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Computational modelling of pentlandite-like structures

The platinum group elements (PGEs) exist in different structures which are known and studied to some extent. The existence of these PGEs in pentlandite-like structure is a promising host phase of these PGEs. In this study Vienna Ab-initio Simulation Package (VASP) density functional theory code was used to investigate phase stability of the PGEs, M_9S_8 ($M = Ru, Pd, Os, Pt, Ir$ and Rh), pentlandite-like structures. The phase stability was investigated by calculating heat of formation, elastic properties, density of states (DOS) and phonon dispersion curves. The calculated heats of formation predicted that the stability decreased as: $Os_9S_8 > Ru_9S_8 > Ir_9S_8 > Rh_9S_8 > Pt_9S_8 > Pd_9S_8$. These indicated that the formation stability increases with an increasing period and decreasing group on the periodic table. Elastic properties of these pentlandite-like systems were calculated and we found that Rh_9S_8 , Ir_9S_8 , Pd_9S_8 and Os_9S_8 were mechanically stable, whereas Pt_9S_8 and Ru_9S_8 were unstable. The density of state of Ru_9S_8 and Pt_9S_8 appeared to have high contribution of electrons at Fermi level which suggested that Ru_9S_8 and Pt_9S_8 are unstable. The partial density of states showed that the atoms at tetrahedral sites lower the stability in the pentlandite-like systems. The phonon dispersion curves indicated that Os_9S_8 , Ir_9S_8 and Rh_9S_8 have no negative modes at the gamma point suggesting stability, while the other structures are unstable. Thus the Os_9S_8 , Ir_9S_8 and Rh_9S_8 are the most stable phases. These findings provided new knowledge that established the stability of the PGEs existence in a pentlandite-like structure that could be applicable in geological search of such phases.

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