Unraveling Unusual Torquoselectivity in Ring-Opening Electrocyclic Reactions: A DFT Perspective

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Supplementary Information

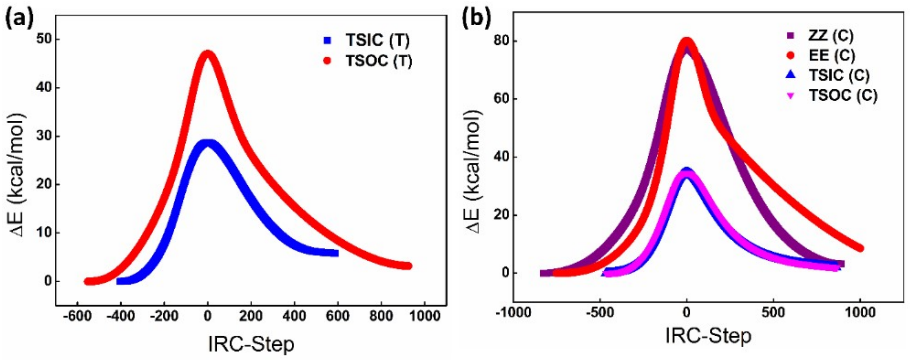

Figure S1. The variation of relative energy (ΔE) along the IRC. (C) and (T) stands for Cis- and Trans- perfluoro-3,4-dimethylcyclobutene systems.

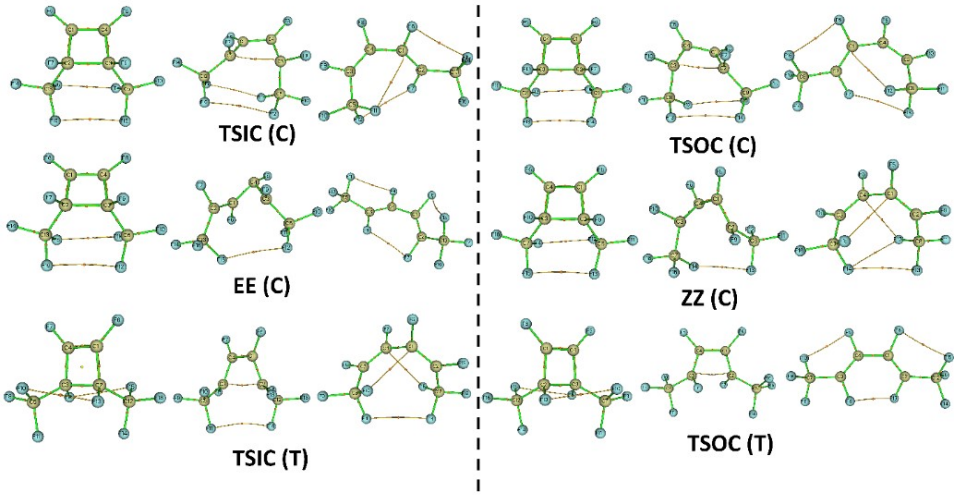

Figure S2. Molecular graph snapshots for inward conrotatory (TSIC) and outward conrotatory (TSOC) reverse minima, transition state, and forward minima are presented in the left, middle, and right panels, respectively for both Cis- and Trans- perfluoro-3,4-dimethylcyclobutene systems. The small red spheres denote the bond critical points (BCPs).

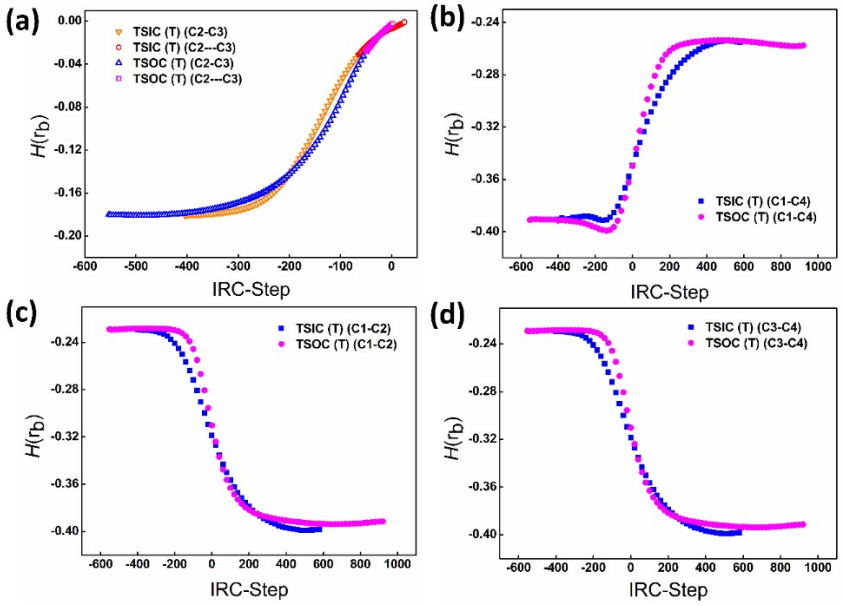

Figure S3. The variation of total local energy density ($H(r_b)$) along the IRC for different BCPs for Trans- perfluoro-3,4-dimethylcyclobutene system.

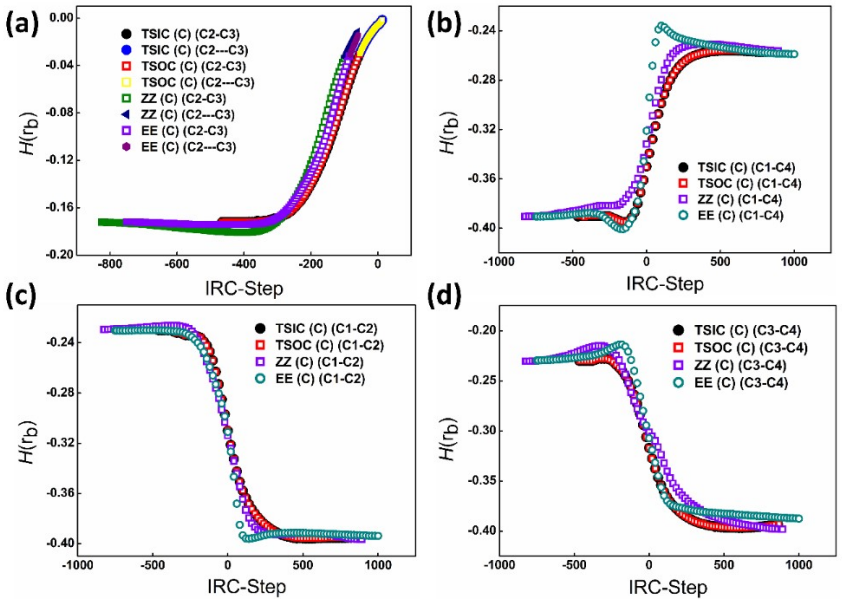

Figure S4. The variation of total local energy density ($H(r_b)$) along the IRC for different BCPs for Cis- perfluoro-3,4-dimethylcyclobutene system.

