QUANTUM CHEMICAL CALCULATIONS OF AN INHIBITOR BASED ON MALEIC ACID, MONOETHANOLAMINE AND PHOSPHATE ACID

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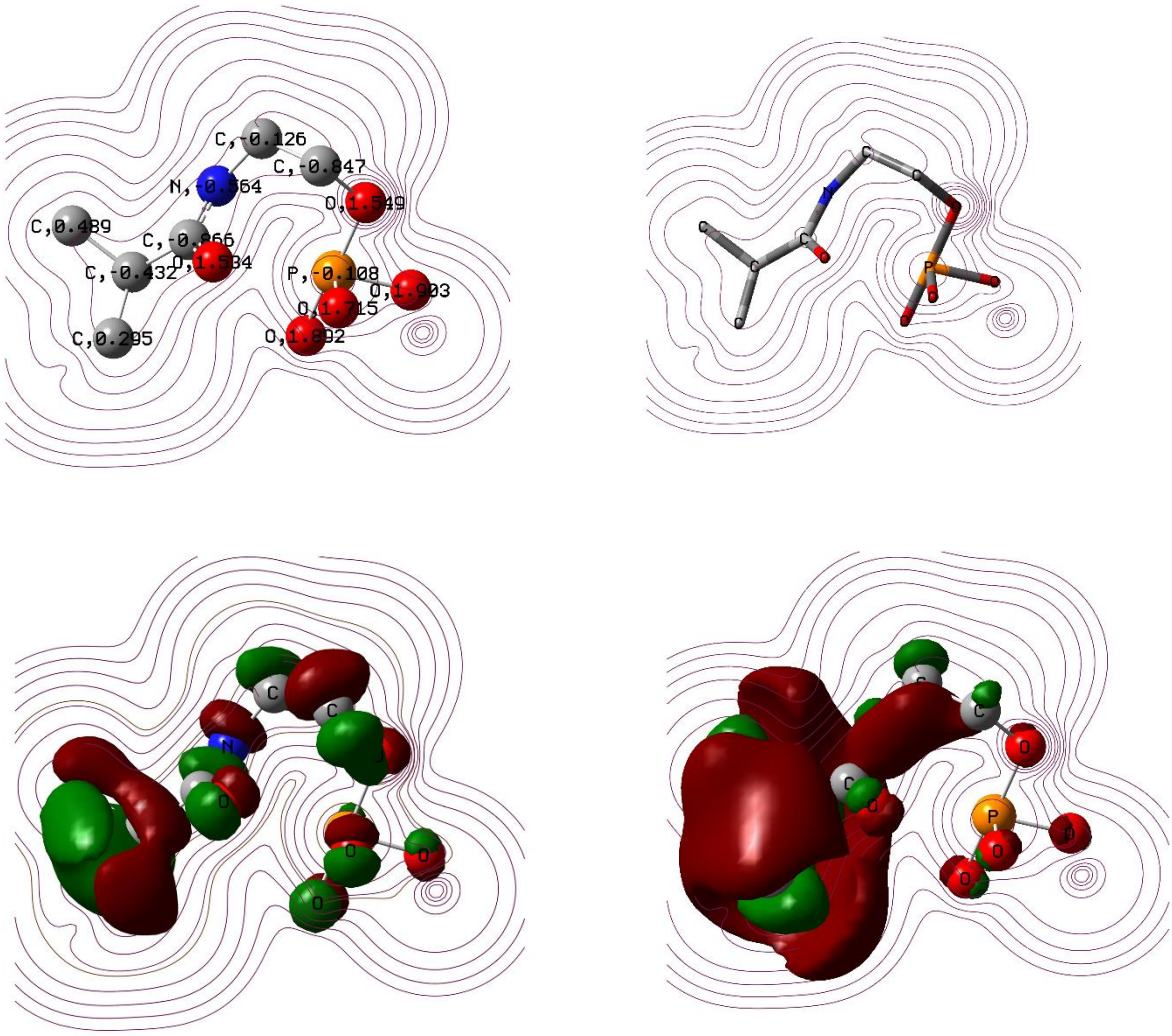
Introduction. One of the best ways to protect metals from corrosion is the use of corrosion inhibitors. The use of inhibitors can only slow down corrosion, but cannot completely stop it[1,2]. Corrosion is one of the processes that cause great damage not only to industry, but also to material and spiritual heritage. According to their types, corrosion inhibitors are divided into anodic, cathodic and mixed corrosion inhibitors [3,4]. In general, there are several types of corrosion, which are characterized by the source of origin and properties. In preventing corrosion, the use of corrosion inhibitors can allow us to use structures for a relatively longer period of time, but it cannot completely eliminate this problem [5,6].

Experimental part The geometries of the studied compounds were generated using the Avogadro software package, and then fully optimized using the Popl basis set - RHF/6-31G(d, p) using GaussView 6.0.16 software. The results of GaussView 6.0.16 calculations using the DFT (B3LYP) method, using the Mulliken method and

the frontier molecular orbital (FMO) approximation to calculate the charges on all atoms, were visualized using the Avogadro program. Comparing the values of electronic charges obtained from the calculation by these methods, it was concluded that the donor atoms with the highest value of negative charge in all calculated molecules can be coordinated.



HOMO = -2,058 eV

LUMO = 4,34 eV

Figure 1. Figure 1 shows the distribution of charge in atoms and localization of frontier orbitals.

The electron density in the HOMO of Figure 1 is located on the oxygen and secondary nitrogen atoms of the -C=O group (Figure 1.). The energies of the LUMO and HOMO states are also very different for this ligand. Therefore, in Figure 1, it

also creates a strong field, and according to Pearson's principle of "hard and soft acids and bases", the oxygen and secondary nitrogen atoms of the -C=O group compete as spectator ligands.

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