Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Synthesis of nanoparticles of zeolitic imidazolate framework ZIF-94 using inorganic deprotonators

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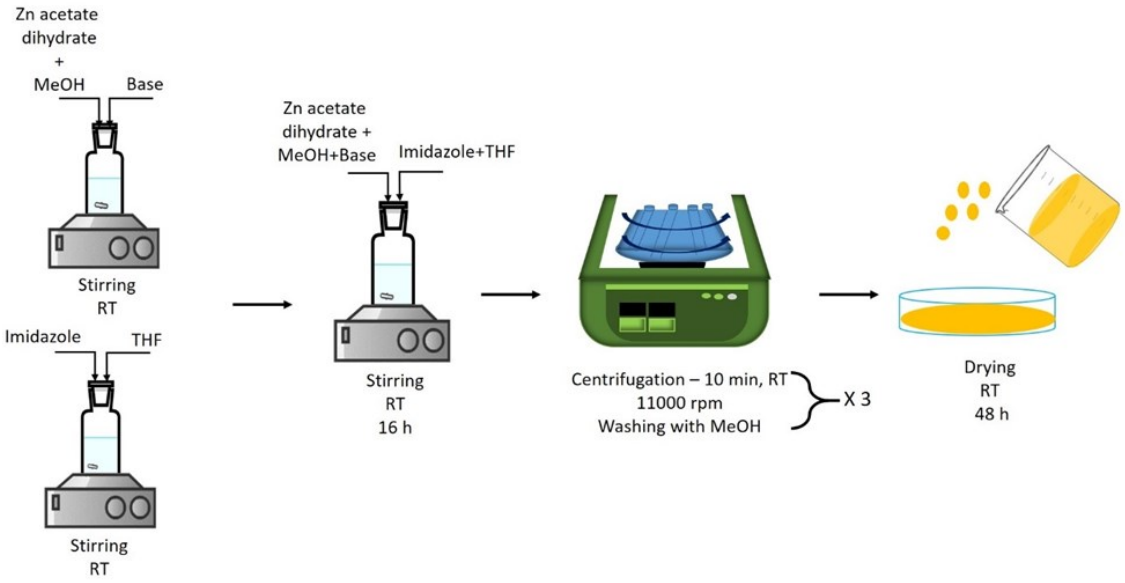

Fig. S1. Experimental scheme of the modified original method of ZIF-94 synthesis.

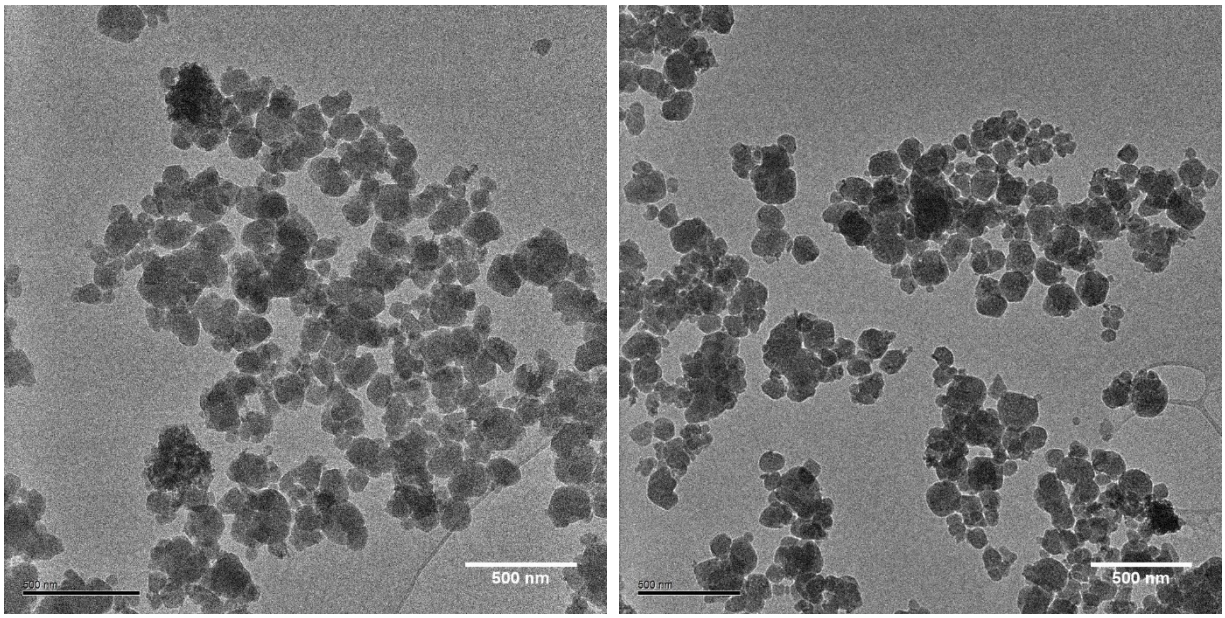

Fig. S2. TEM images of product A4.

