

## Supporting Information

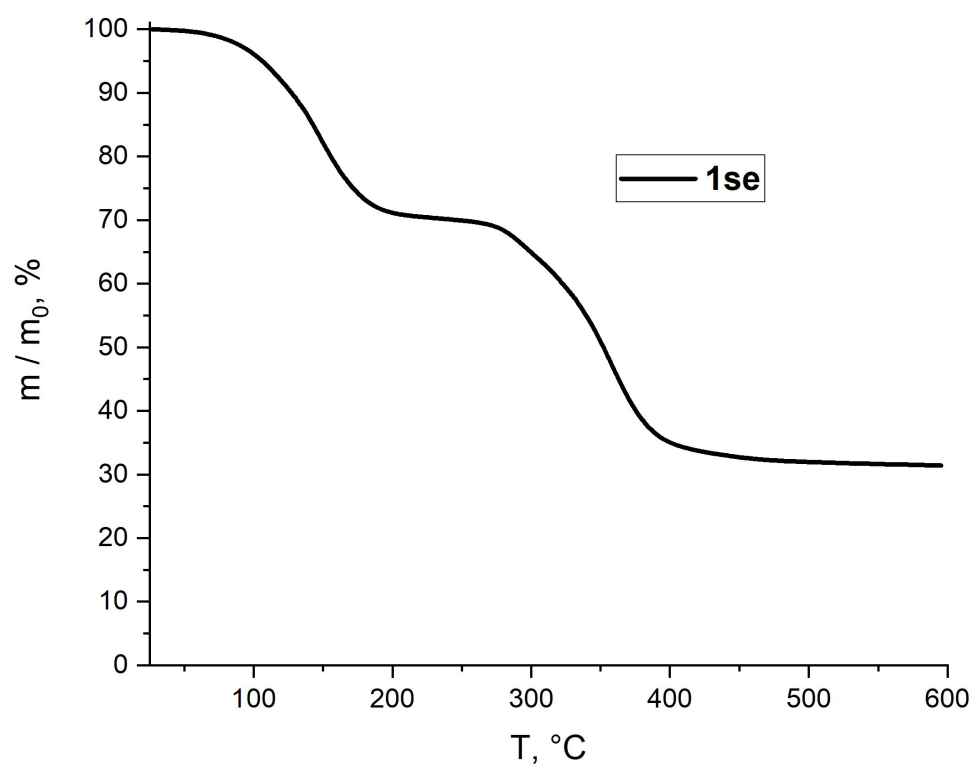
### **A Selenium Functionalized Metal-Organic Framework for Enhanced CO<sub>2</sub> Volumetric Uptake and Sorption Selectivity**