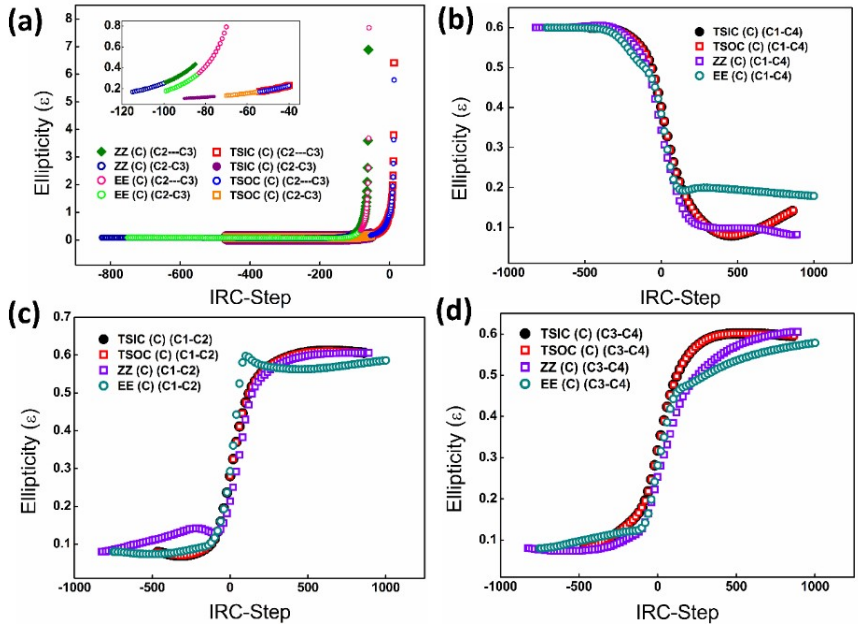

Figure S5. The variation of ellipticity (ε) along the IRC for different BCPs for Cis-perfluoro-3,4-dimethylcyclobutene system.

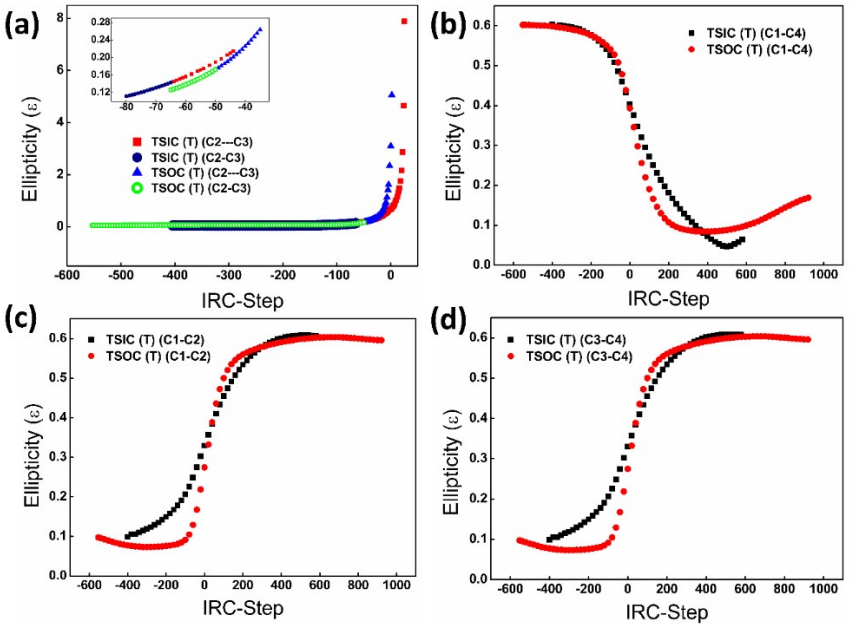

Figure S6. The variation of ellipticity (ε) along the IRC for different BCPs for Trans-perfluoro-3,4-dimethylcyclobutene system.

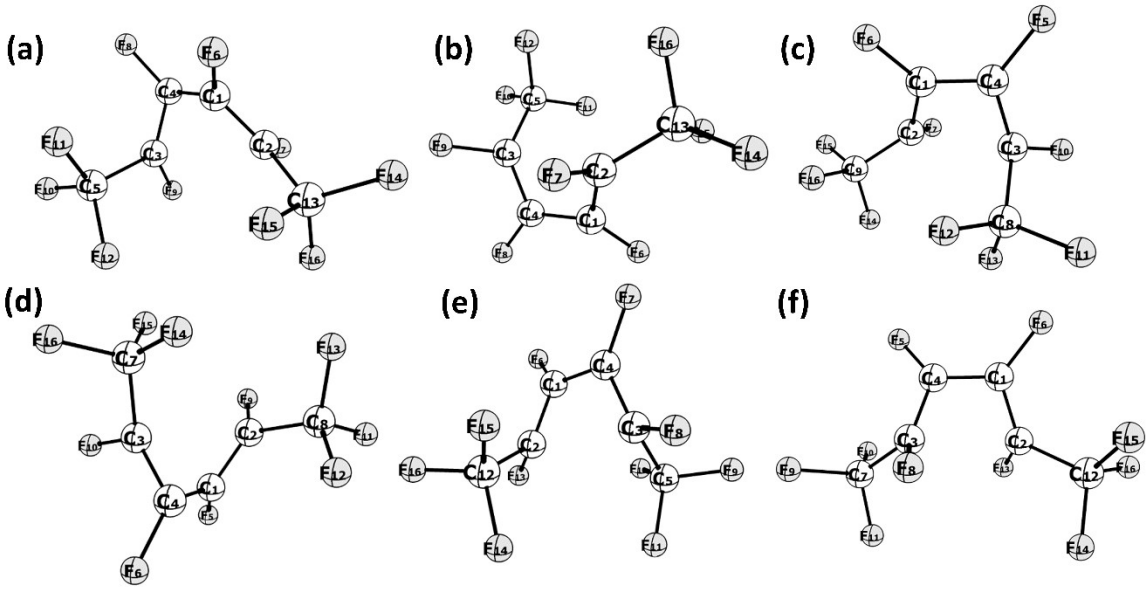

Figure S7. Transition states of Reactions 1-6 (a-f, a:R(Cis)-E,E; b:R(Cis)-Z,E; c:R(Cis)-E,Z; d:R(Cis)-Z,Z; e:R(Trans)-Z,Z; f:R(Trans)-E,E). Atomic numbering has been added to facilitate comparison.

