

Supporting information for

**One-step synthesis of a highly homogeneous SBA-NHC hybrid material:
en route to single-site NHC-metal heterogeneous catalysts with high
loadings**

Mansuy Rocquin,^a Mickaël Henrion,^a Marc-Georg Willinger,^b Philippe Bertani,^c

Michael J. Chetcuti,^a Benoît Louis*^d and Vincent Ritleng*^{a,e}

e-mail: blouis@unistra.fr, vrigleng@unistra.fr

^a Laboratoire de Chimie Organométallique Appliquée, UMR CNRS 7509, Ecole européenne de Chimie, Polymères et Matériaux, Université de Strasbourg, 25 rue Becquerel, 67087 Strasbourg, France.

^b Department of Inorganic Chemistry, Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, Berlin 14195, Germany.

^c Laboratoire de RMN et Biophysique des Membranes, Institut de Chimie, UMR CNRS 7177, Université de Strasbourg, 1 rue Blaise Pascal, 67000 Strasbourg, France.

^d Laboratoire de Synthèse, Réactivité Organiques et Catalyse, Institut de Chimie, UMR CNRS 7177, Université de Strasbourg, 4 rue Blaise Pascal, 67000 Strasbourg, France.

^e Institut d'Etudes Avancées de l'Université de Strasbourg (USIAS), 5 allée du Général Rouvillois, 67083 Strasbourg, France.

Characterization of 1-(2,6-Diisopropylphenyl)-3-[3-(triethoxysilyl)propyl]-imidazolium Iodide (1)

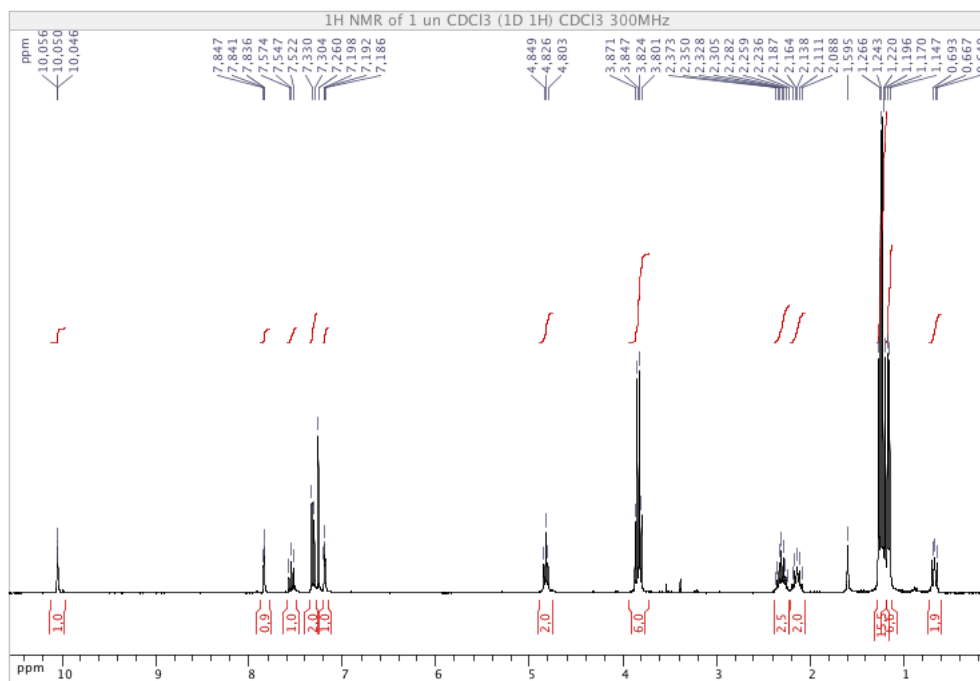


Figure S1a. ¹H NMR spectrum of 1 in CDCl₃.

