

**Dimethyl carbonate synthesis from carbon-di-oxide by ceria-zirconia catalysts prepared using templating method: Characterization, parametric optimization and chemical equilibrium modeling**

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**Supporting Information**

**Table S1. Physical properties and the pure components parameters [Piñeroa et al., 2007].**

	Methanol	CO <sub>2</sub>	DMC	H <sub>2</sub> O
MW (g/mol)	32.042	44.01	90.60	18.02
T <sub>c</sub> (K)	512.6	304.2	548.0	647.3
P <sub>c</sub> (MPa)	8.096	7.382	4.500	22.09
<i>K</i>	-0.16816	0.04285	0.38462	-0.06635
<i>Ω</i>	0.565	0.225	0.385	0.344

**Table S2. Temperature dependence of binary interaction parameters  $k_{ij}$  and  $l_{ij}$  [Bustamante et al., 2012].**

System	$k_{ij}$	$l_{ij}$
CO <sub>2</sub> (1) + methanol (2)	$k_{12} = -0.04889 + 0.000142 T$	$l_{12} = 0.11655 - 0.00049 T$
	$k_{21} = -0.32186 + 0.001202 T$	$l_{21} = 0.0034067 - 3 \times 10^{-5} T$
CO <sub>2</sub> (1) + water (2)	$k_{12} = 3.06296 - 0.009680 T$	$l_{12} = 0$
	$k_{21} = -0.35981 + 0.000859 T$	$l_{21} = 0$
CO <sub>2</sub> (1) + DMC (2)	$k_{12} = -0.00432 + 0.000010 T$	$l_{12} = 8.2567 \times 10^{-5} + 1.47 \times 10^{-6} T$
	$k_{21} = -0.03110 + 0.000080 T$	$l_{21} = 0.0002787 - 2.67 \times 10^{-6} T$
methanol (1) + water (2)	$k_{12} = -0.61880 + 0.001570 T$	$l_{12} = 0$
	$k_{21} = -0.39211 + 0.000815 T$	$l_{21} = 0$
DMC (1) + methanol (2)	$k_{12} = -0.03545 + 0.000282 T$	$l_{12} = 0$
	$k_{21} = 0.03595 - 0.000035 T$	$l_{21} = 0$
DMC (1) + water (2)	$k_{12} = -0.34043$	$l_{12} = -9.22 \times 10^{-5}$
	$k_{21} = -0.0796$	$l_{21} = 1.942 \times 10^{-4}$

**Table S3. Values of  $K_{eq}$  for DMC synthesis by direct  $CO_2$  conversion using  $Ce_{0.5}Zr_{0.5}O_2$  at different temperatures and constant pressure,  $P=150$  bar.**

<b>T (K)</b>	<b><math>y_{o,MeOH}</math></b>	<b><math>y_{o,CO_2}</math></b>	<b><math>X_{eq,MeOH}</math>, experimental</b>	<b><math>y_{eq,MeOH}</math></b>	<b><math>y_{eq,CO_2}</math></b>	<b><math>y_{eq,DMC}</math></b>	<b><math>y_{eq,H_2O}</math></b>	<b><math>K_{eq}</math> (l/mol)</b>
373	0.697797	0.302203	0.004043	0.696515	0.302261	0.000612258	0.0006123	$6.811 \times 10^{-8}$
393	0.708692	0.291308	0.008680	0.705990	0.291469	0.001270488	0.0012705	$3.629 \times 10^{-7}$
413	0.718828	0.281172	0.0055832	0.717130	0.281295	0.000787461	0.0007875	$1.713 \times 10^{-7}$
433	0.728283	0.271717	0.0016944	0.727780	0.271759	0.000230430	0.0002304	$1.823 \times 10^{-8}$
453	0.737123	0.262877	0.0004182	0.737002	0.262888	0.000054981	0.0000550	$1.327 \times 10^{-9}$