Pushing the limits of concertedness. A waltz of wandering carbocations.

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Contents

1 IRCs

Intrinsic Reaction Coordinate calculations (IRCs) provide a simple way of exploring the potential energy surface (PES) of a reacting system, locating the minimum energy path connecting reactant, transition state and products. It helps ensuring that a given transition state structure corresponds to the desired transformation (as this path is followed from TS to reactants and products both) and also can provide information about hidden intermediates or other features of the PES.

1.1 IRCs perfomed on the complete terpene and its simplified structure, system B, ensuring the maintainance of the triterpene reactivity.

As it has been demonstrated before,[1–3] partial simplification of the terpene structures, in strategic positions, allows for the analysis of the chemical behaviour of these species at a lower computational cost without significantly altering the reactivity of the system or the accuracy of the reactivity predictions. We find that this is also the case in the system under study, as truncation of the two cyclohexane rings in **system A** by replacing them with methyl groups in **system B** leads to very similar optimized structures for minima and transition states, as well as intrinsic reaction coordinate (IRC) profiles (see Figure S1)

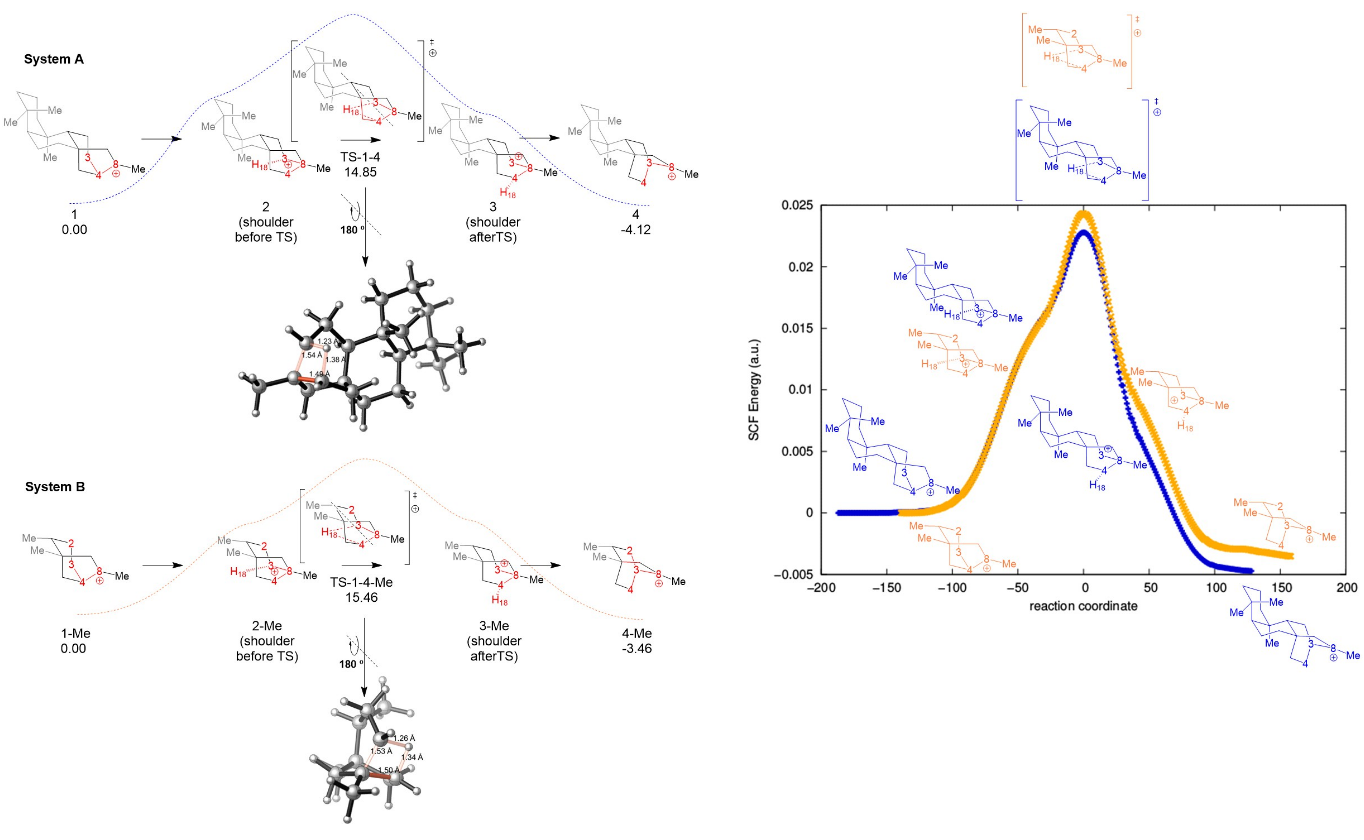


Figure S1 IRCs performed on the terpene proposed by Tantillo et al. (blue) and its simplification (R=Me) (yellow) at the B3LYP/6-31+G(d,p) computational level (gas phase). The blue line corresponds to the terpene while the yellow line corresponds to its simplified structure.

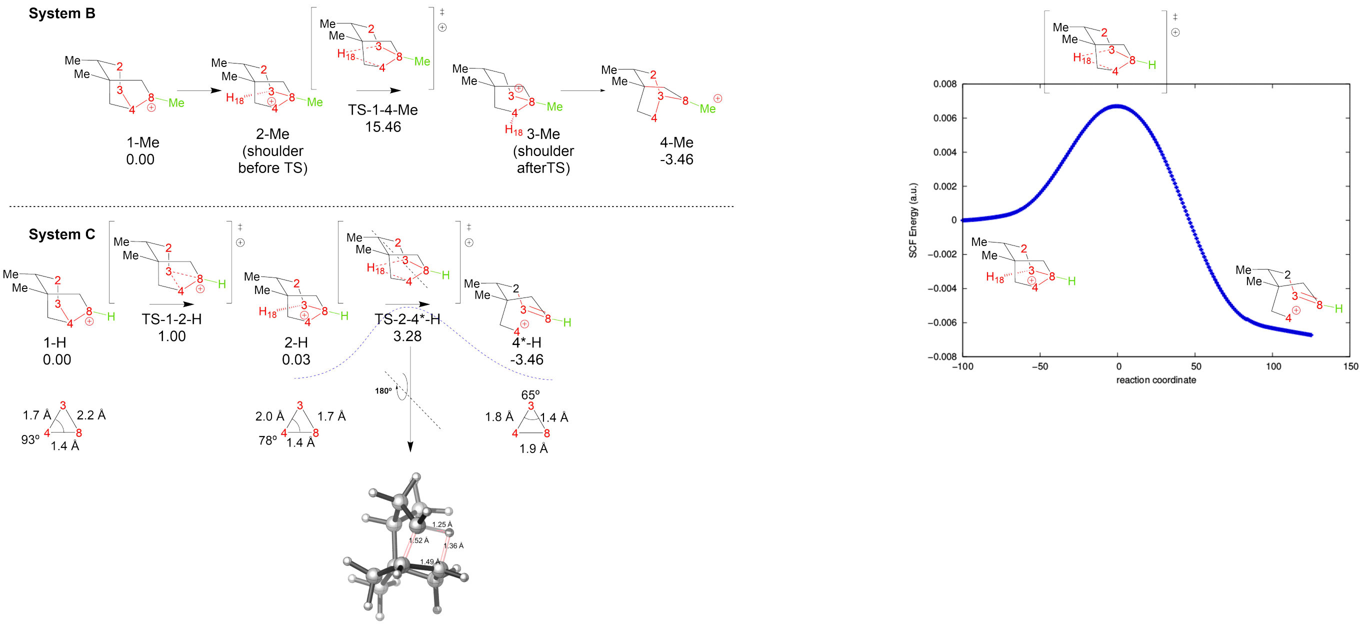


Figure S2 IRC performed on **sytem C**, for the **2**⟶**4*** transformation at the B3LYP/6-31+G(d,p) computational level.

1.2 IRCs corresponding to system C.

The structural modification transforming **system B** into **system C**, involving the replacement of a methyl group by a hydrogen to yield a secondary carbocation, resulted in changes in the mechanism. The main feature is that now we have a two-step process where just a single transition structure could be found before. This is a result of **2-H** becoming an actual minimum in the PES, instead of just a shoulder on the IRC. Once the transition state for the H-shift has been reached, the C4-C8 bond breaks, but a C3-C4 bond is not formed, with the result that the product obtained from the reaction of **1-H** is **4*-H** instead of a hypotetical **4-H**.

To ensure the connection between the minima **2-H** and **4*-H**, **system C**, we ran another IRC starting from **TS-2-4*-H**.

2 Structural analysis of intermediates in system B and system C

The structures of **1-Me** and **4-Me** seem to belong to classical carbocations, as expected by their tertiary nature. However, a detailed analysis of the interatomic distances results indicative of the delocalization of the electron density of the C-C bonds over the carbenium center. Thus, the C8-C4 and C3-C4 distances in **1-Me** are 1.5 and 1.6 Å, respectively, while the C3-C4, C2-C3 and C3-C8 distances in **4-Me** are 1.6, 1.6 and 1.4 Å, respectively. The C-C-C angles, however, do not deviate significantly from the expected sp^3 value (109°), as depicted in Figure S3. The values of 101.4° for C3-C4-C8 in **1-Me** or 99° for C4-C3-C8 in **4-Me** reinforce that delocalization through hyperconjugation is strong. Even if these structures cannot be considered non-classical carbocations, the electron delocalization found marked them as a strategical point in the goal of pushing the limits of concertedness. Thus, the strategy of destabilizing these tertiary species towards secondary ones can achieve two goals: 1) making them more reactive and 2) equipping them with a greater number of chemically equivalent atoms. These two facts together are expected to improve their willingness to evolve through more chemical events.

Despite the analysis of the IRC indicating that our starting hypothesis for **system C** was not accurate -we did not find any extra chemical event and the process went from concerted to stepwise - interesting patterns are found from the structural analysis of the intervening carbocations. On the one hand, the bond distances do not suffer a dramatic change, the values for C3-C4, C3-C8 and C4-C8 are 1.7, 2.2, 1.4 Å in **1-H**, 2.0, 1.7, 1.4 Å in **2-H** and 1.8, 1.4, 1.9 Å in **4*-H**. The comparison between bond distances reveals that even if there are some changes, the bond distances get elongated, but for the putative double bond (C4-C8 in the reactant region, C3-C8 in the product region), they are not extremely significant. However, when we look at the angles instead, differences emerge. Thus C3-C4-C8 sharpens to 93° in **1-H** and even to 78° in **2-H**, what's more in **4*-H** C3-C4-C8 is only of 44°, 55° less than in its homologous **4-Me**.

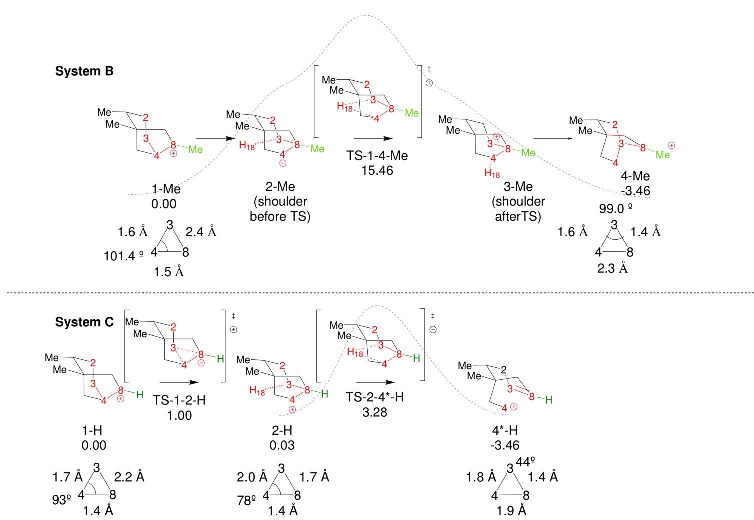


Figure S3 Analysis of some of the representative geometric parameters in reactants and products for **system B**. Optimizations were performed at the B3LYP/6-31+G(d,p) computational level.

3 Analysis of the variation of the main internal coordinates on non-recrossing trajectories

As described in the main text, analysis of internal coordinates (we focus on C–C and C–H distances) can provide information about the connectivity of the atoms and, as a result, about the structures that are visited along a given trajectory. In the following subsections, we provide a comprehensive representation of most C–C and C–H distances of interest along time for all the non-recrossing trajectories calculated.

