

Supporting Information for Kinetics and Mechanism of the Oxidation of Thiourea Dioxide by Iodine in a Slightly Acidic Medium

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Table S1: Initial Concentrations of the Reactants in Different Kinetic Runs

No.	[TDO] ₀ /mM	[I ₂] ₀ /mM	[Γ] ₀ /mM	pH	ages of TDO/s
1-3	0.3	1.23	0.1	4.0	362, 78289, 170892
4-6	0.3	1.23	0.1	4.0	255062, 349479, 431574
7-11	0.6	0.61	0.1	4.0	397, 11905, 34974, 80732, 117522
12-15	0.6	0.61	0.1	4.0	203178, 260952, 346865, 434120
16-18	0.8	1.20	0.01, 0.02, 0.04	3.8	362
19-21	0.8	1.20	0.06, 0.08, 0.1	3.8	362
22-24	0.3	1.22	0.01, 0.02, 0.04	3.6	362
25-27	0.3	1.22	0.06, 0.08, 0.1	3.6	362
28-30	0.3, 0.6, 0.8	1.19	0.1	3.6	362
31-34	1.2, 1.6, 2.1, 3.0	1.19	0.1	3.6	362
35-37	3.0, 2.1, 1.6	1.19	0.1	3.8	362
38-41	1.2, 0.8, 0.6, 0.3	1.19	0.1	3.8	362
42-44	3.0, 2.1, 1.6	1.21	0.1	4.0	362
45-48	1.2, 0.8, 0.6, 0.3	1.21	0.1	4.0	362
49-51	3.0, 2.1, 1.2	1.19	0.1	4.2	362
52-54	0.8, 0.6, 0.3	1.19	0.1	4.2	362
55-57	3.0, 2.1, 1.2	1.19	0.1	4.4	362
58-61	1.0, 0.8, 0.6, 0.3	1.19	0.1	4.4	362
62-64	0.6	2.895, 2.172, 1.448	0.1	3.6	362
65-68	0.6	0.965, 0.734, 0.302, 0.151	0.1	3.6	362
69-71	0.6	2.413, 1.800, 1.206	0.1	3.8	362
72-75	0.6	0.814, 0.573, 0.302, 0.161	0.1	3.8	362
76-78	0.6	2.413, 1.800, 1.216	0.1	4.0	362
79-82	0.6	0.814, 0.613, 0.312, 0.151	0.1	4.0	362
83-85	0.6	2.350, 1.810, 1.186	0.1	4.4	362
86-88	0.6	0.804, 0.603, 0.292	0.1	4.4	362

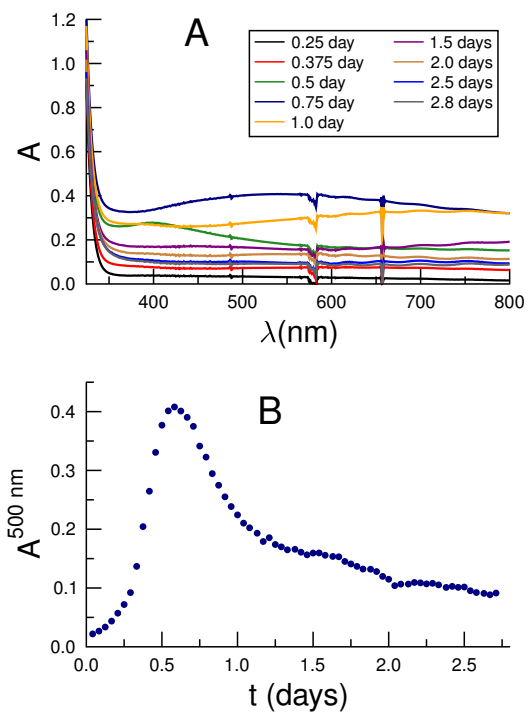


Figure S1: A: Spectral changes of TDO solution at pH = 2 during the course of ageing. $[\text{TDO}]_0 = 0.22 \text{ M}$. B: Absorbance–time plot at $\lambda = 500 \text{ nm}$.

