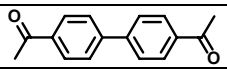
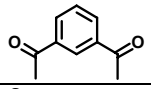
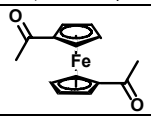
Supplementary Information

A new route to porous monolithic organic frameworks *via* cyclotrimerization

By *Marcus Rose*, *Nicole Klein*, *Irena Senkovska*, *Christian Schrage*, *Philipp Wollmann*, *Winfried Böhlmann*, *Bertram Böhringer*, *Sven Fichtner*, and *Stefan Kaskel**

Table S1: *Porosity of OFC-2 to OFC-4*

		Specific surface area (BET, p/p_0=0.3) / m^2g^{-1}	
Linker	OFC-	A	B
	2	650	12 (565[a])
	3	8	273
	4	40	399

[a]Synthesis in a solution (toluene) instead of a solvent-free melt.

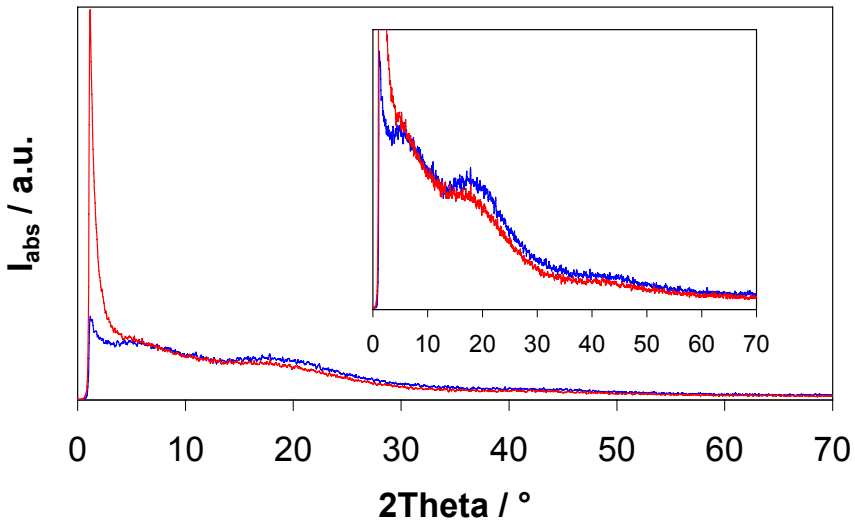


Figure S1. Powder XRD patterns for OFC-1A (blue) and OFC-1B (red) confirming an amorphous structure for the products of both synthetic routes.

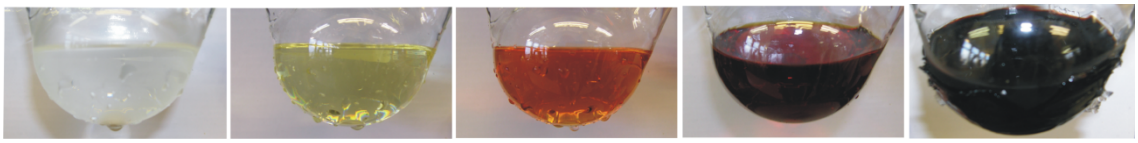


Figure S2. Photographs of the OFC-1A synthesis in solution (0.2 g 14DAB in 60 ml Ethanol/Toluene (5:1)), taken directly after the addition of different amounts of $SiCl_4$ (from the left to the right image: 0 ml, 8 ml, 10 ml, 12 ml, 12 ml after 30 min).

