8th Workshop on Fast Ion - Atom Collisions

September 1 - 3, 2004, Debrecen, Hungary

Program & Abstracts

Debrecen, 2004

Bond rearrangement caused by sudden single and multiple ionization of water molecules

Itzik Ben-Itzhak, A. Max Sayler, Matt Leonard, Jack W. Maseberg, Eric Wells, Mark A. Smith, Jiangfan Xia, Pengqian Wang, Kevin D. Carnes and Brett D. Esry

J.R. Macdonald Laboratory, Physics Department, Kansas State University, Manhattan, KS 66506, USA

Bond rearrangement, namely the dissociation of water into $H_2^+ + O^{q+}$ following sudden ionization by swift proton and highly charged ion impact, was investigated. Single ionization by fast proton impact exhibits a strong isotopic effect, the dissociation of $H_2O^+ \rightarrow H_2^+ + O$ being about twice as likely as $D_2O^+ \rightarrow D_2^+ + O$, with $HDO^+ \rightarrow HD^+ + O$ in between. This suggests that the bond-rearrangement does not happen during the slow dissociation, but rather during the very fast ionization, and thus H_2^+ should also be produced when the water molecule is multiply ionized. We observed that the $H_2^+ + O^+$ and $H_2^+ + O^{2+}$ production in 1 MeV/amu $F^{7+} + H_2O$ collisions are $0.209\pm0.006\%$ and $0.0665\pm0.003\%$, respectively, of the main double-ionization dissociation product, $H_2O^{2+} \rightarrow H^+ + OH^+$. This ratio is similar to the triple to double ionization ratio in similar collisions with atomic targets thus suggesting that the bond-rearrangement fraction out of each ionization level is approximately constant. Similar dissociation channels in the heavier water isotopes, expected to be smaller, are under study. Finally, the fragmentation of HDO exhibits very strong isotopic preference for breaking the OH bond over the OD bond.

Supported by the Chemical Sciences, Geosciences and Biosciences Division, Office of Basic Energy Sciences, Office of Science, U.S. Department of Energy.

Young's interference effect in the autoionization of atoms colliding with molecules

R.O. Barrachina† and M. Žitnik‡

† Centro Atómico Bariloche and Instituto Balseiro, 8400 Bariloche, Río Negro, Argentina

‡ J. Stefan Institute, Jamova 39, P. O. Box 3000, SI 1000 Ljubljana, Slovenia

We study the post-collision interaction (PCI) effects produced on the autoionization of an atom colliding with a molecule. We show that an oscillatory pattern might appear in the emission spectra. This effect can be ascribed to a Young interference effect due to the interaction of the emitted electron with the structured multi-center cluster. We finally discuss the condition under which this effect might be experimentally observed.

The triple differential cross section and interference effects of electron-impact ionization of molecules

J. Gao, *D.H. Madison* and J.L. Peacher

Laboratory for Atomic, Molecular and Optical Research, Physics Department, University of Missouri-Rolla, Rolla, Missouri 65409-0640, USA

The Highest Occupied Molecular Orbital (HOMO) is important for chemical reactions and some biological processes. Electron impact ionization of molecules (e,2e) is an effective probe for studying the important molecular interactions. Recently the interference effect in diatomic molecules has also received considerable attention. For high incident-energy (keV range) electron-impact ionization, the Plane Wave Impulse Approximation (PWIA), which was developed in the 1970's, provided a good understanding of the experimental differential cross section data. However for lower incident-electron energies, no accurate theory exists to describe the ionization process. We have developed a Three-body Distorted Wave (3DW) approach which treats all continuum electrons as distorted waves and which also includes the final state electron-electron interaction (correlation) to all orders of perturbation theory. In addition, we have developed the Distorted Wave Impulse Approximation (DWIA) which is a distorted wave version of the PWIA. Both theories will be used to calculate triple differential cross sections and to study the interference effects for electron-impact ionization of the nitrogen molecule.

A kiadásért felel: Sulik Béla
Szedés, tördelés: Orbán Andrea
Sokszorosítás, fűzés: REXPO Kft., Debrecen
Debrecen, 2004. augusztus