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Interaction of Ag($5s$) and Ag($5p$) with noble gas atoms

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Synopsis We investigate the interaction of ground and excited states of silver atom with all the noble gases, including helium. Born-Oppenheimer potential energy curves are calculated with quantum chemical techniques and spin-orbit effects in the excited states are included. We compare with experimentally available spectroscopic data, as well as previous calculations. The assignment of vibrational levels in the one experiment we compare with, may have to shift up by one unit.

There's a great deal of interest in trapping and cooling of atomic and molecular species, ostensibly for detailed manipulation of interatomic interactions, and precise spectroscopy [1]. Cold and ultracold atomic and molecular ensembles are also employed as prototypes to simulate many-body quantum condensed-phase matter, study processes far from equilibrium, and to create quits for quantum logic operations. Nearly all of the current focus has been on cooling and trapping of alkali metal atoms and associated molecular species due to availability of accessible cycling transitions for laser cooling in such species. The paradigm shift to trapping other atoms occurred with the advent of general-purpose magnetic and off-resonant optical trapping schemes in recent years.

One such atom is silver which has been trapped in a magneto-optical trap, and in a buffer-gas cooled magnetic trap. It was found that in a high density He buffer gas cooled trap, Ag has a sizeable propensity to undergo three-body recombination (Ag-He $\rightarrow$ AgHe (v=0,J)* + He $\rightarrow$ AgHe(0,0) + He) and form van der Waals (vdW) complexes [2]. This process of formation of weakly-bound molecules shows up as a loss of Ag atoms from the trap.

In this work, we will describe the molecular states resulting from the interaction of Ag($5s$) and Ag($5p$) with all the noble gases. The spin-orbit interaction cannot be neglected in systems involving silver. Its effect is to split the ^2P state of Ag into the doublet $^2P_{1/2}$ and $^2P_{3/2}$ at 29552.1 cm^{-1} and 30472.7 cm^{-1}, respectively, separated by 920.6 cm^{-1}. In the Ag-NG complexes, the effect of the SO interaction is to mix the $A\ ^2\Pi$ and $B\ ^2\Sigma^+$ state into a $^2\Pi_{3/2}$ state (dissociating to $^2P_{3/2}$) and a $^2\Pi_{1/2}$ and $^2\Sigma_{3/2}$ state (dissociating to $^2P_{1/2}$).

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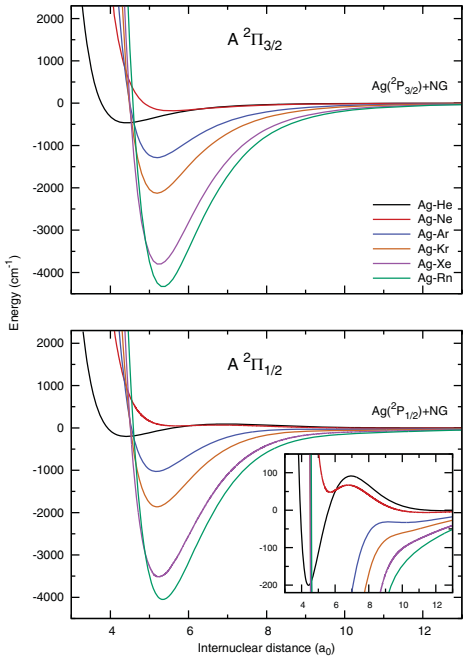

Figure 1. Potential energy curves of the $^2\Pi_{1/2}$ state of the Ag($5p$)-NG complexes. The effect of the spin-orbit interaction is visible in the inset [3].

The potential energy curves (PECs) of the $X\ ^2\Sigma^+$ and $A\ ^2\Pi$ states were calculated using the spin-unrestricted coupled cluster method with single, double, and perturbative triple excitations (UCCSD(T)), as implemented in the MOLPRO 2009.1 package. Comparison is made with available experimentally observed vibrational transitions.

References

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