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**Near-Infrared Radiation Induced Conformational Change and
Hydrogen Atom Tunneling of 2-Chloropropionic Acid
in Low-Temperature Ar Matrix**

SUPPORTING INFORMATION

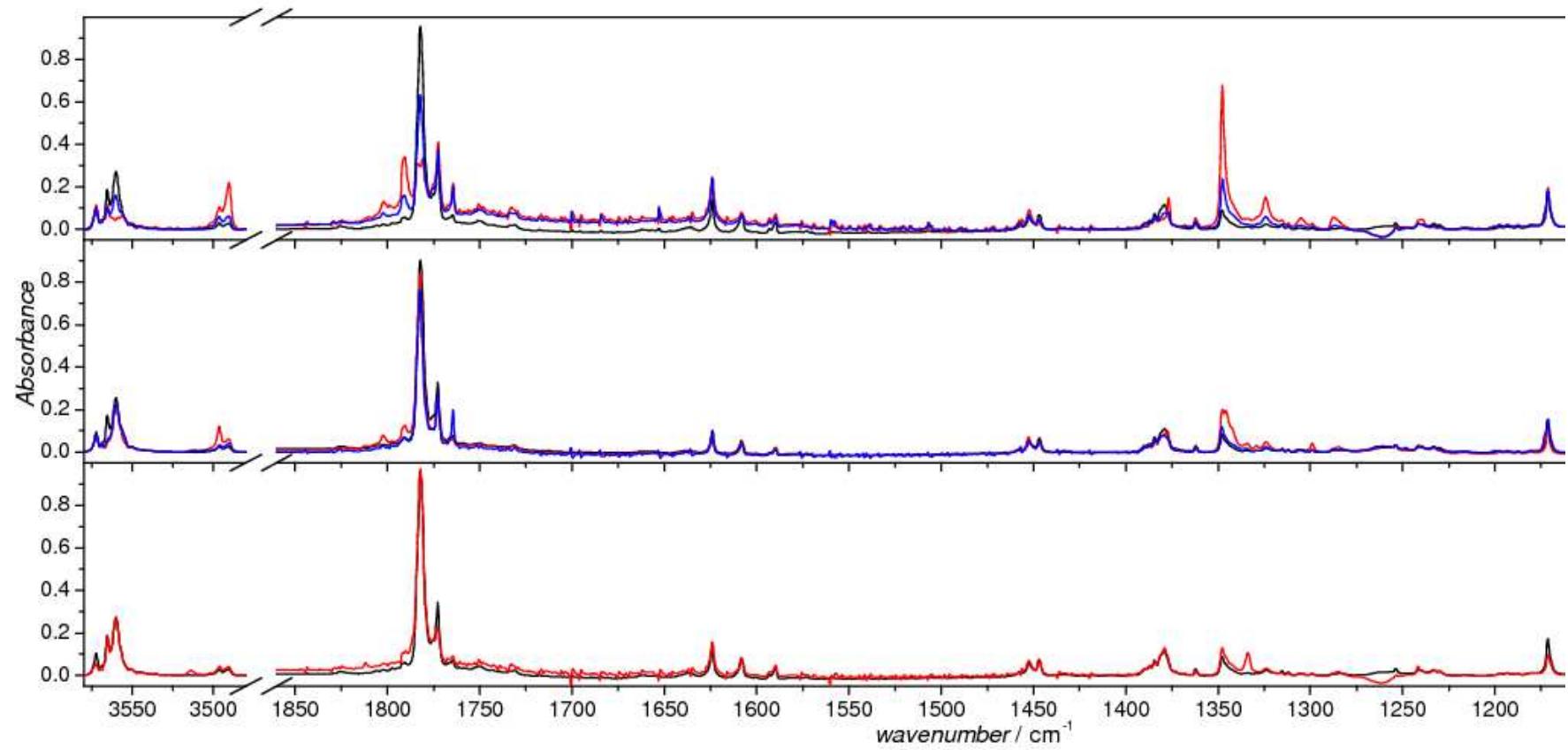


Figure S1. Full-range MI-IR spectra *S*-(-)-2-chloropropionic acid before and after NIR laser irradiation. a: Spectrum obtained after deposition in the dark (black), after 6951 cm^{-1} (red), and after subsequent 6782 cm^{-1} (blue) NIR laser irradiation. b: Spectrum obtained after deposition in the dark (black), after 6961 cm^{-1} (red), and after subsequent 6766 cm^{-1} (blue) NIR laser irradiation. c: Spectrum obtained after deposition in the dark (black) and after 6775 cm^{-1} (red) NIR laser irradiation.

