Mapping the entirety of optical transitions in the singly excited regime of hydrogen and its isotopes with rotational resolution

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Synopsis Here we present rotationally resolved measurements of the complete emission spectrum of molecular hydrogen and its isotopes in the far and extreme ultraviolet spectral range, the regime of singly excited molecular states, over a large interval of excitation energies with very small bandwidth. Due to its completeness, this allows a new and intuitive presentation of the various processes and transitions involved with a special emphasis on their interaction. Scarcely investigated distinct features are clearly separated and reported in its completeness for the first time.

As the simplest neutral molecule, hydrogen plays the role as the most fundamental prototype system in molecular physics and spectroscopy. As the most abundant molecule in the universe, the exact knowledge of its properties is of great importantance for all astrophysical observations and calculations [1].

In spite of its simplicity in structure its emission spectrum already contains a wide array of molecular features after excitation of its electronic states. The large variety of its singly excited individual states with a high degree of couplings and crossings continues to be a field of steadily improving calculations and measurements [2, 3].

The combination of the very small bandwidth and continuous tunability of modern synchrotron radiation sources with a high secondary fluorescence resolution in the vacuum ultraviolet regime is now able to monitor the full process from excitation to final radiative deexcitation with vibrational and rotational resolution. When performed over a large interval of excitation energies reaching all accessible states and covering the complete set of possible emissions, the data can be presented in the form of excitation energydependant emission spectra next to each other, one spectrum for each excitation energy. The resulting map disentangles not only the processes from each other, but also allows a unique view on their interaction at the boundaries.

In the case of hydrogen, several elemental molecular mechanisms such as the Franck-Condonprinciple, vibrational band progressions or dissociation limits can be immediately identified. At the same time more distinct and less investigated features like the influence of highly ionic bound states or dissociative continuum emissions, also called Condon diffraction bands [4, 5], are revealed. The influence of nuclear mass becomes apparent at first glance by comparing hydrogen with its isotope deuterium, in particular in competitions between fluorescence, dissociation and ionization.



Figure 1. A fragment of the emission map containing part of the vibrational progressions from the B and C electronic states of hydrogen (Lyman and Werner band) with various upper and lower vibrational states up to the dissociation limit of the ground state X (solid line). Below, the dissociative continuum is seen culminating in Lyman- α fluorescence from atomic fragments after dissociation including predissociation resonances.

References

- [1] A. Broadfoot et al. 1979 Science 204 979
- [2] L. Wolniewcz et al. 2006 J. Mol. Spectrosc. 238 118
- [3] M. Glass-Maujean *et al.* 2016 J. Mol. Spectrosc. 320 33
- [4] E. Condon 1928 Phys. Rev. 32 858
- [5] H. Schmoranzer et al. 1978 Phys. Rev. A 18 1472

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