Supporting Information

A Perfluorinated Covalent Triazine-based Framework for Highly Selective and Water-tolerant CO$_2$ Capture

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CO$_2$/$N_2$ selectivity calculation by the ideal adsorption solution theory (IAST)
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**CO₂/N₂ selectivity calculation by the ideal adsorption solution theory (IAST)**

The experimental adsorption isotherms were firstly fitted using the single-site Langmuir model:

\[ q_i = q_{i,sat} \frac{b_i p_i}{1 + b_i p_i} \]

where

- \( b_i \) = Langmuir constant, Pa\(^{-1}\)
- \( p_i \) = bulk gas phase pressure of species i, Pa
- \( q_i \) = molar loading of species i, mmol g\(^{-1}\)
- \( q_{i,sat} \) = saturation capacity of species i, mmol g\(^{-1}\)

According to the ideal adsorption solution theory (IAST) proposed by Myers and Prausnitz,\(^1\) the adsorption selectivity, \( S_{ads} \), for binary mixtures of 1 and 2, is defined as

\[ S_{ads} = \frac{q_1 / q_2}{p_1 / p_2} \]

In this study, selectivity calculations were carried out for CO₂/N₂ binary mixtures with N₂ molar fraction ranging from 70% to 100%, which is typical composition range of flue gases.