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Ab-Initio Calculations of the Dissociation Energy and Periodic Properties of the Heavy P-block Dimers

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Abstract. Molecular orbital calculations within the ab-initio frame work using SBK-basis set at the RHF level are reported for heavy P-block dimers of the fourth (Ga_2, Ge_2, As_2, Se_2 and Br_2), fifth (In_2, Sn_2, Sb_2, Te_2 and I_2) and sixth (Tl_2, Pb_2 and Bi_2) rows. The results of the molecular orbital interpreted and correlated in terms of equilibrium bond length, bond order, bonded valence, total valence, total energy, nuclear energy, electronic energy, electron-electron energy, electron-nuclear energy, nuclear-nuclear energy and dissociation energy. The effect of d-orbital on the ground state properties is also reported. The results indicate that method used gives fairly satisfactory predication of the molecular properties.