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Extended Abstract
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Advanced chemistry: 2019 -Fascinating boron-nitrogen-containing heteroaromatic compounds: Electronic structure analysis- Anna Chrostowska

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The heteroaromatic compounds contain boron (B), nitrogen (N) are a family of heterocycles which are isoelectronic and isostructural to the family of conventional organic homologs such as mono-nitrogen containing benzene, naphthalene and heterocycles such as pyrrole, indole and iso. -indole. Their development significantly increases the structural diversity and potential utility of aromatic compounds, but the properties and reactivity of these B'-aromatic heterocycles have not been fully explored. Ultraviolet photoelectronic spectroscopy (UV-PES) is a well-established technique for the gas phase in molecules of ionization energies. These experimental data are supported by the Coherence for Quantitative Calculations, which provide the PE bands for the basic information on the electronic structure and connectivity of any other technique. Boron (B) -nitrogen (N), which contains heteroaromatic compounds of the field in our research, has been chosen exclusively for the advantages and wide applicability of this approach.

Huge developments in the chemistry of organoboranes and related compounds over the past two years have greatly contributed to recent advances in synthetic organic chemistry. The chemistry of boron-containing heterocycles is diverse. A boron atom containing a variety of heteroaromatic compounds, for example for borazaromatics, has been studied, mainly because of their interesting physical and chemical properties. A number of boron derivatives have been synthesized and evaluated for their potential use in the treatment of cancer. In some cases, various boron reagents with heterocycles of the reaction intermediates as their derivatives.

Boron nitride is a thermally and chemically resistant refractory compound of boron and nitrogen with the chemical formula BN. It is a similar structure of a carbon network with various isoelectronic crystal forms. The hexagonal shape corresponding to graphite is the most stable and softest of the bn polymorphs, and is therefore used as a lubricant and additive to cosmetic products. The diamond-like cubic variety (sphalerite structure) is called c-BN; It is softer than diamond, but its thermal and chemical stability is higher. The BN wurtzite of the rare modification is similar to the lonsdaleite but slightly softer than the cubic shape. Due to their excellent thermal and chemical stability, boron nitride ceramics are traditionally used as high

temperature equipment pieces. Boron nitride has potential use in nanotechnology.

Heterocyclic compounds can be usefully classified according to their electronic structure. Saturated heterocycles behave like acyclic derivatives. Thus, piperidine and tetrahydrofuran are conventional amines and ethers, with modified steric profiles. Consequently, the study of heterocyclic chemistry focuses on unsaturated derivatives in particular, and the implications of the preponderance of work and applications in unconstrained 5 and 6-membered cycles. Included are pyridine, thiophene, pyrrole and furan. Another large class of heterocycles refers to those fused to benzene nuclei. For example, the fused benzene analogs of pyridine, thiophene, pyrrole and furan are related to quinoline, benzothiophene, indole and benzofuran. The Fusion's two benzene rings give rise to a third large family of compounds. The heterocycles analogues mentioned above are compounds of this third family: acridine, dibenzothiophene, carbazole and dibenzofuran, rewardment. Unsaturated rings can be classified according to the union of the heteroatom with the conjugated pi system.

The electronic structure calculations did not start with the so-called "ab initio" calculations. The Underlying Findings date back to the 1930s with an understanding of the quantum nature of bonding in solids, Hartree and Fock approximations and Bloch's theorem. Semi-empirical electronic structure calculations using nuclear materials, for example, close bond calculations. These value calculations should not be overlooked. However, in what follows, we focus on the "ab initio" calculations, ie the functional density theory (DFT).

This work is partly presented on 2nd European Congress on Advanced Chemistry on May 09-10, 2019 held at Stockholm, Sweden

In this article, we use it, most people in the materials science community, as a synonym for DFT calculations. The popularity of these methods comes from the fact that, as we will see, they provide quantitative results on many properties of solids without any adjustable parameters, but both conceptual and technical difficulties remain. New paradigm in materials science in general, and they are now accepted as very powerful tools in scientific research and cause radiation. The presentation is divided as follows. The methodologies and tools are briefly presented in the first section. The next two sections focus on some examples of ab initio results in the field of nuclear materials, metals and alloys on one hand and insulating materials on the other.

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