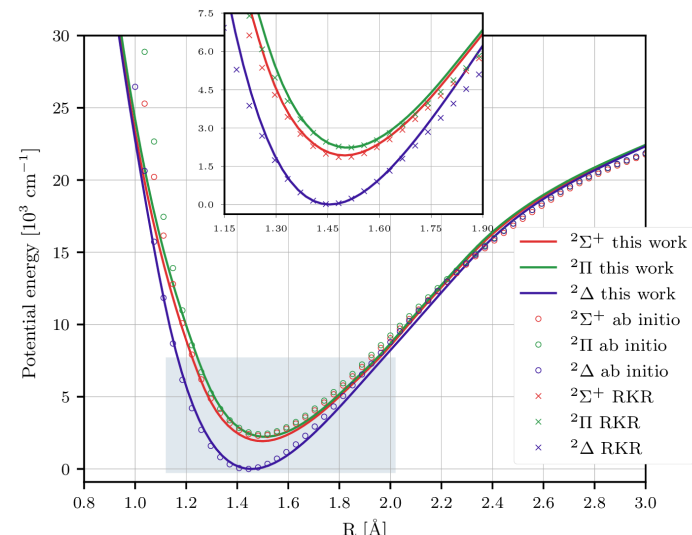
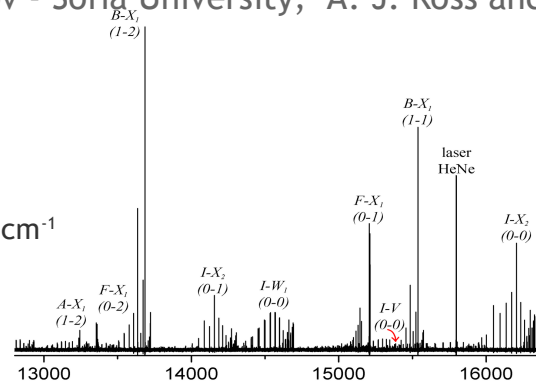


A coupled-channels model describing the low-lying $^2\Delta$, $^2\Sigma^+$ and $^2\Pi$ electronic states of nickel monohydride with experimental accuracy

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- Fully quantum-mechanical model
- Pointwise potential energy curves and coupling functions
- 5 channels, 3 strongly mixed low-lying electronic states
- > 4000 assigned lines, > 730 energy terms, uncertainty 0.01 cm^{-1}



Potential energy curves (PECs)

Solve nuclear Schrodinger equation

Computed energy eigenvalues and wavefunctions

Fit to the observations

Optimised PECs and coupling curves

Compute spectrum

Spectrum line list (quantum numbers, frequency, intensity)

Coupling curves

Experimental data

- The procedure started from RKR and ab initio functions.
- The iterative non-linear least squares fit used SVD, gradually incorporating spin-rotation and BO breakdown terms.

