

Supporting Information for

A Novel Partitioning Scheme for the Application of the Distortion/Interaction – Activation Strain Model to Intramolecular Reactions

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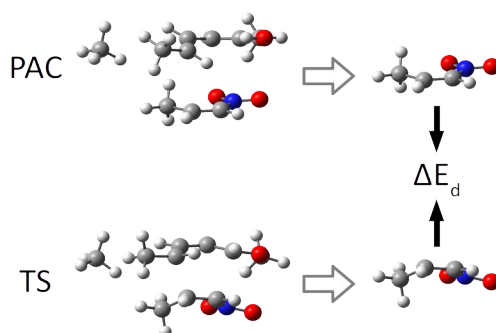
1. Testing the validity of the $\Delta E_i \approx \Delta E_i$ (R1-R2) approximation

As explained in the main text, we use a 2-reacting/1-spectator model system to corroborate that the total interaction energy can be approximated as just the interaction between the two reagents. In this case, we studied the Diels-Alder reaction between 1-methoxy-1,3-pentadiene and 1-nitro-1-propylene in the presence of methane (see Fig. 4 of main text and below). Herein is described the way to calculate all the energy contributions:

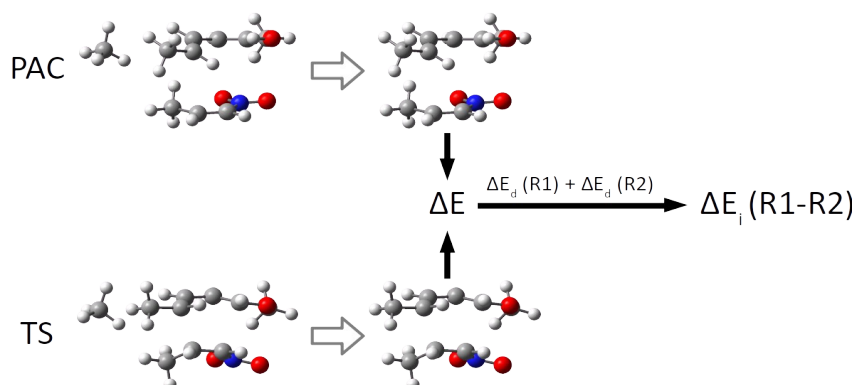


1) Optimize the pre-association complex (or PAC, in which the three molecules are linked by van der Waals forces) and the transition state, and obtain $\Delta E^\ddagger$ by difference. We use the pre-association complex as reference and not the three reagents at infinite distance because we want to extrapolate this model system to intramolecular reactions, and in that case the reaction centers cannot be at infinite distance.

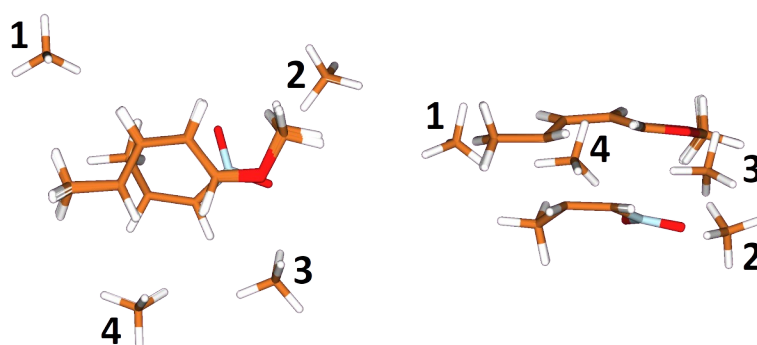
2) The **individual** ΔE_d for a given molecule is calculated by erasing the two other molecules and performing a single-point calculation. Add the values for the three molecules to get the **total** ΔE_d . Finally, the **total** ΔE_i can be extracted by calculating $\Delta E_d - \Delta E^\ddagger$.



3) Computing the **pair-wise** ΔE_i between two molecules requires erasing the third molecule and performing a single-point calculation, to obtain a physically meaningless ΔE . Subtracting this value to the sum of the two ΔE_d yields the pair-wise ΔE_i . The difference between the total ΔE_i and the sum of the three pair-wise yields the non-local ΔE_{disp} term.



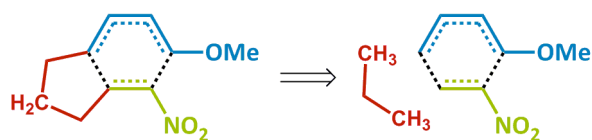
We tested the effect of placing the methane molecule at different positions around the diene-dienophile couple (see below), changing the NO₂ by a CF₃ (to reduce the polarization of the electron density), and increasing the basis set to the augmented aug-cc-pVDZ (to more accurately describe long-range interactions).



Positions above the diene or below the dienophile were not tested, as they do not represent plausible positions for a connector (at those places it will not be able to bind the two reagents). As the results were very similar for all situations, we selected position 1 for the rest of the systems, as it is the most similar to the position of the connector in our molecules. The results displayed in the table below (where R1 accounts for the pentadiene, R2 for the propylene and C for the methane) show that, as there is no strong interaction between the spectator and the two reacting molecules, the pair-wise interaction energy can recover more than 90% of the total interaction energy.

Entry	S1	S2	S3	S4	S5	S6
C	Methane (position 1)	Methane (position 2)	Methane (position 3)	Methane (position 4)	Methane (position 1)	Methane (position 1)
EWG	NO ₂	NO ₂	NO ₂	NO ₂	NO ₂	CF ₃
Basis set	cc-pVDZ	cc-pVDZ	cc-pVDZ	cc-pVDZ	aug-cc-pVDZ	cc-pVDZ
$\Delta E^{\ddagger}$	17.42	16.80	17.36	17.17	15.91	19.60
ΔE_d (R1)	15.49	15.47	15.56	15.53	15.62	16.74
ΔE_d (R2)	13.32	13.16	13.44	13.16	13.01	13.08
ΔE_d (C)	0.00	0.00	0.02	0.00	0.00	0.00
ΔE_d	28.81	28.63	29.02	28.70	28.64	29.82
ΔE_i (R1-R2)	-11.30	-11.10	-11.40	-11.14	-12.73	-10.72
ΔE_i (R1-C)	0.15	-0.02	-0.03	-0.11	0.16	0.36
ΔE_i (R2-C)	-0.02	-0.01	0.05	0.11	0.04	0.07
ΔE_{disp}	-0.23	-0.69	-0.29	-0.39	-0.20	0.08
ΔE_i	-11.39	-11.82	-11.67	-11.53	-12.73	-10.22
ΔE_i (R1-R2) / ΔE_i	99.2%	93.9%	97.7%	96.6%	100.0%	105.0%

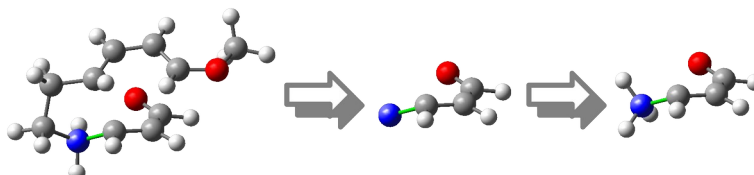
Other plausible fragmentation scheme in the original molecule would have led to 1-methoxy-1,3-butadiene, 1-nitroethylene and propane (see figure below). We tested this possibility, and also the Diels-Alder reaction of this diene-dienophile couple in the presence of 1,3-propanediol. Only for the case of 1,3-propanediol, we also placed it in position 3, so it can interact via hydrogen bonding with NO₂ and OMe. These results show that the differences in the two fragmentation schemes (entries S1 and S7) are rather small, and that this approximation fails if there exists a strong interaction between the spectator/connector and the reaction centers (entries S8 and S9).



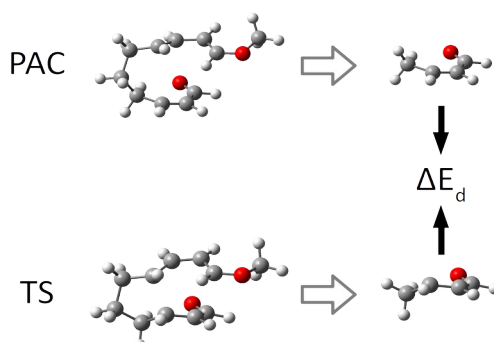
Entry	S7	S8	S9	S10
C	Propane (position 1)	1,3-Propanediol (position 1)	1,3-Propanediol (position 3)	1,3-Propanediol (position 3)
EWG	NO ₂	NO ₂	NO ₂	NO ₂
Basis set	cc-pVDZ	cc-pVDZ	cc-pVDZ	aug-cc-pVDZ
$\Delta E^\ddagger$	11.89	12.25	12.66	11.35
ΔE_d (R1)	11.95	12.80	10.90	10.98
ΔE_d (R2)	10.14	10.11	10.26	10.02
ΔE_d (C)	0.00	0.02	0.80	0.83
ΔE_d	22.09	22.93	21.96	21.83
ΔE_i (R1-R2)	-10.06	-10.65	-7.75	-8.88
ΔE_i (R1-C)	0.04	-0.15	1.29	1.10
ΔE_i (R2-C)	-0.03	0.03	-1.41	-1.19
ΔE_{disp}	-0.15	0.09	-1.43	-1.51
ΔE_i	-10.20	-10.68	-9.30	-10.48
ΔE_i (R1-R2) / ΔE_i	98.6%	99.7%	83.3%	84.7%

2. Procedure to divide molecule fragments

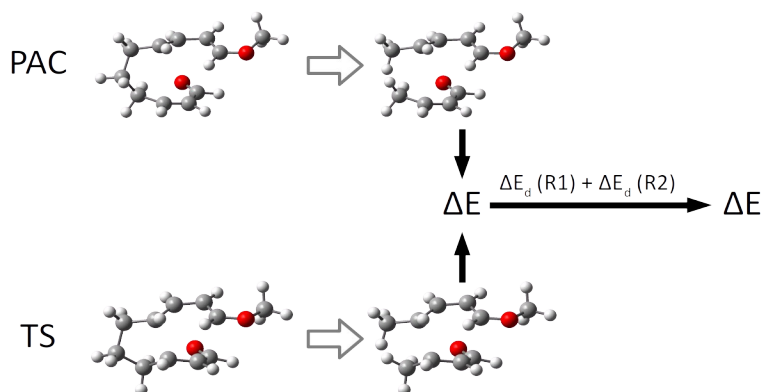
Our method, applied to the Diels-Alder reaction of 1,3,8-nonatrienes, requires replacing the alkyl chain that works as connector to methyl groups. The optimal way to do this involves deleting all the atoms of the molecule except those of the fragment whose ΔE_d will be calculated (or fragments, for ΔE_i) and the carbon atom(s) directly attached to it (see image below, atom in blue). Then, hydrogen atoms are added to build the methyl groups, and their positions are optimized, keeping frozen the rest of the molecule. This allows the description of the distortion of the bond that links the connector and the reaction center(s) (image below, bond in green).



The procedure to calculate the distortion and interaction energies is very similar to the one used for the methane model previously described. First, calculate ΔE_d (R1) and ΔE_d (R2) by erasing the rest of the molecule, this is the connector and the other reaction center, and replacing it using the procedure listed above. We still refer the initial structure as "PAC" in the pictures below, although it is not a complex but a single molecule.



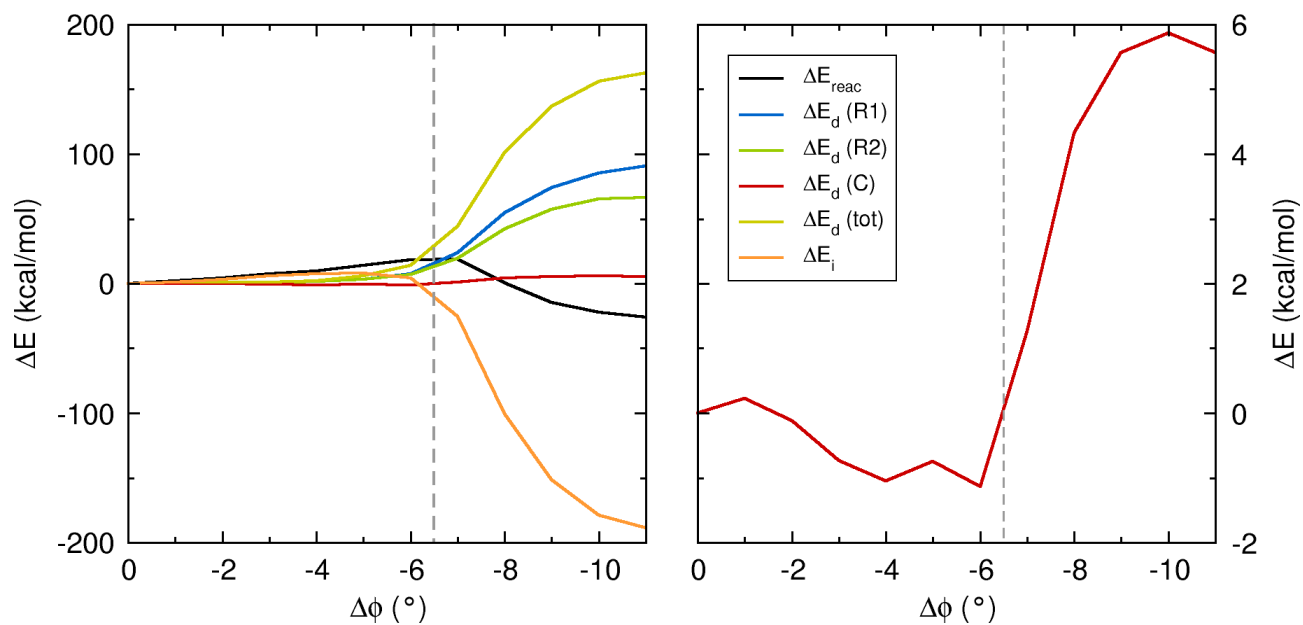
Second, ΔE_i is calculated by erasing the corresponding part of the connector, obtaining ΔE and then using the previously found values for ΔE_d (R1) and ΔE_d (R2):



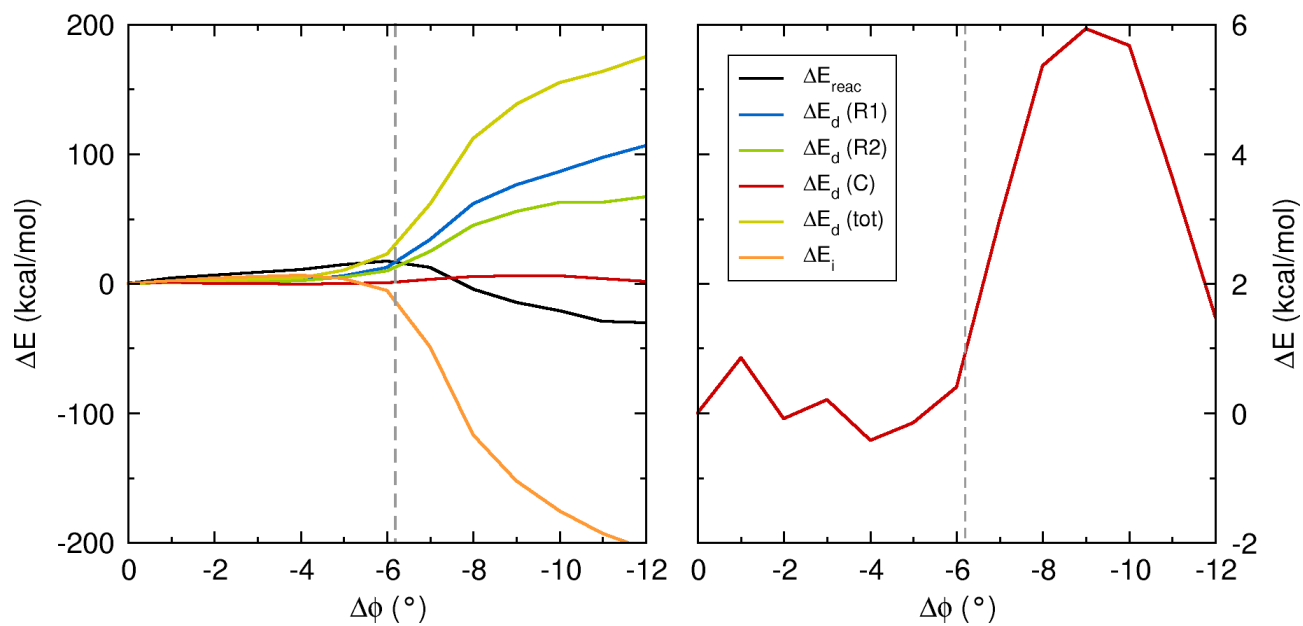
Finally, ΔE_d (C) is given by $\Delta E^\ddagger - \Delta E_d$ (R1) - ΔE_d (R2) - ΔE_i .

