

## عنوان مقاله:

Theoretical Study of the Properties of Adenine Amino Acid Tetomers with C<sub>60</sub>

## محل انتشار:

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## نویسنده:

.Saeedeh Moghadasi - Department of Education and training, District One, Shahr-E-Rey, Tehran, Iran

## خلاصه مقاله:

In this research at the Adenine tautomers and their fullerene derivatives were optimized. NBO calculations and NMR for the tautomers and their Fullerene derivatives were carried out at the B<sup>3</sup>lyp/6-31G\* quantum chemistry level. The core and the valence electrons of atoms were compared. Other cases examined in this study, resonance energy, chemical potential ( $\mu$ ), chemical hardness ( $\eta$ ), Energy Gap, Chemical Hardness, Chemical Potential, Dipole moment parameters between Adenine tautomers and their fullerene derivatives were calculated. This organic base as a chemical component of DNA and RNA plays an important role in our body. In this study of fullerenes, we used a nano carrier. The data in tables and graphs and shapes were compared and discussed.

## کلمات کلیدی:

adenine, Fullerenes, NBO, NMR, IR

## لینک ثابت مقاله در پایگاه سیویلیکا:

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