Synthesis and Characterization of Diborane Compounds. Alexander Damme, Holger Braunschweig, Department of Inorganic Chemistry, Julius-Maximilians University Würzburg, Germany
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The oxidative addition of B–B bonds of diboranes(4) to late transition metal centres affording bis(boryl)complexes \([L_2M(BR_2)_2]\) [1,2] is of great importance because it constitutes the key step in metal-mediated diboration reactions of unsaturated substrates under both homogeneous [3,4] and heterogeneous [5] conditions. Based on facile oxidative addition of B–Br and B–I bonds to Pt(0) centres [6], we became interested in the reactivity of diboranes(4) \(Br_2B_2R_2\) (\(R = \text{NMes}, \text{Mes}\)) towards low-valent phosphine platinum complexes. We have now successfully accomplished the synthesis of two different types of diboryl(4) complexes of platinum. Oxidative addition of one B–Br bond of \(Br_2B_2(N\text{Me}_3)\) to \([\text{Pt}(\text{PEt}_3)_2]\) enabled the isolation of the corresponding diboryl(4) species trans-\([\text{Et}_2\text{Pt}(\text{Br})(\text{NMes})(\text{NMes})]\)} in reasonable yields. Similarly, the reaction of \(Br_2\text{BMe}_2\) with \([\text{Pt}(\text{PEt}_3)_2]\) yields trans-\([\text{Et}_2\text{Pt}(\text{Br})(\text{Mes})(\text{Mes})(\text{Br})]\)}, which features a dative bond from the platinum to the second boron atom, resulting in a distorted square-pyramidal geometry of the platinum centre [7]. In course of this reaction the released phosphine \(\text{PEt}_3\) reacts with one equivalent of diborane(4) forming a mixture of the sp²–sp³ isomeric monophosphine-diborane adducts \(\text{MesBrB–B(PEt}_3\text{)BrMes}\) (1) and \(\text{Mes}_2\text{B–B(PEt}_3\text{)BrBr}\) (2). The main product 2 displays an uncommon B–Br–B bridge and the presence of a dative B–Br bonding interaction to the sp³ boron centre. Reaction of the bulkier phosphine \(\text{PMeCy}_2\) with the diborane(4) affords a similar mixture of adducts of which the main product is the 1,1-dimesityl adduct \(\text{Mes}_2\text{B–B(PEt}_3\text{)Br}\), formally a product of phosphine-induced 1,2-rearrangement of mesityl and bromine ligands [8].

Until recently the diborane component of diboryl-bridged \(ansa\)-complexes has been limited to the amino-substituted \(B(N\text{Me}_3)_2\)-B(N\text{Me}_3) fragment. We have now isolated the new \([2]\text{boraferrocenophane (Fe(}c_5\text{C}_5\text{H}_5\text{)–B(Mes)(Mes)–B(Mes)(–c_5\text{C}_5\text{H}_5)}\)]) which can be readily prepared by the salt metathesis reaction of 1,1'-dilithioferrocene with \(\text{Cl}_2\text{B}_2\text{Mes}_2\) [9].

Keywords: boron compounds; platinum coordination compounds; ferrocene compounds

Acesulfame has been used as a non-caloric artificial sweetener since 1988 [1]. Its coordination properties are important because acesulfame has potential donor atoms which can form coordination bonds with metal ions [2].

The title compound, \(\text{C}_2\text{H}_8\text{Ba}_2\text{Na}_2\text{O}_9\text{S}_8\), is a one dimensional coordination polymer and can be formulated as \([\text{Ba(acs)}_2\text{H}_2\text{O}]\). The compound crystallizes in the centrosymmetric monoclinic space group \(P2_1/c\) with \(a = 8.2223(3), b = 18.9945(6), c = 11.7819(4)\), \(\beta = 123.902(2)\)° and \(Z = 4\). The \(\text{Ba}^{2+}\) ion, surrounded by O- and N-atoms, has nine coordination and the complex forms a polymer that extends parallel to the \(a\)-axis. The molecular structure is stabilized by \(\text{O}\cdots\text{H}–\text{O} and \text{C}–\text{H}–\text{O}\) intermolecular hydrogen bonds.

The geometric parameters which are obtained from X-ray diffraction and the theoretical parameters for the asymmetric unit which are calculated by using density functional theory (B3LYP) with the 6-31G basis sets are compared.

Furthermore, molecular electrostatic potential map and frontier molecular orbital calculations together with experimental and theoretical IR studies were made for this structure.

Keywords: Acesulfamato ligand; Density functional theory; Barium (II) complex