Normal coordinates analysis for the M(NH3)42+ complex ions in D4h and Td symmetries. Simplified molecular models

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A normal coordinates analysis for the M(NH3)42+ complex ions iN Td symmetry (M = Zn, Cd, Co) and in D4h symmetry (M = Cu, Pd, Pt) has been undertaken on the basis of a General Valence Force Field (GVFF), using simplified molecular models. Throughout the course of the present work, we have relaxed the point mass approximation for the NH3-ligands in order to investigate, on a quantitative basis, some relevant ligand - framework coupling vibrations. The simplest molecular model able to accomplish this purpose is to treat the ammino group, in a linear ligator approximation. We show that these model calculations provide a satisfactory set of vibrational frequencies as well as consistent sets of force constants.