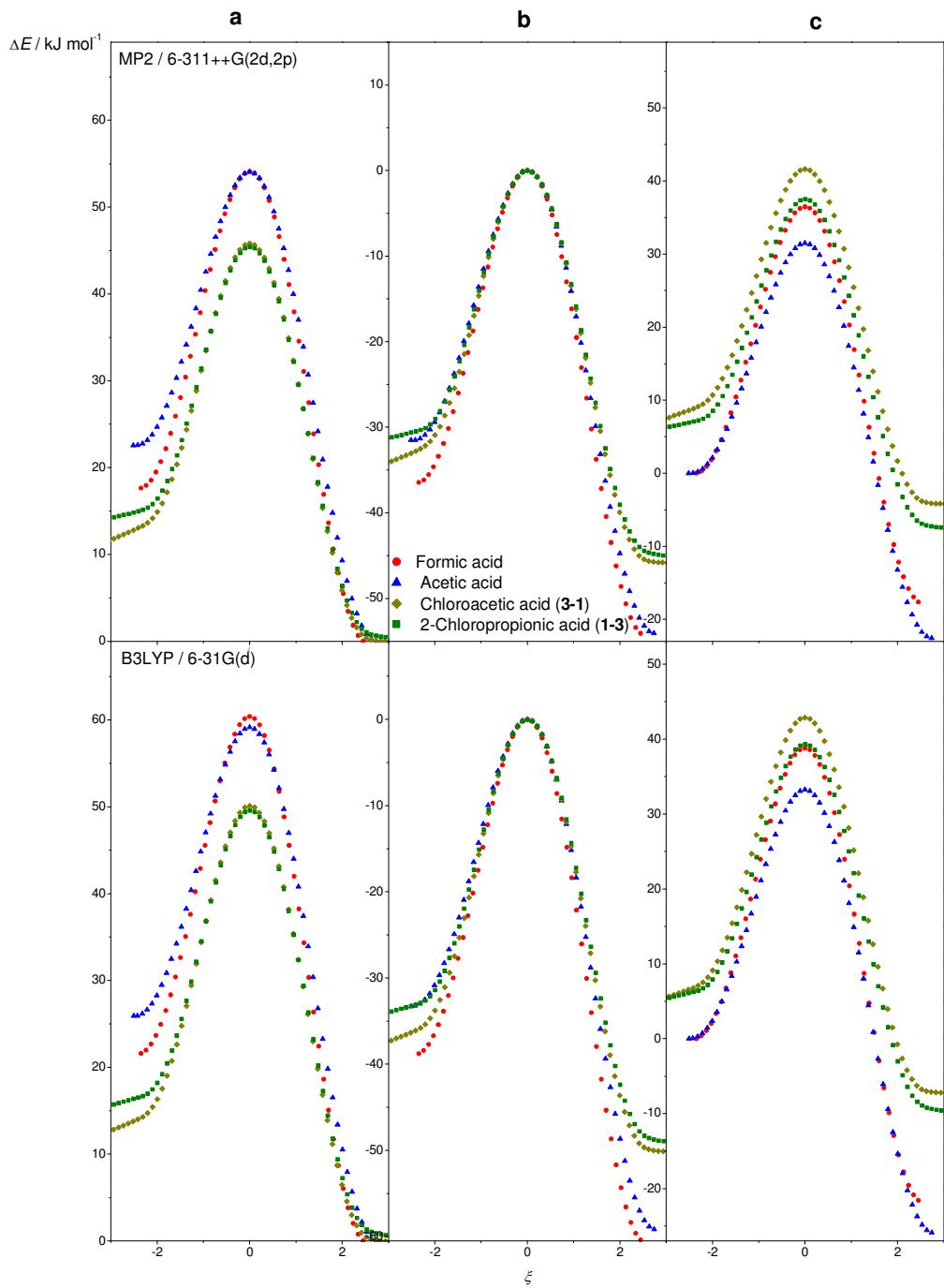


Figure S2. Intrinsic reaction paths of cis \rightarrow trans conversions of formic, acetic, chloroacetic and 2-chloropropionic acids as obtained at the B3LYP/6-31G* and the MP2/6-311++G** levels of theory. The reference (zero) energy is set to the **a**: *trans* minimum, **b**: saddle point, **c**: *cis* minimum.

