Supporting information

Prediction of the mechanochemical reactivity of triarylmethane-based mechanophores using the Constrained Geometries Simulate External Force method.

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General Methods for CoGEF Study:

Gaussian software was used to perform CoGEF calculations according to earlier published methods.[1] Gaussian calculations and chemical structures were set up in GaussView, saved as .com files, and then imported into Gaussian. DFT was first used to optimise the geometry at the B3LYP/6-31G* level of theory. The energy at every step was then calculated stepwise using the optimised geometry. The distance between the terminal anchor atoms of the truncated structure was raised in steps of 0.1 Å[2,3] starting from the equilibrium geometry of the unconstrained molecule (relative energy = 0 kJ/mol), and the energy was minimised at each step. The energy profile calculation was automatically performed. Calculations were run until a chemical transformation was predicted to occur, as evidenced by the rupture of a covalent bond.

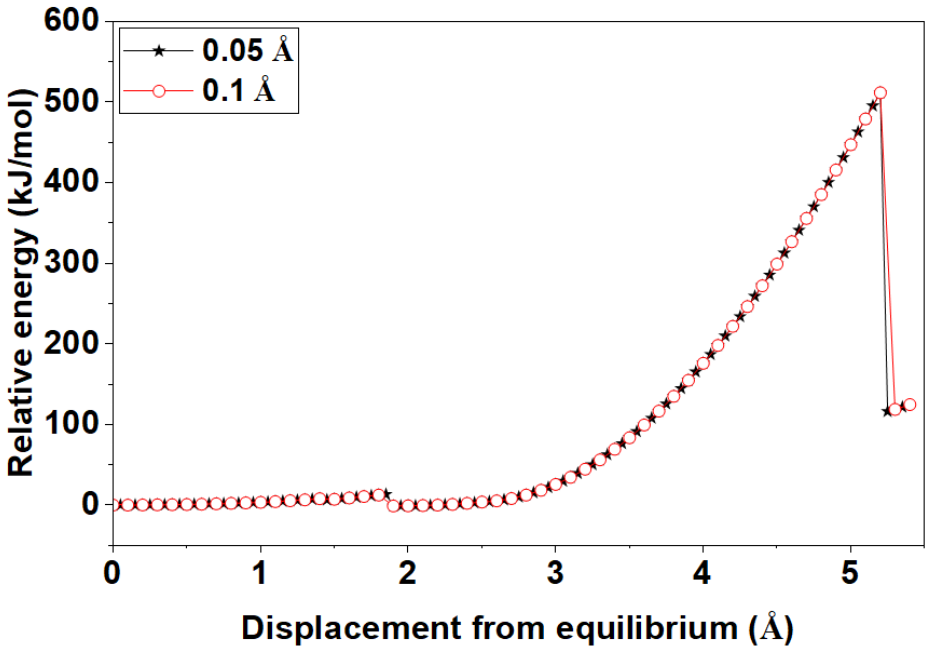


Figure S1: CoGEF curve using 0.05 Å and 0.1 Å step size increments during elongation for model **A** mechanophore. The results show minimal difference in the calculation outcome for the two chosen step sizes.

Table S1: The Comparison of CoGEF step sizes for model **A** mechanophore.

Step size	E_{max} (kJ/mol)	F_{max} (nN)
0.1 Å	511	5.41
0.05 Å	511	5.43

Determination of F_{max}: The predicted maximum force for each mechanochemical transformation was calculated from the slope (ΔE/ΔD) of the energy–displacement curve between adjacent points. ΔE is the energy difference of the molecule between two points of deformation. ΔD refers to the change in the distance between two anchor atoms during elongation. F_{max} typically corresponds to the displacement just before a discontinuity in the relative energy profile. Thus, the slope between the two data points before the sudden energy decrease is used to determine F_{max}. To calculate force in nN (or nJ/m), the slope value is divided by the Avogadro constant.

Determination of E_{max}: The maximum energy relative to the energy of the unconstrained molecule at equilibrium is reported as E_{max}. The value of E_{max} is determined from the CoGEF curve at the displacement corresponding to F_{max}. This usually indicates that E_{max} is the

maximum relative energy on the CoGEF curve; however, it is the relative energy at the inflexion point when the CoGEF profile has no discontinuities.

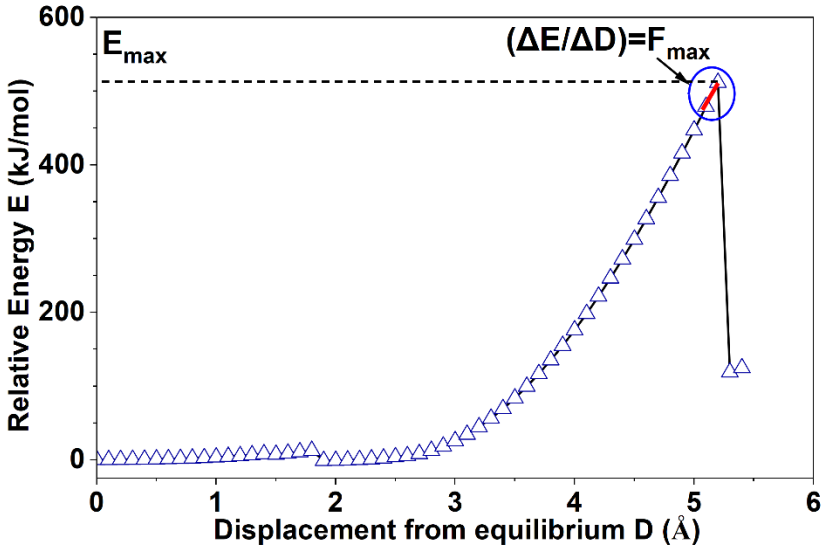


Figure S2: Relative energy (E) profile as a function of displacement from equilibrium, D in CoGEF calculation model A. The red line shows the segment from which F_{max} was calculated for A.

Determination of Rupture Bond Length and Bond Angle (α, β, and γ): Using structural models from CoGEF calculations at the displacement corresponding to F_{max}, rupture bond length and bond angle were computed using the previously said method. The coordinates of the two terminal atoms that provide the distance constraint in the CoGEF computation were used to approximate the external force vector.

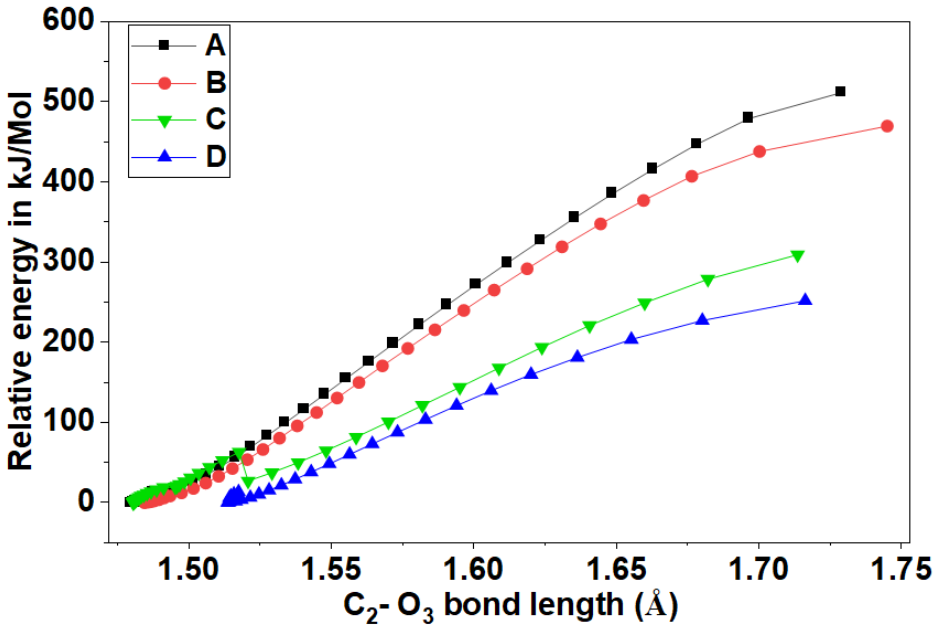


Figure S3: Relative energy vs the $C_2 – O_3$ rupture bond length plot from CoGEF calculation for all model mechanophores in the vacuum phase.

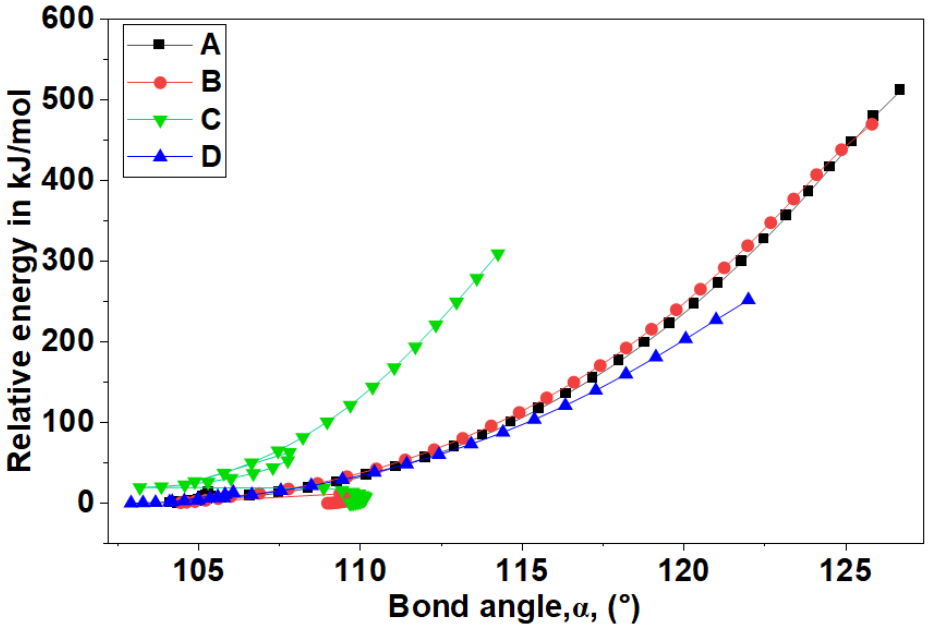
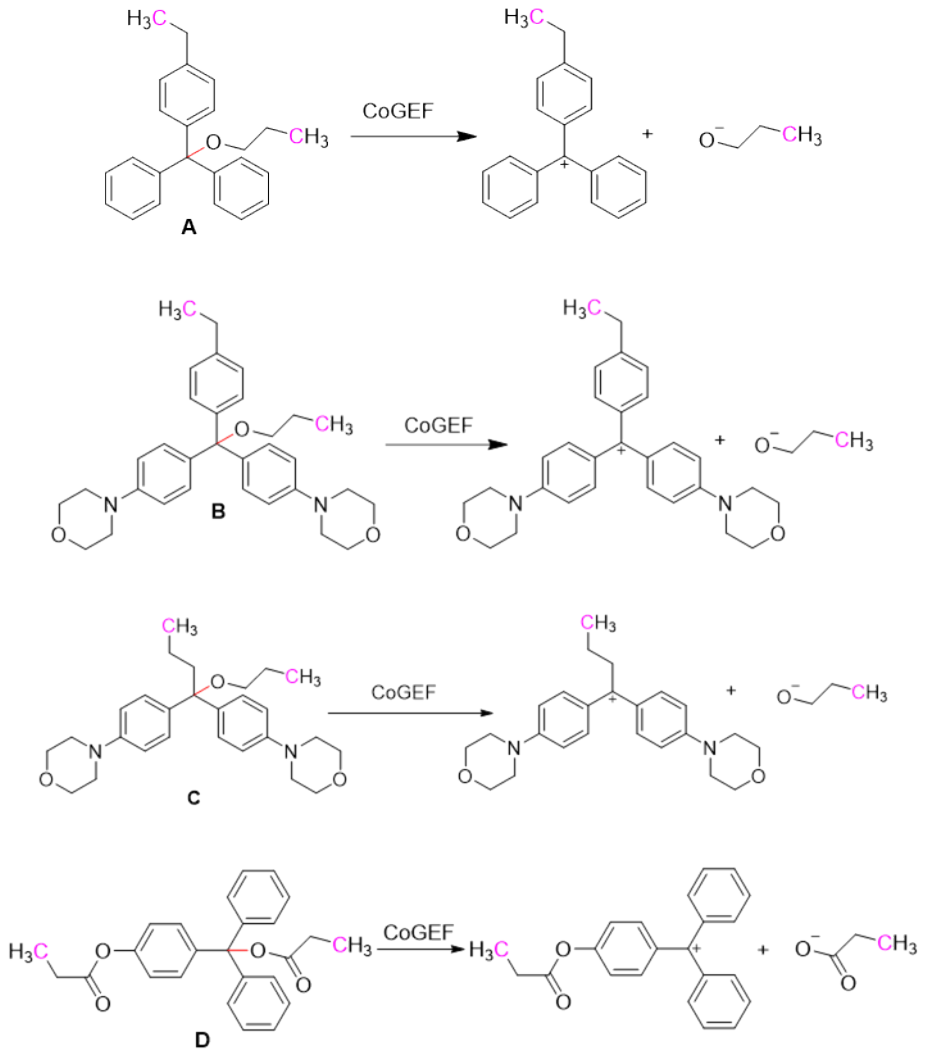


Figure S4: Relative energy vs the rupture bond angle (α) plot from CoGEF calculation for all model mechanophores in the vacuum phase.