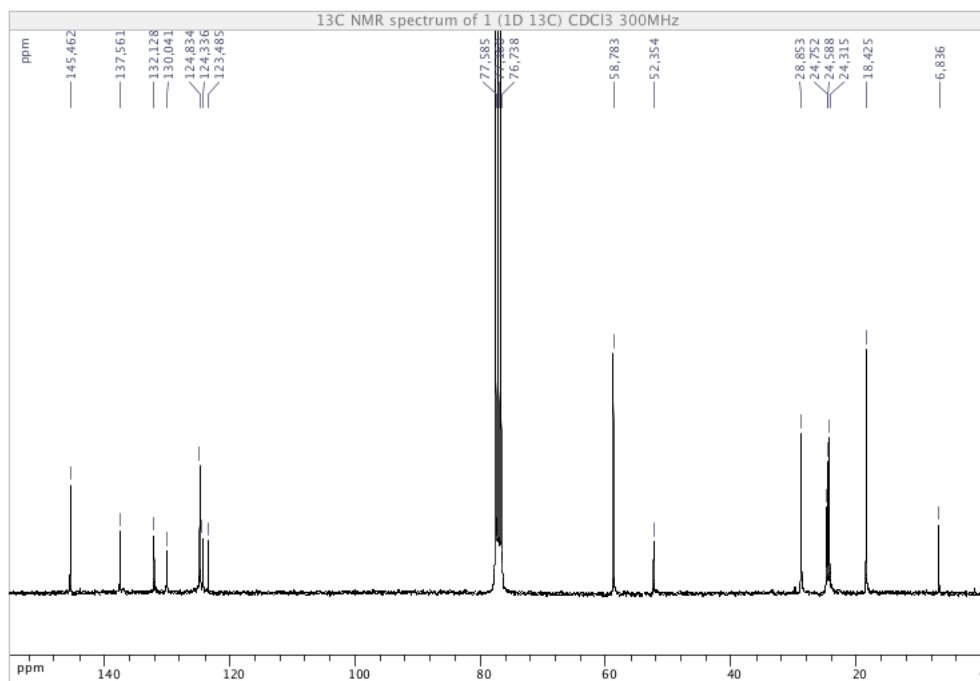


Figure S1b. ¹³C {¹H} NMR spectrum of 1 in CDCl₃.

Characterization of the Hybrid SBA-NHC (2)

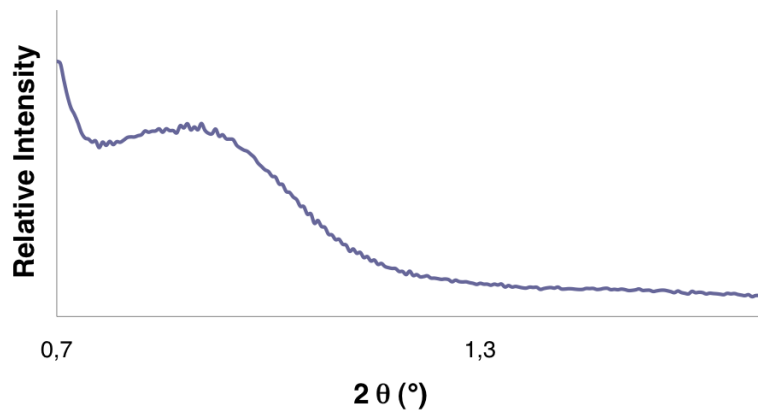


Figure S2a. Small-Angle Powder XRD Pattern of **2**.

