SUPPORTING INFORMATION

A facile synthesis of alkylated nitrogen heterocycles catalysed by 3D mesoporous aluminosilicates with cage type pores in aqueous medium

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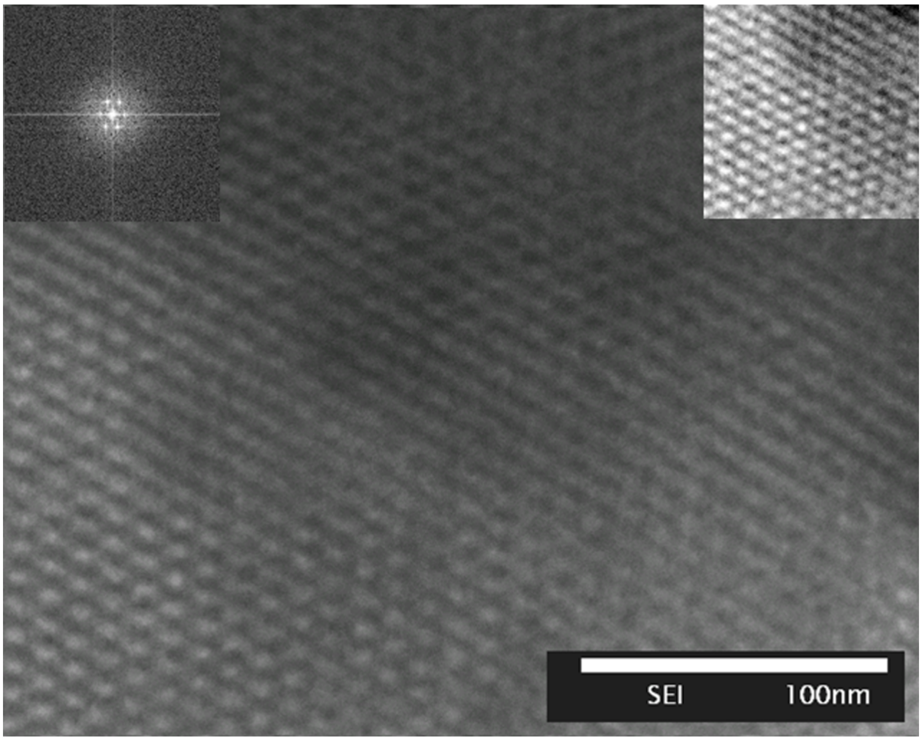

Figure S1: Representative HRTEM image of AlKIT-5 sample. The excellent three-dimensional mesoscopic order of AlKIT-5 was confirmed by HRTEM. The sample exhibits highly ordered mesoporous networks with a well-ordered mesopores and walls, which is characteristics of well-ordered KIT-5 mesoporous silica. The inset figures, displaying the corresponding fast Fourier transform (FFT) and inverse fast Fourier transform (IFFT) pattern of Figure 1S, respectively, confirm the presence of the cubic three dimensional mesoporous network in the sample.

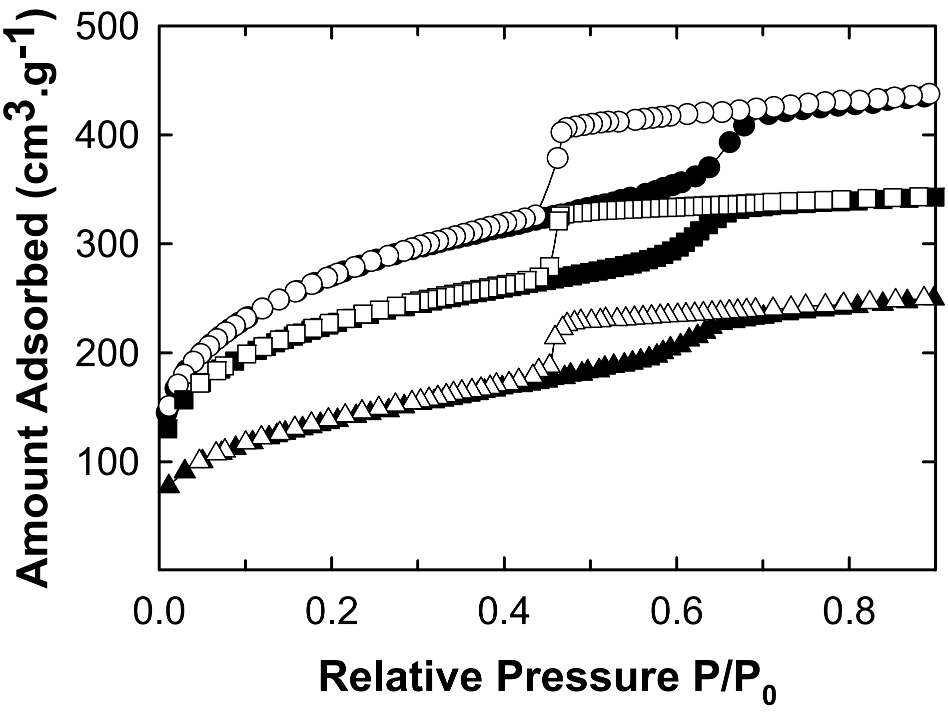

Figure S2. Nitrogen adsorption–desorption isotherms of AlKIT-5 samples before and after the reaction: (●) AlKIT-5(10); SA: 989 m^2/g, PV: 0.68 cm^3/g, (■) AlKIT-5(10) after calcined at 540°C; SA: 810 m^2/g, PV: 0.54 cm^3/g, and (▲) AlKIT-5(10) after dried at 100°C SA: 498 m^2/g, PV: 0.43 cm^3/g. (open symbols: desorption; closed symbols: adsorption).

