Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information: Reactivity of presolvated electrons with supercritical CO_2 in water

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The radiolytic yield of e^-_{hyd} in CO_2-water system

The equations for calculating the Radiolytic yield of e^-_{hyd} are as below:

$$G(t) = \frac{A_{e^-_{aq}}(\lambda t)}{\varepsilon_\lambda \cdot d \cdot F \cdot D} \tag{1a}$$

where d is optical path–length, D – dose, and the dose factor F is:

$$F = \rho_{sol} \times \frac{p \times \frac{Z_{solute}}{M_{solute}} + (100-p) \times \frac{Z_{H_2O}}{M_{H_2O}}}{\frac{100 \times Z_{H_2O}}{M_{H_2O}}} \tag{1b}$$

Where ρ_{sol} is the density of the solution, p is the solute weight fraction per 100 g. of solution, Z_{solute} and Z_{H_2O} are the number of electrons per molecule for the solute and H_2O, respectively, M_{solute} and M_{H_2O} are the molecular weights of the solute and H_2O respectively, and the extinction coefficients of e^-_{hyd} are well known in previous articles.

The physico-chemical properties of the CO_2 solutions

Table S1: at 25°C.

P, bar	$c^{25°C}_{CO_2}$, M	$\rho^{25°C}_{sol}$, kg/m^3	p	f_s	$F^{25°C}$, kg/m^3
1.0	0.033	996.4	0.0015	0.001	997
9.1	0.290	999.6	0.013	0.005	1000
13.6	0.421	1001.2	0.019	0.008	1001
22.3	0.654	1004.1	0.029	0.012	1003
35.0	0.943	1007.8	0.041	0.017	1008
47.0	1.164	1010.9	0.051	0.021	1010
50.5	1.220	1011.6	0.053	0.022	1011
57.3	1.316	1013.0	0.057	0.024	1013
63.6	1.380	1014.0	0.060	0.026	1014
70.2	1.395	1015.0	0.060	0.026	1015
80.8	1.414	1016.2	0.061	0.026	1016
90.9	1.432	1016.9	0.062	0.026	1017
98.0	1.443	1017.2	0.062	0.026	1017
118.2	1.473	1016.9	0.064	0.027	1017

Table S2: at 35°C.

P, bar	$c_{CO_2}^{35°C}$, M	$\rho_{sol}^{35°C}$, kg/m^3	p	f_s	$F^{35°C}$, kg/m^3
2.0	0.05	993.4	0.002	0.001	1001
11.5	0.29	996.4	0.013	0.005	1005
18.7	0.44	998.5	0.020	0.008	1007
31.8	0.70	1001.9	0.031	0.013	1012
45.0	0.92	1004.9	0.040	0.017	1016
58.8	1.10	1007.3	0.048	0.020	1019
72.0	1.23	1009.1	0.054	0.023	1022
82.0	1.27	1009.9	0.055	0.023	1022
92.0	1.29	1010.4	0.056	0.024	1022
105.0	1.31	1011.1	0.057	0.024	1023

where f_s is the electron fraction of CO_2, p is the weight fraction of the solute, and F is a dose factor based on the electron density of the solution. The CO_2 concentrations at different pressures were determined according to c = f (P) dependence. Measurements were taken at different temperatures for a variety of pressures, so the pressures for different temperatures are not the same.

