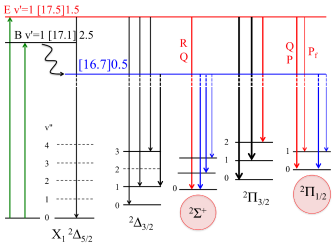
OBSERVATION OF SOME $\Omega = 1/2$ ELECTRONIC STATES OF NICKEL DEUTERIDE, NiD, WITH LASER-INDUCED FLUORESCENCE

AMANDA J. ROSS, PATRICK CROZET, *UMR 5306, ILM University Lyon 1 and CNRS, Villeurbanne, France*; ALLAN G. ADAM, *Department of Chemistry, University of New Brunswick, Fredericton, NB, Canada*; DENNIS W. TOKARYK, *Department of Physics, University of New Brunswick, Fredericton, NB, Canada*.



The five lowest-lying electronic states of nickel hydride (NiH) are usually labeled $^2\Delta_{5/2}$, $^2\Pi_{3/2}$, $^2\Delta_{3/2}$, $^2\Sigma^+_{1/2}$ and $^2\Pi_{1/2}$, although there is significant mixing between them. These states arise from the d^9 electron configuration of Ni^+, perturbed by an H^- ligand. A variety of vibrational levels has been observed in each, and the aggregate data set has been well modelled as a 'supermultiplet' by the Field group[a].

For the deuterated isotopologue NiD, only the $^2\Delta_{5/2}$, $^2\Pi_{3/2}$ and $^2\Delta_{3/2}$ states have been reported in the literature. A multi-isotope supermutiplet fitting including both the NiH and (more limited) NiD data[b] provided predictions for the two $\Omega = 1/2$ states of the NiD supermultiplet. Experimental observation was needed to validate (and improve) the model.

We report on laser-induced fluorescence experiments conducted both at the University of New Brunswick and at Université Lyon 1 in which the $^2\Sigma^+_{1/2}, v = 0, 1, 2$ and $^2\Pi_{1/2}, v = 0, 1$ levels of NiD were identified and rotationally analyzed. The existing multi-isotope supermultiplet model proved remarkably accurate in predicting the energy and structure of these $\Omega = 1/2$ states. In addition, a higher-lying $\Omega = 1/2$ electronic state [16.7]0.5 has been identified in NiD, with no obvious analogue in NiH. The [16.7]0.5-$^2\Sigma^+_{1/2}$ and [16.7]0.5-$^2\Pi_{1/2}$ transitions proved to be a rich source of information about the two lower states.

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[a] J. A. Gray, M. Li, T. Nelis and R. W. Field, J. Chem. Phys. **95**, 7164 (1991)

[b] M. Abbasi, A. Shayesteh, P. Crozet and A. J. Ross, J. Mol. Spectrosc. **349**, 49 (2018)