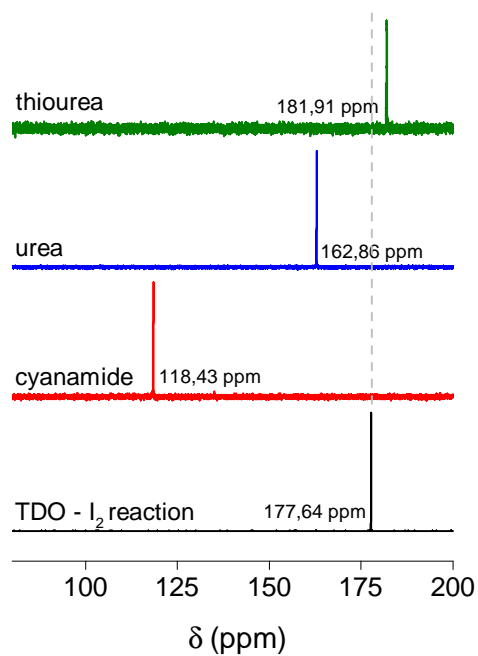


Figure S2: ^{13}C -NMR spectrum of the end product of the TDO-iodine reaction. Conditions are as follows: $[\text{TDO}]_0 = 0.1385 \text{ M}$, $T_{\text{I}_2}^0 = 0.032 \text{ M}$, $T_{\text{I}^-}^0 = 0.1 \text{ M}$. Reference spectrum of urea, thiourea, cyanamide are also indicated.

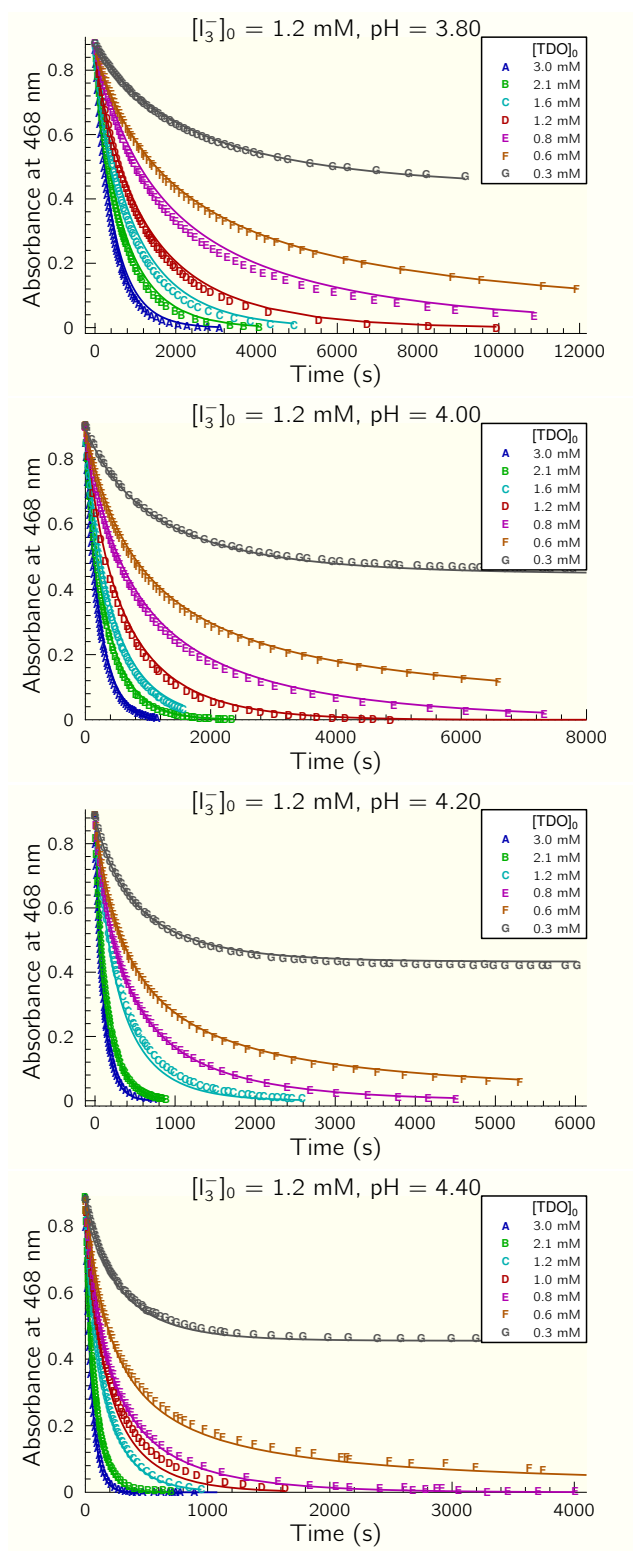


Figure S3: Measured and calculated kinetic curves. TDO dependence.

