Supplementary Material (ESI) for Journal of Material Chemistry

Cyclotricatechylene based porous crystalline material: synthesis and applications in gas storage

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1. ^{1}H NMR spectrum of compound BE

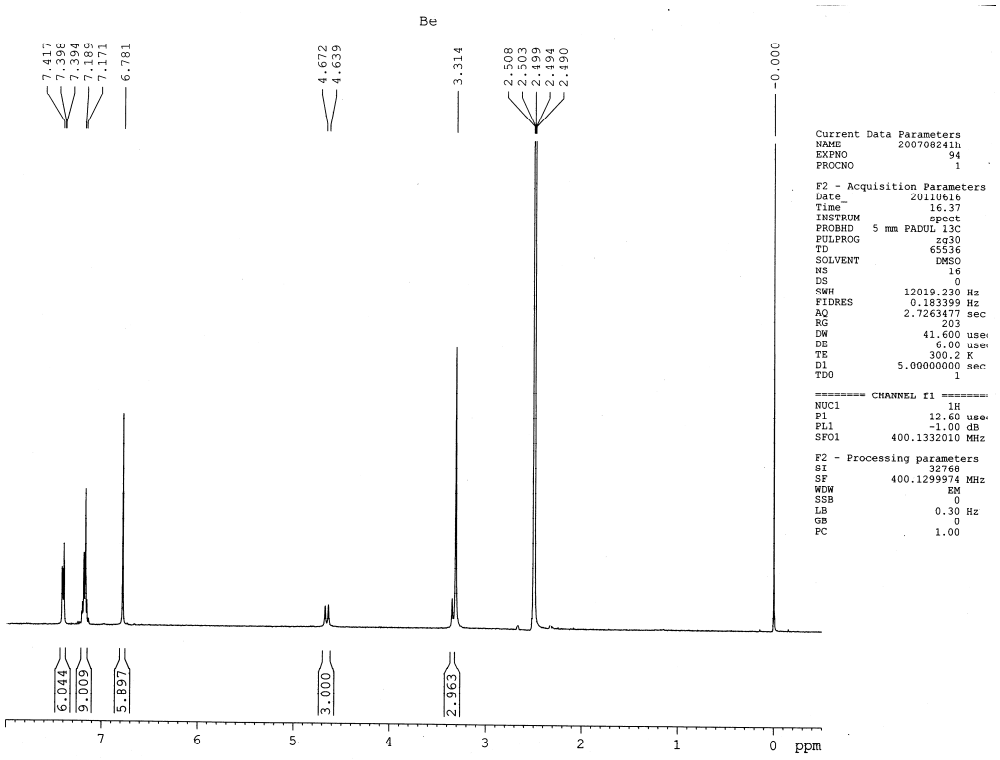

Fig. S1 ^{1}H NMR spectrum of compound **BE**

2. FT-IR spectral profiles

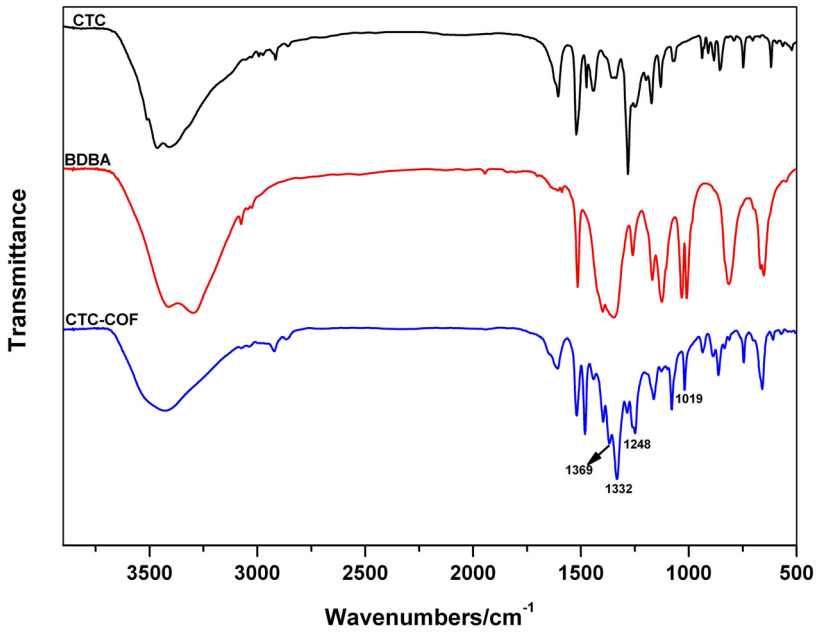

Fig. S2 FT-IR spectra of CTC (black), BDBA (red) and **CTC-COF** (blue).

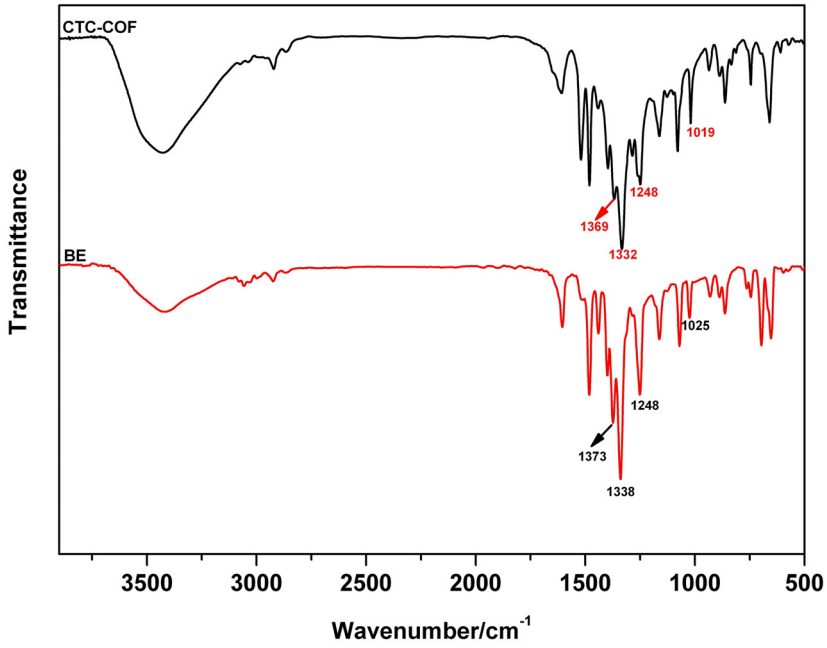

Fig. S3 FT-IR spectra of **CTC-COF** (blue) and **BE** (red)

Table S1: Peak assignment for FT-IR spectrum of **CTC-COF**. Notes are provided to correlate the spectra and compare with that of model compound **BE**.

Peak (cm^{-1})	**Assignment and Notes**
3340.8 (m)	O-H stretch from the end $B(OH)_2$ or OH groups
3065.6 (w)	Aromatic C-H stretch
2986.5 (w)	C-H stretching from aromatic phenyl groups
2920.1 (w)	
2863.5 (w)	
1616.5(w)	C=C stretch for aromatics
1521.0 (m)	Phenyl ring C=C vibrational mode
1480.8 (m)	C=C vibrational modes for CTC units
1369.3 (s)	B-O stretch, characteristic band for boroxoles, in BE it is 1372.7
1332.6 (s)	B-O stretch, in BE is 1337.8
1248.7 (s)	C-O characteristic stretch for boroxoles, in be it is 1247.9
1161.5 (m);	C-H in plane bending modes

1078.6 (m)	
1019.2 (m)	B-C stretch, in BE is 1025.1
861.3 (m)	C-H out of plane bands for *p*-substituted aromatic
833.1 (m)	
807.7 (w)	C-H out of plane bending modes
744.8 (m)	
659.7 (m)	
610.8 (w)	

