BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

Homogeneous continuous flow nitration of *O*-methylisouronium sulfate and its optimization by kinetic modeling

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Beilstein J. Org. Chem. **2024,** *20,* 2408–2420. doi:10.3762/bjoc.20.205

Additional information

Part 1. Effect of molar ratio

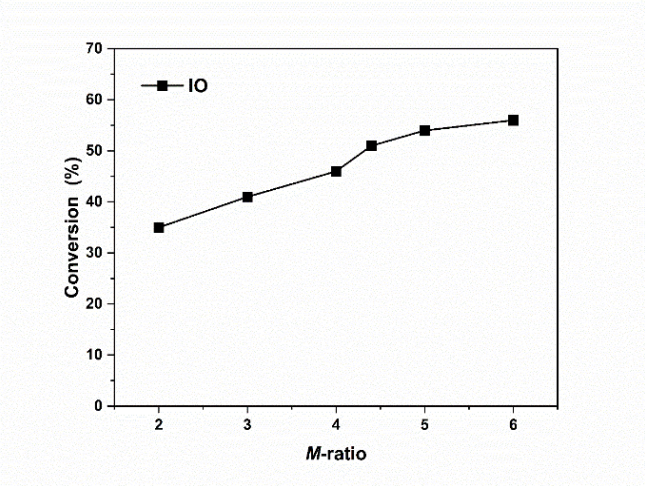

Figure S1: Variation of NIO conversion with HNO_3 molar ratio. The conversion was determined by high performance liquid chromatography (HPLC).

Part 2. Determination of the reaction orders

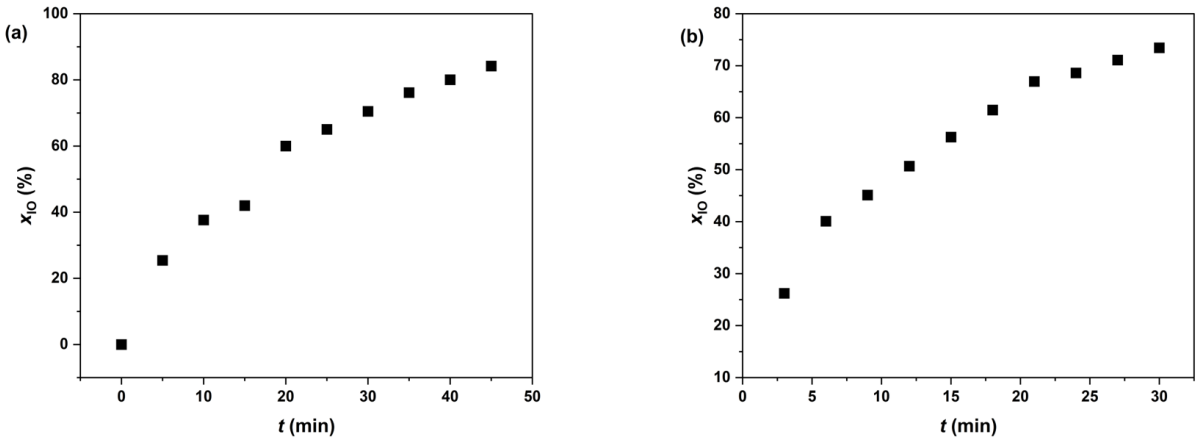

Figure S2: (a) x_{IO} versus reaction time (t). (b) x_{IO} versus reaction time t. Determination of IO reaction order conditions: reaction temperature (T) = 0 °C; initial concentration of reactants in reaction mixture: c_{IO0} = 1 mol/L, c_{HNO_30} = 15 mol/L. Determination of HNO_3 reaction order conditions: reaction temperature (T) = 10 °C; initial concentration of reactants in reaction mixture: c_{IO0} = 1 mol/L, c_{HNO_30} = 4.4 mol/L. The conversion was determined by high performance liquid chromatography (HPLC).

