Ab initio study of relative energy, charge distribution, and NICS for fullerenes C_{36} and its cationic, and its anionic forms

S. Moradi*, B. Alimadadi+, S. Behmanesh*, A. Madadi*, Z. Farahani+,
and K. Keshvari+

**Department of Chemistry, Islamic Azad University, Tehran North Branch, Tehran, Iran*
+Department of Chemistry, School of Science, Azzahra University, Vanak, Tehran, Iran

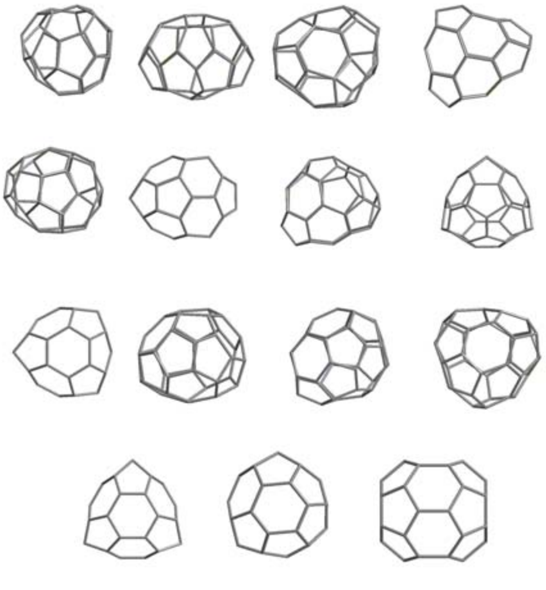
Fullerenes are characterized with presence of 12 five-membered rings and varying number of six-membered rings in their structures.

Fullerenes (C_n) with sizes n=58, 56…etc., have been observed in C_{60} collisions with fast highly charged atomic ions, electrons and laser pulses. The knowledge of the structured properties and binding energies, and charge distribution and aromatic properties of these fullerenes are essential to understand the fragmentation trends and, in particular, why fullerenes with a certain number of carbon atoms appear more frequently than others. In present study C_{36} and its $C_{36}^{+\cdot}$, C_{36}^{2+}, $C_{36}^{3+\cdot}$, C_{36}^{2-} charged forms have been considered for ab initio calculations. The geometries of all neutral species considered in this work were fully optimized at HF/6-31G*. Then geometries were reoptimized in the frame work of the density functional theory (DFT).

For the charged species, geometry optimizations were preformed at the B3LYP/6-31G* basis sets. Two different spin multiplicities were considered in the case of charged species.

NICS values were taken form GIAO-SCF/3-21G and GIAO-B3LYP/6-31G* levels using optimized B3LYP/6-31G* geometries. In these calculations only closed-shell singlet states considered.

The results and discussions for each structure with figures and tables are shown later.



Scheme fullerene structure C36

[1] X. Lu, Z. Chen, W. Thiel, P. Schleyer, R. Huang, L. Zheng, *J. Am.Chem. Soc.* **126**, 14871 (2004).
[2] E.A. Rohifing, D.M. Cox, A. Kaldor, *J. Chem. Phys.* **81**, 3322 (1984).
[3] T. Gao, R.E. Smalley, G.E. Scuseria, *J. Chem. Phys.* **99**, 351 (1993).
[4] J.M. Xiao, M.H. Lin, Y.N. Chiu, M.Z. Fu, S.T. Lai, N.N. Li, *J. Mol. Struct. (THEOCHEM)* **428**, 149–154 (1998).

Ab initio study of relative energy, charge distribution, and NICS for fullerenes C_{38} and its cationic, and its anionic forms

S. Moradi *, Z. Farahani^{+}, A. Madadi*, B. Alimadadi^{+}, K. Keshvari^{+}, and S. Behmanesh*

**Department of Chemistry, Islamic Azad University, Tehran North Branch, Tehran, Iran*
$^{+}$*Department of Chemistry, School of Science, Azzahra University, Vanak, Tehran, Iran*

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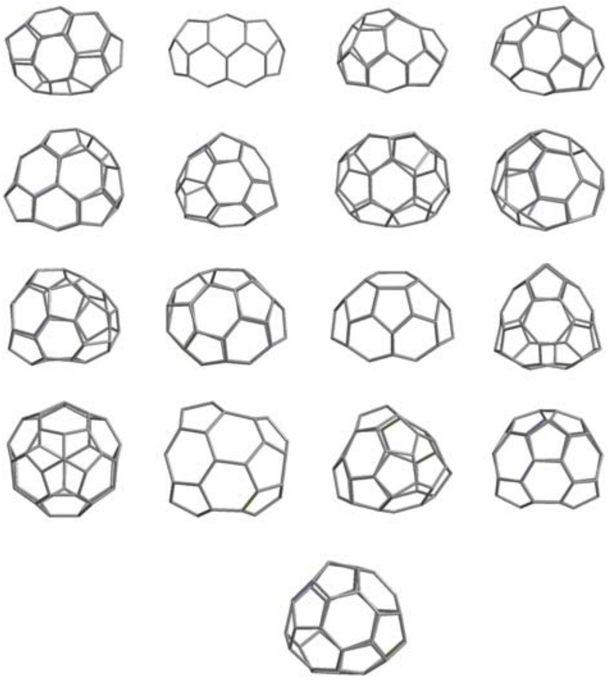

Scheme fullerene structure C38

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[1] X. Lu, Z. Chen, W. Thiel, P. Schleyer, R. Huang, L. Zheng, *J. Am.Chem. Soc.* **126**, 14871 (2004).

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