Characterization of the spectral signal of the double-well broad potential curve of NaH D state

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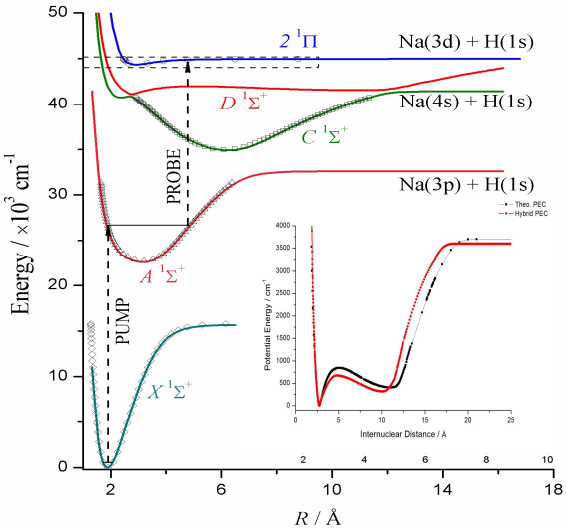
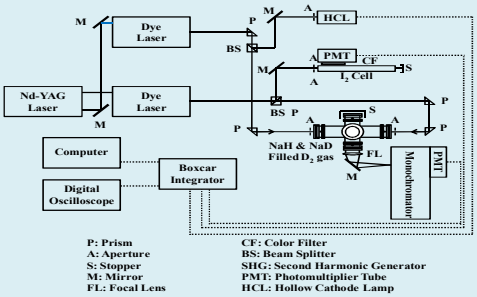
Abstract

Using pulsed optical-optical double resonance fluorescence depletion spectroscopy, many ro-vibrations of the NaH $D^1\Sigma^+$ state have been observed. The *ab initio* calculations show that the adiabatic potential energy curve of the NaH $D^1\Sigma^+$ state has a very shallow double-well structure, with completely different well widths giving different rotational constants and vibrational spacing, while the high-energy region is another very wide potential well confined by an outer turning points of ion interaction (characterized by the 1/R leading term). In this potential well, the rotation constant and vibration spacing have significantly different characteristics in different energy ranges, from which we can deduce the interaction force between NaH diatomic molecules. Due to predissociation, the linewidths of some rotational vibrational energy levels are more than ten times wider than those of conventional depletion signals. In this presentation, we construct a hybrid potential curve modified from a theoretical curve to better represent the observed ro-vibration energy levels.

Experiment

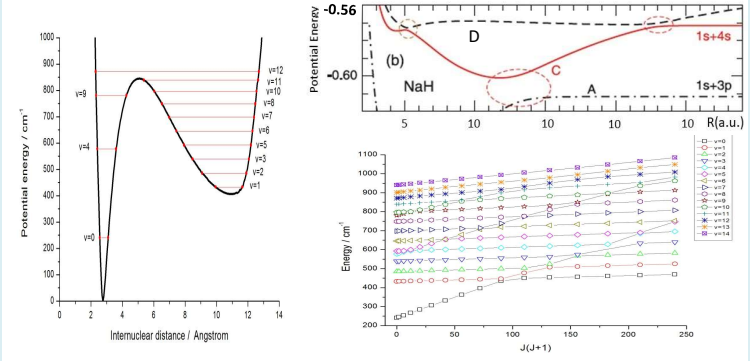


Potential energy curves of the $^1\Sigma^+$ state of X, A , C and D for NaH.



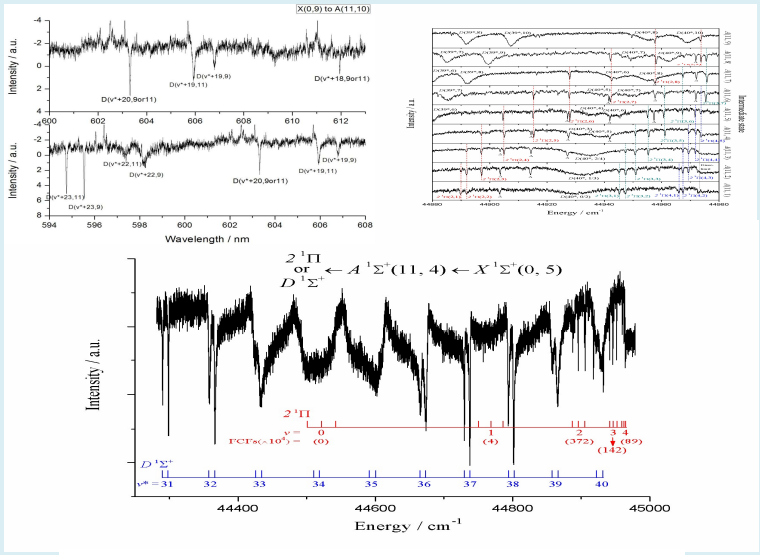
Schematic diagram for experiment

Theoretical Analysis

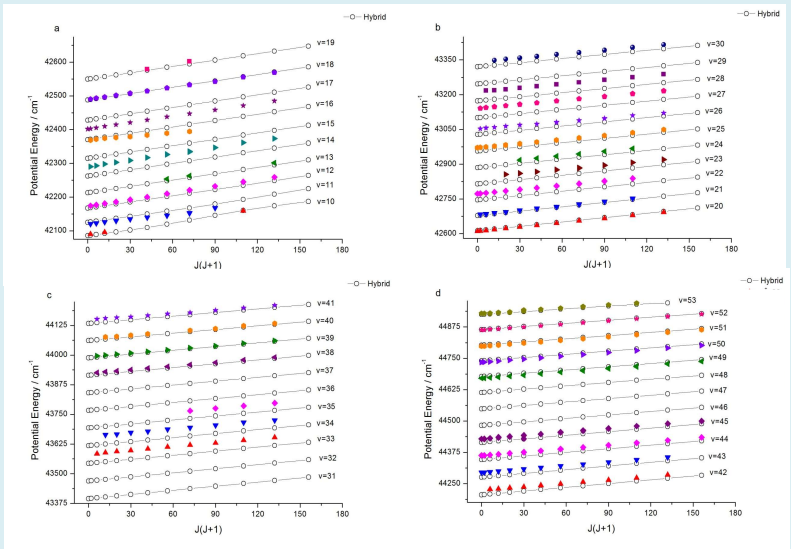


Theoretical D state double-well potential curve[1] with ro-vibrational levels.

Results and Discussion



OODR spectra to explain the insertion of the vibrational levels.



Ro-vibrational Eigen values vs. J(J+1) from the hybrid potential (circle) and observed (color points).

Conclusions

- A total of 555 ro-vibrational energy levels of the NaH $D^1\Sigma^+$ and states was observed of $0 \le v \le 53$, $1 \le J \le 12$.
- A hybrid potential curve modified from a theoretical curve was constructed to better represent the observed ro-vibration energy levels.
- Due to predissociation, the linewidths of some ro-vibrational levels are more than ten times wider than those of conventional depletion

Reference:
[1] Aymar, M.; Deiglmayr, J.; Dulieu, O., Systematic Trends in Electronic Properties of Alkali Hydrides. *Can. J. Phys.* **2009,** *87* (5), 543-556.