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The effect of group substituent on the biological activity of antidiabetic Vanadium(IV) Complex (BMOV: bis (maltolato) oxovanadium)(Theoretical study)

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Abstract:Metals and metal complex have assumed key part in the advancement of present day chemotherapy. Metals can assume an essential part in adjusting the pharmacological properties of known medications after coordinating to a metal. Vanadium containing organic compounds have indicated extensive guarantee as available prodrugs that lighten the vast majority of the symptoms of diabetes. One of the biochemical mechanisms for insulin refinement by these compounds is that they hinder and inhibit PTPs "protein tyrosine phosphatases" that direct adversely on insulin receptor. In this work, we building and designing five derivative complexes in addition to standard (BMOV) and characterization the geometrical shape and crystal structure of a standard vanadium complex BMOV, [Bis(maltolato)oxovanadium(IV)] and its derivative depending on the DFT "density functional theory" survey of the title complexes were performed using the Gaussian 03 program. Crystal structure information, Mulliken charges allocation, complex biological effectiveness, frontier molecular orbital energies (HOMO, LUMO) of the complexes, stability, and polarity were discussed.

Keywords:Diabetes mellitus (DM); protein tyrosine phosphatases (PTPs); organic vanadium complex; density functional theory (DFT); HOMO, LUMO energies.

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