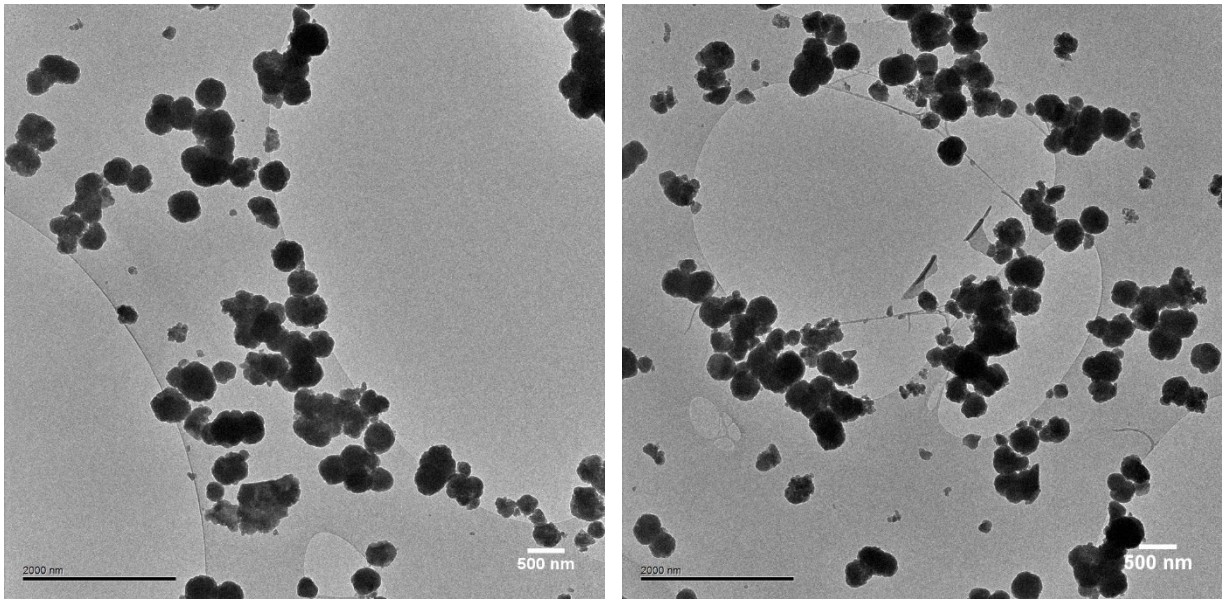

Fig. S3. TEM images of product B.

Miller indices calculation

The interplanar distance d, in the set of (*hkl*) of the materials having cubic unit cell with lattice parameter a is obtained from the equation

$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

Combining the above equation with Bragg's law ($\lambda = 2d\sin\theta$), gives

$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2} = \frac{4\sin^2\theta}{\lambda^2}$$

Rearranging gives

$$\sin^2\theta = \left(\frac{\lambda^2}{4a^2}\right)(h^2 + k^2 + l^2)$$

Where, $\frac{\lambda^2}{4a^2}$ is a constant and $\sin^2\theta$ is proportional to the value of $h^2 + k^2 + l^2$, which can take only integral values except few such as 7, 15 for which the combination of *hkl* is not possible. Taking all these into consideration observed value of $sin^2\theta$ satisfies the *hkl* values for body cantered cubic structure.

