EXOMOL: MOLECULAR LINE LISTS FOR ASTROPHYSICAL APPLICATIONS. A THEORETICAL LINE LIST FOR NICKEL HYDRIDE.

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Exomol (www.exomol.com) is a database of molecular line lists which can be used for spectral characterisation and simulation of astrophysical enviroments such as exoplanets, brown dwarfs, cool stars and sunspots[a]. New line lists for about 30 small molecules of astrophysical interest which currently lack a complete spectroscopic coverage are being generated. The list includes diatomics (e.g., C_2, O_2, AlO), triatomics (e.g., H_2S, C_3, SO_2), tetratomics (e.g., PH_3, HOOH, H_2CO) and a few larger molecules (most notably CH_4 and HNO_3). We report progress on a new theoretical line list for nickel hydride NiH. The spectra of transition-metal hydrides such as NiH are very complicated due to the large-number of low-lying electronic states, to the importance of correlation, relativistic and spin-orbit effects and of the various couplings between angular momenta. In our study potential energy curves and the relevant couplings were computed *ab initio* and the corresponding coupled-surface ro-vibronic problem was solved using an expansion in Hund's case *(a)* wave functions. Potential curves and couplings were then refined semi-empirically using the available experimental spectroscopic data [b].

[a] J. Tennyson and S. N. Yurchenko, Mon. Not. R. Astron. Soc. (submitted)

[b] Vallon R., S.H. Ashworth, P. Crozet, R.W. Field, D. Forthomme, H. Harker, C. Richard and A.J. Ross, J. Chem. Phys. A **113**, 13159-13166 (2009)