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Complete collision data set for electrons scattering on molecular hydrogen and its isotopologues

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Cross sections resolved in the rovibrational levels of the target are required for determining the properties and dynamics of many low-temperature plasmas. We have applied the Molecular Convergent Close-Coupling (MCCC) method to produce a comprehensive set of vibrationally-resolved cross sections for electron collisions with molecular hydrogen and its isotopologues comprised of more than 57,000 entries [1]. This complete collision data set is available to the research community via the LXCat database and the dedicated MCCC database (mccc-db.org). For H_2 the data set includes transitions from all 14 vibrational levels of the ground electronic state to all vibrational levels of 18 excited electronic states (all states in the $n = 2, 3$ shells) with similar datasets for each of the isotopologues. We are working on producing a vibrationally resolved set of cross sections for scattering on the electronically excited $c\,^3\Pi_u$, $a\,^3\Sigma_g^+$, $B\,^1\Sigma_u^+$, $C\,^1\Pi_u$, and $EF\,^1\Sigma_g^+$ states of all H_2 isotopologues with first results already available [2] as well as producing a dataset of fully resolved rovibrational cross sections. An overview of the available MCCC dataset will be presented and an example of modelling calculations based on the MCCC dataset will be given for collisional-radiative (CR) modelling [3].

The MCCC dataset allows for a detailed investigation of dissociation processes of H_2 and its isotopologues by electron impact. In low-temperature plasmas, electron-impact dissociation proceeds almost exclusively via excitation of the dissociative $b\,^3\Sigma_u^+$ state. The latest measurements for dissociation of the ground vibrational level of H_2 are in excellent agreement with MCCC calculations [4]. However, in the absence of similar measurements for vibrationally-excited or isotopically substituted H_2, cross sections for dissociation of these species must be determined by theory alone. We have recently [5] identified large discrepancies (up to a factor of 3) between MCCC cross sections and the recommended and widely used R-matrix cross sections [6] for dissociation of vibrationally-excited H_2, D_2, T_2, HD, HT, and DT, with disagreement in both the isotope effect and dependence on an initial vibrational level. The source of the discrepancies and the consequences for plasma models which have incorporated the previously recommended data will be discussed.

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