Table S1. Miller indices calculation from observed value of $sin^2\theta$

Peak position (2theta, °)	$sin^2\theta$	$\frac{sin^2\theta}{sin^2\theta_{min}}$	$\frac{sin^2\theta}{sin^2\theta_{min}} \times 2$	$h^2 + k^2 + l^2$	*hkl*
7.49607	0.00427	1	2	2	110
10.59482	0.00852	1.99	3.99	4	200
12.9714	0.01276	2.99	5.97	6	211
14.98033	0.01699	3.98	7.95	8	220
16.73979	0.02119	4.96	9.92	10	310
18.36299	0.02546	5.96	11.9	12	222
19.85083	0.02971	6.95	13.9	14	321
21.24348	0.03398	7.95	15.9	16	400
23.77762	0.04244	9.93	19.9	20	420

27.08645	0.05484	12.8	25.7	26	431

Particle size calculation through Scherrer equation

Table S2. The particle size and average particle size of all the samples calculated using Scherrer equation, at the values of 2-theta for different peaks and K equals to 0.94

	Peak position (2theta)	FWHM	Crystal Size (nm) (Kλ/β cos θ)	Average Size (nm)
Original Method	7.48	0.23	36.29	31±4
	10.56	0.28	29.75	
	12.95	0.25	32.83	
	14.97	0.26	31.82	
	16.73	0.33	25.71	
Product A.1	7.47	0.25	32.60	31±1
	10.53	0.28	30.19	
	12.91	0.27	31.24	
	14.92	0.28	29.94	
	16.68	0.29	29.85	
Product A.2	7.47	0.28	29.85	29±1
	10.53	0.30	28.04	
	12.91	0.29	29.21	
	14.92	0.29	29.18	
	18.30	0.29	29.13	
Product A.3	7.51	0.25	33.20	33±1
	10.58	0.26	31.58	
	12.96	0.25	33.33	
	14.96	0.25	33.33	
	18.33	0.25	33.90	
Product A.4	7.46	0.22	38.26	38±2
	12.92	0.21	38.80	
	14.93	0.21	39.76	
	18.31	0.21	39.65	
	19.78	0.24	34.45	
Product B	7.60	0.39	21.17	16±3
	10.68	0.49	16.94	
	13.07	0.52	15.98	
	15.09	0.56	15.04	
	19.91	0.73	11.53	

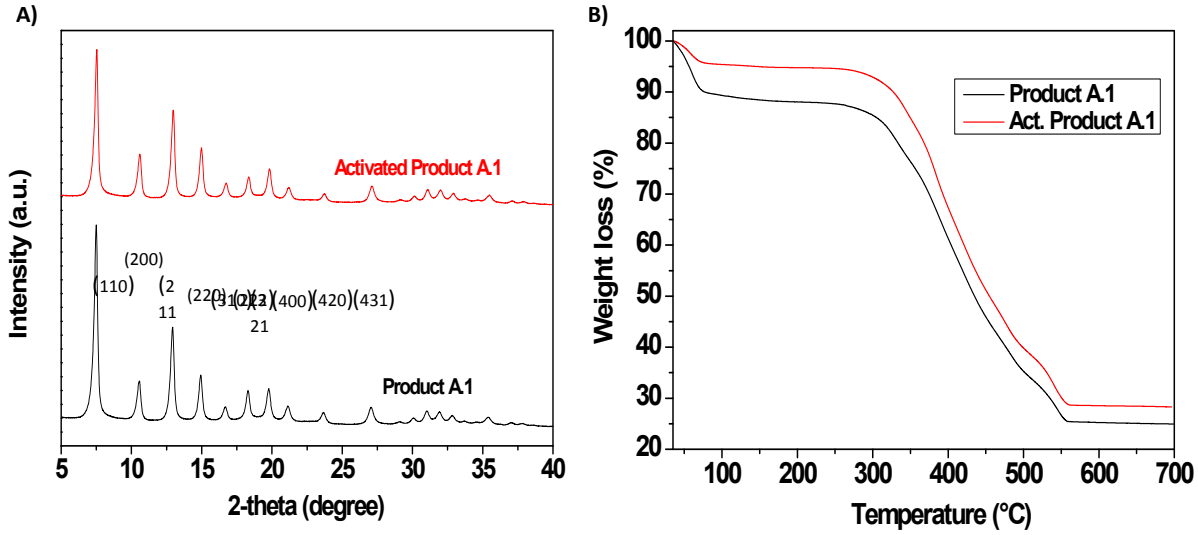

Fig. S4. XRD pattern and TGA curve of product A.1 activated at 200 ºC for 8 h compared with that of non-activated product A.1

Table S3. Pore volume of all the samples calculated using N_2 adsorption data

Sample	Pore Volume (cm^3/g)
Original Method	0.23
Product A.1	0.09
Product A.2	0.16
Product A.3	0.19
Product A.4	0.16
Product B	0.16