Supplementary Materials

Supporting Information for MW Synthesis of ZIF-7. The Effect of Solvent on Particle Size and Hydrogen Sorption Properties

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1. Crystal Structure of ZIF-7 and ZIF-7 III Phases

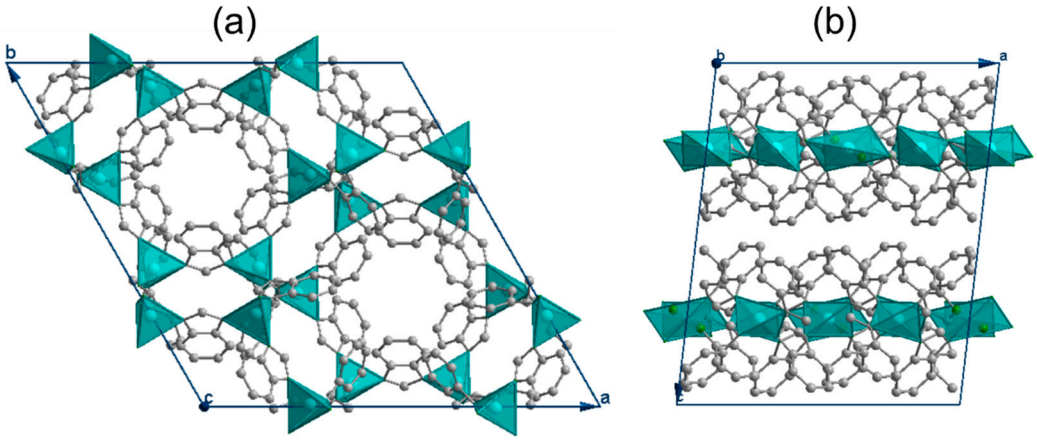

Figure S1. Schematic representation of ZIF-7 (**a**) and ZIF-7 III (**b**) unit cells. Blue tetrahedra represent Zn coordination with nitrogen atoms and gray–carbon atoms. Crystallographic ages are provided on the cell edges.

2. Profile Analysis Data

Table S1. Details of the profile analysis of the synthesized samples.

Sample Designation	Space Group	Lattice Constants				Agreement Factors		
		a, Å	b, Å	c, Å	β, °	GOF	R_p,%	R_{wp},%
ZIF-7 DEF	C2/c (15)	16.0902(17)	16.0635(15)	19.710(2)	96.299(6)	1.52	13.80	18.74
ZIF-7 DMF	R-3 (148)	22.9642(11)	22.9642(11)	15.6754(9)	90	1.34	13.89	18.94
ZIF-7 D/P	C2/c (15)	16.051(3)	16.052(3)	19.642(2)	96.376(10)	1.83	12.36	16.69
	R-3 (148)	22.9938(17)	22.9938(17)	15.6740(16)	90			
ZIF-7 D/P TEA	R-3 (148)	22.9892(17)	22.9892(17)	15.6753(14)	90	1.14	10.59	14.95

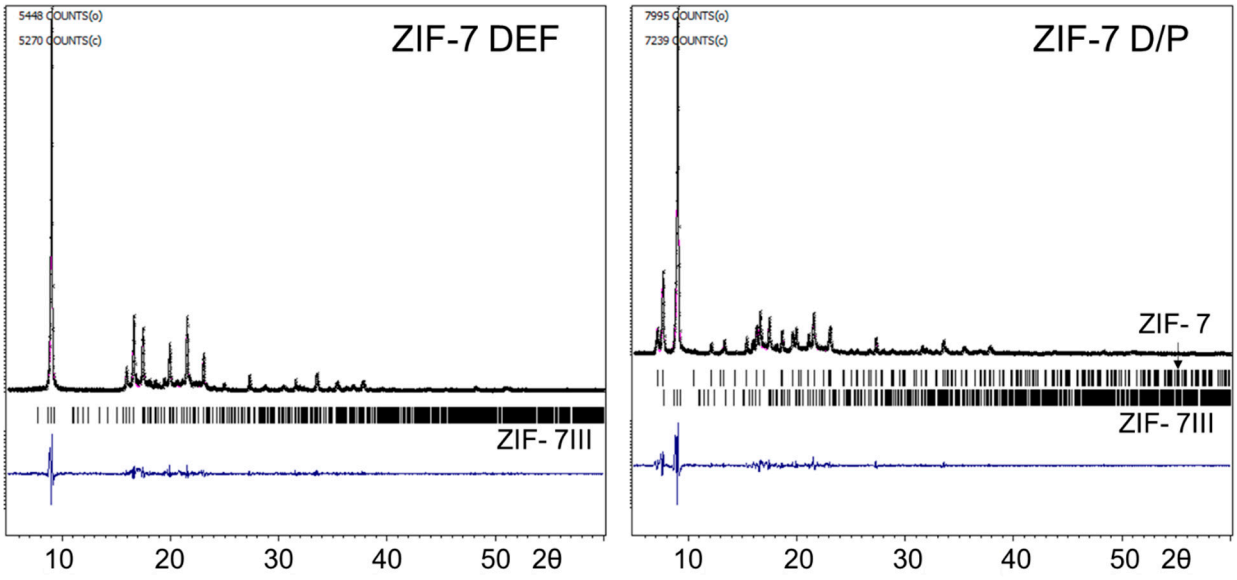

Figure S2. Powder XRD patterns of samples of ZIF-7 DEF (left one) and ZIF-7 D/P (right one): observed (black), calculated (magenta), and their difference (dark blue). The short vertical bars indicate the Bragg positions of the reflections (obtained using the Jana2006 program package).

