Supporting Information

Covalent Triazine Frameworks prepared from 1,3,5-tricyanobenzene

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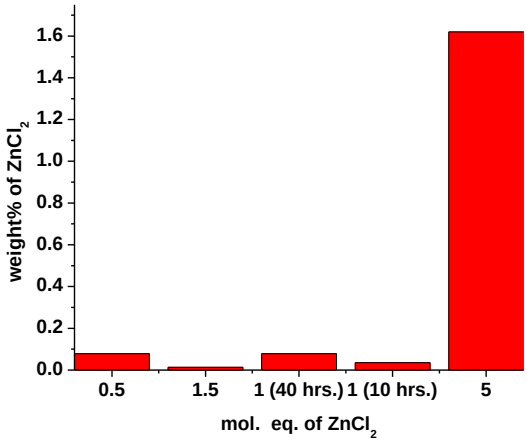

Figure S1: ICP measurements of materials prepared from different mol. eq. of $ZnCl_2$.

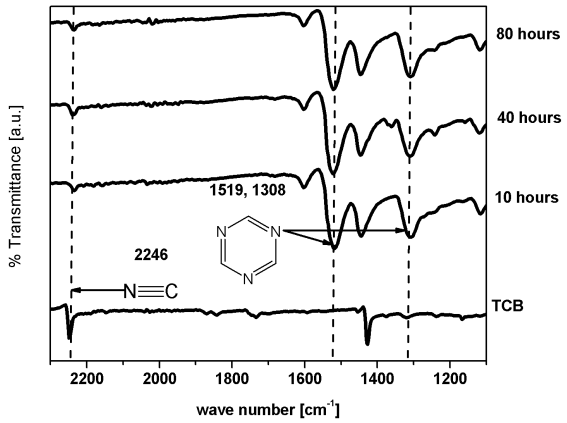

Figure S2: FT-IR spectra of 1,3,5-tricyanobenzene (TCB) and CTF-0 frameworks synthesized with 1 mol. eq. $ZnCl_2$ at 400 °C and various reaction times.

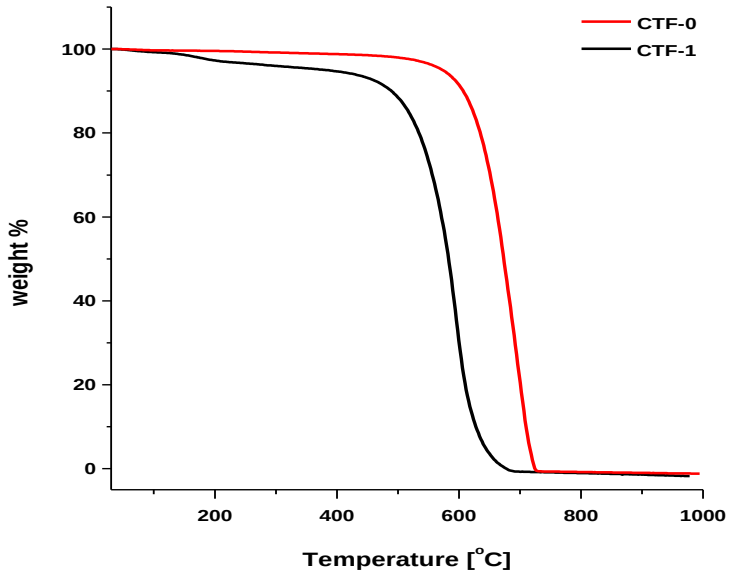

Figure S3: Thermogravimetric analysis of a representative framework heated under oxygen atmosphere (heating rate of 10 °K.min^{-1}). The TGA plot of CTF-1 (black curve) is given for comparison[S1].