3.1 System B.

In this section we provide the same plots included in the main text (variation of C3-C4, C3-C8, C3-H18, C4-H18, C4-C8 with time in the full time-frame, see Figures S4-S6) to which we add plots for C4-H19, C7-H25, C2-H16, C5-H20, C7-H26, C3-H17, C2-H15, C5-H21, C2-C3, C8-C7, and C4-C5, see Figures S7-S8. The variation with time of C3-H18, C4-H18, C3-C8, C3-C4 and C4-C8 are key indicators of the studied triple shift rearrangement evolution, while the other bonds provide valuable information as to whether the reactivity of the system is confined to the expected triple shift or if other chemical events are also taking place, after or instead this triple shift. If those bonds located in the proximity of the active core of the molecule stay inaltered with time, we can asume that we face a *confined* reactivity (see Figure S9 for the identification of the most relevant bonds), if they change significantly with time, however, new chemical events must be present along the reaction paths.

We will not discuss here the variation of C3-C4, C3-C8, C3-H18, C4-H18 and C4-C8, as it has been done in detail in the main text; we just include here the corresponding plots in the full time frame in order to ensure that once the reactant or product basin has been reached, the expected values for these variables are maintained and the system does not evolve further (See Figures S4 and S5).

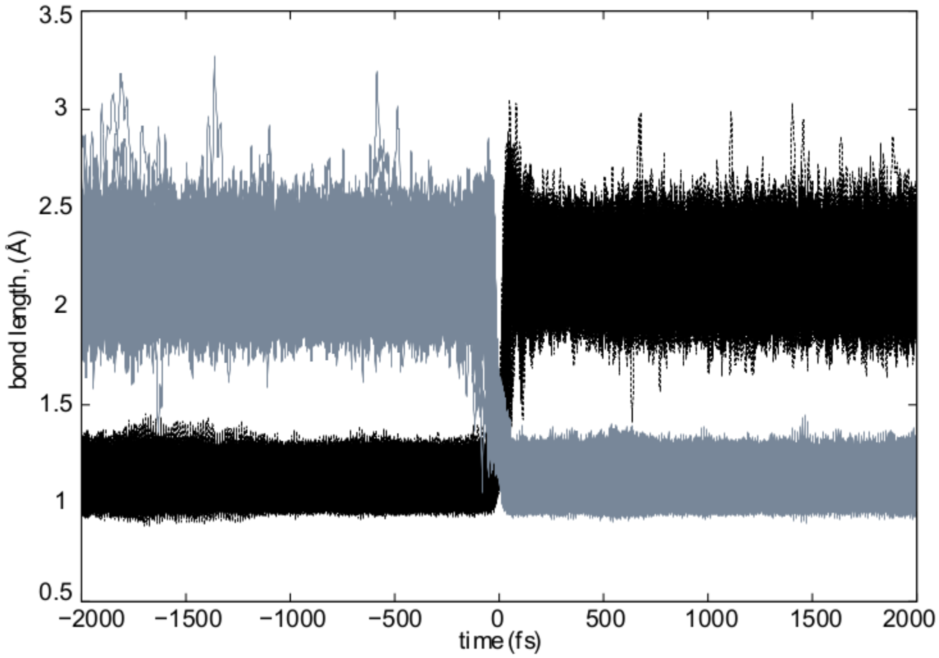


Figure S4 Variation of C3-H18 (black lines) and C4-H18 (grey lines) distances with time along the non-recrossing trajectories, in the full time-frame.

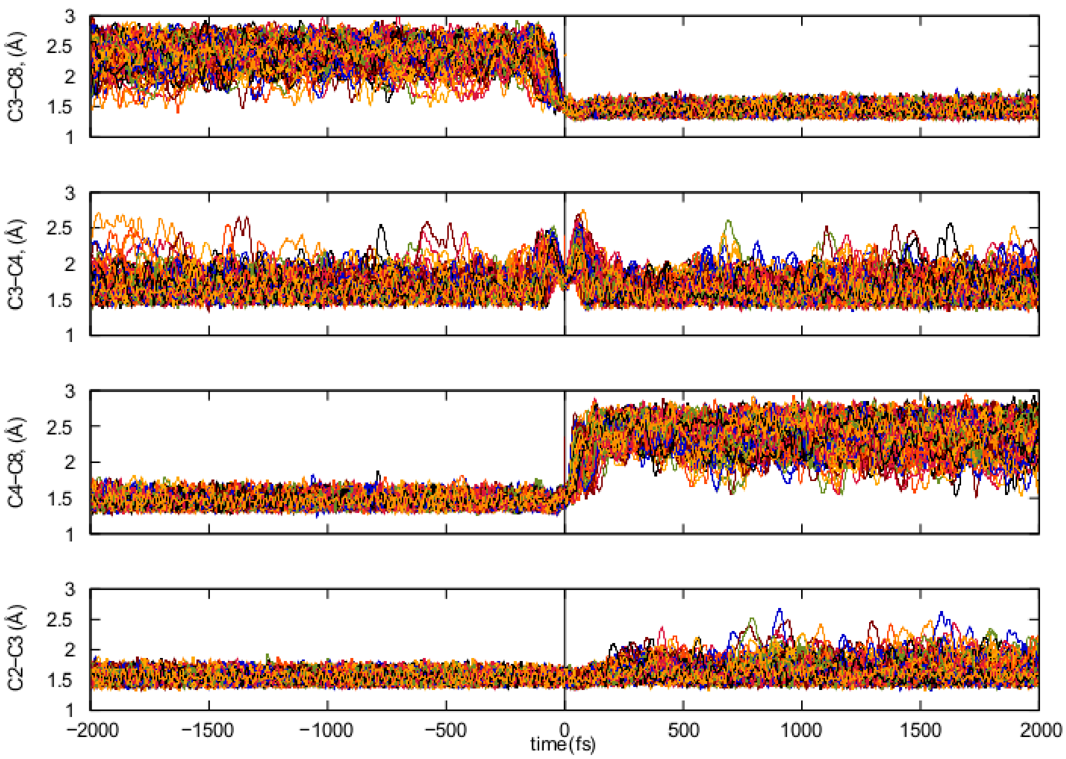


Figure S5 Variation of C3-C8, C3-C4, C4-C8 and C2-C3 distances along the non-recrossing trajectories in the full time-frame.

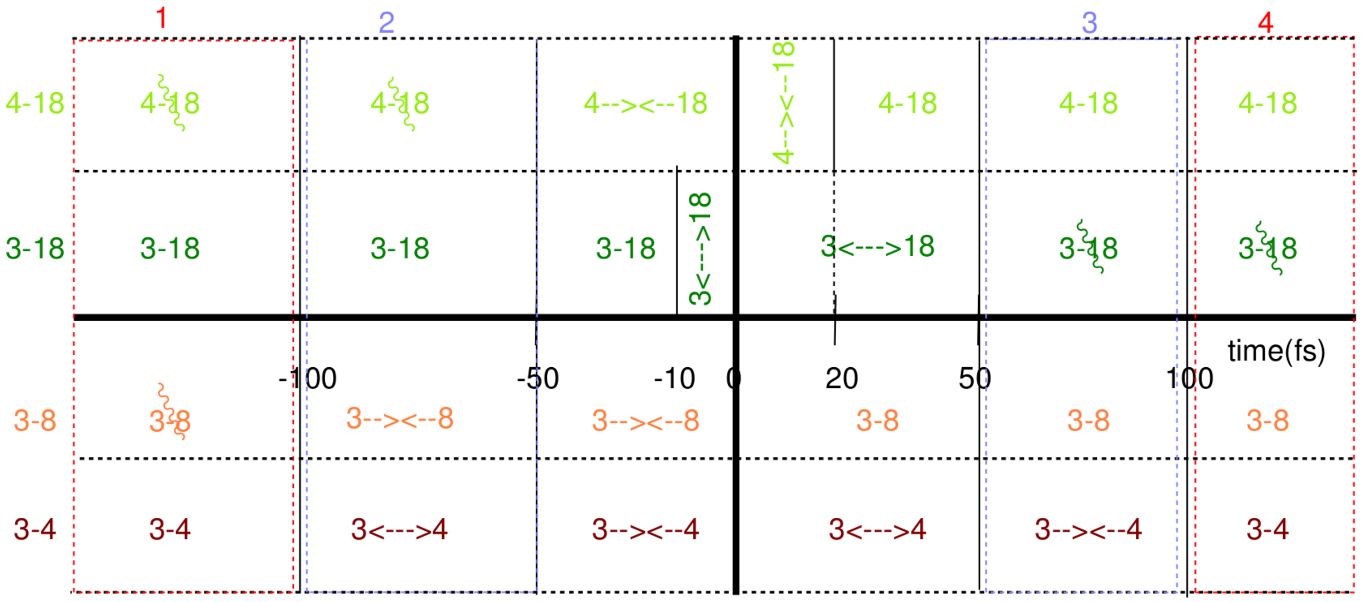


Figure S6 Analysis of the evolution of the main internal coordinates related to the triple shift (C3-H18, C4-H18, C3-C4 and C3-C8) with time. In the vertical axis we have indicated the internal coordinates and in the horizontal axis their variation with time. A hyphen indicates that the atoms are within what is considered a bonding distance (See the Computational Methods section), arrows pointing towards the same direction represent a bond formation while arrows pointing in opposite directions represent a bond breaking process. Moreover, a wavy line represents a bond that has been broken.

In Figure S6 we show a simplified picture of the variation of the main bond distances with time on **system B**, summarizing the discussion presented in the main paper.

In Figures S7 and S8 we have plotted the variation with time of those distances closest to the reactive core.

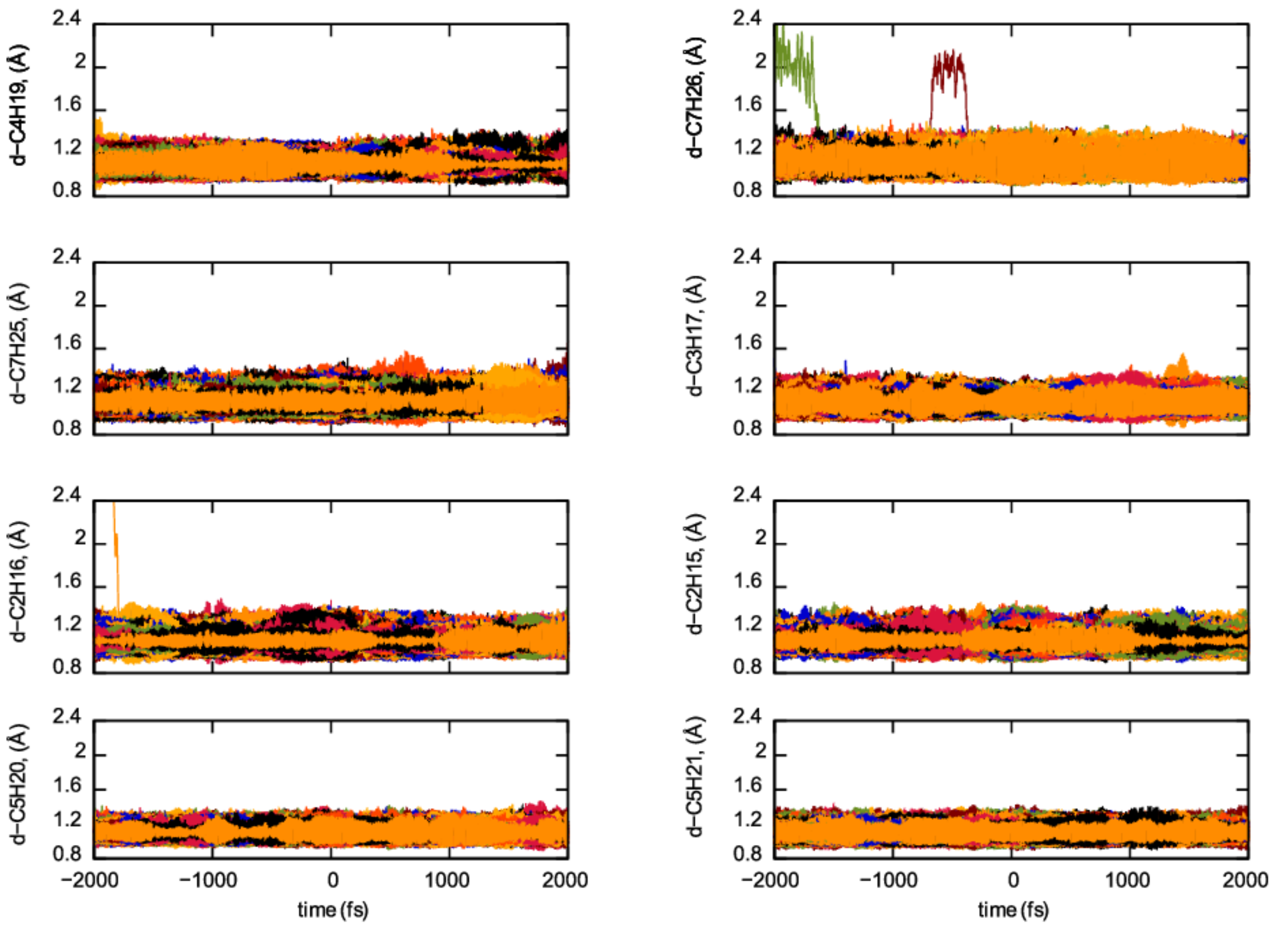


Figure S7 Variation of different C-H distances along trajectories in the full time frame.

