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Elemental factorial study on one-cage pentagonal face nanostructure congeners

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ABSTRACT

A full factorial design with two factors applied on the family of 81 dodecahedrane congeners is presented. One of the factors used four levels (the layers of the structure), while the other factor used three levels (the atom as Boron, Carbon, or Nitrogen, with the same atom for the layer). Ten calculated properties were input for investigation of the link between properties and structural features. Boron, Carbon or Nitrogen were considered as a reference atom. The models with determination coefficient near 1 comprised 22 to 44 distinct factors. The complexity of the models increases from boron taken as a reference to carbon taken as reference. Therefore, along with the less complexity with the factorial analysis (here elements were accounted in a trinomial scale), alternatives for the reference should also be sought (the available software packages for this type of regression do not check when the table of transformation from multinomial data type to binomial variables is built).

1. Introduction

Dodecahedrane ($C_{20}H_{20}$), a chemical spherical compound with high symmetry, has in each vertex a carbon atom that bonds three neighboring carbon atoms and one hydrogen atom [1]. The compound was first synthesized at the Ohio State University in 1982 [1–3] but theoretical studies in regards of group theory, graph theory, or molecular orbital theory were conducted since 1975 [4–7]. The dodecahedrane is a Platonic structure [8] and the compound and/or its derivatives have been investigated in theoretical [9–12] and experimental [13–16] settings. Substitution of all hydrogen atoms in $C_{20}H_{20}$ led to development of several compounds such as $C_{20}F_{20}$ (perfluorododecahedranes), $C_{20}Cl_{20}$, $C_{20}(OH)_{20}$ or $C_{20}Br_{20}$ [17]. Perfluorododecahedranes, which initially was reported as unstable [17], was successfully produced by Banfalvi in milligram quantities [18]. Dodecahedrane complexes were also of scientific interest as endo- ($X@C_{20}H_{20}$, where X = H, He, Ne, Ar, Li, Li^+, Be, Be^+, Be^{2+}, Na, Na^+, Mg, Mg^+, and Mg^{2+} [19] or X = C^{4-}, N^{3-}, O^{2-}, F^-, Ne [20]) or exo-hedral ($XC_{20}H_{20}$, X = H^+, H, N, P, C^-, Si^-, O^+, S^+ [21]) complexes. Dodecahedrane is of scientific interest due to its stability given by its high symmetry, covalent bond angles (108 °C) closest to the ideal tetrahedral bond angle (109.5°) and its C—C bound close to that of diamond (1.54 Å) [20]. Substitution of hydrogen atoms in dodecahedrane have been reported in the scientific literature [17,18,2020] but no study has investigated the substitution of carbon atoms. Furthermore, if the carbon atoms are substituted by other atom(s), the dodecahedrane become a congener [22]. An analysis of the link between the type of the atom and the properties in dodecahedrane may provide useful information on the diversity and stability of these structures. A theoretical study was conducted with the full factorial design to investigate the effects of factors and/or their interactions on ten calculated properties using the full class of dodecahedrane congeners when the molecule is seen as a four layered structure, as well as to investigate the effect on each layer when formed by carbon, boron or nitrogen.

2. Methodology

2.1. One-cage pentagonal faces nanostructures

The elementary unit of one-cage pentagonal faces structure (Fig. 1) was used to construct the full class of compounds using three atoms from the same period to assure the formation of at least three bonds (Boron, Carbon, and Nitrogen). The elementary structure was seen as a four layer structure (see Fig. 1) with each layer being occupied by one type of atom (Boron, Carbon or Nitrogen).

The full class of congeners obtained by this method was constructed based on the one-cage pentagonal faces structure

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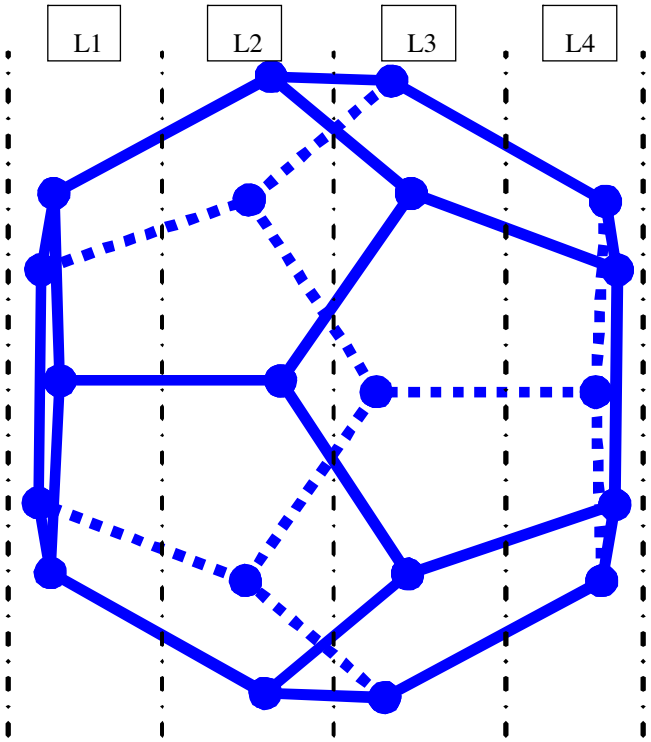

Fig. 1. Layers (L) on one-cage pentagonal faces structure.

presented in Fig. 1 and comprises 81 structures ($3^4 = 81$, where 3 is the type of the atom and 4 are the number of layers). Due to the symmetry and freedom of movement and rotation, just 45 structures are distinct (see Table 1).

