Electronic Supplementary Material (ESI) for Dalton Transactions

Comparative study of structure, thermal stability and dielectric property for a ferroelectric MOF $[Sr(\mu\text{-}BDC)(DMF)]_\infty$ with its solvent-free framework

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Gas adsorption of 3

Figure S1a is the N_2 adsorption-desorption isotherms of **3** at 77 K under the low pressure (under 1 atm), which shows a reversible and hysteretic type-Π isotherm character. The Brunauer-Emment-Teller (BET) apparent surface areas were calculated as 5.9 $m^2 \cdot g^{-1}$ which is too small and the averaged pore width was calculated as ~50 Å (ref. Figure S1b). However, the single crystal structure studies revealed that the diameter for the maximum trigonal channel in **1** is 3.4 Å when the DMF molecules therein are removed. Thus, the pores with averaged width ~50 Å should be the clearance gaps between adjacent particles.

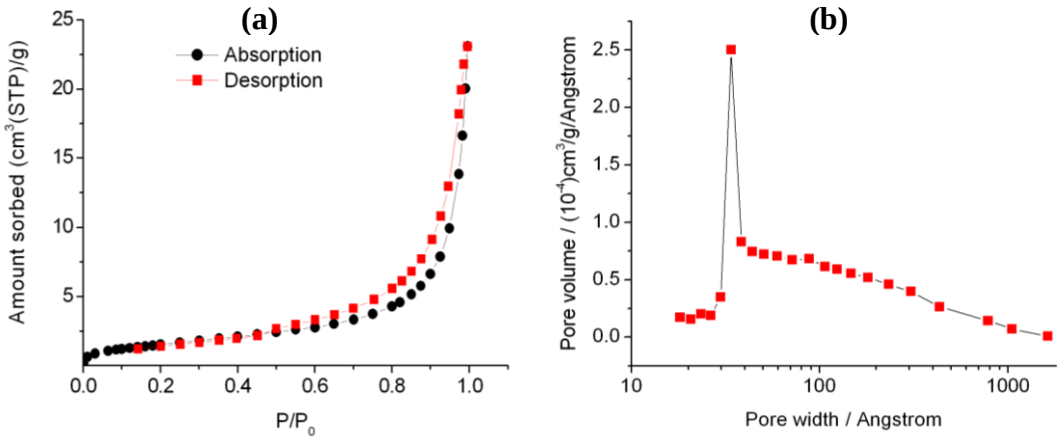

Figure S1 (a) The isotherm for the adsorption and desorption of N_2 on activated **3** at 77 K and (b) pore size distribution.

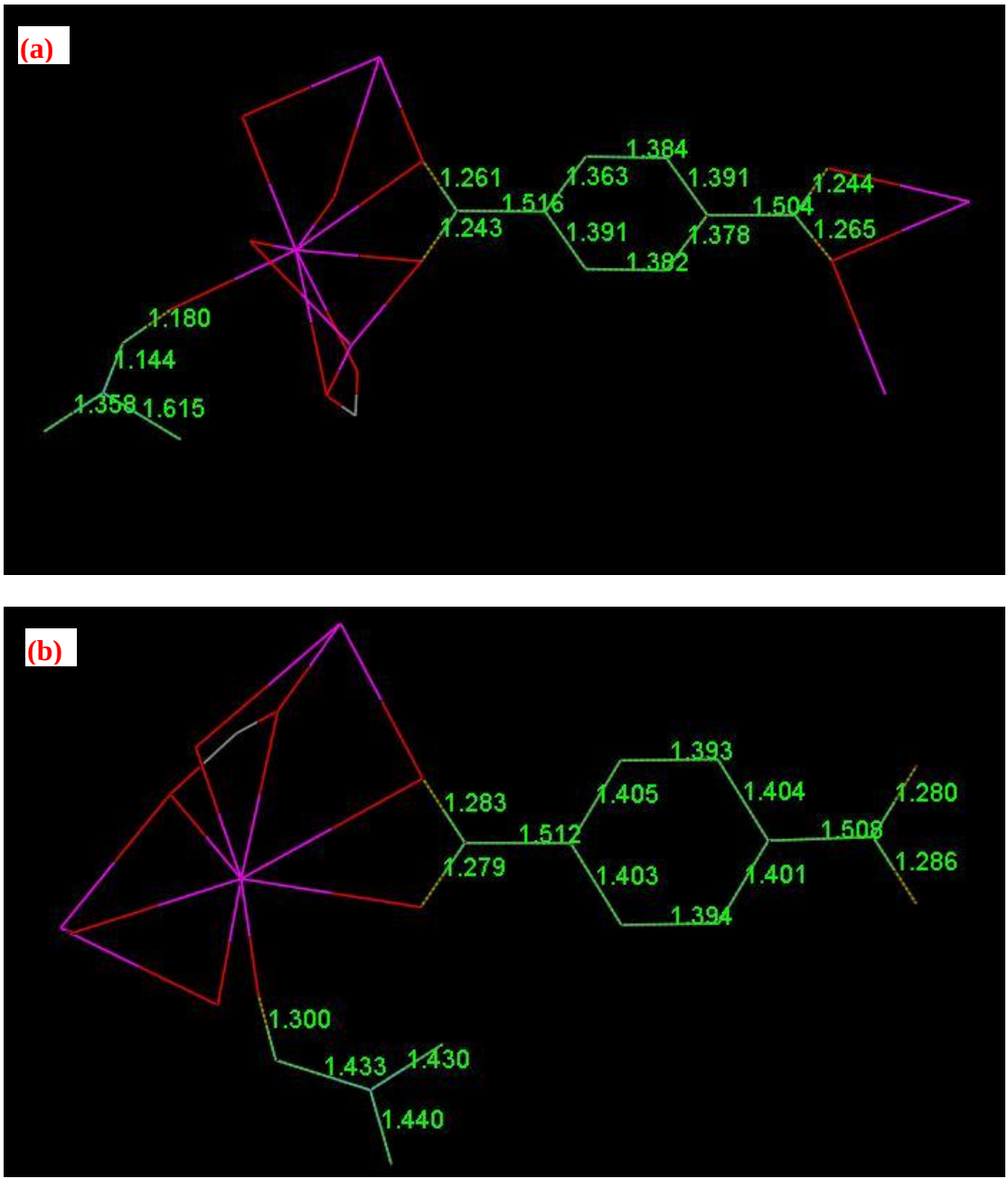

Figure S2 Bond distances in BDC^{2-} and DMF moieties obtained from (a) X-ray single crystal structure analysis at 293 K and (b) crystal structure optimization using the ***Materials Studio*** program.