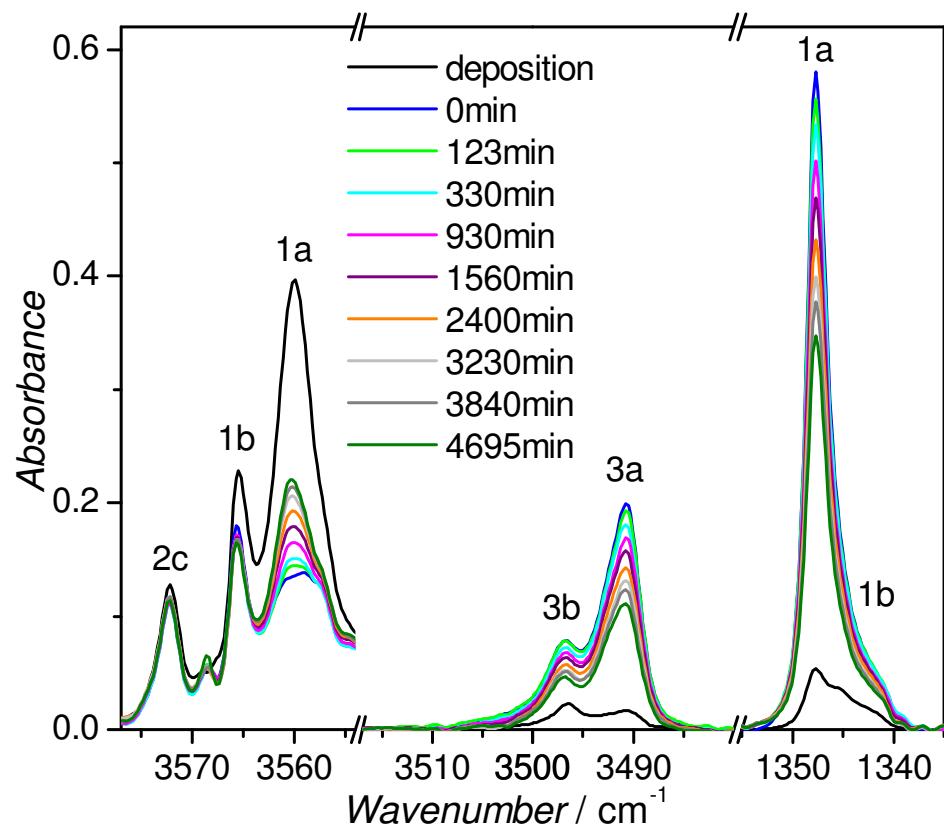


Figure S3. The dark process observed after the NIR irradiation of the OH stretching overtone of **1a**.