3. IRC analysis of structures 1-4 and 6-12

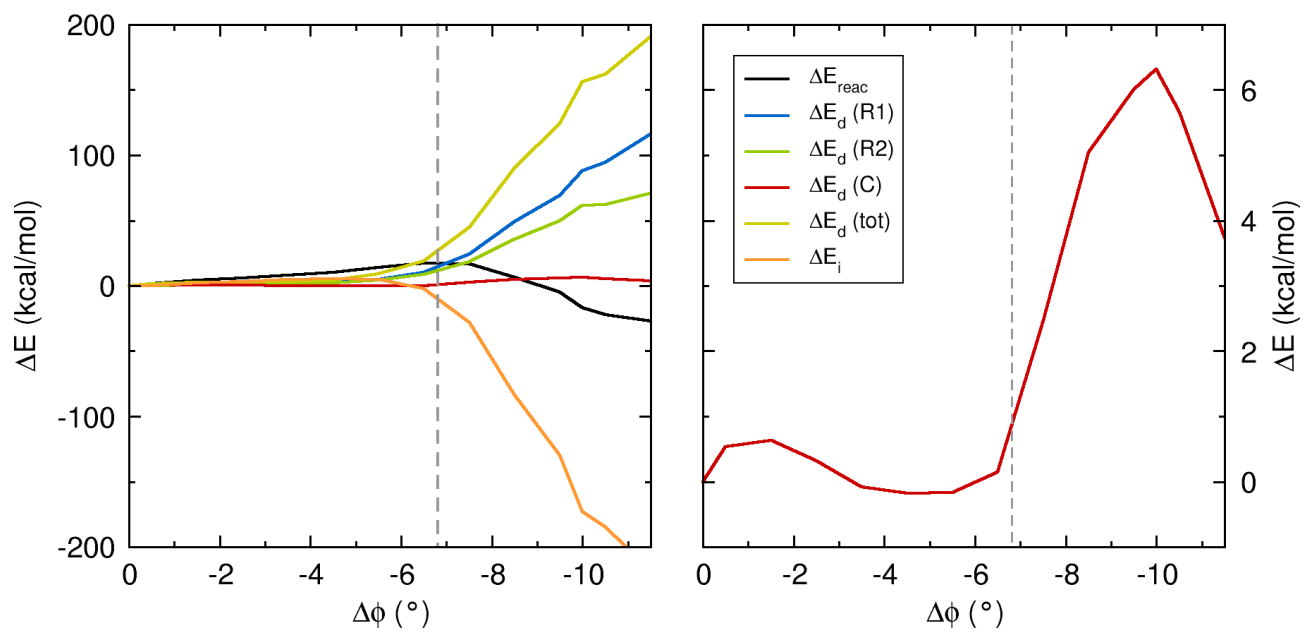
Entry 1 (EWG=Br, 3-carbon connector)



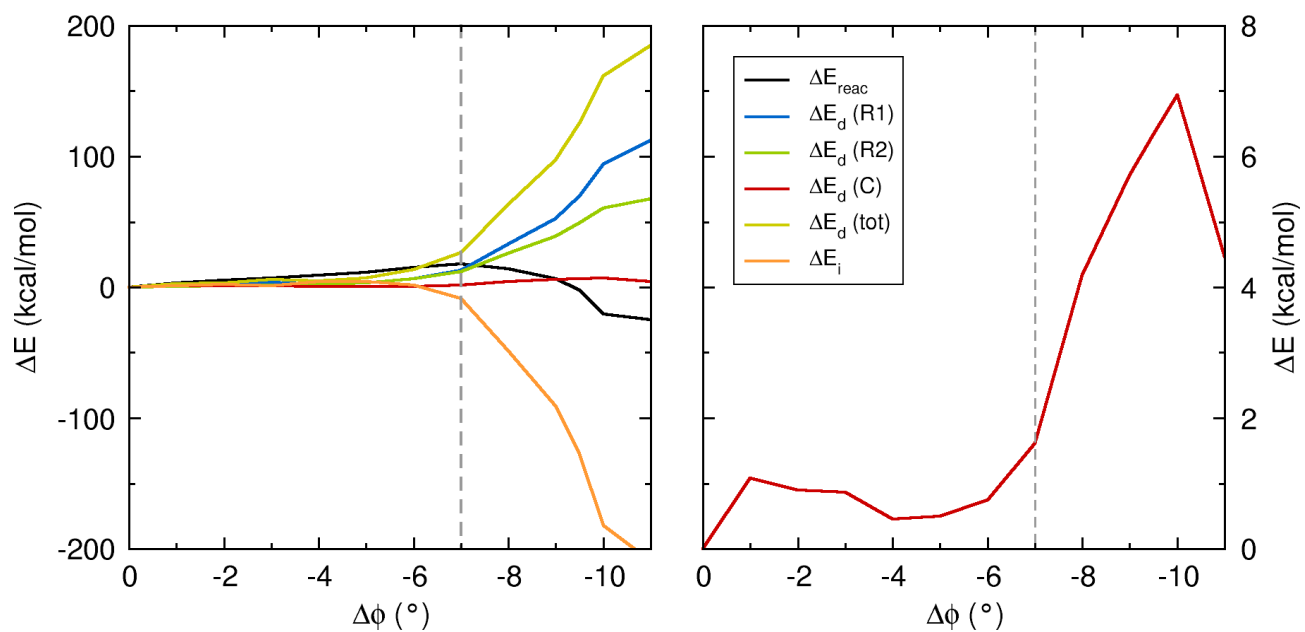
Entry 2 (EWG=CF₃, 3-carbon connector)



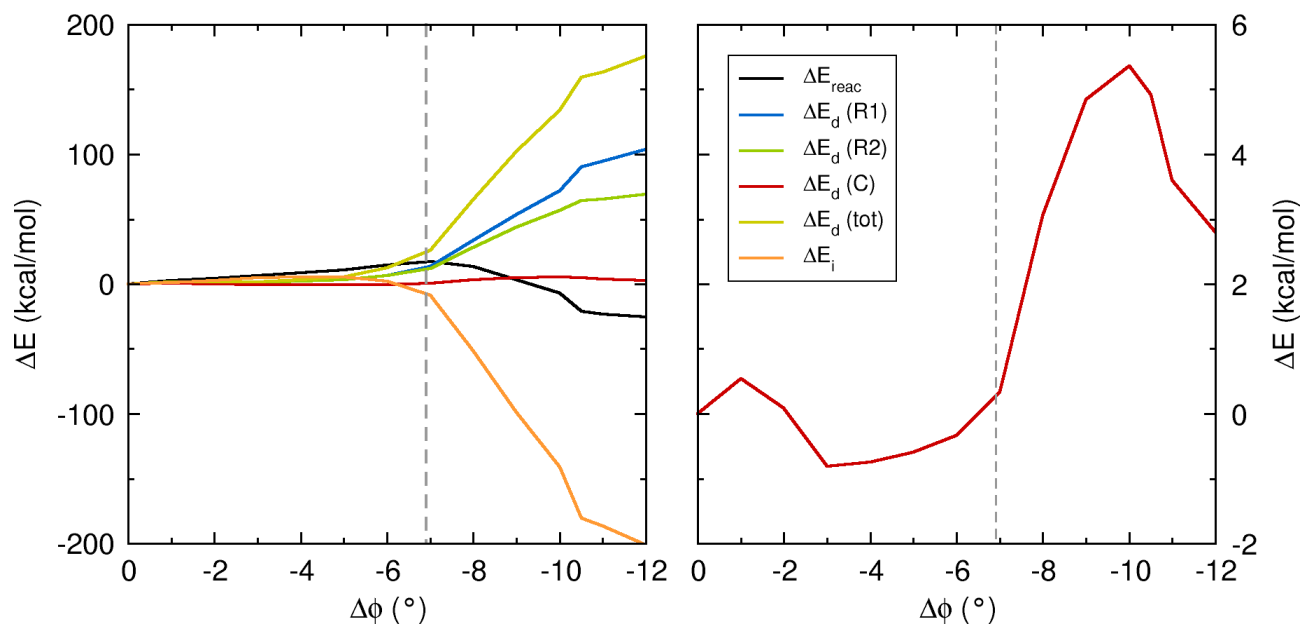
Entry 3 (EWG=CO₂Me, 3-carbon connector)



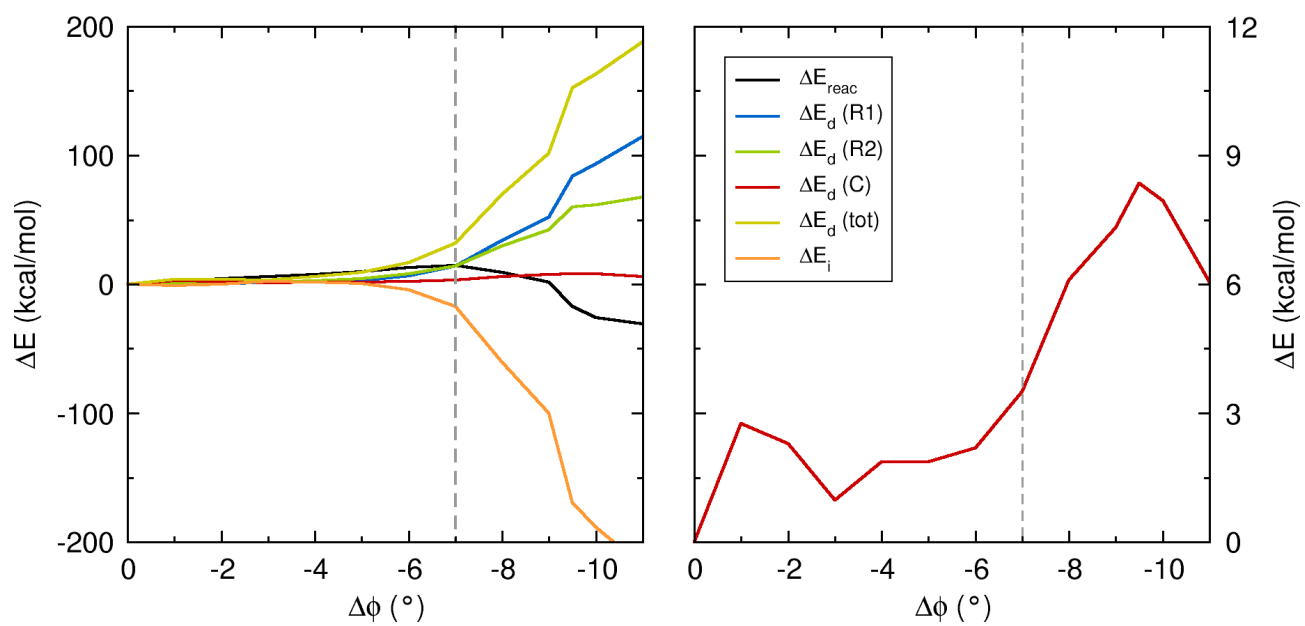
Entry 4 (EWG=COMe, 3-carbon connector)



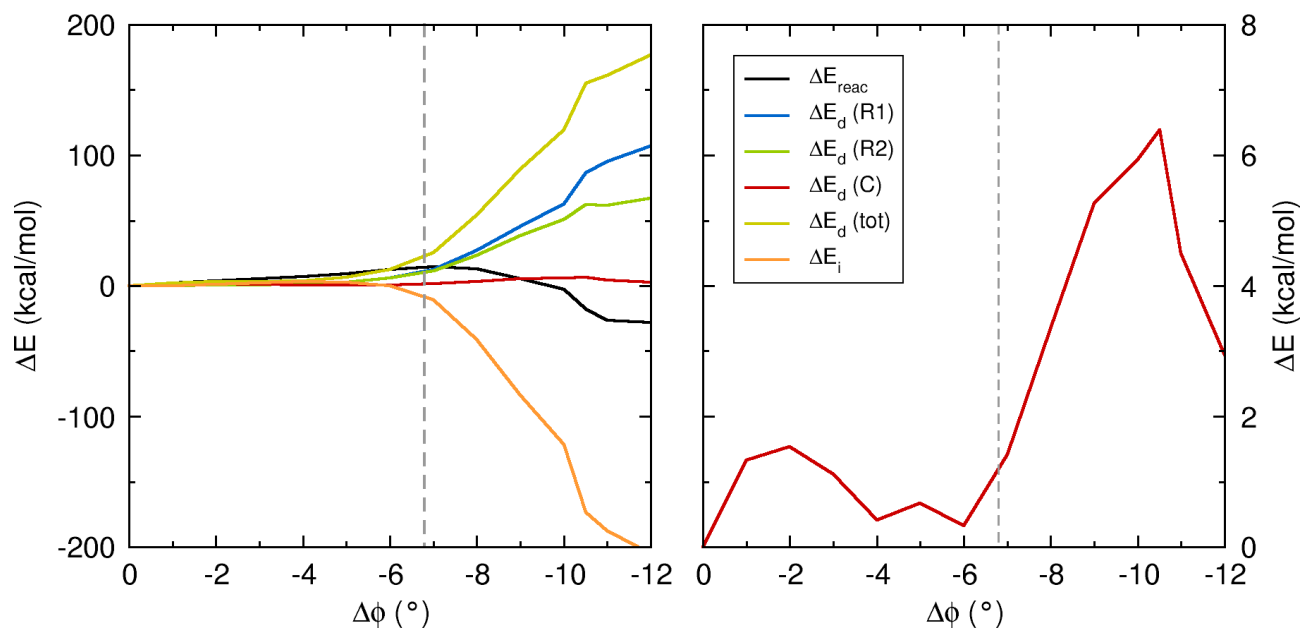
Entry 6 (EWG=SO₂Me, 3-carbon connector)



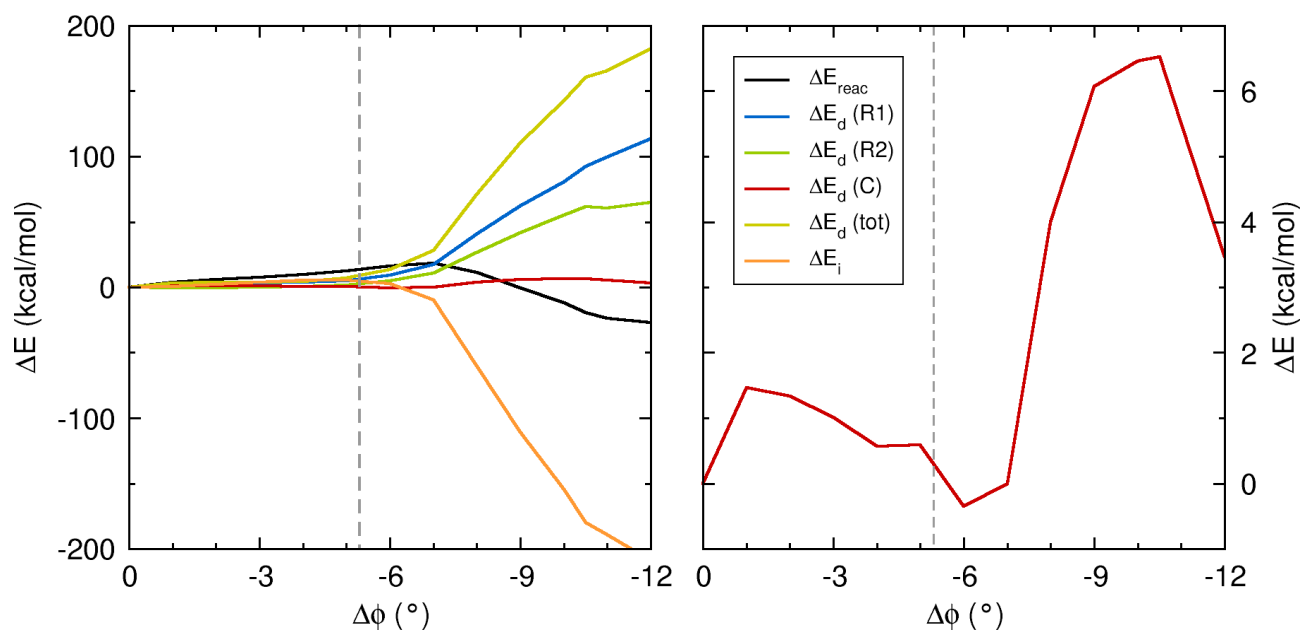
Entry 7 (EWG=NO₂, 3-carbon connector)



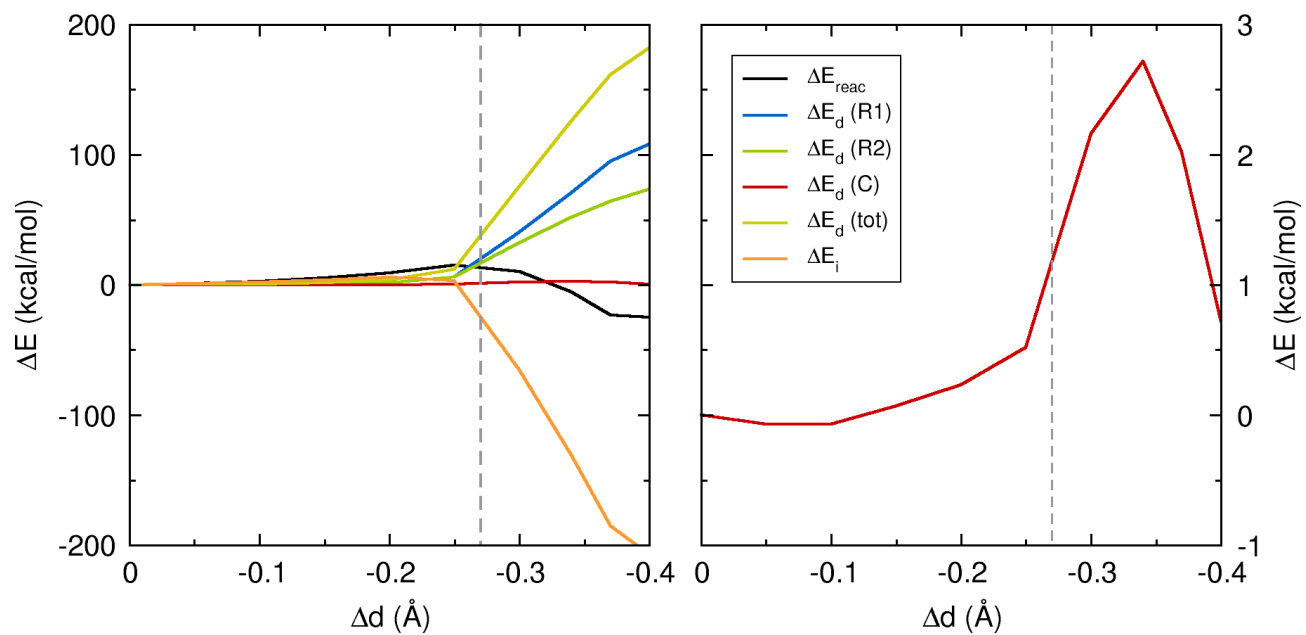
Entry 8 (EWG=SO₂F, 3-carbon connector)