Scheme S1: Proposed mechanophore structures and their heterolytic cleavage products after CoGEF calculation.

Molecular orbitals study for models mechanophore:

We have performed the molecular orbitals analysis using the directly obtained geometries, and also did it with an independent optimized structure of the carbocation, anion and radical. From the data, we get the value in au units; then we convert it to eV units by multiplying by 27.21.

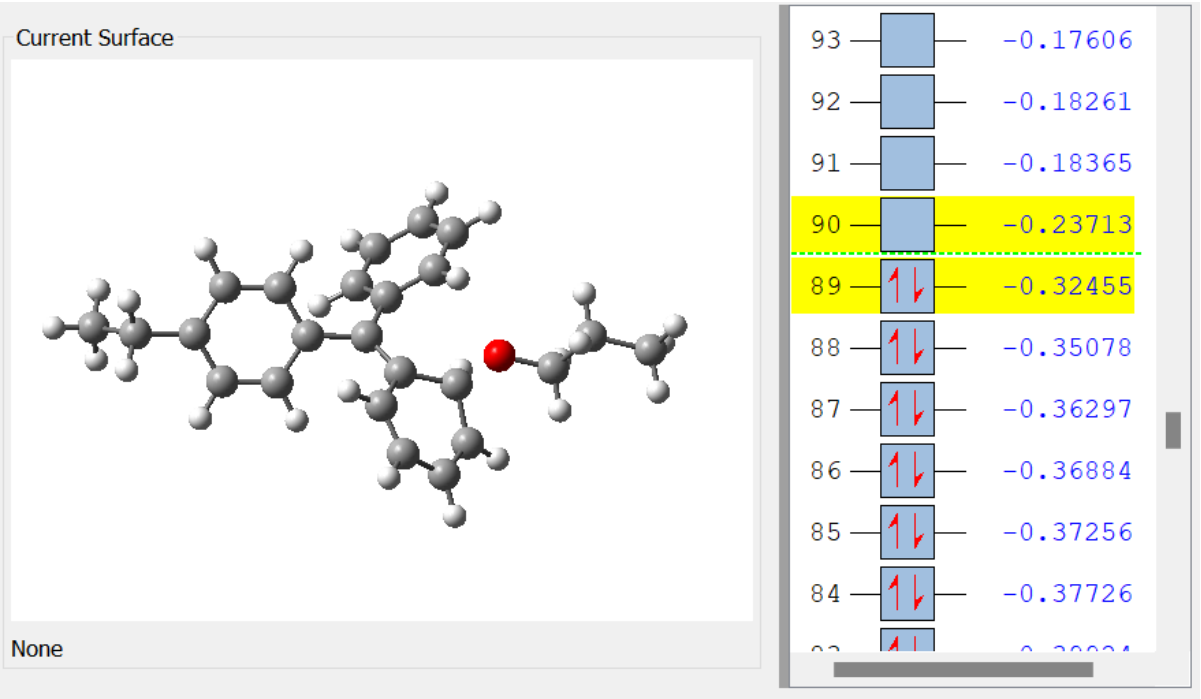


Figure S5: MO diagram for model **A** after C-O bond rupture. HOMO and LUMO have been displayed in yellow. HOMO: -8.83 eV and LUMO: -6.45 eV

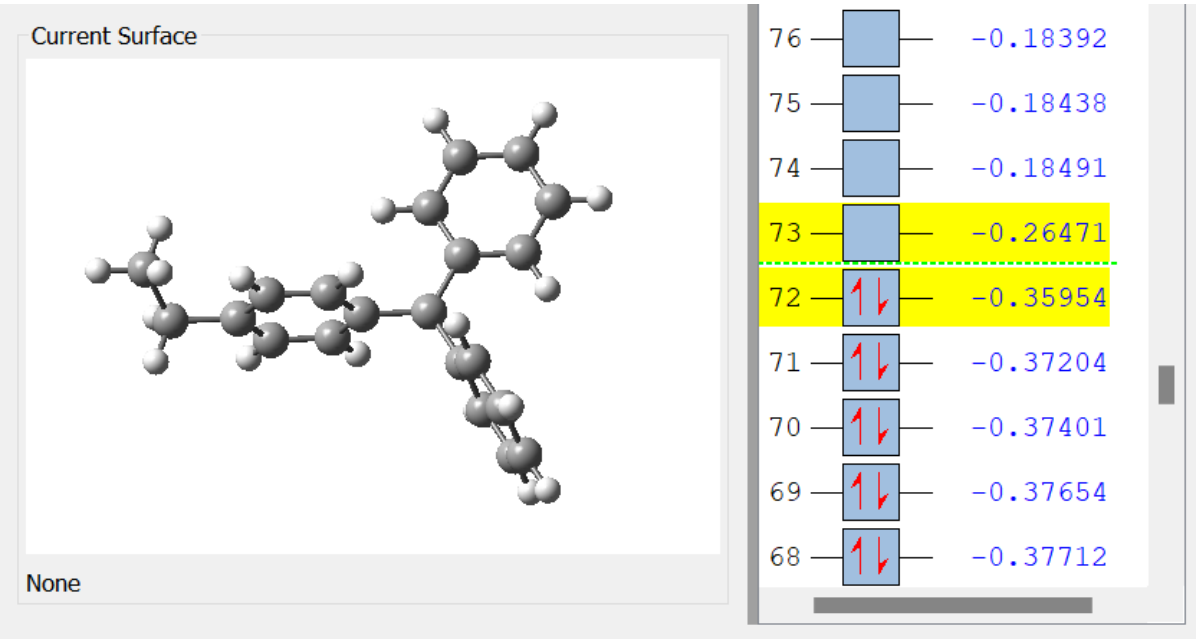


Figure S6: MO diagram for the independent carbocation of model **A**. HOMO and LUMO have been displayed in yellow. HOMO: -9.78 eV and LUMO: -7.20 eV

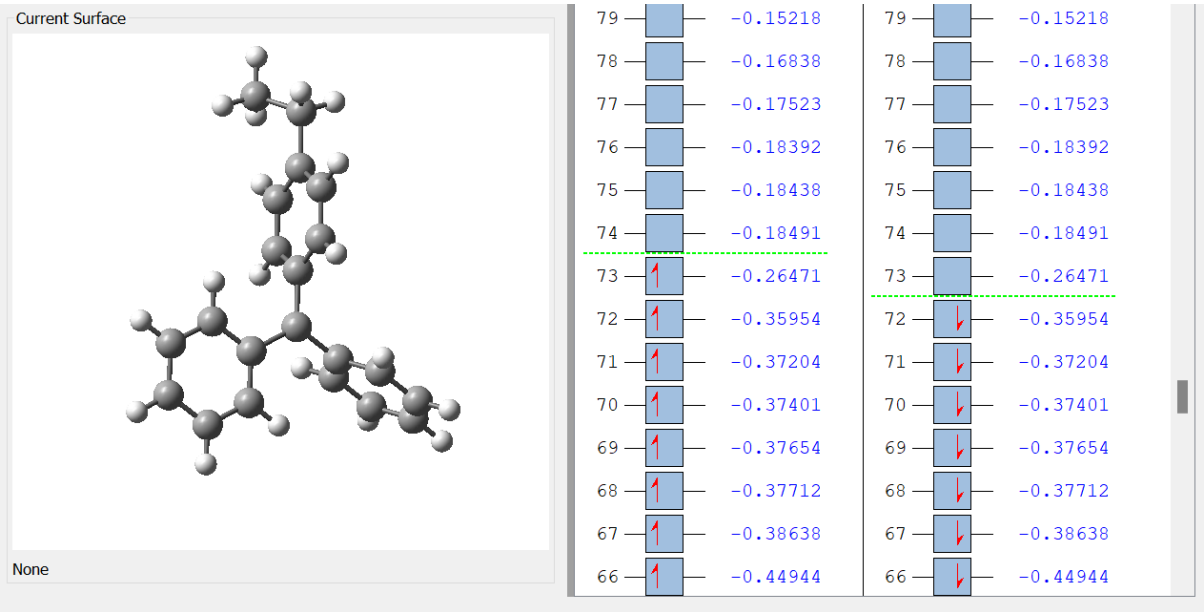


Figure S7. MO diagram for radical fragment from model **A**. SOMOs are reported for the alpha (left) and beta (right) electron spin configuration.

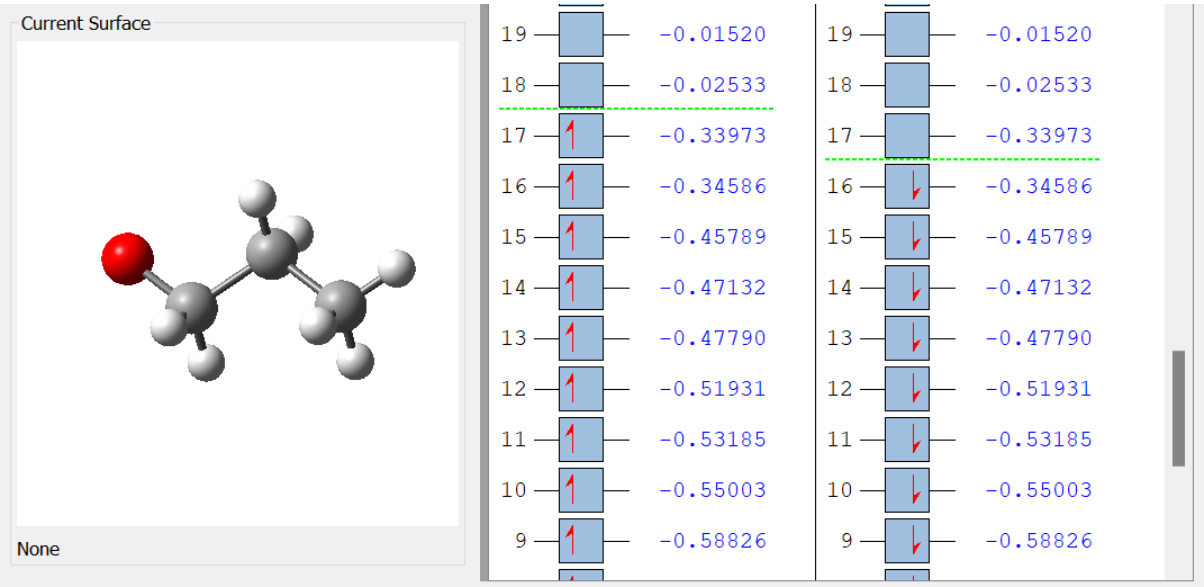


Figure S8. MO diagram for alkoxy radical fragment from model **A**. SOMOs are reported for the alpha (left) and beta (right) electron spin configuration.

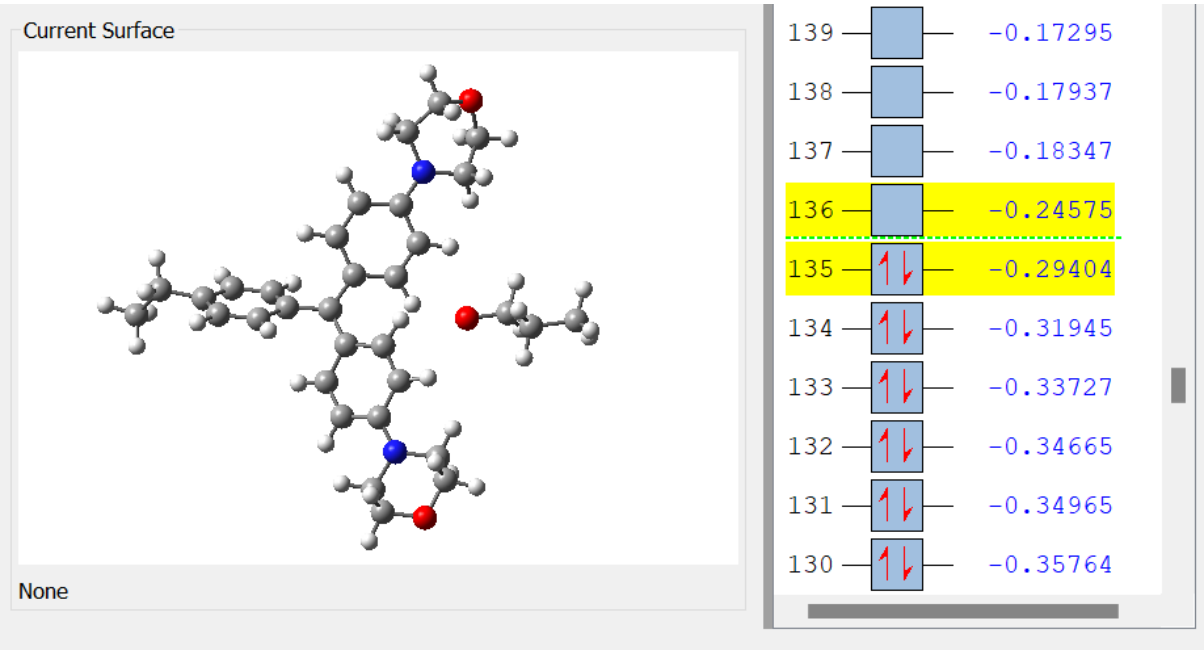


Figure S9: MO diagram for model **B** after C-O bond rupture. HOMO and LUMO have been displayed in yellow. HOMO: -8.00 eV and LUMO: -6.69 eV