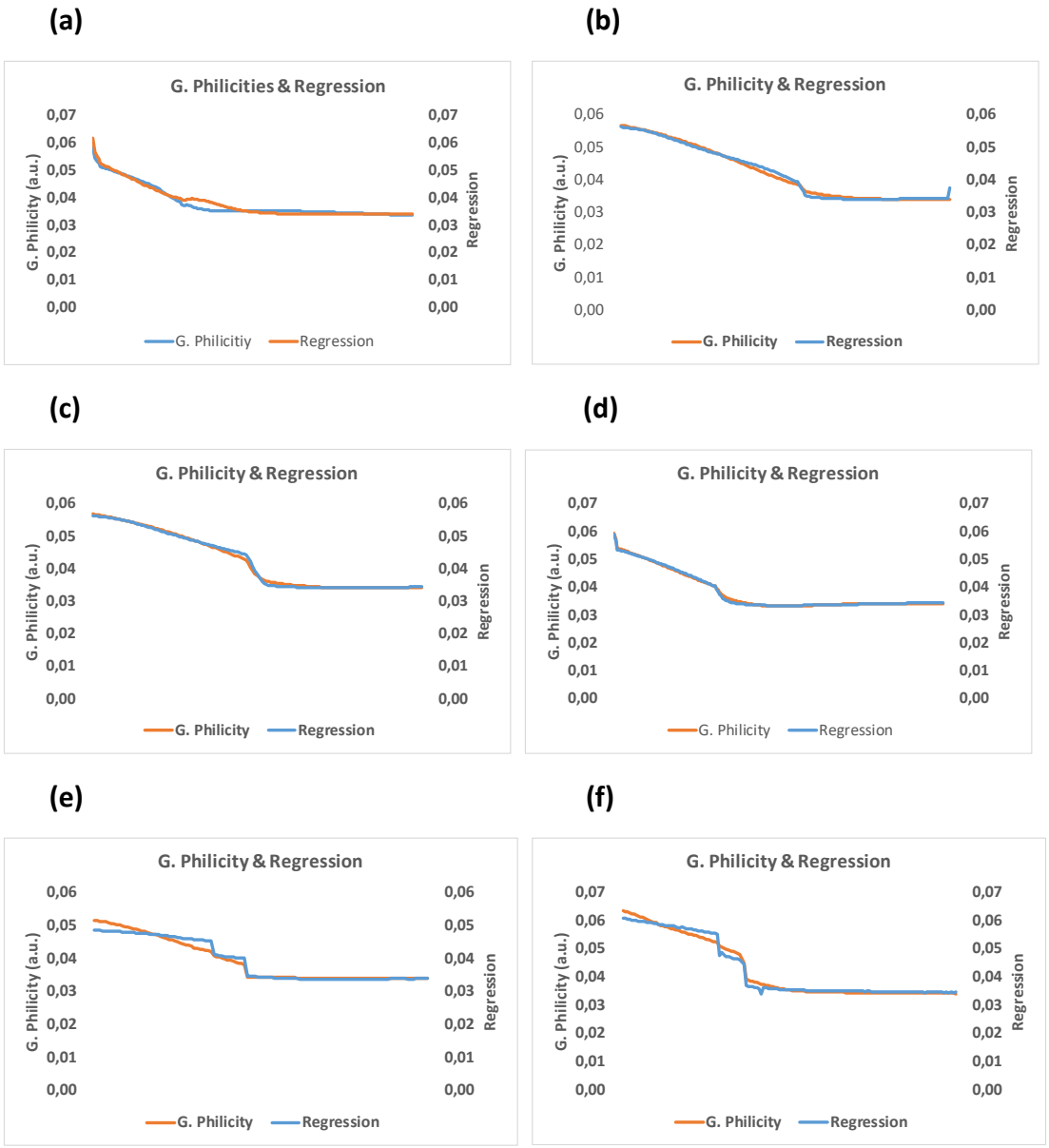

Figure S8. Global electrophilicity and multiple regression analysis for reactions 1–6 along the segment of the reaction path between the reactants and the transition state (Range 1).

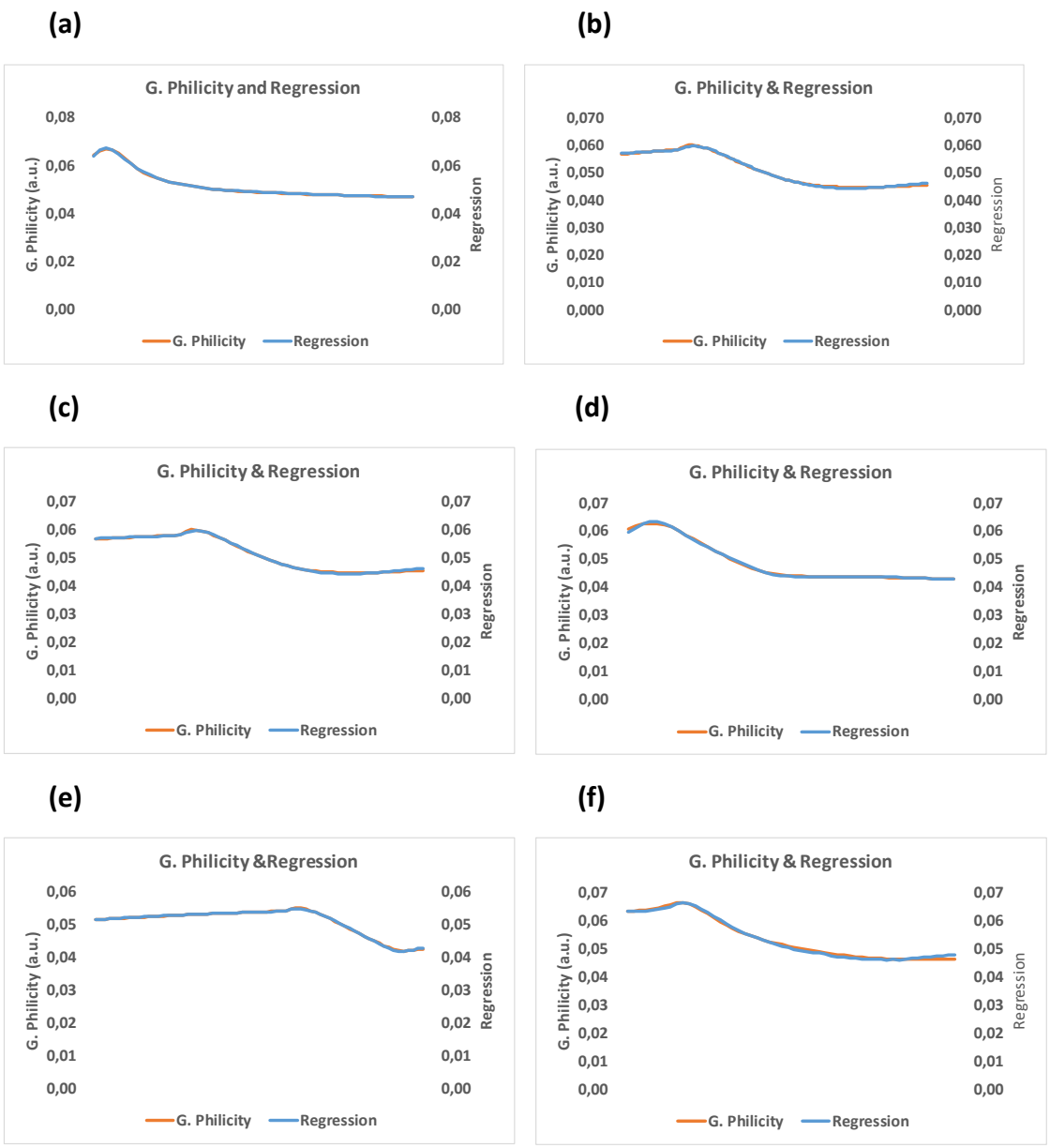

Figure S9. Global electrophilicity and multiple regression analysis for reactions 1–6 along the segment of the reaction path between the transition state and the products (Range 2).

