Electronic structure and theoretical prediction of the formation of cold BaAlk+ (Alk= Na, K, Rb, Cs) molecular ions complexes

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The emerging field of ultracold ion-atom mixtures, comprising alkali-metal atoms and alkaline-earth-metal ions, has opened pathways for manipulating and creating ultracold molecular ions. Motivated by recent experimental studies on ultracold mixtures of Ba+ ions immersed in alkali-metal atoms, this paper focused on studying and conducting a comparative spectroscopic analysis of $BaAlk^+$ (Alk=Na, K, Rb, Cs) molecular ions. Our approach involves first a computational scheme without spin-orbit coupling, based on multi-reference configuration interaction (MRCI) and semi-empirical pseudo-potential theory of the atomic cores Ba^{2+}, Na^+, K^+, Rb^+, and Cs^+ utilizing extended and optimized basis sets. We have determined the adiabatic potentials and their corresponding relative spectroscopic constants, electric dipole moments, vibrational level spacings, and radiative lifetime. Following this initial analysis, we incorporated the spin-orbit operator into the valence MRCI calculations using optimized relativistic spin-orbit pseudopotentials. This incorporation allows us to generate Ω molecular states, which are then split into $\Lambda - S$ states, enabling a deeper understanding of the electronic structure of the studied molecular ions. The obtained results could be explored to investigate the formation of these molecular ions from ion–atom collision systems through stimulated Raman adiabatic processes. Our results are important for the experimental realization of cold molecular ion formation.