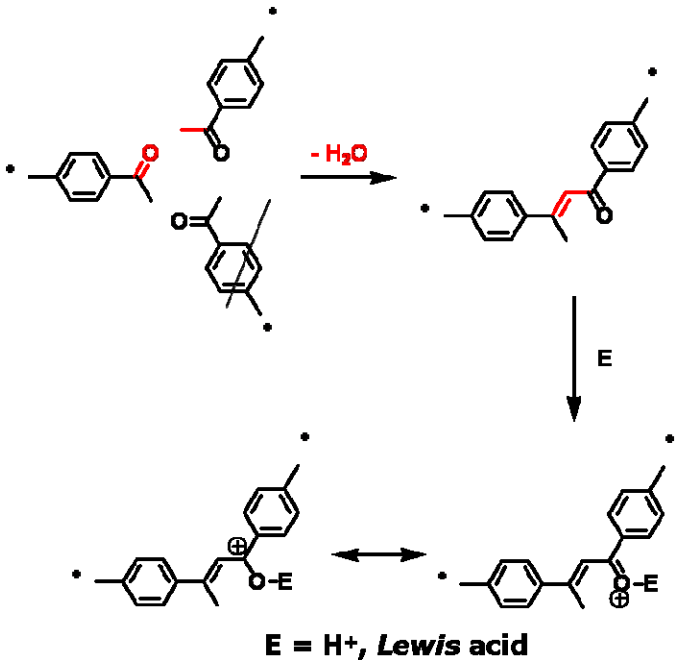


Figure S3. Dimerization reaction of two acetyl groups as a conceivable side reaction to the cyclotrimerization. Reaction with an electrophil E (e.g. *Lewis* acid or proton) can lead to a partial oxidation of the π-electron system and the resulting black color.

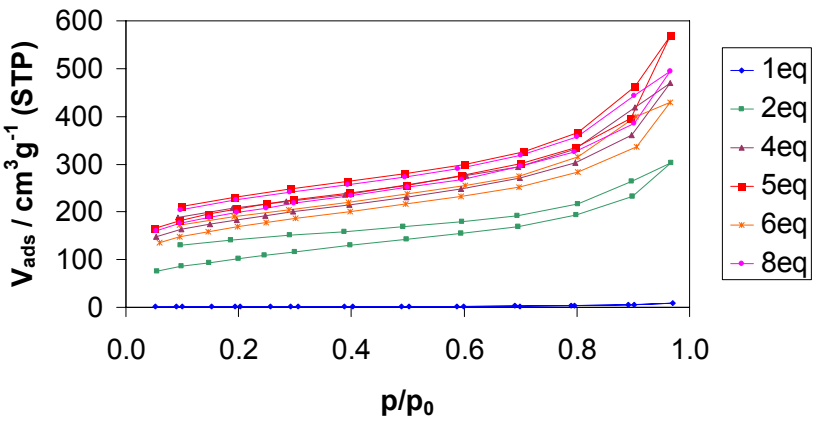


Figure S4. Porosity of OFC-1A in dependence of the amount of 4-toluene sulfonic acid relative to the educt amount.

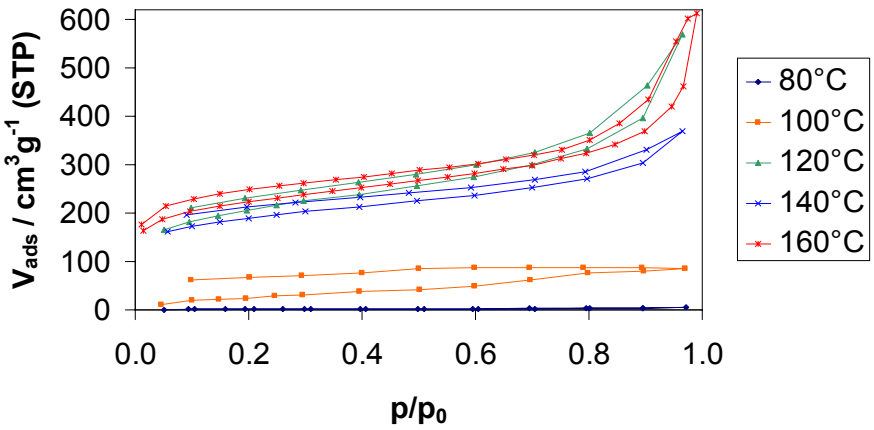


Figure S5. Porosity of OFC-1A in dependence of the reaction temperature.

