Electronic Supplementary Information (ESI) for " Meta-studtite stability in aqueous solutions. Impact of HCO_3^-, H_2O_2 and ionizing radiation on the dissolution and speciation".

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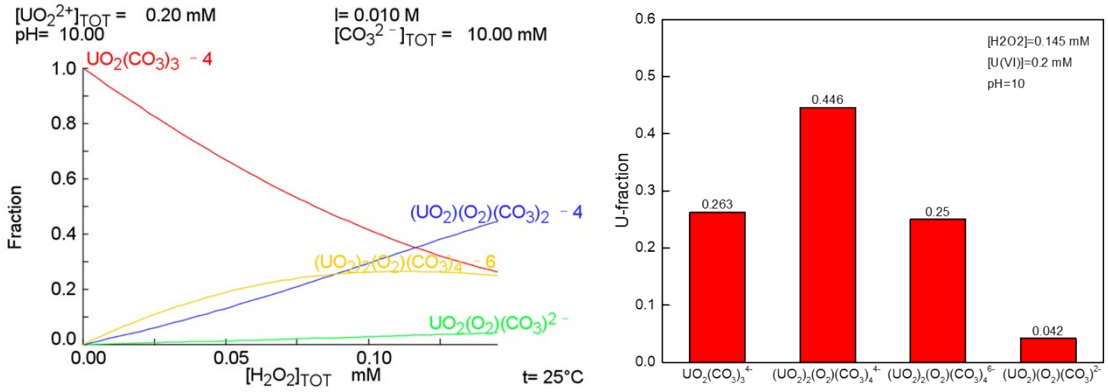

Figure S1. Plot of the uranyl fraction vs. total peroxide concentration calculated by Medusa[5] using the equilibrium constants reported for complexes formed in the ternary U(VI)-peroxide-carbonate system (left).[1] The effect of ionic strength (I=0.01 mol / kg (H_2O)) was accounted for using the simplified HKF (Helgeson-Kirkham-Flowers) model.[2,3,4] Column diagram represents the relative ratio for species formed at $[H_2O_2]_{tot}$ = 0.145 mM (right).

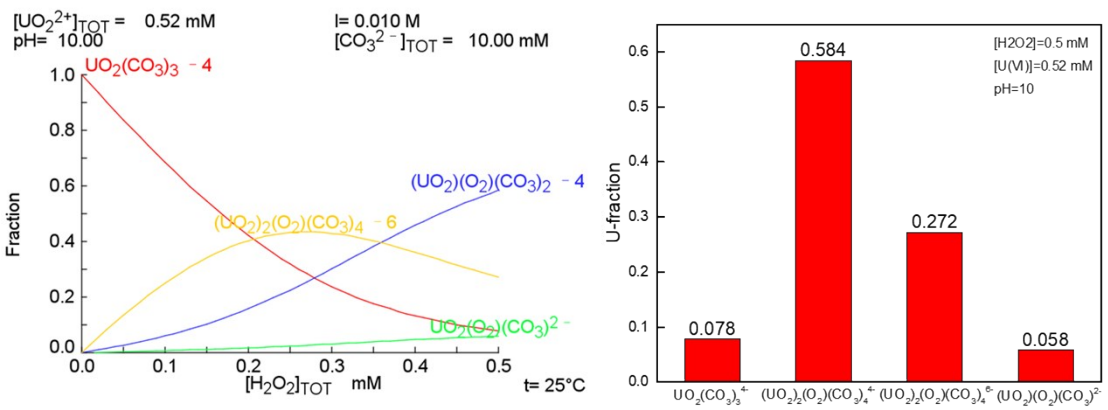

Figure S2. Plot of the uranyl fraction vs. total peroxide concentration calculated by Medusa[5] using the equilibrium constants reported for complexes formed in the ternary U(VI)-peroxide-carbonate system (left).[1] The effect of ionic strength (I=0.01 mol / kg (H_2O)) was accounted for using the simplified HKF (Helgeson-Kirkham-Flowers) model.[2,3,4] Column diagram represents the relative ratio for species formed at $[H_2O_2]_{tot}$ = 0.5 mM (right).

