Quantum Modelling of AgHMoO4, CsHMoO4 and AgCsMoO4 Chemistry in the Field of Nuclear Power Plant Safety

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Abstract : In a major nuclear accident, the released fission products (FPs) and the structural materials are likely to influence the transport of iodine in the reactor coolant system (RCS) of a pressurized water reactor (PWR). So far, the thermodynamic data on cesium and silver species used to estimate the magnitude of FP release show some discrepancies, data are scarce and not reliable. For this reason, it is crucial to review the thermodynamic values related to cesium and silver materials. To this end, we have used state-of-the-art quantum chemical methods to compute the formation enthalpies and entropies of $AgHMoO_4$, $CsHMoO_4$, and $AgCsMoO_4$ in the gas phase. Different quantum chemical methods have been investigated (DFT and CCSD(T)) in order to predict the geometrical parameters and the energetics including the correlation energy. The geometries were optimized with TPSSh-5%HF method, followed by a single point calculation of the total electronic energies using the CCSD(T) wave function method. We thus propose with a final uncertainty of about 2 kJmol⁻¹ standard enthalpies of formation of $AgHMoO_4$, $CsHMoO_4$, and $AgCsMoO_4$.

Keywords : nuclear accident, ASTEC code, thermochemical database, quantum chemical methods
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