Rydberg resonances in photofragmentation of H_2: From spectroscopy to collisions

J. Zs. Mezei[a,b], I. F. Schneider[a,c], Ch. Jungen[a]

[a] *Laboratoire Aimé Cotton, CNRS/Université Paris-Sud, Orsay, France*
[b] *Institute for Nuclear Research, Hungarian Academy of Sciences, Debrecen, Hungary*
[c] *Laboratoire Ondes & Milieux Complexes, CNRS/Université du Havre, Le Havre, France*

Resonances are a spectacular and challenging phenomenon in molecular physics. They occur when two or more open and closed channels interfere. Theoretically resonance phenomena may be accounted for by Multichannel Quantum Defect Theory (MQDT) in an elegant and efficient way [1].

We report theoretical photoionization cross sections for diatomic hydrogen excited from its electronic ground state, either from the ground vibrational level (v''=0) or from excited vibrational levels (v''>0) [2]. Our MQDT calculations take account of the full manifold of Rydberg states and their interactions with the electronic continuum. We show that the photoionization cross section is dominated by resonance effects, in the sense that autoionization resonances produce the major fraction of the averaged cross section. Indeed, inclusion of these resonances leads to an increase by an order of magnitude of the photoionization rate with respect to the contribution of the flat continuum [3], a fact that might have significant consequences in the framework of current astrophysical models [4].

The present work is focused on the case v''=1,N''=1 and specifically deals with the Q transitions (N'=N'') which account for roughly one third of the total photoabsorption cross section. The extension of this study to the P- and R-transitions ($\Delta N = -1$ and 1 respectively) requires the simultaneous treatment of the two photoinduced decay processes ionization (I) and dissociation (D), both of which are far stronger than in the case of the Q transitions. The interconversion of electronic and nuclear energy is mediated by bound states embedded in the "I+D" continua. This is taken into account by MQDT [1], which treats discrete series of states and multiple fragmentation continua in a unified fashion. Here we discuss the predissociated levels corresponding to 3pπD $^1\Pi_u$ $v' > 3$, N'=1,2, and we compare their calculated resonance profiles with those measured recently with different techniques at two synchrotron devices [5, 6].

Acknowledgments. The authors acknowledge the French Agence Nationale pour la Recherche and Triangle de la Physique for financial support within the SUMOSTAI and SpeCoRyd contracts.

[1] Ch. Jungen, "Elements of Quantum Defect Theory", in M. Quack and F. Merkt (editors), *Handbook of High Resolution* ☐*Spectroscopy* **2011**, 471.

[2] J. Zs. Mezei, I. F. Schneider, E. Roueff and Ch. Jungen, *Phys. Rev. A* **2012**, 85, 043411.

[3] A. L. Ford, K. K. Docken, and A. Dalgarno, *ApJ* **1975**, 200, 788.

[4] C. M. Coppola, S. Longo, M. Capitelli, F. Palla, and D. Galli, *ApJ. Suppl. Ser.* **2011**, 193, 7.

[5] G. D. Dickenson, *et al, J. Chem. Phys.* **2010**, 133, 144317.

[6] J. Zs. Mezei, I. F. Schneider and Ch. Jungen, *in preparation.*