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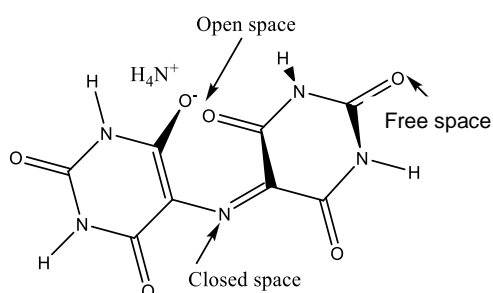
Stability of murexide-metal ion complexes in aqueous medium: A preliminary study using classical and quantum mechanics

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Murexide is an ammonium salt of purpuric acid, which is a reddish violet compound and serves as a metallochromic indicator. Although murexide is used as a suitable complexing agent for a large number of metal ions experimentally, there were not much expounded data available for its complexes. Hence, this is an attempt to explicate the stability of the structures of murexide-metal ion complexes in water, especially at three different binding sites (as given in Figure 1) using molecular mechanics (MM) and quantum mechanics (QM) techniques. Aluminium, iron, copper and zinc (Al^{3+} , Fe^{3+} , Cu^{2+} , Zn^{2+}) murexide complexes have been analyzed.



Optimized structure of murexide was generated using Gaussian 09 software on LINUX operating system with 6-31g (d) basis set and Hartree-Fock method in aqueous medium. Metal oriented structure in a befitting site was used for QM and MM simulations. Software packages were used for QM and MM simulations are Gaussian 09, GROMACS respectively in the LINUX operating system.

Figure 1. Structure of murexide indicating possible metal binding sites

Appraisal of the stability of metal complexes was carried out regarding intermolecular interaction energies in MM and Gibb's free energy change in QM. The outcome of MM and QM techniques upholds that metal ion-murexide complexation does occur as the resultant intermolecular interaction energies and change in Gibb's free energies were negative except at the closed site of Murexide- Zn^{2+} interaction in QM. The resultant trends in the stability of the metal-murexide complexes were as follows:

QM: $\text{Al}^{3+} > \text{Zn}^{2+} > \text{Cu}^{2+} > \text{Fe}^{3+}$ MM: $\text{Al}^{3+} > \text{Cu}^{2+} > \text{Zn}^{2+} > \text{Fe}^{3+}$

Despite the small variations in the trends in the stability of metal-murexide complexes, it confirms the surmise that a molecular mechanics method is sufficient for these studies and yields structural, dynamical, thermodynamic properties without much computational cost.

Keywords: Free energy, molecular dynamics, murexide-metal ion complexes