SUPPORTING INFORMATION
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Topological Investigation of the Reaction Mechanism of Glycerol Carbonate Decomposition by Bond Evolution Theory.

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Table S1. Selected single point electronic energies for the transition states and products as a function of the atomic basis set. Calculations were performed at the CCSD(T) and MP2 levels of approximation on MP2/6-311G(d,p) optimized geometry. In parentheses are given the TS1-to-TS2(a-b), TS1-to-TS3, P1-to-P2, and P1-to-P3 energy differences.

S1A. CCSD(T) energies

	cc-pVDZ	aug-cc-pVDZ	cc-pVTZ	aug-cc-pVTZ	cc-pVQZ
TS1	76.0	74.1	77.8	76.8	77.4
TS2a	82.9 (6.9)	79.8 (5.7)	83.9 (6.1)	82.7 (5.9)	83.6 (6.2)
TS2b	84.7 (8.7)	80.7 (6.6)	85.1 (7.3)	83.8 (7.0)	84.8 (7.4)
TS3	77.7 (1.7)	77.6 (3.5)	78.4 (0.6)	78.3 (1.5)	78.7 (1.3)
R1	-8.3	-3.3	-2.7	-1.1	-2.2
R2	17.8 (26.1)	20.4 (23.7)	19.8 (22.5)	20.8 (21.9)	19.9 (22.1)
R3	14.2 (22.5)	12.7 (16.0)	12.2 (14.9)	11.9 (13.0)	11.6 (13.8)

S1B. MP2 energies

	cc-pVDZ	aug-cc-pVDZ	cc-pVTZ	aug-cc-pVTZ	cc-pVQZ
TS1	71.6	71.7	72.3	68.7	71.0
TS2a	80.5 (9.0)	79.5 (7.8)	80.2 (7.9)	76.4 (7.7)	78.7 (7.6)
TS2b	82.5 (10.9)	80.6 (8.9)	81.4 (9.1)	77.1 (8.4)	79.6 (8.6)
TS3	73.7 (2.1)	73.5 (1.8)	73.4 (1.1)	73.1 (4.4)	73.2 (2.1)
R1	-8.3	-3.3	-2.7	-1.1	-2.2
R2	17.8 (26.1)	20.4 (23.7)	19.8 (22.5)	20.8 (21.9)	19.9 (22.1)
R3	14.2 (22.5)	12.7 (16.0)	12.2 (14.9)	11.9 (13.0)	11.6 (13.8)

Table S2. Basin Populations (in e) and IRC coordinates (RX, Bohr AMU$^{1/2}$) along the TS1 reaction pathway.

	SSD-I		SSD-II		SSD-III		SSD-IV	
Basins	Reactant	Last point	First point	Last point	First point	Last point	First point	Product
LP(O1)	4.65	5.16	5.77	5.48	5.49	5.41	5.41	5.06
LP(O3)	4.64	4.83	4.83	5.23	6.11	5.41	5.37	5.16
LP(O6)	5.34	5.43	5.41	5.33	5.31	5.20	5.18	5.08
SB(C4,C5)	2.00	2.10	2.11	2.24	2.23	2.21	2.22	2.08
SB(O1,C5)	1.35	0.59	-	-	-	-	-	-
SB/DB(O3,C4)	1.36	1.37	1.41	1.48	1.51	2.11	2.14	2.41
DB(C2,O6)	2.68	2.54	2.54	2.64	2.67	2.77	2.78	2.84
SB/DB(O1,C2)	1.66	1.82	1.82	2.21	2.22	2.57	2.59	2.84
SB(C2,O3)	1.64	1.48	1.46	0.92	-	-	-	-
SB(H1,C4)	2.07	2.00	2.00	1.73	1.70	1.56	-	-
SB(H1,C5)	-	-	-	-	-	-	1.60	1.98
IRC	-9.42	-2.36	-2.22	-0.28	-0.14	1.53	1.66	14.00

Table S3. Basin Populations (in e) and IRC coordinates (RX, Bohr AMU$^{1/2}$) along the TS2a reaction pathway.

	SSD-I		SSD-II		SSD-III		SSD-IV	
Basins	Reactant	Last point	First point	Last point	First point	Last point	First point	Product
LP(O1)	4.68	5.12	5.80	5.50	5.54	5.30	5.27	5.03
LP(O3)	4.64	4.76	4.79	4.96	6.28	6.19	5.50	5.33
LP(O6)	5.27	5.37	5.37	5.29	5.28	5.14	5.20	5.03
SB(C2,O3)	1.68	1.57	1.55	1.32	-	-	-	-
SB(C4,C5)	1.98	2.07	2.08	2.14	2.14	2.05	2.03	1.91
SB(O1,C5)	1.38	0.68	-	-	-	-	-	-
SB(O3,C5)	-	-	-	-	-	-	0.70	1.04
DB(C2,O6)	2.66	2.55	2.55	2.64	2.63	2.78	2.72	2.84
SB(O3,C4)	1.33	1.31	1.31	1.21	1.21	1.05	1.05	1.02
SB/DB(O1,C2)	1.66	1.79	1.80	2.12	2.11	2.61	2.64	2.81
IRC	-15.31	-3.63	-3.40	-1.13	-0.91	3.40	3.63	16.56

Table S4. Basin Populations (in e) and IRC coordinates (RX, Bohr $AMU^{1/2}$) along the TS2b reaction pathway.