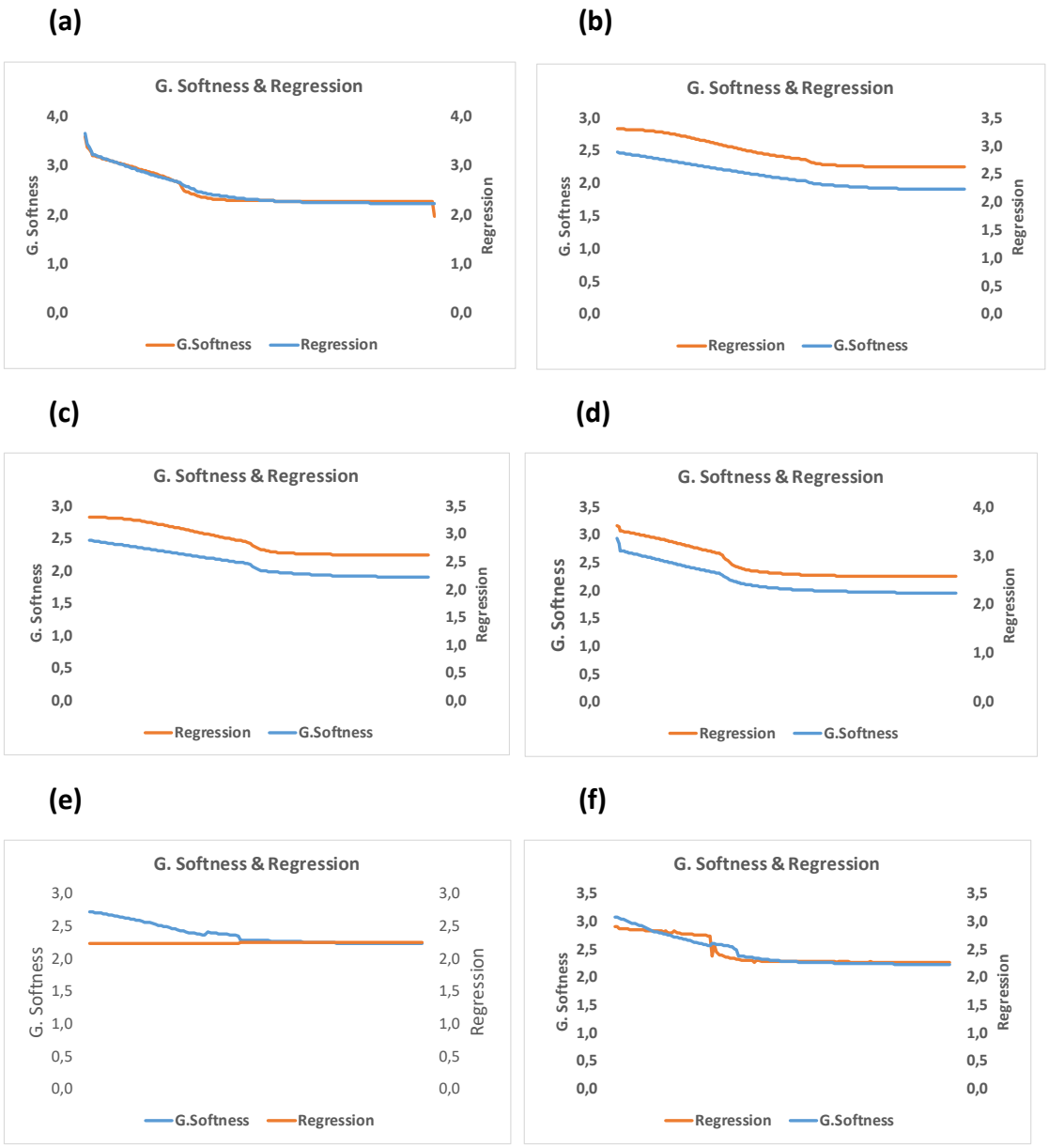

Figure S10. Global Softness and multiple regression analysis for reactions 1–6 (figures a-f respectively) along the segment of the reaction path between the reactants and the transition state (Range 1).

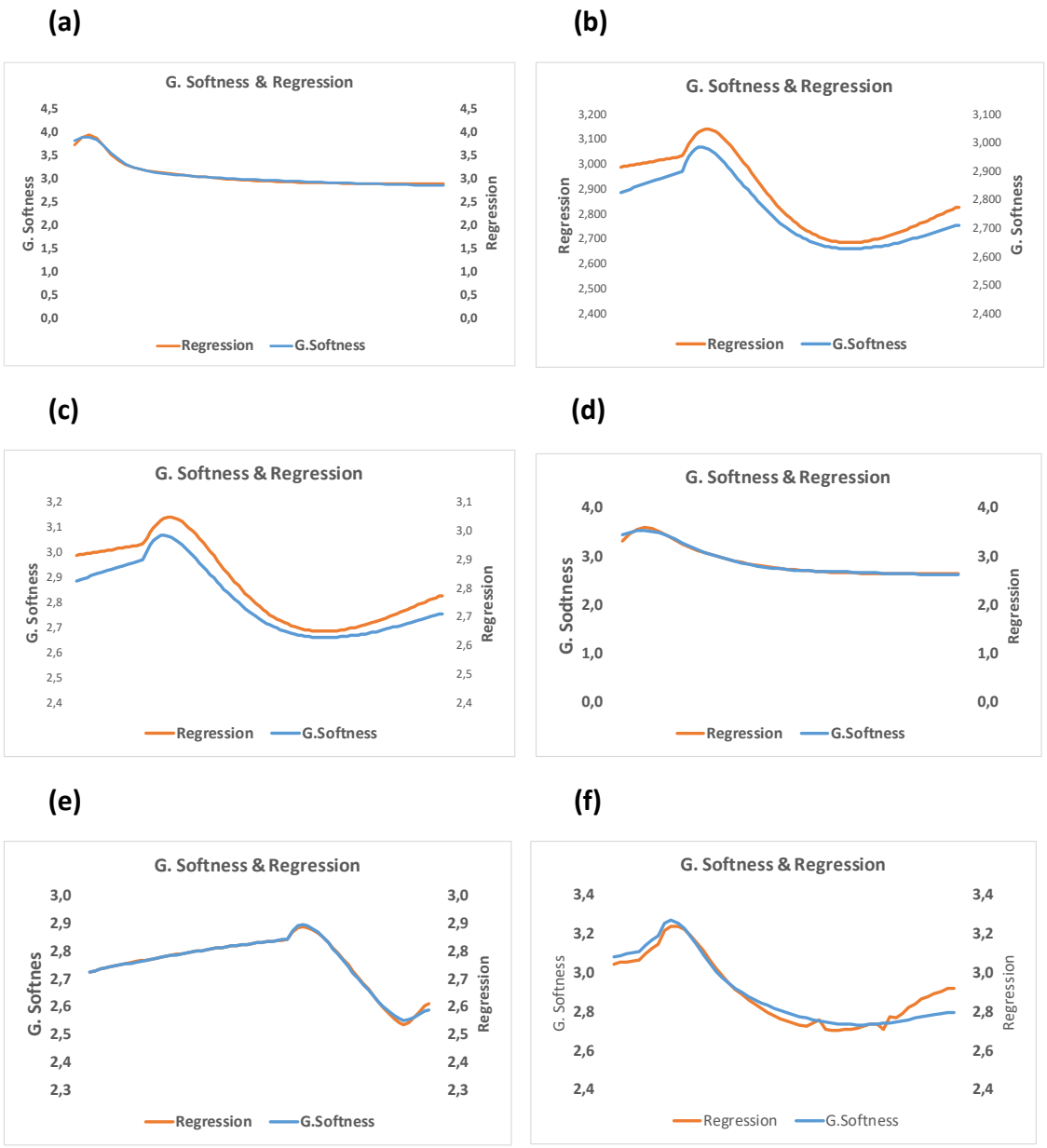

Figure S11. Global Softness and multiple regression analysis for reactions 1–6 (figures a-f respectively) along the segment of the reaction path between the transition state and the products (Range 2).