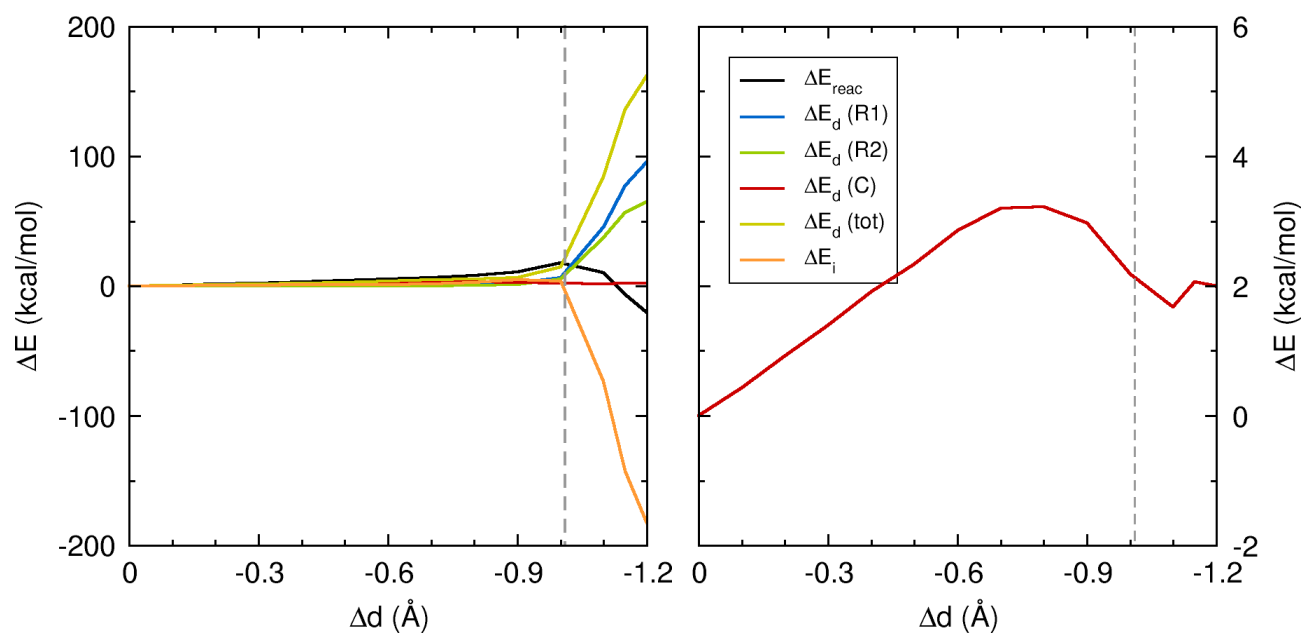
Entry 9 (EWG=(*p*-CHO)Ph, 3-carbon connector)



Entry 10 (EWG=CHO, 4-carbon connector)

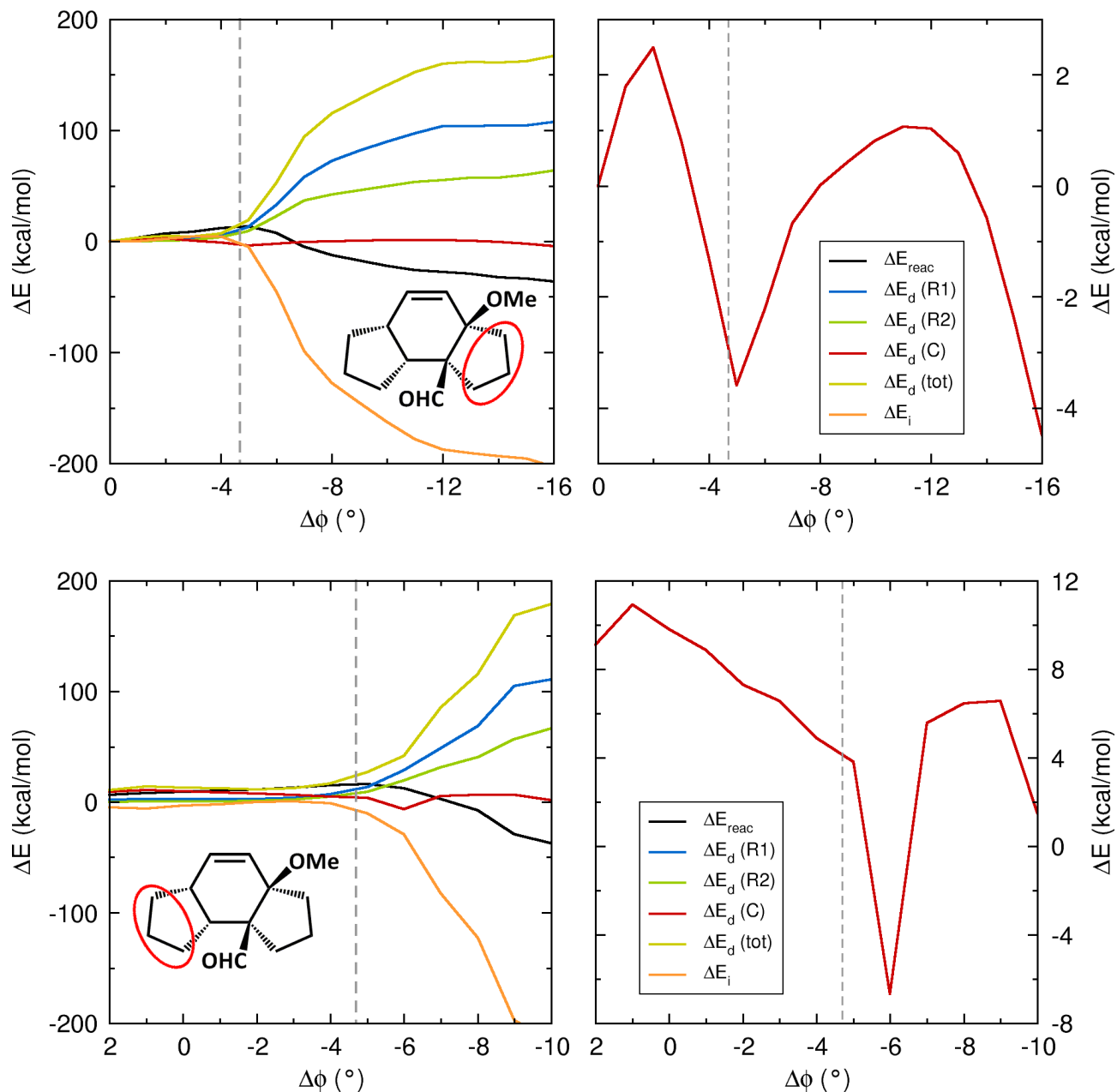


Entry 11 (EWG=CHO, 5-carbon connector)



Entry 12 (EWG=CHO, 2x 3-carbon connector)

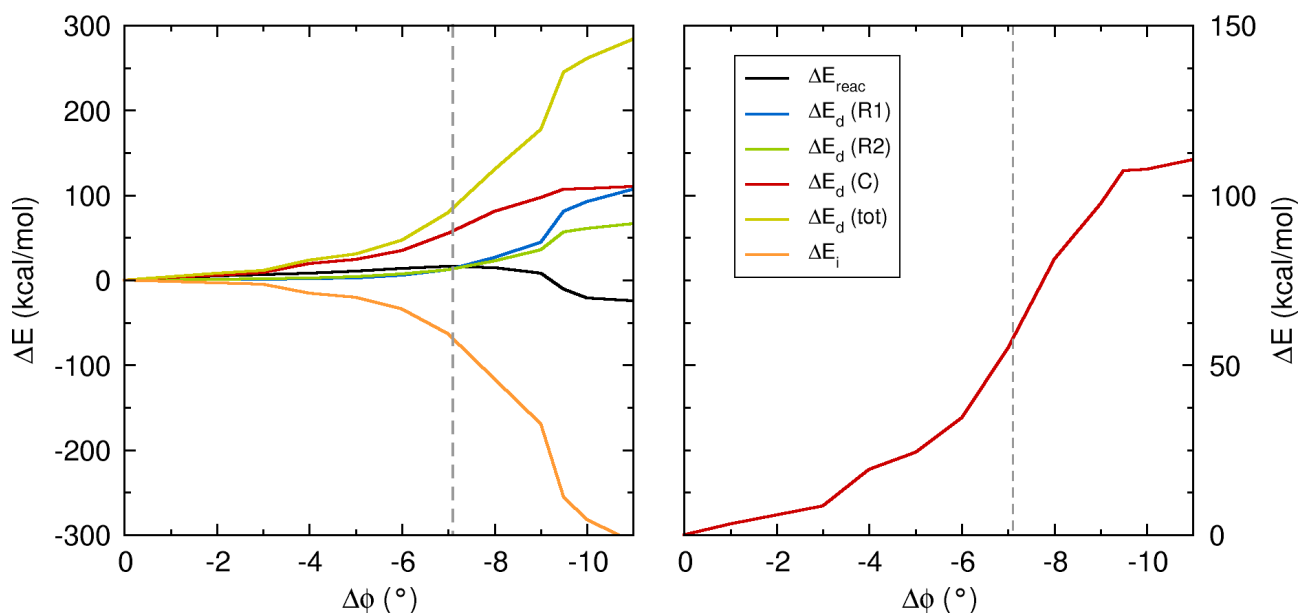
For this situation, one might project the IRC onto the angle compression of the two connectors separately. As shown in the pictures below, the results are clearly different for each connector, which shows the difficulty of this procedure to accurately describe transannular reactions.



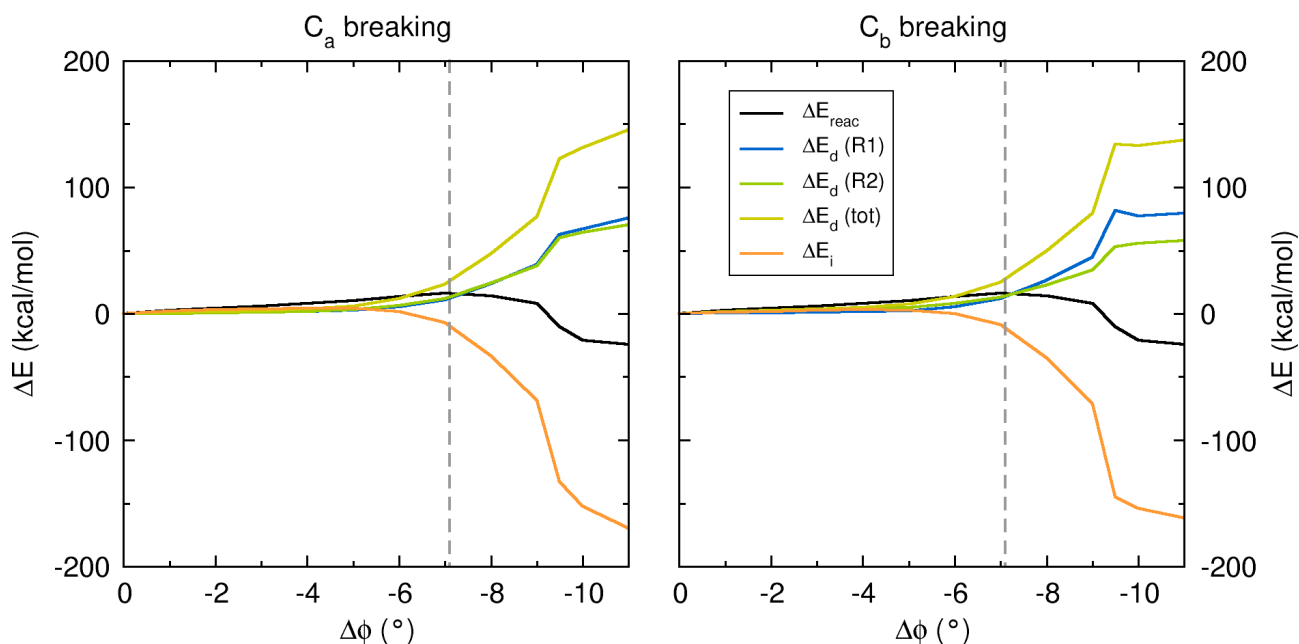
In the latter case, the selected angle experiences an increase of 2° before it starts decreasing, which explains why the x axis does not start in 0. The initial $0^\circ \rightarrow 2^\circ$ is not shown.

4. IRC analysis using former approaches

We carried out the IRC analysis for entry 5 (EWG=CHO) using Houk's and Bickelhaupt's approaches, to compare how do they compare in relation to our approach. For Houk's approach, we used the substitution scheme proposed in entry 5b of the main text, this is replacing the diene and the dienophile by two vinyl groups:

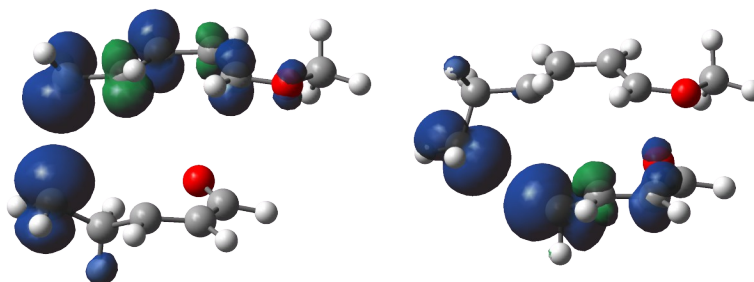


As it was discussed in the main text, this approach widely overestimates the value of ΔE_d (C), and therefore it cannot provide an accurate value of ΔE_i . For Bickelhaupt's approach, we analyzed the effect of cleaving the two inert $\text{CH}_2\text{-CH}_2$ bonds of the connector separately:



Also discussed in the main text, the C_a cleavage leads to an underestimation of ΔE_d (R1), while C_b cleavage provides results more similar to our approach. We analyzed the spin density of the fragments at the

position of the TS (shown below, C_a cleavage at left and C_b cleavage at right; each fragment corresponds to a separate calculation), observing that the delocalization of the unpaired electron over the diene for C_a cleavage is larger than its delocalization over the dienophile for C_b cleavage. This delocalization causes a spurious perturbation of the electron density of the diene, leading to less reliable results.



5. Geometries of minima and TS

5.1. Structures for the methane model

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entryS1.PAC.xyz

C	0.248784	-1.375415	0.485638
H	0.477443	-1.112502	1.520247
C	-1.161229	-1.361488	0.080509
H	-1.885936	-1.590412	0.871454
C	1.237116	-1.756185	-0.347107
H	1.023120	-2.092388	-1.365309
C	-1.634278	-1.096117	-1.147084
H	-0.924309	-0.809990	-1.931950
C	-0.546263	1.956147	-0.861283
H	-1.184609	2.057294	-1.744378
C	0.721804	1.648646	-1.142822
H	1.123583	1.494904	-2.140799
N	1.739838	1.450712	-0.126425
O	2.832840	1.103363	-0.525582
O	1.453803	1.631888	1.044820
C	2.970142	-1.457721	1.209783
H	2.697849	-0.415407	1.432195
H	4.060071	-1.561867	1.220353
H	2.523251	-2.130560	1.960980
O	2.552551	-1.827253	-0.092938
C	-1.183980	2.168027	0.475203
H	-1.031545	1.284088	1.110682
H	-0.710062	3.008275	1.001642
H	-2.256913	2.361456	0.361391
C	-3.080652	-1.167289	-1.531876
H	-3.444474	-0.200884	-1.918455
H	-3.243208	-1.907871	-2.331153
H	-3.704822	-1.450049	-0.672888
C	-4.584116	0.030082	1.677608
H	-4.571098	-1.061698	1.797298
H	-3.560223	0.391679	1.514395
H	-5.207132	0.294407	0.813706
H	-4.997364	0.490431	2.583748

33

entryS1.TS.xyz

C	-0.323623	-1.522397	-0.187209
H	-0.543467	-1.797492	-1.218056
C	1.006497	-1.262196	0.163919

H	1.766764	-1.413697	-0.608046
C	-1.365277	-1.245821	0.681147
H	-1.213036	-1.187325	1.758152
C	1.392255	-0.599533	1.330499
H	0.747964	-0.708680	2.206848
C	0.637304	1.263736	0.958888
H	0.962853	1.583454	1.954346
C	-0.757876	1.168468	0.886407
H	-1.400736	1.258908	1.757133
N	-1.502834	1.316682	-0.316626
O	-2.712155	1.466311	-0.202941
O	-0.930430	1.245638	-1.403077
C	-3.028493	-1.378444	-0.985980
H	-2.504318	-0.622969	-1.588051
H	-4.105772	-1.191270	-1.018187
H	-2.810362	-2.391867	-1.359383
O	-2.661215	-1.276758	0.389329
C	1.507607	1.783256	-0.164697
H	1.402463	1.178200	-1.070031
H	1.204256	2.808730	-0.425170
H	2.559268	1.806678	0.152353
C	2.853499	-0.424109	1.657118
H	3.030492	0.487598	2.248581
H	3.222762	-1.274608	2.250913
H	3.459238	-0.361867	0.741412
C	4.363635	-0.557193	-1.987059
H	4.208101	-1.570064	-1.592839
H	3.434667	0.021750	-1.903187
H	5.156482	-0.060141	-1.413445
H	4.659457	-0.618232	-3.041658