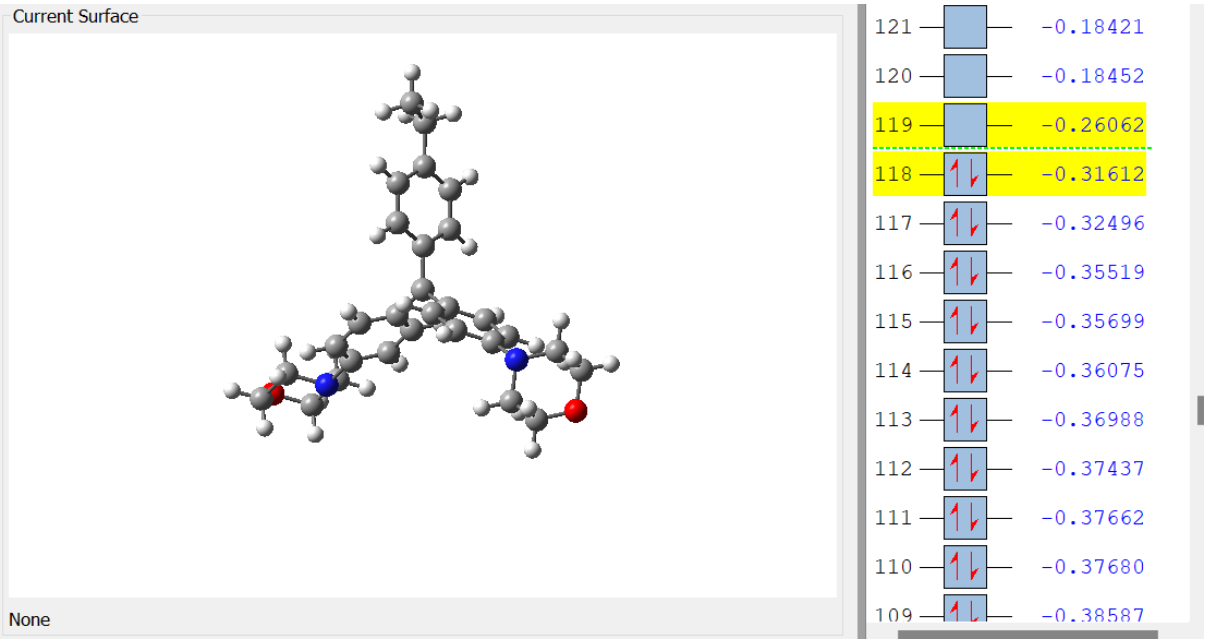


Figure S10: MO diagram for the independent carbocation from model **B**. HOMO and LUMO have been displayed in yellow. HOMO: -8.60 eV and LUMO: -7.09 Ev

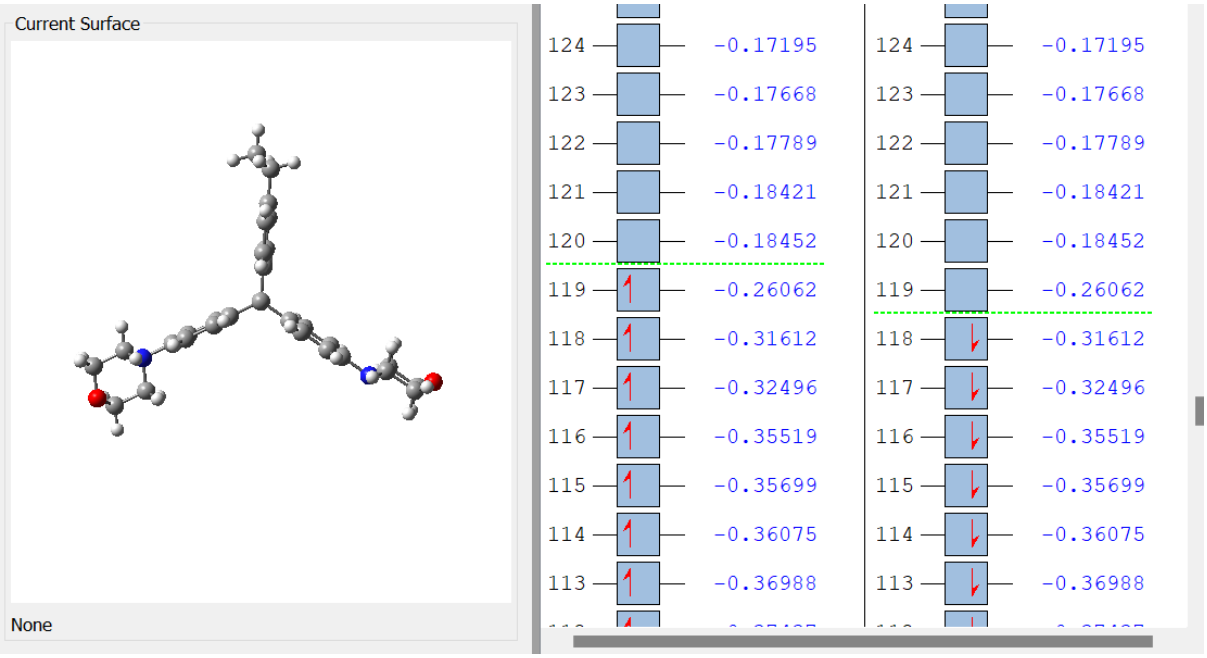


Figure S11. MO diagram for radical fragment from model **B**. SOMOs are reported for the alpha (left) and beta (right) electron spin configuration.

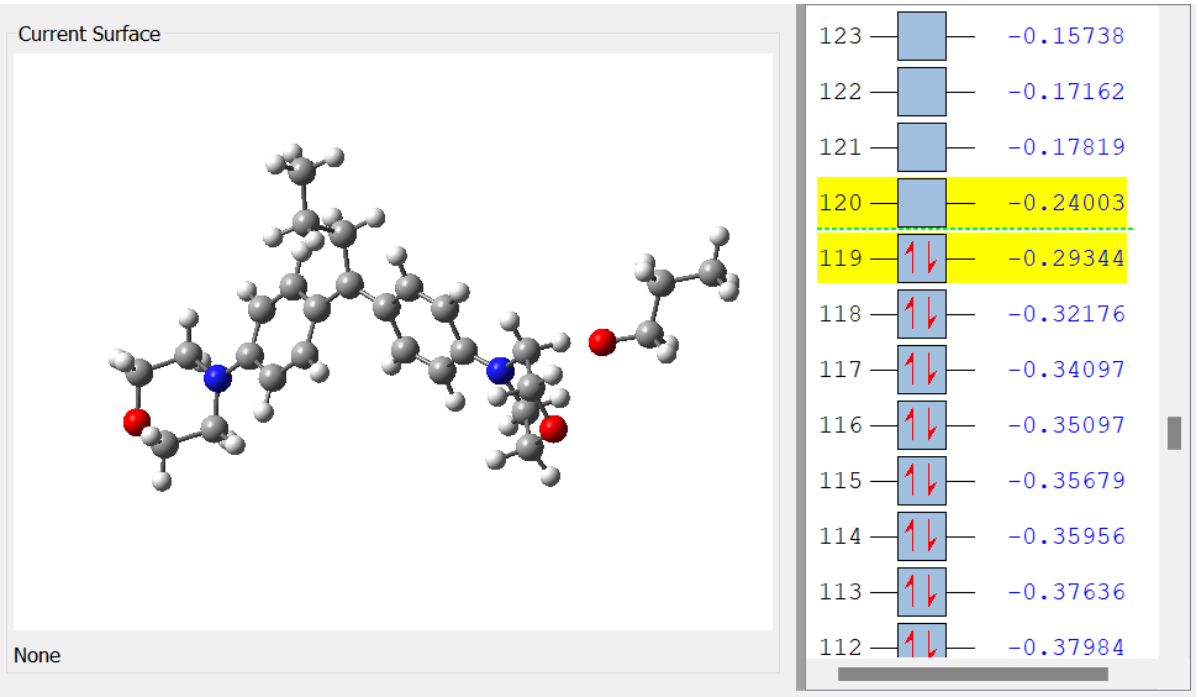


Figure S12: MO diagram for model **C** after C-O bond rupture. HOMO and LUMO have been displayed in yellow. HOMO: -7.98 eV and LUMO: -6.53 eV

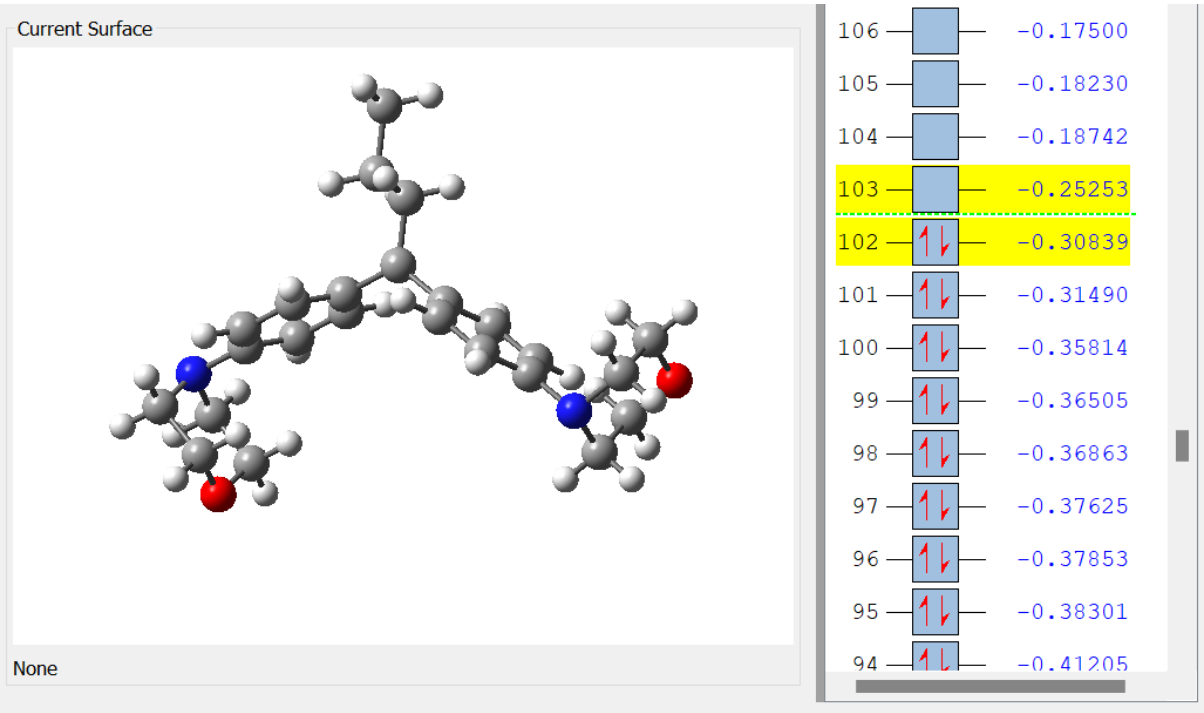


Figure S13: MO diagram for the independent carbocation from model **C**. HOMO and LUMO have been displayed in yellow. HOMO: -8.39 eV and LUMO: -6.87 eV

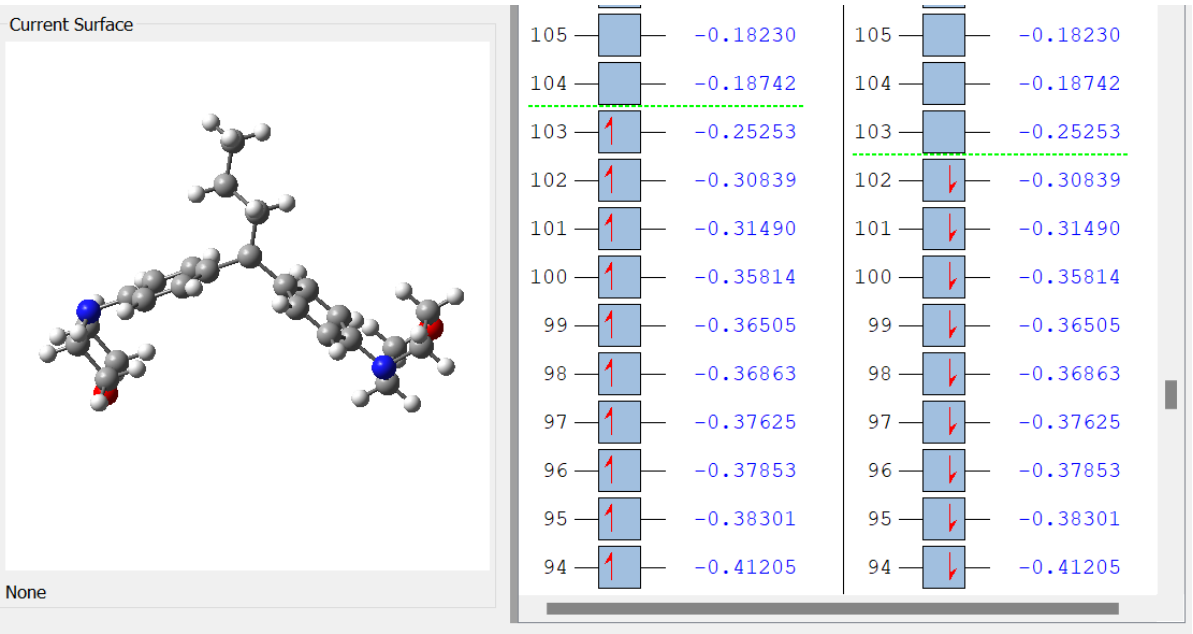


Figure S14. MO diagram for radical fragment from model **C**. SOMOs are reported for the alpha (left) and beta (right) electron spin configuration.

