Structure Optimization and IR Frequency Interpretation of Fe₆(OH)₁₈(H₂O)₆ Nano Particles by DFT Calculations

Lakmal Jayaratna¹, Athula Bandara², M. Vithanaqe¹ and R. Weerasooriya³

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

γ-Fe₂O₃ nanoparticles were synthesised by the co-precipitation method and these particles are in 5-20 nm range in size. Plausible molecular structures (Figure 1) of γ-Fe₂O₃ were examined by density functional theory (DFT) using the cluster modelling method. Cluster configurations and IR frequency calculations of Fe₆(OH)₁₈(H₂O)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 to 1024 cm⁻¹ (Figure 2). However, OH stretching frequencies at (1640), 3000, 3500 cm⁻¹ of γ-Fe₂O₃ is significantly different due to H-bonding nature.

Figure 1. Structure of Fe₆(OH)₁₈(H₂O)₆ cluster. Region a: cluster cavity, b: Fe²⁺ bonded water, c: O-OH bond.

Figure 2. Comparison of experimentally derived and calculated vibrational frequencies of succinic acid - γ-Fe₂O₃ nanoparticles.