

Hydrogenation of *trans,trans*-muconic acid to bio-adipic acid: mechanism identification and kinetic modelling

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Table S1. Experimental data taken at different temperatures for *trans,trans*-muconic acid hydrogenation on Pt/C 5% at 4 bar of s hydrogen.

Time (s)	Temperature (K)	ttMA (mol l ⁻¹)	cHDA (mol l ⁻¹)	tHDA (mol l ⁻¹)	AA (mol l ⁻¹)	H ₂ (mol l ⁻¹)
0	323	6.96E-02	0.00E+00	0.00E+00	0.00E+00	2.73E-03
1200		4.80E-02	1.47E-03	1.45E-02	5.69E-03	2.73E-03
2400		3.55E-02	8.39E-04	1.82E-02	1.50E-02	2.73E-03
3600		2.07E-02	1.46E-03	2.22E-02	2.52E-02	2.73E-03
4500		7.56E-03	3.59E-03	2.96E-02	2.89E-02	2.73E-03
5400		6.47E-04	3.53E-03	2.26E-02	4.28E-02	2.73E-03
7200		0.00E+00	2.12E-03	8.51E-03	5.90E-02	2.73E-03
10800		6.96E-05	0.00E+00	0.00E+00	6.95E-02	2.73E-03
14400		0.00E+00	0.00E+00	0.00E+00	6.96E-02	2.73E-03
0	333	6.96E-02	0.00E+00	0.00E+00	0.00E+00	2.59E-03
1200		4.35E-02	1.13E-03	1.63E-02	8.67E-03	2.59E-03
1800		3.09E-02	1.83E-03	2.21E-02	1.48E-02	2.59E-03
2400		2.29E-02	2.76E-03	2.10E-02	2.29E-02	2.59E-03
3000		1.98E-02	2.82E-03	1.95E-02	2.75E-02	2.59E-03
4500		7.66E-04	2.72E-03	1.48E-02	5.13E-02	2.59E-03
6900		1.33E-03	0.00E+00	0.00E+00	7.00E-02	2.59E-03
9000		0.00E+00	0.00E+00	0.00E+00	7.00E-02	2.59E-03
0	343	6.96E-02	0.00E+00	0.00E+00	0.00E+00	2.47E-03
600		4.85E-02	6.87E-04	8.05E-03	1.24E-02	2.47E-03
1200		3.01E-02	3.32E-03	1.27E-02	2.34E-02	2.47E-03
2400		1.10E-02	1.86E-03	1.82E-02	3.85E-02	2.47E-03
3600		0.00E+00	0.00E+00	0.00E+00	6.96E-02	2.47E-03
6000		0.00E+00	0.00E+00	0.00E+00	6.96E-02	2.47E-03
7200		0.00E+00	0.00E+00	0.00E+00	6.96E-02	2.47E-03

Table S2. Calculated values for the different models with 95% confidence interval and regression metrics.

