Calculation of a line list for MnH for brown dwarf and exoplanetary applications

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Calculation of a line list for manganese hydride (MnH) for brown dwarf and exoplanetary applications.

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Manganese Hydride in astronomy
To date, there are no astrophysical detections of MnH. However, as is pointed out by Halfen & Ziurys (2008), the cosmic abundance of manganese is of the same order as chromium: since chromium hydride (CrH) has found itself in a myriad of astronomical settings, it is quite possible that MnH could still be detected. The calculation of the line list presented in this poster hence opens up this possibility.

In addition to calculating a line list for the main isotopologue 55MnH, line lists have been calculated for 53MnH and 55MnD. The 55Mn isotopoe (stable) is of interest in supernova explosions (Iwamoto et al. 2009). Additionally Lugmair & Shukolyukov (1998) have investigated if the 53Mn and 53Cr isotopes can be used to determine timescales for solar system objects such as chondrites and meteorites. Also, since the possibility of using CrH and CrD spectra to infer the age of brown dwarfs has been postulated (Pavlenco et al. 2008) it was hence decided to generate line lists for the 55MnD isotopologue.

Methodology
The calculation of line lists for transition metal containing (open d shells) diatomic molecules is a hugely challenging problem due to the myriad of low-lying coupled electronic states with high multiplicity (2S+1).

Following experience with calculating such a line list for CrH, a line list for the diatomic molecule of MnH has been calculated which encompasses the first low-lying bonding 10 electronic states. A systematic series of high-level MRCI calculations was firstly undertaken (>200) in order to produce the most continuous and accurate ab initio curves.

Using experimental data available for both the septuplet and quintet electronic states, ab initio Potential Energy Curves (PECs) were then refined. For the X σ+ and AΠ states, spectroscopic constants were taken from Gordon et al. (2005) and Gengeler et al. (2007) respectively and the program PGOPHER (Western 2010 & 2015) was used to convert these into a list of rovibronic energies. For the aΣ+, bΠ, cΣ+, dΠ and eΣ+ states, term values determined from Fourier Transform Spectrometer measurements from the work of Balfour et al. (1990, 1992) were used.

The program DUO which solves the coupled rovibronic Schrödinger equation was then used to calculate a refined line list which contains ~48 000 rovibronic states and ~5 million transitions. This line list includes states up to J = 50 and energy levels up to 32 000 cm⁻¹ which should be adequate for temperatures up to 3000 K.

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