Mononuclear and binuclear dioxidomolybdenum(VI) complexes of ONO appended aroylhydrazone: Crystal structures, interaction energy calculation and cytotoxicity

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Abstract

Mono- and binuclear *cis*-MoO_2 complexes (**1**-**3**) having the general formula [MoO_2(ISF)D] (D = H_2O (complex **1**), DMSO (complex **2**) and 4,4'-bipyridine (complex **3**) ISF = 3,5-diiodosalicyaldehyde-2-furoichydrazide) have been synthesized and fully characterized by different physico-chemical methods. The molecular structures were confirmed unambiguously by single crystal X-ray diffraction studies. The octahedral geometry around the Mo(VI) central atom is satisfied by O, N, O donor atoms of dideprotonated dianionic hydrazone moiety, two oxido oxygens and oxygen/nitrogen atoms of the coordinated solvent molecules. The asymmetric unit of complexes **1** and **2** contains one molecule whereas complex **3** contains only half of the molecule. The 4,4'-bipyridine molecule acts as a linker that links the two asymmetric MoO_2D moieties to form the binuclear dioxidomolybdenum(VI) in complex **3** with Mo···Mo non-bonding distance of 12.01(10) Å. The relevance of hydrogen bonding and non-bonding interactions in the construction of supramolecular architectures were investigated. The upshots of single crystal studies were reproduced with the aid Hirshfeld surface studies. The pre-eminence of dispersion energy component over other components was established by interaction energy calculations and the energy framework analysis. The average

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