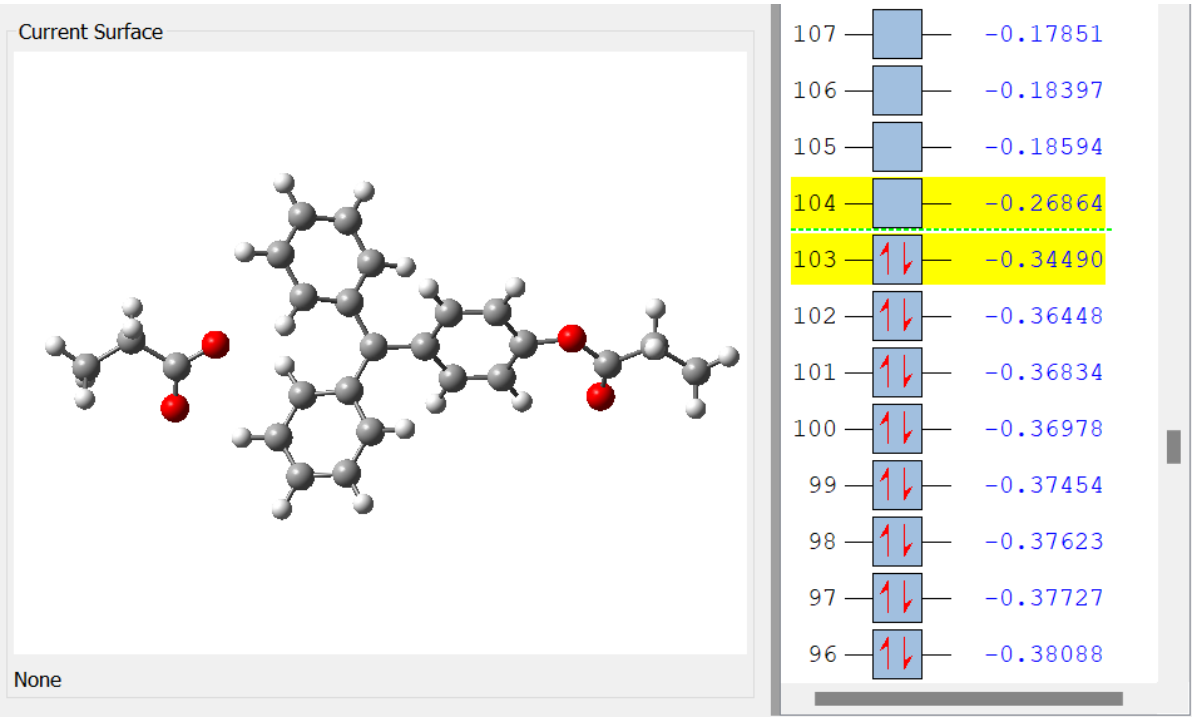


Figure S15: MO diagram for model **D** after C-O bond rupture. HOMO and LUMO have been displayed in yellow. HOMO: -9.38 eV and LUMO: -7.31 eV

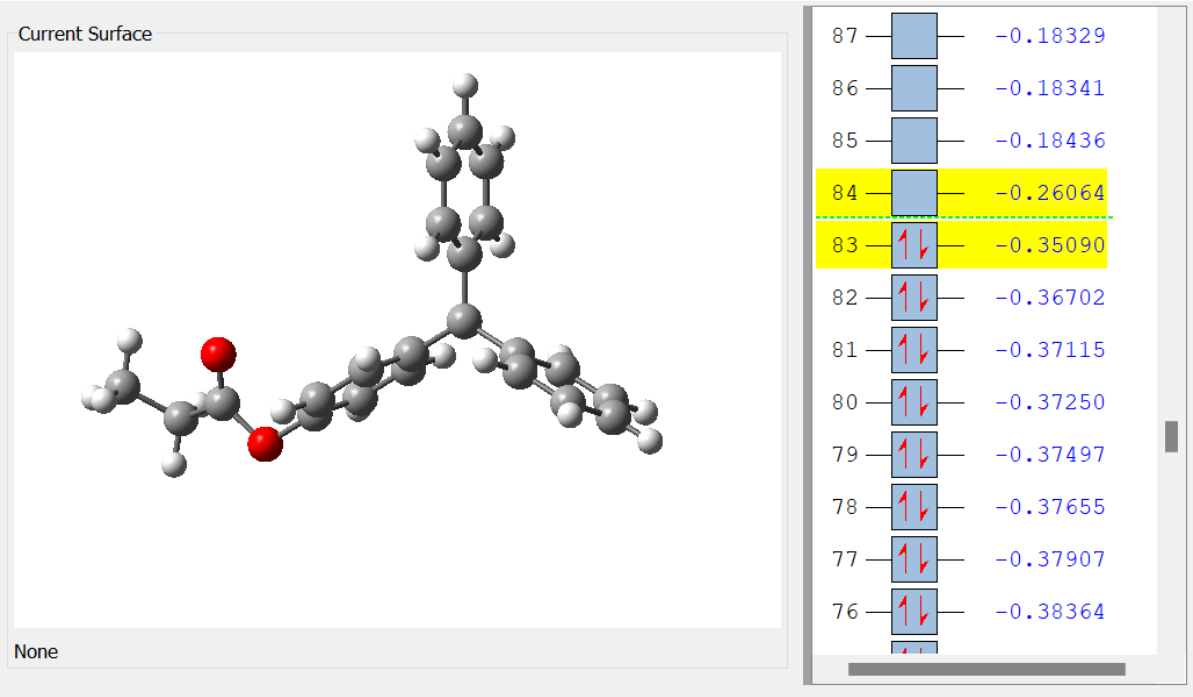


Figure S16: MO diagram for the independent carbocation from model **D**. HOMO and LUMO have been displayed in yellow. HOMO: -9.54 eV and LUMO: -7.09 eV

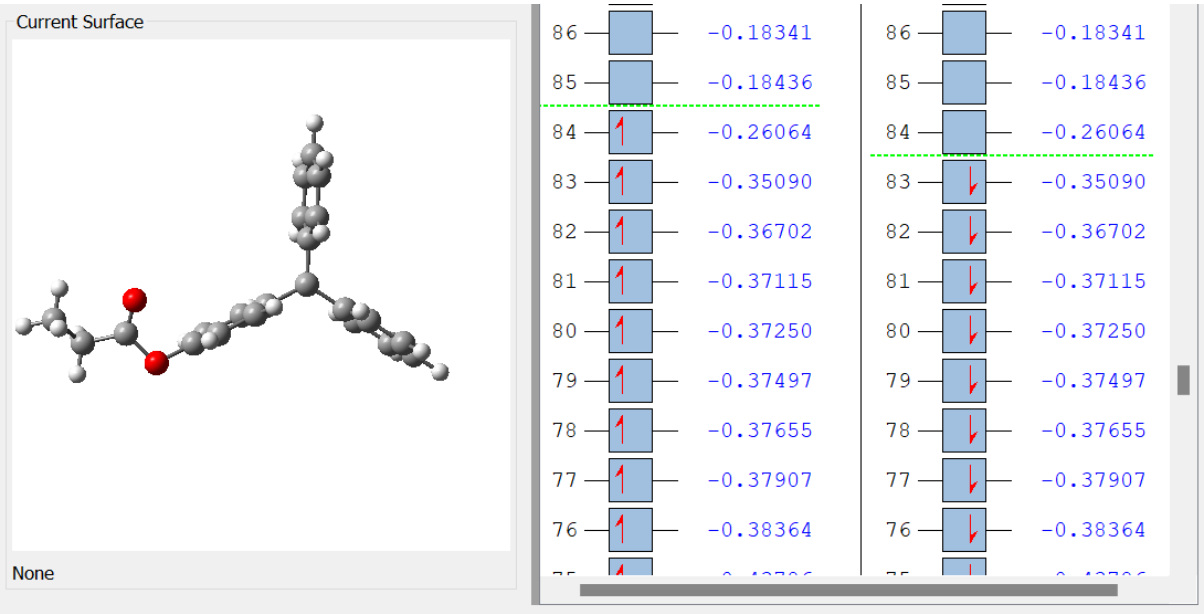


Figure S17. MO diagram for radical fragment from model **D**. SOMOs are reported for the alpha (left) and beta (right) electron spin configuration.

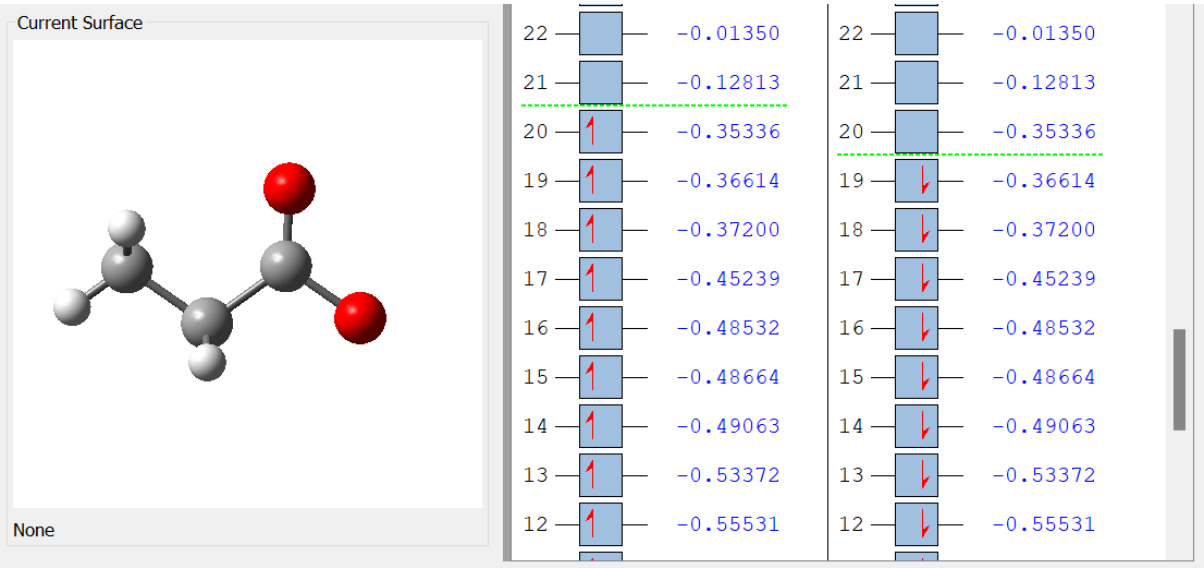


Figure S18. MO diagram for propionate radical fragment from model **D**. SOMOs are reported for the alpha (left) and beta (right) electron spin configuration.

