Topological analysis of the bonds in incomplete cuboidal [Mo_3S_4] clusters.

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Streszczenie

The nature of the bonding interactions within the trinuclear [$Mo_3S_4Cl_3(PH_3)_6$]$^+$ cluster with an [M_3X_{13}] structural type has been investigated using the present topological theories of the chemical bond. The values of the electron density at the Mo–Mo and Mo–ligand bond critical points (bcps) are small, making a topological description of the bond using the electron density as the scalar function difficult. The characteristics of the different bonds can be better understood using the delocalization index, $\delta(A, B)$, or through a topological analysis of the electron localization function (ELF), $\eta(r)$. The delocalization indexes involving the Mo and S centers within the [Mo_3S_4] cluster core are in good agreement with the predominant covalent character of the Mo–Mo and Mo–S bonds. The [Mo_3S_4] unit is unambiguously identified as a chemical entity in the first ELF bifurcation diagram, and futher increasing the $\eta(r)$ value separates the the Mo–S and S valence domains from that of the [Mo_3] core, which further splits into three disynaptic V(Mo, Mo) basins and one trisynaptic V(Mo, Mo, Mo) basin. Calculations of the basin populations and their covariances suggest the existance of a delocalized Mo-(μ_2-S)-Mo bond. Analysis of the orbital contribution to the V(Mo, Mo) and V(Mo, Mo, Mo) basins enables us to establish a relationship between the topological and the MO picture of the bond.

Adres publiczny

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