Part 3. Apparent reaction rate

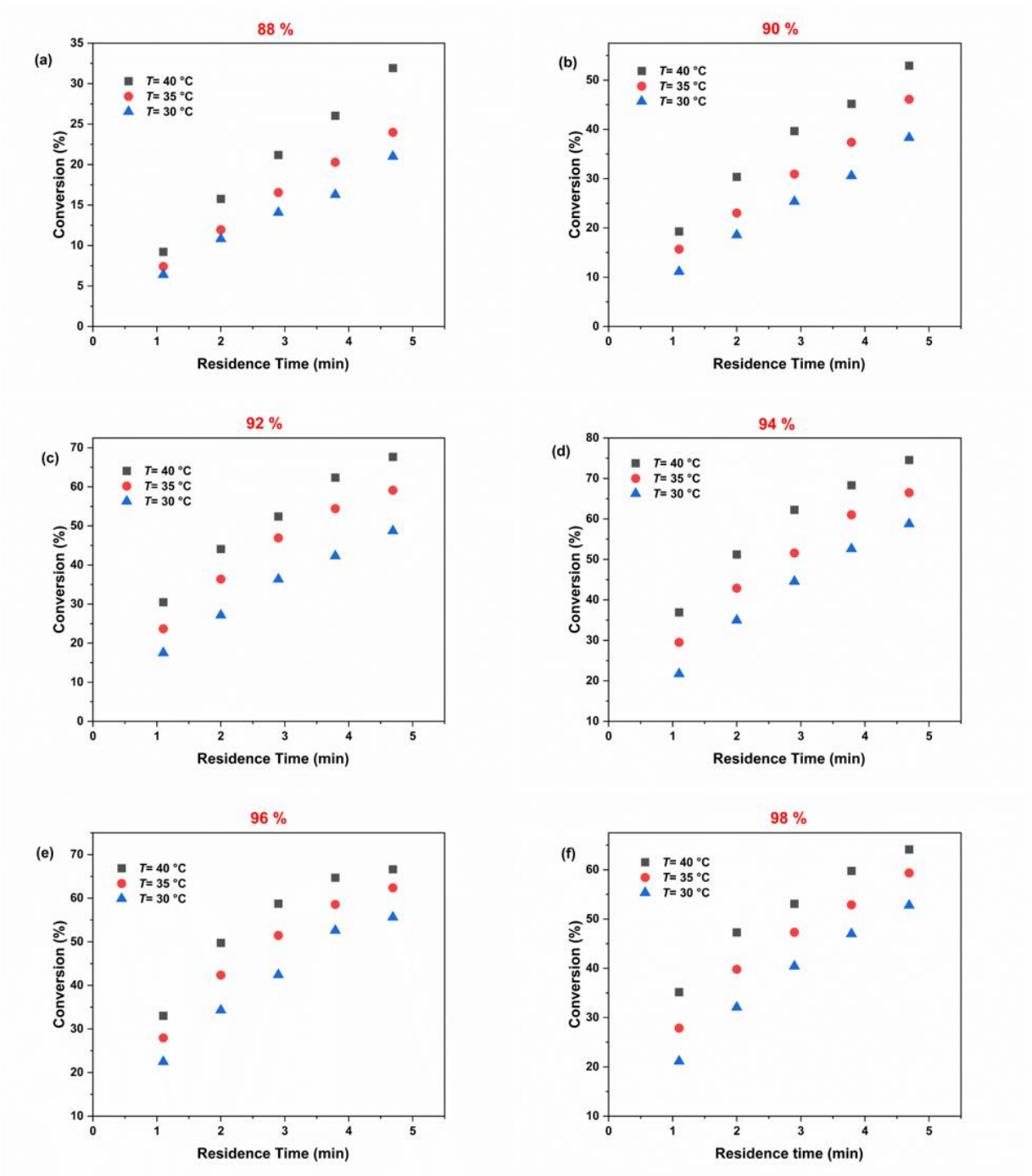

Figure S3: Variation of x_{IO} with t at different temperatures (30 °C, 35 °C, 40 °C) and different H_2SO_4 mass fractions (88%, 90%, 92%, 94%, 96%, 98%).

