Exomol: molecular line lists for astrophysical applications. An *ab initio* study of the eight lowest electronic states of chromium hydride

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Chromium hydride CrH is a molecule of astrophysical interest not least for its pivotal role in the classification of L type brown dwarfs within the widely accepted classification scheme of Kirkpatrick [1]. CrH has also been identified in sunspot data [2] and it has been proposed that theoretically CrH & CrD could be of use in distinguishing brown dwarfs, stars and planets of similar luminosity and mass profiles [3]. Experimentally CrH is well characterised, however on the theoretical side, there is no accurate or complete line list for this molecule available. It is our goal to bridge this gap as part of the ExoMol project [4]. Here we present the first stage of this work, where we use accurate *ab initio* methods to calculate potential energy curves (PECs), dipole moment curves, spin-orbit (SO) and other couplings between the eight lowest electronic states of CrH covering approximately 0.1 Hartree (20000 cm^{-1}). We use the Multi Reference Configuration interaction (MRCI) method as implemented in the *ab initio* quantum-chemistry package MOLPRO. Some promising results will be presented based on the pVTZ basis set. Different convergence problems during the CI step will be discussed. The *ab initio* PECs and SO curves are then used to evaluate the rovibronic energies of CrH by means of the computer programme Duo, which is based on Hund's case (a) and accounts for all couplings explicitly. The next step will be to empirically refine the *ab initio* PECs and SO curves by fitting to the available experimental energies or transition line positions. The refined curves together with *ab initio* (transition) dipole moments will be used to produce a hot line list for CrH.

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