VIBRATIONAL SPECTRA OF THE $MLCl_2$ COMPLEX FROM THEORETICAL CALCULATIONS

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The geometric and vibrational parameters (harmonic and anharmonic frequencies) of the $MLCl_2$ [M= Mn, Fe, Co, Ni, Cu, Zn, Cd, Hg; L= Ethylenediamine (en)] donor-acceptor complexes have been studied by using HF and MPW1PW91+iop(3/76=00572004280)/gen methods. Binding, reorganization, atomization, HOMO-LUMO and ionization potential energies have also been calculated with the same method. SQM calculations have been performed by using anharmonic frequencies and experimental data. The obtained results were found to be in good agreement with the corresponding experimental findings.