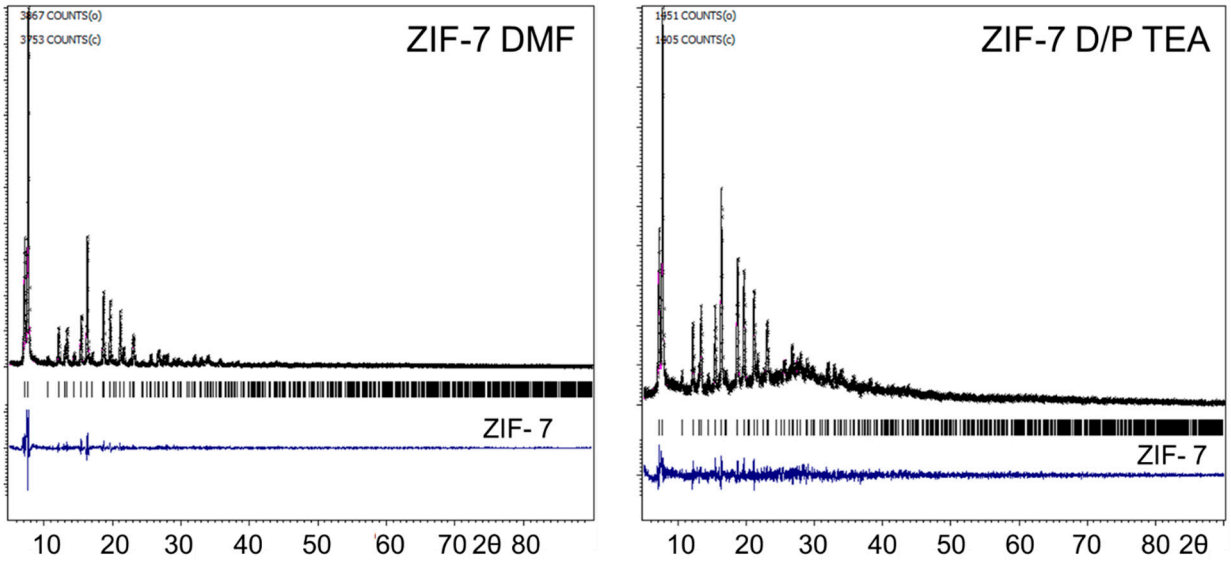

Figure S3. Powder XRD patterns of samples of ZIF-7 DMF (left one) and ZIF-7 D/P TEA (right one): observed (black), calculated (magenta), and their difference (dark blue). The short vertical bars indicate the Bragg positions of the reflections (obtained using the Jana2006 program package).

Sample ZIF-7 DMF TEA was obtained from Zinc nitrate and bIm in a DMF solution with a TEA additive. Molar ratio Zn:PhIm:TEA was 1:2:2.6. Synthesis conditions were the same as we used for the ZIF-7 DMF sample.

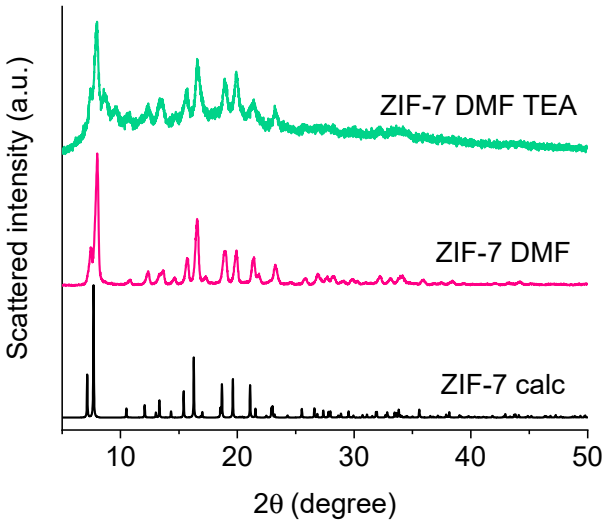

Figure S4. Powder XRD patterns of samples ZIF-7 DMF (pink one) and ZIF-7 DMF TEA (green one). Powder profile ZIF-7 calc was calculated according to crystallographic data (COD ID 412899).

