Supporting Information

Tuning of the Optical Properties and Lewis Acidity of Dibenzopnictogenaborins by Modification on Bridging Main Group Elements

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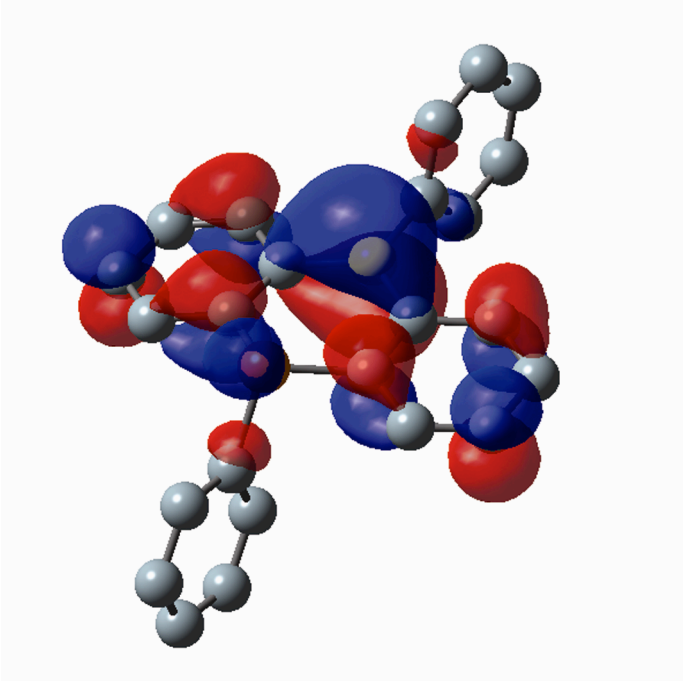
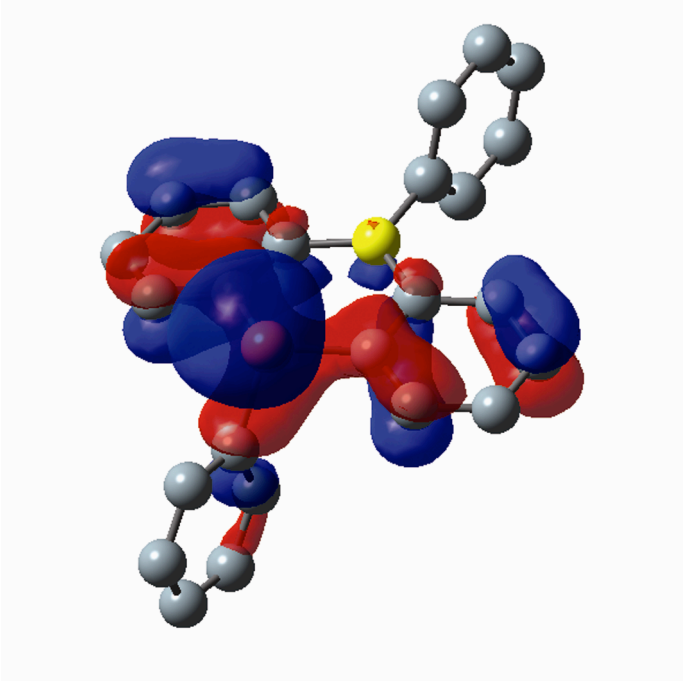
Orbital plots (isovalue: 0.03)
All the calculations were carried out at B3LYP/6-31G(d) level of theory using Gaussian 03 program package. Orbital plots were generated by GaussView 3.09.[1] In order to reduce computation time, mesityl groups on boron atoms were replaced by phenyl groups.