33

entryS1.adduct.xyz

C	-0.140890	-1.118776	1.086377
H	-0.666170	-2.068541	0.997758
C	1.191129	-1.038792	1.049259
H	1.811319	-1.931069	0.930708
C	-0.887089	0.175674	1.273909
H	-0.617228	0.566100	2.274887
C	1.837951	0.318772	1.130925
H	1.615032	0.742535	2.128690
C	1.167112	1.271105	0.098019
H	1.490178	2.295542	0.337435
C	-0.378572	1.237006	0.280698
H	-0.767061	2.217769	0.572627

N	-1.064380	0.990139	-1.042079
O	-1.379996	1.969526	-1.677932
O	-1.222011	-0.157125	-1.405132
C	-2.966268	-1.043309	1.018857
H	-2.684267	-1.530963	0.071819
H	-4.034756	-0.797808	0.989267
H	-2.788234	-1.735208	1.860408
O	-2.296554	0.185528	1.190919
C	1.617353	0.960558	-1.332030
H	1.403378	-0.086155	-1.593874
H	1.104418	1.609661	-2.055158
H	2.695191	1.139355	-1.435940
C	3.354719	0.257001	0.982504
H	3.796751	1.264205	0.951371
H	3.797492	-0.283125	1.831433
H	3.643228	-0.273066	0.063046
C	0.805528	-3.015244	-1.902950
H	0.625024	-3.715402	-1.076094
H	0.084067	-2.189211	-1.850303
H	1.826442	-2.617492	-1.821861
H	0.698503	-3.545485	-2.857921

33

entryS2.PAC.xyz

C	-0.732521	1.354992	-0.690460
H	-0.104533	1.178324	-1.565982
C	-2.158387	1.032685	-0.809316
H	-2.576710	1.092350	-1.821449
C	-0.199570	1.900061	0.420793
H	-0.821947	2.157126	1.281927
C	-2.979405	0.664965	0.186269
H	-2.564821	0.550382	1.194376
C	-1.248245	-2.034884	0.385474
H	-2.155524	-2.276671	0.946980
C	-0.265211	-1.532010	1.136644
H	-0.323489	-1.346704	2.205710
N	1.021417	-1.130711	0.597953
O	1.778283	-0.579342	1.372729
O	1.273605	-1.360503	-0.572434
C	1.998125	1.979961	-0.401548
H	1.996818	0.916507	-0.684746
H	2.985953	2.252869	-0.015455
H	1.754918	2.598357	-1.282109
O	1.079039	2.234458	0.646691
C	4.759787	-0.423604	-0.654620

H	4.519992	-0.124316	-1.683785
H	3.831931	-0.641565	-0.111787
H	5.300978	0.389765	-0.153475
H	5.395196	-1.318296	-0.679087
C	-4.443747	0.393808	0.021825
H	-5.049153	1.077911	0.637481
H	-4.701920	-0.628906	0.342740
H	-4.753924	0.513967	-1.025844
C	-1.261550	-2.295197	-1.087201
H	-0.532767	-3.077610	-1.344424
H	-0.952089	-1.396523	-1.637655
H	-2.261906	-2.603556	-1.412134

33

entryS2.TS.xyz

C	-0.480085	-1.440946	0.852637
H	0.205574	-1.474575	1.698401
C	-1.777484	-0.959039	1.064888
H	-2.049191	-0.697897	2.092224
C	-0.003851	-1.693384	-0.422444
H	-0.676786	-1.897843	-1.254500
C	-2.644065	-0.563780	0.044238
H	-2.545278	-1.068292	-0.920379
C	-1.648676	1.073936	-0.665853
H	-2.419584	1.187840	-1.434787
C	-0.436484	0.643327	-1.219098
H	-0.344314	0.310238	-2.248616
N	0.837287	0.931178	-0.659014
O	1.814217	0.702344	-1.362852
O	0.920218	1.355050	0.492016
C	2.257583	-1.770246	0.240576
H	2.148761	-0.785812	0.716760
H	3.213548	-1.817652	-0.289192
H	2.200858	-2.570432	0.995840
O	1.251214	-1.969287	-0.752764
C	4.427859	1.105628	1.034380
H	4.115550	0.732916	2.019558
H	3.550767	1.197613	0.381603
H	5.153971	0.409280	0.593611
H	4.901473	2.088053	1.158914
C	-4.047164	-0.116470	0.365601
H	-4.740327	-0.971646	0.353699
H	-4.417957	0.614146	-0.369737
H	-4.097967	0.346407	1.361777
C	-1.752450	2.077793	0.461147

H	-1.239386	3.008847	0.177218
H	-1.269786	1.713936	1.373066
H	-2.807219	2.310850	0.660019

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entryS2.adduct.xyz

C	-0.619214	1.651250	-0.557784
H	-0.130958	2.283345	-1.297343
C	-1.905065	1.306339	-0.655784
H	-2.524258	1.646867	-1.489314
C	0.123226	1.137764	0.647736
H	-0.347313	1.598070	1.538648
C	-2.490808	0.391862	0.388492
H	-2.469353	0.925677	1.357717
C	-1.565319	-0.848172	0.558090
H	-1.891488	-1.382574	1.463079
C	-0.104927	-0.376329	0.819396
H	0.239038	-0.681249	1.812797
N	0.853460	-1.095066	-0.098868
O	1.343382	-2.117606	0.324947
O	1.043210	-0.636145	-1.205237
C	2.150346	2.110449	-0.259728
H	2.061005	1.617550	-1.240868
H	3.209484	2.150889	0.021836
H	1.759590	3.140966	-0.319733
O	1.513422	1.364065	0.755418
C	4.132426	-0.758030	0.003742
H	4.873463	-0.044722	-0.381642
H	3.534528	-1.161205	-0.823508
H	3.459498	-0.251871	0.709465
H	4.648246	-1.579614	0.516758
C	-3.940754	0.017620	0.099351
H	-4.579698	0.910712	0.149794
H	-4.319475	-0.713746	0.828679
H	-4.050040	-0.413014	-0.906444
C	-1.691699	-1.812468	-0.624839
H	-1.003557	-2.661781	-0.513629
H	-1.462062	-1.305097	-1.573153
H	-2.710253	-2.217970	-0.674120

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entryS3.PAC.xyz

C	0.226585	-0.921285	-1.336809
H	-0.077427	-0.312746	-2.190477
C	1.665466	-1.085121	-1.101600

H	2.304212	-1.031056	-1.991596
C	-0.701978	-1.527584	-0.571950
H	-0.416111	-2.193781	0.246017
C	2.259006	-1.281655	0.085397
H	1.637804	-1.284348	0.988721
C	1.366948	1.719836	0.873749
H	2.087719	1.493336	1.665312
C	0.106144	1.411686	1.187497
H	-0.215574	0.963429	2.124044
N	-1.010838	1.616169	0.283815
O	-2.096066	1.226238	0.670936
O	-0.815275	2.151380	-0.793024
C	-2.552600	-0.674962	-1.741479
H	-2.235889	0.374231	-1.646485
H	-3.643118	-0.736713	-1.664992
H	-2.222120	-1.078291	-2.713433
O	-2.038490	-1.463607	-0.681930
C	-1.696844	-1.629269	2.710582
H	-2.024346	-2.590241	2.292462
H	-2.165726	-1.480917	3.691892
H	-1.994998	-0.823789	2.026489
H	-0.604085	-1.641001	2.831442
C	1.901039	2.320016	-0.387938
H	1.488254	3.327679	-0.539190
H	1.585197	1.726024	-1.255847
H	2.995340	2.372274	-0.353298
C	3.729082	-1.501720	0.273230
H	4.162111	-0.759008	0.963096
H	4.265301	-1.437602	-0.684171
H	3.930887	-2.492401	0.711375

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entryS3.TS.xyz

C	-0.240414	-0.693980	1.600646
H	0.037366	-0.170874	2.514846
C	-1.599221	-0.802490	1.285092
H	-2.312848	-0.408468	2.014866
C	0.747019	-1.063848	0.703291
H	0.564538	-1.775691	-0.101939
C	-2.086312	-1.142105	0.020771
H	-1.467429	-1.801854	-0.592915
C	-1.501251	0.486371	-1.041630
H	-1.926524	0.032097	-1.942773
C	-0.100785	0.492536	-1.090458
H	0.458260	-0.054679	-1.843435

N	0.716386	1.446868	-0.430105
O	1.904880	1.467938	-0.734281
O	0.232391	2.178537	0.431493
C	2.462403	0.082458	1.851177
H	1.891973	1.019420	1.787347
H	3.520220	0.280025	1.655152
H	2.342491	-0.377433	2.844916
O	2.047492	-0.832528	0.837509
C	2.720138	-1.710097	-2.163096
H	2.968294	-2.335493	-1.295721
H	3.492430	-1.827865	-2.933899
H	2.668161	-0.661605	-1.839529
H	1.753996	-2.029202	-2.580962
C	-2.332532	1.618195	-0.479427
H	-2.100430	2.549774	-1.017157
H	-2.113723	1.796895	0.577267
H	-3.401095	1.400604	-0.612795
C	-3.568285	-1.303617	-0.204507
H	-3.848869	-1.058031	-1.240391
H	-4.145929	-0.654097	0.468875
H	-3.878241	-2.343705	-0.019949

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entryS3.adduct.xyz

C	-0.620693	-1.758699	0.330863
H	-0.303841	-2.530376	1.030715
C	-1.905959	-1.448297	0.147742
H	-2.699619	-1.959847	0.697767
C	0.379340	-1.007328	-0.506649
H	0.191381	-1.285097	-1.562257
C	-2.254725	-0.341560	-0.813711
H	-1.955132	-0.666855	-1.828299
C	-1.390080	0.911098	-0.491000
H	-1.504068	1.614548	-1.329420
C	0.113279	0.509991	-0.446866
H	0.678991	1.004100	-1.243114
N	0.763565	1.041379	0.806179
O	1.306374	2.121785	0.720690
O	0.667178	0.389648	1.823148
C	2.157317	-2.075478	0.755438
H	1.759780	-1.760861	1.733077
H	3.252662	-2.022944	0.781186
H	1.861202	-3.118452	0.548436
O	1.759459	-1.197539	-0.275165
C	3.673735	0.921566	-1.681332

H	4.381387	0.214002	-1.231030
H	4.220681	1.656527	-2.285877
H	3.120120	1.434327	-0.884514
H	2.975691	0.360319	-2.315812
C	-1.870302	1.619094	0.779167
H	-1.223943	2.475099	1.018540
H	-1.866508	0.934465	1.639608
H	-2.887067	2.005863	0.634025
C	-3.749213	-0.039137	-0.845690
H	-3.970293	0.826181	-1.488182
H	-4.133686	0.175020	0.162132
H	-4.302976	-0.904316	-1.237383

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entryS4.PAC.xyz

C	-0.672127	-1.499684	-0.653438
H	-1.396690	-1.295046	-1.443911
C	0.729530	-1.669212	-1.051846
H	0.892103	-2.059162	-2.064083
C	-1.087960	-1.645770	0.619882
H	-0.391629	-1.923674	1.415792
C	1.809305	-1.383912	-0.308568
H	1.663919	-0.939521	0.682628
C	1.027708	1.712791	-0.495726
H	2.049954	1.776010	-0.109898
C	0.093223	1.684347	0.457589
H	0.287358	1.706014	1.526748
N	-1.328383	1.581519	0.182797
O	-2.051035	1.448035	1.150091
O	-1.716035	1.626710	-0.972091
C	-3.348098	-1.192453	0.171564
H	-3.138801	-0.226931	-0.312738
H	-4.276449	-1.119989	0.747809
H	-3.444823	-1.982198	-0.592379
O	-2.333855	-1.527719	1.102493
C	3.688462	0.640513	2.213905
H	3.829445	-0.441980	2.100933
H	2.614420	0.867682	2.234714
H	4.163902	1.161060	1.372119
H	4.146687	0.975233	3.152745
C	0.854398	1.666555	-1.980695
H	0.352836	2.579087	-2.335364
H	0.206065	0.828313	-2.266479
H	1.827813	1.569819	-2.475555
C	3.223803	-1.623532	-0.740856

H	3.735275	-2.326905	-0.063619
H	3.811936	-0.691067	-0.727001
H	3.263295	-2.041444	-1.756850

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entryS4.TS.xyz

C	-0.511566	0.290245	1.682171
H	-1.299790	-0.187590	2.262703
C	0.796564	-0.192861	1.807734
H	0.967077	-0.989914	2.537533
C	-0.847042	1.210200	0.703375
H	-0.103618	1.874144	0.262625
C	1.822957	0.103630	0.910245
H	1.777131	1.067943	0.399566
C	1.130585	-0.842946	-0.770331
H	1.982362	-0.441707	-1.330530
C	-0.066529	-0.229939	-1.157689
H	-0.104801	0.620371	-1.832549
N	-1.344381	-0.848619	-1.054239
O	-2.262980	-0.322034	-1.668162
O	-1.488725	-1.834956	-0.335141
C	-3.169186	0.846631	0.903903
H	-3.026738	-0.228598	0.726629
H	-4.054680	1.193420	0.363046
H	-3.281540	1.048877	1.981146
O	-2.076568	1.598485	0.378333
C	2.673362	2.523257	-1.634615
H	2.413225	3.178182	-0.792805
H	1.782376	1.970382	-1.961441
H	3.452038	1.815595	-1.320005
H	3.045803	3.131427	-2.467846
C	1.255001	-2.311692	-0.427482
H	0.919677	-2.920755	-1.280625
H	0.629539	-2.584694	0.427207
H	2.304557	-2.560250	-0.220509
C	3.223899	-0.397662	1.147835
H	3.805564	0.335928	1.727473
H	3.760033	-0.563033	0.199974
H	3.220370	-1.344528	1.706959

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entryS4.adduct.xyz

C	-0.442345	0.655872	1.636555
H	-1.212024	0.751065	2.400580
C	0.781759	0.201771	1.914177

H	1.062500	-0.095969	2.927471
C	-0.703534	1.058940	0.209264
H	-0.048313	1.924814	-0.010714
C	1.775651	0.070337	0.789680
H	1.984325	1.085965	0.404408
C	1.120590	-0.707689	-0.387587
H	1.779008	-0.593696	-1.262252
C	-0.237030	-0.043806	-0.760176
H	-0.218826	0.358589	-1.778200
N	-1.328899	-1.082585	-0.839076
O	-1.532788	-1.568712	-1.928871
O	-1.897968	-1.397850	0.184035
C	-3.030937	1.407269	0.792761
H	-3.161252	0.403197	1.225920
H	-3.949353	1.691082	0.264506
H	-2.849187	2.140636	1.597487
O	-2.010549	1.425156	-0.181105
C	2.597670	2.262701	-2.063017
H	2.463022	3.042049	-1.302004
H	1.637415	1.764769	-2.253196
H	3.330922	1.526050	-1.708727
H	2.957570	2.718499	-2.993620
C	1.002427	-2.203478	-0.081380
H	0.494762	-2.731781	-0.900208
H	0.432468	-2.372876	0.843844
H	2.000423	-2.646371	0.028099
C	3.101684	-0.534852	1.237430
H	3.601252	0.133769	1.952960
H	3.780105	-0.688301	0.384392
H	2.952311	-1.504540	1.734065

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entryS6.PAC.xyz

C	0.169702	-1.648675	-0.636734
H	-0.141959	-1.327480	-1.632409
C	1.588539	-1.511519	-0.282397
H	2.308176	-1.648105	-1.099511
C	-0.711205	-2.225701	0.202014
H	-0.392237	-2.614168	1.172443
C	2.067607	-1.264288	0.946346
H	1.351297	-1.063553	1.752129
C	0.710095	1.724988	0.466615
H	1.598535	1.687472	1.105335
C	-0.438356	1.367492	1.043485
H	-0.470855	1.081342	2.096117

C	-2.556397	-2.044673	-1.231435
H	-2.432321	-0.961409	-1.371860
H	-3.621858	-2.297326	-1.206831
H	-2.066156	-2.581771	-2.060765
O	-2.021189	-2.454354	0.010807
C	0.951448	2.135468	-0.953946
H	1.325267	1.267087	-1.523204
H	0.051080	2.508680	-1.451389
H	1.733154	2.906286	-0.993998
C	3.519771	-1.259738	1.315301
H	3.821977	-0.298849	1.763367
H	3.734718	-2.038795	2.064390
H	4.155147	-1.446356	0.437717
C	4.455805	1.126922	-1.127319
H	4.604259	0.368424	-1.907046
H	3.554142	0.879463	-0.551535
H	5.326875	1.137832	-0.459900
H	4.339588	2.112532	-1.596010
C	-1.777016	1.333068	0.385482
F	-2.510350	0.304772	0.844117
F	-1.720268	1.198843	-0.955644
F	-2.490413	2.447881	0.623976

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entryS6.TS.xyz

C	0.087813	-1.692598	0.493980
H	0.345739	-1.785283	1.548514
C	-1.249134	-1.470168	0.144508
H	-1.985241	-1.413137	0.952200
C	1.094482	-1.575303	-0.455673
H	0.885429	-1.754404	-1.508054
C	-1.645342	-1.084612	-1.130958
H	-1.038318	-1.423791	-1.973581
C	-0.693738	0.807688	-1.282953
H	-1.031644	0.834286	-2.322379
C	0.680569	0.633154	-1.107925
H	1.321151	0.474209	-1.975391
C	2.845832	-1.697431	1.122284
H	2.466482	-0.816193	1.658820
H	3.940028	-1.665877	1.089875
H	2.517095	-2.616622	1.634231
O	2.414591	-1.697767	-0.227424
C	-1.506017	1.648251	-0.325324
H	-1.263472	1.403413	0.717208
H	-1.279409	2.714880	-0.476876