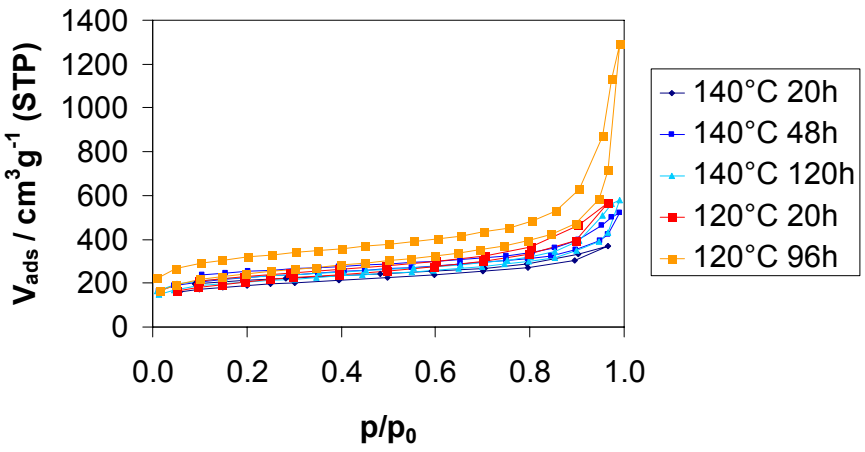


Fig. S6. Porosity of OFC-1A in dependence of the amount of the reaction time.

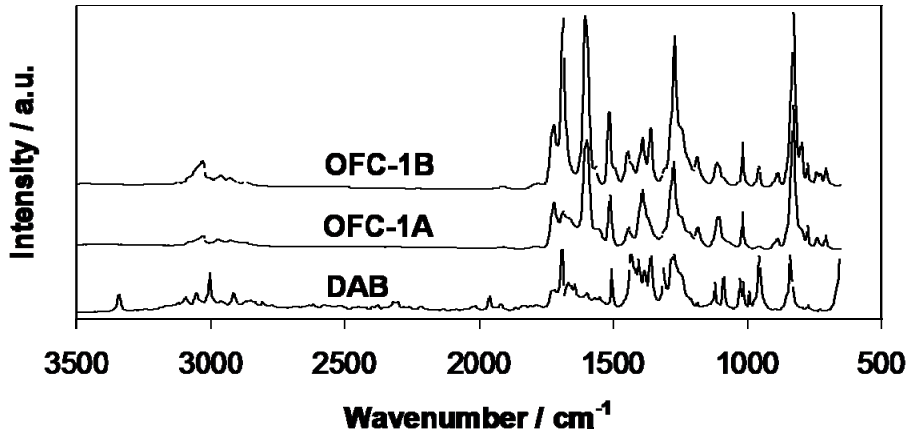


Figure S7. FTIR spectra of 1,4-diacetylbenzene (bottom), OFC-1A (middle) and OFC-1B (top) measured in diffuse reflexion mode.

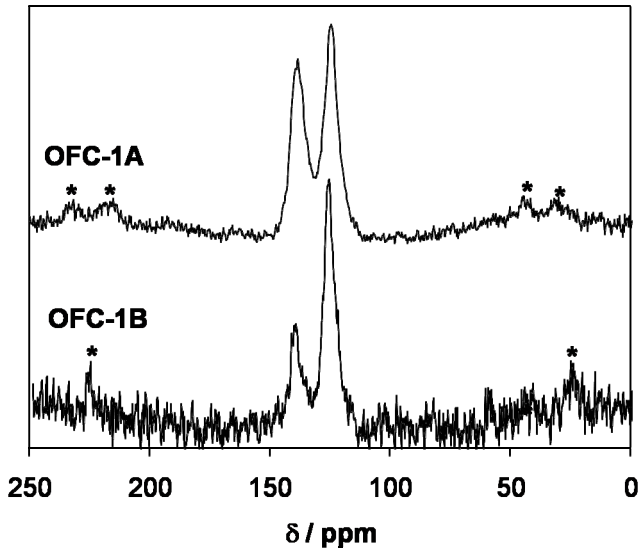


Figure S8. ^{13}C CP MAS NMR spectra of OFC-1A and -1B revealing aromatic carbon atoms.