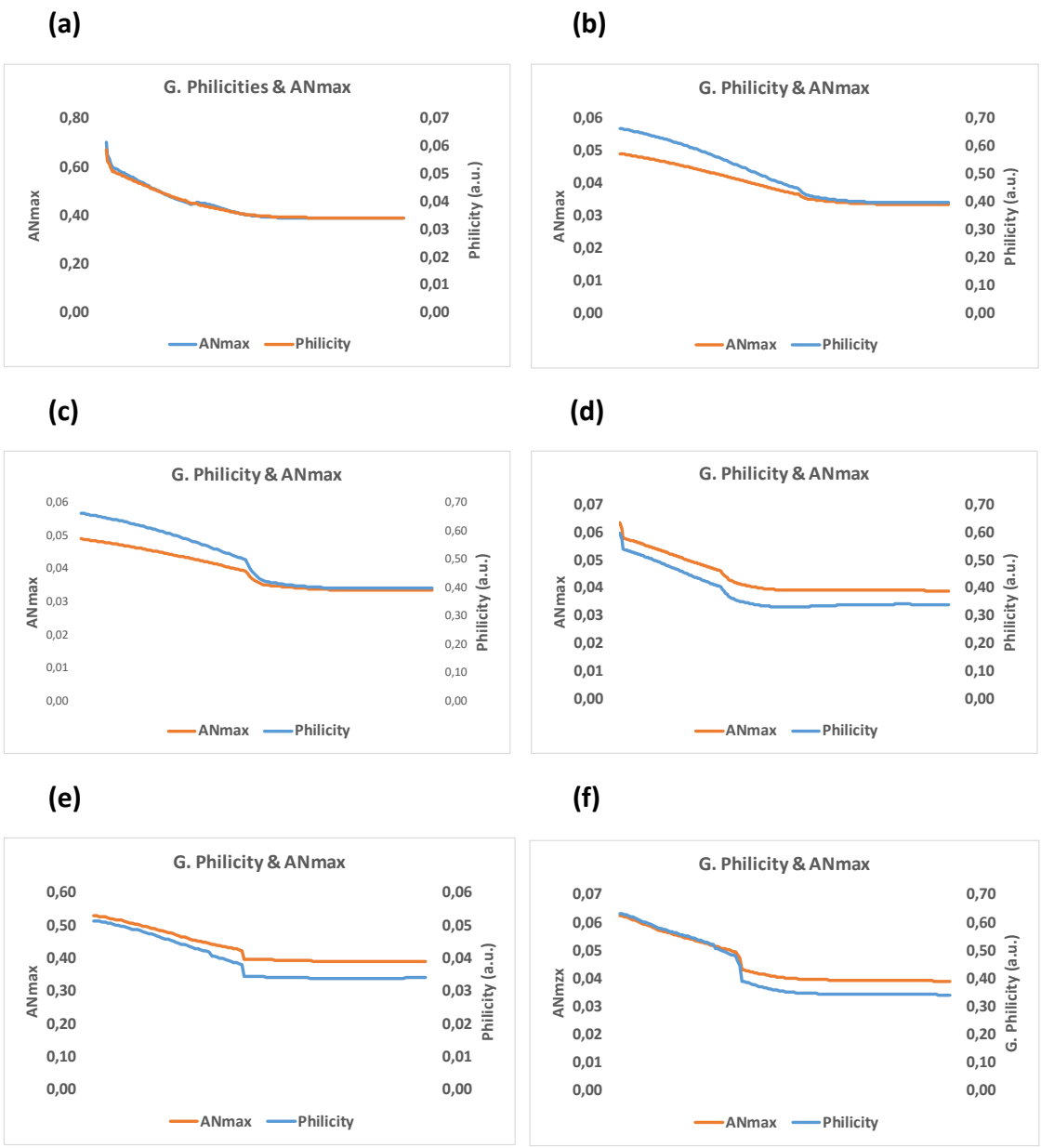

Figure S12. Global electrophilicities and Maximum Charge variation for reactions 1–6 (figures a-f respectively) along the segment of the reaction path between the reactants and the transition state (Range 1).

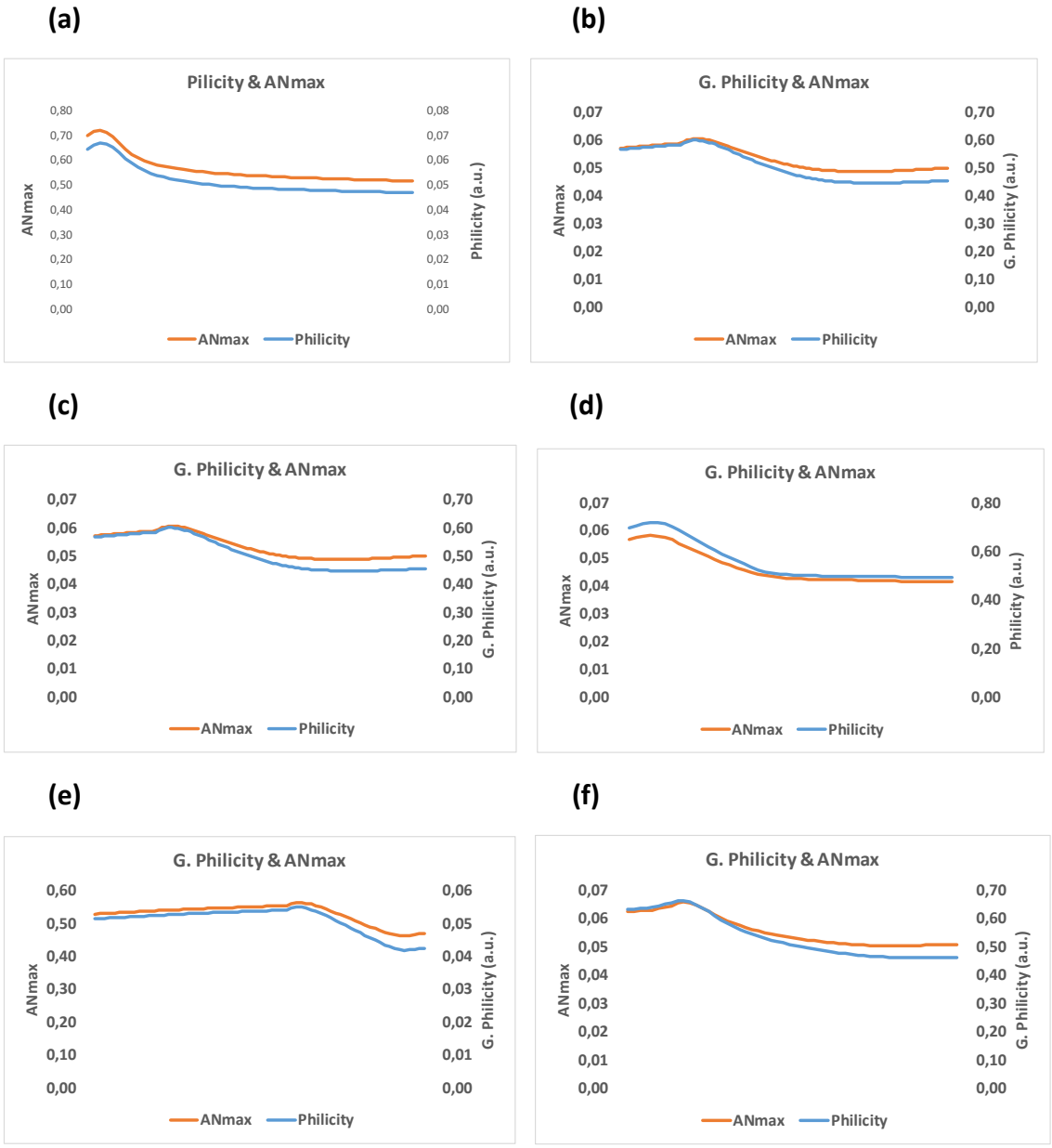

Figure S13. Global electrophilicities and Maximum Charge variation for reactions 1–6 (figures a-f respectively) along the segment of the reaction path between the transition state and the products (Range 2).