Parameter		LHHW_17P	LHHW_15P	LHHW_13P	LHHW_13 (case 3)
K_{itMA}	[L mol ⁻¹]	1.49E+01 ±190%	6.97E+01 ±35%	9.40E+00 ±0.01%	9.85E+00 ±0.12%
K_{cHDA}	[L mol ⁻¹]	4.86E+03 ±81%	9.16E+02 ±56%	3.44E+04 ±0.03%	4.95E+04 ±0.03%
K_{itHDA}	[L mol ⁻¹]	5.81E+00 ±500%	1.00E+00 ±43%	2.28E+01 ±0.04%	2.52E+01 ±0.05%
K_{aa}	[L mol ⁻¹]	6.53E+01 ±133%	3.57E+01 ±35%		
K_{H2}	[L mol ⁻¹]	4.20E+02 ±400%	1.02E+00 ±96%		
A_{h02}	[s ⁻¹]	4.72E+00 ±93%	3.86E+00 ±27%	8.86E-06 ±5000%	1.00E-01 ±0.10%
E_{ah02}	[J mol ⁻¹]	1.20E+05 ±146%	7.41E+04 ±34%	2.75E+04 ±0.02%	2.73E+04 ±0.06%
A_{h23}	[s ⁻¹]	4.35E+00 ±43%	2.31E+00 ±46%	1.39E-01 ±0.04%	2.40E-01 ±0.13%
E_{ah23}	[J mol ⁻¹]	2.96E+04 ±264%	1.23E+04 ±140%	4.01E+04 ±0.09%	3.97E+04 ±0.04%
A_{i12}	[s ⁻¹]	2.98E+00 ±63%	5.51E+00 ±42%	2.23E+01 ±0.005%	2.30E+01 ±0.03%
A_{i21}	[s ⁻¹]	5.43E-01 ±306%	3.61E+00 ±65%	5.17E+00 ±0.03%	5.02E+00 ±0.00%
E_{ai12}	[J mol ⁻¹]	4.03E+04 ±116%	1.63E+05 ±119%	2.95E+04 ±0.04%	2.60E+04 ±0.02%
E_{ai21}	[J mol ⁻¹]	1.17E+05 ±43%	2.24E+05 ±83%	7.63E+05 ±0.03%	8.25E+05 ±0.02%
A_{h13}	[s ⁻¹]	8.63E+00 ±19%	5.74E+00 ±18%	8.66E+00 ±0.02%	8.89E+00 ±0.03%
E_{ah13}	[J mol ⁻¹]	8.59E+04 ±33%	8.37E+04 ±27%	3.89E+04 ±0.04%	4.67E+04 ±0.06%
A_{h01}	[s ⁻¹]	6.45E+00 ±25%			
E_{ah01}	[J mol ⁻¹]	7.77E+04 ±60%			
SSE		2.51E-04	5.38E-04	7.76E-04	7.71E-04
R ²		99.49%	98.90%	98.43%	98.42%

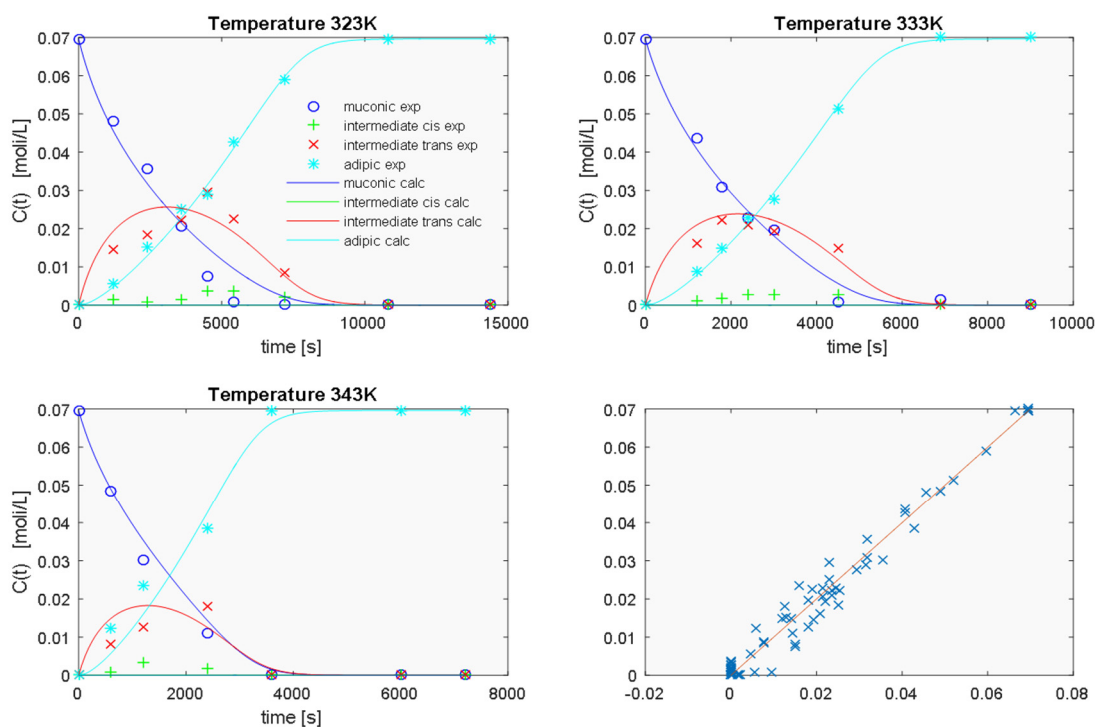


Figure S1: Results of the regression with the model LHHW_13P (case3).