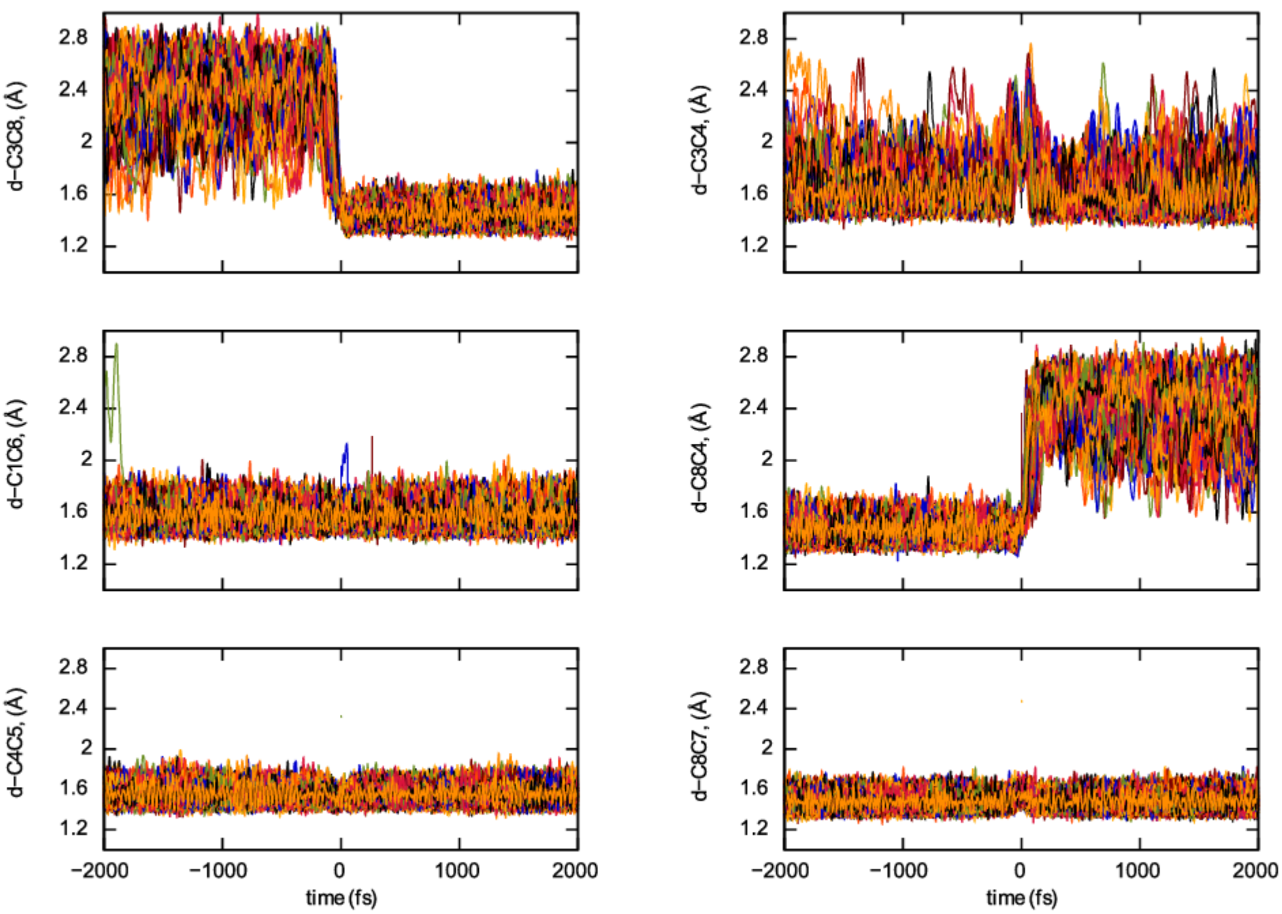


Figure S8 Variation of different C-C distances along trajectories in the full time frame.

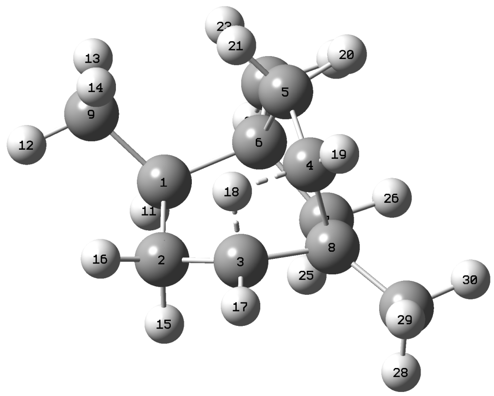


Figure S9 Atom labels on **TS-1-4-Me**.

When the system is in the product region (from 0 to 2000 fs), if the trajectory follows the expected path, C2-C3 and C3-C4 turn pseudo-equivalent (Figure S8), so that there is a non simultaneous dance of atoms 4 and 2 between being bonded-non-bonded to atoms 3 and 8 (see Figure 4 in the Manuscript, blue labels and arrows indicate the corresponding vibrations , which explains the variability observed on these bond distances at the product region.

The remaining interatomic distances acquire the expected values (see Figure S7 and S8) with just three exceptions: C7-H26 and C1-C6. These two bond distances reach a value of more than 2 Å in two independent trajectories (see Figure S7, top left) on the reactant region. In one of them this large separation is caused by the breaking of the C7-H26 bond, induced by the reversible migration of H26 from C7 to C8, as sketched in Figure S10 (red arrows). In the other, H26 migrates from C7 to C8 resulting in the breaking of the C7-H26 bond again, but instead of reverting to the initial structure, the system evolves through the migration of C1 from C6 to C7 instead, thus leading to an alternative tertiary carbocation (Figure S10 (green arrows)).

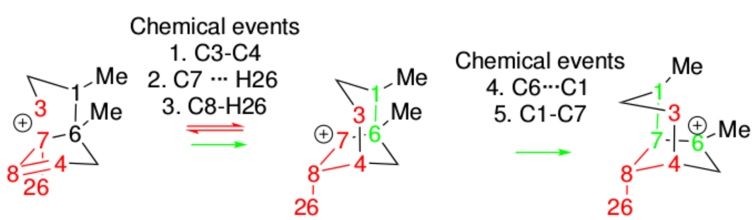


Figure S10 Analysis of the two “abnormal” trajectories on the reactant region. We have chosen red arrows to represent one of them and green to represent the other. Only those atoms that are actively participating on these reactions are highlighted.

3.2 System C

Analogously to **System B**, we performed an analysis of the evolution of key interatomic distances with time for **system C**. Nevertheless, we are not including those plots here, since they are not very informative. As already commented in the main text, significantly more chemical events are taking place in this system, and following a reduced set of internal coordinates does not provide enough information to characterize them. In Figure S11 we represent the variation with time of the C3-H18 and C4-H18 distances. The fluctuations of these values exceed those expected for a simple C3-C4 H-shift, and clearly indicate that further migrations are taking place.

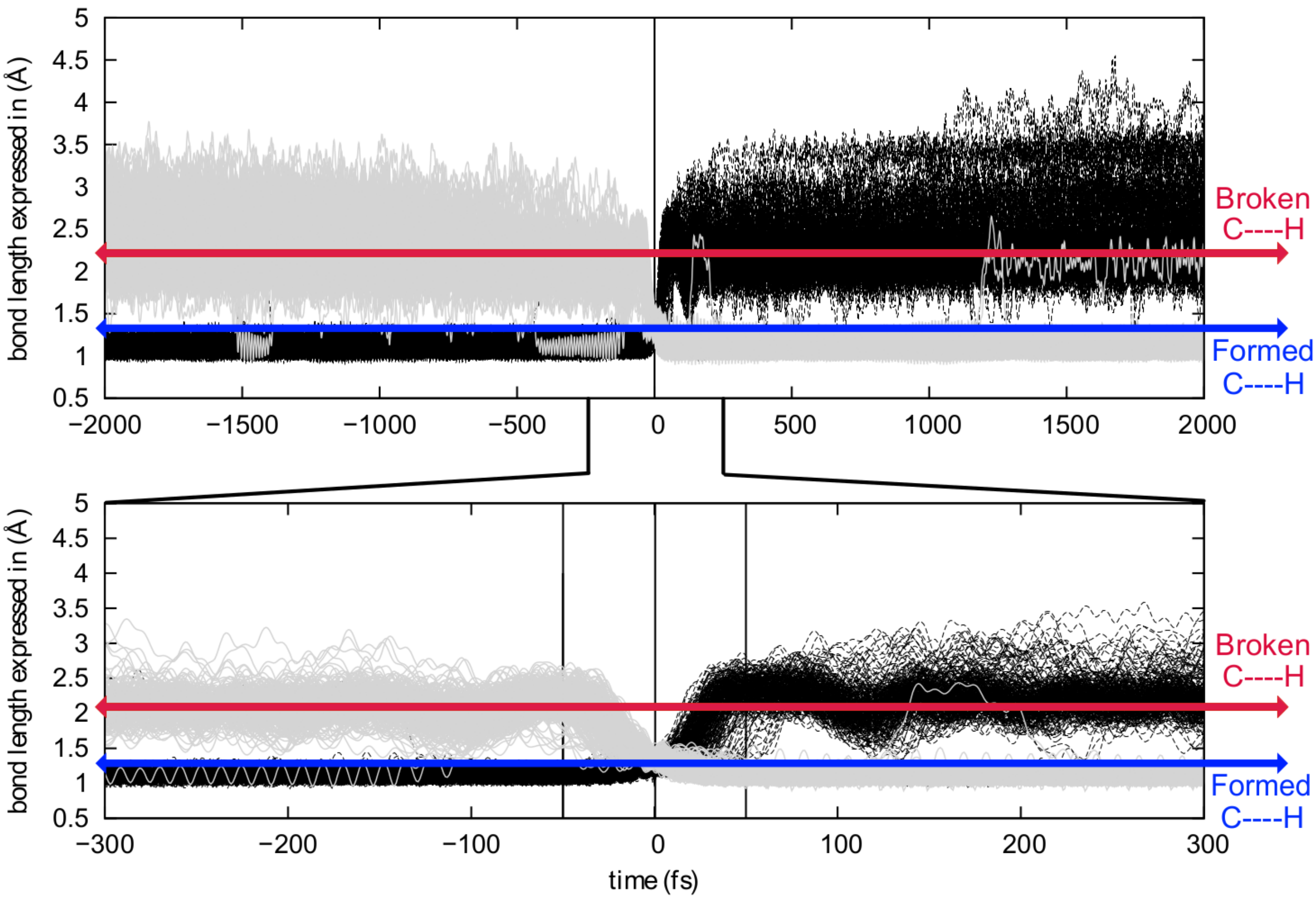


Figure S11 Analysis of the evolution of C3-H18 (black) and C4-H18 (grey) between -2000 and 2000 fs (top) and between -300 and 300 fs (bottom): the red lines indicate the minimum distance for a C-H bond, according to the criteria stablished in Molden.

At this point we found more efficient to inspect all trajectories with the goal of identifying the chemical events and structures along them. The overwhelming number of chemical events found, led us to choose two points in time (1000 and 2000 fs) and systematically examine the structures reached at them. In the manuscript, we have already presented which are the most common structures at these time frames, as well as the chemical events responsible for their interconversion. Here, we provide a more detailed description of the chemistry leading to those structures that are not so common but are relevant nonetheless.

3.2.1 Analysis of the interconversion of the different structures found at 1000 and 2000 fs on those trajectories that do not recross.