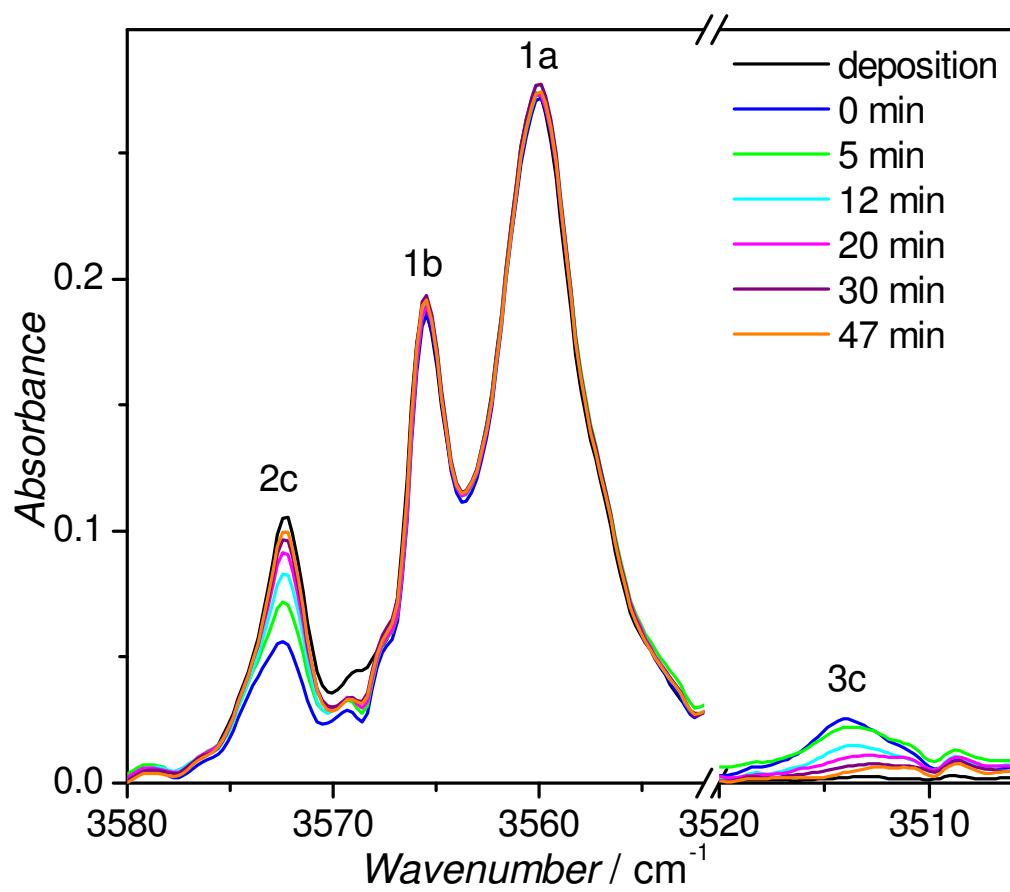


Figure S4. The dark process observed after the NIR irradiation of the OH stretching overtone of **2c**.