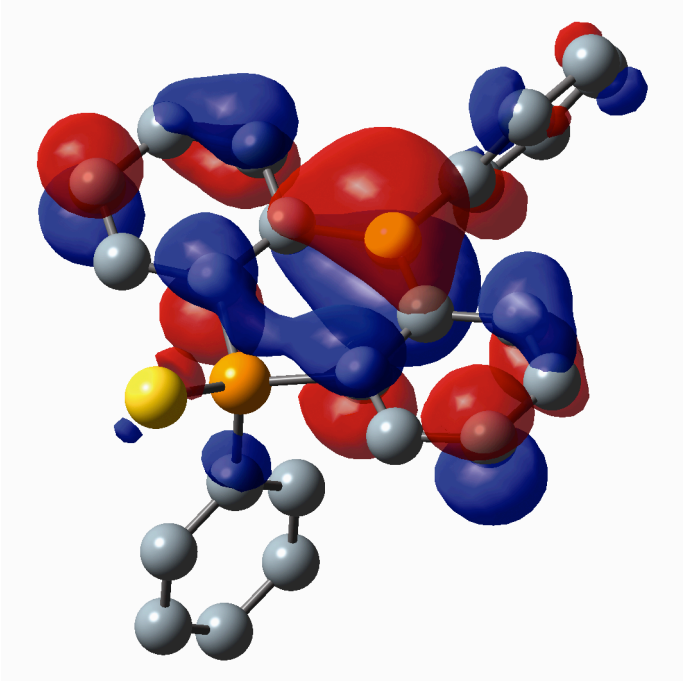
LUMO of **1**



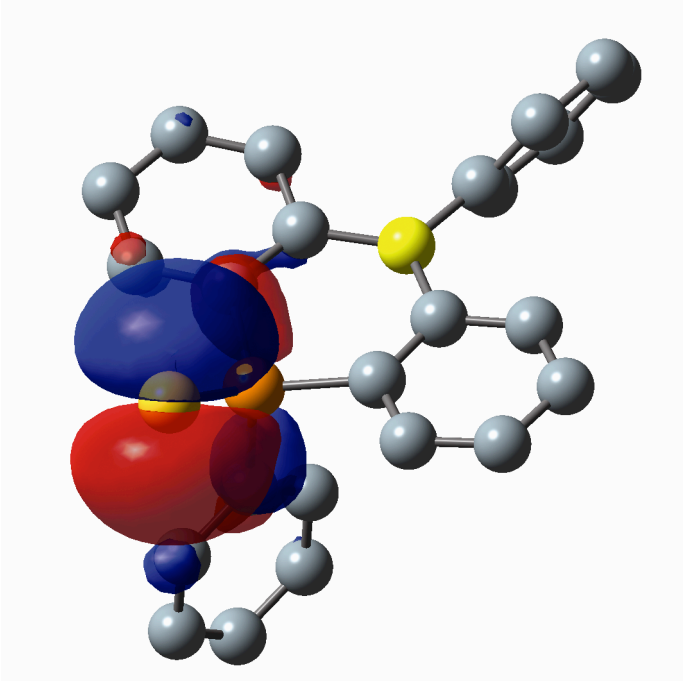
HOMO of **1**



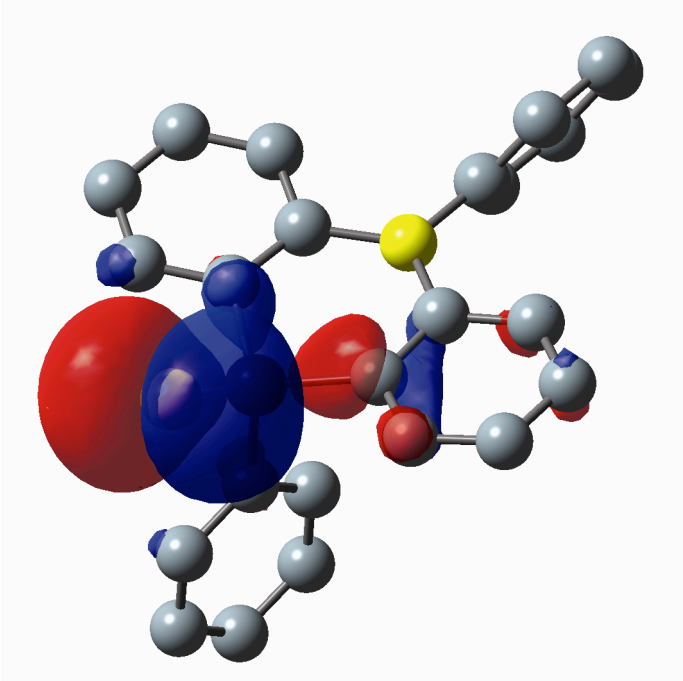
