Szeged Matrix Property Indices as Descriptors to Characterize Fullerenes

Lorentz JÄNTSCHI[1,2] and Sorana D. BOLBOACĂ[3,*]

[1] *Technical University of Cluj-Napoca, Department of Physics and Chemistry, 103-105 Muncii Bldv., RO-400641, Cluj-Napoca, Romania*
[2] *Babeş-Bolyai University, Doctoral Studies - Chemistry, 11 Arany Janos str., RO-400028, Cluj-Napoca, Romania*
[3] *Iuliu Haţieganu University of Medicine and Pharmacy, Department of Medical Informatics and Biostatistics, 6 Louis Pasteur str., RO-400349, Cluj-Napoca, Romania*

Abstract. Fullerenes are class of allotropes of carbon organized as closed cages or tubes of carbon atoms. The fullerenes with small number of atoms were not frequently investigated. This paper presents a detailed treatment of total strain energy as function of structural feature extracted from isomers of C_{40} fullerene using Szeged Matrix Property Indices (SMPI). The paper has a two-fold structure. First, the total strain energy of C_{40} fullerene isomers (40 structures) was linked with SMPI descriptors under two scenarios, one which incorporate just the SMPI descriptors and the other one which contains also five calculated properties (dipole moment, scf-binding-energy, scf-core-energy, scf-electronic-energy, and heat of formation). Second, the performing models identified on C_{40} fullerene family or the descriptors of these models were used to predict the total strain energy on C_{42} fullerene isomers. The obtained results show that the inclusion of properties in the pool of descriptors led to the reduction of accurate linear models. One property, namely scf-binding-energy proved a significant contribution to total strain energy of C_{40} fullerene isomers. However, the top-three most performing models contain just SMPI descriptors. A model with four descriptors proved most accurate model and show fair abilities in prediction of the same property on C_{42} fullerene isomers when the approach considered the descriptors identified on C_{40} as the predicting descriptors for C_{42} fullerene isomers.

Keywords: nano structure-property relationship; C_{40} fullerene; C_{42} fullerene; Szeged Matrix Property Indices (SMPI).

* Corresponding author: phone: +40750774506; e-mail: sbolboaca@umfcluj.ro