Table S1: Elemental analysis results

Entry	$ZnCl_2$ (mol eq.)	Time (h)	Temp (°C)	% Eyperimental			% Theory		
				% C	% H	% N	% C	% H	% N
1	0.5	40	400	66.4	2.7	22.1	70.6	2.0	27.4
2	1	10	400	66.4	2.6	22.1	70.6	2.0	27.4
3	1	40	400	65.6	2.4	22.3	70.6	2.0	27.4
4	1.5	40	400	65.9	2.5	22.0	70.6	2.0	27.4
5	5	20/20	400/600	63.5	2.7	14.8	70.6	2.0	27.4
6[a]	1	40	400	72.8	3.2	19.3	75.0	3.1	21.9

[a] This entry is the original CTF-1 framework synthesized from 1 mol. eq. of $ZnCl_2$ at 400 °C for 40 hours.[S1]

Structural modeling: A hexagonal unit cell (P-6) was chosen based on powder diffraction pattern with parameters a, b = 7.3 Å and c = 3.3 Å. Computer modeling of the network and XRD peaks simulation was carried out using Materials Studio 4.3 software.

Table S2: Fractional atomic coordinates of CTF-0 framework calculated from Material Studio Software.

CTF-0 framework			
Hexagonal, P-6 a = b = 7.3 Å, c = 3.3 Å			
atoms			
C1	0.11222267	0.55611362	0.50000000
C2	0.22337626	0.77662566	0.50000000
C3	0.55947788	0.44051211	0.50000000
N1	0.45309503	0.22655101	0.50000000

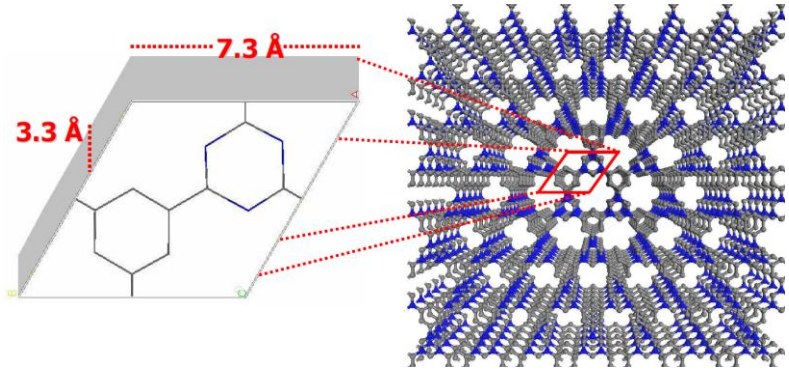

Figure S4: Stacking of the eclipsed CTF-0 framework with P-6 hexagonal unit cell of described dimensions.