H	-2.583554	1.503260	-0.480830
C	-3.096905	-0.865547	-1.463088
H	-3.225922	-0.069922	-2.213791
H	-3.542897	-1.781162	-1.882262
H	-3.672328	-0.588175	-0.568006
C	-4.362980	0.259307	2.096245
H	-4.447646	-0.834385	2.050315
H	-3.335374	0.560421	1.855037
H	-5.054577	0.709512	1.372368
H	-4.617471	0.602723	3.106636
C	1.404728	1.307579	0.006862
F	2.721097	1.032418	-0.019255
F	1.304817	2.655779	-0.041611
F	0.966237	0.968077	1.243933

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entryS6.adduct.xyz

C	-0.290976	-1.795053	0.037508
H	-0.124501	-2.567521	0.789010
C	-1.510672	-1.373208	-0.304470
H	-2.413402	-1.770043	0.167179
C	0.864635	-1.224090	-0.738904
H	0.714122	-1.552471	-1.781811
C	-1.619057	-0.286791	-1.343672
H	-1.223569	-0.684885	-2.298009
C	-0.673378	0.877976	-0.931107
H	-0.695671	1.618972	-1.745221
C	0.793960	0.344147	-0.846347
H	1.307586	0.593380	-1.787207
C	2.420253	-1.987488	0.938421
H	1.962097	-1.256331	1.620324
H	3.510598	-1.935123	1.050655
H	2.085421	-3.000500	1.220528
O	2.141736	-1.715089	-0.419969
C	-1.209427	1.568393	0.329944
H	-1.249698	0.874982	1.180745
H	-0.594539	2.427111	0.620470
H	-2.223858	1.943665	0.136849
C	-3.059073	0.153437	-1.588482
H	-3.102543	1.020935	-2.263917
H	-3.631656	-0.664888	-2.048623
H	-3.563536	0.422919	-0.649482
C	1.627570	1.076764	0.184331
F	1.219244	0.872234	1.453212
F	2.923778	0.742614	0.138950

F	1.582682	2.408512	-0.028237
C	-4.348424	-0.208683	2.064975
H	-4.643492	0.814333	1.797597
H	-4.701325	-0.437274	3.078382
H	-4.795216	-0.916137	1.354165
H	-3.254518	-0.293069	2.029604

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entryS7.PAC.xyz

C	1.064746	-1.357142	-0.148765
H	1.233640	-1.299836	-1.224311
C	-0.310699	-1.625087	0.278385
H	-0.983299	-1.939747	-0.525391
C	2.092497	-1.179497	0.702955
H	1.962403	-1.252201	1.786033
C	-0.823291	-1.525017	1.514743
H	-0.225219	-1.206341	2.372211
C	-0.535832	1.632523	1.500369
H	-0.704774	1.747544	2.571136
C	0.678360	1.808043	0.998873
H	1.594408	2.063647	1.525263
H	-1.864367	-1.788499	1.708282
H	-1.367937	1.369378	0.847528
C	-3.376823	0.068610	-0.892158
H	-2.284090	0.210081	-0.934820
H	-3.789677	0.621344	-1.751709
N	0.904214	1.653140	-0.438569
O	2.041828	1.858083	-0.816343
O	-0.022908	1.334777	-1.151248
C	3.707255	-0.860499	-0.972772
H	3.149797	-0.055101	-1.472948
H	4.781508	-0.652386	-1.016831
H	3.493928	-1.825028	-1.462544
O	3.375669	-0.921663	0.404379
C	-3.712952	-1.412466	-1.032676
H	-3.293018	-1.839468	-1.955376
H	-3.316488	-1.990637	-0.181882
H	-4.802781	-1.569852	-1.054702
C	-3.925996	0.658206	0.403498
H	-3.474219	0.163107	1.279242
H	-3.723323	1.737405	0.480266
H	-5.016297	0.518982	0.471523

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entryS7.TS.xyz

C	1.047671	-1.430700	-0.226606
H	1.257666	-1.540005	-1.289631
C	-0.295139	-1.514893	0.189174
H	-1.039676	-1.700207	-0.588269
C	2.039880	-0.998335	0.623170
H	1.916456	-1.002676	1.705474
C	-0.739696	-1.168481	1.460252
H	-0.084374	-1.329345	2.318229
C	-0.486924	0.848024	1.551375
H	-0.666826	0.919465	2.625163
C	0.767915	1.222386	1.102040
H	1.636655	1.475317	1.700552
H	-1.804639	-1.273340	1.680260
H	-1.333268	1.072884	0.903567
C	-3.348519	0.181998	-0.898165
H	-2.252339	0.303630	-0.887112
H	-3.695057	0.711513	-1.800210
N	0.938528	1.496624	-0.282082
O	2.024911	1.930292	-0.650256
O	0.006658	1.249787	-1.043459
C	3.617713	-0.675857	-1.094156
H	2.946602	0.003522	-1.636367
H	4.645032	-0.303048	-1.150785
H	3.566576	-1.694416	-1.510289
O	3.290459	-0.694899	0.293160
C	-3.713566	-1.295315	-1.007282
H	-3.261580	-1.761810	-1.895538
H	-3.373844	-1.858263	-0.121435
H	-4.804366	-1.429820	-1.077316
C	-3.960693	0.837360	0.336421
H	-3.620956	0.340537	1.260892
H	-3.690206	1.901401	0.407621
H	-5.059630	0.769739	0.316878

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entryS7.adduct.xyz

C	0.728269	-1.620797	-0.471188
H	1.038403	-1.964504	-1.458334
C	-0.513852	-1.797447	-0.017494
H	-1.272745	-2.291430	-0.627864
C	1.738423	-0.963659	0.430412
H	1.944917	-1.646499	1.274303
C	-0.864061	-1.321418	1.364335
H	-0.471909	-2.048320	2.097829
C	-0.275750	0.072183	1.669111

H	-0.267912	0.236684	2.754693
C	1.134889	0.297036	1.117256
H	1.851839	0.650021	1.864346
H	-1.952844	-1.291887	1.510599
H	-0.935518	0.830178	1.228174
C	-3.023367	0.479953	-0.895287
H	-1.950755	0.233193	-0.839163
H	-3.142504	1.066114	-1.820956
N	1.141455	1.404141	0.090328
O	2.104829	2.135575	0.088835
O	0.222851	1.455404	-0.705173
C	3.036199	-0.296300	-1.491148
H	2.144284	0.269236	-1.802912
H	3.916983	0.346683	-1.608104
H	3.143653	-1.175771	-2.148261
O	2.995224	-0.685500	-0.127564
C	-3.854852	-0.795079	-0.990431
H	-3.568702	-1.402830	-1.861645
H	-3.733223	-1.419599	-0.089223
H	-4.928031	-0.564018	-1.081612
C	-3.412438	1.344892	0.299179
H	-3.306934	0.788007	1.245783
H	-2.781260	2.244062	0.361965
H	-4.461924	1.671674	0.230827

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entryS8.PAC.xyz

C	-1.888189	-1.209019	-0.134851
H	-2.102915	-0.834734	-1.137687
C	-0.480486	-1.436044	0.209099
H	0.175497	-1.672086	-0.635908
C	-2.887459	-1.491601	0.722522
H	-2.688914	-1.937475	1.700598
C	0.051833	-1.373679	1.438082
H	-0.549236	-1.089194	2.306019
C	-0.233502	1.865660	1.459116
H	-0.195002	2.090405	2.524931
C	-1.365080	2.028613	0.788819
H	-2.324006	2.374764	1.165244
H	1.102556	-1.610779	1.613404
H	0.659612	1.502203	0.950364
C	2.846557	0.253107	-0.706011
H	1.767408	0.451486	-0.810284
H	3.367988	0.820262	-1.493917
N	-1.418425	1.719968	-0.640327

O	-2.490320	1.901057	-1.184431
O	-0.422239	1.299055	-1.190268
C	-4.601197	-0.745465	-0.692116
H	-4.135459	0.242300	-0.830124
H	-5.691252	-0.649268	-0.650817
H	-4.318438	-1.398740	-1.533931
O	-4.206354	-1.321768	0.540632
C	3.080491	-1.230955	-0.922995
H	2.697590	-1.537345	-1.912808
H	2.534064	-1.809495	-0.153290
C	3.343799	0.738120	0.653150
H	2.887532	0.108857	1.448513
H	2.999586	1.770916	0.825699
O	4.746732	0.762590	0.755048
H	5.054146	-0.070871	0.367023
O	4.479746	-1.484417	-0.827909
H	4.627094	-2.435556	-0.894205

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entryS8.TS.xyz

C	-1.722058	-1.456375	0.007557
H	-1.911572	-1.737304	-1.027696
C	-0.388801	-1.461353	0.460944
H	0.371109	-1.765945	-0.262859
C	-2.731226	-0.892719	0.755264
H	-2.628263	-0.721281	1.826147
C	0.023230	-0.908897	1.668239
H	-0.650524	-0.937180	2.526217
C	-0.252771	1.096103	1.433062
H	-0.114535	1.340886	2.487119
C	-1.489912	1.373116	0.878512
H	-2.386069	1.710583	1.388485
H	1.083136	-0.958801	1.928281
H	0.614702	1.227680	0.788189
C	2.726934	0.179553	-0.817945
H	1.630205	0.264505	-0.902741
H	3.157054	0.573710	-1.752615
N	-1.598270	1.414106	-0.539030
O	-2.666411	1.771615	-1.021495
O	-0.631975	1.052577	-1.206398
C	-4.281633	-0.866032	-1.018472
H	-3.599307	-0.289189	-1.656705
H	-5.305629	-0.504173	-1.152377
H	-4.230548	-1.940247	-1.256109
O	-3.975428	-0.652535	0.357898

C	3.098572	-1.285678	-0.679452
H	2.702434	-1.864357	-1.533626
H	2.652681	-1.699145	0.247260
C	3.238193	1.028417	0.343676
H	2.898273	0.573136	1.301119
H	2.790521	2.033440	0.291982
O	4.633421	1.204728	0.329557
H	5.008789	0.332529	0.134890
O	4.518092	-1.384833	-0.623841
H	4.760671	-2.306812	-0.475830

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entryS8.adduct.xyz

C	1.503691	1.396977	-0.976919
H	1.673167	1.269697	-2.046500
C	0.469049	2.089048	-0.492794
H	-0.260509	2.556430	-1.157183
C	2.487240	0.825121	0.008963
H	2.976753	1.670625	0.524587
C	0.323798	2.197858	0.999711
H	1.089931	2.888340	1.396038
C	0.496899	0.811837	1.650829
H	0.526655	0.906651	2.744129
C	1.749773	0.076352	1.162276
H	2.480197	-0.131673	1.949641
H	-0.649196	2.619042	1.285069
H	-0.378805	0.202374	1.387746
C	-2.432970	-0.267961	-0.963203
H	-1.355988	-0.150183	-1.159665
H	-2.936105	-0.513822	-1.912256
N	1.408666	-1.296470	0.636219
O	2.187773	-2.184878	0.886278
O	0.420935	-1.408578	-0.066212
C	3.278178	-0.753632	-1.638540
H	2.255747	-1.161999	-1.644195
H	3.989639	-1.587037	-1.596426
H	3.441276	-0.191472	-2.573425
O	3.541738	0.059203	-0.505854
C	-2.966971	1.051065	-0.436447
H	-2.807947	1.856923	-1.176424
H	-2.417793	1.322969	0.487104
C	-2.646557	-1.421062	0.013761
H	-2.263409	-1.121988	1.014494
H	-2.050996	-2.289040	-0.300788
O	-3.989884	-1.839165	0.082914

H	-4.513463	-1.030121	0.179178
O	-4.354720	0.900105	-0.155980
H	-4.679342	1.712472	0.250353

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entryS9.PAC.xyz

C	2.793449	-0.784706	-0.154356
H	3.214616	-0.920339	0.842405
C	3.582446	-0.010006	-1.119304
H	4.661635	0.010122	-0.938070
C	1.600651	-1.314568	-0.471047
H	1.163216	-1.221469	-1.467154
C	3.101260	0.664342	-2.172925
H	2.029022	0.710119	-2.380323
C	1.227057	2.553354	-0.295857
H	1.144649	3.133369	-1.214626
C	0.212653	1.794216	0.096125
H	-0.750512	1.624605	-0.384540
H	3.772249	1.179147	-2.861782
H	2.147114	2.593711	0.287057
N	0.349944	1.023956	1.336266
O	-0.601132	0.316592	1.644829
O	1.365748	1.106644	1.988392
C	1.195914	-2.216757	1.676944
H	1.361399	-1.260461	2.195050
H	0.392880	-2.771720	2.173049
H	2.122237	-2.813341	1.682314
O	0.762790	-2.001911	0.342032
H	-0.904845	-1.114635	-0.375236
O	-1.213894	-0.596000	-1.136382
C	-2.485922	-1.079816	-1.514601
H	-2.425884	-2.142408	-1.813866
H	-2.780129	-0.506069	-2.407475
C	-3.543810	-0.917095	-0.427809
H	-4.438452	-1.497657	-0.708425
H	-3.166048	-1.369017	0.509160
C	-3.969448	0.522087	-0.164262
H	-4.399182	0.952678	-1.083567
H	-4.770756	0.526731	0.599141
O	-2.909975	1.371383	0.217295
H	-2.336604	0.878965	0.826245

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entryS9.TS.xyz

C	-2.687721	0.866320	-0.361571
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H	-3.128604	1.468911	0.431035
C	-3.398067	-0.279602	-0.770404
H	-4.367088	-0.445789	-0.292947
C	-1.404225	1.135518	-0.769555
H	-0.920425	0.673187	-1.631668
C	-2.870678	-1.305395	-1.542707
H	-2.073713	-1.094774	-2.257530
C	-1.606692	-2.196249	-0.233363
H	-1.397353	-3.002802	-0.937139
C	-0.557503	-1.341830	0.062666
H	0.372866	-1.241576	-0.492858
H	-3.526582	-2.132526	-1.820263
H	-2.313961	-2.418799	0.565039
N	-0.580124	-0.605985	1.263636
O	0.422058	0.090922	1.523664
O	-1.557864	-0.642876	1.999588
C	-1.031082	2.666492	0.992718
H	-1.286523	1.899137	1.737052
H	-0.174636	3.251985	1.340884
H	-1.886224	3.333573	0.803526
O	-0.607499	2.053804	-0.225813
H	1.180257	0.860581	-0.483206
O	1.491167	0.486879	-1.324471
C	2.870991	0.769945	-1.436543
H	3.024104	1.818224	-1.755512
H	3.258288	0.123821	-2.240643
C	3.649038	0.520025	-0.149898
H	4.663612	0.936721	-0.266213
H	3.175433	1.093331	0.670222
C	3.774588	-0.942370	0.264059
H	4.270420	-1.509219	-0.541232
H	4.433818	-1.002696	1.151879
O	2.543648	-1.581641	0.502758
H	1.993191	-0.983211	1.035896

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entryS9.adduct.xyz

C	-2.678561	0.861038	-0.606347
H	-3.132103	1.792928	-0.267091
C	-3.406486	-0.168206	-1.045425
H	-4.496239	-0.116834	-1.071937
C	-1.182012	0.727431	-0.634483
H	-0.840369	0.691428	-1.683053
C	-2.694021	-1.410844	-1.501554
H	-2.227299	-1.222051	-2.484637

C	-1.601820	-1.814132	-0.492425
H	-0.969014	-2.605590	-0.914032
C	-0.712936	-0.645124	-0.060725
H	0.341601	-0.772929	-0.325593
H	-3.391315	-2.246946	-1.640853
H	-2.096497	-2.215025	0.401137
N	-0.712687	-0.494245	1.440401
O	0.333850	-0.139104	1.958484
O	-1.750066	-0.644687	2.044140
C	-0.995393	2.450388	1.073216
H	-1.584838	1.772974	1.708732
H	-0.147440	2.830558	1.655685
H	-1.631507	3.296787	0.767317
O	-0.451231	1.796355	-0.064299
H	1.279080	1.326332	-0.813093
O	1.664904	0.716928	-1.464668
C	3.070105	0.813054	-1.402352
H	3.400813	1.844212	-1.628462
H	3.459165	0.167685	-2.206256
C	3.667949	0.376116	-0.068204
H	4.730605	0.673011	-0.052836
H	3.179370	0.935051	0.752185
C	3.591933	-1.119323	0.224635
H	4.001988	-1.682263	-0.629603
H	4.232514	-1.347447	1.097501
O	2.284442	-1.606643	0.427900
H	1.872549	-1.067338	1.121596

5.2. Structures for the intramolecular reactions

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entry01-adduct.xyz

C	-0.271258	1.967932	-0.871133
H	-0.459547	2.587566	-1.753031
C	0.979727	1.815513	-0.431860
H	1.804210	2.319489	-0.938753
C	-1.473582	1.383450	-0.188349
H	-2.074809	2.233662	0.182806
C	1.303800	0.987238	0.787640
H	1.210908	1.637838	1.679133
C	0.254750	-0.108719	0.994551
C	-1.150418	0.488284	1.036772
H	-1.138471	1.120272	1.940365
C	-2.309634	-0.534098	1.123100