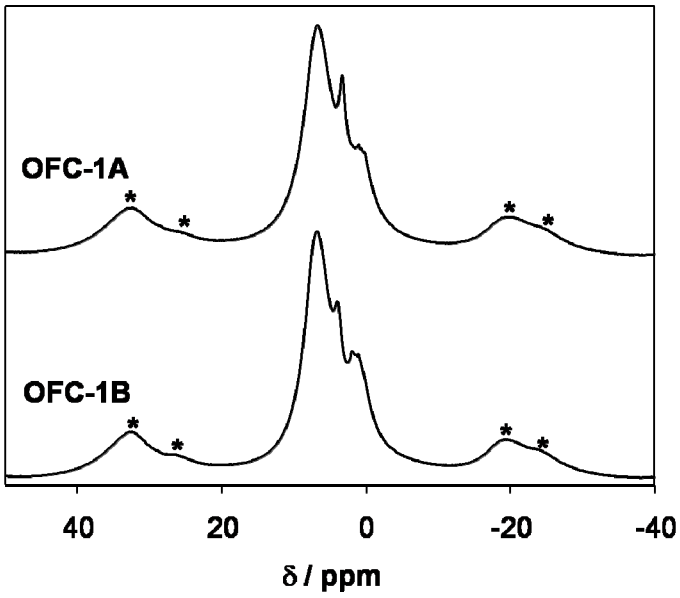


Figure S9. ^{1}H MAS NMR spectra of OFC-1A and -1B reveal aromatic and aliphatic C-H groups indicating an incomplete cross-linking.

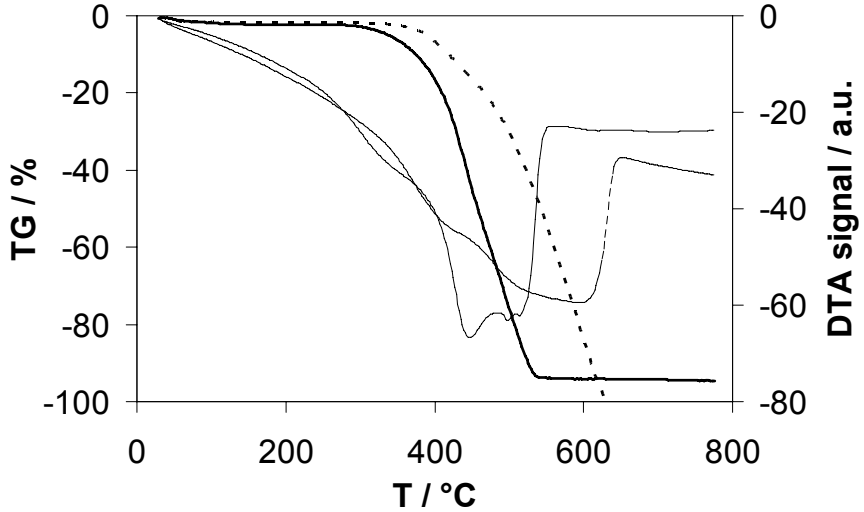


Figure S10. DTA (small lines) and TG (bold lines) of OFC-1A (filled lines) and OFC-1B (dashed lines).

Table S2. Results of the EDX analysis (wt-%).

OFC-1A		OFC-1B	
C	97.35	C	98.43
O	1.34	O	1.57
N	1.17	S	0
Na	0.13		

Table S3. Results of the elemental analysis and comparison with theoretical values (wt-%). [a]Estimated as the non C,H atoms (residue).

