SUPPLEMENTARY MATERIAL

for

Radiation-induced chemistry in the C_2H_2–H_2O system at cryogenic temperatures: a matrix isolation study

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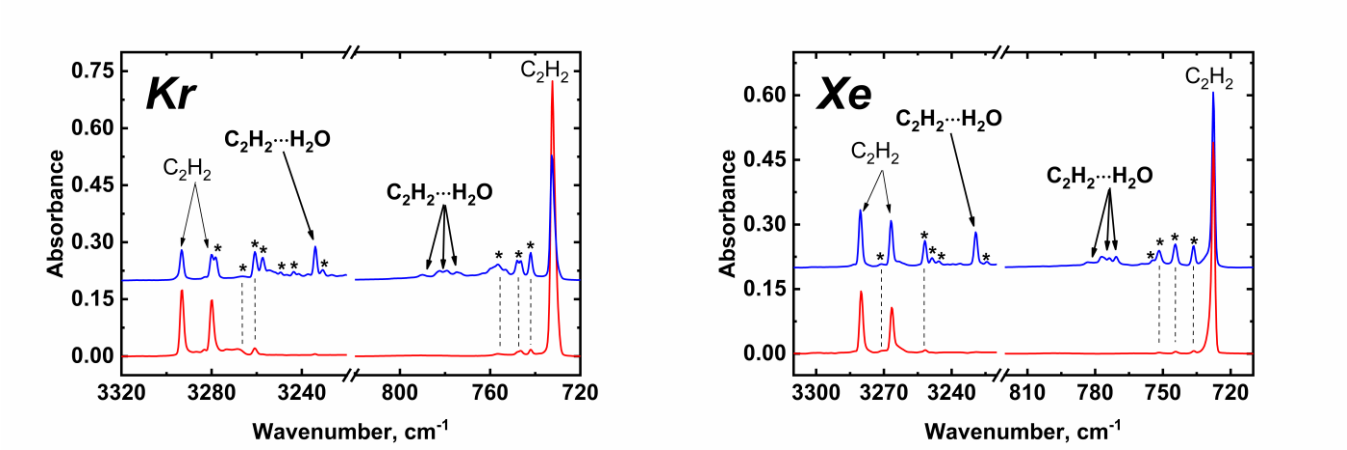

Figure S1. Fragments of FTIR spectra of the deposited $^{12}C_2H_2/H_2O$/Ng 1:1:1000 (upper traces) and $^{12}C_2H_2$/Ng 1:1000 (lower traces) matrices. Ng = Kr (left panel) or Xe (right panel). Spectra were recorded at 5 K. Absorptions due to acetylene associates ($(^{12}C_2H_2)_n$) are marked with asterisks.

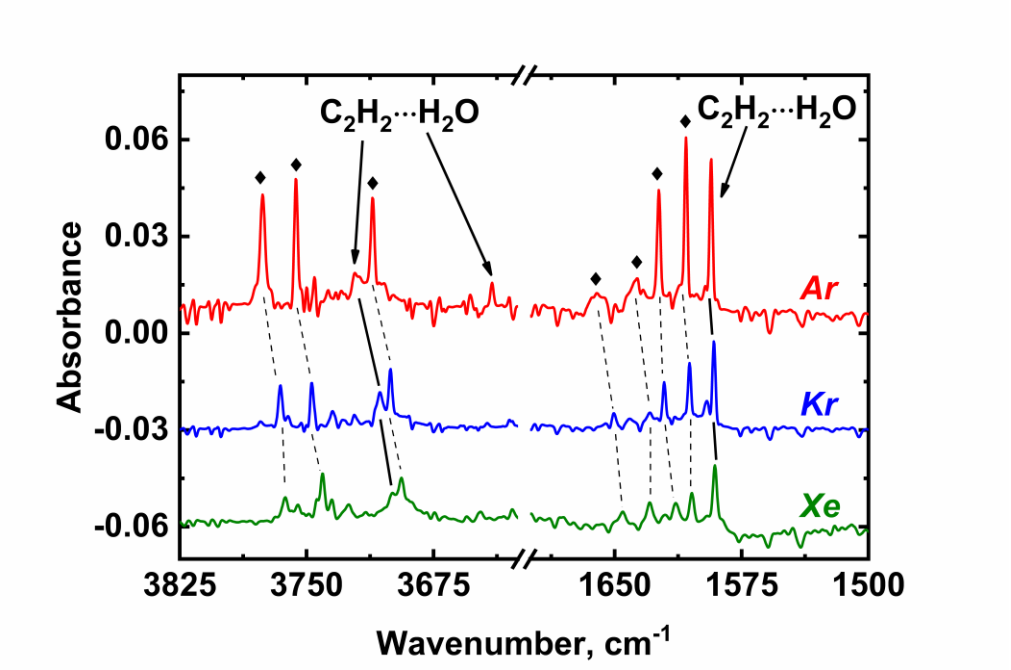

Figure S2. Fragments of FTIR spectra of the deposited $^{12}C_2H_2/H_2O$/Ng 1:1:1000 matrices. Ng = Ar, Kr, and Xe. Spectra were recorded at 5 K. Absorptions due to matrix-isolated H_2O molecules (multiple bands are due to hindered rotation) are marked with diamonds.

