Supporting information

Kinetics and thermodynamics of the decarboxylation of 1,2-glycerol carbonate to produce glycidol: computational insights

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Table S1. Thermodynamics of polymer vs. cyclic carbonate formation.

	Enthalpy (kcal/mol)		Free Energy (kcal/mol)	
	Polymer	Cyclic Carbonate	Polymer	Cyclic Carbonate
Ethylene carbonate	-21.2	-15.1	-0.4	-3.8
Propylene carbonate	-21.2	-15.7	0.5	-4.2
Chloropropylene carbonate	-22.1	-13.8	0.1	-2.5
Styrene carbonate[†]	-22.8	-14.8	-0.8	-3.4
Cyclopentene carbonate*	-15.8	-14.5	7.1	-5.8
Indene carbonate*	-21.1	-18.2	1.5	-6.6
Cyclohexene carbonate*	-22.6	-16.7	3.4	-4.6
Trimethylene carbonate	-23.1	-11.7	-2.6	-0.8
1,2-Glyercol carbonate	-21.3	-16.2	0.6	-4.3
1,2-Glycerol carbonate, methyl ether	-22.1	-15.3	0.0	-3.9
1,3-Glycerol carbonate	-22.3	-9.0	-0.5	1.7
1,3-Glycerol carbonate, methyl ether	-20.9	-8.2	0.7	2.8

Average of 4 iterations unless noted. * Calculated from 1-mer + CO_2 + epoxide → 2-mer. [†] Average of 3 iterations (until 4-mer).

Table S2. Metric parameters for dimethyl carbonate, 1,2- and 1,3-glycerol carbonates, and propylene and trimethylene carbonates.

	DMC			Glycerol				PC/TMC			
	O-C-O (°)	**C=O (Å)**	**C-O (Å)**	**O-C-O (°)**	**O-C-C (°)**	**C=O (Å)**	**C-O (Å)**	**O-C-O (°)**	**O-C-C (°)**	**C=O (Å)**	**C-O (Å)**
1,2-Carbonate	110.0	1.206	1.332	108.8	102.3 101.6	1.183	1.370 1.362	108.8	101.4 102.6	1.183	1.364 1.366
1,3-Carbonate				116.0	108.5 110.9	1.187	1.352 1.357	116.6	109.9 109.9	1.189	1.353 1.353
Enthalpy difference, 1,2-1,3, kcal/mol		N.A.			-7.3				-9.0		