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Hot temperatures line lists for metal hydrides

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Abstract

The ExoMol project is an ERC funded project set up with the purpose of calculating high quality theoretical molecular line list data to facilitate the emerging field of exoplanet and cool star atmospheric characterisation [1].

Metal hydrides are important building blocks of interstellar physical chemistry. For molecular identification and characterisation in astrophysical sources, one requires accurate and complete spectroscopic data including transitional frequencies and intensities in the form of a line list. The *ab initio* methods offer the best opportunity for detailed theoretical studies of free diatomic metal hydrides and other simple hydride molecules. In this contribution we present progress on theoretical line lists for AlH, CrH, MgH, NiH, NaH and TiH obtained from first principles, applicable for a large range of temperatures up to 3500 K.

Among the hydrides, AlH is of special interest because of a relatively high cosmic abundance of aluminium. The presence of AlH has been detected in the spectra of M-type and S-type stars as well as in sunspots (See [2] and references therein).

CrH is a molecule of astrophysical interest; under the classification scheme developed by Kirkpatrick et al [3], CrH is of importance in distinguishing L type brown dwarfs. It has been proposed that theoretical line-lists of CrH and CrD could be used to facilitate a 'Deuterium test' for use in distinguishing planets, brown dwarfs and stars [5] and also it has been speculated that CrH exists in sunspots [4] but a higher-quality hot-temperature line-list is needed to confirm this finding.

The presence of MgH in stellar spectra is well documented through observation of the $A\,^2\Pi \rightarrow X\,^2\Sigma^+$ and $B'\,^2\Sigma^+ \rightarrow X\,^2\Sigma^+$ transitions. Different spectral features of MgH have been used as an indicator for the magnesium isotope abundances in the atmospheres of different stars from giants to dwarfs including the Sun, to measure the temperature of stars, surface gravity, stars' metal abundance, gravitational, as well as for a deuterium test (see [6] and references therein). MgH is an important part of stellar atmospheric models.

NiH is predicted to be the most common nickel-bearing molecule [7] and was indentified in sunspot spectra around 15 000 cm^{-1} (646 cm) over 40 years ago [8]. Knowledge of ^{58}NiH/^{60}NiH isotopologue ratio in stellar spectra is used to test models of supernovae and star formation [9].

The spectra of metal hydrides such can be very complicated due to the large-number of interacting electronic states, to the importance of electron correlation, relativistic and spin-orbit effects and of the various couplings between angular momenta. Via the use of the Born-Oppenheimer approximation, the Schrödinger equation describing the state of a molecule can be factorised into an 'electronic' component and a nuclear (i.e., rotational-vibrational) component. The former is solved using the *ab initio* quantum chemistry package MOLPRO, yielding potential energy, dipole and transition moment, and spin-orbit curves. The resulting coupled-surface ro-vibronic problem was then solved using the in-house computer program DUO, which is based on expansion in Hund's case (a) wave functions. Potential curves and couplings were then refined semi-empirically using the available experimental spectroscopic data.

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