3. Spectra of ^{11}B MAS NMR and ^{13}C CP-MAS NMR

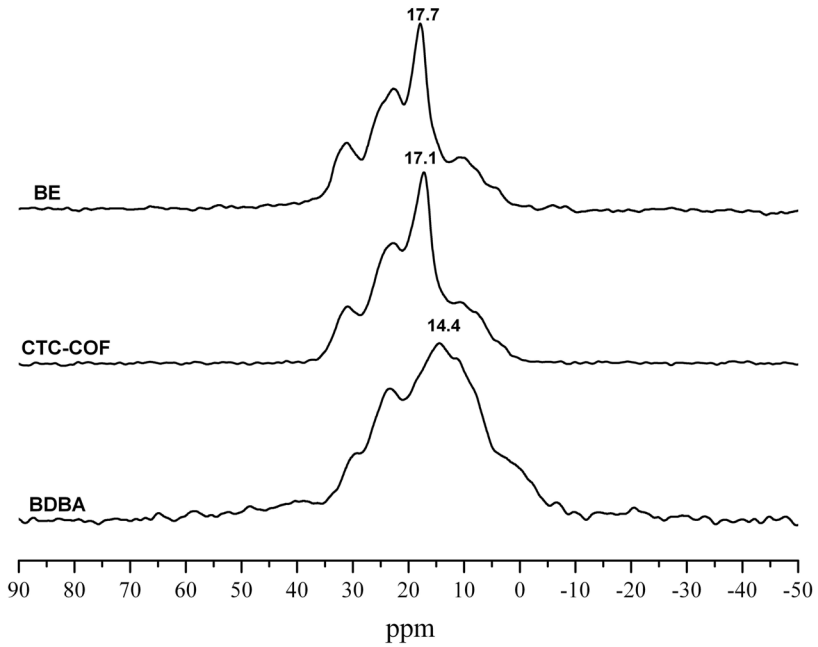

Fig. S4 ^{11}B MAS NMR spectra of BE, **CTC-COF** and BDBA.

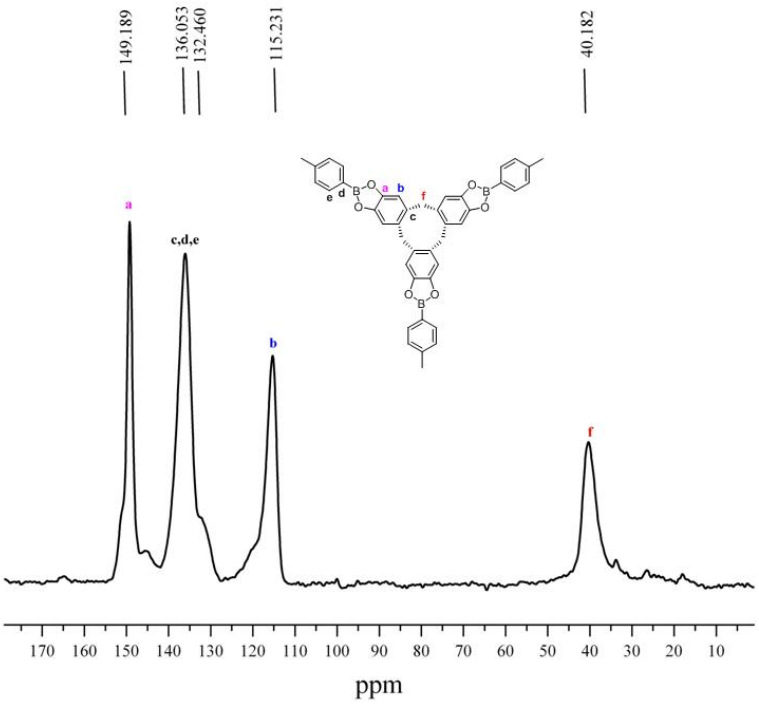

Fig. S5 ^{13}C CP-MAS NMR spectrum of **CTC-COF**.

