

Supporting Information

for

Oxidation of a Levitated 1-Butyl-3-methylimidazolium Dicyanoborate ([BMIM][DCBH]) Droplet by Nitrogen Dioxide

Michael Lucas,¹ Stephen J. Brotton,¹ Jan A. P. Sprenger,² Maik Finze,² Shiv K. Sharma,³ Ralf I. Kaiser*¹

¹ Department of Chemistry, University of Hawaii at Manoa, Honolulu, HI 96822, USA

² Julius-Maximilians-Universität Würzburg, Institute for Inorganic Chemistry, Institute for Sustainable Chemistry & Catalysis with Boron (ICB), Am Hubland, 97074 Würzburg, Germany

³ Hawaii Institute of Geophysics and Planetology, University of Hawaii at Manoa, Honolulu, HI 96822, USA

Corresponding Author

*E-mail: ralfk@hawaii.edu

Analysis of 1-butyl-3-methylimidazolium dicyanoborate

Elemental analysis calculated for C₁₀H₁₇BN₄ (204.15 g mol⁻¹): C 58.85, H 8.40, N 27.45%; found: C 58.91, H 8.49, N 27.53%.

¹H NMR (400.13 MHz, Aceton-d₆): *d* = 8.87 (s br, 1H, NCHN), 7.64 (dd, 1H, ³*J*(¹H, ¹H) ≈ 1.75 Hz, NCHCHN), 7.58 (dd, 1H, ³*J*(¹H, ¹H) ≈ 1.75 Hz, NCHCHN), 4.25 (t, 2H, ³*J*(¹H, ¹H) = 7.38 Hz, NCH₂), 3.95 (s, 3H, NCH₃), 1.84 (m, 2H, NCH₂CH₂), 1.31 (m, 2H, CH₂CH₂CH₃), 0.93 (q, 2H, ¹*J*(¹H, ¹¹B) = 94.0 Hz, BH), 0.87 (t, 3H, ³*J*(¹H, ¹H) = 7.45 Hz, CH₂CH₃) ppm.

¹¹B NMR (128.38 MHz, Aceton-d₆): *d* = -41.8 (t, 1B, ¹*J*(¹H, ¹¹B) = 92.6 Hz, BH).

¹³C{¹H} NMR (100.62 MHz, Aceton-d₆): *d* = 135.5 (s, 1C, NCHN), 133.4 (q, 2C, ¹*J*(¹¹B, ¹³C) = 60.8 Hz, BCN), 123.3 (s, 1C, NCHCHN), 121.9 (s, 1C, NCHCHN), 48.9 (s, 1C, NCH₂), 35.5 (s, 1C, NCH₃), 31.2 (s, 1C, NCH₂CH₂), 18.6 (s, 1C, CH₂CH₃), 12.3 (s, 1C, CH₂CH₃) ppm.

Analytical Instruments and Details

The NMR spectra were recorded at 25 °C in acetone-d₆ on a Bruker DPX 400 spectrometer. ¹H and ¹³C chemical shifts were calibrated against the residual solvent signal and the solvent signal, respectively (*d* (¹H): (CD₂H)(CD₃)CO 2.05 ppm; *d* (¹³C): (CD₃)₂CO 29.84 ppm and 206.26 ppm).

Elemental analysis (C, H, N) were performed with a a Elementar Vario MICRO cube instrument (Elementar Analysensysteme, Germany).