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Quantum chemical modeling of molecular and electronic structure of 5,7-dihydroxy-4,8-dimethyl-2-oxo-2*H*-chromene-6-carboxylic acid and its metal complexes

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Abstract

Quantum chemical modeling of 3,7-dihydroxy-4,8-dimethyl-2-oxo-2*H*-chromene-6-carboxylic acid (H_2L), its anionic forms, metal complexes $ZnL(H_2O)_2$, $AlLNO_3$, $CuL(H_2O)_2$, $FeL(NO_3)$ and complex anions $AlL(NO_3)_2^-$ and $AlL(NO_3)_2(H_2O)_2^-$ was performed by the DFT/B3LYP method. The NBO method was used to calculate interatomic distances, interbond angles and atomic charges.

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