Experimental Charge Density Study on Vitamin B12

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A high resolution X-ray diffraction dataset (sin θ/λ=1.2Å^{-1}, 100K MoKα CCD, Rint 3.6% for 98 205 unique reflections) of vitamin B12 propanol solvate was interpreted in terms of the multipole formalism [1,2]. The structure was refined to full convergence, first using a fixed model density composed of invariom pseudoatoms [3] with standard radial functions, followed by a fit of all parameters including multipole populations restricted by local site symmetries and chemical equivalencies. This model was modified, in subsequent refinement cycles, by implementing bound-atom radial functions projected from theoretical molecular densities [4]. The results of the two refinements and DFT calculations were compared in terms of local topological properties and d-orbital populations of the Co site.

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