THE NEW 2D CHEMISTRY OF BORON

Josep M. Oliva-Enrich[a], Maxime Ferrer[b,c], Rubén López-Sánchez[a], Ibon Alkorta[b], José Elguero[b]

[a] Physical Chemistry Institute "Rocasolano" (CSIC), 28006 Madrid, Spain
[b] Instituto de Química Médica (CSIC), 28006 Madrid, Spain
[c] PhD Programme in Theoretical Chemistry and Computational Modelling, Doctoral School, Universidad Autónoma de Madrid, 28049 Madrid, Spain

Isolation of 2D boron and borane sheets, the latter isoelecronic and quasi-isostructural to graphene, call for the possibility of developing a new 2D boron chemistry. Planarity in borane molecules is very unusual. Theoretical models and counting rules have also been developed for 2D borane systems. By means of the {C=C} ↔ {B(H_2)B} transformation one can transform any conjugated open or closed (polycyclic) hydrocarbon C_nH_m into the corresponding isostructural and isoelectronic borane B_nH_{m+n} by substituting every 2π electrons for a perpendicular H_2 moiety and all carbon atoms by boron atoms. For instance the singlet-triplet gaps in naphthalene and anthracene are smaller as compared to the equivalent planar boranes, respectively; hence, if ever synthesized these planar boranes could be stable. We will show several examples where planarization enhances stability and provides new directions within 2D boron chemistry: (i) benzene analogues R-Ph, (ii) polycyclic conjugated hydrocarbons, and (iii) ferroborane, the latter an analogue of ferrocene from a structural and electronic point of view.