Table S1. Total energy difference and its component analysis between different conformations of cis- and trans- perfluoro-3,4-dimethylcyclobutene systems. Units are in kcal/mol. (The values in parentheses indicate the percentage contribution to the overall interactions)

	ΔE	ΔE_x	ΔE_c	ΔT_s	ΔE_e	ΔE_{xc}	ΔE_s	ΔE_q
EE (C)	80.17	42.34 (7.16)	4.62 (0.78)	-96.98 (16.39)	130.18 (22.00)	46.96 (7.94)	110.32 (18.64)	-160.33 (27.10)
ZZ (C)	77.32	40.28 (7.33)	4.12 (0.75)	-86.66 (15.76)	119.59 (21.76)	44.39 (8.08)	106.18 (19.32)	-148.45 (27.01)
TSIC (C)	34.63	27.91 (7.50)	3.59 (0.96)	-71.47 (19.20)	74.59 (20.04)	31.51 (8.46)	61.62 (16.55)	-101.58 (27.29)
TSOC (C)	34.63	27.92 (7.50)	3.59 (0.96)	-71.50 (19.21)	74.62 (20.04)	31.51 (8.46)	61.57 (16.54)	-101.56 (27.28)
TSIC (T)	28.63	25.84 (9.24)	2.63 (0.94)	- 49.64 (17.75)	49.80 (17.81)	28.47 (10.18)	51.02 (18.25)	-72.19 (25.82)
TSOC (T)	47.00	29.91 (6.48)	5.00 (1.08)	- 66.03 (14.31)	78.11 (16.92)	34.92 (7.56)	108.23 (23.45)	-139.34 (30.19)

Table S2. Regression equations for the linear relationship between global and local electrophilicity for the studied reactions. The regressions include two variables (C2 and C3). Range 1 and Range 2 correspond to the reaction paths from reactants to the transition state, and from the transition state to the products, respectively. The "points" field corresponds to the number of data points used to perform the regression.

Reaction	Range 1	points	Range 2	points
1	ω = -0.020545 + 6.66585·ω(2) -4.9902·ω(3)	52	ω = 0.029869 + 8.14304·ω(2) - 4.88528·ω(3)	181
2	ω = 0.000704 + 8.36606·ω(2) + 0.021475·ω(3)	105	ω = 0.029838 – 0.06876·ω(2) +4.25769·ω(3)	165
3	ω = 0.001254 + 8.18234·ω(2) + 0.10148·ω(3)	59	ω = 0.02963 + 0.36798·ω(2) +3.77536·ω(3)	149
4	ω = -0.01825 + 5.7542·ω(2) – 6.5639·ω(3)	46	ω = 0.02963 + 6.40114·ω(2) - 2.08507·ω(3)	204
5	ω = 0.004843 – 7.81214·ω(2) + 15.6526·ω(3)	68	ω = 0.03038 – 612.983·ω(2) + 615.976·ω(3)	121
6	ω = -0.00243 – 144.548·ω(2) + 153.525·ω(3)	54	ω = -0.00243 + 144.548·ω(2) + 153.525·ω(3)	54

Table S3. Regression equations for the linear relationship between global and local electrophilicity for the studied reactions. The regressions include four variables (C1–C4). Range 1 and Range 2 correspond to the reaction paths from reactants to the transition state, and from the transition state to the products, respectively. The "points" field corresponds to the number of data points used to perform the regression.

Reaction	Range 1	points	Range 2	points
1	$\omega = 0.005154 + 3.81916\cdot\omega(1) + 1.57623\cdot\omega(2) + 0.38138\cdot\omega(3) + 3.58031\cdot\omega(4)$	52	$\omega = 0.007251 + 1.73109\cdot\omega(1) + 2.9087\cdot\omega(2) + 2.0894\cdot\omega(3) + 1.9476\cdot\omega(4)$	181
2	$\omega = 0.012484 + 9.37502\cdot\omega(1) + 20.1703\cdot\omega(2) + 11.84821\cdot\omega(3) + 6.41566\cdot\omega(4)$	105	$\omega = 0.01035 + 1.72657\cdot\omega(1) + 3.8288\cdot\omega(2) + 1.18759\cdot\omega(3) + 1.39067\cdot\omega(4)$	165
3	$\omega = 0.01808 - 9.13706\cdot\omega(1) + 19.9137\cdot\omega(2) + -11.6633\cdot\omega(3) + 6.37219\cdot\omega(4)$	59	$\omega = 0.01047 + 1.8546\cdot\omega(1) + 3.7772\cdot\omega(2) + 1.20928\cdot\omega(3) + 1.2485\cdot\omega(4)$	149
4	$\omega = 0.00367 - 0.2792\cdot\omega(1) + 4.14923\cdot\omega(2) + 2.40954\cdot\omega(3) + 2.08421\cdot\omega(4)$	46	$\omega = -0.00011 + 3.3924\cdot\omega(1) + 1.3380\cdot\omega(2) + 4.8109\cdot\omega(3) + 1.28517\cdot\omega(4)$	204
5	$\omega = -0.00141 + 280.248\cdot\omega(1) - 316.463\cdot\omega(2) + 323.916\cdot\omega(3) + 3.58122\cdot\omega(4)$	68	$\omega = 0.007617 - 29.599\cdot\omega(1) - 15.2442\cdot\omega(2) - 10.1804\cdot\omega(3) - 33.2426\cdot\omega(4)$	121
6	$\omega = 0.00516408 + 3.8202\cdot\omega(1) + 1.57508\cdot\omega(2) + 0.379697\cdot\omega(3) - 278.084\cdot\omega(4)$	54	$\omega = -0.005419 - 1119.62\cdot\omega(1) + 1147.53\cdot\omega(2) - 1139.52\cdot\omega(3) + 1121.58\cdot\omega(4)$	54

Table S4. Standard errors of the coefficients for the multiple linear regressions: global electrophilicity vs. local electrophilicity.

	Range 1			Range 2		
Reaction	Independ.	C2	C3	Independ.	C2	C3
1	0.0012	0.16	0.12	0.0002	0.62	0.66
2	0.0006	0.53	0.60	0.0002	0.39	0.44
3	0.0009	0.77	0.90	0.0001	0.32	0.36
4	0.0012	0.15	0.21	0.0001	0.15	0.15
5	0.0007	66	86	0.0002	1036	1036
6	0.0009	166	165	0.0009	166	166

Table S5. Standard errors of the coefficients for the multiple linear regressions: global electrophilicity vs. local electrophilicity.

	Range 1					Range 2				
Reaction	**Independ.**	**C1**	**C2**	**C3**	**C4**	**Independ.**	**C1**	**C2**	**C3**	**C4**
1	0.0011	0.27	0.20	0.17	0.14	0.0002	0.01	0.15	0.12	0.09
2	0.0035	2.27	2.89	2.78	1.23	0.0003	0.12	0.12	0.11	0.09
3	0.0050	2.99	3.78	3.64	1.63	0.0004	0.12	0.10	0.10	0.08
4	0.0017	0.93	0.57	0.72	0.52	0.0012	0.22	0.29	0.33	0.16
5	0.0017	136	158	158	136	0.0001	91	121	121	91
6	0.0007	770	892	893	770	0.0007	770	893	893	770

Table S6. Autocorrelation (coefficient of determination, R^2) of the local electrophilicity variables in the linear regressions for the reactions in Range 1.