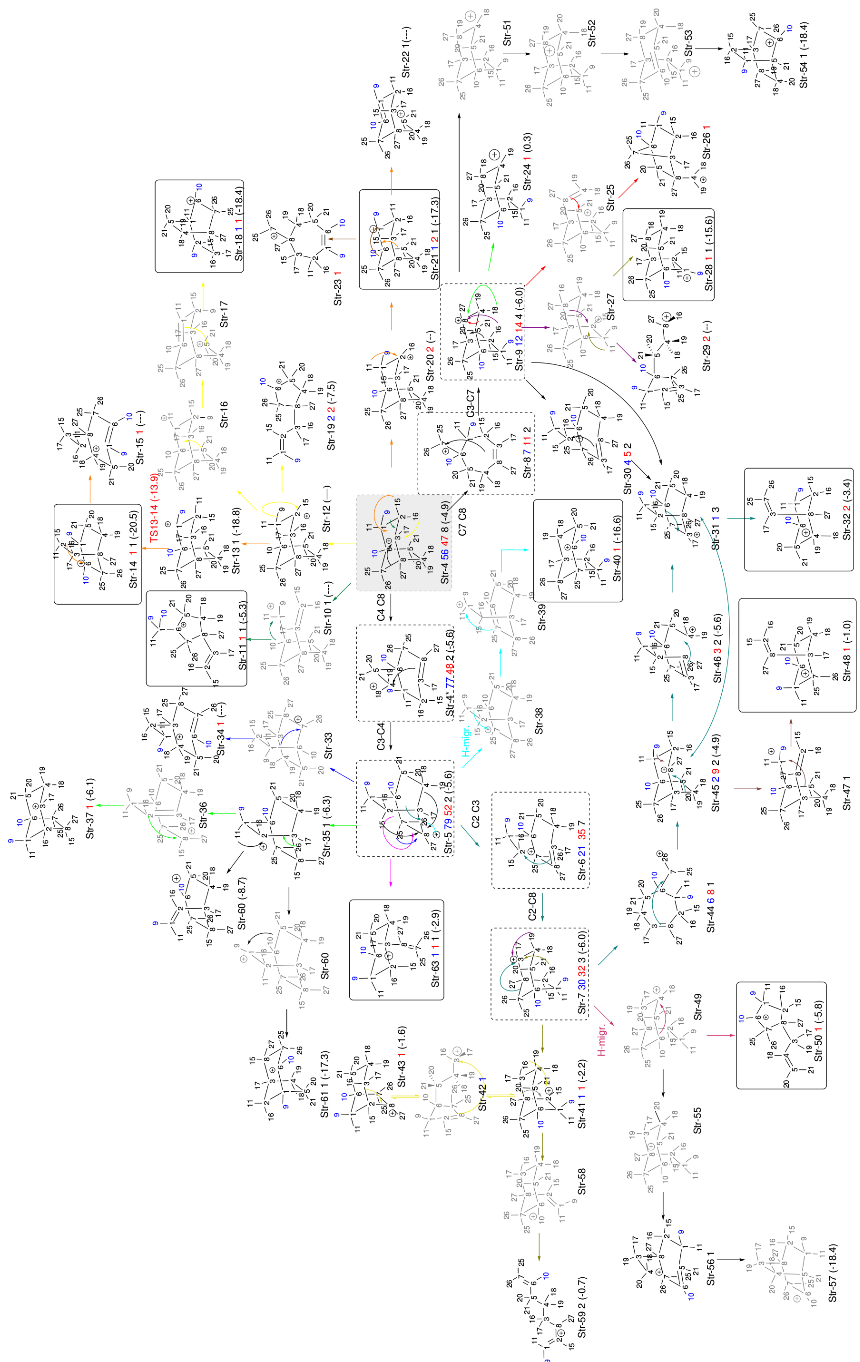


Figure S12 Highly branched reaction paths obtained from the trajectories under study, depicted as sequences of structures with a defined conectivity. We use the prefix Str on their names to avoid confusion with other numbers used in the representation. Below each of those, a number in blue indicates how many times this structure appears at exactly the 1000 fs time step of a trajectory, a number in red how many times it does at 2000 fs and in black at 4000fs. With dashed squares, we have highlighted those structures most frequently encountered, while we have used solid squares to indicate tertiary carbocations (surprisingly, they are not among those structures most frequently encountered at either 1000 or 2000 fs). All black structures in the scheme were used as starting point of geometry optimizations. For those where the optimization preserved connectivity (they are actual minima on the potential energy surface), their energies relative to **1-H** are noted between parentheses. The numbers (9,10) in blue on the structures represent the methyl groups that keep their structural integrity along the trajectory.

Here, we will focus our analysis on the interconversion among the carbocations found at 2000 fs, because the initial chemical events responsible for their formation are common to those found at 1000 fs.

As predicted by the MEP obtained through an IRC calculation from **TS-2-4*-H**, **4** can advance to **4*** through the breaking of C4-C8 bond, but then, unexpectedly, **4*** keeps evolving through the formation of a C4-C3 bond, leading to **5**. Carbocation **5**, on its turn, can evolve through five alternative paths:

1. Breaking of the C6-C7 bond, leading to tertiary carbocation **63** (-2.9 kcal/mol), represented by a pink arrow.

2. Migration of H25 from C7 to C8 concluding with the formation of secondary carbocation **33**, then C1-C6 bond breaking leading to **34** (blue arrows). **34** is not a minimum on the PES, and a geometry optimization starting from this structure leads to a tertiary carbocation through the formation of a bond between C7 and C1.

3. Migration of H26 from C7 to C8 yielding secondary carbocation **38**, then C1-C6 bond cleavage leading to **39** and finally C1-C7 bond formation, leading to tertiary carbocation **40**, (-16.6 kcal/mol) represented by light blue arrows.

4. Migration of H15 from C2 to C8 leading to **35**. The latter progresses then through the migration of C8 from C3 to C2, concluding in **7**, represented by light-green arrows.

5. Cleavage of the C2-C3 bond furnishing **6**. Then, the formation of the C2-C8 bond leads to **7**. This structure can further evolve through the breaking of the C7-C8 bond to **44**, not a minimum on the PES, which then results in **45**, through the formation of a bond between C3 and C7, as represented by bluish green arrows.

Now, secondary carbocation **45** can keep progressing through two different paths:

1. C4-C3 bond cleavage towards **46** (-5.6 kcal/mol), then C4-C8 bond formation leading to intermediate **31** (detected at 1000 and 4000 fs but not at 2000 fs, all our attempts to optimize this structure concluded in **46**). Finally, **31** can evolve through a C6-C7 bond break furnishing **32** (-3.4 kcal/mol), represented by bluish green arrows.

2. C1-C2 bond breaking leading to **47** (an intermediate not found at either 1000 or 2000 fs) and subsequent migration of C5 from C6 to C1 that results in **48** (-1.0 kcal/mol), represented by purple arrows.

At the same time, **7** can evolve towards **41** through the migration of H16 from C2 to C3 (represented by an olive green arrow). **41** can then evolve towards **42** through the breaking of the C3-C8, which would then progress to (**43** through the formation of a bond between C2 and C3. Another path for the evolution of **7** implies the migration of H19 from C4 to C3 towards **49**; then **49** is transformed into tertiary carbocation **50** (-5.8 kcal/mol) by the breaking of the C5-C6 bond, (represented by dark-magenta arrows).

Returning to structure **4**, we find that it can also evolve through other four alternative paths, which at some point ramify, leading to a total of nine possible mechanisms:

1. Cleavage of the C1-C2 bond, leading to structure **10** (not found at either of the chosen time points, but found along some trajectories), which could further evolve towards tertiary carbocation **11** (-5.3 kcal/mol), through the migration of methyl 10 from C6 to C1, represented by green arrows.

2. Migration of H16 from C2 to C3, leading to secondary carbocation **12**. **12** can then evolve to **19** (-7.5 kcal/mol) through cleavage of the C1-C6 bond, or follow a more complex path, involving the migration of H11 from C1 to C2, followed by the migration of C5 from C6 to C1. This last cation can keep evolving through the cleavage of the C1-C2 bond, leading to **15**. **15** is not a minimum on the PES, and a geometry optimization starting from it leads to a structure that will be discussed below. Another alternative for the evolution of **12** involves the migration of C9, followed by the breaking of the C5-C6 bond and the subsequent formation of a bond between C5 and C1, which would result in the formation of another tertiary carbocation, **18** (-18.4 kcal/mol), represented by yellow arrows. Two structures appear along the latter path (**16** and **17**), which have not been identified at any of the chosen time points.

3. Migration of H15 between C2 and C3, followed by the migration of H11 from C1 to C2. This results in tertiary carbocation **21** (-17.3 kcal/mol), which can further evolve through the cleavage of the C7-C6 bond to the non-classical primary carbocation **23**, represented by brown arrows. As expected, **23** is not a minimum on the PES and it converts into **21** upon geometry optimization.

4. Cleavage of the C7-C8 bond, and subsequent formation of a bond between C7 and C3, which leads to **9**, as represented by the black arrow. **9** constitutes a confocal point that opens 4 new possible paths:

   (a) H18 migration from C4 to C8 leading to a secondary carbocation **24** (0.3 kcal/mol) (green arrow).

   (b) C5-C4 bond break followed by C5-C8 bond formation towards **26** (red arrows).

   (c) H16 migration from C2 to C8, leading to a non detected secondary carbocation that can further evolve through the C3-C8 bond break concluding with **29** (purple arrows).

   (d) C2-C3 bond break leading to **30**, this structure can further evolve through the C2-C8 bond formation leading to **31** which, despite not being identified, connects this path with that derived from **4*** (black arrows).

Along these paths we have identified several carbocations (as described in the Computational Methods section) that have been used as the starting point for geometry optimizations. Most of them are real minima on the PES but others might better be described as transient structures: specifically **6**, **8**, **12**, **15**, **20**, **23**, **26**, **29**, **30**, **34** and **44**, because during its optimization **6** evolves backwards towards **30**, **23** evolves backwards towards **21** and **26** towards **4** as well as **8**, **30** evolve backwards towards **9**, **44** evolves furnishing **45**. The carbocations that have not been listed here evolve towards species that had not been previously identified along the trajectories, S13 .

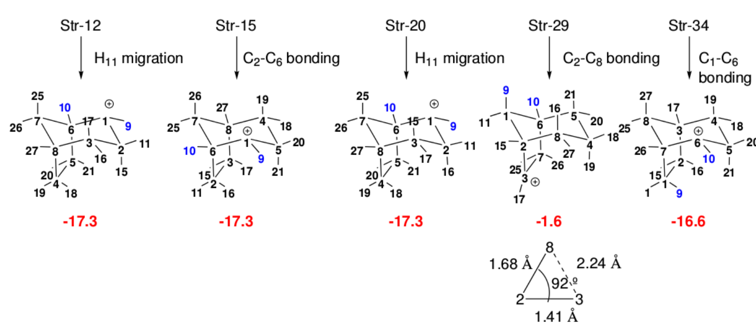


Figure S13 Minima obtained from the optimization of carbocations found along the trajectories run for 2000 fs.

Then, we performed an analysis of the geometry of all primary and secondary carbocations. This analysis allowed us to classify this minima as non-classical carbocations because of the acute C-C-C angles and the elongated bond distances (see Figure 7-C in the Manuscript and Figure S13 at the bottom). Among the tertiary carbocations a distinction should be made, as their relative stability seems strongly dependent upon their structure. Those carbocations featuring a C-C bond paralell to the p orbital of the carbocation are more stable than those that do not posses this feature. We attribute this stabilization to the electron delocalization of the σC-C bond on the vacant orbital of the carbocation.

The emergence of a new set of various carbocationic structures led us to conclude that the reactivity of **system C** is wider than expected, and the consideration of a limited, even long, time-frame (2000 fs) could be a handicap in the perspective gained of the PES of the cited system. So, in an attempt to identify if that handicap was a real issue, we decided to explore those trajectories that recrossed towards products in order to check whether new structures keep appearing.

3.2.2 Analysis of the trajectories run for 2000 fs that recrossed towards products.

The detailed analysis of those trajectories that recross towards products led us to find 74 already known structures, but also a set of new carbocations specifically 5 tertiary, 2 secondary and 3 primary and one structure resembling a TSS corresponding to a hydrogen migration. For this trajectories the most matched structures are coincident with those found in the trajectories that do not recross, i.e. **4***, **4**, **5**, **6**, **7**, **9**. Curiously, even if **8** is found at all the time-points it cannot be designated as a frequent structure.