LUMO of **2**



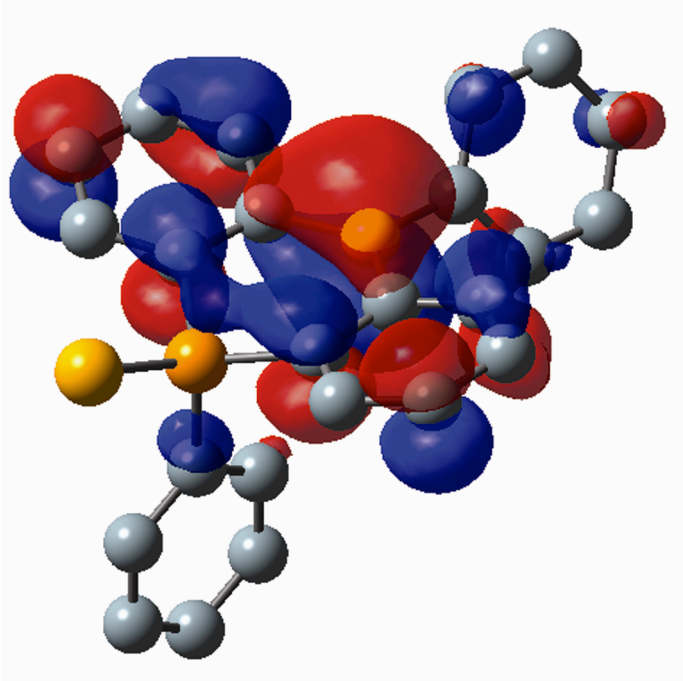
HOMO of **2**



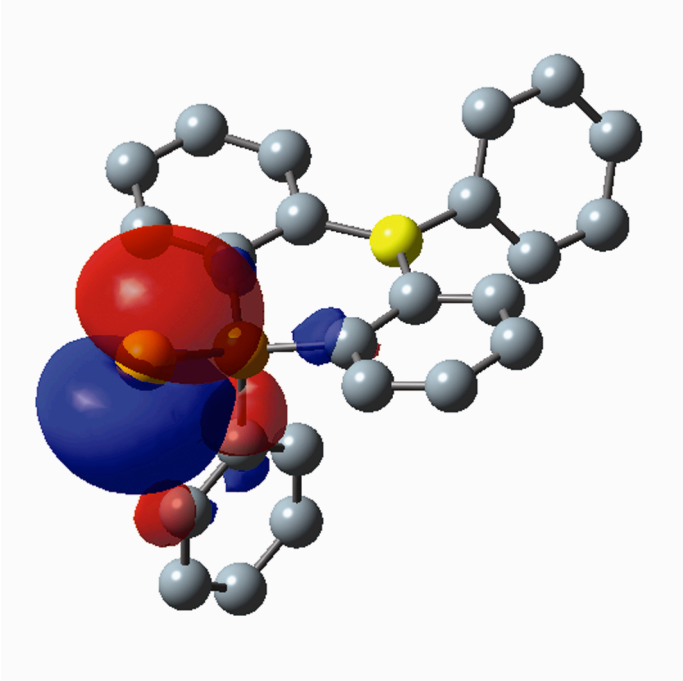
NHOMO of **2**



