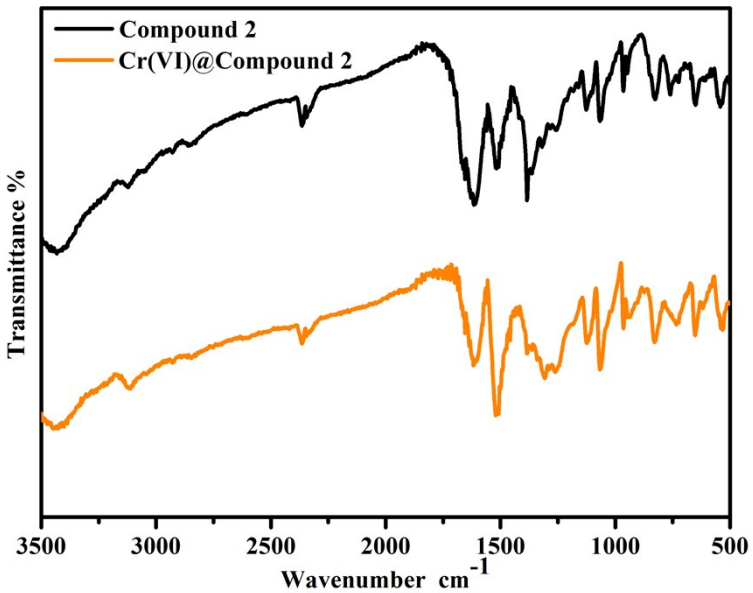


**Figure. S17** IR spectra for: (a) as-synthesized **2** (black curve); (b) **2** containing $Cr_2O_7^{2-}$ obtained in a $2\times10^{-3}$ mol $L^{-1}$ $K_2Cr_2O_7$ aqueous solution for 72 hours. The peaks of $ClO_4^-$ significantly reduced, even disappeared, indicating that the $ClO_4^-$ ions were replaced by $Cr_2O_7^{2-}$ anion ions (orange curve).

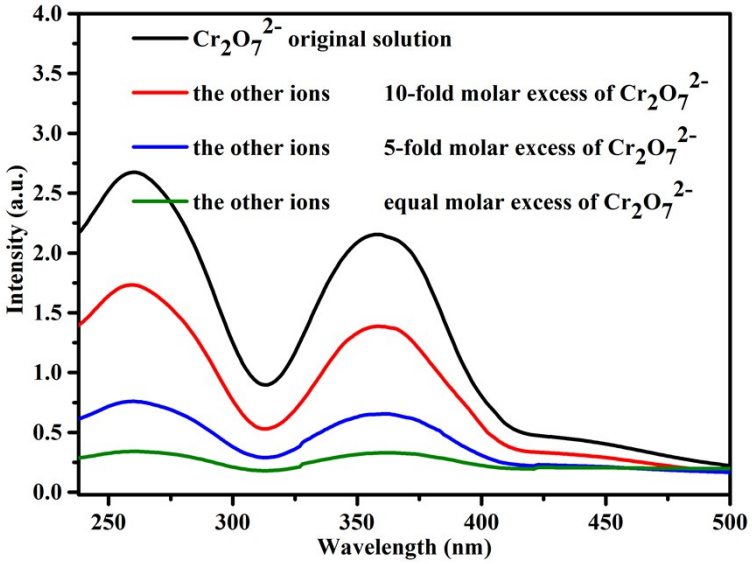


**Figure. 18** The UV-vis absorbance spectra of $Cr_2O_7^{2-}$ on the selective trapping of **1**. a) The $Cr_2O_7^{2-}$ UV-vis absorbance spectra of the mixed solution containing $Cl^-$, $Br^-$, $NO_3^-$ equal-fold molar excess of $Cr_2O_7^{2-}$ after 24 hours (green line); b) The $Cr_2O_7^{2-}$ UV-vis absorbance spectra of the mixed solution containing $Cl^-$, $Br^-$, $NO_3^-$ 5-fold molar excess of $Cr_2O_7^{2-}$ after 24 hours (blue line); c) The $Cr_2O_7^{2-}$ UV-vis absorbance spectra of the mixed solution containing $Cl^-$, $Br^-$, $NO_3^-$, $SO_4^{2-}$, $ClO_4^-$ and $BF_4^-$ 10-fold molar excess of $Cr_2O_7^{2-}$ after 24 hours (red line); The $Cr_2O_7^{2-}$ UV-vis absorbance spectra of $10\times10^{-3}$ mol $L^{-1}$ $Cr_2O_7^{2-}$ solution (black line).

**Table. S1** Comparison of chromate detection limits among MOF.

| MOFs | Detection limit | Ref. |
|---|---|---|
| $[Eu_7(mtb)_5(H_2O)_{16}]\cdot NO_3\cdot 8DMA\cdot 18H_2O$ | 0.56 ppb | 1 |
| $Eu^{3+}$@MIL-124 | 7.8 ppb | 2 |
| $[Cd(TIPA)](ClO_4^-)_2$ | 8.0 ppb | This work |
| $[Ag(m3\text{-}abtz)]\cdot(NO_3)\cdot(0.125H_2O)$ | 9.88 ppb | 3 |
| $[Zn_7(TPPE)_2(SO_4^{2-})_7](DMF\cdot H_2O)$ | 27.0 ppb | 4 |
| $[Eu_2L1.5(H2O)2EtOH]\cdot DMF$ | 0.52 ppm | 5 |
| [Zn(btz)]n | 0.52 ppm | 6 |
| $[Ln(Hpzbc)_2(NO_3)]\cdot H_2O$ | 1.04 ppm | 7 |

**References**


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