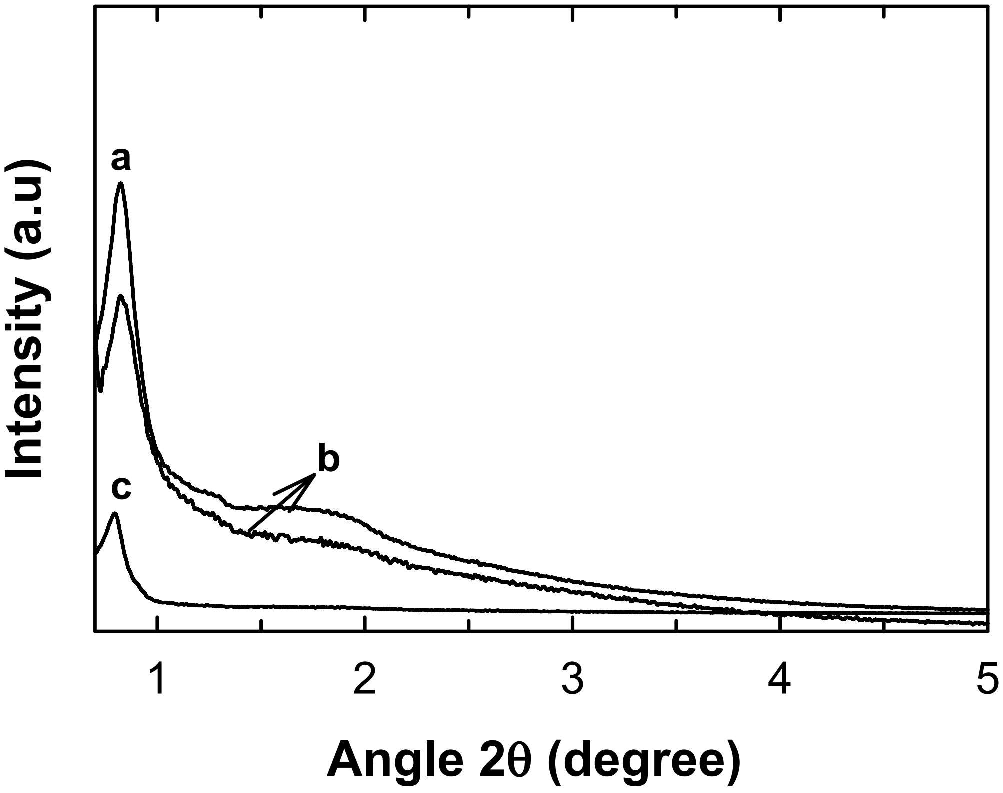

Figure S3: Low angle powder X-ray diffraction patterns of AlKIT-5 samples before and after the reaction: (a) AlKIT-5(10), (b) AlKIT-5(10) after calcined at 540°C, and (c)AlKIT-5(10) after dried at 100°C.

The importance of water as a solvent in the synthesis of alkylated heterocycles:

To achieve truly environmentally benign chemical syntheses, it is an important task to treat water-insoluble organic materials in water as well as to treat water-unstable materials in water.[1] The use of water as a solvent has effectively been shown to increase the rate and yield of many organic reactions.[2] Even reactions with water-insoluble reactants have generated successful results, proving that water solubility is not necessary.[3] It is thought that the increased rate and yield are due the hydrophobic nature of the reagents, since their repulsion from water would enhance the collisions between organic molecules and increase their ground-state energies, leading to an increase in the rate of the reaction.[3] If a reaction proceeds "on water",[2,3] then replacement of environmentally unfriendly, potentially dangerous, and/or expensive organic solvents with water would be beneficial.

[1] S. Azoulay, K. Manabe, S. Kobayashi *Org. Lett.*, 2005, *7*, 4593.

[2] (a) P. A. Grieco, *Organic Synthesis in Water*; Blackie Academic & Professional: London, 1998. (b) C. J. Li, T. H. Chan, *Organic Reactions in Aqueous Media*; John Wiley: New York, 1997.

[3] The terminology "on water" is commonly used to refer to the water-based reaction of water-insoluble organic substrates. See, for example: (a) S. Narayan, J. Muldoon, M. G. Finn, V. V. Fokin, H. C. Kolb, K. B. Sharpless, *Angew. Chem., Int. Ed.* 2005, *44*, 3275. (b) J. E. Klijn, J. B. N. Engberts, *Nature* 2005, *435*, 746. (c) M. C. Pirrung, *Chem. Eur. J.* 2006, *12*, 1312.