Pt(II) complexes with linear diamines. I – Vibrational study of Pt-diaminopropane

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Abstract

A conformational analysis of the $Pt(dap)Cl_2$ complex (dap = 1,3-diaminopropane) was performed by vibrational spectroscopy (FTIR, Raman and INS), coupled to quantum mechanical methods within the Density Functional Theory (DFT) and Effective Core Potential (ECP) approaches.

A complete spectral assignment of the system was achieved, due to the combined use of all available vibrational spectroscopic techniques. A good agreement was found between experimental and theoretical results, as well as with reported data for analogous complexes (e.g., cisplatin).