The distinct structures of this family of nano-cages were study using full-factorial analysis design. The flowchart of the applied approach is depicted in Fig. 2. The cages were initially drawn with HyperChem software (geometry was initially optimized with PM3; Hypercube Inc. USA). The geometry of the cages was refined at a Hartree-Fock (RHF) level of theory [23–25] with 3–21G basis set, and further refined by Möller-Plesset [26] untill the second order (MP2) with 6–31G* basis set [27] using Spartan software (v.10, Wavefunction Inc. USA). The properties included in the full factorial analysis were calculated after geometry optimization (MP2 based calculations).

2.2. Full-factorial analysis on dodecahedrane congeners

The main issue in the proposed approach is related with the management of a large system of equations that must be solved (for one cage, with disregards of the symmetry, the system square matrix contains 729 variables). The implemented approach operates with the type of the atom (a quality) and accordingly the multinomial problem was translated into a multi-binomial problem [28]. As example, 'atom type' (as Boron, Carbon or Nitrogen) on a certain layer in Fig. 1 is a trinomial variable. The presence of a certain atom (e.g. B) was encoded with 1 (other atoms with 0), and thus the problem is translated from trinomial to tri-binomial when all three atoms are considered. One atom was taken as a refer-

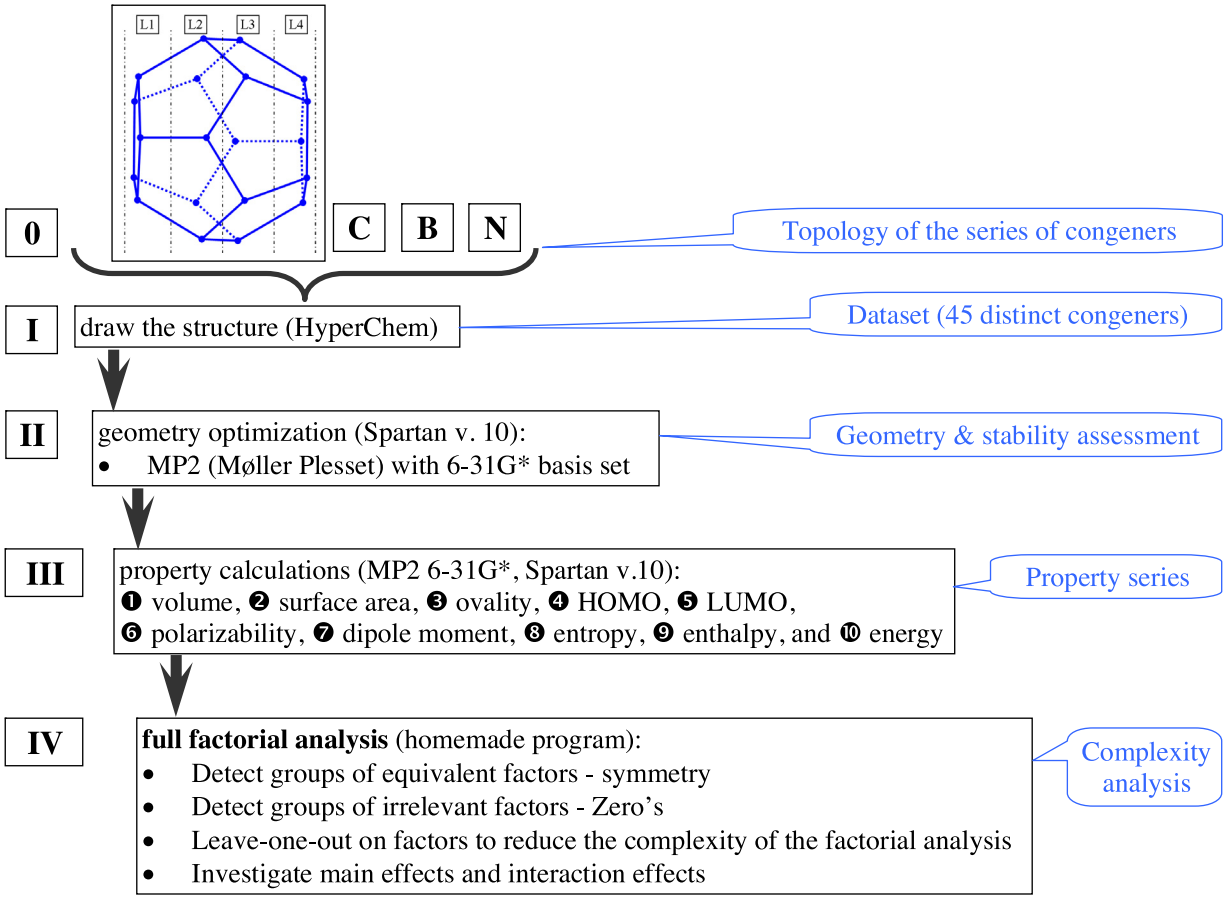

Fig. 2. Full factorial analysis flowchart on one-cage pentagonal faces structures with the same atom per layer (Boron or Carbon or Nitrogen). HOMO stands for highest occupied molecular orbital and LUMO is the lowest unoccupied molecular orbital.

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