

MS43-P3 **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 $[L_nM(BR_2)_2]$ [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) $Br_2B_2R_2$ ($R = NMe_2, Mes$) towards low-valent phosphine platinum complexes. We have now successfully accomplished the synthesis of two different types of diboranyl(4) complexes of platinum. Oxidative addition of one B–Br bond of $B_2Br_2(NMe_2)$ to $[Pt(PiPr_3)_2]$ enabled the isolation of the corresponding diboranyl(4) species $trans-[(iPr_3P)_2Pt(Br)\{B(NMe_2)B(NMe_2)Br\}]$ in reasonable yields. Similarly, the reaction of $Br_2B_2Mes_2$ with $[Pt(PEt_3)_3]$ yields $trans-[(Et_3P)_2Pt(Br)\{B(Mes)B(Mes)Br\}]$, 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 PEt_3 reacts with one equivalent of diborane(4) forming a mixture of the sp^2-sp^3 isomeric monophosphine-diborane adducts $MesBrB-B(PEt_3)BrMes$ (**1**) and $Mes_2B-B(PEt_3)Br_2$ (**2**). The main product **2** displays an uncommon B–Br–B bridge and the presence of a dative B–Br bonding interaction to the sp^2 boron centre. Reaction of the bulkier phosphine $PMeCy_2$ with the diborane(4) affords a similar mixture of adducts of which the main product is the 1,1-dimesityl adduct $[Mes_2B-B(PEt_3)Br_2]$, formally a product of phosphine-induced 1,2-rearrangement of mesityl and bromine ligands [8].

Until recently the diborane component of diborane-diyl bridged *ansa*-complexes has been limited to the amino-substituted $B(NMe_2)-B(NMe_2)$ fragment. We have now isolated the new [2]boraferrocenophane $[Fe(\eta^5-C_5H_4)-B(Mes)-B(Mes)-(\eta^5-C_5H_4)]$ which can be readily prepared by the salt metathesis reaction of 1,1'-dilithioferrocene with $Cl_2B_2Mes_2$ [9].

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MS43-P4 **Experimental and DFT Studies on Poly[okta- μ_3 -acesulfamato-O,O':N,O';O',N:O,O-tetraaquatetrabarium(II)] Complex.** Güneş Demirtaş,^a Necmi Dege,^a Hasan Yıçbudak,^b Ömer Yurdakul^b and Orhan Büyükgüngör^a ^aOndokuz Mayıs University, Faculty of Arts and Sciences, Department of Physics, 55139 Samsun-Turkey. ^bOndokuz Mayıs University, Faculty of Arts and Sciences, Department of Chemistry, 55139 Samsun-Turkey.
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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, $C_{32}H_{40}Ba_4N_8O_{36}S_8$, is a one dimensional coordination polymer and can be formulated as $[Ba(acs)_2H_2O]_n$. The compound crystallizes in the centrosymmetric monoclinic space group $P2_1/c$ with $a = 8.2223(3)$, $b = 18.9945(6)$, $c = 11.7819(4)$ Å, $\beta = 123.902(2)^\circ$ and $Z = 4$. The 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 $OZH\cdots O$ and $CZH\cdots O$ 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.

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