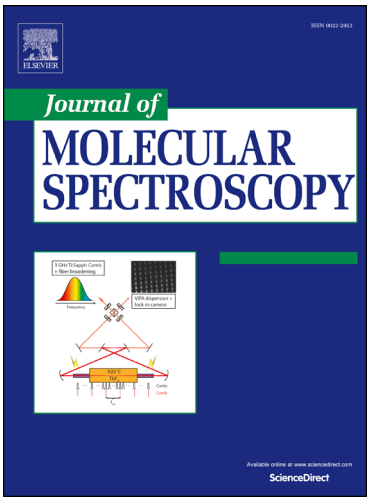

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Observation of low-lying electronic states of NiD with multi-isotope analysis

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Abstract.

Resolved laser induced fluorescence spectra of ^{58}NiD, recorded at Doppler resolution between 11000 and 18000 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 $Ni^+(3d^9)D^-$ 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(Ω = 5/2) v = 1, I(Ω = 3/2) v = 0 and E(Ω = 3/2) v = 1 at 16664.8, 17367.3 and 17508.1 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 Ω =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}NiH (wbere som Ω =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 Ni^+ atomic properties. Born-Oppenheimer breakdown terms were included in the model. The equilibrium bond lengths for ^{58}NiH/^{58}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