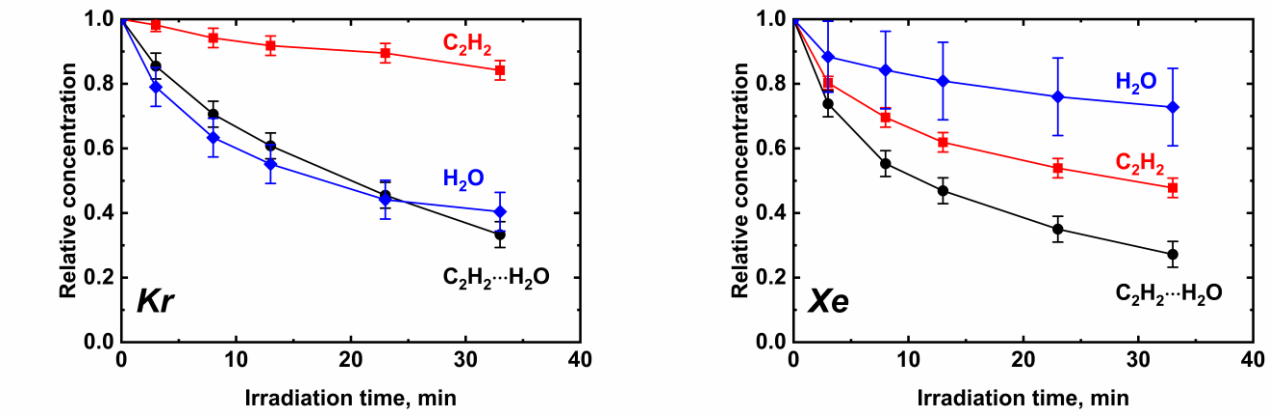

Figure S3. Kinetics of radiation-induced decay of C_2H_2 and H_2O isolated molecules and $C_2H_2\cdots H_2O$ complexes in Kr (left panel) and Xe (right panel) matrices.

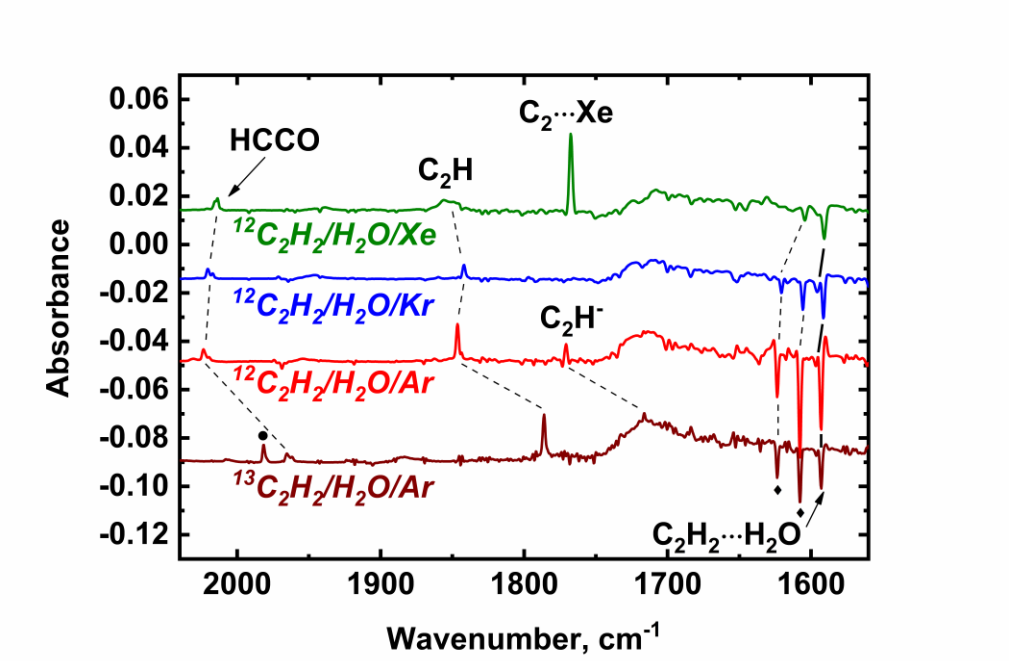

Figure S4. Fragments of the difference FTIR spectra of the C_2H_2/H_2O/Ng 1:1:1000 samples (Ng = Ar, Kr, and Xe) showing the result of *X*-irradiation (all spectra represent the samples irradiated to a maximum dose in each experiment). Spectra were recorded at 5 K. Absorptions due to matrix-isolated H_2O molecules (multiple bands are due to hindered rotation) are marked with diamonds. Absorption due to $^{13}C_4H$ is marked with a bullet. Please note that the broad "hump"-like feature in 1740–1710 cm^{-1} is not related to the sample, but is an external artefact (see e.g. Saenko E. V., Feldman V. I., 2016, Phys. Chem. Chem. Phys., 18, 47, 32503).

