Sulfur and Selenium Activation by Frustrated NHC/$B(C_6F_5)_3$ Lewis Pairs; Conformational Flexibility of Products

Dirk Holschumacher, Constantin G. Daniliuc, Peter G. Jones, and Matthias Tamm

Institut für Anorganische und Analytische Chemie, Technische Universität Braunschweig, Postfach 3329, 38023 Braunschweig, Germany

Reprint requests to Prof. Dr. M. Tamm. Fax: +49-531-391-5387. E-mail: m.tamm@tu-bs.de

Z. Naturforsch. **2011**, *66b,* 371 – 377; received February 18, 2011

Frustrated Lewis pairs consisting of N-heterocyclic carbenes (NHC) and the borane $B(C_6F_5)_3$ react with elemental sulfur or selenium to give products of the type NHC-*E*-$B(C_6F_5)_3$, where *E* is S or Se. Three such products, two with sulfur and one with selenium, were characterized by X-ray diffraction and shown to exhibit considerable conformational flexibility, as revealed by differing torsion angles in the atom sequence N–C–*E*–B–C_{ipso}–C_{ortho}. In the sulfur derivatives, the S–B bonds are all long (*ca.* 2.05 Å), and the C–S bonds (*ca.* 1.73 Å) are clearly lengthened compared to imidazole-2-thiones. The Se–B distance of 2.2111 Å is the first selenone-borane bond length to be determined by X-ray analysis.

Key words: N-Heterocyclic Carbenes, Frustrated Lewis Pairs, Sulfur, Selenium