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Electronic Structure and Bonding in Complex Biomolecule

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For over a century vitamin B_{12} and its enzyme cofactor derivates have persistently attracted research efforts for their vital biological role, unique Co-C bonding, rich red-ox chemistry, and recently their candidacies as drug delivery vehicles *etc.* However, our understanding of this complex metalorganic molecule's efficient enzyme activated catalytic power is still controversial. We have for the first time calculated the electronic structure, Mulliken effective charge and bonding of a whole Vitamin B_{12} molecule without any structural simplification by first- principles approaches based on density functional theory using structures determined by high resolution X-ray diffraction. A partial density of states analysis shows excellent agreement with X-ray absorption data and has been used successfully to interpret measured optical absorption spectra. Mulliken bonding analysis of B_{12} and its derivatives reveal noticeable correlations between the two axial ligands which could be exploited by the enzyme to control the catalytic process. Our calculated X-ray near edge structure of B_{12} and its derivates using Slater's transition state theory are also in good agreement with experiments. The same approach has been applied to other B_{12} derivatives, ferrocene peptides, and recently DNA molecules.