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Using density functional to evaluate isotopic shifts in the lead compounds

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Abstract

In the present work, at the level of B3LYP/SDD and BP86/TZ2P+ theory quantum-chemical calculations of clusters of sulfur compounds of divalent and tetravalent lead, and lead sulfide have been carried out. It has been shown that this level of theory is applicable for estimation of geometrical parameters, Raman and IR spectra, and thermodynamic characteristics of sulfur and lead compounds. It has been shown that there exists correlation between the experimental and computed characteristics of lead sulfide. The effect of the isotopic shift of lead and sulfur on the change of thermodynamic parameters and Raman spectra for lead sulfide has been estimated.