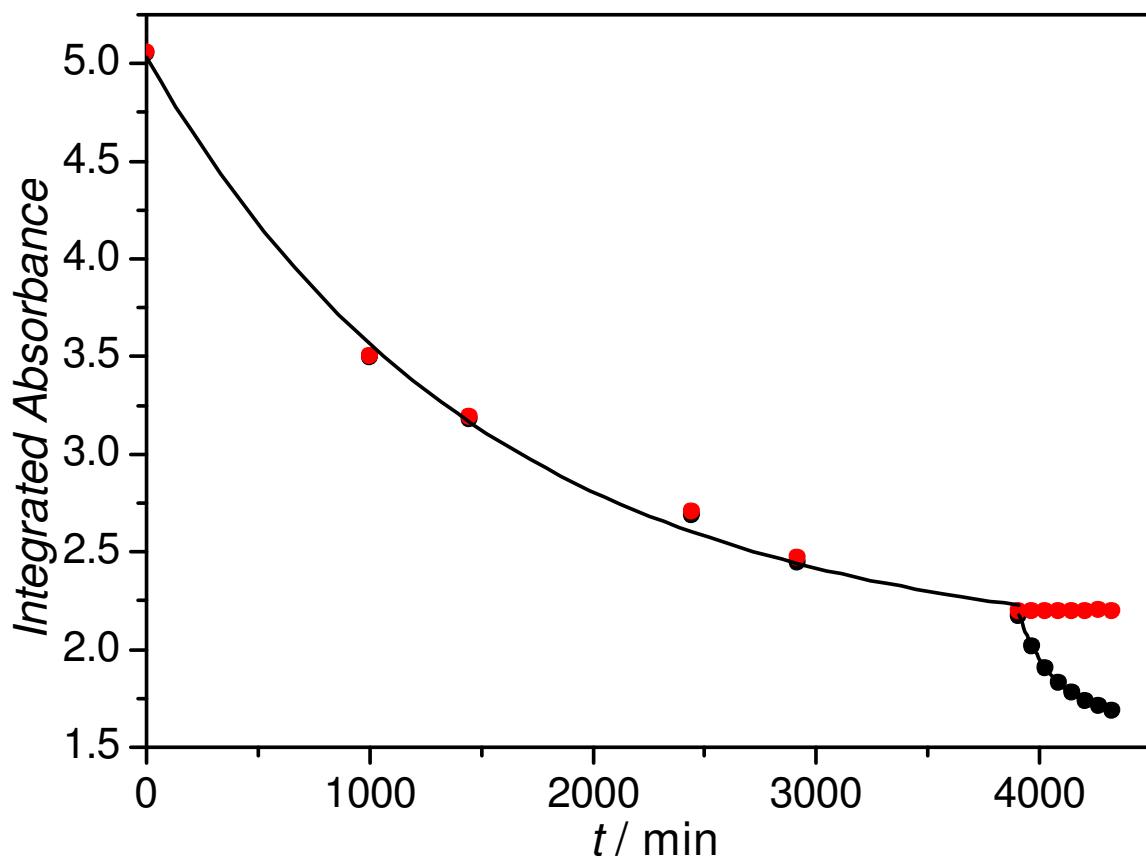


Figure S5. Decay of the integrated absorbance of ν_1 band of **1a**. In the first 3908 minutes the IR source of the spectrometer was turned on only during the short measurements. After 3908 minutes the IR source was continuously on. Black dots are the direct measurements, red dots are corrected by the effect of the IR source.

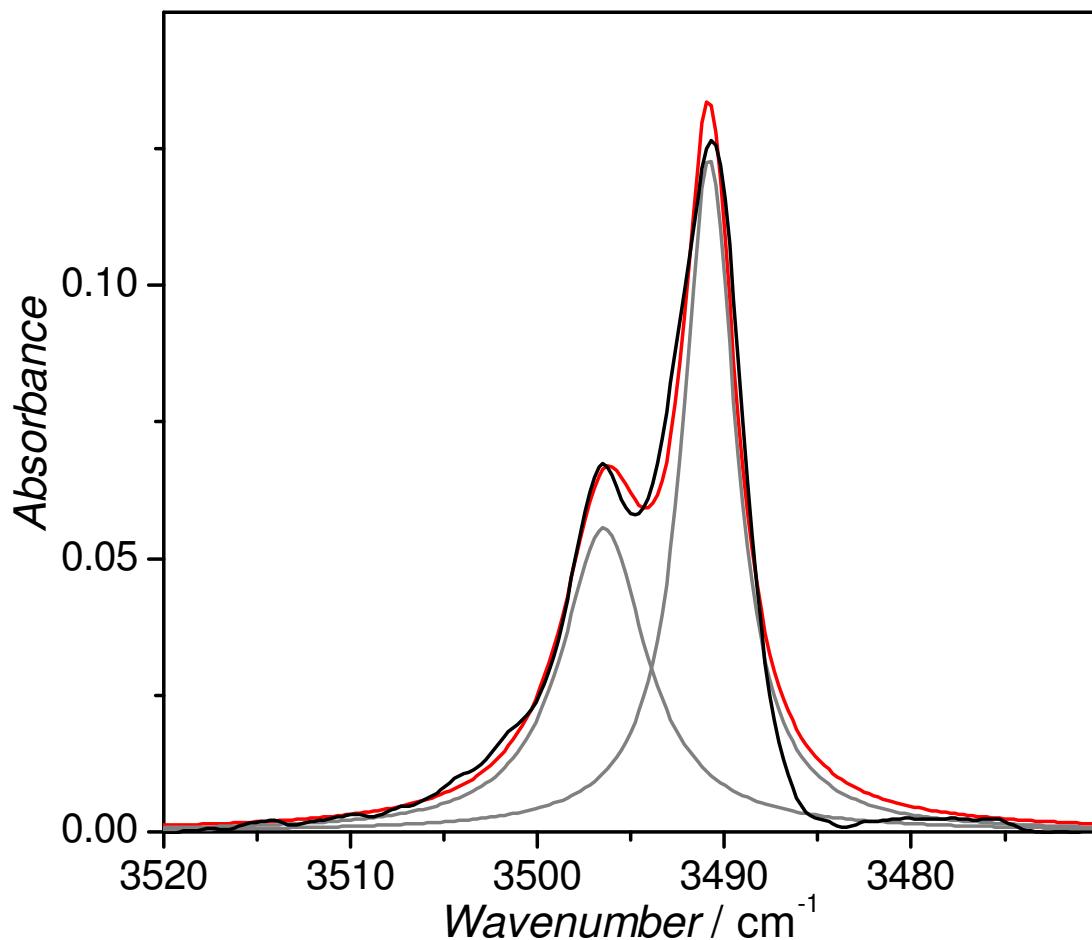


Figure S6. Example of a Lorentzian band fit of the ν_1 band of **3a** and **3b**. Black curve: measured spectrum, grey: fitted Lorentzians, red: sum of fitted Lorentzians.