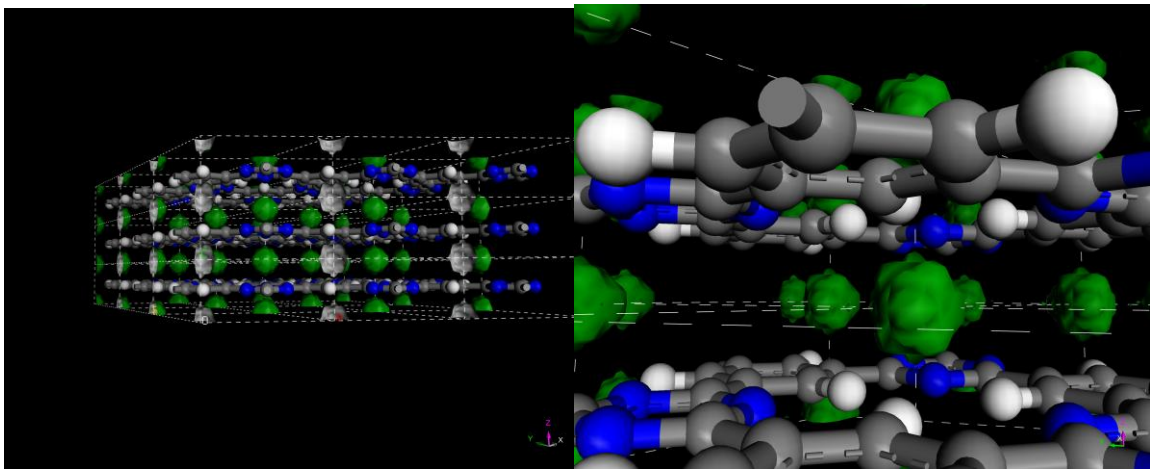

Figure S5: Stacking of the eclipsed CTF-0 framework with a Connolly surface (green, 1.65 Å radius) showing the non-connected pores of the ideal structure.

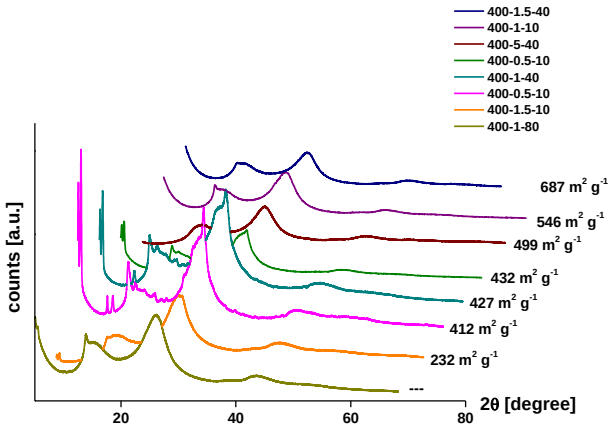

Figure S6: PXRD pattern of CTF-0s prepared at 400 °C with different monomer/$ZnCl_2$ ratios and reaction times.

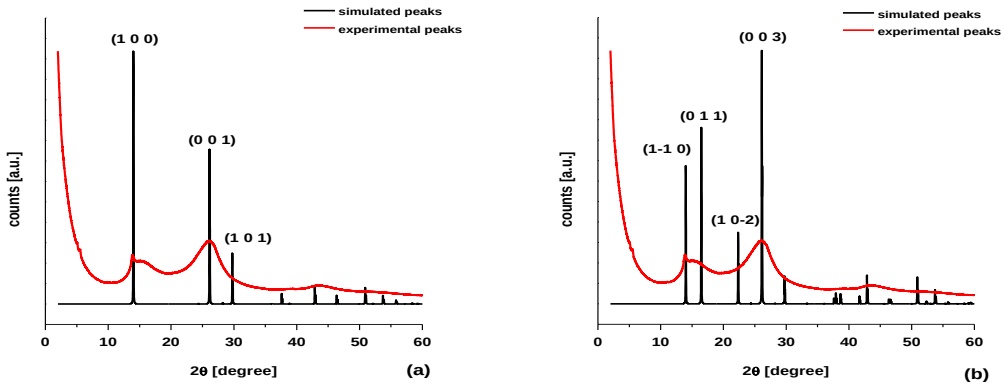

Figure S7. Experimental PXRD pattern of CTF-0-400-80-1 along with the simulated patterns for CTF-0 in eclipsed (a) and staggered (b) packing.

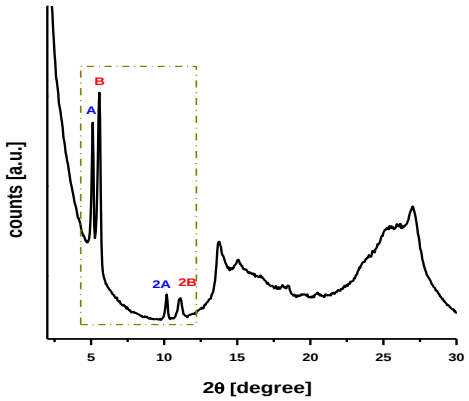

Figure S8: XRD diffractogram of CTF-0-400-40-1 showing additional sharp diffraction peaks at low angles.