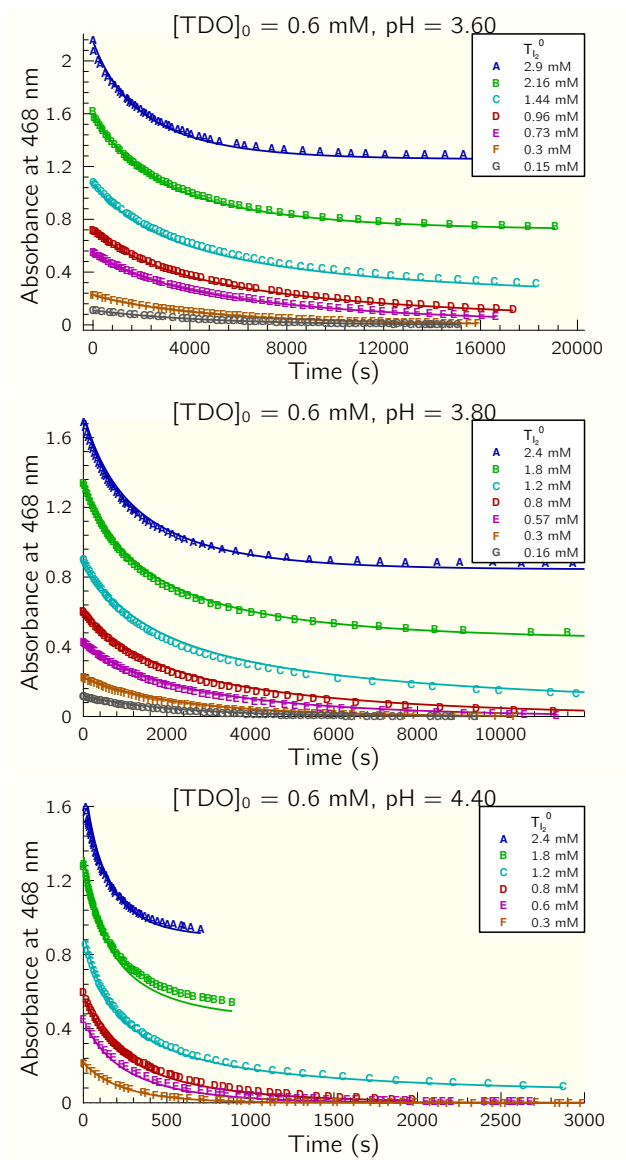


Figure S4: Measured and calculated kinetic curves. Iodine dependence.