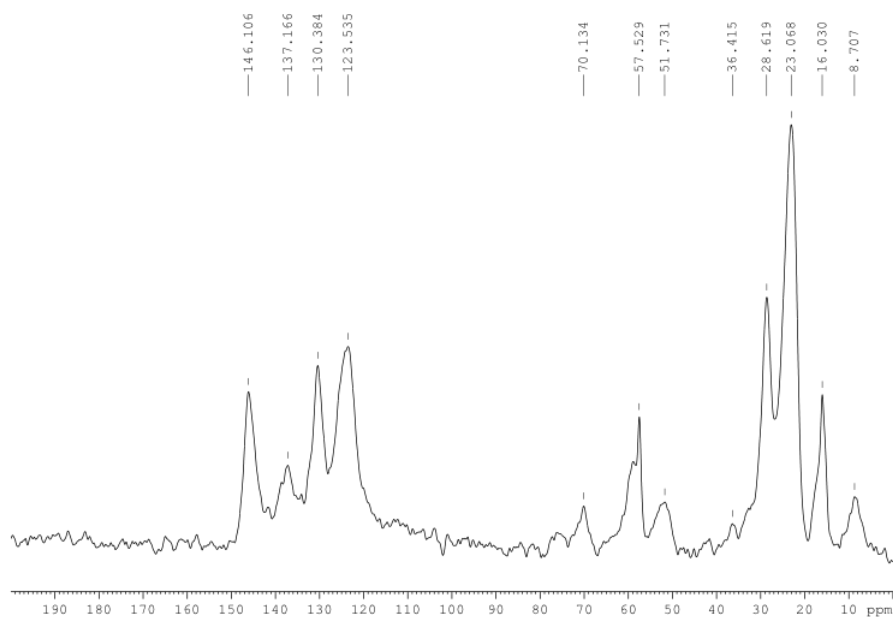


Figure S2b. ^{13}C CP-MAS NMR spectrum of **2**.^{1,2}

(1) 102400 scans were accumulated with a recycle delay of 3 s.

(2) Peaks at 70, 59, 58 and 16 ppm correspond to residual template agent present in micropores and to Si-OEt signals that arise from surfactant removal by extraction with EtOH (see Fig. S3a).

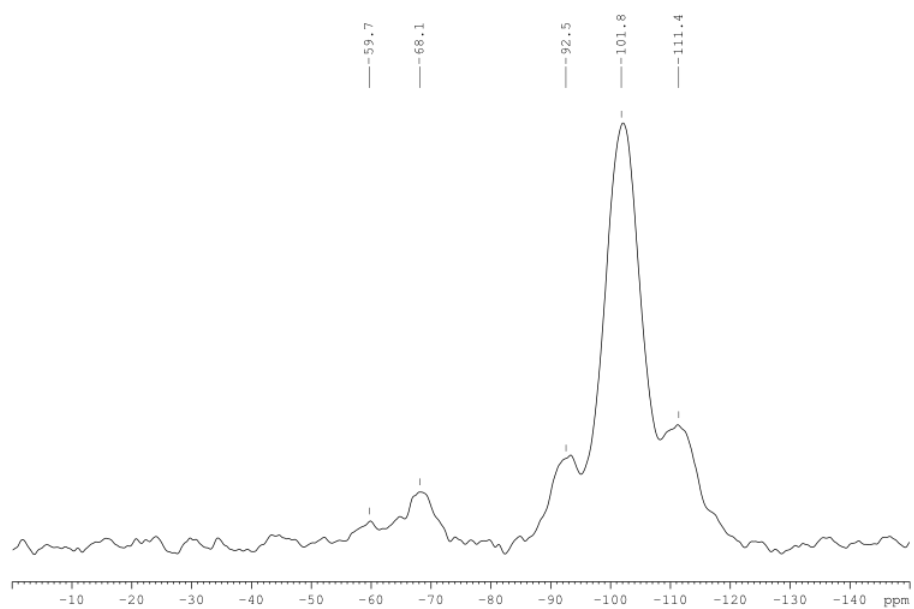


Figure S2c. ^{29}Si CP-MAS NMR spectrum of **2**.³

(3) 32768 scans were accumulated with a recycle delay of 5 s.

