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Photodissociation of cold $RbBa^+$ ions produced in a hybrid cold atom-ion trap

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Synopsis The formation and destruction processes of cold $RbBa^+$ molecular ions are modelled in the context of their experimental observation in hybrid setups merging cold atom and cold ion traps.

Investigating atom-ion interactions in hybrid setups merging a cold atom trap and a cold ion trap has revealed to be one of the novel developments of research on ultracold matter. Beside elastic or inelastic binary collisions, charge exchange, or three-body collisions, the formation of cold molecular ions has been directly observed by one group [1], while they are predicted to be created in most experiments of this kind [2].

Here we present a theoretical investigation about the possible destruction of $RbBa^+$ molecular ions by a photodissociation mechanism, due to the many lasers involved in the experimental setup of Ref. [3]. The potential energy curves (PEC) and all the relevant permanent and transition electric dipole moments (PEDM and TEDM, respectively) of $RbBa^+$ are calculated in a semiempirical methodology which has been already used in our group to describe a number of diatomic systems [4]. Both atoms are represented as a one-electron system, where the valence electron is moving in the field of a relativistic effective core potential (ECP) with a core polarization potential (CPP) correction. The $RbBa^+$ electronic structure is thus reduced to an effective two-electron problem. The re-maining two valence electrons are considered to calculate the Hartree-Fock and the excitation determinants, in an atom-centered Gaussian ba-sis set, through the usual self-consistent field methodology. Finally, a full configuration inter-action (FCI) is achieved.

With this data we computed the state-to-state absorption cross section, $\sigma_{\Lambda vj}(\nu)$, of a $RbBa^+$ rovibrational level (v,j) in the Λ electronic state induced by a laser with frequency ν. Following Ref. [3] we focused on photodissociation by a 1064 nm laser towards accessible electronic states Λ', reaching continuum states with angular momentum j' and energy $\varepsilon=\hbar k$. The corresponding process is illustrated in Figure 1.

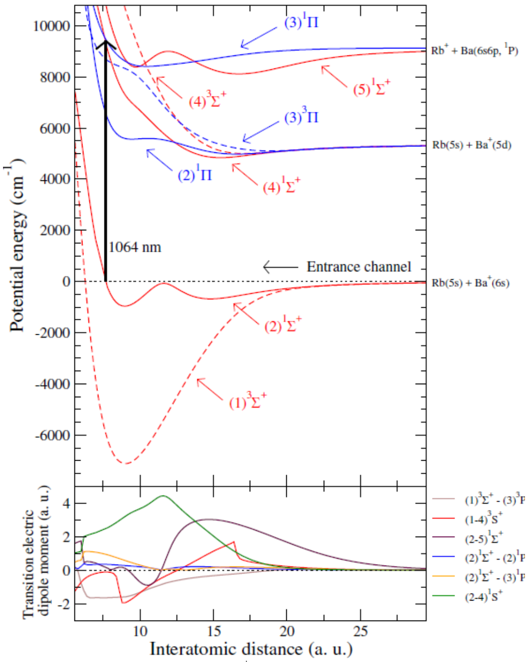

Figure 1. Computed $RbBa^+$ potential energy curves and transition dipole moments. The suggested transition (black arrow) corresponds to an initial weakly-bound molecular ion assumed to be created by three-body collision (see Ref. [3])

Preliminary results indicate that the lifetime of the molecular ions is strongly limited by the presence of laser light in the experiment, in agreement with the findings of Ref. [5].

References

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