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Full Factorial Analysis on One-Cage Pentagonal Faced Nanostructures

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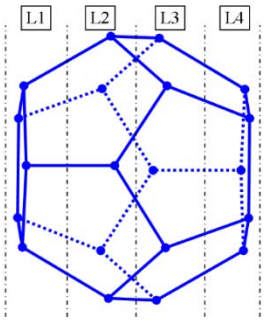
Dodecahedrane is a chemical compound with high symmetry, which has in each vertex a carbon atom that bonds three neighboring carbon atoms and one hydrogen atom [1]. In fact, dodecahedrane is only one representative of a series of congeners, which allow conducting a stability study in the series.
The elementary unit of one-cage pentagonal face structure was used to construct the whole class of compounds using three atoms from the same period which allow formation of at least three bonds: boron, carbon, and nitrogen. The elementary structure was split in four layers and on each layer one atom could take places (either C = carbon, N = nitrogen, B = boron).



A total number of 81 structures (3^4) could be constructed based on four layers (L1-L4) and three levels (C, N, B) but due to symmetry, just 45 of them are distinct.
The distinct structures of this family of cages were taken into study. Full factorial analysis (including all 45 congeners) was applied on distinct one-cage structures to characterize the family. In the first step of the analysis, the geometry of structures was optimized with Spartan software (v.10) using Møller Plesset method (MP2 level of theory) with 6-31G* (polarized valence split) basis set. In the second step of the analysis, the values of the following properties were calculated with Spartan software: volume, surface area, ovality, HOMO energy, LUMO energy, polarizability, dipole moment, entropy, enthalpy, and energy (at zero point). In the third step, full factorial analysis was conducted for three distinct cases, with C, N, or B as reference and other two atoms as factors [2]. A program was implemented for full factorial analysis and its applicability is presented. The first model in the full factorial analysis takes all factors and all possible interactions between factors that lead to a model with a determination coefficient of one (always true in the full factorial analysis). A stepwise backward method is implemented to withdraw from the model the less influential factors or interactions and to calculate the models characteristics. Good models with goodness-of-fit higher than 0.95 were obtained on the investigated structures with factors that ranged from two (enthalpy with C and N, respectively as reference) to twenty-seven (HOMO energy with C as reference). The highest correlation coefficient was obtained for energy as property of interest in models with four factors and any of the investigated atoms as reference (r = 0.9999). The highest correlation coefficient was obtained when carbon atom was the reference in 67% of cases.

References

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