Topological characterization of a complete set of small sized graphene sheets using molecular descriptors

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Introduction

Graphenes are very thin layers formed by hexagonal networks of carbon atoms that possess special mechanical, electrical and optical properties. There is a growing interest in the study and exploitation of graphene, expressed in numerous recent studies, being studied both theoretically and practically. For the counting of small sized graphenes please see [1]. Here, graphenes were theoretically investigated using molecular descriptors. The complete set of 22 graphene conformers with 5 cycles of 6 connected carbon atoms was subjected to the study.

Theoretical study

The Zagreb index family was used in the first instance (for a recent study using Zagreb indices please see [2]). The SMPI (from Szeged Matrix Property Indices, please see [5]) family of descriptors has been used in the second instance.

Results and discussion

The analysis showed that in the case of the analyzed graphenes, the degeneracy of the Zagreb indices is very high. In addition, when the first Zagreb index is degenerate, the structures can still be discriminated by the second Zagreb index. However, when the second Zagreb index is also degenerate, the entire Zagreb index family built with expressions involving vertex degree on adjacent ones is degenerate. In general, topological descriptors have a low power of discrimination in classes of conformers (for more details please see [3] and [4]). Moreover, for a pair of conformers even the extended Hückel energy is degenerate. In this case the resolution can be obtained with descriptors generated from molecular geometry. The SMPI discriminated all 22 conformers adequately.

Conclusions

In the case of graphenes is not recommended the characterization with Zagreb indices. It is recommended to use SMPI for graphene discrimination.

References

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