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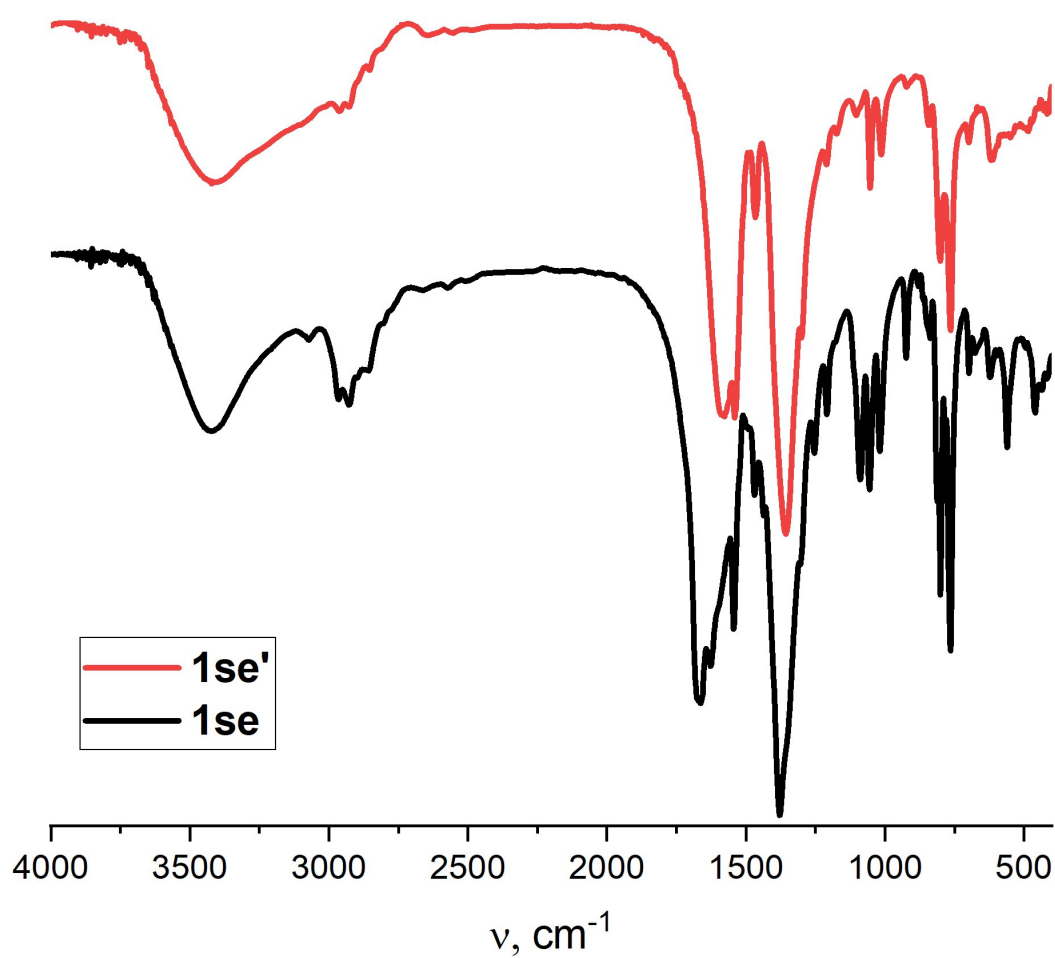
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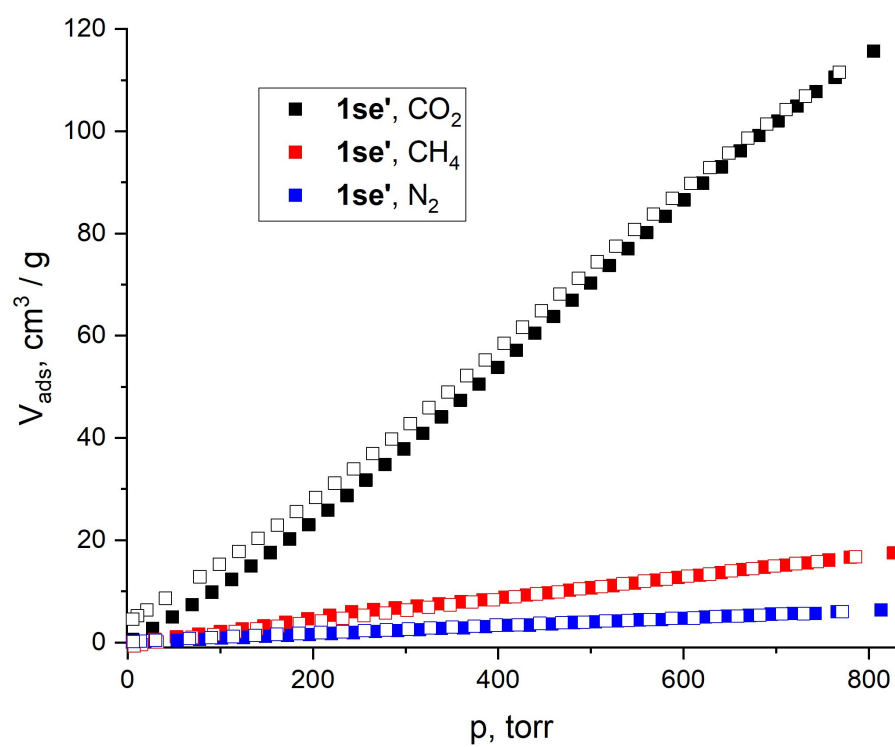
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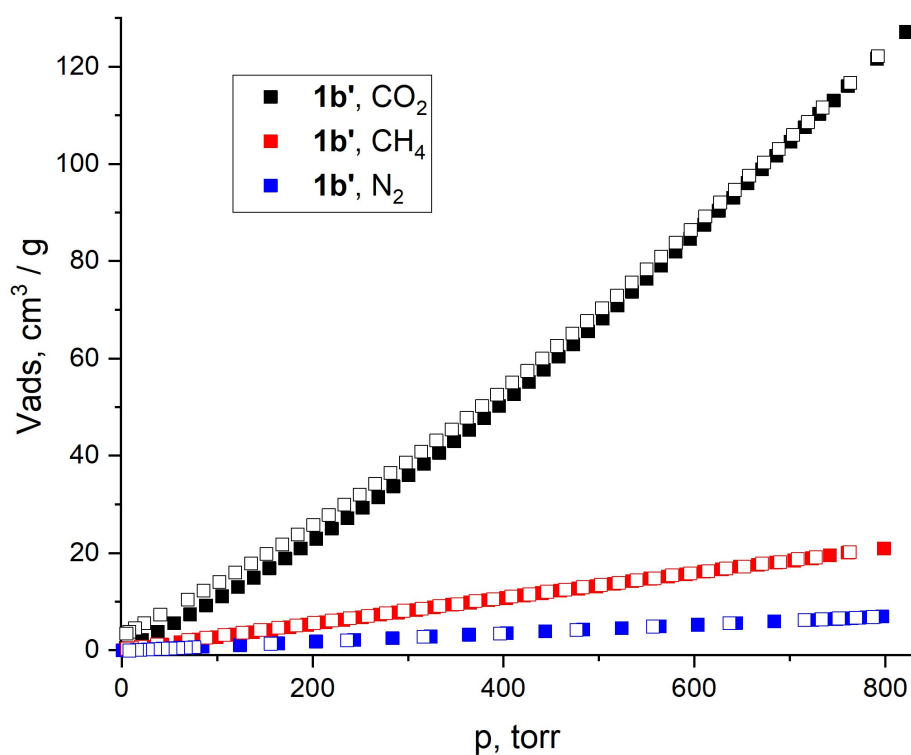
**Figure S1.** TG plot of the synthesized **1se** (black line).