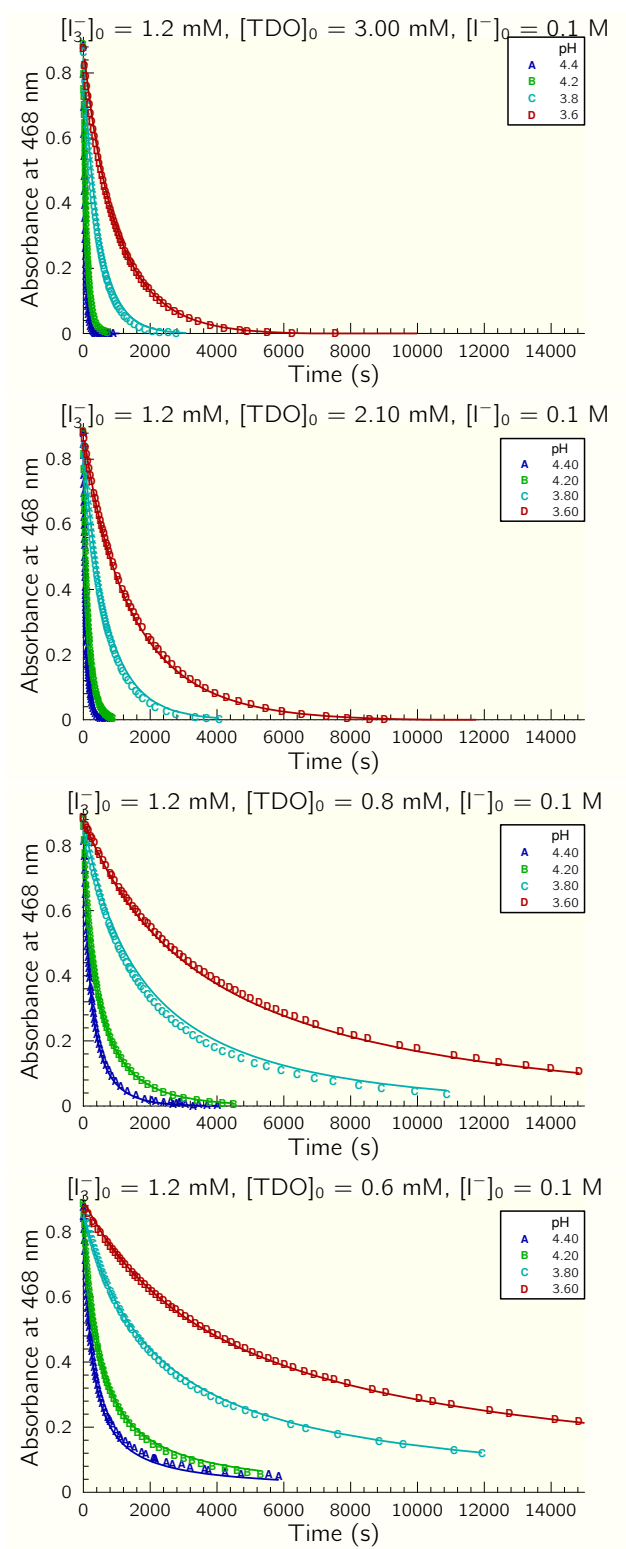


Figure S5: Measured and calculated kinetic curves. pH dependence.

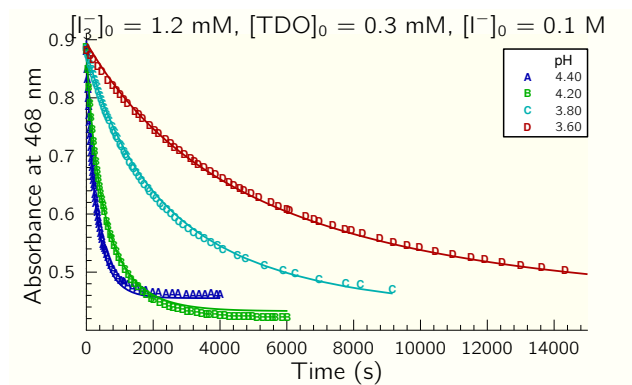


Figure S6: Measured and calculated kinetic curves. pH dependence in iodine excess.

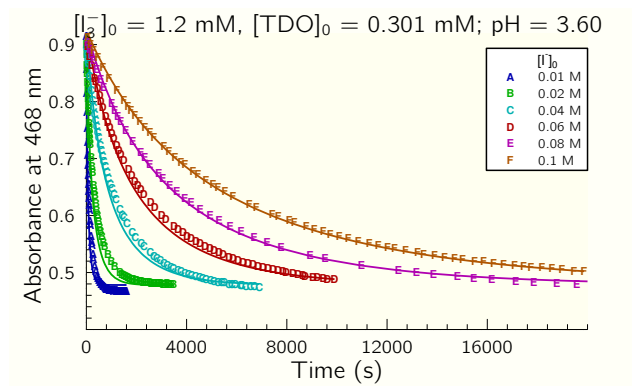


Figure S7: Measured and calculated kinetic curves. Iodide ion dependence.