H	-1.922936	-1.551141	0.970191
H	-2.795933	-0.514646	2.107635
C	-2.416393	0.536071	-1.057833
H	-2.997754	1.146837	-1.763642
H	-1.835953	-0.200617	-1.632744
C	-3.287281	-0.161612	-0.009165
H	-4.041585	0.548950	0.365024
H	-3.824702	-1.034038	-0.404504
H	0.481075	-0.659891	1.915059
O	2.612657	0.464749	0.862282
C	3.362070	0.342858	-0.329607
H	4.145206	-0.398395	-0.124289
H	3.846916	1.296302	-0.604323
H	2.756249	-0.013010	-1.176328
Br	0.457005	-1.501105	-0.399587

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entry01-reagent.xyz

C	-0.418332	-1.330776	-1.138513
H	-0.026136	-0.897833	-2.065977
C	-1.780058	-0.933004	-0.770047
H	-2.463218	-0.668264	-1.578292
C	0.383638	-2.130623	-0.421966
H	-0.013165	-2.610071	0.482025
C	-2.168434	-0.828756	0.513426
H	-1.474638	-1.021446	1.334827
C	0.624398	1.028533	1.165688
C	1.520851	0.075948	1.412618
H	1.406576	-0.430917	2.379250
C	2.687056	-0.351225	0.571842
H	2.665434	0.174456	-0.394765
H	3.601596	-0.020909	1.093883
C	1.825187	-2.389986	-0.738193
H	1.997964	-3.473033	-0.856406
H	2.077491	-1.914488	-1.700379
C	2.778639	-1.867070	0.346357
H	2.581860	-2.392161	1.297668
H	3.810575	-2.123029	0.061045
H	-0.176617	1.299452	1.851254
O	-3.382162	-0.480185	0.988636
C	-4.368211	-0.188468	0.022891
H	-5.281109	0.060340	0.574707
H	-4.551634	-1.058864	-0.629120
H	-4.066197	0.668882	-0.601226
Br	0.584575	2.049769	-0.426920

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entry01-TS.xyz

C	0.634679	-1.543536	-1.113840
H	0.909252	-1.315928	-2.148426
C	-0.726522	-1.600688	-0.806107
H	-1.448727	-1.468874	-1.611184
C	1.632205	-1.500736	-0.143456
H	1.490651	-2.096944	0.761806
C	-1.143432	-1.485469	0.516587
H	-0.523364	-1.863840	1.328887
C	-0.222440	0.470612	0.974474
C	1.144623	0.226800	1.048520
H	1.428246	-0.230727	2.005856
C	2.264576	1.009568	0.406455
H	1.948288	1.360673	-0.587467
H	2.492351	1.901043	1.014231
C	3.050752	-1.143239	-0.509232
H	3.742621	-1.979952	-0.329932
H	3.086075	-0.909325	-1.585068
C	3.481720	0.097629	0.292427
H	3.799738	-0.204060	1.304902
H	4.337457	0.604179	-0.176420
H	-0.873325	0.459239	1.845651
O	-2.430718	-1.400034	0.930836
C	-3.407173	-1.123000	-0.056516
H	-4.347809	-0.961344	0.481515
H	-3.522763	-1.976239	-0.745421
H	-3.147698	-0.219775	-0.629087
Br	-0.862262	1.704414	-0.343783

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entry02-adduct.xyz

C	-0.187563	-1.724027	1.092385
H	-0.467110	-2.199963	2.036891
C	1.082261	-1.394597	0.850691
H	1.872890	-1.569192	1.583401
C	-1.282160	-1.479970	0.090877
H	-1.449349	-2.433127	-0.442691
C	1.445611	-0.696953	-0.439939
H	1.411246	-1.428107	-1.275551
C	0.370168	0.350206	-0.760726
C	-0.952089	-0.402349	-1.004702
H	-0.796886	-0.934517	-1.954702
C	-2.235166	0.452963	-1.136606

H	-2.150004	1.388622	-0.569534
H	-2.437696	0.724524	-2.181680
C	-2.638454	-1.058387	0.679282
H	-3.191115	-1.908764	1.103577
H	-2.485780	-0.314080	1.474889
C	-3.339878	-0.409474	-0.514580
H	-3.659498	-1.190852	-1.224225
H	-4.228434	0.173546	-0.237282
C	0.255485	1.442444	0.298914
F	-0.629569	1.150435	1.274208
F	1.408031	1.726510	0.906940
F	-0.180195	2.587538	-0.267640
H	0.672447	0.879833	-1.675900
O	2.718917	-0.099800	-0.421051
C	3.755150	-1.035550	-0.587218
H	4.701884	-0.483887	-0.544162
H	3.677871	-1.548848	-1.563993
H	3.753613	-1.802970	0.207519

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entry02-reagent.xyz

C	-0.139893	-1.602941	0.995189
H	-0.444322	-1.253302	1.987366
C	1.276781	-1.414514	0.682963
H	1.953044	-1.261409	1.524307
C	-1.099687	-2.066646	0.181994
H	-0.835872	-2.459528	-0.807820
C	1.736776	-1.317379	-0.578252
H	1.072269	-1.416115	-1.439035
C	-0.281378	1.179090	-1.080631
C	-1.455700	0.576549	-1.282664
H	-1.606687	0.143800	-2.279413
C	-2.640149	0.456119	-0.365209
H	-2.378234	0.749984	0.660261
H	-3.387697	1.182429	-0.728814
C	-2.559652	-1.968885	0.505585
H	-3.059367	-2.944101	0.385429
H	-2.671721	-1.673714	1.561873
C	-3.283753	-0.938940	-0.378730
H	-3.323093	-1.306238	-1.419392
H	-4.328626	-0.858761	-0.041986
C	0.144973	1.870225	0.176292
F	-0.239794	1.249699	1.306269
F	1.484618	1.974501	0.227145
F	-0.341643	3.123075	0.253150

H	0.462398	1.237100	-1.876608
O	2.999307	-1.080324	-0.982306
C	3.942199	-0.829055	0.039231
H	4.896679	-0.632702	-0.460711
H	4.044643	-1.701113	0.706241
H	3.640405	0.049040	0.633070

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entry02-TS.xyz

C	-0.660193	-1.674363	0.913190
H	-0.990389	-1.594942	1.953652
C	0.716556	-1.643527	0.682502
H	1.386224	-1.604865	1.540820
C	-1.621696	-1.532608	-0.084313
H	-1.431082	-1.996257	-1.055108
C	1.205777	-1.367067	-0.590685
H	0.627587	-1.643082	-1.470914
C	0.191389	0.621832	-0.930520
C	-1.175974	0.354157	-0.982307
H	-1.522654	0.045631	-1.975432
C	-2.267417	1.024428	-0.175703
H	-1.934442	1.190247	0.859583
H	-2.495029	2.011159	-0.611266
C	-3.061706	-1.273576	0.294828
H	-3.733875	-2.054021	-0.091133
H	-3.136575	-1.290593	1.393464
C	-3.491391	0.115074	-0.217663
H	-3.836771	0.037694	-1.262320
H	-4.330600	0.517128	0.367632
C	0.743356	1.507197	0.131166
F	0.365870	1.155775	1.376257
F	2.092353	1.520754	0.122114
F	0.357309	2.793437	-0.017885
H	0.777778	0.655253	-1.848080
O	2.505110	-1.223868	-0.921890
C	3.444306	-1.171464	0.137082
H	4.414767	-0.970235	-0.329342
H	3.483772	-2.136202	0.668696
H	3.202586	-0.366169	0.845032

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entry03-adduct.xyz

C	0.945165	-1.851362	-0.926269
H	1.301378	-2.347227	-1.834451
C	-0.294074	-2.084010	-0.490284

H	-0.952221	-2.773631	-1.024689
C	1.930465	-0.995084	-0.189198
H	2.682358	-1.687348	0.233227
C	-0.846067	-1.437289	0.755830
H	-0.577677	-2.052780	1.630873
C	-0.192920	-0.050339	0.990764
C	1.337096	-0.196589	1.010090
H	1.560336	-0.755451	1.931687
C	2.110693	1.145700	1.024950
H	1.469470	1.957576	0.649628
H	2.432831	1.426868	2.036841
C	2.713958	0.032000	-1.022394
H	3.486930	-0.439029	-1.646914
H	2.021391	0.588224	-1.668581
C	3.287752	0.952685	0.057051
H	4.119955	0.444098	0.571238
H	3.672269	1.903217	-0.337132
C	-0.687599	0.937425	-0.041271
O	-0.221994	1.120125	-1.140735
H	-0.549569	0.311051	1.964969
O	-2.257184	-1.382224	0.801377
C	-2.930071	-1.057010	-0.399426
H	-3.748529	-0.366114	-0.151772
H	-3.357986	-1.962822	-0.861826
H	-2.271607	-0.577107	-1.141858
O	-1.764463	1.607788	0.407840
C	-2.347425	2.501904	-0.535877
H	-2.736173	1.943436	-1.400203
H	-3.161945	3.007567	-0.008053
H	-1.603923	3.225776	-0.894631

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entry03-reagent.xyz

C	0.312379	-1.495789	-0.940856
H	0.539654	-1.225498	-1.978122
C	-1.108388	-1.467818	-0.576867
H	-1.828485	-1.705923	-1.362177
C	1.337210	-1.785937	-0.127250
H	1.133445	-2.096862	0.905164
C	-1.533179	-1.100931	0.645341
H	-0.833414	-0.789191	1.424494
C	0.683810	1.470024	1.144383
C	1.961016	1.067807	1.203181
H	2.377736	0.935711	2.210045
C	2.930713	0.793223	0.093526

H	2.453505	0.934984	-0.883706
H	3.728298	1.550252	0.188960
C	2.774491	-1.688589	-0.544981
H	3.279583	-2.656751	-0.388555
H	2.813352	-1.475443	-1.625632
C	3.568001	-0.603555	0.199174
H	3.677430	-0.881758	1.262218
H	4.586544	-0.574845	-0.216845
C	-0.095124	1.665756	-0.099956
O	0.301356	1.597014	-1.240072
H	0.125112	1.646461	2.064811
O	-2.804426	-1.029126	1.090722
C	-3.807342	-1.437459	0.187783
H	-4.760224	-1.357805	0.722409
H	-3.645806	-2.479131	-0.136416
H	-3.828406	-0.786892	-0.702665
O	-1.380719	1.935737	0.207786
C	-2.246902	2.040045	-0.913890
H	-2.203848	1.115272	-1.508306
H	-3.250714	2.195441	-0.504789
H	-1.953557	2.882320	-1.555908

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entry03-TS.xyz

C	-0.952942	-1.294125	1.134699
H	-1.193152	-0.972969	2.152113
C	0.388145	-1.562700	0.852537
H	1.116604	-1.478970	1.658666
C	-1.943396	-1.170351	0.154380
H	-1.890632	-1.851442	-0.699393
C	0.819840	-1.632326	-0.465103
H	0.139163	-1.918690	-1.264507
C	0.061133	0.497318	-1.091672
C	-1.338092	0.391922	-1.044071
H	-1.759127	-0.005057	-1.977636
C	-2.298865	1.355087	-0.371909
H	-1.897690	1.667911	0.600480
H	-2.411822	2.253434	-1.000721
C	-3.319934	-0.675359	0.547836
H	-4.093050	-1.436396	0.366685
H	-3.314236	-0.463118	1.628359
C	-3.626290	0.623619	-0.217031
H	-4.028370	0.386061	-1.216730
H	-4.384121	1.228739	0.300456
C	0.798721	1.221399	-0.063538

O	0.370296	1.573883	1.017528
H	0.605713	0.283737	-2.009338
O	2.092567	-1.750373	-0.878671
C	3.108045	-1.581661	0.092999
H	4.056856	-1.591953	-0.454047
H	3.091297	-2.407837	0.822141
H	2.995384	-0.621871	0.617660
O	2.092295	1.438628	-0.426304
C	2.860328	2.139937	0.541607
H	2.917297	1.572911	1.483405
H	3.857703	2.263553	0.106006
H	2.410756	3.118286	0.761584

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entry04-adduct.xyz

C	0.450637	-1.972248	-0.516023
H	0.721965	-2.743058	-1.244098
C	-0.823598	-1.844534	-0.141743
H	-1.582679	-2.516449	-0.546717
C	1.570190	-1.170459	0.071387
H	2.158524	-1.874578	0.689202
C	-1.275442	-0.820005	0.866996
H	-1.204555	-1.258130	1.877433
C	-0.344298	0.420791	0.856183
C	1.121005	-0.018850	1.016773
H	1.201871	-0.384759	2.052107
C	2.158002	1.112750	0.793330
H	1.709750	1.930758	0.210134
H	2.513552	1.541766	1.740270
C	2.563392	-0.536852	-0.915008
H	3.237842	-1.280202	-1.364444
H	2.011485	-0.023494	-1.713393
C	3.289566	0.477542	-0.029491
H	3.989651	-0.052259	0.637812
H	3.868378	1.219307	-0.596733
C	-0.624183	1.261852	-0.383107
O	-0.071368	1.064281	-1.443410
H	-0.629382	1.029822	1.729014
O	-2.642406	-0.444115	0.748956
C	-3.210780	-0.469166	-0.546089
H	-4.088937	0.190055	-0.516536
H	-3.547596	-1.481580	-0.824997
H	-2.517294	-0.107910	-1.323847
C	-1.632468	2.373552	-0.208780
H	-1.153652	3.178116	0.374006

H	-1.937788	2.767232	-1.185271
H	-2.493089	2.017787	0.375116

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entry04-reagent.xyz

C	-0.191221	-1.404916	0.912383
H	-0.483263	-1.133554	1.932581
C	1.234868	-1.258992	0.611472
H	1.930762	-1.338589	1.447858
C	-1.154250	-1.767550	0.052953
H	-0.882825	-2.076217	-0.964365
C	1.683966	-0.941841	-0.616088
H	1.000897	-0.787857	-1.454170
C	-0.395495	1.558379	-0.922374
C	-1.633217	1.083145	-1.142693
H	-1.909590	0.923169	-2.194109
C	-2.733715	0.784705	-0.168134
H	-2.379075	0.907620	0.861840
H	-3.513328	1.546380	-0.346795
C	-2.614747	-1.714742	0.384330
H	-3.097942	-2.680165	0.159956
H	-2.726898	-1.538060	1.466277
C	-3.359712	-0.604166	-0.374676
H	-3.388991	-0.842021	-1.452742
H	-4.406092	-0.590569	-0.033574
C	0.229923	1.820323	0.403099
O	-0.334523	1.633576	1.463700
H	0.240965	1.758684	-1.789331
O	2.963198	-0.727432	-0.998189
C	3.948741	-0.908913	-0.002987
H	4.915998	-0.734015	-0.486160
H	3.911964	-1.932997	0.403686
H	3.810032	-0.190378	0.822630
C	1.647423	2.351759	0.350178
H	1.641099	3.355497	-0.104537
H	2.054550	2.412172	1.365721
H	2.276960	1.708606	-0.283629

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entry04-TS.xyz

C	-0.516930	-1.381687	0.942772
H	-0.842612	-1.283936	1.981633
C	0.859640	-1.368890	0.704375
H	1.528916	-1.306935	1.561537
C	-1.485287	-1.289076	-0.066135

H	-1.271106	-1.818186	-0.999220
C	1.345396	-1.139101	-0.570472
H	0.751013	-1.354937	-1.455093
C	0.116479	0.933559	-0.913260
C	-1.223559	0.502144	-0.958740
H	-1.528816	0.189624	-1.967597
C	-2.388311	1.134039	-0.214854
H	-2.088393	1.371138	0.813216
H	-2.672366	2.071704	-0.719190
C	-2.946120	-1.179815	0.328697
H	-3.520983	-2.057056	-0.002338
H	-3.003750	-1.144599	1.427717
C	-3.526566	0.122472	-0.244942
H	-3.848437	-0.034217	-1.288693
H	-4.408039	0.457309	0.319741
C	0.693848	1.559142	0.269432
O	0.138177	1.537483	1.362196
H	0.696547	0.970146	-1.836328
O	2.639265	-0.968398	-0.905863
C	3.581352	-0.946800	0.151868
H	4.555991	-0.759367	-0.311606
H	3.599279	-1.915899	0.675986
H	3.353416	-0.147226	0.874020
C	2.049636	2.221111	0.095166
H	1.905775	3.207322	-0.373763
H	2.518166	2.366835	1.076231
H	2.698399	1.633016	-0.570365

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entry05-adduct.xyz

C	0.048418	1.829731	0.443900
H	0.214579	2.663285	1.133325
C	-1.199725	1.507431	0.096786
H	-2.041954	2.084693	0.484135
C	1.266307	1.166625	-0.122936
H	1.750802	1.917204	-0.774959
C	-1.509931	0.377234	-0.851974
H	-1.507220	0.762167	-1.885958
C	-0.405092	-0.710692	-0.774692
C	0.973547	-0.077214	-1.009549
H	0.959669	0.255244	-2.059275
C	2.180783	-1.026365	-0.788953
H	1.873807	-1.912372	-0.217806
H	2.600546	-1.379785	-1.740766
C	2.335737	0.715626	0.882702

H	2.897179	1.562308	1.304183
H	1.862326	0.156342	1.700072
C	3.200539	-0.218582	0.033837
H	3.837360	0.381336	-0.637135
H	3.861950	-0.860523	0.631316
C	-0.575418	-1.490390	0.508885
O	0.151382	-1.440598	1.470906
H	-1.472010	-2.155974	0.517732
H	-0.626559	-1.428176	-1.583905
O	-2.799901	-0.194719	-0.692521
C	-3.376862	-0.154754	0.595866
H	-4.124168	-0.959064	0.629727
H	-3.887285	0.803984	0.788321
H	-2.640686	-0.320043	1.400666

