IFS PRO - 09

Structure Optimization and IR Frequency Interpretation of $Fe_6(OH)_{18}(H_2O)_6$ Nano Particles by DFT Calculations

Lakmal Jayarathna[1], Athula Bandara[2], M. Vithanage[1] and R. Weerasooriya[3]

[1]Chemical and Environmental Systems Modeling Laboratory, Institute of Fundamental Studies, Kandy
[2]Department of Chemistry, Faculty of Science, University of Peradeniya
[3]Nano Team, Institute of Fundamental Studies, Kandy

γ-Fe_2O_3 nanopratciles were syntheised by the co-precipitation method and these particles are in 5-20 nm range in size. Plausible molecular structures (Figure 1) of γ - Fe_2O_3 were examined by density functional theory (DFT) using the cluster modelling method. Cluster configurations and IR frequency calculations of $Fe_6(OH)_{18}(H_2O)_6$ were performed using the DFT hybride B3LYP function with 6-31G (*d, p*) basic set. The average bond lengths of Fe-Fe and bulk Fe-O entities as 2.93 Å and 1.92 Å, respectively. The calculated bond lengths are comparable with the crystallographic data. Vibrational frequency calculations and experimental data are in good agreement with the observations in the range of 900 cm^{-1} to1024 cm^{-1} (Figure 2). However, OH stretching frequencies at (1640), 3000, 3500 cm^{-1} of γ -Fe_2O_3 is significantly different due to H-bonding nature.

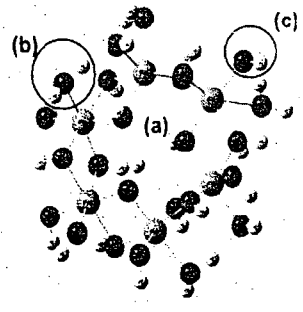

Figure 1. Structure of $Fe_6(OH)_{18}(H_2O)_6$ cluster. Region **a**: cluster cavity, **b**: Fe^{2+} bonded water, **c**: O-OH bond.

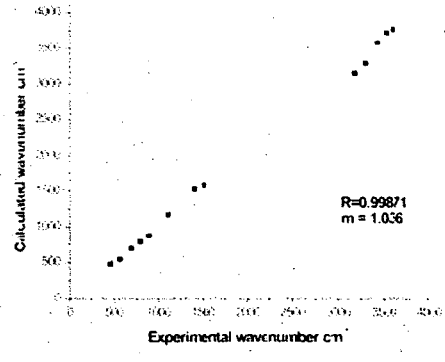

Figure 2. Comparison of experimentally derived and calculated vibrational frequencies of succinic acid - γ – Fe_2O_3 nanoparticles.