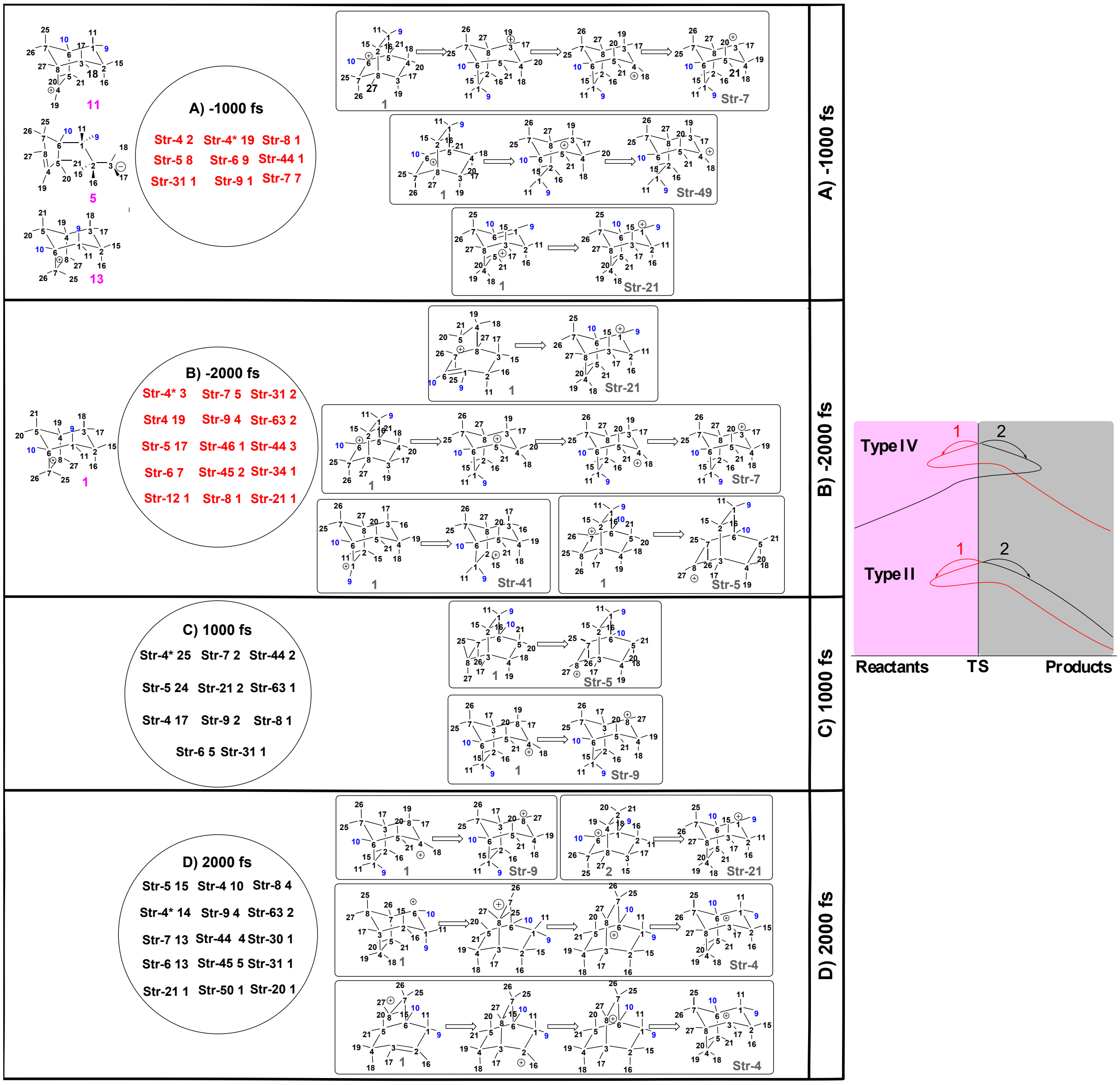


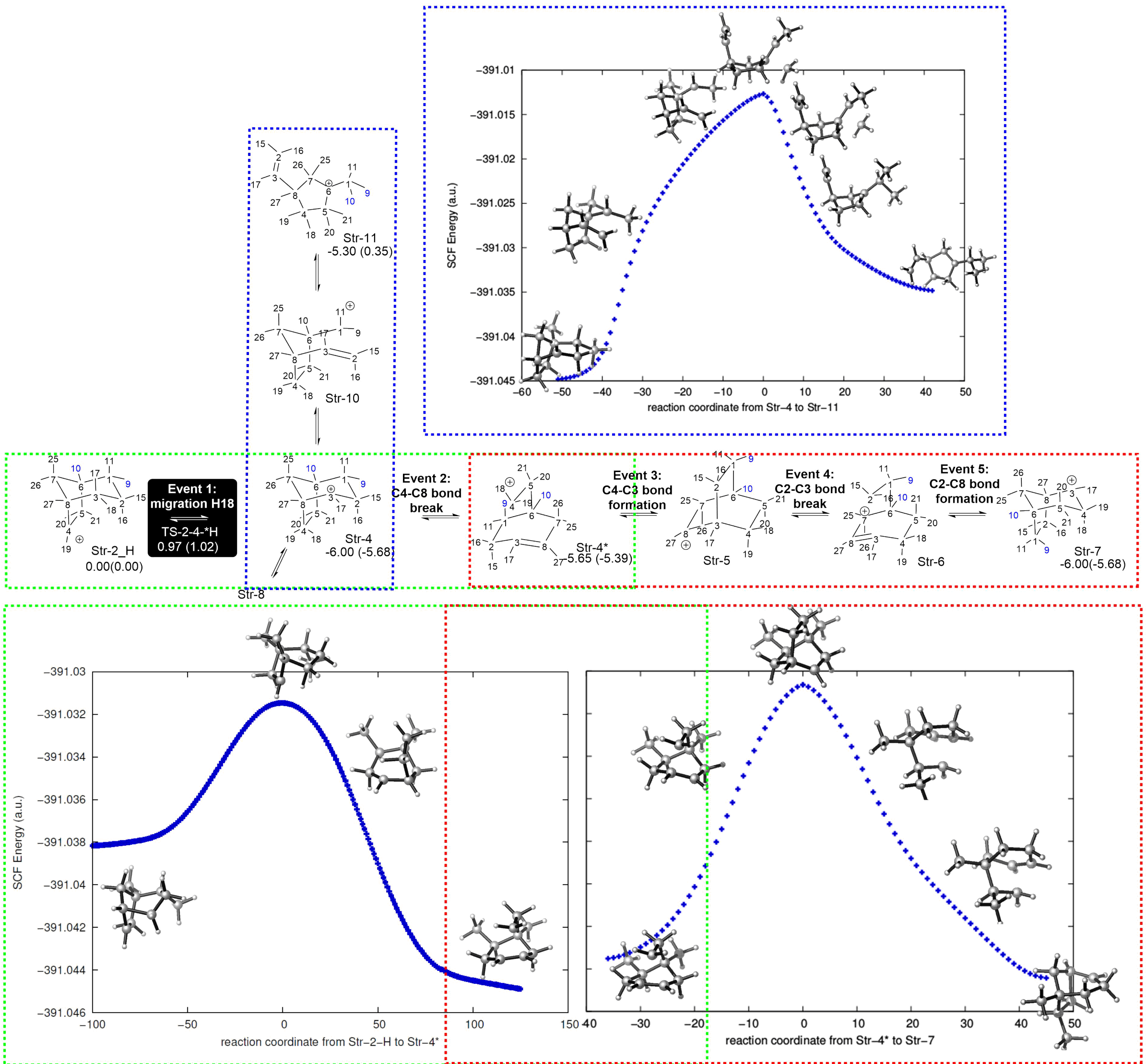
Figure S14 Structures obtained from the analysis of those trajectories that recross towards products. In red and black, inside circles, we indicate those structures found in the negative and positive time frames. Numbers in pink and grey indicate structures obtained in the reactant and product basin, respectively.

Later, given the fact that new structures appear on those trajectories that recross and consequently that the reactivity of **system C** has not blossomed in its totallity at 2000 fs, a second set of 4000 fs trajectories was also acquired. The trajectories were run using B3LYP/6-31+G(d,p) in the gas phase. When we consider a larger time frame (4000 fs x2) some of the already introduced primary and secondary carbocations are found again (see Figure S12, black numbering), but some seem to have further progressed towards a tertiary carbocation. Even if new tertiary species have emerged in this new time-frame, we find cases were the tertiary carbocations can further evolve into other tertiary carbocations, as already mentioned. This indicates that if the system is allowed longer sampling times, it will eventually fall in a potential well reaching a thermodinamically controlled ratio of tertiary carbocations (those more stable and constituting

real potential wells).
Consequently, long time frames are needed so that the system can reach the potential wells. If we were to shorten the sampling time we would be reducing our knowledge on the PES and we would be artificially stopping the reactivity of the system that still would have not reached a potential well. Moreover extending more the time-frame of the trajectories would be allowing more and more carbocations to appear since the potential reactivity of this highly fluxional system has not blossomed in its totality, not all the potential migrations of this molecule have been seen. The subtle structural modification proposed onto **system B** seems to have made these players (carbocations) to lose their expected tempo towards a wandering melody.

3.2.3 Connecting the trajectory results with stationary points in the PES

We calculated the stationary points (i.e. minima and transition states), and the corresponding IRCs for several TSSs, for structures corresponding to a representative dynamics trajectory. This trajectory (summarized by line drawings in the figure below; starting at the **Str-2-H** to **Str-4** enclosed in green) seldom visits the three structures for which a relatively high barrier is predicted on the potential energy surface (enclosed in blue). Structures accessed by transition state structures for which lower barriers are predicted (enclosed in red; one IRC shown) are accessed more frequently. These structures are interconverted by elementary steps (in terms of the potential energy surface) that involve more than one ”distinct chemical event”, as expressed in the manuscript.



Traj 112:
Energies reported relative to 2_H
b3lyp/6-31G** Rel. FE (Rel SCF)
Activation SCF Energy ts4-7: 2.87 kcal/mol
Activation SCF Energy ts4-11: 20.26 kcal/mol

Figure S15 In this plot the structures visited in a representative dinamycs trajectory are plotted using black structures and arrows. The IRCs conneting these structures at the PES are plotted in blue and the correspondence between the sections of the trajectory and the structures visited along the IRCs indicated through dashed colored squares. The trajectories were started at **TS-2-4-*H**, indicated in black.

References

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4 Gaussian 09 full reference

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5 Cartesians

1
SCF Energy: -781.799601021
Num. Imaginary Frequencies: 0

C	3.167708	-0.476280	-0.059936
C	1.613173	-0.583155	-0.258250
C	0.761276	0.706971	0.038639
C	1.386384	1.884888	-0.762396
C	2.892130	2.059248	-0.516149
C	3.667130	0.775863	-0.825661
H	1.510421	-0.721856	-1.347764
H	1.228948	1.707279	-1.836278
H	0.875341	2.825331	-0.523266
H	3.262341	2.873850	-1.149160
H	3.078266	2.380311	0.515508
H	3.589620	0.574216	-1.903962
H	4.734448	0.920653	-0.618549
C	-0.682858	0.433214	-0.548429
C	0.967527	-1.829132	0.376111
H	1.588957	-2.711384	0.203920
H	0.886316	-1.725353	1.464712
C	-0.413232	-2.089815	-0.236316
C	-1.365263	-0.894816	-0.088325
C	3.626091	-0.436669	1.415084
H	3.212208	-1.272035	1.990051
H	4.716868	-0.525458	1.460336
H	3.360193	0.487665	1.930628
C	3.844572	-1.704918	-0.714369
H	3.486392	-1.867022	-1.737916
H	4.927116	-1.547217	-0.766162
H	3.684642	-2.626526	-0.146232
C	0.717573	1.109638	1.532133
H	1.649810	1.580159	1.841993
H	-0.068139	1.849914	1.714407
H	0.556405	0.267947	2.209342
C	-2.662742	-1.105914	-0.947720
H	-2.975727	-2.164672	-0.820302
H	-0.494944	0.291589	-1.621876
C	-1.692552	1.621094	-0.455913
H	-1.162840	2.574152	-0.392617
C	-2.711510	1.569926	0.696487
C	-3.730729	-0.353230	-0.277070
H	-2.599446	-0.943716	-2.029881
C	-5.062470	-0.088306	-0.832700
H	-5.674864	-0.972602	-0.577202
H	-5.553802	0.769844	-0.367162
H	-5.065561	-0.014736	-1.923377
C	-3.257750	0.091424	1.024169
C	-2.024998	-0.784366	1.314103
H	-4.027664	0.186754	1.794642
H	-2.335317	-1.776497	1.664693
H	-1.392068	-0.343069	2.081108
H	-0.282142	-2.306030	-1.305732
H	-0.876107	-2.981565	0.208049
H	-2.248335	1.671672	-1.401921
H	-3.557237	2.233810	0.497670
H	-2.270859	1.870610	1.651351

