Supporting Information

For

Experimental Evidence of Sensitivity of the High Harmonic Generation to the Hydrogen Bonding

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S1. Parameters used for numerical simulation of the HHG spectra:

Pulse Parameters:

Intensity (I) = 1×10^{14} W/cm^2

Frequency (ω) = 0.056 a.u. (~813 nm)

Number of cycles in the $\sin^2$ envelop ($n_{envelop}$) = 46 cycles

Total pulse duration (T_P) = 124.8 fs

Code Parameters:

Spatial grid size (X_{lim}) ≈ 410 a.u.

Extent of mask function (X_0) = 273.0 a.u.

Step size of Spatial grid (dx) = 0.2 a.u.

Time Step Size (dt) = 0.1 a.u.

Potentials Used:

(All equations are written in atomic unit)

Acetonitrile: $$U(x) = -0.01 - \frac{0.08}{\sqrt{(x-0.54)^2+0.001}} - \frac{0.14}{\sqrt{(x-2.81)^2+6.14}}$$

Chloroform: $$U(x) = -0.01 - \frac{0.03}{\sqrt{(x-0.74)^2+0.005}} - \frac{0.21}{\sqrt{(x-0.50)^2+0.005}}$$

Acetonitrile + Chloroform: $$U(x) = -0.02 - \frac{0.09}{\sqrt{(x-0.72)^2 + 0.01}} - \frac{0.10}{\sqrt{(x-0.49)^2 + 0.001}}$$

As 62 femtosecond is the obtained FWHM of the experimental Gaussian pulse, we have used 124 fs as the full duration of the pulse in simulation. 1D-MEPs were computed along the respective bond direction. Further discussion of the MEP-based HHG simulations will be given in our future publications.Here, we note that ionization potentials obtained from MEP-based calculations (0.198 a.u. for acetonitrile, 0.590 a.u. for chloroform, and 0.437 a.u. for the hydrogen bonded complex) are different from the reported values in literature.We believe that this difference originates from the MEP-based calculations. We are further improving the MEP-based formalism and our future publications would address these issues.