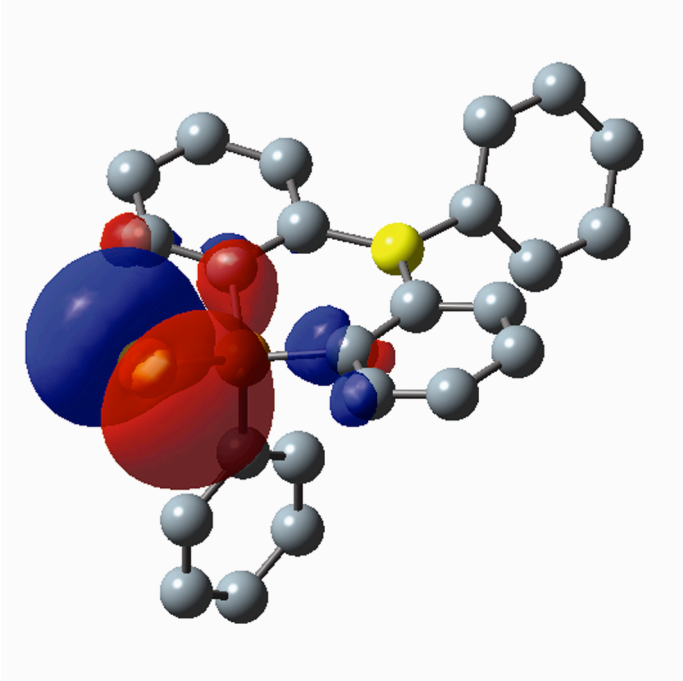
LUMO of **3**



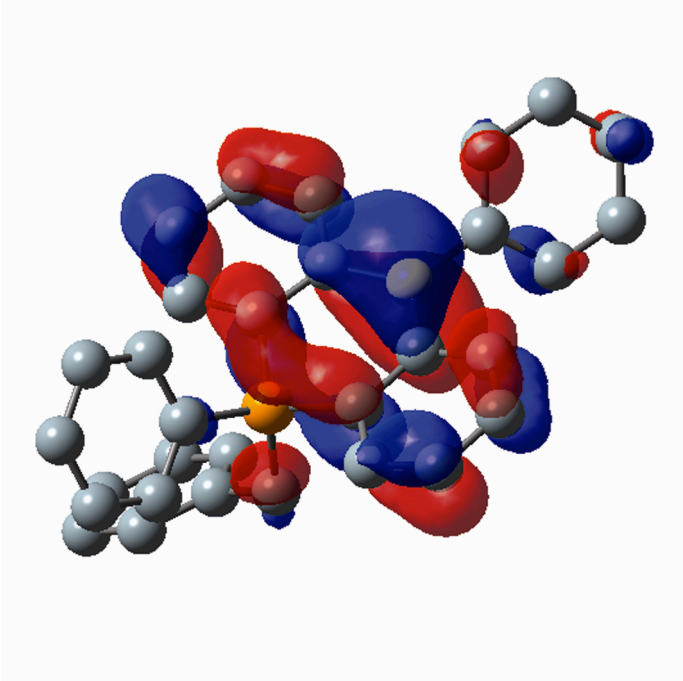
HOMO of **3**



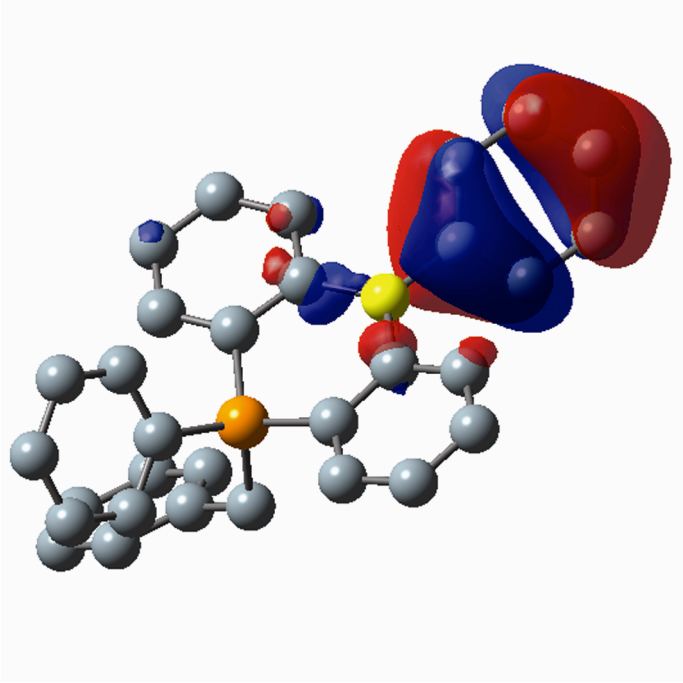
NHOMO of **3**