TS-1-4
SCF Energy: -781.776780986
Num. Imaginary Frequencies: 1
Imaginary Frequency: -407.6808

C	3.180932	-0.454678	-0.076103
C	1.632668	-0.555140	-0.314684
C	0.773879	0.699065	0.095277
C	1.393402	1.950999	-0.587664
C	2.894952	2.112529	-0.310625
C	3.681276	0.864011	-0.721593
H	1.549065	-0.584271	-1.413934
H	1.248259	1.868128	-1.674740
H	0.867389	2.861055	-0.271033
H	3.267576	2.981164	-0.865354
H	3.068294	2.342602	0.747431
H	3.619627	0.757606	-1.814317
H	4.744568	0.996325	-0.487653
C	-0.653247	0.465403	-0.525512
C	0.981057	-1.861718	0.179818
H	1.599357	-2.719334	-0.096617
H	0.914834	-1.882960	1.274829
C	-0.410437	-2.054772	-0.440962
C	-1.360226	-0.881003	-0.162585
C	3.606824	-0.533561	1.406827
H	3.201339	-1.425159	1.897247
H	4.698136	-0.602202	1.469680
H	3.307735	0.336796	1.993678
C	3.883888	-1.616659	-0.817677
H	3.548698	-1.693928	-1.858719
H	4.965656	-1.446414	-0.832295
H	3.720539	-2.584388	-0.333522
C	0.709064	0.949301	1.623672
H	1.568723	1.523164	1.969618
H	-0.172155	1.542691	1.899323
H	0.693382	0.030565	2.213956
C	-2.666507	-0.941726	-0.997382
H	-3.075567	-1.959260	-1.020001
H	-0.461979	0.371145	-1.601301
C	-1.632234	1.676212	-0.372558
H	-1.213946	2.466221	0.255475
C	-3.017427	1.310418	0.152294
C	-3.646197	-0.041585	-0.232619
H	-2.524215	-0.620338	-2.033412
C	-5.112689	-0.040201	-0.626441
H	-5.512269	-1.057972	-0.596057
H	-5.718058	0.583397	0.039040
H	-5.232579	0.335228	-1.646779
C	-3.231677	-0.141196	1.195591
C	-1.941766	-0.920817	1.288225
H	-3.962784	-0.062005	2.000923
H	-2.249424	-1.948050	1.532863
H	-1.277593	-0.585985	2.082523
H	-0.297954	-2.156570	-1.528652
H	-0.867453	-2.988902	-0.089571
H	-1.820008	2.140704	-1.347481
H	-3.764295	2.101329	0.246045
H	-2.826101	1.170325	1.357014

4
SCF Energy: -781.804946879
Num. Imaginary Frequencies: 0

C	3.139440	-0.382356	-0.222260
C	1.580884	-0.543930	-0.320065
C	0.716796	0.678277	0.162790
C	1.227908	1.961605	-0.549744
C	2.740084	2.176248	-0.398913
C	3.528880	0.960215	-0.895561
H	1.399736	-0.588964	-1.407437
H	0.996309	1.888073	-1.622678
H	0.688981	2.841234	-0.172697
H	3.033977	3.063871	-0.970725
H	2.996079	2.398646	0.643651
H	3.369808	0.861354	-1.979313
H	4.603983	1.129048	-0.759656
C	-0.742002	0.403033	-0.361361
C	1.026120	-1.865106	0.248814
H	1.651535	-2.704847	-0.064643
H	1.052871	-1.867338	1.344118
C	-0.402850	-2.131489	-0.249907
C	-1.377181	-0.974416	0.035528
C	3.700485	-0.454433	1.215232
H	3.385165	-1.369926	1.727074
H	4.795103	-0.468371	1.178995
H	3.411722	0.393417	1.838662
C	3.816385	-1.510499	-1.036438
H	3.398697	-1.586070	-2.047430
H	4.887216	-1.304193	-1.137695
H	3.724849	-2.489082	-0.555105
C	0.766985	0.910241	1.694408
H	1.633852	1.510199	1.971224
H	-0.105972	1.464726	2.053630
H	0.830480	-0.013384	2.271835
C	-2.636094	-1.101540	-0.845041
H	-3.211374	-2.021140	-0.618495
H	-0.623185	0.348581	-1.452628
C	-1.767625	1.531352	-0.081777
H	-1.468587	2.177902	0.748123
C	-3.177711	0.952813	0.389151
C	-3.563256	0.024181	-0.655841
H	-2.418580	-1.202118	-1.922017
C	-4.757191	0.212056	-1.493163
H	-4.900622	-0.566957	-2.243000
H	-5.643712	0.289403	-0.845996
H	-4.692357	1.195971	-1.984272
C	-2.917012	0.163830	1.721228
C	-1.898405	-0.980048	1.498663
H	-3.868712	-0.207098	2.111971
H	-2.372552	-1.949235	1.690345
H	-1.073469	-0.898661	2.204190
H	-0.358351	-2.292947	-1.336278
H	-0.794717	-3.059756	0.185514
H	-1.911913	2.177431	-0.951348
H	-3.895654	1.763467	0.532792
H	-2.548449	0.906559	2.434819

1-Me
SCF Energy: -430.379354431
Num. Imaginary Frequencies: 0

H	-1.578079	-0.171164	-1.722548
C	-1.305080	-0.462644	-0.699522
C	-0.724225	0.816666	-0.012849
C	-0.201338	0.482080	1.408943
H	-0.904558	-0.093001	2.013786
H	0.037493	1.398654	1.961519
C	0.632415	1.187646	-0.703816
H	0.676365	1.179646	-1.799331
H	0.900271	2.223266	-0.405766
C	1.664033	0.365084	-0.050527
C	1.084679	-0.310694	1.100085
H	1.777227	-0.523801	1.918442
H	1.530754	-2.327540	0.258025
C	0.641700	-1.722006	0.451307
H	0.085151	-2.194081	1.267261
C	-0.219035	-1.566930	-0.812359
H	-0.689089	-2.530112	-1.033684
H	0.432661	-1.358131	-1.671282
C	3.057352	0.246554	-0.491744
C	-2.583725	-1.001736	-0.032275
C	-1.705142	1.992853	-0.042618
H	-1.246035	2.898231	0.369535
H	-2.029898	2.213471	-1.065020
H	-2.597585	1.782177	0.551168
H	-2.979924	-1.835557	-0.619257
H	-2.409862	-1.373542	0.982829
H	-3.369105	-0.244138	0.020319
H	3.539153	-0.666993	-0.133744
H	3.181566	0.376069	-1.569904
H	3.593691	1.085307	-0.010100

TS-1-4-Me
SCF Energy: -430.354979114
Num. Imaginary Frequencies: 1
Imaginary Frequency: -426.4630

C	1.573029	0.090154	-0.099048
C	-0.769114	0.772134	-0.121640
C	-0.297322	0.719647	1.361815
C	-1.358987	-0.609846	-0.566681
C	-0.241015	-1.698252	-0.664282
C	1.037864	-1.328213	0.070474
C	1.029276	-0.006260	1.297856
C	0.579607	0.980077	-0.861272
C	3.061633	0.262887	-0.344631
H	0.912005	2.021514	-0.787000
H	0.527080	0.728824	-1.925455
C	-1.760898	1.913436	-0.369014
H	-0.053274	1.729411	1.720635
H	-1.739851	-0.454592	-1.582304
H	-1.016602	0.293390	2.063688
H	-0.604872	-2.669772	-0.318687
H	0.077730	-1.839044	-1.704467
H	0.682454	-1.305226	1.277448
H	1.818245	-2.080833	0.196486
H	1.708727	-0.124629	2.142536
C	-2.532642	-1.113713	0.289280
H	-1.316817	2.878460	-0.103833
H	-2.049162	1.956783	-1.424142
H	-2.673954	1.797320	0.221283
H	-2.987401	-1.991843	-0.178911
H	-2.222541	-1.413389	1.297487
H	-3.316916	-0.359529	0.390766
H	3.359576	1.297680	-0.153141
H	3.662710	-0.389552	0.296526
H	3.304279	0.032714	-1.386061

4-Me
SCF Energy: -430.383540145
Num. Imaginary Frequencies: 0

C	-1.467093	0.221226	-0.516641
C	-1.398030	-0.242158	0.854551
C	-0.789308	-1.666083	1.000736
C	0.511741	-1.800733	0.173316
C	0.942433	-0.430646	-0.411793
C	-0.223058	0.066253	-1.290307
C	1.086523	0.566021	0.793458
C	-0.312734	0.800399	1.419383
H	1.712427	0.051909	1.532798
H	-2.340862	-0.133067	1.394839
C	-2.662395	0.875507	-1.072384
H	-0.609099	-1.817884	2.068949
H	-1.538421	-2.403726	0.699697
H	0.370631	-2.513412	-0.646896
H	1.321729	-2.197533	0.792383
C	2.226885	-0.579113	-1.233650
H	-0.329659	0.627457	2.500741
H	-0.655611	1.828972	1.262826
H	-0.450337	-0.659023	-2.096133
H	-0.017826	0.997623	-1.839715
C	1.762915	1.904434	0.461202
H	3.064771	-0.863710	-0.589241
H	2.115118	-1.361535	-1.991748
H	2.499138	0.347355	-1.747003
H	-2.498075	1.354106	-2.038611
H	-3.437971	0.097972	-1.179689
H	-3.085765	1.587341	-0.351702
H	1.790125	2.542896	1.350049
H	2.794690	1.765278	0.130825
H	1.227716	2.458338	-0.319588

1-H
SCF Energy: -391.037131606
Num. Imaginary Frequencies: 0

H	1.421242	0.668149	-1.515543
C	0.905728	0.765378	-0.551693
C	0.627331	-0.689121	-0.049501
C	-0.135370	-0.662759	1.304818
H	0.281453	0.035573	2.032191
H	-0.144585	-1.656274	1.769113
C	-0.477314	-1.315022	-0.976680
H	-0.378362	-1.187786	-2.059969
H	-0.504913	-2.413947	-0.804152
C	-1.748536	-0.872907	-0.405720
C	-1.559494	-0.291491	0.873246
H	-2.383385	-0.291803	1.586356
H	-2.505003	1.560451	-0.088179
C	-1.505835	1.266767	0.236941
H	-1.283126	1.783557	1.176782
C	-0.428812	1.514036	-0.825443
H	-0.248732	2.593223	-0.868384
H	-0.816539	1.241375	-1.813372
H	-2.708988	-0.924361	-0.918884
C	1.827858	1.582740	0.371390
C	1.893749	-1.549315	-0.020460
H	1.663147	-2.580004	0.269521
H	2.377779	-1.573796	-1.002295
H	2.620334	-1.163247	0.698407
H	2.084294	2.529217	-0.113388
H	1.363601	1.827637	1.332423
H	2.765956	1.062194	0.577990

TS-1-2-H
SCF Energy: -391.036546425
Num. Imaginary Frequencies: 1
Imaginary Frequency: -144.5274

C	0.925210	0.793950	-0.505244
C	-0.401323	1.543317	-0.814601
C	-1.538832	1.189380	0.140052
C	-1.517692	-0.411172	0.972705
C	-0.073230	-0.735292	1.301680
C	0.626209	-0.685095	-0.091089
C	-0.515845	-1.211719	-1.021079
C	-1.768838	-0.763006	-0.351787
C	1.797127	1.576233	0.491867
C	1.879492	-1.562654	-0.158517
H	1.481414	0.740101	-1.448873
H	2.115579	2.520625	0.040898
H	2.702244	1.026819	0.762979
H	1.269048	1.825861	1.418727
H	-0.719041	1.352668	-1.843234
H	-0.249580	2.626215	-0.741595
H	-2.540039	1.454328	-0.198922
H	-1.396997	1.635176	1.130092
H	-2.301542	-0.339551	1.721966
H	-0.049780	-1.752215	1.715540
H	0.365054	-0.073393	2.050447
H	2.314598	-1.548807	-1.163021
H	1.646043	-2.602313	0.093862
H	2.646955	-1.219766	0.540258
H	-0.433858	-0.937414	-2.076565
H	-0.565529	-2.314358	-0.986071
H	-2.758240	-0.797631	-0.800410

