Radioactive $RaAg^+$ molecular ion: electronic structure, formation schemes, and propsects for precision measurements

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We present a theoretical investigation of the formation of the radioactive molecular ion $RaAg^+$. As a basis for comparison, we first conducted a systematic study of the electronic structure of the $X^1\Sigma$ ground state of radium-alkali-metal molecular ions, $RaAlk^+$ (Alk = Li, Na, K, Rb, Cs and Ag). The ground-state potential energy curves and permanent dipole moments (PDMs) are computed using high-level quantum chemistry methods, specifically the coupled cluster approach with single, double, and perturbative triple excitations [CCSD(T)], in combination with large Gaussian basis sets and small-core relativistic energy-consistent pseudopotentials. Subsequently, we determined the excited state potential energy curves and dipole moments of eight λ–S states and fourteen Ω states for $RaAg^+$ using the multireference configuration interaction method with Davidson correction (MRCI+Q). The spectroscopic parameters of the bound states are extracted, and spin-orbit coupling effects are explicitly accounted for in our calculations. Additionally, we employed coupled-channel calculations to estimate the nearest-neighbor density of magnetic-field-induced Feshbach resonances in ultracold Ra^+ + Ag collision systems. The present results may be useful for creating a quantum simulator using ultracold Ra^+ ions and Ag atoms.

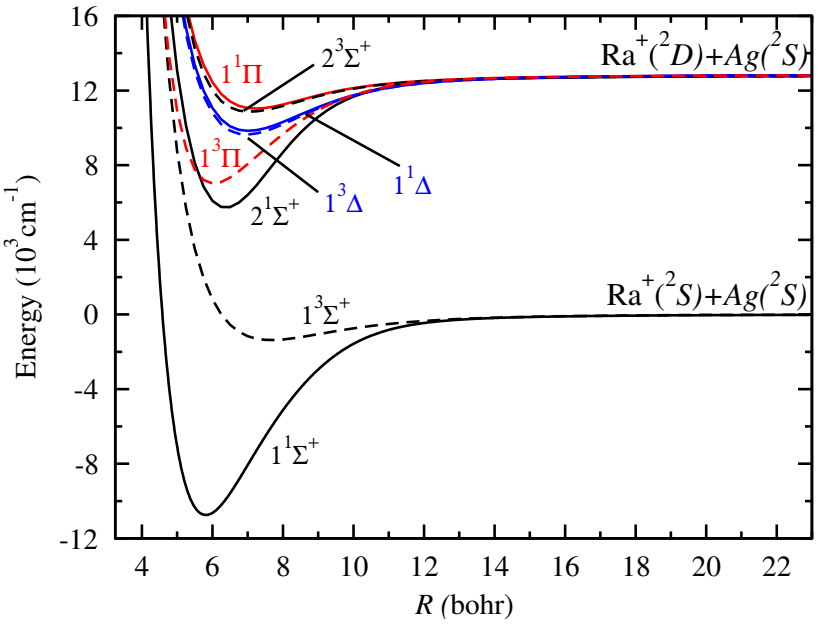

Figure 1: Potential energy curves for the ground and exited states using MRCI+Q and aug-cc-pwCV5Z.

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