

# Contents of the data files:

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## Two-photon ionization of H2

- "H2-2photon-cs-ADZ.txt": Stationary two-photon cross sections for ionization of H2 (model ADZ). First column: Photon energy (eV). Second column: Cross sections in atomic units.
- "H2-2photon-cs-ATZ-R{30|50}.txt": Stationary two-photon cross sections for ionization of H2 (model ATZ, two different R-matrix radii 30 and 50 a.u.). First column: Photon energy (eV). Second column: Cross sections in atomic units.
- "H2-2photon-yields-ADZ-RMT.txt": Ionization rates for ionization of H2 (model ADZ). First column: Photon energy in atomic units. Second column: Yield in (atomic unit of time)<sup>-1</sup>.
- "H2-2photon-yields-ATZ-RMT.txt": Ionization rates for ionization of H2 (model ADZ). First column: Photon energy in atomic units. Second column: Yield in (atomic unit of time)<sup>-1</sup>.

## One-photon ionization of H2

- "H2-beta-fixed.dat": Fixed nuclei asymmetry parameter for one-photon ionization of H2 at equilibrium geometry. First column: Photon energy in eV. Other columns: Values of the beta parameter beta2 for ionization to individual final ionic states of H2<sup>+</sup>.
- "H2-beta-averaged.dat": Vibrationally averaged asymmetry parameter for one-photon ionization of H2. First column: Photon energy in eV. Second column: Values of the beta parameter beta2 averaged over vibronic levels.

## One-photon ionization of H2O

- "H2O-beta-raw.txt": Asymmetry parameter for one-photon ionization of H2O (model L). First column: Photon energies in eV. Other columns: Values of the beta parameter beta2 for ionization to individual final ionic states of H2O<sup>+</sup>.
- "H2O-beta-smoothed.txt": Smoothed asymmetry parameter for one-photon ionization of H2O (model L). First column: Photon energies in eV. Other columns: Values of the smoothed beta parameter beta2 for ionization to individual final ionic states of H2O<sup>+</sup>.
- "H2O-cs-L-raw.txt": Cross sections for one-photon ionization of H2O (model L). First column: Photon energies in eV. Other columns: Values of partial cross sections for ionization to individual final ionic states of H2O<sup>+</sup>.
- "H2O-cs-L-smoothed.txt": Smoothed cross sections for one-photon ionization of H2O (model L). First column: Photon energies in eV. Other columns: Values of smoothed partial cross sections for ionization to individual final ionic states of H2O<sup>+</sup>.
- "H2O-cs-RMT.txt": Ionization rates for ionization of H2O by a linear pulses of three different orientations. First column: Photon energy in atomic units. Other columns: Ionization rates in (atomic unit of time)<sup>-1</sup> for polarization in X, Y, Z.
- "H2O-cs-S-raw.txt": Cross sections for one-photon ionization of H2O (model S). First column: Photon energies in eV. Other columns: Values of partial cross sections for ionization to individual final ionic states of H2O<sup>+</sup>.
- "H2O-cs-S-smoothed.txt": Cross sections for one-photon ionization of H2O (model S). First column: Photon energies in eV. Other columns: Values of smoothed partial cross sections for ionization to individual final ionic states of H2O<sup>+</sup>.

## Strong field ionization of H2O

- "H2O-strong-field.txt": Time-dependent electric field pulse. First column: Time in atomic units. Second column: Electric field intensity in atomic units.
- "H2O-strong-field-spectrum.txt": Energy spectrum of the time-dependent electric field pulse. First column: Photon energy (spectral component) in eV. Second column: Real part of Fourier transform of the electric field intensity. Third column: Imaginary part of Fourier transform of the electric field intensity.
- "H2O-strong-field-yield-HF-xy-{X,A,B}.dat": Ionization yields for ionization of H2O into ionic states X, A, B by pulses in xy plane (model A). First column: Orientation of the pulse (degrees). Second column: Yield.
- "H2O-strong-field-yield-HF-xz-{X,A,B}.dat": Ionization yields for ionization of H2O into ionic states X, A, B by pulses in xz plane (model A). First column: Orientation of the pulse (degrees). Second column: Yield.
- "H2O-strong-field-yield-HF-yz-{X,A,B}.dat": Ionization yields for ionization of H2O into ionic states X, A, B by pulses in yz plane (model A). First column: Orientation of the pulse (degrees). Second column: Yield.
- "H2O-strong-field-yield-Cl-xy-{X,A,B}.dat": Ionization yields for ionization of H2O into ionic states X, A, B by pulses in xy plane (model B). First column: Orientation of the pulse (degrees). Second column: Yield.
- "H2O-strong-field-yield-Cl-xz-{X,A,B}.dat": Ionization yields for ionization of H2O into ionic states X, A, B by pulses in xz plane (model B). First column: Orientation of the pulse (degrees). Second column: Yield.
- "H2O-strong-field-yield-Cl-yz-{X,A,B}.dat": Ionization yields for ionization of H2O into ionic states X, A, B by pulses in yz plane (model B). First column: Orientation of the pulse (degrees). Second column: Yield.
- "H2O-RMT-intensity-{HF|Cl}.txt": Field-intensity dependence of the ionization yields into states X, A, B by pulses parallel to selected axis. First column: Intensity (10<sup>14</sup> W/cm<sup>2</sup>). Other columns: Yields.
- "Additional\_figures\_H2O\_strong\_field.pdf": Figures with additional data from the letter to the reviewers. These include: (i) comparisons of the state-dependent ionization yields for polarizations parallel with the coordinate axes for calculations for various inner region sizes and B-spline density and those where the field coupling between the ion states (both in the inner and the outer region) has been removed; (ii) Field-strength dependence of the ionization yields for polarizations parallel with the coordinate axes calculated for two different sizes of the inner region (15 vs 50 a.u.).