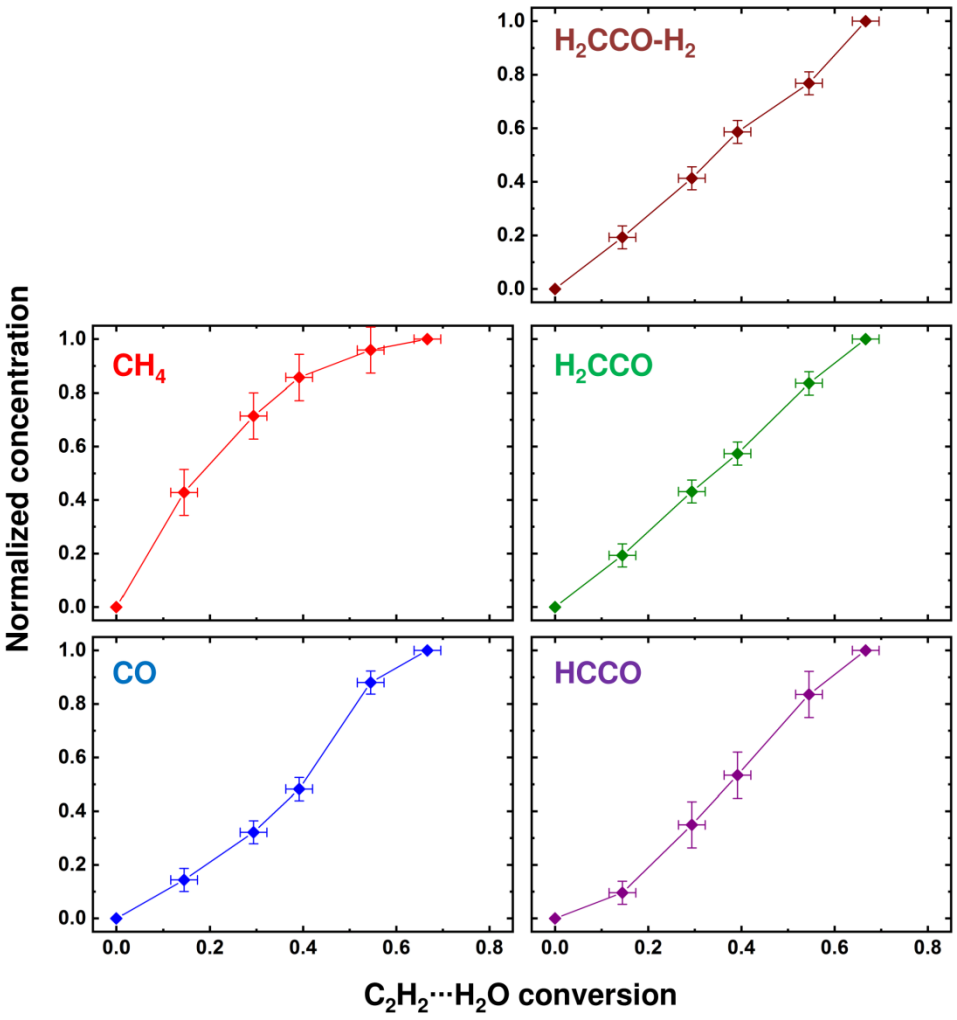

Figure S5. Build-up profiles of CH_4, CO, H_2CCO, HCCO, and H_2CCO–H_2 generated under radiolysis of C_2H_2/H_2O/Kr 1:1:1000 sample.