4. Thermal gravimetric analysis (TGA)

Powder-like sample of **CTC-COF** was heated at a constant rate of 10 ºC /min under nitrogen from 25 ºC to 900 ºC. As shown in **Fig. S6**, guest molecules are steadily lost upon heating, the framework is stable up to 520 ºC.

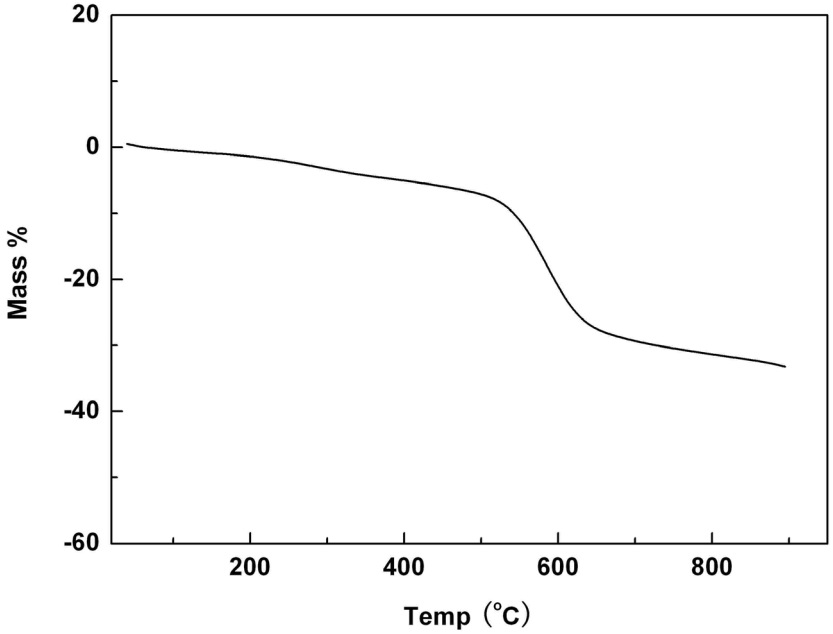

Fig. S6 TGA measurement of **CTC-COF.**

5. BET plot of the nitrogen adsorption measurement

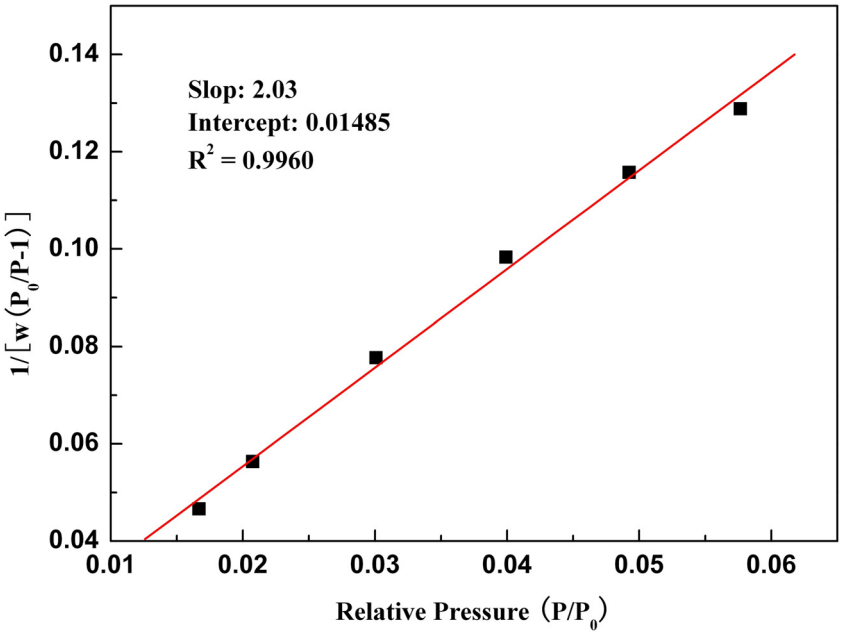

Fig. S7: BET plot of **CTC-COF**.