**Figure S2.** IR spectra of the synthesized **1se** (black line) and activated **1se'** (red line).



(a)



(b)

**Figure S3.** Gravimetric  $\text{CO}_2$ ,  $\text{CH}_4$  and  $\text{N}_2$  adsorption and desorption isotherms for **1se'** (a) and **1b'** (b) at 273 K.

**Table S1.** Textural characteristics of **1se'**.

Model	$A_{\text{BET}}$ ( $\text{m}^2 \cdot \text{g}^{-1}$ )		Model	$V_{\text{pore}}$ ( $\text{cm}^3 \cdot \text{g}^{-1}$ )
Langmuir	1570		Gourvich $\text{N}_2$ adsorption at $p/p_0 = 0.95$	0.57
BET	1504		DFT model	0.42
DFT	1352			

**Table S2.** The comparison of porosities between the isorecticular **1t'**, **1se'** and **1b'**.

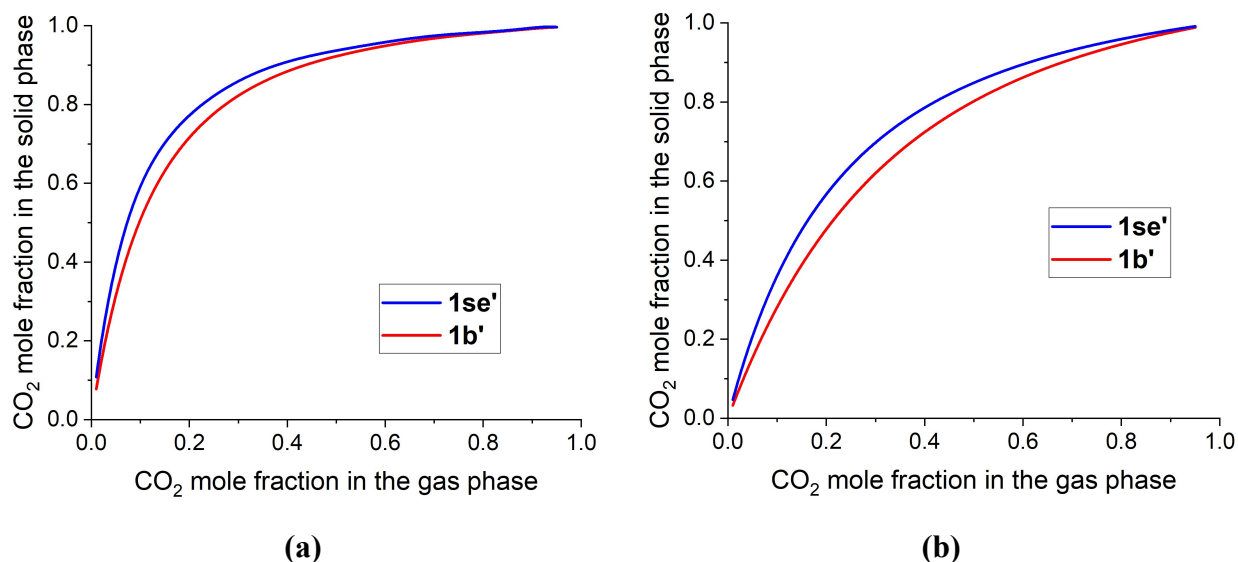
Compound	aperture, $\text{\AA}^2$ (from the X-ray data)	$V_{\text{pore}}$ , $\text{cm}^3 \cdot \text{g}^{-1}$ (from the X-ray data)	$V_{\text{pore}}$ , $\text{cm}^3 \cdot \text{cm}^{-3}$ (experimental)
<b>1t'</b> [from Ref. 30]	5 x 8	0.68	0.64
<b>1se'</b>	5 x 8	0.55	0.60
<b>1b'</b>	6 x 8	0.75	0.62

