Investigation of the cooperative-effects of Lewis- and Brønstedt acids in homogeneously catalyzed OME fuel synthesis by inline-NMR monitoring

Supporting Information

-

Patrick Endres,^{a,b} Timo Schuett,^{a,b} Stefan Zechel,^{a,b} Martin D. Hager,^{a,b,c,d} Robert Geitner*^e and Ulrich S. Schubert*^{a,b,c,d}

а	Patrick Endres, Timo Schuett, Julian Kimmig, Dr. Stefan Zechel, Dr. Martin D. Hager, Prof. Dr. Ulrich S. Schubert Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena,
	Humboldtstr. 10, 07743 Jena, Germany
b	Patrick Endres, Timo Schuett, Julian Kimmig, Dr. Stefan Zechel, Dr. Martin D. Hager, Prof. Dr. Ulrich S. Schubert
	Jena Center for Soft Matter (JCSM),
	Friedrich Schnier University Jena, Dhiles Friedrich State St
	Philosophenweg 7,
	07743 Jena, Germany
С	Dr. Martin D. Hager, Prof. Dr. Ulrich S. Schubert
	Center for Energy and Environmental Chemistry Jena (CEEC Jena),
	Friedrich Schiller University Jena,
	Philosophenweg 7a, 07743 Jena, Germany
	E-mail: ulrich.schubert@uni-jena.de
d	Dr. Martin D. Hager, Prof. Dr. Ulrich S. Schubert
	Helmholtz Insitute for Polymers in Energy Applications Jena (HIPOLE Jena),
	Lessingstraße 12-14, 07743 Jena, Germany
е	JunProf. Dr. Robert Geitner
	Institute for Chemistry and Bioengineering
	Technical University Ilmenau
	Weimarer Str. 32, 98693 Ilmenau, Germany
	E-mail: robert.geitner@tu-ilmenau.de

Table of contents

1.	NMR measurement cycle	S1
2.	NMR measurements at selected reaction times	S2
3.	Kinetic fitting of molar share over time	S3

1. NMR measurement cycle

The NMR measurements were started with an initial shim on sample, and then ¹H NMR spectra were acquired. This process was repeated ten times before conducting another shim on sample. This entire cycle of measurements and shimming was repeated up to a maximum of 50 times. (Fig. S1)



Figure S1: Analytic cycle of the online NMR measurements.

2. ¹H NMR measurements at selected reaction times



Figure S2: ¹H NMR spectrum after reactor loading, dimethoxy methane 150 g, trioxane 44.4 g, ZnCl₂ 17.5 mmol L⁻¹, 20 °C (43 MHz).



Figure 3: ¹H NMR spectrum after 20 min prior to the addition of the Brønsted acid catalyst, dimethoxy methane 150 g, trioxane 44.4 g, ZnCl₂ 17.5 mmol L⁻¹, 20 °C (43 MHz).



Figure 4: ¹H NMR spectrum after 120 min at equilibrium conditions, dimethoxy methane 150 g, trioxane 44.4 g, triflic acid 13.5 mmol L⁻¹, ZnCl₂ 17.5 mmol L⁻¹, 20 °C (43 MHz).

3. Kinetic fitting of molar share over time



Figure 6: Experimentally extracted concentrations of OME_x over time with kinetic fits, dimethoxy methane 150 g, trioxane 44.4 g, triflic acid 13.5 mmol L⁻¹, ZnCl₂ 2.9 mmol L⁻¹, 20 °C.