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Quantum-chemical study of the structure and properties of isotropically pure selenides and tellurides of lead

© **Nikolay B. Egorov**,[1]* **Oleg Kh. Poleschuk**,[2+] **Ivan I. Zherin**[2] and **Alexander L. Ivanovsky**[3]
[1] *Department of Chemical Technology of Rare, Scattered, and Radioactive Elements. Tomsk Polytechnical University. Lenin St., 30. Tomsk, 634050. Russia. Phone: +7 (3822) 41-91-07. E-mail: egorov@tpu.ru*
[2] *Department of Organic Chemistry. Tomsk State Pedagogical University. Komsomolskiy St., 75. Tomsk, 634041. Russia. Phone: +7 (3822) 59-14-54. E-mail: poleshch@tspu.edu.ru*
[3] *Laboratory of Quantum Chemistry and Spectroscopy of the Institute of Solid State Chemistry. UrDRAS. Pervomayskaya St., 91. Ekaterinburg, 620990. Russia. Phone: +7 (343) 374-53-31. E-mail: ivanovskii@ihim.uran.ru*

*Supervising author; +Corresponding author

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Abstract

In the present work at the level of the theory B3LYP/SDD and BP86/TZ2P+ quantum-chemical calculations of compounds of selenium and tellurium, and lead chalcogenides have been conducted. It is shown that this level of theory is applicable in estimating the geometrical parameters, the Raman spectra and IR spectra and thermodynamic characteristics of compounds of lead chalcogenides. It is shown that there are dependencies between the experimental and calculated characteristics of sulfide, selenide and lead telluride. The effect of isotope shift of lead, selenium and tellurium on the change of thermodynamic parameters and the Raman spectra for the lead chalcogenides was estimated.