Trans-dichlorotetrakis (1H-pyrazole-κN2) copper (II): Synthesis, crystal structure, hydrogen bonding graph-sets, vibrational and DFT studies

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Description
The copper complex $[Cu(HPrz)_4]Cl_2$ (HPrz = Pyrazole) was synthesized and its structure was characterized by FT-IR, Raman and single-crystal X-ray diffraction (XRD) techniques. The structural conformers, optimized geometric parameters, normal mode frequencies and corresponding vibrational assignments of the compound were examined by means of the density functional theory (DFT) method, the Becke-3-Lee–Yang–Parr (B3LYP) functional, the 6-311+G(3df,p) and lanl2dz basis sets. Reliable vibrational assignments were investigated by the potential energy distribution (PED) analysis. The compound crystallizes in the monoclinic space group C2/c with the unit cell parameters *a* = 13.5430 (10) Å, *b* = 9.1480 (10) Å, *c* = 14.6480 (10) Å and *β* = 116.7° (5). There is a good agreement between the theoretically predicted structural parameters and vibrational frequencies and those obtained experimentally. The …