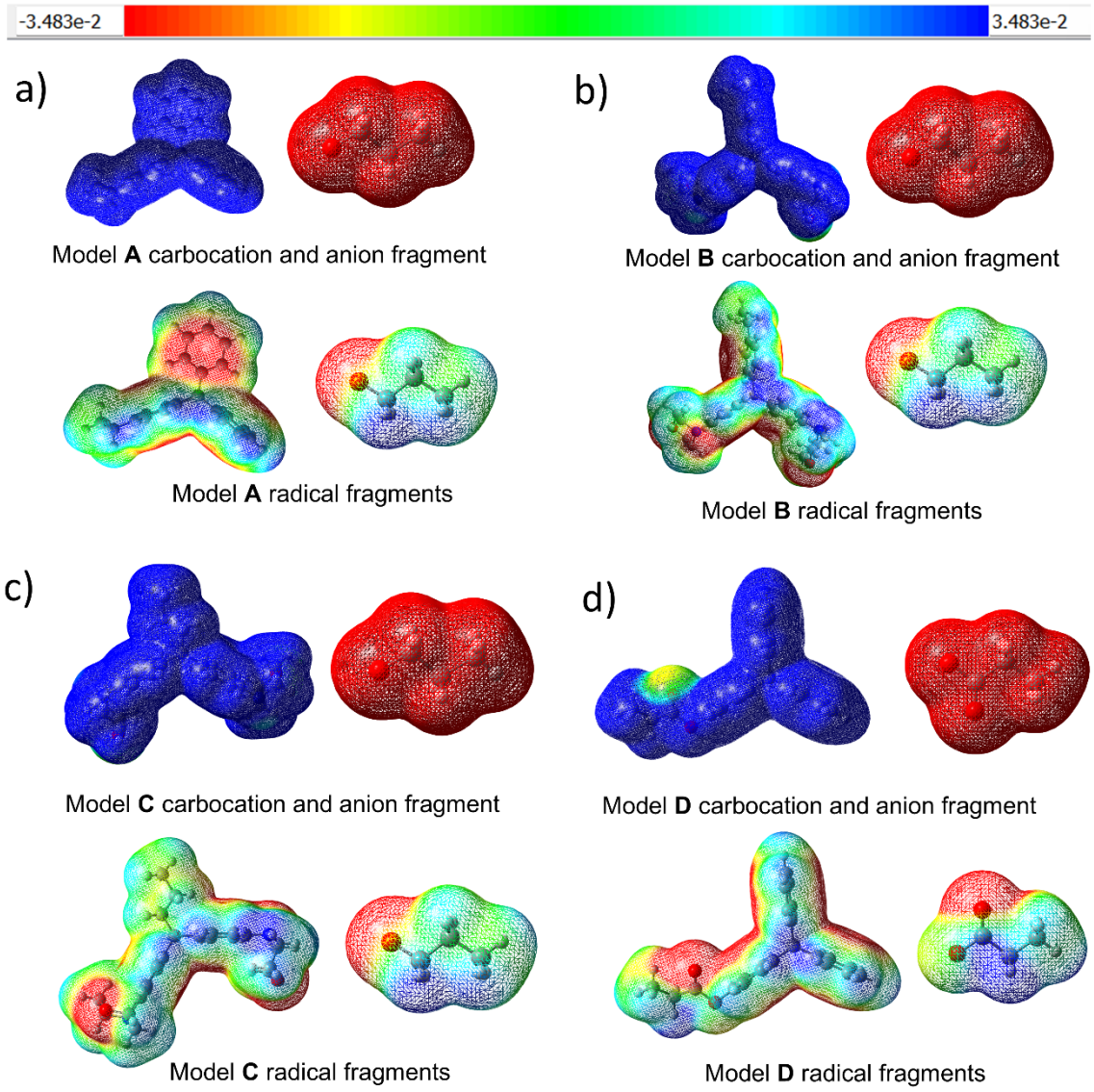


Figure S19: a-d) Electrostatic potential surface (ESP) mapping isolated carbocation and anion fragments (heterolytic cleavage), and isolated radical fragments (homolytic cleavage) for models **A**, **B**, **C** and **D** mechanophore.

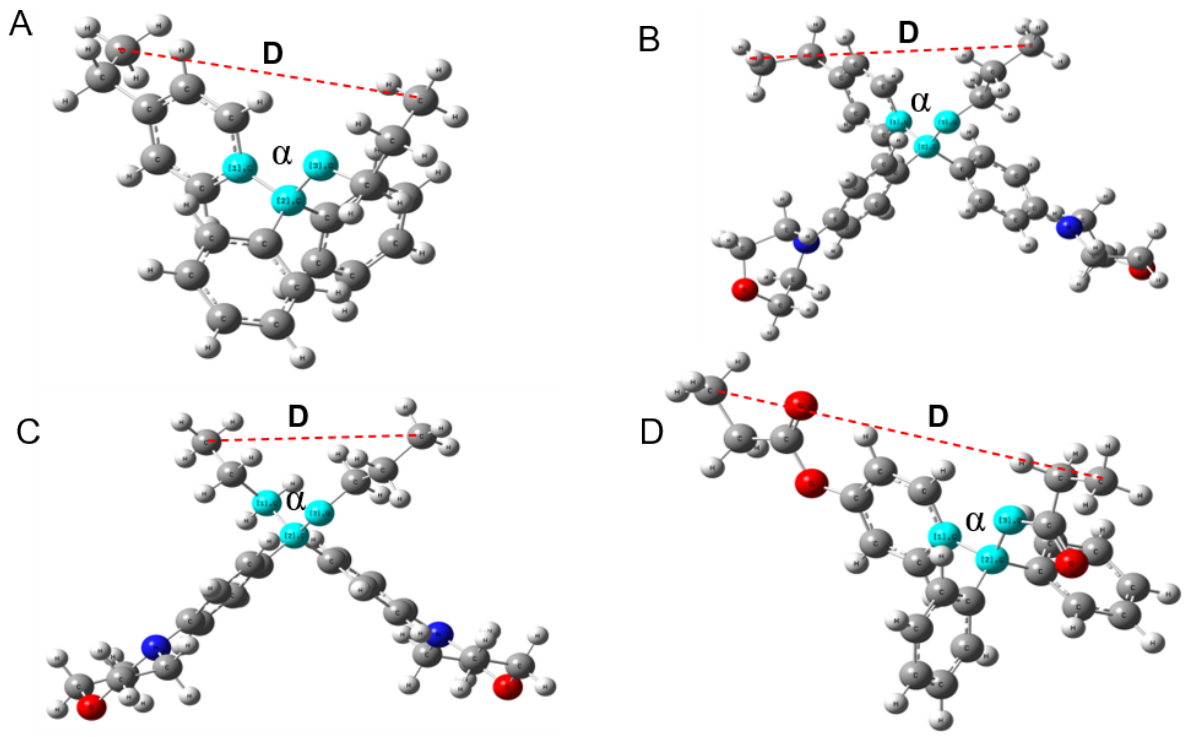


Figure S20: 3D structure of proposed **A**, **B**, **C**, and **D** mechanophores. The angle of the C_1, C_2, and O_3 atoms, which is denoted as a sky blue colour, is α.

Table S2: Change of C_2-O_3 bond length and the C_1-C_2-O_3 bond angle for all models during CoGEF calculation in vacuum.

Model	**At equilibrium, the C_2-O_3 bond length (Å)**	**Before rupture, the C_2-O_3 bond length (Å)**	**After bond rupture, the distance between C_2 and O_3, (Å)**	**At equilibrium, the C_1-C_2-O_3 bond angle, α (°)**	**Before rupture, the C_1-C_2-O_3 bond angle, α (°)**
A	1.48	1.73	3.44	104.1	126.7
B	1.48	1.74	3.40	109.0	125.8
C	1.48	1.71	3.43	109.7	114.3
D	1.51	1.71	4.93	102.9	122.0