Experimental	**OFC**		**Theoretical composition**			
	1A	**1B**		**100% CT = $C_{10}H_6$**	**100% Dim = 50% CT = $C_{10}H_8O$**	**0% Reaction (14DAB) = $C_{10}H_{10}O_2$**
C	82.9	87.0	C	95.2	83.3	74.1
H	4.9	4.9	H	4.8	5.6	6.2
O[a]	n.d.	8.1	O	-	11.1	19.7
H/C ratio in %	5.9	5.6		5.0	6.7	8.4
O[a]/C ratio in %	n.d.	9.3		0.0	13.3	26.6
N	1.0					
Na	0.1					

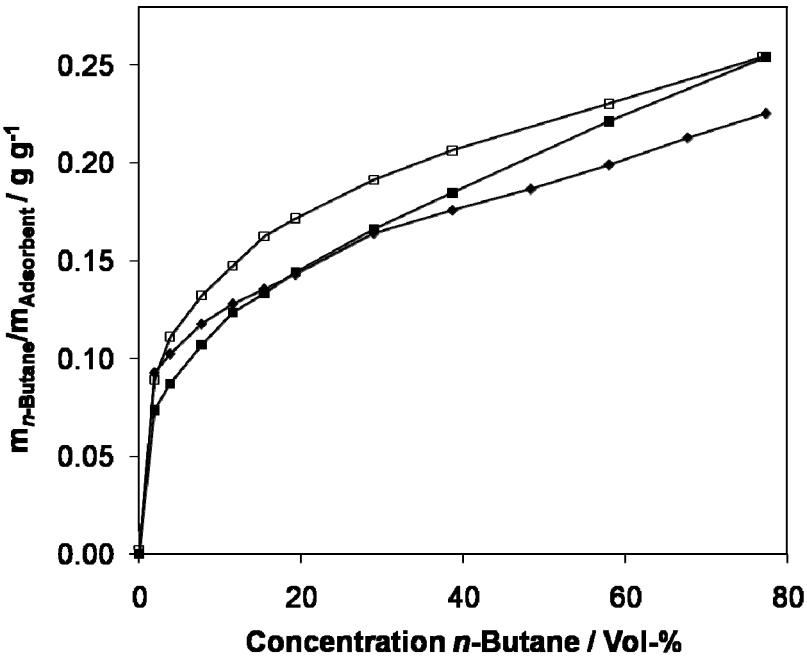


Figure S11. *n*-Butane physisorption isotherms of OFC-1A (diamonds) and OFC-1B (squares) measured at 30 °C. Filled symbols denote adsorption and empty symbols denote desorption, respectively.