Particle size for the sample ZIF-7 D/P TEA was calculated according to the Williamson-Hall analysis:

$$D = \lambda/b \cdot 10 = 1.5406/0.3378 \cdot 10 = 46 \text{ nm}$$

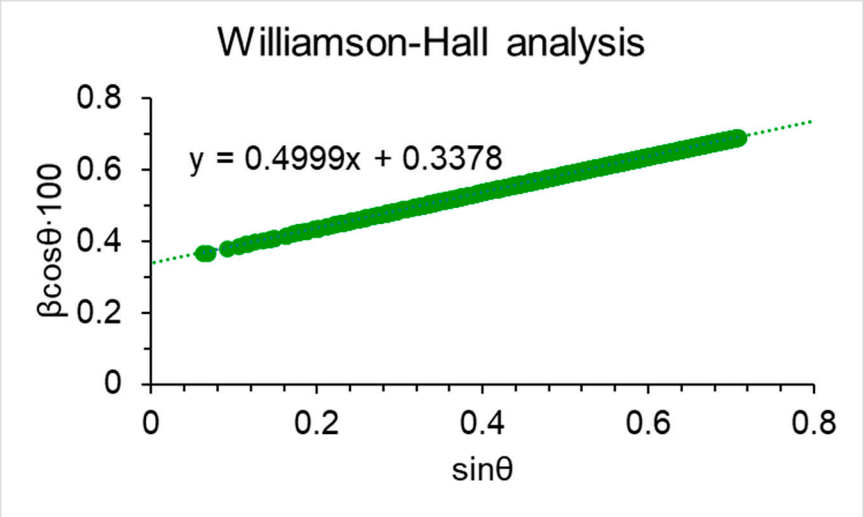

Figure S5. Plot of the Williamson-Hall analysis of the profile of the ZIF-7 D/P TEA sample.

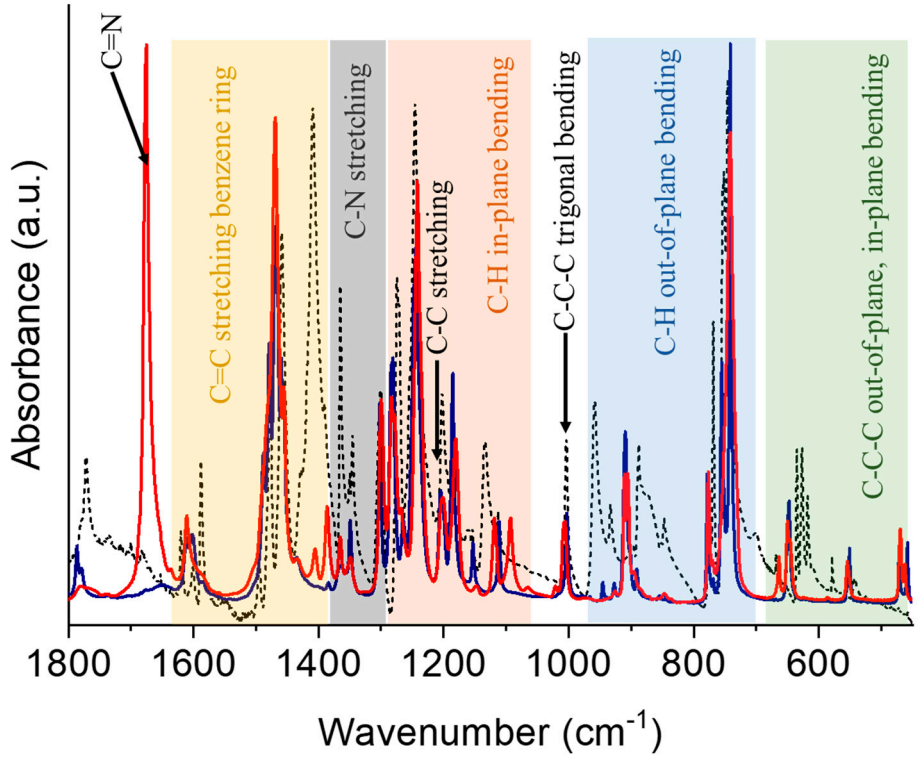

Figure S6. FTIR-spectra of samples ZIF-7 DEF (dark blue, ZIF-7 III phase) and ZIF- DMF (red, ZIF-7 phase).

Table S2. Assignments of observed peaks on experimental FTIR spectra of ZIF-7 DEF (designated as ZIF-7 III) and ZIF-7-DMF (designated as ZIF-7).

Assignment	Observed FTIR, cm^{-1}	
	ZIF-7	ZIF-7 III
C-C-C out-of-plane bending		455
C-C-C out-of-plane bending	467	467
C-C-C out-of-plane bending	555	550
C-C-C in-plane bending	645	650
C-C-C out-of-plane bending	665	
C-H out-of-plane bending	740	740
C-H out-of-plane bending		755
C-H out-of-plane bending	775	775
C-H out-of-plane bending	905	905
C-C-C trigonal bending	1005	1005
C-H in-plane bending	1090 1115	1110
C-H in-plane bending		1155
C-H in-plane bending	1180 1200	1185 1200
C-C stretching	1240	1240
C-H in-plane bending	1275	1275
C-N stretching	1300	1300
C-N stretching	1350	1350
C-N stretching	1365	1365

C=C stretching benzene ring	1390	
C=C stretching benzene ring	1405	
C=C stretching benzene ring	1455	1455
C=C stretching benzene ring	1470	1470
C=C stretching benzene ring	1605	1600
		1610
C=N	1675	
N-H in plane bending + C-C-C out-of-plane bending		1785