2-H
SCF Energy: -391.038177057
Num. Imaginary Frequencies: 0

C	-1.757077	-0.626753	-0.298703
C	0.645097	-0.658308	-0.149463
C	0.020049	-0.850487	1.271645
C	0.908342	0.858853	-0.446211
C	-0.424279	1.589477	-0.778112
C	-1.610044	1.058235	0.025572
C	-1.436162	-0.607807	1.071493
C	-0.530015	-1.122266	-1.057035
H	-2.766675	-0.819337	-0.649035
H	-0.592673	-2.216651	-1.104683
H	-0.467137	-0.755184	-2.083748
C	1.913494	-1.496200	-0.337713
H	0.076731	-1.911399	1.574798
H	1.511879	0.881939	-1.360876
H	0.473557	-0.276477	2.082333
H	-0.335577	2.661322	-0.571524
H	-0.663232	1.495357	-1.840538
H	-1.516422	1.366803	1.080625
H	-2.605298	1.398719	-0.264707
H	-2.169469	-0.541331	1.872297
C	1.702732	1.597158	0.644103
H	1.719660	-2.555700	-0.139810
H	2.286358	-1.409313	-1.362981
H	2.713934	-1.174336	0.334452
H	2.037771	2.567983	0.267796
H	1.108399	1.793101	1.544438
H	2.595367	1.043088	0.947703

TS-2-4*-H
SCF Energy: -391.031466692
Num. Imaginary Frequencies: 1
Imaginary Frequency: -428.8707

C	-0.917547	-0.825558	-0.463025
C	0.401499	-1.643156	-0.659841
C	1.635221	-0.960297	-0.087518
C	1.457348	0.403399	1.086941
C	0.013875	0.815825	1.283683
C	-0.616634	0.677895	-0.134502
C	0.558270	1.142145	-1.040261
C	1.785842	0.528050	-0.365487
C	-1.845110	-1.528986	0.541435
C	-1.864929	1.551399	-0.295702
H	-1.431359	-0.818268	-1.430734
H	-2.133757	-2.512270	0.158304
H	-2.765979	-0.965557	0.710544
H	-1.368060	-1.692795	1.515101
H	0.631623	-1.763706	-1.725456
H	0.306103	-2.650983	-0.247044
H	2.579187	-1.505060	-0.039117
H	1.416341	-0.951023	1.145249
H	2.234748	0.487596	1.845986
H	0.060805	1.873319	1.580088
H	-0.507610	0.280543	2.079136
H	-2.268322	1.469443	-1.309958
H	-2.656975	1.266539	0.402022
H	-1.627851	2.604894	-0.114328
H	0.446536	0.824987	-2.081388
H	0.654907	2.232907	-1.036367
H	2.782644	0.855132	-0.646382

4*-H
SCF Energy: -391.046773441
Num. Imaginary Frequencies: 0

C	1.777427	0.332156	-0.739040
C	1.627608	-0.974160	-0.274317
C	1.578099	0.194093	1.153366
C	0.144566	0.698998	1.324437
C	-0.551641	0.699734	-0.069758
C	0.573105	1.173526	-1.026580
C	-0.921879	-0.762001	-0.475943
C	0.303327	-1.695597	-0.269905
C	-2.153736	-1.346981	0.227004
H	2.525486	-1.576933	-0.152254
H	2.776657	0.708336	-0.947980
H	1.886694	-0.642761	1.785363
H	2.367391	0.942917	1.254438
H	0.173428	1.714800	1.729509
H	-0.401065	0.079197	2.039962
C	-1.754074	1.646366	-0.117069
H	-2.047000	-1.345287	1.317887
H	-3.063470	-0.798330	-0.026055
H	-2.304635	-2.385860	-0.083749
H	0.218011	-2.266303	0.663222
H	0.359173	-2.450273	-1.064791
H	0.813222	2.233382	-0.889803
H	0.290716	1.043787	-2.080070
H	-1.144132	-0.731244	-1.550666
H	-2.486180	1.402339	0.657021
H	-1.439694	2.683220	0.040741
H	-2.261419	1.592207	-1.085945

Str-4
SCF Energy: -391.044878906
Num. Imaginary Frequencies: 0

C	-1.038378	-0.764864	-0.296067
C	0.170080	-1.769297	-0.145777
C	1.406866	-1.143318	-0.681592
C	1.521497	0.464055	1.296432
C	0.089030	1.061588	1.178431
C	-0.485758	0.689122	-0.211762
C	0.735620	0.702494	-1.128926
C	1.967813	-0.002430	-0.086264
C	-2.176378	-1.125530	0.658447
C	-1.533359	1.709715	-0.697902
H	-1.408446	-0.888928	-1.322608
H	-2.507017	-2.154089	0.484658
H	-3.042126	-0.476829	0.498865
H	-1.878305	-1.047446	1.708584
H	-0.049991	-2.709472	-0.654329
H	0.321380	-1.980181	0.920542
H	1.881638	-1.545416	-1.575435
H	1.555461	-0.386621	1.985683
H	2.230753	1.202694	1.674740
H	0.147664	2.151770	1.252951
H	-0.558173	0.730098	1.992889
H	-1.926204	1.448270	-1.685581
H	-2.375665	1.748498	-0.001873
H	-1.108307	2.716276	-0.752729
H	0.571052	0.299193	-2.133632
H	1.257296	1.656172	-1.256622
H	2.946791	0.306800	-0.446222

Str-4*
SCF Energy: -391.046773454
Num. Imaginary Frequencies: 0

C	0.921708	0.761857	-0.476378
C	-0.303590	1.695315	-0.270323
C	-1.627744	0.973241	-0.273818
C	-1.577872	-0.192906	1.153700
C	-0.144541	-0.698231	1.324688
C	0.551667	-0.699706	-0.069506
C	-0.572932	-1.174082	-1.026279
C	-1.777268	-0.332687	-0.739957
C	2.153592	1.347204	0.226301
C	1.754166	-1.646239	-0.116270
H	1.143835	0.730787	-1.551118
H	2.303900	2.386188	-0.084390
H	3.063477	0.798961	-0.027118
H	2.047138	1.345323	1.317210
H	-0.359867	2.449621	-1.065492
H	-0.218014	2.266273	0.662589
H	-2.525774	1.575923	-0.152471
H	-1.886579	0.643389	1.786390
H	-2.367088	-0.941917	1.254355
H	-0.173566	-1.713843	1.730249
H	0.401406	-0.078242	2.039813
H	2.261623	-1.592507	-1.085113
H	2.486158	-1.401693	0.657768
H	1.439915	-2.683055	0.042049
H	-0.290228	-1.044773	-2.079780
H	-0.812968	-2.233937	-0.889283
H	-2.776481	-0.709100	-0.948612

Str-7
SCF Energy: -391.047232442
Num. Imaginary Frequencies: 0

C	-0.687115	-0.922688	-0.537344
C	0.801763	-1.223059	-0.805987
C	1.959932	-0.034395	0.217968
C	1.268512	0.250839	1.511674
C	-0.192818	0.753236	1.354650
C	-0.756373	0.570871	-0.075996
C	0.221458	1.252014	-1.061322
C	1.476548	0.406938	-1.018296
C	-1.340609	-1.963320	0.379571
C	-2.170930	1.148879	-0.169619
H	-1.188936	-0.965788	-1.511999
H	-1.290588	-2.960856	-0.067559
H	-2.397966	-1.732287	0.533448
H	-0.860090	-2.014700	1.362156
H	1.084212	-1.604378	-1.789640
H	1.241460	-1.929740	-0.091437
H	2.934286	-0.519719	0.255004
H	1.347155	-0.625134	2.164928
H	1.902240	1.011372	1.994288
H	-0.243052	1.816844	1.606884
H	-0.830900	0.237708	2.076928
H	-2.581050	1.032720	-1.178307
H	-2.851081	0.654009	0.530223
H	-2.172616	2.216391	0.072623
H	-0.179823	1.270672	-2.079341
H	0.452612	2.285949	-0.780059
H	2.151938	0.391053	-1.869931

Str-9
SCF Energy: -391.034542612
Num. Imaginary Frequencies: 0

C	1.071218	0.865384	-0.542074
C	-0.399560	0.708076	-0.967071
C	-1.203285	-0.088795	0.084528
C	-0.636675	-1.522904	0.193123
C	0.894711	-1.619661	-0.053104
C	1.680541	-0.388695	-0.057516
C	-3.633704	0.362196	0.573845
C	-2.678689	-0.112297	-0.228792
C	1.296487	2.035673	0.476523
C	3.093564	-0.437188	0.355653
H	1.696143	1.134338	-1.416010
H	0.921796	2.951498	0.015534
H	2.350169	2.182625	0.719531
H	0.739985	1.860400	1.400150
H	-0.458490	0.199179	-1.938512
H	-0.837469	1.699438	-1.109631
H	-1.073431	0.410173	1.055155
H	-0.843472	-1.930274	1.187150
H	-1.140890	-2.180968	-0.520729
H	1.055418	-1.902305	-1.122768
H	1.384266	-2.420671	0.509884
H	3.699912	0.382398	-0.032631
H	3.088966	-0.358146	1.458734
H	3.548457	-1.408964	0.137916
H	-4.681234	0.317992	0.293673
H	-3.404855	0.810368	1.538251
H	-2.952930	-0.557817	-1.186390

Str-11
SCF Energy: -391.037626587
Num. Imaginary Frequencies: 0

C	2.156193	-0.500529	0.411947
C	-4.039405	-0.426279	0.468001
C	-2.907589	-0.436456	-0.239566
C	-1.037621	1.261669	-0.753064
C	0.450241	1.323556	-0.358083
C	0.797730	-0.014948	0.148875
C	-0.431291	-0.806833	0.318672
C	-1.620145	0.195813	0.208947
C	2.608948	-1.169130	-0.949915
C	3.166962	0.575178	0.847936
H	2.108565	-1.309540	1.149718
H	2.660014	-0.434644	-1.757350
H	1.957699	-1.994789	-1.243242
H	3.612800	-1.564714	-0.775775
H	-4.945356	-0.889048	0.090299
H	-4.102838	0.047323	1.444943
H	-2.887295	-0.919226	-1.218224
H	-1.133512	0.930062	-1.793929
H	-1.537650	2.227597	-0.666367
H	0.576961	1.958689	0.546481
H	1.163432	1.736294	-1.080297
H	3.316325	1.336315	0.076937
H	2.853204	1.067436	1.773031
H	4.132175	0.098555	1.035597
H	-0.450194	-1.463178	-0.577894
H	-0.417995	-1.488379	1.175893
H	-1.770476	0.649001	1.197673

Str-12
SCF Energy: -391.063625428
Num. Imaginary Frequencies: 0

C	0.839081	0.787702	-0.010863
C	-0.302774	1.739613	-0.014788
C	-1.669844	1.218386	-0.504162
C	-1.544820	-0.779484	1.090913
C	-0.012041	-0.915091	1.262859
C	0.630397	-0.633569	-0.231377
C	-0.600207	-0.942590	-1.121878
C	-1.773362	-0.309291	-0.365614
C	2.175957	1.341857	0.295478
C	1.864529	-1.490358	-0.515153
H	0.031515	2.637236	-0.557644
H	2.137504	2.351691	0.706837
H	2.720013	1.380526	-0.664248
H	2.770159	0.685067	0.936430
H	-0.357268	2.106057	1.026534
H	-2.464478	1.715442	0.059981
H	-1.810466	1.495887	-1.554282
H	-1.980627	-0.093604	1.823010
H	-2.011112	-1.755490	1.253770
H	0.325943	-1.934742	1.471330
H	0.400527	-0.286749	2.058838
H	2.308253	-1.228385	-1.481156
H	2.637839	-1.401624	0.251991
H	1.569653	-2.541701	-0.562970
H	-0.476518	-0.559862	-2.140384
H	-0.702216	-2.030309	-1.188379
H	-2.740218	-0.642496	-0.752147

Str-14
SCF Energy: -391.067044890
Num. Imaginary Frequencies: 0

C	-0.657147	-0.622931	0.000050
C	0.243318	-0.972579	-1.270502
C	1.600738	-0.231455	-1.261085
C	1.601160	-0.232375	1.260593
C	0.243790	-0.973615	1.269861
C	-0.787133	0.831437	0.000358
C	0.480779	1.586489	0.000569
C	1.691272	0.654571	0.000071
C	-1.956430	-1.427267	-0.000065
C	-2.077020	1.536353	0.000272
H	-0.333155	-0.765717	-2.176706
H	-1.728316	-2.496182	-0.000466
H	-2.564177	-1.223773	-0.887518
H	-2.563926	-1.224381	0.887696
H	0.370371	-2.058208	-1.215885
H	2.429920	-0.944339	-1.267471
H	1.707754	0.384712	-2.159441
H	2.430401	-0.945199	1.266237
H	1.708389	0.383147	2.159367
H	-0.332357	-0.767517	2.176444
H	0.370935	-2.059188	1.214368
H	-2.670341	1.209536	-0.867273
H	-2.670807	1.209020	0.867298
H	-1.981873	2.622746	0.000581
H	0.455312	2.274204	-0.863953
H	0.455418	2.273269	0.865856
H	2.616482	1.236107	0.000129