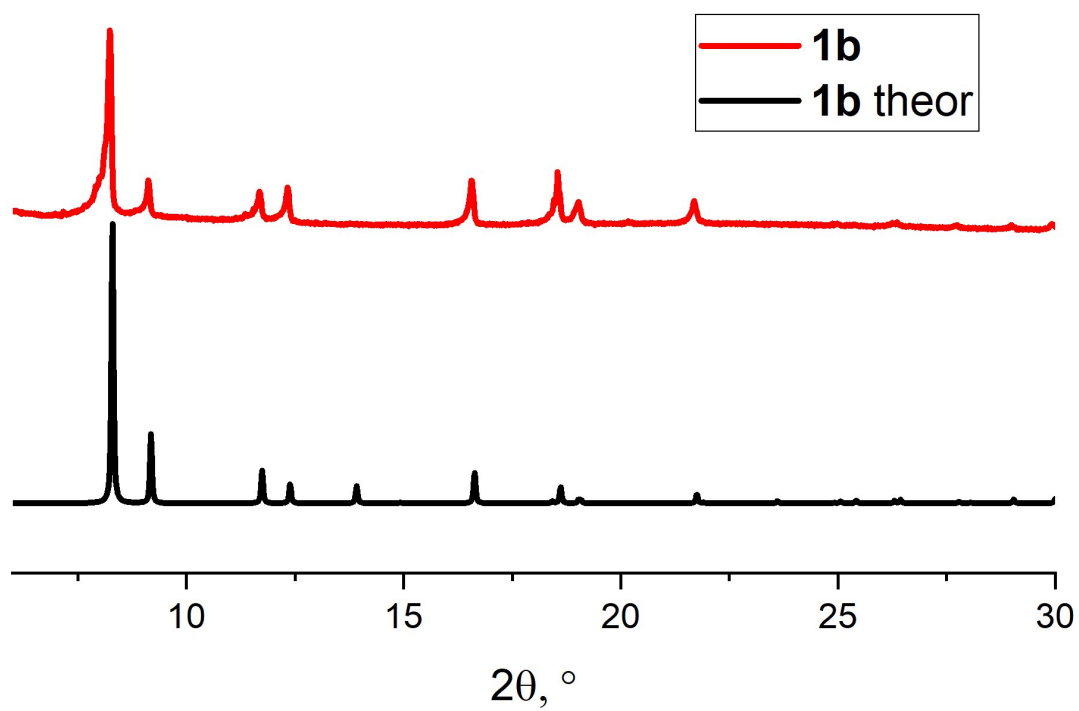
**Table S3.** Calculated virial coefficients for  $\text{CO}_2$  isosteric heats of adsorption and virial Henry constants determination.