Input data to Optimize for Model A

```
%nprocshared=20
%mem=2GB
%chk=Benzo_opt.chk
# opt b3lyp/6-31g* geom=connectivity

Benzo_opt

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 C          -0.32161498   0.66352247   0.19851452
 C           0.18844597  -0.78820326   0.28428541
 C           1.39274505  -1.14159180  -0.33858229
 C          -0.54816338  -1.75342984   0.98306545
 C           1.86004453  -2.46024559  -0.26536212
 H           1.95504927  -0.40282461  -0.87055843
 C          -0.08097156  -3.07284149   1.05763438
 H          -1.46737469  -1.48351054   1.45945105
 C           1.12314200  -3.42595854   0.43312388
 H           2.77940537  -2.72953381  -0.74194309
 H          -0.64339561  -3.81098323   1.59127558
 H           1.48011240  -4.43318848   0.48987381
 C           0.15656869   1.29789807  -1.12158462
 C          -0.63581455   1.20443514  -2.27387144
 C           1.38590826   1.97096229  -1.17034826
 C          -0.20309197   1.79052600  -3.47200054
 H          -1.57082978   0.68638363  -2.23883518
 C           1.81782063   2.55573297  -2.36923194
 H           1.99466965   2.03853637  -0.29209496
 C           1.02211850   2.46765718  -3.51912205
 H          -0.80928092   1.72070182  -4.35094869
 H           2.75505036   3.07029879  -2.40578153
 H           1.34999930   2.91758091  -4.43345629
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 C          -2.53785756   1.76882344   0.79817005
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H	1.66321923	-0.68766088	0.60512251
C	1.50656226	-0.69680611	2.74688817
H	1.80666602	-1.71857422	2.84369772
H	1.89459807	-0.13123638	3.56872991
H	0.43771720	-0.63682099	2.74648772
O	0.19237373	1.41491768	1.29978826

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51

Input data to Scan for Model A in 0.1 Å step size

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%mem=2GB
%chk=Benzo_scan.chk
opt=modredundant b3lyp/6-31g* geom=connectivity

Benzo_scan

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C	2.61031700	-1.33679600	-0.83224300
C	0.75512900	-2.60242400	0.04906300
C	3.31259700	-2.52510400	-1.06439600
H	3.07533200	-0.39059500	-1.08433000
C	1.45546600	-3.79076100	-0.18053100
H	-0.23439300	-2.64185400	0.48821600
C	2.73628400	-3.75817500	-0.74312100
H	4.30913000	-2.48380700	-1.49329700
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C	1.10115600	0.96748700	-2.23745700
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H	0.56882800	2.58100600	0.69950900
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Input data to Scan for Model A in 0.05 Å step size

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C	-0.90315569	4.05489462	-0.36476200
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C	-0.34466469	5.30186162	-0.03148800
C	-2.90213269	5.22454162	-1.14494700
H	-2.66486769	3.09003262	-1.16488100
C	-1.04500169	6.49019862	-0.26108200
H	0.64485731	5.34129162	0.40766500
C	-2.32581969	6.45761262	-0.82367200
H	-3.89866569	5.18324462	-1.57384800
H	-0.58878269	7.44012562	-0.00025600
H	-2.86817969	7.38002062	-1.00625600
C	-0.45054469	1.56458962	-0.94304900
C	-0.69069169	1.73195062	-2.31800800
C	-0.36797869	0.25666362	-0.43473300
C	-0.85867769	0.62318962	-3.15667800
H	-0.75189669	2.72841862	-2.74077600
C	-0.54249769	-0.85049638	-1.26985800
H	-0.15836369	0.11843162	0.61895800
C	-0.79027769	-0.67267938	-2.63609700
H	-1.04406669	0.77634162	-4.21548200
H	-0.47836069	-1.85156538	-0.85432100
H	-0.92387869	-1.53191538	-3.28579400
C	1.37128631	2.96249562	0.04825500
C	2.08531831	2.88128562	1.25194400
C	2.08150131	3.24829862	-1.13034600
C	3.47161931	3.07560462	1.27135400
H	1.54875031	2.67153462	2.16674100
C	3.46308531	3.44514662	-1.10400400
H	1.55562831	3.31770462	-2.07647700
C	4.18682331	3.35864062	0.09828500

H	4.00336331	3.01027362	2.21742800
H	3.98790231	3.66969862	-2.02906700
C	5.69438831	3.52521562	0.11685100
H	6.00617131	3.93808462	1.08524000
H	5.99352131	4.25623562	-0.64611900
C	6.44817131	2.19954762	-0.13269200
H	7.53331831	2.35573662	-0.11375600
H	6.19539231	1.45767762	0.63344400
H	6.18035431	1.77595162	-1.10747300
C	-1.92737569	2.21939562	1.73672100
H	-2.38456969	1.44785162	1.10135200
H	-2.46377869	3.16156862	1.57738500
C	-1.98431169	1.81631362	3.20947300
H	-3.04194169	1.80184162	3.50960100
H	-1.49788369	2.60250862	3.80114900
C	-1.33655669	0.45697262	3.51189300
H	-1.42265469	0.20861162	4.57599700
H	-1.81962469	-0.34607438	2.94050300
H	-0.27419669	0.46808362	3.24958100
O	-0.51797569	2.38307562	1.38850000

1 2 1.0 13 1.0 24 1.0 51 1.0
2 3 1.5 4 1.5
3 5 1.5 6 1.0
4 7 1.5 8 1.0
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7 9 1.5 11 1.0
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15 18 1.5 19 1.0
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34 35 1.0 36 1.0 37 1.0

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41 42 1.0 43 1.0 44 1.0 51 1.0
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44 45 1.0 46 1.0 47 1.0
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47 48 1.0 49 1.0 50 1.0
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B 37 47 S 120 0.050000

Input data to Scan for Model A in solvent

%nprocshared=20
%mem=2GB
%chk=Benzo_scan_solvent.chk
opt=modredundant b3lyp/6-31g* scrf=(solvent=ethanol) geom=connectivity

Benzo_scan_solvent

0 1

C	0.57545100	-0.05499800	0.08556300
C	1.33373400	-1.34760700	-0.27913300
C	2.58437800	-1.31958100	-0.92411100
C	0.84388700	-2.59136600	0.16120200
C	3.30546300	-2.49882400	-1.15050800
H	3.00177800	-0.37576700	-1.25481900
C	1.56272100	-3.77044200	-0.06129600
H	-0.10702500	-2.63739800	0.67901600
C	2.79569600	-3.73008000	-0.72428900
H	4.26494100	-2.45108600	-1.65571700
H	1.15993000	-4.71781200	0.28288900
H	3.35248900	-4.64457100	-0.90186200
C	0.80179500	1.12290100	-0.89052200
C	0.93986400	0.93248200	-2.27734600
C	0.75526200	2.43970100	-0.39992400
C	1.04431800	2.02702200	-3.14506100
H	0.97065800	-0.06970700	-2.68921600
C	0.86572900	3.53390000	-1.26474900
H	0.62771000	2.59965500	0.66374600
C	1.01213200	3.33290900	-2.64287700
H	1.15216800	1.85541800	-4.21150000
H	0.83298400	4.54148900	-0.86187300
H	1.09675900	4.18071700	-3.31511600

C	-0.95012000	-0.28991700	0.18115900
C	-1.66432700	-0.02565800	1.35854600
C	-1.66191000	-0.75772800	-0.93816000
C	-3.05070700	-0.22066100	1.41153700
H	-1.13124400	0.32488800	2.23156700
C	-3.04356900	-0.95270300	-0.87962100
H	-1.13690200	-0.97858100	-1.86154200
C	-3.76698900	-0.68444500	0.29718400
H	-3.58066100	-0.01282600	2.33762800
H	-3.56782300	-1.32147400	-1.75731500
C	-5.27354400	-0.85529800	0.34517600
H	-5.58119800	-1.11100900	1.36721600
H	-5.56849700	-1.69789400	-0.29365900
C	-6.03615700	0.41001300	-0.10849500
H	-7.11952000	0.24938000	-0.06188400
H	-5.78971200	1.26489100	0.53193700
H	-5.77460400	0.67533600	-1.13949100
C	2.39775800	0.54398000	1.74030100
H	2.81101500	1.30848800	1.06926000
H	2.94309300	-0.39150800	1.57458700
C	2.51531000	0.97850000	3.19989400
H	3.58534100	1.00688400	3.44874600
H	2.06591700	0.20151500	3.83223800
C	1.87433400	2.34060800	3.50531800
H	2.01394800	2.61128000	4.55816300
H	2.32344000	3.13286400	2.89301400
H	0.79922200	2.32234400	3.29982600
O	0.97409100	0.34477900	1.45442900

1 2 1.0 13 1.0 24 1.0 51 1.0
2 3 1.5 4 1.5
3 5 1.5 6 1.0
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24 25 1.5 26 1.5
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41 42 1.0 43 1.0 44 1.0 51 1.0
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44 45 1.0 46 1.0 47 1.0
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47 48 1.0 49 1.0 50 1.0
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B 47 37 S 60 0.100000

Input data to Optimize for Model B

%nprocshared=20
%mem=2GB
%chk=Tr_opt.chk
opt b3lyp/6-31g* geom=connectivity

Tr_opt

0 1

C	-3.56100155	0.21658416	0.00000000
C	-2.16584155	0.21658416	0.00000000
C	-1.46830355	1.42433516	0.00000000
C	-2.16595755	2.63284416	-0.00119900
C	-3.56078255	2.63276616	-0.00167800
C	-4.25838355	1.42456016	-0.00068200
H	-4.11076055	-0.73573284	0.00045000
H	-1.61633355	-0.73592884	0.00131500
H	-1.61575755	3.58498716	-0.00125800
H	-4.11090455	3.58504716	-0.00263100
C	0.07169619	1.42444720	0.00088786
C	0.58471222	0.15825983	0.71165091
C	0.97978338	-0.95026446	-0.03772490

C	0.65592856	0.12028198	2.10402573
C	1.44541675	-2.09693048	0.60561850
H	0.92397720	-0.91995674	-1.13549990
C	1.12127524	-1.02704666	2.74769179
H	0.34513851	0.99422048	2.69473510
C	1.51578733	-2.13543808	1.99844837
H	1.75666734	-2.97077496	0.01515435
H	1.17728259	-1.05677864	3.84554220
C	0.58586470	1.44231410	-1.45063256
C	1.67919720	2.23838660	-1.79321689
C	-0.04022882	0.66164940	-2.42212176
C	2.14581204	2.25410289	-3.10758812
H	2.17295456	2.85345899	-1.02703646
C	0.42624476	0.67774372	-3.73717306
H	-0.90161881	0.03367085	-2.15203521
C	1.51902400	1.47401270	-4.07970228
H	3.00740561	2.88161077	-3.37780918
H	-0.06760522	0.06217859	-4.50299817
C	2.03415137	1.49208735	-5.53088011
H	3.10330951	1.44965353	-5.53038433
H	1.64390491	0.64692572	-6.05843060
C	1.57215326	2.78763575	-6.22349262
H	2.01673301	3.63039978	-5.73666859
H	1.87229416	2.76964924	-7.25037719
H	0.50643401	2.86301160	-6.16466263
C	2.09600504	2.53147203	1.00135521
H	2.60195883	3.40472727	0.64591738
H	2.46696244	1.66995743	0.48649289
C	2.34540224	2.37316669	2.51275869
H	2.86817945	1.45732756	2.69398414
H	1.40837639	2.35717585	3.02911792
C	3.19100757	3.55599989	3.02016115
H	3.37766571	3.43781360	4.06710467
H	4.12156352	3.58142045	2.49260128
H	2.66132416	4.47060395	2.85332320
O	0.58451075	2.67287963	0.74253311
C	3.40090346	-3.61015214	2.85689134
C	1.12373408	-4.33947405	3.20421907
C	3.86648238	-4.75657411	3.50070892
H	3.82997411	-3.60164242	1.87672505
C	1.58949434	-5.48664629	3.84786474
H	0.48431883	-3.82798126	3.89300298
H	4.46941299	-4.43418900	4.32377789
H	1.19719441	-6.32858780	3.31670068
C	-6.49572828	1.58022376	1.19741071
C	-6.49579138	1.27139139	-1.19897614
C	-7.89055677	1.58148876	1.19748292
H	-6.18021245	0.79406527	1.85109610
C	-7.89121818	1.27214051	-1.19886853
H	-6.17920691	2.05760799	-1.85207470
H	-8.20588252	2.50806307	1.62983661
H	-8.20796210	0.34621147	-1.63156784
N	-5.79838351	1.42481646	-0.00093409
N	2.02939813	-3.40184607	2.70838832
O	-8.58832861	1.42704032	-0.00071157

O	2.96069478	-5.69506661	3.99587610
H	3.79296007	-2.76800795	3.38791373
H	4.50684957	-5.26768661	2.81252735
H	1.16069096	-5.49537954	4.82814602
H	0.51985362	-4.66149962	2.38170590
H	-6.17867120	2.50611284	1.62996616
H	-8.20742368	0.79607581	1.85141094
H	-6.18010915	0.34538071	-1.63227622
H	-8.20706001	2.05830788	-1.85238578

1 2 1.5 6 1.5 7 1.0
2 3 1.5 8 1.0
3 4 1.5 11 1.0
4 5 1.5 9 1.0
5 6 1.5 10 1.0
6 66 1.0
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11 12 1.0 22 1.0 49 1.0
12 13 1.5 14 1.5
13 15 1.5 16 1.0
14 17 1.5 18 1.0
15 19 1.5 20 1.0
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17 19 1.5 21 1.0
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19 67 1.0
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22 23 1.5 24 1.5
23 25 1.5 26 1.0
24 27 1.5 28 1.0
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27 29 1.5 31 1.0
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29 32 1.0
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32 33 1.0 34 1.0 35 1.0
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35 36 1.0 37 1.0 38 1.0
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39 40 1.0 41 1.0 42 1.0 49 1.0