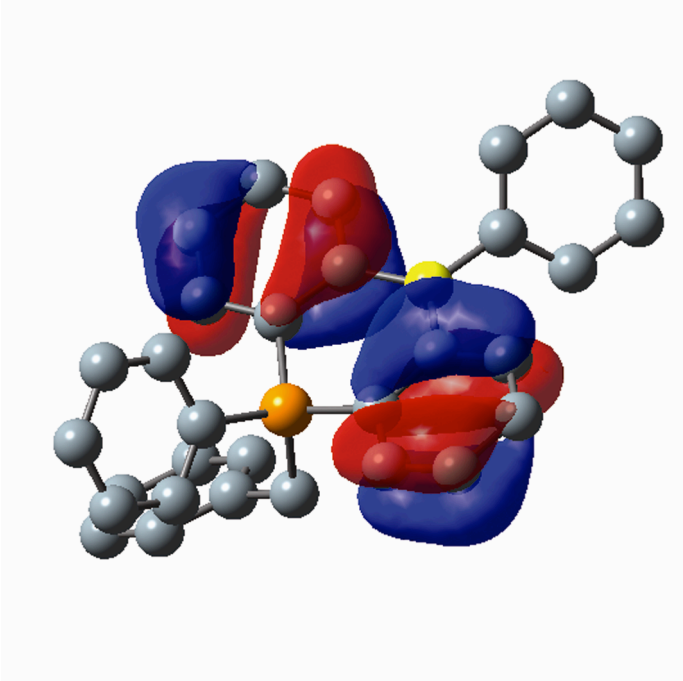
LUMO of **4**



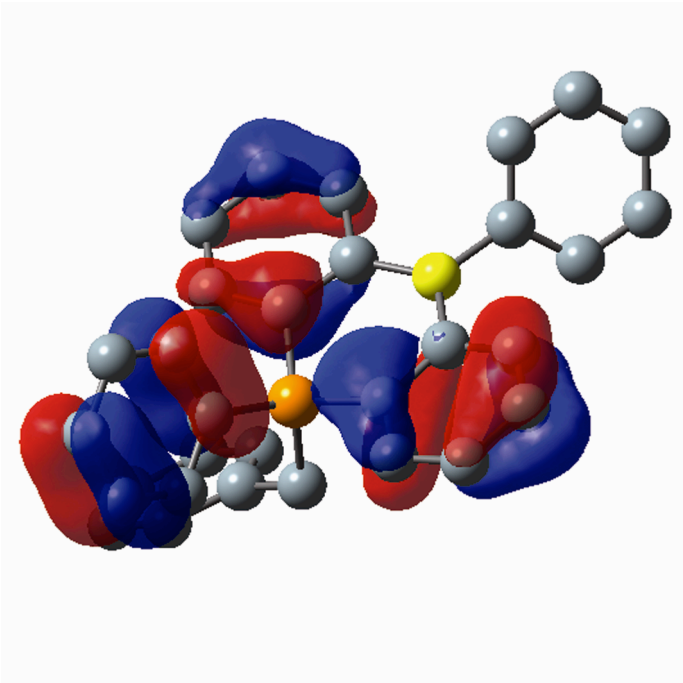
HOMO of **4** (a π orbital of the *B*-Ph group)



