

## Modeling RbCs Spectra, Photoassociation, and Cold Molecule Formation

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This talk will describe how spectroscopic information can help design a route from cold atoms to cold molecules. In particular I will discuss computational work and analysis of spectra in support of experiments to produce cold RbCs molecules by the DeMille group at Yale [1]. The goal is to produce molecules in the  $J = 0, v = 0$  level of the ground electronic state for use as qubits in an optical lattice [2]. At present, the favored strategy is to excite photoassociation resonances (PAR) just below the  $\text{Rb}(5S)+\text{Cs}(6P_{1/2})$  threshold, let them decay to appropriate  $a$  or  $X$  state levels, and then induce a Raman transition via mixed  $A/b$  state levels to  $X(v = 0)$ . Many PARs have been cleanly observed and matched reasonably well to eigenvalues calculated from fitted potentials, as reported in [1].

The model potentials were constructed from a) an analysis of spectroscopic data on the  $A^1\Sigma^+$  and  $b^3\Pi$  states, as reported in [3] and extended since; b) long range dispersion coefficients from [4], slightly adjusted to optimally fit the data; and c) *ab initio* calculations [5] for electronic states with no spectroscopic data. Franck-Condon factors calculated for radiative decay of the PARs indicate which ground state levels will be populated in the first step. Of particular interest are two possible routes to intermediate energy levels of the highly mixed  $A$  and  $b$  states, from which it is estimated that the  $X(v = 0)$  state can be reached by a single stimulated decay. Namely, a) decay of a PAR at the inner turning point of the  $A/b$  state to an  $X$  state level bound by more than  $1,000\text{ cm}^{-1}$ , followed by reexcitation to an intermediate  $A$  state level; and b) decay of a PAR to  $a^3\Sigma^+$  levels, followed by reexcitation to  $A/b$  state levels at the inner turning point of the  $a$  state. Experiments are now beginning to confirm the possibilities of scheme b). We are also attempting to improve our knowledge of the  $a$  state potential from data on reexcitation of  $a$  state levels to mixed  $A/b$  levels, which are relatively well known from [3].

The detection of the  $X$  state levels and design of the Raman process depend on accurate knowledge of the  $A$  and  $b$  states. Because of possible analogies to similar experiments on other alkali dimers, we briefly review the current status of the analysis of spectroscopic data on these states in RbCs. Our “standard model” includes non-relativistic  $^S\Lambda$  (case a) potentials characterized in the low energy regime by Dunham-RKR expansions together with diagonal and off-diagonal spin-orbit functions. For the latter, Morse-type functions are used to reproduce the known asymptotic limit, and the minimum at  $R$  somewhat greater than  $R_e$ , such as has been obtained in every alkali dimer studied so far. The discrete variable representation (DVR) numerical method is used to calculate eigenvalues for these highly mixed states. Unfortunately, for the  $\approx 1,000$  presently available experimental term values, including very few  $|\Omega|=1$  and no  $|\Omega|=2$  levels, we find that fits to this standard model exhibit an rms residual of roughly  $0.2\text{ cm}^{-1}$  as compared with experimental errors of perhaps  $0.005\text{ cm}^{-1}$ . These persistent discrepancies are a matter for further study when more data are available. Also, to better characterize  $|\Omega| = 1$  PARs, it would be useful to have accurate experimental data on the  $(1)^1\Pi$  and  $(2)^3\Sigma^+$  states of RbCs.

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