MOF	Virial coefficients for $\text{CO}_2$ (Standard Error)			
	$A_0$	$A_1$	$A_2$	$B_0$
<b>1se'</b>	-2391.36 (0.29 %)	-43720.52 (1.5 %)	4892414 (2.7 %)	14.45192 (0.16 %)
<b>1b'</b>	-2290,35 (1.1 %)	-24036,42 (3.0 %)	-	14,084 (0.61 %)

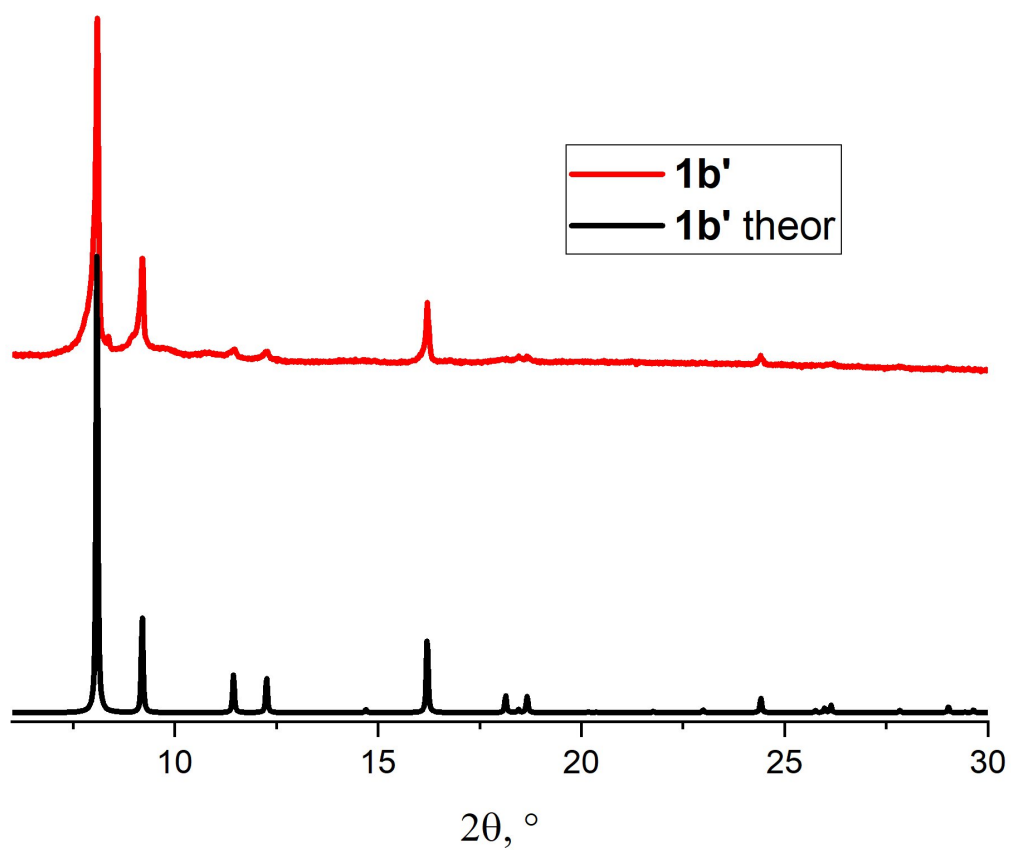
**Table S4.** Fit parameters of the isotherms for IAST calculations.

Gas	Parameters (Standard Error)	
	<b>1se'</b>	<b>1b'</b>
CO <sub>2</sub>	(273K) Freundlich isotherm o = 0,00484 (0.31 %) t = 0,88159 (0.70 %)	(273K) Freundlich isotherm o = 0,00535 (0.19 %) t = 0,80858 (0.60 %)
	(298 K) Freundlich isotherm o = 0,00199 (0.15 %) t = 0,89456 (0.34 %)	(298 K) Freundlich isotherm o = 0,00203 (0.23 %) t = 0,91471 (0.56 %)
CH <sub>4</sub>	(273K) Henry isotherm k = 0,0007040 (0.11 %)	(273K) Henry isotherm k = 0,0008734 (0.13 %)
N <sub>2</sub>	(273K) Henry isotherm k = 0,0002607 (0.24 %)	(273K) Henry isotherm k = 0,0002862(0.15 %)

**Figure S4.** Dependences of adsorbed CO<sub>2</sub> mole fraction in MOF on CO<sub>2</sub> mole fraction in gas phase for binary gas mixtures: CO<sub>2</sub>/N<sub>2</sub> **(a)** and CO<sub>2</sub>/CH<sub>4</sub> **(b)** at 273K and total P = 1 bar.



**Figure S5.** PXRD pattern of the synthesized compound **1b** (red line) compared to the theoretical one (black line).



**Figure S6.** PXRD pattern of the synthesized compound **1b'** (red line) compared to the theoretical one for **1b'** (black line).