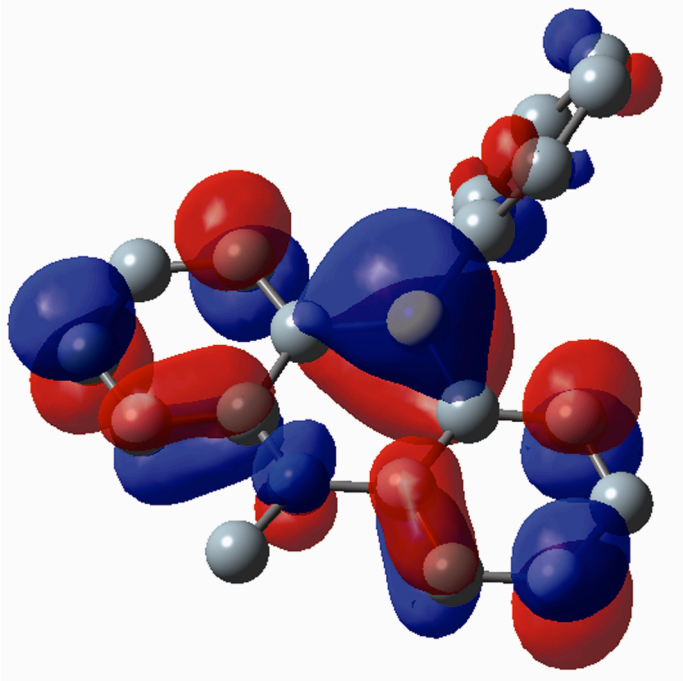
The highest π orbital of **4**



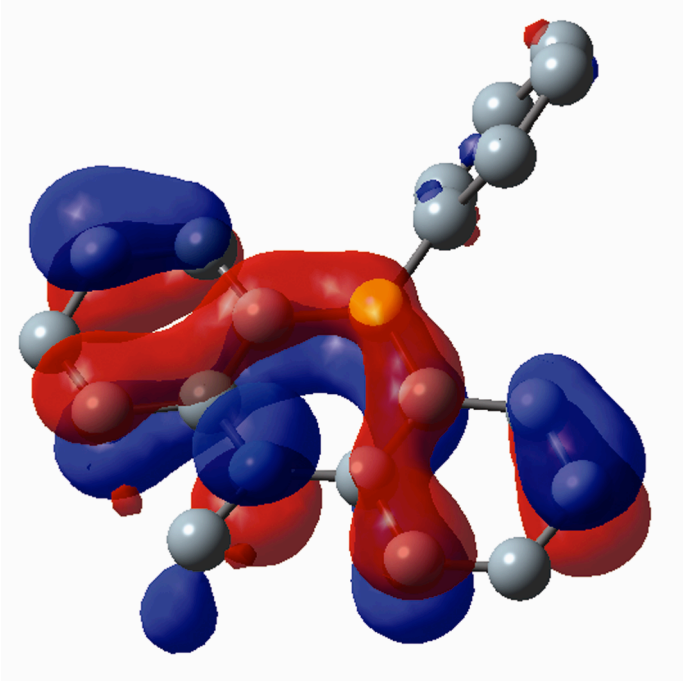
The second highest π orbital of **4**



LUMO of **7**



HOMO of **7**



Reference for Supporting Information

(1) GaussView, Version 3.09, Dennington II, Roy; Keith, Todd; Millam, John; Eppinnett, Ken; Hovell, W. Lee; and Gilliland, Ray; Semichem, Inc., Shawnee Mission, KS, 2003.