6. Simulation and calculation of crystal packing

Table S2: Refined crystal data

Formula	$C_{60}H_{36}B_6O_{12}$
Formula weight	1013.78
Crystal system	Trigonal
Space group	*P*-3*m*1
Unit cell dimensions	$a = b = 25.0645$ Å $c = 4.2989$ Å
Cell volume	2338.87 Å^3

Table S3: Fractional atomic coordinates

Atom	x	y	z
C1	0.55638	0.38826	1.20405
C2	0.54748	0.34038	-3.98469
C3	0.59625	0.34775	1.82702
C4	0.46388	0.44021	1.89250
C5	0.58635	0.29317	0.63838
C6	0.52400	0.47600	0.78145
B1	0.54943	0.45057	0.53624
O1	0.51685	0.39176	1.40862
H1	0.50315	0.29735	-3.98872
H2	0.53847	0.26923	0.55038
H3	0.61512	0.30756	0.42729
H4	0.43562	0.39304	1.80528

Simulation of crystal packing

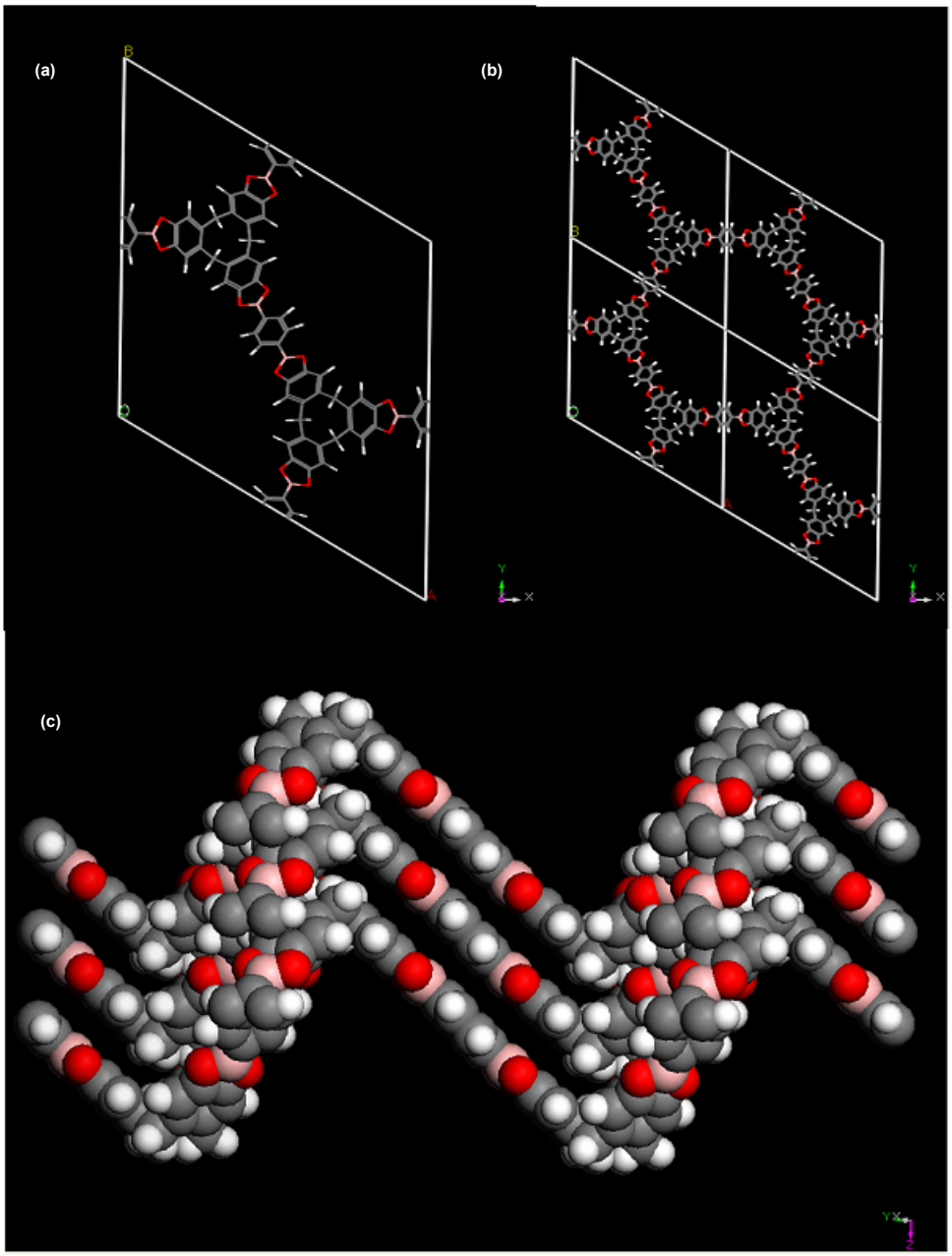

Fig. S8: Simulation of crystal lattice of the unit cell calculated in an eclipsed arrangement: a) Top view in AB plane, b) crystal structure of four unit cells in AB plane, c) side view of the eclipsed crystal lattice packing of **CTC-COF**.

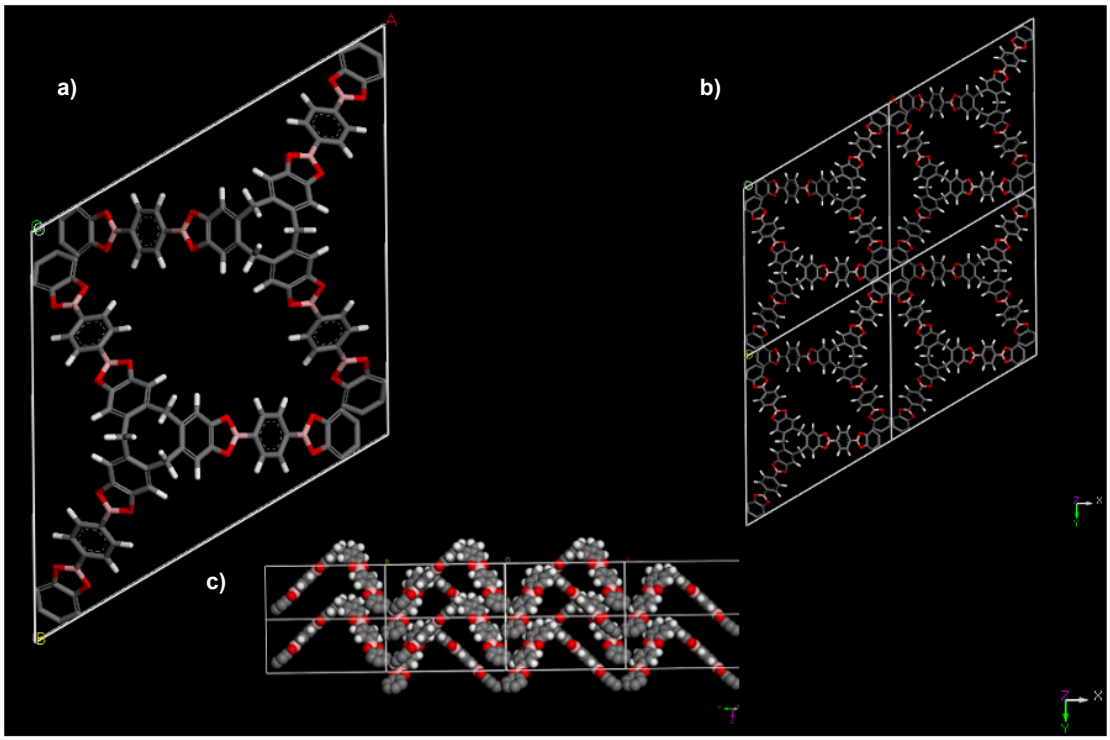

Fig. S9: Simulation of crystal lattice of the unit cell calculated in the staggered arrangement: a) Top view in AB plane, b) crystal structure of four unit cells in AB plane, c) side view of the eclipsed crystal lattice packing of **CTC-COF**.