Title:	In-Depth Experimental and Computational Investigations for Remarkable Gas/Vapor Sorption, Selectivity, and Affinity by a Porous Nitrogen-Rich Covalent Organic Framework
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Abstract:	Porous nitrogen-rich covalent organic frameworks (COFs) are most challenging materials for selective CO2 capture, separation, and conversion for a substantive impact on the environment and clean energy application. On the other hand, separation of industrial cyclic congeners (benzene/cyclohexane) by the host–guest interaction through π-electron-rich and -deficient centers in a COF is the key. On the basis of the strategic design, a triazine-based benz-bis(imidazole)-bridged COF (TBICOF) has been synthesized under polycondensation conditions and structurally characterized by various analytical techniques. Because of the presence of a benz-bis(imidazole) ring, TBICOF exhibits permanent stability and porosity in the presence of acid and base monitored by the wide-angle X-ray pattern and N2 sorption studies. The enhanced CO2 uptake of 377.14 cm3 g–1 (73.4 wt %) at 195 K confirms its high affinity toward the framework. CO2 sorption is highly selective over N2 and CH4 because of very strong interactions between CO2 and triazine and benz-bis(imidazole)-functionalized pore walls of TBICOF as clearly evident from the isosteric heat of adsorption and ideal adsorbed solution theory calculation, which is higher than other reported functionalized metal–organic frameworks or COFs. Interestingly, TBICOF also behaves as a heterogeneous organocatalyst for chemical fixation of CO2 into cyclic carbonates under ambient conditions. The π-electron-deficient triazine and benz-bis(imidazole) moieties have been utilized for selective sorption and separation of benzene (641.9 cm3 g–1) over cyclohexane (186.2 cm3 g–1). Computational studies based on density functional theory and grand canonical Monte Carlo molecular simulations further support the selectivity of CO2 (over N2 and CH4) and benzene (over cyclohexane).
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