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QSAR relationships The changes in the ratio of electrons to the natural charge of atoms in the complexes of glycine and alanine amino acids with intermediates

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Abstract

In this paper, the quantum chemistry calculations related to the structural parameter of the three anions and the resulting complexes with glycine and alanine have been performed. The calculations were carried out using the HF and DFT method and in the base series 6-31G *. Natural Transplantation Orbital (NBO), hybrid capacity for bindings and is obtained. The ratio of the internal electrons, Valance and Reedberg to the natural charge of atoms and its relation with complex stability have been considered.

Keywords: NBO, glycine, alanine, natural charge

1. Introduction