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# Singlet and triplet states dissociation of doubly charged $HDO$ , $H_2O$ and $D_2O$ as a function of internal energy

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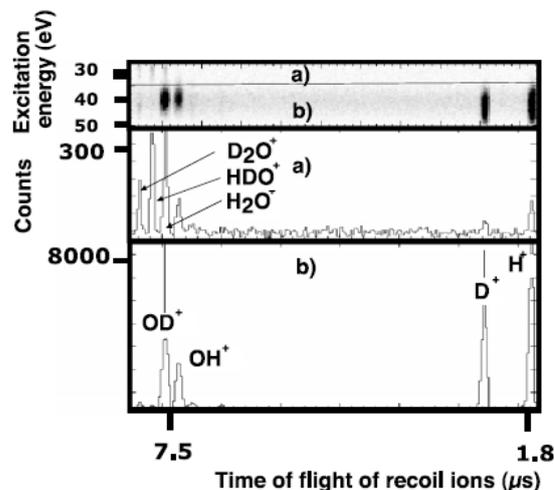
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**Synopsis** The fragmentation of  $HDO^{2+}$ ,  $H_2O^{2+}$  and  $D_2O^{2+}$  is reported as a function of the excitation energy. The doubly charged ions were prepared selectively to triplet or singlet excited states in collisions with  $F^+$  and  $H^+$  at 3 keV, respectively. For  $HDO^{2+}$  the isotopic ratio, ratio of probabilities for the two dissociation channels  $OD^+ - H^+$  over  $OH^+ - D^+$ , was estimated to be  $4.5 \pm 0.8$  using  $H^+$  and  $3.8 \pm 0.8$  using  $F^+$  projectiles. Results are compared with recent calculations.

Fragmentation of doubly charged water or heavy water ions has been studied with a large variety of excitation methods using photons, electrons, slow or fast ion impact. Two-body and/or three-body dissociation schemes have been predicted in theoretical calculations for each molecular energy state. For  $HDO^{2+}$  the isotopic ratio defined as the ratio of probabilities for the two dissociation channels  $\frac{OD^+ - H^+}{OH^+ - D^+}$  was calculated to be 8.6 for the ground triplet state. For the first and second singlet states the ratios were found to be 3 and 15.7, respectively [1]. These calculations showed a strong dependence on the energy and the multiplicity of the  $HDO^{2+}$  molecular state.

In this work, we investigated the fragmentation of  $HDO^{2+}$ ,  $H_2O^{2+}$  and  $D_2O^{2+}$  prepared selectively to singlet or triplet state due to the spin conservation rule using  $H^+ + M \rightarrow H + M^{2+}$  (singlet states) or  $F^+ + M \rightarrow F + M^{2+}$  (triplet states) collisions at 3 keV. M represents the mixture of  $HDO$ ,  $H_2O$  and  $D_2O$ . Excitation energies of singlet and triplet states of the doubly charged parent ions with respect to the neutral ground state have been measured for different dissociation channels using the CIDECE method [2]. The doubly charged parent ions were identified by analyzing the correlation between the charged fragments. For  $HDO^{2+}$ ,  $OD^+ - H^+$  is the dominant dissociation channel for both multiplicities. For this channel the excitation energy of  $HDO^{2+}$  parent ion was measured to be  $42.2 \pm 0.5$  eV and  $40.7 \pm 0.3$  eV in  $H^+$  and  $F^+$  collisions. The isotopic ratio was estimated to be  $4.5 \pm 0.8$  using  $H^+$  and  $3.8 \pm 0.8$  using  $F^+$  projectiles. For  $F^+$  projectiles the discrepancy between the measured and the theoretical isotopic value suggests that the initial vibrational

and rotational states of neutral  $HDO$  play an important role in the dissociation dynamics of the doubly ionized molecules. The good agreement between the measured excitation energy and the calculated electronic energy levels indicates that the molecules are prepared to electronic excited states by electron capture directly from inner orbitals without vibrational energy deposition. This is also confirmed by our KER (kinetic energy release) measurements which are comparable to values obtained in photon ionization.



**Figure 1.**  $H^+ + M \rightarrow H + M^{2+}$  (singlet states) collisions. Top panel: excitation energy ( $E_{exc}$ ) versus time of flight of the recoil ions. (a) Mass spectrum for  $E_{exc} < 34$  eV. (b) Mass spectrum for  $E_{exc} > 34$  eV.

## References

- [1] B. Gervais *et al* 2009 *J. Chem. Phys.* **131** 024302
- [2] S. Martin *et al* 2015 *J. Chem. Phys.* **142** 094306

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