Exomol: molecular line lists for astrophysical applications. A theoretical line list for scandium hydride

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Exomol [1] is creating a database of molecular line lists for astrophysical applications and also comprises several transition-metal-containing (TMC) diatomics. Spectra of open-shell, TMC systems are very complex due to the large number of low-lying interacting electronic states and to the importance of spin-orbit, electron-correlation and relativistic effects. As a result, fully *ab initio* calculations of line positions and intensities with anything approaching experimental accuracy have so far remained elusive. We report in this work progress on a new theoretical line list for scandium hydride ScH. Because of the presence of one *d*-shell electron ScH shows an increased complexity with respect to molecules containing only main-group elements and is fully representative of TMC diatomics. At the same time ScH is amenable to very high-level electronic-structure treatments because of the small number of valence electrons and serves as an ideal benchmark system. We report *ab initio* potential energy curves for all six electronic terms correlating with the lowest-energy dissociation channel as well as the relevant couplings computed at various levels of electronic-structure treatment. The curves where used for the solution of the coupled-surface ro-vibronic problem using an in-house program. Comparison with experimental data is provided when possible.

[1] J. Tennyson and S. N. Yurchenko, Mon. Not. R. Astr. Soc. 425, 21-33 (2012). See also www.exomol.com.