A COUPLED-CHANNELS POTENTIAL FIT DESCRIBING THE LOW-LYING $X^2\Delta$, $^2\Pi$ AND $^2\Sigma^+$ STATES OF NiH TO EXPERIMENTAL ACCURACY

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A direct potential fit to Hund's case (a) potential curves for the low-lying 'supermultiplet' states ($X^2\Delta$, $^2\Pi$, $^2\Sigma^+$) of NiH and to R-dependent spin-orbit and rotational coupling functions has reproduced the experimental term values of ^{58}NiH, ^{60}NiH, ^{62}NiH up to 6500 cm^{-1}, with a root mean square deviation very close to the estimated uncertainty of 0.01 cm^{-1}. Second-order Born-Oppenheimer breakdown corrections to the rotational Hamiltonian had to be included to achieve this result. The spin-orbit interaction A_{so}(R) associated with Ni^+ is large compared to the energy separations between the three electronic states, so that most of the observed rovibrational states are strong mixtures of the Ω-components of the multiplet. This made the fitting procedure particularly difficult, because there were no perturbation-free data to determine the starting values for the model functions. Potential curves were optimized from RKR turning-points generated from earlier work using an effective Hamiltonian approach[a], and the spin-orbit and rotational coupling functions from theoretical predictions[b]. We believe that this model may be reliably extrapolated to higher rotational states, with potential applications in the simulation of high temperature spectra, for example in the context of stellar atmospheres.

[a] M. Abbasi *et al*, J. Mol. Spectrosc. 349 49-59 (2018)
[b] C. Marian, J. Chem. Phys., 93(2) 1176-1186 (1990)