Part 4. Determination of M_C function

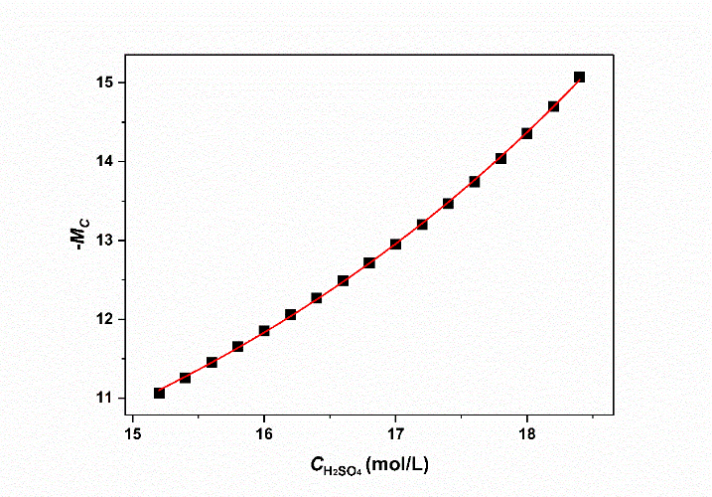

Figure S4: The results of polynomial fitting the data of M_c function at 298K.[1]

Part 5. Values of nM_c and $\lg\left(\frac{c_{NO_2^+}}{c_{HNO_3}}\right)+\lg k_0$ under different temperatures and H_2SO_4 mass fraction

Table S1: Values of nM_c and $\lg\left(\frac{c_{NO_2^+}}{c_{HNO_3}}\right)+\lg k_0$ at different temperatures and H_2SO_4 mass fraction.

Mass fraction of H_2SO_4 (wt %)	Temperature (℃)	$\lg\left(\frac{c_{NO_2^+}}{c_{HNO_3}}\right)+\lg k_0$	nM_c
88	30	11.285	-12.931
	35	11.705	-13.230
	40	12.226	-13.592
90	30	12.015	-13.275
	35	12.431	-13.591
	40	12.947	-14.023
92	30	12.745	-13.871
	35	13.156	-14.146
	40	13.668	-14.567
94	30	13.476	-14.462
	35	13.882	-14.791
	40	14.389	-15.209
96	30	14.206	-15.225
	35	14.607	-15.572
	40	15.110	-16.053
98	30	14.936	-16.026
	35	15.333	-16.393
	40	15.831	-16.859

Part 6. Kinetic model validation experiments under different conditions

Table S2: Kinetic model validation experiments under different conditions

Mass fraction of H_2SO_4 (wt %)	Temperature (°C)	Time (min)	Theoretical conversion (%)	Actual conversion (%)	Errors (%)
94	40	3.5	60	62	2
		6.3	80	81	1
		9.3	90	86	4
	35	4.2	60	62	2
		5.6	70	71	1
		7.6	80	79	1
	30	5.1	60	61	1
		6.8	70	69	1
		9.3	80	78	2
98	40	5.6	60	62	2
		7.4	70	72	2
		10.2	80	78	2
	35	6.0	60	59	1
		8.0	70	70	0
		11.0	80	77	3
	30	6.4	60	61	1
		8.6	70	69	1
		11.7	80	77	3

Part 7. Reaction optimization using kinetic models

Table S3: Reaction optimization using kinetic models.

Mass fraction of H_2SO_4 (wt %)	Temperature (°C)	Time (min)	Theoretical conversion (%)	Actual conversion (%)	Errors (%)
94	45	7.8	90	83.9	6
		10.3	95	85.8	9
		13.7	98	87.6	10
	40	7.6	85	81	4
		12.4	95	87.4	8

References

1. Marziano, N. C.; Tomasin, A.; Traverso, P. G. *Journal of the Chemical Society, Perkin Transactions 2* **1981**, (7), 1070-1075, 10.1039/P29810001070.