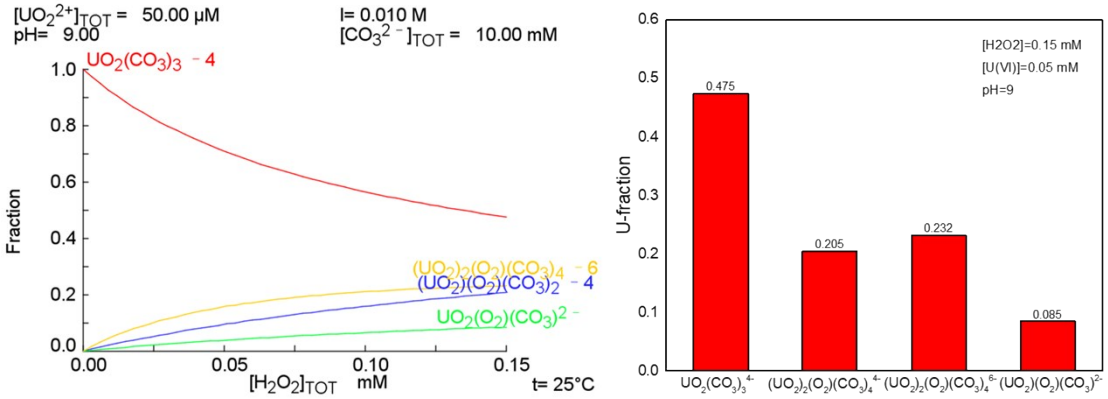

Figure S3. Plot of the uranyl fraction vs. total peroxide concentration for studtite dissolution in HCO_3^- in the presence of H_2O_2 calculated under experimental conditions by Medusa[5] using the equilibrium constants reported for complexes formed in the ternary U(VI)-peroxide-carbonate system (left).[1] The effect of ionic strength (I=0.01 mol / kg (H_2O)) was accounted for using the simplified HKF (Helgeson-Kirkham-Flowers) model.[2,3,4] Column diagram represents the relative ratio for species formed at $[H_2O_2]_{tot}$ = 0.15 mM (right).

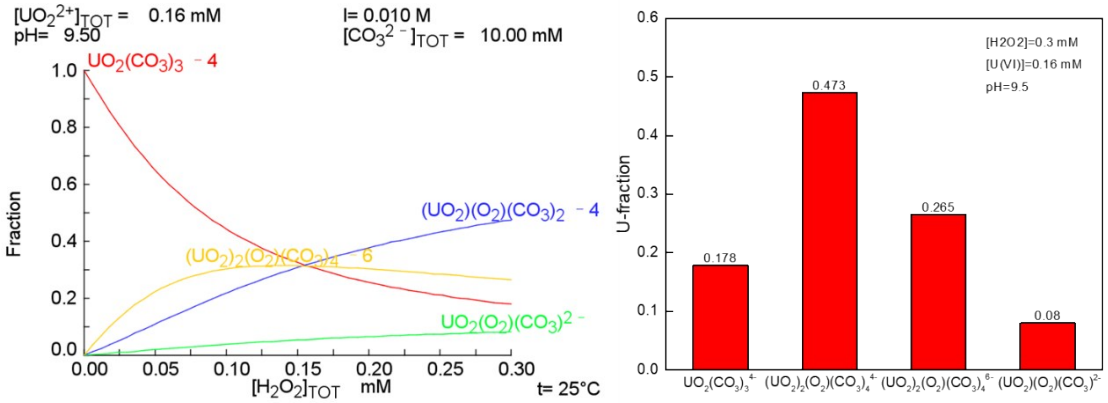

Figure S4. Plot of the uranyl fraction vs. total peroxide concentration for meta-studtite dissolution in HCO_3^- in the presence of H_2O_2 calculated under experimental conditions by Medusa[5] using the equilibrium constants reported for complexes formed in the ternary U(VI)-peroxide-carbonate system (left).[1] The effect of ionic strength (I=0.01 mol / kg (H_2O)) was accounted for using the simplified HKF (Helgeson-Kirkham-Flowers) model.[2,3,4] Column diagram represents the relative ratio for species formed at $[H_2O_2]_{tot}$ = 0.3 mM (right).

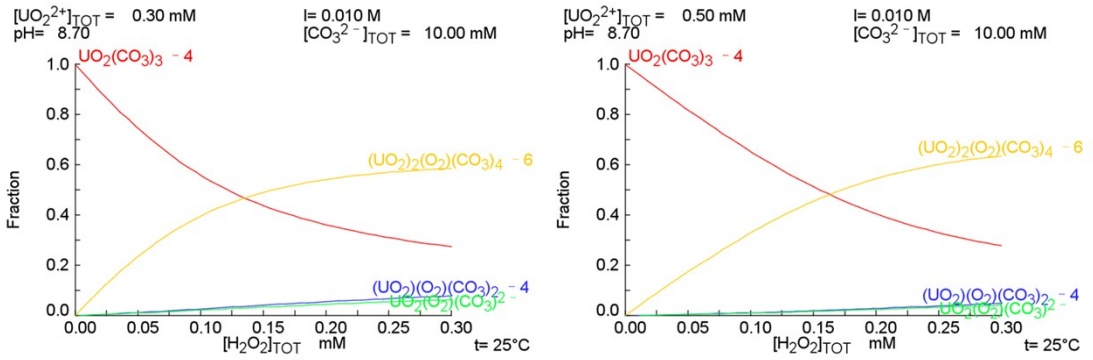

Figure S5. Plots of the uranyl fraction vs. total peroxide concentration for solutions containing 0.3 mM H_2O_2, 10 mM HCO_3^- and 0.3 mM U(VI) (left) and 0.5 mM U(VI) (right) at pH = 8.7 calculated by Medusa[5] using the equilibrium constants reported for complexes formed in the ternary U(VI)-peroxide-carbonate system.[1] The effect of ionic strength (I=0.01 mol / kg (H_2O)) was accounted for using the simplified HKF (Helgeson-Kirkham-Flowers) model.[2,3,4]