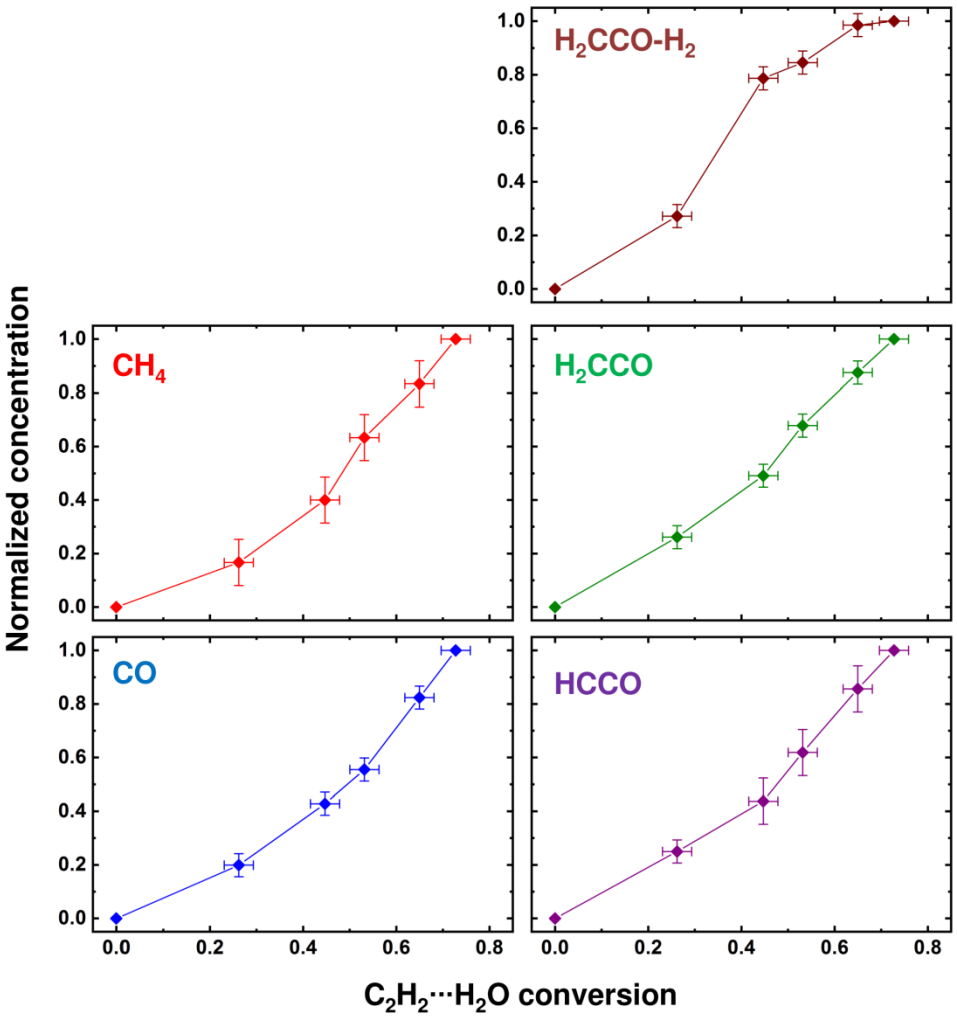

Figure S6. Build-up profiles of CH_4, CO, H_2CCO, HCCO, and H_2CCO–H_2 generated under radiolysis of C_2H_2/H_2O/Xe 1:1:1000 sample.

Table S1. Optimized molecular geometries and corresponding energies for H_2, H_2CCO and $H_2CCO\cdots H_2$ complex obtained via CCSD(T) calculations employing the L2a_3 basis set.*

Atomic number	Cartesian coordinates			Energy, a.u.
	x	y	z	
		H_2		
1	0.00000000	0.00000000	0.37175183	−1.173088
1	0.00000000	0.00000000	−0.37175183	
		H_2CCO		
8	0.00000000	0.00000000	1.93082680	
6	0.00000000	0.00000000	0.76666209	
6	−0.00000000	−0.00000000	−0.55017819	−152.391771
1	0.94212439	0.00000000	−1.07365535	
1	−0.94212439	−0.00000000	−1.07365535	
		$H_2CCO\cdots H_2$: Structure I		
6	0.21512513	1.35710562	0.00000000	
6	−0.76847350	0.48211384	−0.00000000	
1	0.60622507	1.70490635	0.94234699	
1	0.60622507	1.70490635	−0.94234699	−153.565797
8	−1.63724335	−0.29326653	−0.00000000	
1	0.85610678	−2.53918224	0.00000000	
1	0.12203480	−2.41658342	0.00000000	
		$H_2CCO\cdots H_2$: Structure II		
6	1.14656962	−0.38236892	0.00000000	
6	0.60650334	0.81845738	0.00000000	
1	0.49959983	−1.24439056	0.00000000	
1	2.22045877	−0.47427645	−0.00000000	−153.565858
8	0.12811635	1.87996015	0.00000000	
1	−2.30280091	−0.67076974	0.00000000	
1	−2.29844701	0.07338813	0.00000000	

*__Calculation details:__ molecular geometries were fully optimized at the CCSD(T)/L2a_3 level (with only the valence electron are correlated; tolerance of gradient: 10^{-7} a.u.) using a PRIRODA code. More details of the calculation procedure could be found elsewhere (Sosulin I. S., Shiryaeva E. S., Tyurin D. A., Feldman V. I., 2018, J. Phys. Chem. A, 122, 16, 4042).