***N*-Heterocyclic Carbenes as Highly Efficient Catalysts for the Cyclotrimerization of Isocyanates**

Hung A. Duong, Michael J. Cross, and Janis Louie*

Department of Chemistry, University of Utah, 315 South 1400 East, Salt Lake City, UT 84112-0850

SUPPORTING INFORMATION

General information. 1,3-Diisopropyl-4,5-dimethylimidazol-2-ylidene (**iPrIm**), 1,3-bis-(2,4,6-trimethylphenyl)-imidazol-2-ylidene (**IMes**), 1,3-bis-(2,6-diisopropylphenyl)-imidazol-2-ylidene (**IPr**), 1,3-dicyclohexylimidazol-2-ylidene (**ICy**), 1,3-di-*tert*-butylimidazol-2-ylidene (**ItBu**), 1,3-diadamantylimidazol-2-ylidene (**IAd**), 1,3-bis-(2,6-diisopropylphenyl)-4,5-dihydroimidazolin-2-ylidene (**SIPr**) were prepared according to literature procedures.¹ Phenyl isocyanate, 4-methoxyphenyl isocyanate, 2-methylphenyl isocyanate, cyclohexyl isocyanate, and allyl isocyanate were purchased from Aldrich, dried over phosphorous pentoxide, and degassed prior to use.

¹H and ¹³C NMR spectra were recorded on a Varian VXL-300 spectrometer and a Varian VXR-500 spectrometer and referenced to residual protiated solvent (resonances downfield to the standard are reported as positive). All ¹³C NMR spectra were proton decoupled. IR spectra were recorded on a Bruker Tensor 27 spectrometer. HRMS were performed at the mass spectrometry facility at the University of Utah.

General procedure: Under a nitrogen atmosphere, a solution of PhNCO (1:1 v:v in THF) was added to an oven dried round bottom flask containing SIPr (0.1 mol%) and equipped with a magnetic stir bar. The reaction was stirred at room temperature for 30 min. The resulting precipitate was filtered, washed with pentane, and dried *in vacuo* to afford the isocyanurate as a white solid in 99% yield.

Spectra of products **8-11** were compared to reported values.²

Procedure for the synthesis of 1,3,5-tris(4-methoxyphenyl)-1,3,5-triazinane-2,4,6-trione (12): Under a nitrogen atmosphere, a solution of 4-methoxyphenyl isocyanate (1:1 v:v in THF) was added to SIPr (0.1 mol%) and the reaction was stirred at room temperature for 30 minutes. The resulting precipitate was filtered, recrystallized from methylene chloride and hexane, and dried *in vacuo* to afford the isocyanurate as a white solid in 85% yield. Mp: 259.0 – 259.5 °C (lit.^{2c} mp 259 – 260 °C); IR (KBr pellet): 1705 cm⁻¹

(C=O); ^1H NMR (CDCl_3): δ 7.29 (d, J = 9.0 Hz, 2H), 6.98 (d, J = 9.0 Hz, 2H), 3.81 (s, 3H); ^{13}C NMR (CDCl_3): δ 160.1, 149.3, 129.6, 126.5, 114.8, 55.7; HRMS (m/z): calcd for $\text{C}_{24}\text{H}_{21}\text{N}_3\text{O}_6$ (M^+) 447.14303, found 447.14440.

References

- (1) (a) Arduengo, A. J. III; Krafczyk, R.; Schmutzler, R.; Craig, H. A.; Goerlich, J. R.; Marshall, W. J. Unverzagt, M. *Tetrahedron* **1999**, 55, 14523. (b) Böhm, V. P. W.; Weskamp, T.; Gstottmayr, W. K.; Herrmann, W. A. *Angew. Chem. Int. Ed.* **2000**, 39, 1602. (c) Kuhn, N.; Kratz, T. *Synthesis* **1993**, 561.
- (2) (a) Tang, J.; Mohan, T.; Verkade, J. G. *J. Org. Chem.* **1994**, 59, 4931. (b) Weiss, K.; Hoffmann, K. *Z. Naturforsch., Teil B* **1987**, 42, 769. (c) Kogon, I. C. *J. Am. Chem. Soc.* **1956**, 78, 4911.

8

solvent : CDCl₃

8

solvent: CDCl₃

solvent : CDCl_3

solvent : CDCl₃

solvent : CDCl_3

solvent: CDCl_3

solvent : CDCl₃

11

solvent : CDCl₃

12

solvent: CDCl_3

12

solvent: CDCl₃