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The structural properties of a compound formed by pyrocatechines and iron

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Phenolic compounds generally has special smell, are easily soluble in water, organic solvents (alcohols, esters, chloroform, ethyl acetate), and in aqueous solutions of bases, and are colorless or colorful, crystalline and amorphous materials. Phenols form colorful complexes when they form compounds with heavy metals. In this study, the structural properties of a compound formed by pyrocatechines and iron is investigated theoretically.

The optimized geometric parameters (bond lengths, bond and dihedral angles), conformational analysis, normal mode frequencies and corresponding vibrational assignments of the compound are theoretically examined by means of B3LYP hybrid density functional theory (DFT) method together with 6-31+g(d,p) and Cep-121g basis sets. All the calculations were performed by using Gaussian 09.A1 program and GaussView 5.0.8 was used for visualization of the structure and simulated vibrational spectra.

Sum of electronic and zero-point energies of the compound is calculated as -2407.935 a.u. The geometrical parameters calculated from DFT method with the basis set of 6-31+g(d,p) of the compound: The bond lengths of the compound are calculated as C-H (1,09 Å), C-O (1,29 Å), C-C(1,43 Å), O-Fe(1,90 Å), respectively. The angles of the compound is find out as O-Fe-O (90,11°), C-O-Fe(112,81°), C-C-O(120,06°), C-C-C (119,61°), C-C-H (120,78°), respectively. C-O vibration frequencies (frequency values are scaled by 0.9648) of the compound are calculated in the range of 1296-1473. The most intense vibrations of O-C are symmetric frequency at 1360 cm^{-1} and asymmetric at 1473 cm^{-1} frequency. C=C aromatic ring vibrations are calculated at 1340 and 1569 cm^{-1}. C-H aliphatic vibrations are calculated in the range of 3077 and 3107 cm^{-1}. O-Fe vibrations are observed as stretch and twist in the range of 506-571 cm^{-1}.

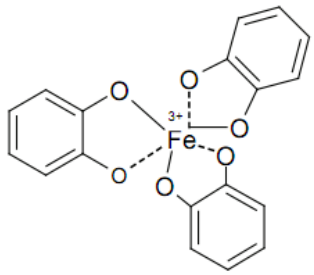

Figure. The complex of Fe^{+3} and Pyrocatechines

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