CP-MAS NMR Characterization of the Pristine SBA-15 (3)

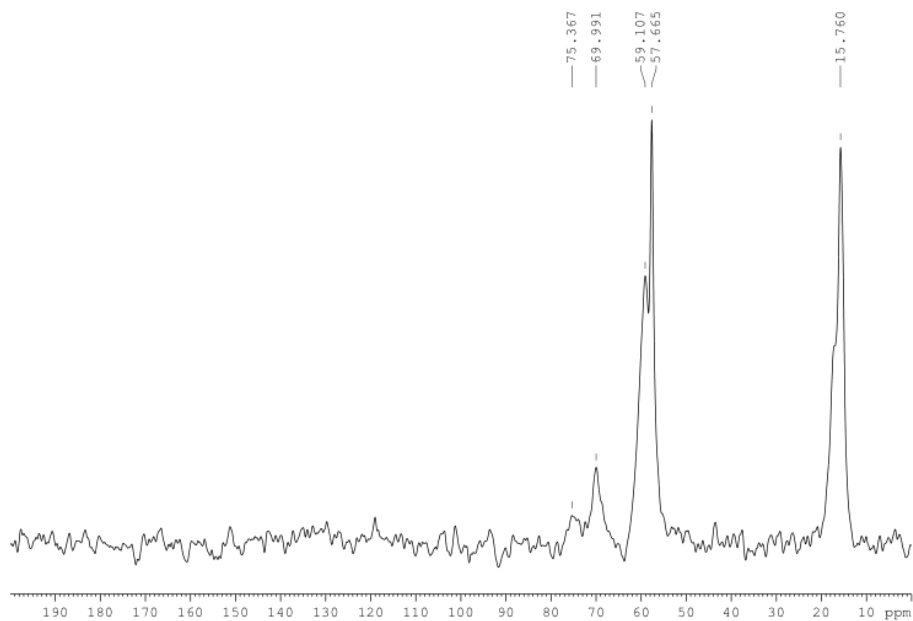


Figure S3a. ^{13}C CP-MAS NMR spectrum of **3**.⁴

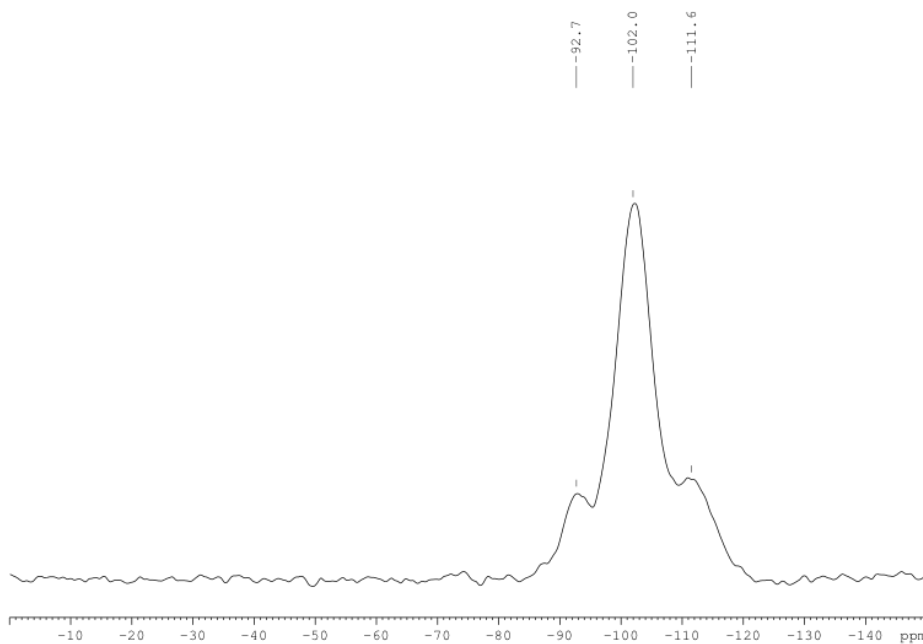


Figure S3b. ^{29}Si CP-MAS NMR spectrum of **3**.⁵

(4) 32100 scans were accumulated with a recycle delay of 3 s.

(5) 32768 scans were accumulated with a recycle delay of 5 s.