Reaction	**C1/C2**	**C2/C4**	**C1/C4**	**C2/C3**	**C2/C4**	**C3/C4**
1	-0,7686	-0.6799	0.8668	0.9529	-0.9693	-0.9452
2	-0.9958	-0.9939	-0.9978	-0.9997	0.9935	-0.9924
3	-0.9951	0.9929	-0.9980	-0.9996	0.9935	-0.9918
4	-0.9754	-0.9163	0.9613	0.9662	-0.9917	-0.9866
5	-0.9977	0.9977	-1.0000	-1.0000	0.9977	-0.9977
6	-0.9915	0.9915	-1.0000	-1.0000	0.9915	-0.9915

Table S7. Autocorrelation (coefficient of determination, R^2) of the local electrophilicity variables in the linear regressions for the reactions in Range 2.

Reaction	**C1/C2**	**C2/C4**	**C1/C4**	**C2/C3**	**C2/C4**	**C3/C4**
1	0.8846	-0.7558	-0.9663	-0.9733	-0.9389	0.8499
2	-0.4824	0.4988	-0.9043	-0.9914	0.0953	-0.6678
3	-0.3276	0.3706	-0.8524	-0.9870	0.6399	-0.6137
4	0.1080	0.1978	-0.5310	-0.9526	-0.8724	0.7033
5	-0.8877	0.8877	-1.0000	-1.0000	0.8877	-0.8877
6	-0.9915	0.9915	-1.0000	-1.0000	0.9915	-0.9915

Table S8. Regression equations for the linear relationship between global and local softness for the studied reactions. Regressions include two variables (C2 and C3). Range 1 and Range 2 correspond to the reaction paths from reactants to the transition state, and from the transition state to the products, respectively. The "points" field corresponds to the number of data points used to perform the regression.

Reaction	Range 1	points	Range 2	points
1	$\eta^{-1} = 9.47549 - 7.75195 \cdot \eta^{-1}(2) - 10.3756 \cdot \eta^{-1}(3)$	52	$\eta^{-1} = 2.1044 + 4.6713 \cdot \eta^{-1}(2) - 2.25571 \cdot \eta^{-1}(3)$	181
2	$\eta^{-1} = -0.126 + 8.75509 \cdot \eta^{-1}(2) + 0.17179 \cdot \eta^{-1}(3)$	105	$\eta^{-1} = 2.09843 + 1.76346 \cdot \eta^{-1}(2) - 0.4192323 \cdot \eta^{-1}(3)$	165
3	$\eta^{-1} = -0.08596 + 8.41364 \cdot \eta^{-1}(2) + 0.388155 \cdot \eta^{-1}(3)$	59	$\eta^{-1} = 2.09605 + 1.70184 \cdot \eta^{-1}(2) - 0.500329 \cdot \eta^{-1}(3)$	149
4	$\eta^{-1} = 7.79347 - 3.94762 \cdot \eta^{-1}(2) - 12.3511 \cdot \eta^{-1}(3)$	46	$\eta^{-1} = 1.8976 + 1.01937 \cdot \eta^{-1}(2) - 4.12792 \cdot \eta^{-1}(3)$	204
5	$\eta^{-1} = 0.22645 + 3.67765 \cdot \eta^{-1}(2) + 4.35427 \cdot \eta^{-1}(3)$	68	$\eta^{-1} = 2.16374 - 1954.86 \cdot \eta^{-1}(2) - 1956.18 \cdot \eta^{-1}(3)$	121
6	$\eta^{-1} = -0.25364 - 224.9 \cdot \eta^{-1}(2) + 234.262 \cdot \eta^{-1}(3)$	54	$\eta^{-1} = 2.13531 - 2514.25 \cdot \eta^{-1}(2) - 2516.3 \cdot \eta^{-1}(3)$	54

Table S9. Standard errors of the coefficients for the multiple linear regressions: global softness vs. local softness.

	Range 1			Range 2		
Reaction	Independ.	C2	C3	Independ.	C2	C3
1	2.5	3.4	3.7	0.015	0.24	0.43
2	0.07	0.36	0.43	0.003	0.06	0.07
3	0.1	0.47	0.58	0.003	0.06	0.07
4	0.89	1.18	1.9	0.011	0.16	0.28
5	0.06	40	40	0.01	391	391
6	0.14	181	181	0.01	448	448

Table S10. Autocorrelation (coefficient of determination, R^2) of the local softness variables in the linear regressions for the reactions in Range 1

Reaction	C1/C2	C2/C4	C1/C4	C2/C3	C2/C4	C3/C4
1	-0.6526	-0.3787	0.9101	0.9291	0.9100	-0.2055
2	-0.9183	0.9303	-0.9818	-0.9833	0.9337	-0.9464
3	-0.9057	0.9202	-0.9855	-0.9810	0.9330	-0.9438
4	-0.9302	-0.7184	0.8902	0.8989	-0.7429	-0.4310
5	-0.9981	0.9981	-1.0000	-1.0000	0.9981	-0.9981
6	-0.9928	0.9928	-1.0000	-1.0000	0.9928	-0.9928

Table S11. Autocorrelation (coefficient of determination, R^2) of the local softness variables in the linear regressions for the reactions in Range 2.

Reaction	C1/C2	C2/C4	C1/C4	C2/C3	C2/C4	C3/C4
1	0.8871	-0.7032	-0.9778	-0.9415	-0.8511	0.6920
2	0.3880	-0.3637	-0.8955	-0.9774	0.0149	0.0024
3	0.3403	-0.3860	-0.9004	-0.9764	0.0704	0.0165
4	0.9317	0.0375	-0.9750	-0.3058	-0.9252	0.0771
5	-0.3670	0.3670	-1.0000	-1.0000	0.3669	-0.3669
6	0.0734	-0.0778	-1.0000	-1.0000	-0.0788	0.0788

Table S12. Regression equations for the linear relationship between global and local softness for the reactions studied. Regressions include four variables (C1–C4). Range 1 and Range 2 correspond to the reaction paths from reactants to the transition state, and from the transition state to the products, respectively. The "points" field corresponds to the number of data points used to perform the regression.

Reaction	Range 1	points	Range 2	points
1	$\eta^{-1} = 1.71172 - 1.80657\cdot\eta^{-1}(1) + 2.3995\cdot\eta^{-1}(2) + 0.567511\cdot\eta^{-1}(3) + 2.63468\cdot\eta^{-1}(4)$	52	$\eta^{-1} = 1.9267 - 2.62351\cdot\eta^{-1}(1) + 2.65464\cdot\eta^{-1}(2) - 0.17453\cdot\eta^{-1}(3) + 3.06096\cdot\eta^{-1}(4)$	181
2	$\eta^{-1} = 1.13626 - 8.5513\cdot\eta^{-1}(1) + 15.1166\cdot\eta^{-1}(2) - 8.41553\cdot\eta^{-1}(3) + 6.13967\cdot\eta^{-1}(4)$	105	$\eta^{-1} = 2.17154 + 0.047076\cdot\eta^{-1}(1) + 1.33755\cdot\eta^{-1}(2) + 0.76002\cdot\eta^{-1}(3) - 0.22559\cdot\eta^{-1}(4)$	165
3	$\eta^{-1} = 1.12152 - 8.46233\cdot\eta^{-1}(1) + 15.018\cdot\eta^{-1}(2) - 8.38483\cdot\eta^{-1}(3) + 6.20373\cdot\eta^{-1}(4)$	59	$\eta^{-1} = 2.2263 - 0.32850\cdot\eta^{-1}(1) + 1.12704\cdot\eta^{-1}(2) + 0.95340\cdot\eta^{-1}(3) + 0.00640\cdot\eta^{-1}(4)$	149
4	$\eta^{-1} = 2.15862 + 0.210233\cdot\eta^{-1}(1) + 0.38441\cdot\eta^{-1}(2) - 1.70479\cdot\eta^{-1}(3) + 3.70961\cdot\eta^{-1}(4)$	46	$\eta^{-1} = 1.74203 - 1.25015\cdot\eta^{-1}(1) - 0.02671\cdot\eta^{-1}(2) + 6.27875\cdot\eta^{-1}(3) + 1.467\cdot\eta^{-1}(4)$	204
5	$\eta^{-1} = -0.182879 + 161.01\cdot\eta^{-1}(1) - 190.309\cdot\eta^{-1}(2) + 198.733\cdot\eta^{-1}(3) + -159.669\cdot\eta^{-1}(4)$	68	$\eta^{-1} = 2.04413 - 4039.99\cdot\eta^{-1}(1) - 1698.5\cdot\eta^{-1}(2) + 1699.96\cdot\eta^{-1}(3) + 4040.3\cdot\eta^{-1}(4)$	122
6	$\eta^{-1} = -0.54457 - 2659.51\cdot\eta^{-1}(1) + 2973.72\cdot\eta^{-1}(2) - 2964.63\cdot\eta^{-1}(3) + 2661.08\cdot\eta^{-1}(4)$	54	$\eta^{-1} = 2.28199 - 196.281\cdot\eta^{-1}(1) - 2120.33\cdot\eta^{-1}(2) + 2122.13\cdot\eta^{-1}(3) + 195.921\cdot\eta^{-1}(4)$	152

