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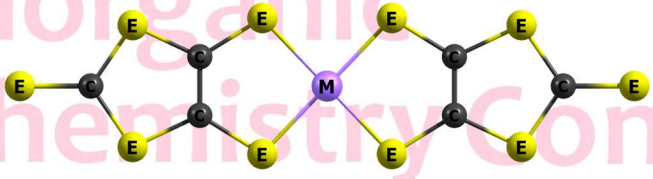
# Strength and nature of metal-dichalcogenolate bond in homoleptic metal bis(1,2-dichalcogenolate) complexes $[M(C_3E_5)_2]^{2-}$ (E=S, Se; M=Ni(II), Pd(II), Pt(II)); A theoretical study

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"Dichalcogenolene" is a general term used to describe unsaturated bidentate ligands in the form of E^E$^{x-}$ units with chalcogen donor atoms (E=S, dithiolene; Se, diselenolene; Te, ditellurolene) and different charges (x=2, 1, 0) [1]. This class of ligands includes ene-1,1- and ene-1,2 dichalcogenolates (where x=2) and also the corresponding oxidized species (neutral and monoanionic). However, the study of 1,2-dichalcogenolene ligands in coordination chemistry has been more extensive, resulting in a greater number of reported complexes [2]. In this work, the interactions between the fragments in homoleptic square-planar $d^8$ metal bis(1,2-dichalcogenolate) complexes $[M(C_3E_5)_2]^{2-}$ (E=S, Se; M=Ni(II), Pd(II), Pt(II)) have been investigated, at BP86/def2-TZVP and M06/def2-TZVP levels of theory. Four types of interaction energies between the fragments as well as the total interaction energies of the complexes [3–5] were calculated and compared. An Energy Decomposition Analysis-Natural Orbital for Chemical Valence (EDA-NOCV) was also performed to study the nature of metal−bis(dichalcogenolate) interactions in these complexes. The results showed that the total interaction energies are decreased by changing the chalcogen atom from sulfur to selenium. The analysis of metal−bis(dichalcogenolate) interaction showed that the orbital interactions have less contribution to the total attractive interactions compared to electrostatic interactions.




**$[M(C_3E_5)_2]^{2-}$**
**E** = S, Se
**M** = Ni(II), Pd(II), Pt(II)

***Keywords:*** 1,2-Dichalcogenolate, Metal Complexes, Interaction Energy, Nature of Bond.

**References**

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