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45 46 1.0 47 1.0 48 1.0

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50 52 1.0 53 1.0 67 1.0 70 1.0
51 54 1.0 55 1.0 67 1.0 73 1.0
52 56 1.0 69 1.0 71 1.0
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54 57 1.0 69 1.0 72 1.0
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58 60 1.0 61 1.0 66 1.0 74 1.0
59 62 1.0 63 1.0 66 1.0 76 1.0
60 64 1.0 68 1.0 75 1.0
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62 65 1.0 68 1.0 77 1.0
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Input data to Scan for Model B

%nprocshared=20
%mem=2GB
%chk=Tr_scan.chk
opt=modredundant b3lyp/6-31g* geom=connectivity

Tr_scan

0 1

C	-2.72731200	-1.24514300	-0.91812900
C	-1.60018000	-0.44216200	-0.77113900
C	-1.23267900	0.08725500	0.47892200
C	-2.04033000	-0.22323400	1.57849100
C	-3.16961400	-1.03915800	1.44304800
C	-3.54343800	-1.56448400	0.19080100
H	-2.99608400	-1.59718800	-1.90794700
H	-1.00675200	-0.21255100	-1.64984000
H	-1.77147100	0.16527600	2.55116000
H	-3.74428600	-1.27624700	2.33050300
C	0.00985700	0.99444500	0.60732700
C	1.30106800	0.25688400	0.22040900

C	2.45365200	0.93087300	-0.22129600
C	1.42073500	-1.12710900	0.43860600
C	3.65232700	0.26129300	-0.46941400
H	2.41935700	2.00139500	-0.39046200
C	2.61106400	-1.81214900	0.20544500
H	0.56546900	-1.68029100	0.80927700
C	3.76154000	-1.13421400	-0.26481900
H	4.49560200	0.82704200	-0.84685300
H	2.65132400	-2.87353400	0.41889700
C	-0.25587800	2.28470500	-0.20087500
C	-0.94878100	3.34619400	0.40532100
C	0.07393200	2.40717500	-1.56125400
C	-1.28093600	4.49458300	-0.31654400
H	-1.22806400	3.25728400	1.44851700
C	-0.26661000	3.55623000	-2.28302300
H	0.60705900	1.60770500	-2.06370700
C	-0.94779400	4.62249900	-1.67560100
H	-1.80930400	5.30375500	0.18155200
H	0.00649300	3.62566500	-3.33304600
C	-1.35016300	5.85092000	-2.46935200
H	-1.33170900	6.73320600	-1.81591800
H	-0.61364800	6.03387200	-3.26289900
C	-2.75357400	5.72263000	-3.10338800
H	-3.51722900	5.56903200	-2.33238800
H	-3.01318500	6.62633100	-3.66748300
H	-2.79535200	4.86770700	-3.78796600
C	1.21638900	2.06370800	2.55294700
H	1.36378100	2.98644900	1.97399300
H	2.12163600	1.45151700	2.45669500
C	0.93512000	2.38559300	4.01883200
H	0.73214400	1.44606700	4.54808900
H	0.01882000	2.98648600	4.08118000
C	2.10392700	3.12997700	4.68438000
H	1.88199000	3.35009200	5.73434100
H	3.02389800	2.53276500	4.65607300
H	2.30880100	4.08288700	4.18037700
O	0.06022100	1.33147800	2.05213200
C	6.22191000	-1.09549700	-0.70562600
C	5.00298300	-3.28015200	-0.59653500
C	7.39571800	-1.98793600	-0.30098100
H	6.34915600	-0.75810000	-1.74675100
C	6.14583700	-3.71437600	-1.51522300
H	5.12115300	-3.74563600	0.39496200
H	7.32818300	-2.22038200	0.77055300
H	5.95672800	-3.34972800	-2.53395800
C	-5.67705700	-2.46164800	1.11893000
C	-4.63803100	-3.58014100	-0.80378700
C	-7.04541700	-2.86144000	0.56288100
H	-5.36160100	-3.20011600	1.87826100
C	-6.02776800	-3.94294100	-1.32138200
H	-3.96172500	-3.42182200	-1.64552200
H	-7.43765000	-2.05344500	-0.07232600
H	-6.02013700	-4.90639000	-1.83555700
N	-4.70334800	-2.35910400	0.02336300
N	4.95374300	-1.81335600	-0.51260200

O	-6.96178900	-4.09535900	-0.21047800
O	7.45087300	-3.23276900	-1.06479500
H	6.23296600	-0.20242900	-0.06973400
H	8.34501300	-1.47925000	-0.48675000
H	6.22015300	-4.80448600	-1.54442500
H	4.06191100	-3.64948700	-1.01992900
H	-5.76629700	-1.48817900	1.60951200
H	-7.75264600	-3.06589100	1.36952900
H	-4.24421100	-4.42533700	-0.21104700
H	-6.39049700	-3.16268700	-2.00700400

1 2 1.5 6 1.5 7 1.0
2 3 1.5 8 1.0
3 4 1.5 11 1.0
4 5 1.5 9 1.0
5 6 1.5 10 1.0
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11 12 1.0 22 1.0 49 1.0
12 13 1.5 14 1.5
13 15 1.5 16 1.0
14 17 1.5 18 1.0
15 19 1.5 20 1.0
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17 19 1.5 21 1.0
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19 67 1.0
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22 23 1.5 24 1.5
23 25 1.5 26 1.0
24 27 1.5 28 1.0
25 29 1.5 30 1.0
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27 29 1.5 31 1.0
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29 32 1.0
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32 33 1.0 34 1.0 35 1.0
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45 46 1.0 47 1.0 48 1.0
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50 52 1.0 53 1.0 67 1.0 70 1.0
51 54 1.0 55 1.0 67 1.0 73 1.0
52 56 1.0 69 1.0 71 1.0
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54 57 1.0 69 1.0 72 1.0
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58 60 1.0 61 1.0 66 1.0 74 1.0
59 62 1.0 63 1.0 66 1.0 76 1.0
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B 45 35 S 60 0.100000

Input data to Scan for Model B in solvent

%nprocshared=20
%mem=2GB
%chk=Tr_scan_solvent.chk
opt=modredundant b3lyp/6-31g* scrf=(solvent=ethanol) geom=connectivity

Tr_opt_solvent

0 1

C	-2.58719100	-1.47586300	-0.87785600
C	-1.45323500	-0.68330900	-0.70324600
C	-1.21683400	0.02078800	0.48989900
C	-2.17145400	-0.10277900	1.51025500
C	-3.30875600	-0.89962700	1.35697000
C	-3.55008000	-1.60716900	0.15451600
H	-2.73157300	-1.97521900	-1.82822800

H	-0.74212600	-0.61480800	-1.52018000
H	-2.01317600	0.41934800	2.44460800
H	-3.99575300	-0.98817100	2.19008800
C	0.01095900	0.94629700	0.63006200
C	1.31644100	0.24804100	0.22421500
C	2.41614000	0.93713300	-0.31719100
C	1.51156100	-1.11097900	0.53480200
C	3.63477700	0.30532400	-0.56931100
H	2.33327900	1.99443800	-0.54184400
C	2.71785300	-1.76255000	0.28786900
H	0.69568100	-1.67783700	0.96980300
C	3.81791900	-1.06936100	-0.27971600
H	4.45262100	0.89488200	-0.96507600
H	2.79525300	-2.81868000	0.51535800
C	-0.29252000	2.24284800	-0.15766600
C	-0.89941500	3.33341700	0.48738200
C	-0.08400200	2.33529500	-1.54575400
C	-1.26497600	4.48096900	-0.22376500
H	-1.08693200	3.27515600	1.55284700
C	-0.45559700	3.48193200	-2.25551500
H	0.37648600	1.51245900	-2.08117700
C	-1.05119300	4.57864000	-1.60905900
H	-1.72331000	5.31244100	0.30563600
H	-0.27572500	3.52614600	-3.32656900
C	-1.48665500	5.80612100	-2.38689300
H	-1.41000900	6.69339900	-1.74527500
H	-0.80422000	5.96733000	-3.23141800
C	-2.93215800	5.69619800	-2.92260000
H	-3.64485500	5.56762800	-2.09963800
H	-3.21135900	6.59899600	-3.47820100
H	-3.03537300	4.83620100	-3.59454700
C	1.23493300	1.98653700	2.57989400
H	1.39516200	2.89889500	1.99008000
H	2.13102800	1.36076900	2.48895400
C	0.96044600	2.33001700	4.04185800
H	0.74068900	1.40189900	4.58515400
H	0.05819200	2.95274100	4.09982000
C	2.14586100	3.05777600	4.69685400
H	1.92850800	3.29457700	5.74399900
H	3.05238600	2.44049200	4.67415900
H	2.36877000	3.99953900	4.18023100
O	0.06769000	1.25962300	2.08267200
C	6.06931500	-1.08803800	-1.36627400
C	5.32113300	-3.04668700	0.00716300
C	6.90845700	-2.16736200	-2.04869500
H	5.60137300	-0.47855900	-2.14664000
C	6.83019800	-3.22028900	0.17152900
H	4.85853400	-3.15083400	0.99444900
H	7.71159800	-1.71086800	-2.63205000
H	7.05887600	-4.22428600	0.53645200
C	-5.81889800	-2.32313100	0.92516200
C	-4.80588500	-3.35561100	-1.12107400
C	-7.11191600	-2.71321000	0.21054800
H	-5.66857800	-2.96396800	1.80776500
C	-5.71827100	-4.51343800	-0.71885700

H	-5.18807600	-2.87528100	-2.03506000
H	-7.31702300	-1.99956800	-0.59782900
H	-5.27240300	-5.05988500	0.12225200
N	-4.68409600	-2.40006200	-0.00853700
N	5.02382000	-1.71088100	-0.53727300
O	-7.06558400	-4.07003000	-0.34500500
O	7.55881500	-3.06949900	-1.09220600
H	6.71772900	-0.42344900	-0.77532100
H	6.27481600	-2.75551600	-2.72489900
H	7.20965800	-2.48907000	0.89687400
H	4.91683900	-3.84683400	-0.63125200
H	-5.92693300	-1.29393800	1.28470400
H	-7.95153100	-2.69932900	0.90953300
H	-5.84639600	-5.20458400	-1.55533900
H	-3.81931000	-3.76837300	-1.35827200

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2 3 1.5 8 1.0
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B 35 45 S 60 0.100000

Input data to Optimize for Model C

%nprocshared=20
%mem=2GB
%chk=Tph-opt.chk
opt b3lyp/6-31g* geom=connectivity

c-opt

0 1
C 0.02193500 1.70181900 0.41583400
C -1.22803100 0.80629000 0.36978100
C -1.52491600 0.12643400 -0.82375100

C	-2.10093400	0.61498000	1.45208200
C	-2.63489100	-0.70846100	-0.93712100
H	-0.86280900	0.25051600	-1.67418100
C	-3.21941900	-0.21553400	1.35063500
H	-1.92732500	1.12256300	2.39409100
C	-3.51591400	-0.89794900	0.15244200
H	-2.79818200	-1.23226700	-1.87108900
H	-3.88399700	-0.30130800	2.20295000
C	1.28958600	0.85463900	0.21824600
C	2.25235600	1.16648800	-0.75448700
C	1.53100000	-0.25395100	1.04242100
C	3.41267000	0.40427200	-0.89203400
H	2.08677100	2.02017400	-1.39808000
C	2.68549200	-1.02804400	0.90732800
H	0.79341200	-0.54297500	1.78560100
C	3.65941200	-0.71105300	-0.06361500
H	4.14869700	0.70182400	-1.63099900
H	2.80781600	-1.89535600	1.54489400
C	-5.03101400	-2.61530600	1.16093600
C	-5.09048100	-2.21999300	-1.26321300
C	-6.52827400	-2.91253200	1.13070500
H	-4.47515400	-3.56618800	1.08071200
C	-6.58679500	-2.54076000	-1.23772000
H	-4.91050700	-1.45084300	-2.01940700
H	-7.10038900	-1.99244000	1.32193500
H	-6.89693200	-3.03600300	-2.16022300
C	5.33249200	-1.83314700	-1.54436700
C	5.21387900	-2.44577400	0.82997300
C	6.83713700	-2.08986100	-1.51747100
H	4.81895500	-2.74619600	-1.89528300
C	6.72246600	-2.70106500	0.79969500
H	4.94321300	-2.05147700	1.81371900
H	7.37463400	-1.15980500	-1.27980300
H	6.99560900	-3.52012400	1.46845200
N	4.85342800	-1.46026300	-0.19838800
N	-4.66407600	-1.71474300	0.04974700
O	7.16227300	-3.11281000	-0.52838200
O	-6.91045300	-3.47051300	-0.16218700
H	7.25850500	-1.78850400	1.09999800
H	4.67912600	-3.40211400	0.68520800
H	5.10809200	-1.03355600	-2.25214600
H	7.18951200	-2.48124200	-2.47414800
H	-6.79621400	-3.66954600	1.87068800
H	-4.76694400	-2.15630400	2.11477600
H	-4.52714000	-3.12478000	-1.55344200
H	-7.16266700	-1.61223500	-1.10913100
C	0.12464200	2.52819900	1.72685300
C	1.29925200	3.52020200	1.76557300
H	0.22071800	1.82884200	2.56793700
H	-0.81566700	3.07498300	1.88342100
C	1.32165100	4.34297600	3.06410900
H	2.24269700	2.97079700	1.65988600
H	1.23770600	4.18971900	0.89890700
H	2.16518500	5.04294000	3.07481600
H	0.40063500	4.92875500	3.18158600

H	1.41613600	3.69385600	3.94419000
C	-1.11377000	3.55668300	-0.84151300
H	-2.06741700	3.03653800	-0.68062400
H	-1.01550300	4.33897200	-0.07484000
O	-0.00542300	2.61587500	-0.74848300
C	-1.06277700	4.17286900	-2.23758400
C	-2.16645600	5.22074400	-2.45322900
H	-1.15187300	3.36732800	-2.97704300
H	-0.07431800	4.62681200	-2.38361300
H	-2.11093300	5.64742000	-3.46065800
H	-3.16393600	4.77984900	-2.33257800
H	-2.07792800	6.04700700	-1.73661100

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Input data to Scan for Model C

%nprocshared=20
%mem=2GB
%chk=C.chk
opt=modredundant b3lyp/6-31g* geom=connectivity

C

0 1

C	0.02193500	1.70181900	0.41583400
C	-1.22803100	0.80629000	0.36978100
C	-1.52491600	0.12643400	-0.82375100
C	-2.10093400	0.61498000	1.45208200
C	-2.63489100	-0.70846100	-0.93712100
H	-0.86280900	0.25051600	-1.67418100
C	-3.21941900	-0.21553400	1.35063500
H	-1.92732500	1.12256300	2.39409100
C	-3.51591400	-0.89794900	0.15244200
H	-2.79818200	-1.23226700	-1.87108900
H	-3.88399700	-0.30130800	2.20295000
C	1.28958600	0.85463900	0.21824600
C	2.25235600	1.16648800	-0.75448700

C	1.53100000	-0.25395100	1.04242100
C	3.41267000	0.40427200	-0.89203400
H	2.08677100	2.02017400	-1.39808000
