Order-Disorder Phase Transition in Hexakis(Imidazole)Metal(II) Complex

Pedro Martín-Zarza[a], Cristina González Silgo[b], Silvana Radescu[b], Eduardo Hernández-Bocanegra[c], Xavier Solans[d], [a]*Departamento de Química Inorgánica.* [b]*Departamento de Física Fundamental II, Universidad de La Laguna.* [c]*Departamento de Física Aplicada II, Universidad del País Vasco.* [d]*Departamento de Cristalografía y Mineralogía, Universidad de Barcelona. Spain.* E-mail: csilgo@ull.es

Imidazole has received considerable attention as a good ligand for a variety of metals. In addition to their ability to serve as models of active sites in metalloenzymes, transition metal complexes of imidazole (Him) could lead to potential applications such as electrochromic displays, photovoltaic cells and biomaterials [1-2].

$Ni(Him)_6SO_4.2H_2O$ undergoes a reversible order-disorder phase transition at 223 K, monitored by differential scanning calorimetry and single-crystal X-ray diffraction. In both phases the $[Ni(Him)]^{2+}$ cation displays $\bar{3}$ symmetry as in other similar complex. SO_4^{2-} anions and one water are disordered, displaying 3.2 site symmetry in the P P $\bar{3}$1c space group. It was of interest that the nature of this transition is due to the water reorientational motion, without space group change. We have estimated ΔH from the configurational entropy. The results are similar to those obtained in thermal analysis in which ΔH=3.529 KJ/mol. The water role is confirmed by analysis of powder samples in which the phase transition is precluded by water loss.

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