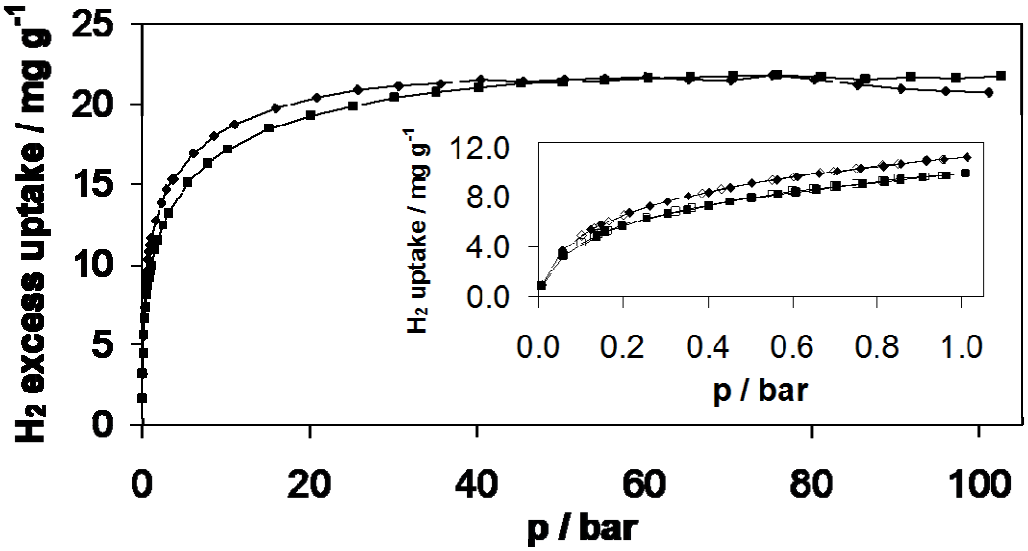


Figure S12. High pressure hydrogen adsorption of OFC-1A (diamonds) and OFC-1B (squares) measured at -196 °C. The inset shows the low pressure hydrogen physisorption isotherm measured up to 1 bar.

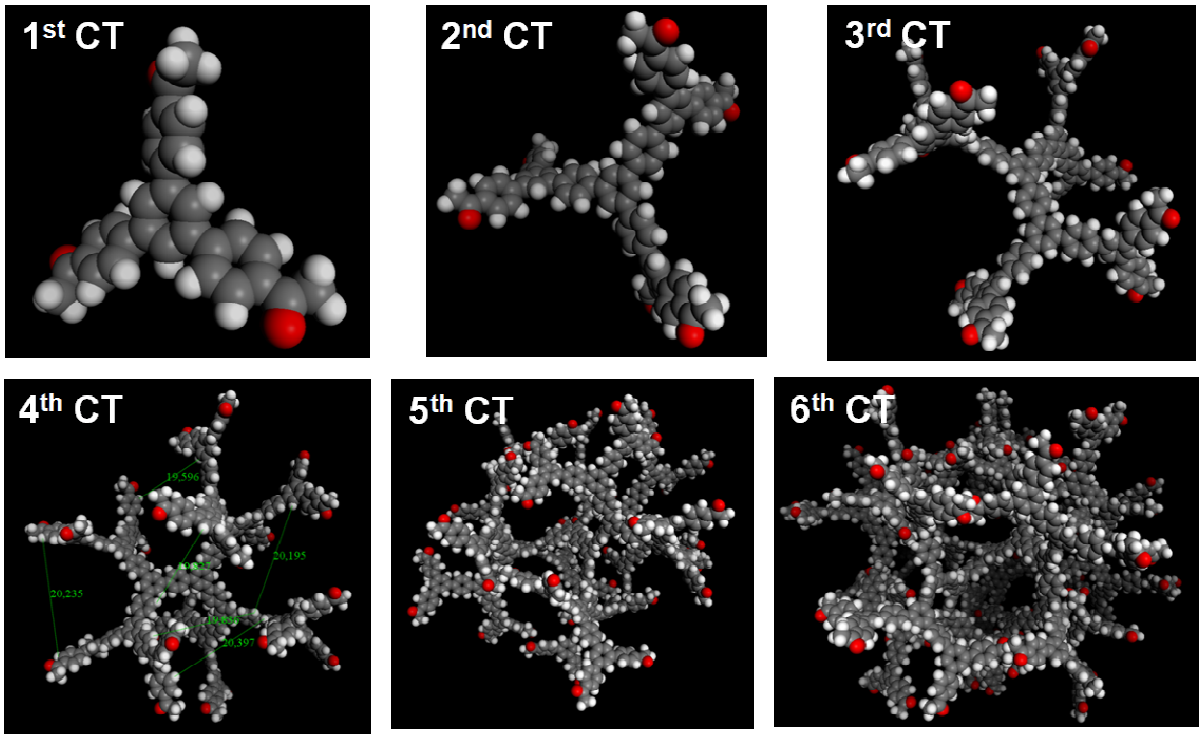


Figure S13. Strucutral simulations of a dendrimer of OFC-1 after different cyclotrimerization steps. Beginning with the 6th reaction step not all acetyl end groups are accessible for further reaction.