C	2.68549200	-1.02804400	0.90732800
H	0.79341200	-0.54297500	1.78560100
C	3.65941200	-0.71105300	-0.06361500
H	4.14869700	0.70182400	-1.63099900
H	2.80781600	-1.89535600	1.54489400
C	-5.03101400	-2.61530600	1.16093600
C	-5.09048100	-2.21999300	-1.26321300
C	-6.52827400	-2.91253200	1.13070500
H	-4.47515400	-3.56618800	1.08071200
C	-6.58679500	-2.54076000	-1.23772000
H	-4.91050700	-1.45084300	-2.01940700
H	-7.10038900	-1.99244000	1.32193500
H	-6.89693200	-3.03600300	-2.16022300
C	5.33249200	-1.83314700	-1.54436700
C	5.21387900	-2.44577400	0.82997300
C	6.83713700	-2.08986100	-1.51747100
H	4.81895500	-2.74619600	-1.89528300
C	6.72246600	-2.70106500	0.79969500
H	4.94321300	-2.05147700	1.81371900
H	7.37463400	-1.15980500	-1.27980300
H	6.99560900	-3.52012400	1.46845200
N	4.85342800	-1.46026300	-0.19838800
N	-4.66407600	-1.71474300	0.04974700
O	7.16227300	-3.11281000	-0.52838200
O	-6.91045300	-3.47051300	-0.16218700
H	7.25850500	-1.78850400	1.09999800
H	4.67912600	-3.40211400	0.68520800
H	5.10809200	-1.03355600	-2.25214600
H	7.18951200	-2.48124200	-2.47414800
H	-6.79621400	-3.66954600	1.87068800
H	-4.76694400	-2.15630400	2.11477600
H	-4.52714000	-3.12478000	-1.55344200
H	-7.16266700	-1.61223500	-1.10913100
C	0.12464200	2.52819900	1.72685300
C	1.29925200	3.52020200	1.76557300
H	0.22071800	1.82884200	2.56793700
H	-0.81566700	3.07498300	1.88342100
C	1.32165100	4.34297600	3.06410900
H	2.24269700	2.97079700	1.65988600
H	1.23770600	4.18971900	0.89890700
H	2.16518500	5.04294000	3.07481600
H	0.40063500	4.92875500	3.18158600
H	1.41613600	3.69385600	3.94419000
C	-1.11377000	3.55668300	-0.84151300
H	-2.06741700	3.03653800	-0.68062400
H	-1.01550300	4.33897200	-0.07484000
O	-0.00542300	2.61587500	-0.74848300
C	-1.06277700	4.17286900	-2.23758400
C	-2.16645600	5.22074400	-2.45322900
H	-1.15187300	3.36732800	-2.97704300
H	-0.07431800	4.62681200	-2.38361300
H	-2.11093300	5.64742000	-3.46065800

H -3.16393600 4.77984900 -2.33257800
H -2.07792800 6.04700700 -1.73661100

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Input data to Scan for Model C in solvent

%nprocshared=20
%mem=2GB
%chk=Tph-scan-ethanol.chk
opt=modredundant b3lyp/6-31g* scrf=(solvent=ethanol) geom=connectivity

C-scan-ethanol

C	0.02194	1.70182	0.41583
C	-1.22803	0.80629	0.36978
C	-1.52492	0.12643	-0.82375
C	-2.10093	0.61498	1.45208
C	-2.63489	-0.70846	-0.93712
H	-0.86281	0.25052	-1.67418
C	-3.21942	-0.21553	1.35064
H	-1.92733	1.12256	2.39409
C	-3.51591	-0.89795	0.15244
H	-2.79818	-1.23227	-1.87109
H	-3.884	-0.30131	2.20295
C	1.28959	0.85464	0.21825
C	2.25236	1.16649	-0.75449
C	1.531	-0.25395	1.04242
C	3.41267	0.40427	-0.89203
H	2.08677	2.02017	-1.39808
C	2.68549	-1.02804	0.90733
H	0.79341	-0.54298	1.7856
C	3.65941	-0.71105	-0.06362
H	4.1487	0.70182	-1.631
H	2.80782	-1.89536	1.54489
C	-5.03101	-2.61531	1.16094
C	-5.09048	-2.21999	-1.26321
C	-6.52827	-2.91253	1.13071

H	-4.47515	-3.56619	1.08071
C	-6.5868	-2.54076	-1.23772
H	-4.91051	-1.45084	-2.01941
H	-7.10039	-1.99244	1.32194
H	-6.89693	-3.036	-2.16022
C	5.33249	-1.83315	-1.54437
C	5.21388	-2.44577	0.82997
C	6.83714	-2.08986	-1.51747
H	4.81896	-2.7462	-1.89528
C	6.72247	-2.70107	0.7997
H	4.94321	-2.05148	1.81372
H	7.37463	-1.1598	-1.2798
H	6.99561	-3.52012	1.46845
N	4.85343	-1.46026	-0.19839
N	-4.66408	-1.71474	0.04975
O	7.16227	-3.11281	-0.52838
O	-6.91045	-3.47051	-0.16219
H	7.25851	-1.7885	1.1
H	4.67913	-3.40211	0.68521
H	5.10809	-1.03356	-2.25215
H	7.18951	-2.48124	-2.47415
H	-6.79621	-3.66955	1.87069
H	-4.76694	-2.1563	2.11478
H	-4.52714	-3.12478	-1.55344
H	-7.16267	-1.61224	-1.10913
C	0.12464	2.5282	1.72685
C	1.29925	3.5202	1.76557
H	0.22072	1.82884	2.56794
H	-0.81567	3.07498	1.88342
C	1.32165	4.34298	3.06411
H	2.2427	2.9708	1.65989
H	1.23771	4.18972	0.89891
H	2.16519	5.04294	3.07482
H	0.40064	4.92876	3.18159
H	1.41614	3.69386	3.94419
C	-1.11377	3.55668	-0.84151
H	-2.06742	3.03654	-0.68062
H	-1.0155	4.33897	-0.07484
O	-0.00542	2.61588	-0.74848
C	-1.06278	4.17287	-2.23758
C	-2.16646	5.22074	-2.45323
H	-1.15187	3.36733	-2.97704
H	-0.07432	4.62681	-2.38361
H	-2.11093	5.64742	-3.46066
H	-3.16394	4.77985	-2.33258
H	-2.07793	6.04701	-1.73661

B 35 44 S 75 0.100000

Input data to Optimize for Model D

%nprocshared=20
%mem=2GB
%chk=Tph-opt.chk

opt b3lyp/6-31g* geom=connectivity

Tph-opt

0 1

C	-0.58518387	0.82317152	0.30972700
C	-1.24932447	2.21175119	0.27517692
C	-1.48121185	2.85710229	-0.94830048
C	-1.62077282	2.83122201	1.47483939
C	-2.07751408	4.12613916	-0.96789734
H	-1.20346577	2.38272374	-1.86742658
C	-2.21548218	4.09854843	1.45503221
H	-1.44961417	2.33547344	2.40830779
C	-2.44189576	4.74749765	0.23471732
H	-2.25389536	4.62106204	-1.89996923
H	-2.49666736	4.57073974	2.37312927
H	-2.89203435	5.71799527	0.22075707
C	-1.09787746	0.04785227	1.53567942
C	-2.23172858	-0.76917336	1.42704284
C	-0.43068666	0.16340065	2.76204671
C	-2.70896156	-1.45766429	2.54953363
H	-2.73451086	-0.86656321	0.48665678
C	-0.91040332	-0.52227954	3.88518571
H	0.44381544	0.77676257	2.84161728
C	-2.05369276	-1.32501326	3.78144084
H	-3.57365920	-2.08232364	2.46651074
H	-0.40364128	-0.43262519	4.82220466
C	-0.93936543	0.05228086	-0.97388736
C	-2.16028429	0.29487857	-1.61564256
C	-0.04417798	-0.88865217	-1.50036778
C	-2.48515345	-0.39684861	-2.78883837
H	-2.84532497	1.00881689	-1.20867551
C	-0.36886946	-1.58172589	-2.67452057
H	0.88687173	-1.07778832	-1.00622844
C	-1.58940451	-1.33545647	-3.31966792
H	-3.41788338	-0.20800976	-3.27947966
H	0.31491464	-2.30050226	-3.07805117
H	-1.83714314	-1.86404769	-4.21760272
C	-2.68124687	-4.45614478	5.69863256
C	-1.67850986	-5.40131161	6.38607321
H	-3.21850046	-4.99275590	4.94654303
H	-3.36858715	-4.07617118	6.42642340
H	-2.20739570	-6.21478072	6.83698777
H	-0.99086752	-5.78161979	5.65981740
H	-1.14063500	-4.86372664	7.13954238
O	-2.55122306	-2.00762750	4.93486933
O	0.83413628	0.97571213	0.39882573
C	2.70058392	1.45987432	-1.30659852
C	2.68925151	1.75141527	-2.81883456
H	2.97026318	0.43726240	-1.14158561
H	3.41204620	2.09736476	-0.82389659
H	3.66197209	1.56925329	-3.22599014
H	1.97632870	1.11425693	-3.29835652
H	2.41993202	2.77378860	-2.98243620
C	1.29779581	1.72154586	-0.72842284

O	0.55564207	2.59492527	-1.24979227
C	-1.92147548	-3.28432458	5.05008094
O	-0.74821099	-3.45024989	4.62342987

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Input data to Scan for Model D

%nprocshared=20
%mem=2GB
%chk=Tph-scan.chk
opt=modredundant b3lyp/6-31g* geom=connectivity

Tph-scan

0 1

C	1.22633200	0.02924700	-0.08704900
C	1.79308500	1.30300600	-0.74282000
C	3.15616200	1.40456500	-1.08677900
C	0.96939700	2.42499500	-0.94367700
C	3.66774400	2.58712100	-1.62981300
H	3.81752900	0.56975300	-0.90091200
C	1.48414800	3.60837800	-1.48403700
H	-0.07973800	2.37701400	-0.68001000
C	2.83505100	3.69312600	-1.83385700
H	4.72076300	2.64303300	-1.88720800
H	0.82716900	4.45992500	-1.63084900
H	3.23527200	4.60958700	-2.25623500
C	-0.31628700	-0.01944900	-0.14749100
C	-0.94690500	-0.32710600	-1.36764400
C	-1.12013800	0.25250200	0.96704700
C	-2.33537800	-0.35987200	-1.46524000
H	-0.35128800	-0.55156900	-2.24488100
C	-2.52014600	0.21807500	0.88878200
H	-0.65290800	0.49208000	1.91155400
C	-3.11636500	-0.08920800	-0.33621200
H	-2.82819800	-0.59793800	-2.40024900
H	-3.12406600	0.42639900	1.75821900
C	1.77281500	-1.30267600	-0.63071400
C	2.23908800	-1.43296200	-1.94802800
C	1.68708400	-2.45538900	0.16933300
C	2.63418600	-2.68221400	-2.44424300
H	2.30252300	-0.56278900	-2.59039500
C	2.08889000	-3.69837400	-0.32228900
H	1.30177900	-2.37504600	1.17962200
C	2.56691100	-3.81778700	-1.63343600
H	2.99705200	-2.76080300	-3.46432700
H	2.02465900	-4.57426700	0.31564800
H	2.87855000	-4.78418800	-2.01659300
C	-6.86653800	-0.13602400	-0.33419900
C	-8.04451700	0.09421100	0.61651900
H	-6.88791400	-1.14856900	-0.75850500
H	-6.90866700	0.54464100	-1.19474400
H	-8.99223500	-0.05384300	0.08909200
H	-8.00787800	-0.59778600	1.46338800

H	-8.02967000	1.11008600	1.02299900
O	-4.51134600	-0.16595300	-0.58339200
O	1.50366800	0.12596800	1.39803500
C	2.68308200	0.28386200	3.44813900
C	4.03344800	0.11727800	4.15078900
H	1.93000900	-0.39903100	3.86221800
H	2.28098700	1.29512700	3.59757500
H	3.93139900	0.31323700	5.22313100
H	4.42279900	-0.89711600	4.01963200
H	4.77630600	0.80773500	3.74039700
C	2.76351300	0.04181400	1.95471600
O	3.79645600	-0.20043600	1.32729800
C	-5.52601100	0.05286500	0.33673400
O	-5.34329600	0.35472400	1.51734000

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B 35 44 S 60 0.100000

Input data to Scan for Model D in solvent

%nprocshared=20
%mem=2GB
%chk=Tph-scan-ethanol.chk
opt=modredundant b3lyp/6-31g* scrf=(solvent=ethanol) geom=connectivity

Tph-scan-ethanol

0 1

C	1.22633200	0.02924700	-0.08704900
C	1.79308500	1.30300600	-0.74282000
C	3.15616200	1.40456500	-1.08677900
C	0.96939700	2.42499500	-0.94367700
C	3.66774400	2.58712100	-1.62981300
H	3.81752900	0.56975300	-0.90091200
C	1.48414800	3.60837800	-1.48403700
H	-0.07973800	2.37701400	-0.68001000
C	2.83505100	3.69312600	-1.83385700
H	4.72076300	2.64303300	-1.88720800
H	0.82716900	4.45992500	-1.63084900
H	3.23527200	4.60958700	-2.25623500
C	-0.31628700	-0.01944900	-0.14749100
C	-0.94690500	-0.32710600	-1.36764400
C	-1.12013800	0.25250200	0.96704700
C	-2.33537800	-0.35987200	-1.46524000
H	-0.35128800	-0.55156900	-2.24488100
C	-2.52014600	0.21807500	0.88878200
H	-0.65290800	0.49208000	1.91155400
C	-3.11636500	-0.08920800	-0.33621200
H	-2.82819800	-0.59793800	-2.40024900
H	-3.12406600	0.42639900	1.75821900
C	1.77281500	-1.30267600	-0.63071400
C	2.23908800	-1.43296200	-1.94802800
C	1.68708400	-2.45538900	0.16933300
C	2.63418600	-2.68221400	-2.44424300
H	2.30252300	-0.56278900	-2.59039500

C	2.08889000	-3.69837400	-0.32228900
H	1.30177900	-2.37504600	1.17962200
C	2.56691100	-3.81778700	-1.63343600
H	2.99705200	-2.76080300	-3.46432700
H	2.02465900	-4.57426700	0.31564800
H	2.87855000	-4.78418800	-2.01659300
C	-6.86653800	-0.13602400	-0.33419900
C	-8.04451700	0.09421100	0.61651900
H	-6.88791400	-1.14856900	-0.75850500
H	-6.90866700	0.54464100	-1.19474400
H	-8.99223500	-0.05384300	0.08909200
H	-8.00787800	-0.59778600	1.46338800
H	-8.02967000	1.11008600	1.02299900
O	-4.51134600	-0.16595300	-0.58339200
O	1.50366800	0.12596800	1.39803500
C	2.68308200	0.28386200	3.44813900
C	4.03344800	0.11727800	4.15078900
H	1.93000900	-0.39903100	3.86221800
H	2.28098700	1.29512700	3.59757500
H	3.93139900	0.31323700	5.22313100
H	4.42279900	-0.89711600	4.01963200
H	4.77630600	0.80773500	3.74039700
C	2.76351300	0.04181400	1.95471600
O	3.79645600	-0.20043600	1.32729800
C	-5.52601100	0.05286500	0.33673400
O	-5.34329600	0.35472400	1.51734000

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B 35 44 S 75 0.100000
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1. Beyer MK. The mechanical strength of a covalent bond calculated by density functional theory. J Chem Phys 2000; 112: 7307–7312.

2. Wang C, Yang C, Wu J, Wang Z, Yang K. How external forces affect the degradation properties of perfluorooctanoic acid in mechanochemical degradation: a DFT study. RSC Mechanochemistry. 2025;2(5):692-705.

3. Li ZA, Toivola R, Ding F, Yang J, Lai PN, Howie T, Georgeson G, Jang SH, Li X, Flinn BD, Jen AK. Highly Sensitive Built-In Strain Sensors for Polymer Composites: Fluorescence Turn-On Response through Mechanochemical Activation. Advanced Materials 2016 May 17;28(31):6592-7.