Basins	SSD-I		SSD-II		SSD-III		SSD-IV	
	Reactant	Last point	First point	Last point	First point	Last point	First point	Product
LP(O1)	4.63	4.83	4.89	4.97	6.32	6.05	5.44	5.34
LP(O3)	4.63	5.17	5.75	5.62	5.55	5.26	5.28	5.04
LP(O6)	5.31	5.44	5.38	5.39	5.39	5.16	5.16	5.04
SB(C1,O3)	-	-	-	-	-	-	0.69	1.02
SB(C4,C5)	2.00	2.09	2.10	2.13	2.12	2.02	2.01	1.92
SB(O1,C5)	1.38	1.27	1.27	1.23	1.23	1.12	1.12	1.05
SB(O3,C4)	1.67	0.60	-	-	-	-	-	-
DB(C2,O6)	2.66	2.52	2.54	2.54	2.58	2.77	2.77	2.86
SB(O1,C2)	1.63	1.52	1.47	1.21	-	-	-	-
SB/DB(C2,O3)	1.34	1.84	1.86	2.01	2.06	2.63	2.64	2.86
IRC	-12.83	-2.72	-2.53	-1.17	-0.97	3.31	3.45	11.85

Table S5. Basin Populations (in e) and IRC coordinates (RX, Bohr $AMU^{1/2}$) along the TS3 reaction pathway.

| Basins	SSD-I		SSD-II		SSD-III		SSD-IV	
	Reactant	Last point	First point	Last point	First point	Last point	First point	Product
LP(O8)	4.73	4.70	4.65	4.17	2.73	2.46	4.42	4.55
SB(H3,C5)	2.10	2.08	2.09	2.12	-	-	-	-
SB(H6,O8)	1.72	1.74	1.74	1.70	1.78	1.70	1.69	1.68
LP(C5)	-	-	1.59	1.70	1.65	0.71	-	-
P(H3)	-	-	0.53	0.52	-	-	-	-
SB(C7,O8)	1.26	1.05	1.06	1.26	1.25	1.94	-	-
SB(H3,O8)	-	-	-	-	0.53	1.74	1.74	1.70
SB/DB(C5,C7)	2.01	2.04	2.04	2.08	2.10	3.12	3.85	3.69
IRC	10.87	0.86	0.73	0.00	-0.12	-2.44	-2.56	-16.50
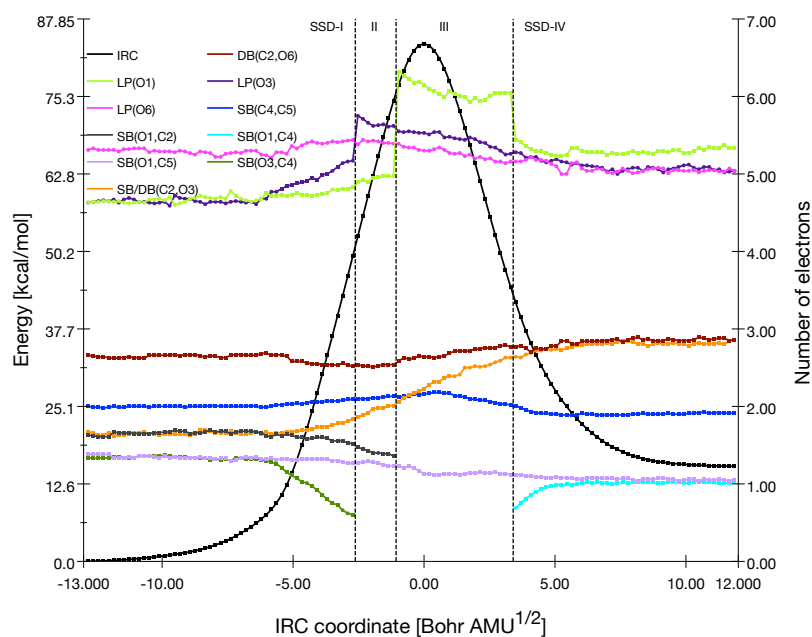
Figure S1. Population evolution (in e) of selected basins along the IRC associated with the TS2b reaction pathway together with the relative potential energy curve.
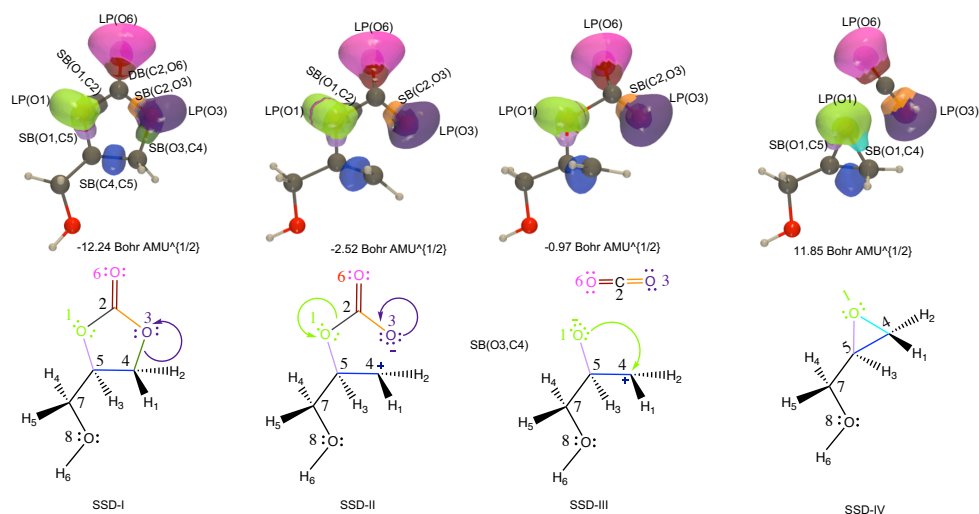

Figure S2. ELF basin isosurfaces (η = 0.75) for specific points of the successive structural stability domains and Lewis structures along TS2b reaction pathway. The color labeling of the basins was performed according to Figure S1 and, for each point, the corresponding intrinsic reaction coordinate is provided.