Supplementary Material

Sucrose Is a Promising Feedstock for the Synthesis of the Platform Chemical Hydroxymethylfurfural

David Steinbach, Andrea Kruse, Jörg Sauer and Philipp Vetter

The molar ratios $y_{i,\ meas}$ of the acid-catalyzed dehydration of sucrose, which were calculated from all concentrations c_i determined experimentally (see Equation S1), are shown in Table S1.

$$y_{i,\ meas} = \frac{c_i}{c_{sucrose,\ start}} \quad \text{(S1)}$$

The molar ratios $y_{i,\ meas}$ of the acid-catalyzed dehydration of glucose or fructose, which were calculated from all concentrations c_i determined experimentally (see Equation S2 and S3), are shown in Table S2.

$$y_{i,\ meas} = \frac{c_i}{c_{glucose,\ start}} \quad (2)$$

$$y_{i,\ meas} = \frac{c_i}{c_{fructose,\ start}} \quad (3)$$

Table S1. Experimentally determined molar ratios $y_{i,\,meas}$ of the acid-catalyzed conversion of sucrose. Feedstock contained 2 wt % sucrose and 0.005 mol/L sulfuric acid.

Temperature [°C]	Residence Time [min]	Fructose [mol/mol]	Glucose [mol/mol]	HMF [mol/mol]	Furfural [mol/mol]	Xylose [mol/mol]	Levulinic Acid [mol/mol]	Formic Acid [mol/mol]	∑ Side Products * [mol/mol]
180	2	0.996	1.064	0.008	0.000	0.000	0.000	0.000	−0.068
	4	0.976	1.035	0.036	0.001	0.000	0.000	0.000	−0.047
	6	0.934	1.030	0.074	0.002	0.000	0.000	0.000	−0.040
	8	0.855	1.058	0.152	0.005	0.000	0.000	0.000	−0.070
	10	0.711	0.930	0.183	0.007	0.000	0.000	0.000	0.171
	12	0.622	0.884	0.255	0.009	0.065	0.005	0.000	0.172
	14	0.454	0.764	0.422	0.013	0.047	0.020	0.015	0.290
	16	0.402	0.751	0.478	0.015	0.048	0.019	0.000	0.300
	18	0.246	0.778	0.588	0.020	0.051	0.038	0.035	0.291
	20	0.145	0.798	0.641	0.024	0.050	0.041	0.029	0.314
	22	0.098	0.792	0.672	0.026	0.054	0.065	0.057	0.308
	24	0.067	0.780	0.669	0.026	0.048	0.058	0.065	0.364
200	2	0.956	1.119	0.054	0.002	0.000	0.000	0.000	−0.132
	4	0.856	1.006	0.130	0.006	0.000	0.000	0.000	0.003
	6	0.750	1.035	0.285	0.014	0.000	0.012	0.000	−0.090
	8	0.484	0.843	0.452	0.025	0.066	0.033	0.029	0.112
	10	0.344	0.973	0.532	0.030	0.000	0.034	0.000	0.099
	12	0.217	0.809	0.597	0.032	0.067	0.039	0.056	0.252
	14	0.052	0.715	0.682	0.041	0.061	0.094	0.085	0.374
	16	0.020	0.667	0.647	0.042	0.056	0.116	0.115	0.469
	18	0.000	0.666	0.626	0.046	0.059	0.165	0.163	0.456
220	2	0.770	1.059	0.181	0.007	0.069	0.000	0.000	−0.073
	4	0.467	0.999	0.392	0.028	0.080	0.020	0.025	0.032
	6	0.262	0.921	0.505	0.042	0.071	0.035	0.055	0.179
	8	0.172	0.941	0.566	0.047	0.079	0.044	0.069	0.168
	10	0.082	0.804	0.623	0.060	0.065	0.069	0.107	0.310
		0.065	0.784	0.563	0.057	0.081	0.097	0.100	0.377
		0.045	0.767	0.569	0.057	0.038	0.099	0.101	0.442
		0.044	0.802	0.558	0.057	0.036	0.104	0.108	0.414
	12	0.027	0.588	0.560	0.065	0.047	0.125	0.138	0.604
	14	0.000	0.458	0.515	0.069	0.043	0.215	0.232	0.715
	16	0.000	0.465	0.501	0.070	0.043	0.250	0.277	0.684
	18	0.022	0.434	0.472	0.065	0.037	0.219	0.248	0.761

* ∑ Side products are calculated from the carbon balance (difference to 100%), assuming that the average sum formula of side products is $C_6H_{12}O_6$.

Table S2. Experimentally determined molar ratios $y_{i,\,meas}$ of the acid-catalyzed conversion of glucose or fructose at 220 °C. Feedstock contained 0.005 mol/L sulfuric acid and either 1.05 wt % glucose or 1.05 wt % fructose.

Feedstock	Temperature [°C]	Residence Time [min]	Fructose [mol/mol]	Glucose [mol/mol]	HMF [mol/mol]	Furfural [mol/mol]	Xylose [mol/mol]	Levulinic Acid [mol/mol]	Formic Acid [mol/mol]	∑ Side Products * [mol/mol]
fructose	220	6	0.224	0.006	0.472	0.039	0.000	0.037	0.037	0.230
		10	0.029	0.005	0.480	0.049	0.000	0.113	0.114	0.331
			0.040	0.003	0.509	0.046	0.000	0.089	0.089	0.320
			0.052	0.002	0.500	0.047	0.000	0.084	0.083	0.323
			0.051	0.006	0.514	0.048	0.000	0.065	0.065	0.326
glucose	220	6	0.000	0.895	0.037	0.004	0.054	0.003	0.004	0.017
		10	0.000	0.647	0.095	0.013	0.056	0.021	0.024	0.179
			0.004	0.827	0.088	0.011	0.035	0.013	0.016	0.029
			0.006	0.729	0.092	0.012	0.037	0.014	0.017	0.118
			0.007	0.794	0.082	0.011	0.056	0.015	0.018	0.047

* ∑ Side products are calculated from the carbon balance (difference to 100 %), assuming that the average sum formula of side products is $C_6H_{12}O_6$.

Table S3. Activation energy EA_n and Arrhenius factor A_n of the n first-order reactions defined according to the model (see Figure 2).

n	A_n [min^{-1}]	EA_n [kJ/mol]
1	7470000	70.6
2	188000	65.4
3	41400	61.6
4	9880	59.4
5	29700	49.1
6	24600	57.3
7	0.0686	10.6
8	2360000	70.9
9	0.0775	8.3