Table S3: Peak positions and corresponding distances from Figure S1 based on copper K-α X-rays radiation with λ = 0.154 nm.

Peaks	2θ (degree)	Distance (nm)
A	5.1	3.5
2A	10.2	1.7
B	5.5	3.2
2B	11.0	1.6

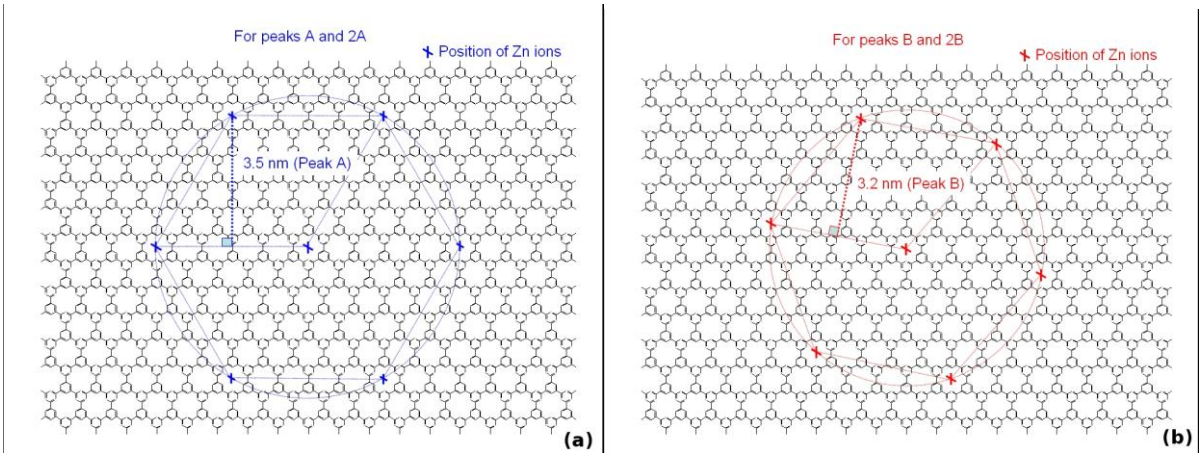

Figure S9: Possible crystalline phase formation by coordination with Zn resulting to the peaks set A (a) and B (b) according to Figure **S3** and Table **S2**.

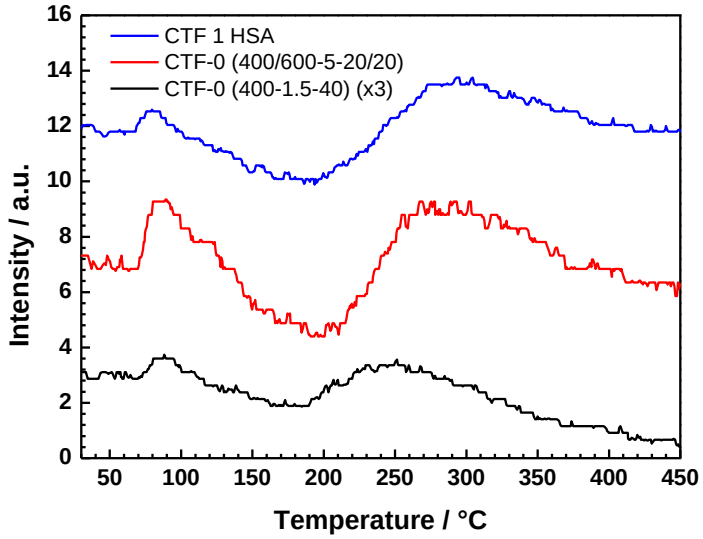

Figure S10: CO_2 Temperature-Programmed Desorption measurements of representative CTF-0 materials and of CTF-1 HSA for comparison.

[S1] Kuhn, P.; Antonietti, M.; Thomas, A. *Angew. Chem. Int. Ed.*, **2008,** 47, 3450-3453.