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entry05-reagent.xyz

C	0.134061	-1.180638	0.901721
H	-0.211715	-0.978526	1.921300
C	1.531825	-0.838771	0.630246
H	2.217783	-0.841050	1.478430
C	-0.752303	-1.656226	0.014958
H	-0.419722	-1.903197	-1.001143
C	1.962095	-0.471637	-0.591649
H	1.277886	-0.404568	-1.439955
C	-0.487221	1.752781	-0.779988
C	-1.623547	1.113291	-1.111280
H	-1.804058	0.960303	-2.184041
C	-2.725699	0.621528	-0.221570
H	-2.469531	0.786264	0.831370
H	-3.606487	1.245619	-0.455409
C	-2.210809	-1.830387	0.310383
H	-2.529893	-2.858465	0.070969
H	-2.377859	-1.678712	1.388947
C	-3.098707	-0.848656	-0.470283
H	-3.041363	-1.069605	-1.550873
H	-4.146519	-1.014035	-0.176502
C	-0.010800	2.024280	0.593196
O	-0.585969	1.731968	1.619364
H	0.979777	2.537459	0.637752
H	0.183002	2.086514	-1.576672
O	3.215015	-0.139899	-0.964080
C	4.200826	-0.188179	0.044325
H	5.147176	0.090101	-0.432010
H	4.280280	-1.202119	0.469946

H	3.970538	0.523149	0.855262
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entry05-TS.xyz

C	-0.170090	-1.224174	0.943127
H	-0.505601	-1.167482	1.981702
C	1.198475	-1.057398	0.706405
H	1.857033	-0.914269	1.562613
C	-1.142568	-1.243043	-0.067010
H	-0.864325	-1.742618	-0.999888
C	1.656545	-0.785418	-0.568879
H	1.082004	-1.056127	-1.452139
C	0.157245	1.172907	-0.872074
C	-1.108784	0.559277	-0.965907
H	-1.339359	0.215633	-1.984564
C	-2.367185	1.032834	-0.257760
H	-2.124068	1.326893	0.770626
H	-2.766748	1.912515	-0.787427
C	-2.606203	-1.322493	0.325265
H	-3.053914	-2.278501	0.016283
H	-2.672957	-1.265618	1.422803
C	-3.352338	-0.128219	-0.286482
H	-3.625041	-0.349270	-1.332608
H	-4.284027	0.091334	0.253513
C	0.617743	1.781696	0.353990
O	0.050952	1.680128	1.434630
H	1.592258	2.326548	0.280495
H	0.771582	1.307478	-1.763178
O	2.908925	-0.453275	-0.913565
C	3.803878	-0.132817	0.135845
H	4.727622	0.208055	-0.343353
H	4.015015	-1.017041	0.757768
H	3.391200	0.668743	0.769714

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entry06-adduct.xyz

C	-0.263937	-2.124017	0.955800
H	-0.484739	-2.735135	1.835214
C	1.000071	-1.806509	0.677225
H	1.814226	-2.149166	1.319062
C	-1.430873	-1.640935	0.146653
H	-1.989507	-2.518129	-0.227777
C	1.384331	-0.944463	-0.504476
H	1.535285	-1.590682	-1.394969
C	0.254684	0.020205	-0.869925

C	-1.034888	-0.801033	-1.083540
H	-0.759253	-1.477361	-1.909112
C	-2.317332	-0.024640	-1.452810
H	-2.092219	0.994824	-1.786125
H	-2.818124	-0.547126	-2.280059
C	-2.424999	-0.747712	0.911130
H	-3.065831	-1.334102	1.585054
H	-1.867357	-0.030060	1.528566
C	-3.219595	-0.026890	-0.191125
H	-4.156063	-0.564649	-0.400176
H	-3.473901	0.994977	0.113533
S	0.130849	1.405134	0.340227
O	-1.147703	2.107841	0.083294
O	0.437274	0.941153	1.706484
H	0.500699	0.547956	-1.805028
C	1.430712	2.534490	-0.159501
H	1.335199	3.369496	0.545633
H	2.390403	2.020688	-0.062834
H	1.228097	2.869602	-1.182976
O	2.577519	-0.216845	-0.286238
C	3.738004	-1.002777	-0.424116
H	3.814131	-1.421635	-1.444063
H	4.597886	-0.348273	-0.237299
H	3.763688	-1.834885	0.299523

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entry06-reagent.xyz

C	-0.475283	-1.671446	1.020812
H	-0.722862	-1.188357	1.970881
C	0.952050	-1.680753	0.707936
H	1.633466	-1.455704	1.528117
C	-1.495033	-2.064801	0.241978
H	-1.302123	-2.565480	-0.714941
C	1.428857	-1.803897	-0.545840
H	0.764855	-1.981556	-1.395649
C	-0.136114	0.901343	-1.195702
C	-1.405491	0.505705	-1.337304
H	-1.638667	0.043479	-2.306540
C	-2.581829	0.642178	-0.412536
H	-2.252236	0.923867	0.596580
H	-3.192647	1.471630	-0.812875
C	-2.920123	-1.719747	0.554861
H	-3.578510	-2.599944	0.471961
H	-2.978177	-1.365009	1.596613
C	-3.462601	-0.617450	-0.372389

H	-3.571589	-1.013109	-1.397627
H	-4.474341	-0.337853	-0.040870
S	0.566452	1.665491	0.253113
O	-0.148959	1.259985	1.482579
O	2.032437	1.500732	0.158306
H	0.622622	0.765981	-1.968386
C	0.219737	3.406777	0.004258
H	0.681912	3.921739	0.856092
H	0.678095	3.723222	-0.939530
H	-0.867358	3.547802	0.001350
O	2.705234	-1.725826	-0.956773
C	3.658384	-1.384459	0.035771
H	3.700673	-2.160146	0.818514
H	4.624860	-1.328549	-0.477004
H	3.403768	-0.409674	0.479538

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entry06-TS.xyz

C	-0.761090	-1.684735	0.987115
H	-1.064686	-1.486215	2.018835
C	0.607111	-1.759645	0.741157
H	1.296526	-1.674883	1.579965
C	-1.731285	-1.568262	-0.015012
H	-1.583838	-2.149300	-0.929174
C	1.086519	-1.651966	-0.562324
H	0.449652	-1.913769	-1.406088
C	0.115306	0.427733	-1.009256
C	-1.264070	0.174057	-1.012921
H	-1.605202	-0.177521	-1.995700
C	-2.353689	0.955068	-0.300114
H	-2.027764	1.218109	0.716245
H	-2.563262	1.886689	-0.852835
C	-3.163058	-1.266118	0.374402
H	-3.845200	-2.079359	0.086470
H	-3.210908	-1.168576	1.470043
C	-3.591281	0.064482	-0.266946
H	-3.934750	-0.108571	-1.300979
H	-4.425408	0.529209	0.277137
S	0.859772	1.427962	0.231394
O	0.201928	1.181803	1.536795
O	2.332251	1.302035	0.121103
H	0.725340	0.390423	-1.911536
C	0.482943	3.123129	-0.227575
H	0.961467	3.747130	0.538209
H	0.915354	3.316191	-1.215894

H	-0.604342	3.260050	-0.220329
O	2.366200	-1.640513	-0.938992
C	3.356429	-1.568304	0.081987
H	3.312365	-2.467432	0.716816
H	4.317144	-1.534722	-0.442451
H	3.225119	-0.654077	0.674632

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entry07-adduct.xyz

C	-0.370401	1.975273	-0.452763
H	-0.633651	2.770525	-1.156408
C	0.906255	1.792698	-0.113654
H	1.690041	2.434377	-0.521535
C	-1.504015	1.184247	0.125820
H	-2.056620	1.874882	0.788889
C	1.341206	0.735297	0.869078
H	1.275991	1.149831	1.890073
C	0.372114	-0.470147	0.875431
C	-1.085905	-0.032418	1.006927
H	-1.171881	0.266517	2.062874
C	-2.127343	-1.139511	0.704300
H	-1.695698	-1.904581	0.042430
H	-2.466037	-1.648459	1.616544
C	-2.533656	0.631135	-0.873590
H	-3.200658	1.414334	-1.260990
H	-2.014111	0.158195	-1.718320
C	-3.263021	-0.424065	-0.040435
H	-3.933541	0.072843	0.680019
H	-3.871905	-1.112149	-0.641925
H	0.668683	-1.150561	1.681021
O	2.679395	0.320973	0.741671
C	3.205215	0.204920	-0.572696
H	3.875968	-0.663189	-0.578448
H	3.779664	1.107291	-0.839779
H	2.424486	0.051449	-1.333275
N	0.627241	-1.280789	-0.364815
O	1.382788	-2.219896	-0.256158
O	0.099803	-0.926123	-1.401510

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entry07-reagent.xyz

C	-0.276494	-1.391025	0.910637
H	-0.574996	-1.118582	1.928591
C	1.151615	-1.236588	0.630921
H	1.806834	-1.098666	1.491367

C	-1.247743	-1.731056	0.048528
H	-0.993183	-2.035141	-0.974338
C	1.648792	-1.125929	-0.615650
H	1.012369	-1.220114	-1.498907
C	-0.171758	1.461213	-0.921519
C	-1.442587	1.086257	-1.101444
H	-1.689607	0.914078	-2.157049
C	-2.601711	0.915828	-0.165142
H	-2.290010	1.030869	0.877950
H	-3.294804	1.742819	-0.400364
C	-2.704459	-1.593868	0.368871
H	-3.258804	-2.511982	0.115313
H	-2.818789	-1.431793	1.452886
C	-3.348268	-0.412097	-0.378472
H	-3.400311	-0.636342	-1.458336
H	-4.388014	-0.299306	-0.035970
H	0.547579	1.581329	-1.727529
O	2.918016	-0.875344	-0.979473
C	3.825745	-0.599325	0.071396
H	4.787161	-0.377675	-0.404090
H	3.933858	-1.472115	0.736444
H	3.480967	0.270493	0.652740
N	0.458951	1.729557	0.362321
O	1.631641	2.051484	0.314290
O	-0.183619	1.613207	1.387219

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entry07-TS.xyz

C	-0.451179	-1.370901	0.940429
H	-0.777439	-1.275719	1.979694
C	0.928202	-1.330950	0.706732
H	1.594035	-1.222417	1.562139
C	-1.427178	-1.299716	-0.061766
H	-1.207848	-1.811705	-1.003172
C	1.418045	-1.140009	-0.572656
H	0.829636	-1.400816	-1.451518
C	0.157218	0.933246	-0.901848
C	-1.178179	0.512583	-0.934867
H	-1.444787	0.210761	-1.956826
C	-2.375742	1.121418	-0.226053
H	-2.116256	1.382876	0.805994
H	-2.669499	2.041993	-0.754913
C	-2.887648	-1.204670	0.331057
H	-3.451098	-2.094666	0.015397
H	-2.948595	-1.148254	1.429017

C	-3.484459	0.077293	-0.271595
H	-3.778123	-0.099540	-1.320252
H	-4.385715	0.398267	0.268725
H	0.796376	1.029629	-1.773481
O	2.682403	-0.894094	-0.910414
C	3.600660	-0.603745	0.141025
H	4.533810	-0.315824	-0.353429
H	3.769309	-1.500509	0.758016
H	3.233014	0.230505	0.753014
N	0.728533	1.528319	0.251947
O	1.851922	2.012809	0.149066
O	0.106302	1.470020	1.308250

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entry08-adduct.xyz

C	-0.350577	-1.862752	0.975706
H	-0.587966	-2.306995	1.946352
C	0.926607	-1.728204	0.604261
H	1.732815	-2.063123	1.255785
C	-1.507614	-1.481508	0.094424
H	-1.827341	-2.408506	-0.414807
C	1.247698	-1.094401	-0.731883
H	0.996809	-1.819569	-1.531899
C	0.271680	0.078186	-0.942343
C	-1.161377	-0.447325	-1.032264
H	-1.173535	-0.981675	-1.994758
C	-2.317112	0.580135	-1.035029
H	-2.047560	1.485494	-0.477474
H	-2.583691	0.885280	-2.055860
C	-2.742676	-0.907472	0.808895
H	-3.362690	-1.694762	1.260253
H	-2.423673	-0.212834	1.597828
C	-3.459085	-0.139920	-0.304995
H	-3.955328	-0.850122	-0.987565
H	-4.223370	0.554305	0.068536
S	0.497192	1.277603	0.414128
O	-0.554694	1.211606	1.418329
O	1.889899	1.413720	0.802343
H	0.568275	0.653048	-1.829889
O	2.557749	-0.643553	-0.976525
C	3.571982	-0.974945	-0.054067
H	3.700727	-2.066898	0.047330
H	4.495633	-0.551505	-0.466396
H	3.386730	-0.522050	0.931736
F	0.147589	2.608146	-0.469403

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entry08-reagent.xyz

C	0.451837	-1.677141	-1.004806
H	0.706190	-1.258357	-1.983939
C	-0.975561	-1.664245	-0.691371
H	-1.661159	-1.511902	-1.525099
C	1.466595	-2.038492	-0.203446
H	1.263706	-2.491174	0.775227
C	-1.449928	-1.698444	0.570148
H	-0.782887	-1.805301	1.429204
C	0.169494	0.955962	1.188469
C	1.440929	0.558726	1.313012
H	1.685310	0.143000	2.300059
C	2.605729	0.651799	0.373412
H	2.279301	0.917843	-0.639890
H	3.223309	1.485731	0.751821
C	2.897988	-1.736874	-0.530553
H	3.533399	-2.630651	-0.420602
H	2.961800	-1.416964	-1.583053
C	3.467911	-0.620369	0.362275
H	3.580780	-0.990589	1.396392
H	4.479871	-0.364848	0.013978
S	-0.549970	1.629715	-0.265961
O	0.176169	1.305779	-1.484406
O	-1.997743	1.526878	-0.178368
H	-0.573111	0.878477	1.982695
O	-2.724647	-1.599240	0.976670
C	-3.688050	-1.362756	-0.035982
H	-3.718391	-2.203329	-0.748588
H	-4.652965	-1.276760	0.474589
H	-3.455504	-0.426996	-0.566544
F	-0.224670	3.200004	0.004556

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entry08-TS.xyz

C	-0.689138	-1.689717	0.962360
H	-0.997124	-1.511790	1.996814
C	0.684923	-1.750480	0.727454
H	1.360059	-1.666240	1.577934
C	-1.666488	-1.584627	-0.035198
H	-1.505204	-2.158332	-0.951875
C	1.185192	-1.640811	-0.563325
H	0.568643	-1.889082	-1.426090
C	0.088284	0.475607	-1.039626

C	-1.277001	0.160604	-1.008217
H	-1.621490	-0.193884	-1.988084
C	-2.370390	0.919056	-0.279968
H	-2.040600	1.186722	0.733504
H	-2.584084	1.852114	-0.824398
C	-3.105804	-1.332209	0.371019
H	-3.762170	-2.163224	0.075456
H	-3.145936	-1.256863	1.468623
C	-3.582650	-0.003335	-0.241045
H	-3.942012	-0.169038	-1.270560
H	-4.418406	0.427446	0.327163
S	0.798731	1.428139	0.206926
O	0.229259	1.134009	1.519594
O	2.240711	1.546758	0.016516
H	0.697480	0.467753	-1.940873
O	2.465382	-1.557610	-0.913632
C	3.426211	-1.387089	0.125563
H	3.449336	-2.278578	0.771024
H	4.389958	-1.269274	-0.379264
H	3.202492	-0.484983	0.709409
F	0.214191	2.918864	-0.142613

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entry09-adduct.xyz

C	2.275390	0.509327	1.608228
H	2.488132	0.294471	2.660158
C	1.600229	1.613277	1.277755
H	1.266601	2.304770	2.053447
C	2.831020	-0.437544	0.584713
H	3.905627	-0.196217	0.495190
C	1.316235	1.957187	-0.163481
H	2.229331	2.403579	-0.596812
C	1.023926	0.674003	-0.987870
C	2.218411	-0.294874	-0.849856
H	3.004556	0.143962	-1.483281
C	1.972516	-1.741979	-1.328907
H	0.924025	-2.028726	-1.155830
H	2.169743	-1.863611	-2.402995
C	2.758829	-1.937413	0.925821
H	3.542192	-2.242492	1.633962
H	1.787764	-2.193408	1.380620
C	2.880479	-2.605325	-0.445781
H	3.924580	-2.539229	-0.794553
H	2.595741	-3.666300	-0.442906
H	0.994615	1.000876	-2.038301

O	0.311929	2.932772	-0.375763
C	-0.715960	3.049506	0.586537
H	-1.556042	3.546328	0.083417
H	-0.405190	3.674761	1.441733
H	-1.062456	2.073897	0.964723
C	-0.363939	0.153671	-0.680026
C	-1.419547	0.566580	-1.502462
C	-0.661819	-0.653662	0.431126
C	-2.732986	0.200286	-1.222560
H	-1.200675	1.201848	-2.362518
C	-1.969341	-1.024727	0.713977
H	0.142312	-0.979445	1.088338
C	-3.014137	-0.594984	-0.111023
H	-3.547944	0.535132	-1.869512
H	-2.211481	-1.648338	1.575783
C	-4.410560	-0.987325	0.195684
O	-4.730539	-1.670165	1.138145
H	-5.175011	-0.598746	-0.520973