CP-MAS NMR Characterization of the Grafted SBA-NHC (4)

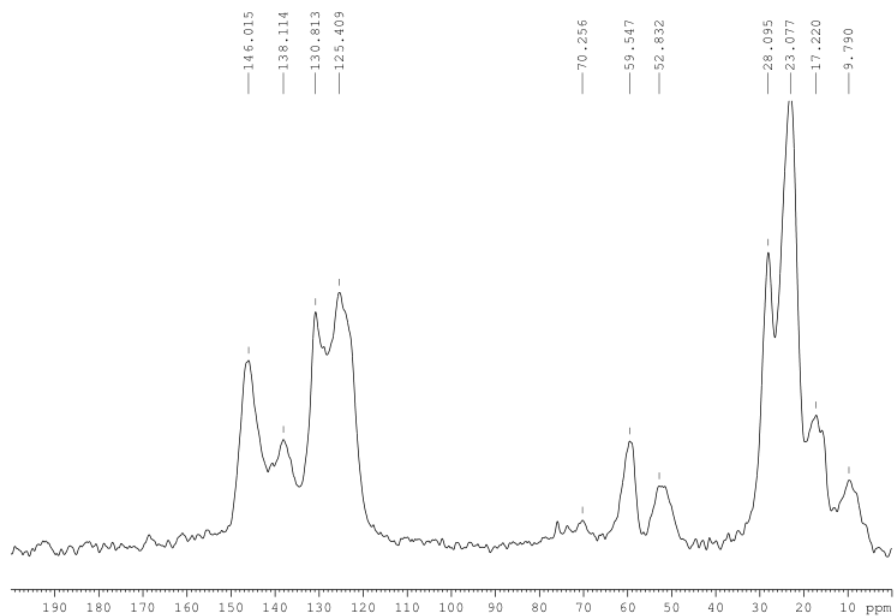


Figure S4a. ^{13}C CP-MAS NMR spectrum of 4.^{6,7}

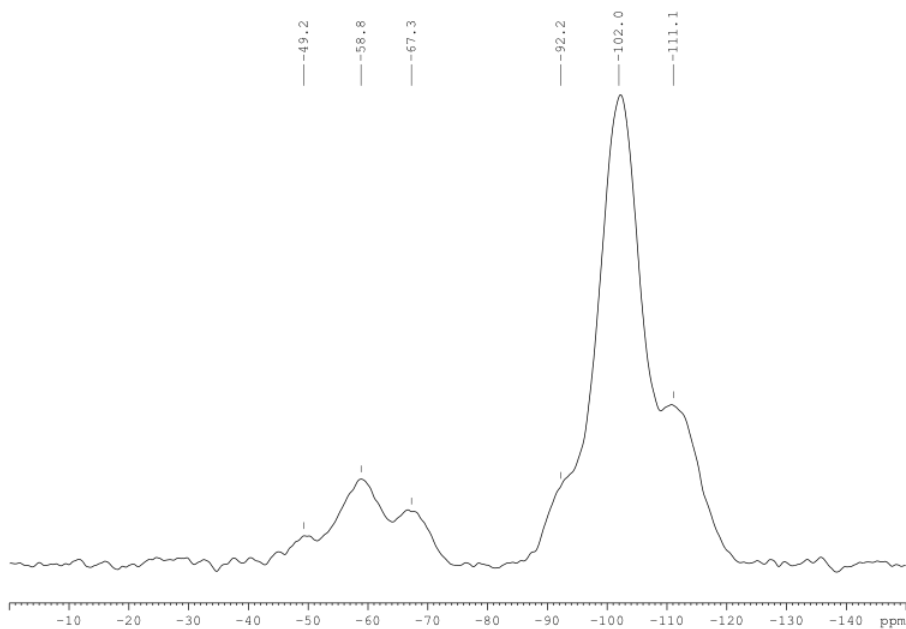


Figure S4b. ^{29}Si CP-MAS NMR spectrum of 4.⁸

(6) 28675 scans were accumulated with a recycle delay of 3 s.

(7) Peaks at 70, 59 and 17 ppm correspond to residual template agent present in micropores and to Si-OEt signals that arise from surfactant removal by extraction with EtOH (see Fig. S3a).

(8) 32768 scans were accumulated with a recycle delay of 5 s.