Table S13. Standard errors of the coefficients for the multiple linear regressions: global softness vs. local softness.

	Range 1					Range 2				
Reaction	**Independ.**	**C1**	**C2**	**C3**	**C4**	**Independ.**	**C1**	**C2**	**C3**	**C4**
1	0.29	0.29	0.48	0.44	0.11	0.04	0.47	0.45	0.51	0.45
2	0.13	0.74	0.49	0.66	0.44	0.025	0.13	0.12	0.11	0.1
3	0.17	0.99	0.64	0.86	0.6	0.03	0.18	0.15	0.13	0.14
4	0.2	0.52	0.52	0.51	0.17	0.095	0.35	0.18	0.13	0.13
5	0.024	156	189	189	156	0.05	879	464	468	879
6	0.15	1111	1352	1352	1111	0.06	150	479	479	150

Cartesian coordinates for transition states

EE (C)

C	-0.15949200	1.25712100	-0.27399100
C	-1.24519200	0.66292100	0.39598200
C	1.05242400	0.15419800	0.68019900
C	1.01155400	1.55150000	0.43818100
C	1.79487400	-0.89423000	-0.15629600
F	-0.23422000	1.33198300	-1.62043500
F	-1.62549800	1.06512900	1.60864700
F	2.03510100	2.24516900	-0.10604600
F	0.76473500	-0.37654100	1.88302400
F	3.01607900	-1.08481200	0.37046900
F	1.92777700	-0.47126300	-1.41726400
F	1.14253500	-2.06435200	-0.15441200
C	-2.13106200	-0.39595400	-0.19836800
F	-3.26265000	0.12947200	-0.71021800
F	-1.48821600	-1.04519600	-1.18606000
F	-2.49104600	-1.28662600	0.74182400

ZZ (C)

C	0.30668600	1.40653800	0.31804000
C	0.93527500	0.17231600	0.56850300
C	-1.32534500	0.41945700	0.02670800
C	-0.53041800	1.26996200	-0.78344700
F	0.44668600	2.48932900	1.10285300
F	-0.98139100	2.23818000	-1.58925200
C	-1.58724700	-1.08970800	-0.06149100
C	2.00440900	-0.44792900	-0.29562400
F	1.00436200	-0.28706700	1.83371400
F	-2.34678700	0.95497400	0.73601000
F	3.21848400	-0.19175400	0.24668600
F	1.99677500	0.05072800	-1.53942200
F	1.87914100	-1.78347100	-0.35884200
F	-0.76511700	-1.68904500	-0.92374900
F	-1.47043900	-1.67316600	1.13914600
F	-2.85061900	-1.26246600	-0.49560400

TSIC (C)

C	-0.27889800	1.45859600	-0.26717800
C	-0.85203200	0.42487800	0.50219500
C	1.39540900	0.16999300	0.44558700
C	1.07103300	1.45663200	-0.01644400
C	1.39995400	-1.10905200	-0.37888900
F	-0.92549100	2.17332000	-1.18874100
F	-0.85541700	0.47449900	1.85773300
F	1.92349500	2.47772900	-0.07139600
F	2.30504000	0.05518800	1.42398700
F	2.66140100	-1.34505300	-0.79515000
F	0.61610200	-1.03503200	-1.46377000
F	1.01384700	-2.16025900	0.36083500
C	-2.03437400	-0.39991900	0.03188400
F	-3.18679500	0.07796500	0.53724300
F	-2.11596400	-0.37758400	-1.30736300
F	-1.90361300	-1.67485900	0.43518300

TSOC (C)

C	0.27888600	1.45866000	-0.26733500
C	0.85201700	0.42508900	0.50228600
C	-1.39501100	0.16992000	0.44573000
C	-1.07098600	1.45663900	-0.01648300
F	-1.92352900	2.47767200	-0.07136300
F	0.92542200	2.17313300	-1.18914000
F	0.85559900	0.47502100	1.85780500
C	-1.39987500	-1.10904600	-0.37887300
C	2.03416300	-0.39999000	0.03189200
F	-2.30445900	0.05507500	1.42431100
F	-2.66132100	-1.34456800	-0.79541700
F	-0.61576200	-1.03524400	-1.46356700
F	-1.01428500	-2.16043600	0.36085800
F	1.90324400	-1.67486600	0.43532800
F	3.18671200	0.07778200	0.53707600
F	2.11558300	-0.37775300	-1.30736900

TSIC (T)

C	0.48680900	1.43314900	0.48468200
C	0.95005300	0.11465700	0.61663600
C	-0.95000700	0.11467700	-0.61659100
C	-0.48669500	1.43315000	-0.48469400
C	-1.77143300	-0.65848400	0.40547500
F	0.83298900	2.43722500	1.28677400
F	-0.83279400	2.43719700	-1.28686100

F	-1.27203400	-0.31810200	-1.84607200
F	-3.07636500	-0.54909500	0.08453700
F	-1.61357600	-0.19919000	1.65480300
F	-1.45588600	-1.96350100	0.38397500
C	1.77135700	-0.65858400	-0.40545700
F	1.27212600	-0.31808100	1.84611800
F	1.45564300	-1.96356400	-0.38400700
F	1.61353200	-0.19921500	-1.65476300
F	3.07630900	-0.54938600	-0.08453800

TSOC (T)

C	0.68169900	1.37984200	-0.08187300
C	1.05829700	0.06867000	-0.43769600
C	-1.05829500	0.06869400	0.43764300
C	-0.68161100	1.37980400	0.08171900
F	-1.53813800	2.37289900	-0.16833000
F	1.53827400	2.37283800	0.16836700
C	-2.31831700	-0.60537800	-0.05826600
F	-0.67277800	-0.48258000	1.61124600
F	-3.32155600	-0.49292500	0.83245400
F	-2.71080400	-0.04644000	-1.21417700
F	-2.09298700	-1.91289600	-0.26492000
C	2.31829800	-0.60542100	0.05827900
F	0.67268700	-0.48265500	-1.61120800
F	2.09306100	-1.91301600	0.26450100
F	2.71050000	-0.04677200	1.21441800
F	3.32169400	-0.49259300	-0.83222200