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entry09-reagent.xyz

C	-1.161543	1.397033	-1.272058
H	-1.076161	0.856557	-2.222831
C	0.102089	1.884968	-0.709008
H	0.912208	2.093615	-1.409173
C	-2.385020	1.539226	-0.741190
H	-2.506901	2.118166	0.182440
C	0.293564	2.008758	0.614669
H	-0.482546	1.730393	1.332109
C	-1.404123	-1.364339	1.735568
C	-2.646790	-1.347095	1.224269
H	-3.458937	-1.322535	1.961067
C	-3.125421	-1.334919	-0.199358
H	-2.287583	-1.196416	-0.894936
H	-3.566606	-2.323038	-0.414864
C	-3.618763	0.913949	-1.320438
H	-4.406708	1.673993	-1.448937
H	-3.383509	0.520888	-2.323539
C	-4.175087	-0.231583	-0.457167
H	-4.532737	0.175381	0.503383
H	-5.057576	-0.651617	-0.962463
H	-1.328342	-1.321606	2.826702
O	1.406179	2.426147	1.255159
C	2.486889	2.804621	0.430993
H	3.289378	3.137147	1.098904

H	2.197508	3.626592	-0.244587
H	2.833089	1.949534	-0.175297
C	-0.100785	-1.357354	1.048375
C	0.990228	-0.792932	1.728723
C	0.114691	-1.877683	-0.242457
C	2.232817	-0.675886	1.119379
H	0.845258	-0.405276	2.739161
C	1.352046	-1.754436	-0.856993
H	-0.689712	-2.402594	-0.755253
C	2.414422	-1.137129	-0.185591
H	3.063789	-0.208685	1.654338
H	1.528247	-2.142612	-1.861337
C	3.730273	-0.994818	-0.850281
O	3.967846	-1.361649	-1.975658
H	4.518719	-0.506167	-0.225483

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entry09-TS.xyz

C	-2.051054	0.549885	-1.539451
H	-1.918284	-0.110482	-2.402768
C	-1.038974	1.481206	-1.289975
H	-0.193716	1.513943	-1.976613
C	-3.070154	0.243077	-0.634008
H	-3.503445	1.071138	-0.066753
C	-0.951398	2.131212	-0.067888
H	-1.836269	2.336636	0.531674
C	-0.884037	0.238124	1.308152
C	-2.113687	-0.406662	1.087310
H	-2.890273	-0.019653	1.759134
C	-2.386468	-1.865391	0.773805
H	-1.698137	-2.262958	0.016381
H	-2.248703	-2.468713	1.685901
C	-3.959932	-0.954384	-0.890674
H	-5.009481	-0.660240	-1.038408
H	-3.623334	-1.442502	-1.819295
C	-3.827594	-1.947678	0.277741
H	-4.501242	-1.650882	1.099000
H	-4.112439	-2.966308	-0.020949
H	-0.872361	0.971322	2.116996
O	0.087835	2.884868	0.342471
C	1.237422	2.905989	-0.489125
H	2.000301	3.466052	0.062698
H	1.016416	3.419014	-1.439689
H	1.605807	1.888099	-0.694598
C	0.450119	-0.188806	0.901642

C	1.554726	0.319483	1.615565
C	0.706871	-1.008030	-0.220973
C	2.855133	0.026603	1.229087
H	1.370292	0.961828	2.478606
C	2.005748	-1.285096	-0.615134
H	-0.124399	-1.388030	-0.812046
C	3.092177	-0.772253	0.106389
H	3.700481	0.426554	1.795739
H	2.214811	-1.902207	-1.490596
C	4.474727	-1.075887	-0.318722
O	4.761129	-1.747767	-1.281618
H	5.270529	-0.627760	0.326320

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entry10-adduct.xyz

C	0.222250	-1.879867	0.128916
C	1.462963	-1.520768	-0.208431
C	1.771965	-0.234009	-0.926628
C	0.681419	0.826377	-0.626764
C	-0.714508	0.251801	-0.908523
C	-1.016867	-1.101360	-0.206358
H	0.871873	1.662529	-1.323118
H	-0.714618	0.040482	-1.992610
H	-1.561439	-1.724028	-0.942567
H	1.750374	-0.416006	-2.014367
C	-1.839370	1.269155	-0.654533
H	-1.702390	1.747023	0.327251
H	-1.790321	2.064642	-1.414281
C	-3.194288	0.564594	-0.681032
H	-4.014406	1.296799	-0.678138
H	-3.281190	0.006569	-1.629128
C	-1.971542	-0.936864	0.984251
H	-1.509071	-0.251006	1.705354
H	-2.101309	-1.905762	1.491191
C	-3.334265	-0.398168	0.514728
H	-3.824070	0.118590	1.353811
H	-3.995010	-1.233648	0.234526
O	3.072214	0.283246	-0.683406
C	3.659389	-0.000440	0.569666
H	4.419542	0.773043	0.742459
H	2.932164	0.024158	1.399155
H	4.155720	-0.985619	0.577477
H	0.067086	-2.836842	0.637543
H	2.300863	-2.187502	0.006944
C	0.914938	1.408942	0.749011

O	0.216481	1.250690	1.720291
H	1.834139	2.038723	0.817603

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entry10-reagent.xyz

C	0.288025	-1.208200	0.943000
C	1.695948	-0.923271	0.644275
C	2.127306	-0.617049	-0.592395
C	-0.122127	1.830207	-0.896630
C	-1.394806	1.398950	-0.944284
C	-0.599791	-1.742397	0.093317
H	0.420625	2.015792	-1.827235
H	-1.837642	1.265844	-1.940222
H	-0.254392	-2.059844	-0.898932
H	1.438573	-0.549860	-1.437988
C	-2.296104	1.106499	0.218219
H	-1.701009	0.739302	1.063421
H	-2.720308	2.066223	0.564354
C	-3.435712	0.149003	-0.131112
H	-4.076319	0.036419	0.758759
H	-4.070210	0.603223	-0.911800
C	-2.056430	-1.977878	0.375814
H	-2.290316	-1.694860	1.415942
H	-2.249845	-3.060432	0.294076
C	-2.997131	-1.241801	-0.599113
H	-3.903529	-1.845332	-0.760928
H	-2.501879	-1.169521	-1.583549
O	3.387992	-0.332413	-0.982952
C	4.377574	-0.379861	0.021716
H	5.329782	-0.147628	-0.467479
H	4.174808	0.363436	0.811142
H	4.427322	-1.381886	0.479437
H	-0.046422	-0.934451	1.950243
H	2.388088	-0.913556	1.487420
C	0.632156	2.073343	0.351569
O	0.168196	2.024729	1.470164
H	1.709734	2.323322	0.199389

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entry10-TS.xyz

C	0.049859	-1.242865	0.992487
C	1.415732	-1.078975	0.738149
C	1.872193	-0.879813	-0.550909
C	0.428164	1.064195	-0.952223
C	-0.897700	0.615562	-0.804830

C	-0.938756	-1.263086	0.003217
H	0.905023	1.047445	-1.933108
H	-1.350518	0.315902	-1.758015
H	-0.665052	-1.700787	-0.962205
H	1.301407	-1.210884	-1.415556
C	-1.900256	1.261781	0.142595
H	-1.610194	1.056935	1.180071
H	-1.848333	2.356425	0.035850
C	-3.325590	0.774493	-0.149778
H	-3.966362	1.026832	0.709482
H	-3.738970	1.317704	-1.015270
C	-2.379281	-1.513847	0.413657
H	-2.499871	-1.251572	1.478269
H	-2.583206	-2.594131	0.331860
C	-3.394614	-0.735502	-0.422028
H	-4.410511	-1.107039	-0.222833
H	-3.201323	-0.942054	-1.487984
O	3.128660	-0.572761	-0.912866
C	4.033212	-0.230243	0.121780
H	4.958498	0.082721	-0.373378
H	3.637361	0.595728	0.734308
H	4.236343	-1.098309	0.768897
H	-0.270100	-1.188332	2.036865
H	2.080286	-0.902177	1.583230
C	1.107307	1.784099	0.105544
O	0.684260	1.903385	1.245434
H	2.100539	2.215796	-0.176997

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entry11-adduct.xyz

C	0.526473	-1.876754	-0.288130
C	1.763536	-1.450603	-0.551640
C	2.078926	-0.033275	-0.943964
C	0.960381	0.922522	-0.465798
C	-0.420900	0.389751	-0.879382
C	-0.728301	-1.049174	-0.384636
H	1.140576	1.878808	-0.991015
H	-0.359061	0.306584	-1.980231
H	-1.312845	-1.528793	-1.193176
H	2.108703	0.031105	-2.044656
C	-1.515559	1.421778	-0.583858
H	-1.475286	1.709583	0.478154
H	-1.269491	2.327644	-1.161428
C	-2.944677	0.976009	-0.917064
H	-3.536645	1.865475	-1.181048

H	-2.945471	0.332383	-1.815266
C	-1.604012	-1.191850	0.877722
H	-1.304512	-0.449019	1.629869
H	-1.395053	-2.181236	1.316899
C	-3.106398	-1.117992	0.591332
H	-3.654731	-1.491015	1.470988
H	-3.340310	-1.815054	-0.234034
O	3.362003	0.419548	-0.534511
C	3.888472	-0.128579	0.656052
H	4.653474	0.574129	1.012639
H	3.126189	-0.253327	1.443975
H	4.365491	-1.107649	0.483016
H	0.379133	-2.929860	-0.026828
H	2.597841	-2.155515	-0.526248
C	-3.647145	0.267696	0.243551
H	-4.721576	0.176536	0.016501
H	-3.573585	0.916524	1.134082
C	1.151950	1.270101	0.993201
O	0.388223	1.026733	1.895371
H	2.098865	1.824668	1.196599

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entry11-reagent.xyz

C	-0.813419	-1.864243	-0.579181
C	-2.045614	-1.070354	-0.631302
C	-2.817193	-0.847638	0.444089
C	0.554832	1.679678	1.293640
C	1.856526	1.710259	0.957355
C	0.047974	-1.867582	0.447700
H	0.289584	1.593037	2.350987
H	2.577016	1.640714	1.783453
H	-0.172562	-1.236526	1.318506
H	-2.646157	-1.361929	1.393210
C	2.467662	1.813512	-0.404495
H	1.684585	1.936147	-1.160791
H	3.093589	2.722821	-0.412375
C	3.357770	0.608218	-0.758316
H	3.838715	0.831182	-1.722303
H	4.174518	0.509627	-0.021029
C	1.384430	-2.547335	0.454585
H	1.478397	-3.202456	-0.427457
H	1.484319	-3.186274	1.347022
C	2.509317	-1.498176	0.454287
H	3.480072	-1.987199	0.637483
H	2.342076	-0.812493	1.302202

O	-3.858282	0.009263	0.541249
C	-4.104192	0.809196	-0.599701
H	-4.904120	1.504920	-0.323419
H	-3.196078	1.364010	-0.892928
H	-4.434334	0.189821	-1.450388
H	-0.551396	-2.430348	-1.480481
H	-2.275982	-0.590983	-1.584252
C	2.574052	-0.707381	-0.854734
H	3.018642	-1.353998	-1.628870
H	1.549070	-0.478145	-1.192387
C	-0.605451	1.730851	0.373650
O	-0.571668	1.869295	-0.830129
H	-1.590520	1.625578	0.889392

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entry11-TS.xyz

C	0.260310	-1.349092	0.936490
C	1.632537	-1.138835	0.746051
C	2.160028	-0.958112	-0.515610
C	0.643126	0.958497	-1.048961
C	-0.670597	0.591052	-0.707667
C	-0.694538	-1.350549	-0.081632
H	0.989698	0.828903	-2.075805
H	-1.272229	0.325137	-1.582931
H	-0.367253	-1.681400	-1.071865
H	1.654360	-1.323617	-1.406938
C	-1.471809	1.338377	0.355212
H	-1.362272	0.867357	1.344206
H	-1.038487	2.340319	0.470510
C	-2.944789	1.459171	-0.038520
H	-3.405292	2.273649	0.542437
H	-2.997334	1.775580	-1.095837
C	-2.113326	-1.758932	0.266676
H	-2.264655	-1.619151	1.350714
H	-2.171443	-2.847205	0.095387
C	-3.284045	-1.096849	-0.476195
H	-4.120761	-1.812272	-0.470133
H	-3.034348	-0.942380	-1.540162
O	3.422377	-0.603195	-0.804415
C	4.231294	-0.167803	0.277438
H	5.160183	0.204017	-0.167823
H	3.733117	0.636378	0.841226
H	4.458079	-1.006041	0.955386
H	-0.099853	-1.348716	1.969493
H	2.246264	-0.938723	1.623445

C	-3.794098	0.203664	0.158419
H	-4.804472	0.409620	-0.230199
H	-3.917020	0.021699	1.241031
C	1.495667	1.730933	-0.167522
O	1.261295	1.975586	1.007013
H	2.445779	2.088578	-0.638004

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entry12-adduct.xyz

C	1.497767	-1.048088	0.456986
H	1.123841	-1.564622	1.355170
C	0.874796	-1.632008	-0.784032
H	1.445779	-2.367362	-1.361662
C	-0.320067	-1.224243	-1.212996
H	-0.747577	-1.617988	-2.139922
C	-1.175794	-0.293527	-0.378515
O	-1.849180	-1.041819	0.637507
C	-2.682866	-2.078175	0.175128
H	-3.172117	-2.505006	1.059363
H	-3.460689	-1.703175	-0.513693
H	-2.107203	-2.870904	-0.331132
C	-2.135590	0.521784	-1.260762
H	-2.991166	0.844149	-0.644482
H	-2.521652	-0.048868	-2.117659
C	3.024190	-1.040941	0.362618
H	3.442406	-2.016723	0.074044
H	3.444951	-0.772953	1.343277
C	-1.293077	1.727979	-1.663159
H	-0.525336	1.417218	-2.391102
H	-1.878358	2.538694	-2.117839
C	3.310741	0.065288	-0.670839
H	4.279006	0.552592	-0.494739
H	3.352259	-0.368031	-1.681549
C	-0.640592	2.125482	-0.336331
H	0.246531	2.759687	-0.451889
H	-1.374901	2.702781	0.251132
C	2.120388	1.052994	-0.567054
H	1.610518	1.137448	-1.538249
H	2.449566	2.063087	-0.286818
C	1.176802	0.459343	0.504620
H	1.506180	0.819488	1.489273
C	-0.321823	0.789753	0.395477
C	-0.919012	0.900354	1.804149
O	-0.302655	0.776835	2.828587
H	-2.002527	1.164390	1.817984

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entry12-reagent.xyz

C	1.917288	-1.323467	0.429144
H	1.334157	-1.087464	1.321118
C	1.303546	-1.832353	-0.655881
H	1.934795	-2.058337	-1.523963
C	-0.126297	-1.867668	-0.930839
H	-0.400126	-2.023744	-1.977333
C	-1.110015	-1.390999	-0.140518
O	-0.851448	-1.177768	1.179256
C	-1.933405	-1.199433	2.094783
H	-1.485424	-1.355058	3.083167
H	-2.479081	-0.244155	2.111184
H	-2.623757	-2.029775	1.876979
C	-2.378818	-0.832482	-0.741651
H	-2.972191	-0.359882	0.052786
H	-3.012542	-1.634082	-1.151592
C	3.312350	-0.791009	0.354594
H	3.791955	-1.147536	-0.571627
H	3.939227	-1.118269	1.199383
C	-2.100055	0.201252	-1.867819
H	-2.062004	-0.322266	-2.835318
H	-2.976779	0.865446	-1.932019
C	3.273267	0.756764	0.345761
H	3.106678	1.121032	1.373462
H	4.263198	1.130224	0.042733
C	-0.801055	1.044109	-1.764015
H	0.033949	0.485495	-2.208102
H	-0.940597	1.937418	-2.397544
C	2.189937	1.368703	-0.565857
H	2.091402	0.791324	-1.498437
H	2.525354	2.380907	-0.855994
C	0.862684	1.546706	0.116075
H	0.918138	1.868867	1.163815
C	-0.390935	1.461802	-0.370962
C	-1.482069	1.855376	0.561648
O	-1.364184	2.029385	1.753691
H	-2.479832	2.003116	0.076955

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entry12-TS.xyz

C	1.492710	-1.128970	-0.543475
H	0.808596	-1.812139	-0.038362
C	1.068495	-0.440161	-1.675821

H	1.845162	-0.001084	-2.313181
C	-0.220254	0.074660	-1.852489
H	-0.314935	0.953095	-2.493995
C	-1.304762	-0.206418	-1.032871
O	-1.439278	-1.471982	-0.589672
C	-2.676782	-1.896312	-0.045631
H	-2.552519	-2.964456	0.160589
H	-2.917824	-1.386376	0.897314
H	-3.490820	-1.749826	-0.773210
C	-2.364201	0.848828	-0.825833
H	-3.037836	0.556310	-0.009232
H	-2.985869	0.962387	-1.730497
C	2.974931	-1.198577	-0.256770
H	3.526239	-1.696175	-1.069083
H	3.139392	-1.796365	0.650443
C	-1.684776	2.187270	-0.497316
H	-1.121789	2.522581	-1.379781
H	-2.454055	2.954002	-0.316715
C	3.503414	0.245574	-0.043139
H	4.330720	0.236200	0.681142
H	3.923571	0.643003	-0.978862
C	-0.725919	2.095909	0.721390
H	0.073863	2.840634	0.601960
H	-1.292194	2.408633	1.615796
C	2.352127	1.164882	0.438759
H	2.014582	1.828976	-0.371821
H	2.695313	1.815813	1.259745
C	1.195255	0.320886	0.906744
H	1.459522	-0.449333	1.638209
C	-0.138991	0.735105	1.030220
C	-0.951560	-0.145921	1.863089
O	-0.665775	-1.290681	2.170158
H	-1.926819	0.294904	2.204513