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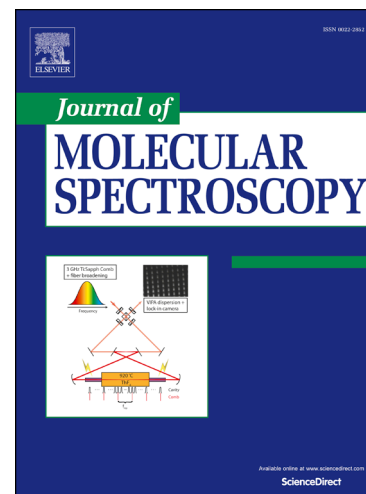
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# Observation of low-lying electronic states of NiD with multi-isotope analysis

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## Abstract.

Resolved laser induced fluorescence spectra of  $^{58}\text{NiD}$ , recorded at Doppler resolution between 11000 and 18000  $\text{cm}^{-1}$  have established more than 200 term energies in two of the three strongly interacting, low-lying states ( $^2\Delta$ ,  $^2\Pi$ ,  $^2\Sigma^+$ ) of NiD, associated with an  $\text{Ni}^+(3d^9)\text{D}^-$  configuration. Our observations span  $v=0-5$  in the lowest spin-orbit component of the ground state,  $X\ ^2\Delta_{5/2}$ ,  $v=0-3$  in  $X\ ^2\Delta_{3/2}$  and  $v=0-1$  in the lower component of the  $W\ ^2\Pi_{3/2}$  state. Collisional processes populate several neighbouring excited states, allowing us also to locate the first rotational levels of  $A(\Omega=5/2)\ v=1$ ,  $I(\Omega=3/2)\ v=0$  and  $E(\Omega=3/2)\ v=1$  at 16664.8, 17367.3 and 17508.1  $\text{cm}^{-1}$  respectively. Spin-orbit and rotation-electronic interactions are strong in NiD (as in NiH), and with no direct observation of either of the  $\Omega=1/2$  states, meaningful representations of the low-lying energy levels is difficult. We have therefore attempted a global, multi-isotope fit to reproduce the term energies of the known term energies of NiD and  $^{58,60,62}\text{NiH}$  (where some  $\Omega=1/2$  levels are known). Dunham-type parameters have been used to represent the unperturbed  $^2\Delta$ ,  $^2\Pi$  and  $^2\Sigma^+$  states, with off-diagonal matrix elements (treating spin-orbit,  $L$ - and  $S$ -uncoupling effects) based on  $\text{Ni}^+$  atomic properties. Born-Oppenheimer breakdown terms were included in the model. The equilibrium bond lengths for  $^{58}\text{NiH}/^{58}\text{NiD}$  are 1.4545(1)/1.4559(1) Å for the  $X\ ^2\Delta$  state and 1.5094(2)/1.5083(2) Å for the  $W\ ^2\Pi$  state.

## Keywords

Laser-induced fluorescence; NiH; NiD; multi-isotope fit; spin-orbit perturbations, Supermultiplet Hamiltonian.

## I INTRODUCTION

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