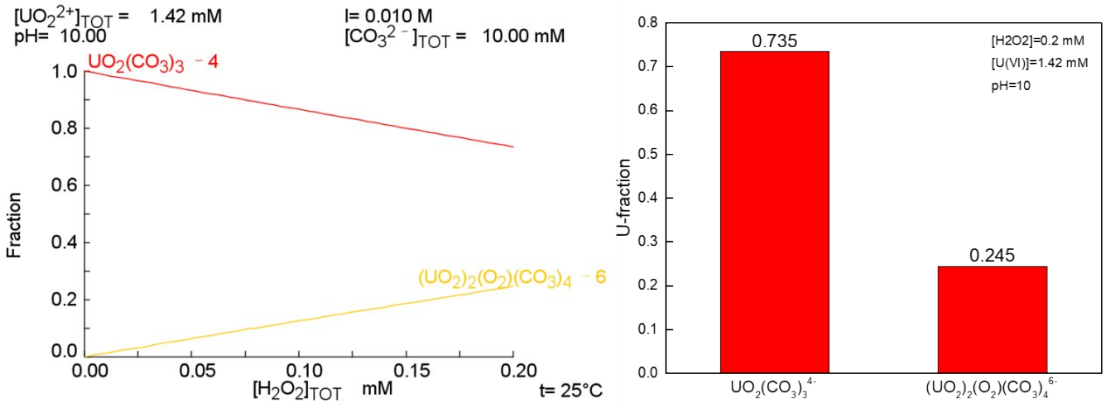

Figure S6. Plot of the uranyl fraction vs. total peroxide concentration for studtite dissolution in the presence of HCO_3^- with gamma-radiation calculated under experimental conditions by Medusa[5] using the equilibrium constants reported for complexes formed in the ternary U(VI)-peroxide-carbonate system.[1] The effect of ionic strength (I=0.01 mol / kg (H_2O)) was accounted for using the simplified HKF (Helgeson-Kirkham-Flowers) model.[2,3,4] Column diagram represents the relative ratio for species formed at $[H_2O_2]_{tot}$ = 0.2 mM (right).

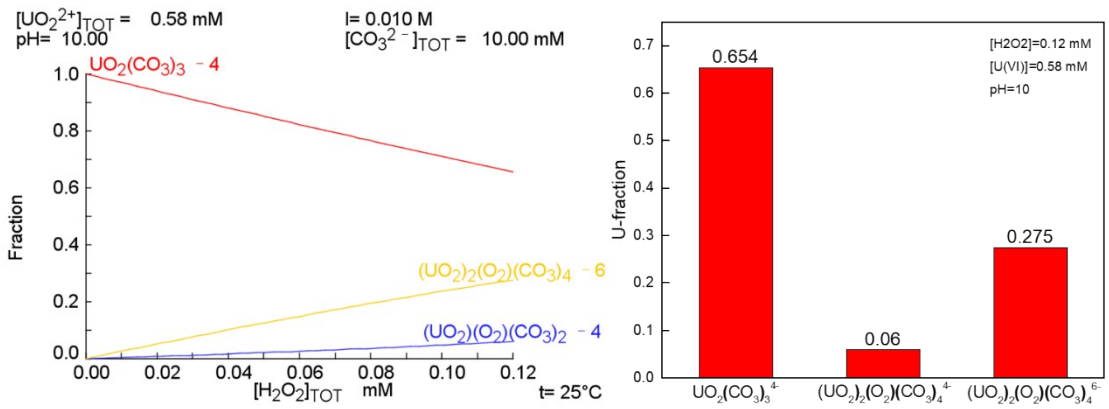

Figure S7. Plot of the uranyl fraction vs. total peroxide concentration for meta-studtite dissolution in the presence of HCO_3^- with gamma-radiation calculated under experimental conditions by Medusa[5] using the equilibrium constants reported for complexes formed in the ternary U(VI)-peroxide-carbonate system[2]. The effect of ionic strength (I=0.01 mol / kg (H_2O)) was accounted for using the simplified HKF (Helgeson-Kirkham-Flowers) model.[2,3,4] Column diagram represents the relative ratio for species formed at $[H_2O_2]_{tot}$ = 0.12 mM (right).

References

1 P. L. Zanonato, P. Di Bernardo, Z. Szabó and I. Grenthe, *Dalt. Trans.*, 2012, **41**, 11635–11641.

2 H. C. Helgeson, D. H. Kirkham and G. C. Flowers, *Am. J. Sci.*, 1981, **281**, 1249–1516.

3 E. H. Oelkers and H. C. Helgeson, *Geochim. Cosmochim. Acta*, 1990, **54**, 727–738.

4 E. L. Shock, E. H. Oelkers, J. W. Johnson, D. A. Sverjensky and H. C. Helgeson, *J. Chem. Soc. Faraday Trans.*, 1992, **88**, 803–826.

5 Medusa - computer program for calculating the composition of equilibrium mixtures by I. Puigdomenech, freely available from https://www.kth.se/che/medusa