Optical cell for liquid–gas system spectroscopy

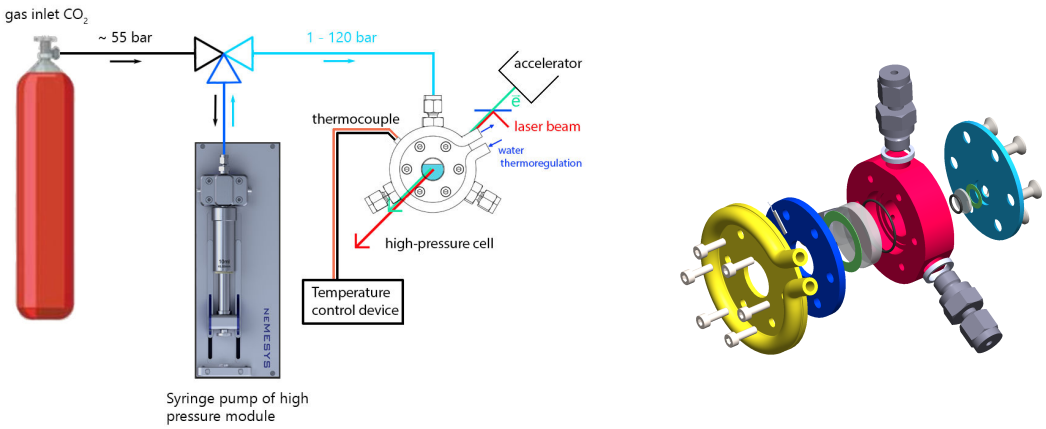

Figure S1: The schematic representation of the experiment setup.

Extra data

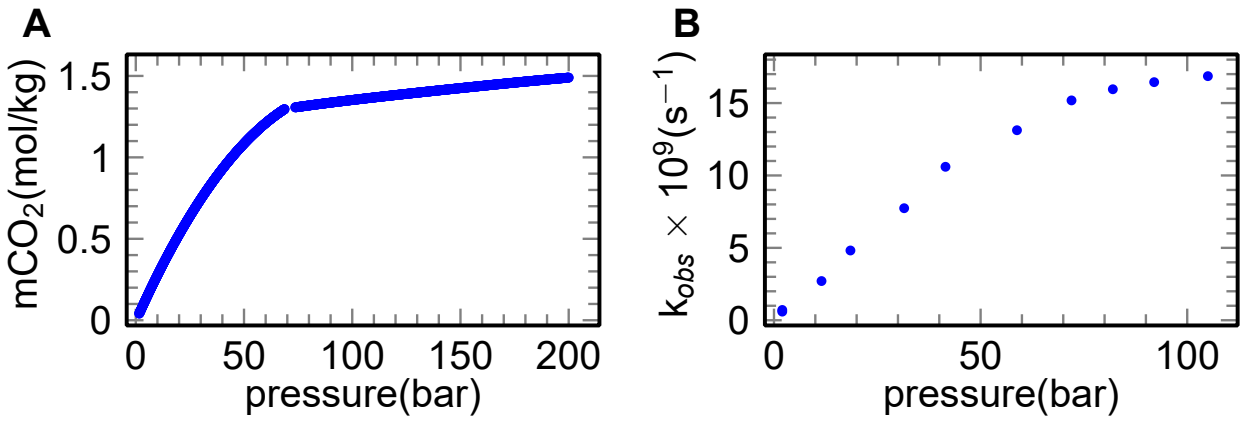

Figure S2: Pulse radiolysis data of a water – CO_2 system at different pressures (A) and comparison with molar concentration(B).

To learn more about the calculation of the molarity of CO_2, refer to this Jupyter notebook: Carbon dioxide solubility in water as a function of pressure and temperature.

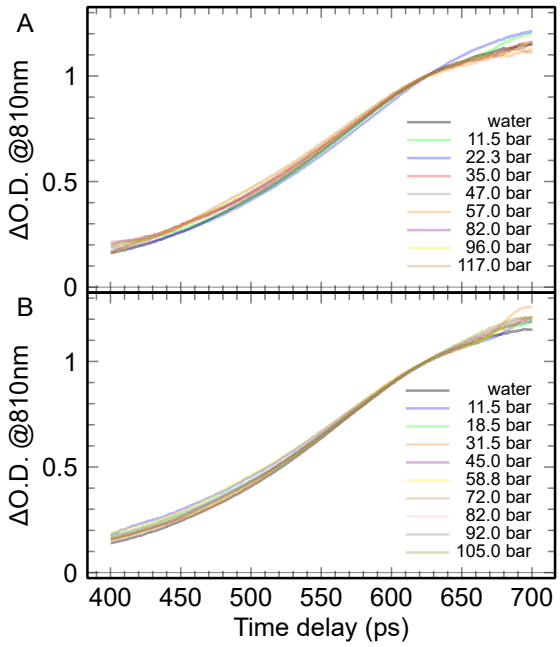

Figure S3: The absorption spectra of e^-_{hyd} electron at 10-20 ps time range after the electron pulse: A – 25°C, B – 35°C.