Str-15
SCF Energy: -391.063625497
Num. Imaginary Frequencies: 0

C	-0.839064	0.787729	-0.010964
C	0.012174	-0.915320	1.262888
C	1.544904	-0.779553	1.090771
C	1.669719	1.218481	-0.504156
C	0.302815	1.739621	-0.014539
C	-0.630359	-0.633594	-0.231305
C	0.600139	-0.942470	-1.121955
C	1.773344	-0.309188	-0.365746
C	-2.176009	1.341845	0.295383
C	-1.864562	-1.490289	-0.515130
H	-0.325662	-1.935054	1.471164
H	-2.769272	0.685622	0.937865
H	-2.721045	1.378963	-0.663786
H	-2.137583	2.352178	0.705546
H	2.011311	-1.755527	1.253522
H	-0.400423	-0.287127	2.058959
H	1.980679	-0.093726	1.822935
H	2.464489	1.715517	0.059817
H	1.810240	1.496056	-1.554274
H	-0.031434	2.637615	-0.556644
H	0.357255	2.105368	1.027036
H	-1.569811	-2.541694	-0.562678
H	-2.637989	-1.401266	0.251832
H	-2.308027	-1.228438	-1.481288
H	0.702204	-2.030164	-1.188636
H	0.476301	-0.559594	-2.140413
H	2.740164	-0.642312	-0.752437

Str-18
SCF Energy: -391.065786367
Num. Imaginary Frequencies: 0

C	-0.117097	-0.618574	0.822325
C	0.815618	-0.935041	-0.505786
C	1.112543	0.407702	-1.213242
C	0.454640	1.876211	0.715642
C	0.477082	0.592829	1.584139
C	-1.318896	-0.356438	0.070757
C	-1.294868	0.874114	-0.753895
C	0.113316	1.491138	-0.736758
C	2.046109	-1.729746	-0.048079
C	-2.457418	-1.292602	0.040402
H	-0.174337	-1.519172	1.436648
H	1.769602	-2.687550	0.400649
H	2.653569	-1.166665	0.665171
H	2.664814	-1.937344	-0.927692
H	0.248502	-1.588309	-1.180520
H	2.131661	0.736206	-0.984310
H	1.056089	0.273378	-2.297837
H	1.424592	2.379608	0.748807
H	-0.282934	2.590437	1.096810
H	-0.090893	0.722685	2.509792
H	1.493687	0.327221	1.883579
H	-3.092229	-1.186347	-0.841199
H	-2.141836	-2.331304	0.180859
H	-3.069200	-1.051066	0.928284
H	-1.677550	0.648622	-1.759747
H	-2.044014	1.564090	-0.324387
H	0.144292	2.367959	-1.387936

Str-19
SCF Energy: -391.039479855
Num. Imaginary Frequencies: 0

C	2.906203	0.237231	0.589420
C	2.111160	-0.657636	-0.010300
C	0.686921	-0.946238	0.385470
C	-0.474606	0.786120	-1.166717
C	-1.582525	1.317229	-0.231698
C	-2.384421	0.151294	0.165178
C	-1.766893	-1.073843	-0.342796
C	-0.319390	-0.702904	-0.764942
C	4.337396	0.507769	0.229440
C	-3.598458	0.200494	0.982600
H	2.506909	0.813359	1.427468
H	4.486187	1.563635	-0.026817
H	4.665373	-0.101761	-0.617361
H	4.996897	0.296129	1.079663
H	2.507180	-1.251638	-0.835657
H	0.596191	-1.998009	0.693224
H	0.419826	-0.343183	1.265730
H	0.459708	1.340957	-1.065238
H	-0.803325	0.876824	-2.207407
H	-2.194152	2.157144	-0.586771
H	-1.163398	1.686500	0.728172
H	-4.095135	1.172500	0.971943
H	-4.290816	-0.613967	0.745955
H	-3.267593	0.006702	2.020716
H	-1.924930	-1.963701	0.277817
H	-2.375284	-1.251659	-1.260896
H	-0.015955	-1.306941	-1.624467

Str-20
SCF Energy: -391.063625391
Num. Imaginary Frequencies: 0

C	0.839048	0.787700	-0.010716
C	-0.303145	1.739514	-0.014136
C	-1.669637	1.218320	-0.504703
C	-1.544959	-0.779144	1.090840
C	-0.012241	-0.915526	1.262889
C	0.630448	-0.633596	-0.231178
C	-0.600008	-0.942748	-1.121848
C	-1.773302	-0.309359	-0.365919
C	2.176001	1.342103	0.295113
C	1.864776	-1.490090	-0.515006
H	0.030856	2.637874	-0.555636
H	2.137411	2.352414	0.705357
H	2.720669	1.379520	-0.664222
H	2.769605	0.686074	0.937419
H	-1.809289	1.495664	-1.554887
H	-0.358294	2.104774	1.027553
H	-2.464907	1.715484	0.058444
H	-1.980264	-0.092655	1.822669
H	-2.011933	-1.754767	1.254254
H	0.325138	-1.935605	1.470606
H	0.400549	-0.287948	2.059312
H	2.308540	-1.227789	-1.480958
H	2.638015	-1.401343	0.252274
H	1.570139	-2.541477	-0.563077
H	-0.476108	-0.560187	-2.140370
H	-0.701922	-2.030480	-1.188240
H	-2.740086	-0.642593	-0.752525

Str-21
SCF Energy: -391.063625536
Num. Imaginary Frequencies: 0

C	0.839070	0.787759	-0.010707
C	-0.302693	1.739742	-0.014350
C	-1.669703	1.218719	-0.503845
C	-1.544994	-0.779792	1.090620
C	-0.012300	-0.916269	1.262596
C	0.630324	-0.633580	-0.231253
C	-0.600150	-0.942051	-1.122190
C	-1.773348	-0.308980	-0.365794
C	2.176023	1.341726	0.295762
C	1.864658	-1.490004	-0.515391
H	0.031648	2.637582	-0.556671
H	2.769371	0.685232	0.937864
H	2.137684	2.351921	0.706252
H	2.720937	1.379209	-0.663476
H	-1.810394	1.496547	-1.553861
H	-0.357086	2.105797	1.027119
H	-2.464376	1.715621	0.060377
H	-1.980430	-0.093965	1.822971
H	-2.011833	-1.755623	1.253092
H	0.325031	-1.936345	1.469993
H	0.400551	-0.288898	2.059157
H	2.308672	-1.227142	-1.481028
H	2.637664	-1.401837	0.252108
H	1.569900	-2.541331	-0.564243
H	-0.476236	-0.558743	-2.140448
H	-0.702250	-2.029711	-1.189333
H	-2.740175	-0.641938	-0.752563

Str-24
SCF Energy: -391.037215296
Num. Imaginary Frequencies: 0

C	0.869865	0.916305	-0.428912
C	-0.561697	1.440404	-0.805037
C	-1.456726	0.173259	-0.892440
C	-1.049871	-0.129117	1.405826
C	0.063839	-1.013421	1.315093
C	0.689438	-0.615635	-0.222474
C	-0.453262	-0.936281	-1.190471
C	-2.187045	-0.203417	0.515604
C	1.589427	1.704059	0.669020
C	1.963749	-1.443183	-0.349125
H	1.497888	0.986774	-1.326247
H	1.740042	2.739110	0.349435
H	2.577042	1.286115	0.886468
H	1.025233	1.740741	1.608564
H	-0.543485	1.939660	-1.777270
H	-0.941733	2.179531	-0.092016
H	-2.282042	0.267127	-1.602670
H	-2.965010	0.527544	0.738262
H	-0.922170	0.788368	1.980415
H	-0.188568	-2.069104	1.207239
H	0.842163	-0.842559	2.057551
H	2.398657	-1.267967	-1.339786
H	2.711976	-1.157626	0.395047
H	1.767430	-2.514234	-0.249664
H	-0.073018	-0.801791	-2.212638
H	-0.847973	-1.953530	-1.117685
H	-2.602725	-1.205996	0.392487

Str-28
SCF Energy: -391.061967838
Num. Imaginary Frequencies: 0

C	-0.953482	0.731268	-0.090209
C	0.139419	1.663292	0.315541
C	1.275182	0.752162	0.856199
C	1.604983	-0.928788	-1.030649
C	0.087652	-0.807539	-1.170715
C	-0.642304	-0.603282	0.345586
C	0.468321	-0.441595	1.406782
C	2.214453	0.271759	-0.275413
C	-2.196606	1.175330	-0.755213
C	-1.719845	-1.645154	0.598027
H	-0.303415	2.263536	1.131010
H	-2.033228	2.010365	-1.440824
H	-2.847904	1.548458	0.052914
H	-2.738327	0.366337	-1.248213
H	0.422520	2.379040	-0.463986
H	2.421693	1.099993	-0.963252
H	1.845993	1.270164	1.629221
H	2.035565	-1.020735	-2.033247
H	1.837505	-1.861868	-0.509267
H	-0.416661	-1.702798	-1.541917
H	-0.153059	-0.020587	-1.899884
H	-2.226052	-1.438309	1.546231
H	-2.473625	-1.676172	-0.193142
H	-1.268768	-2.638374	0.672842
H	-0.005084	-0.207596	2.367545
H	1.057877	-1.349961	1.547150
H	3.178338	-0.026217	0.147197

Str-29
SCF Energy: -391.039554342
Num. Imaginary Frequencies: 0

C	0.445868	0.950394	-0.614237
C	-1.013448	0.624951	-1.002626
C	-1.029674	-0.744569	-1.365436
C	-1.278695	-0.638926	1.398815
C	0.264076	-0.567765	1.437626
C	0.893395	-0.403592	0.034402
C	0.195121	-1.418365	-0.934905
C	-1.903492	0.339829	0.397522
C	0.664016	2.241198	0.175709
C	2.410922	-0.587466	0.081702
H	0.992891	1.054089	-1.563508
H	1.729460	2.381944	0.378948
H	0.142224	2.261934	1.135797
H	0.330639	3.106032	-0.406337
H	-1.605124	1.333531	-1.582927
H	-1.896899	1.368593	0.772348
H	-1.867925	-1.239496	-1.856480
H	-1.694247	-0.421962	2.387914
H	-1.596060	-1.661017	1.162190
H	0.651819	-1.477364	1.908211
H	0.591774	0.264211	2.068722
H	2.865025	-0.438082	-0.904036
H	2.866981	0.127173	0.773366
H	2.675448	-1.591323	0.429116
H	0.781932	-1.472269	-1.879585
H	0.072405	-2.454341	-0.601430
H	-2.928873	0.084216	0.126260

Str-32
SCF Energy: -391.035021062
Num. Imaginary Frequencies: 0

C	-0.976496	-0.798415	-0.397530
C	0.510236	-0.940826	0.139784
C	2.756639	0.299078	0.244794
C	0.670328	1.482688	-0.559159
C	-0.800732	1.700616	-0.206483
C	-1.587220	0.471500	-0.002969
C	3.498579	-0.799263	0.081913
C	1.251836	0.387780	0.366852
C	-1.790031	-2.080238	-0.217502
C	-2.946788	0.557287	0.547555
H	-0.831019	-0.605165	-1.484692
H	-1.995503	-2.278209	0.839417
H	-1.221103	-2.929204	-0.604131
H	-2.740985	-2.051731	-0.757051
H	1.031386	-1.555091	-0.598213
H	0.454968	-1.519656	1.066662
H	3.263832	1.259875	0.330715
H	1.211913	2.425127	-0.441750
H	0.786540	1.185498	-1.609062
H	-1.344246	2.271470	-0.985048
H	-0.934682	2.332128	0.687668
H	-3.298258	1.578929	0.694716
H	-3.653074	-0.013146	-0.070050
H	-2.948968	0.025596	1.514868
H	4.579873	-0.730011	0.023242
H	3.082041	-1.799983	0.012349
H	1.039180	0.722329	1.396836

Str-34
SCF Energy: -391.062901649
Num. Imaginary Frequencies: 0

C	-0.161655	1.503027	-0.203634
C	-1.460928	0.995667	0.481045
C	-1.757543	-0.404298	-0.115172
C	-1.174253	-1.527506	0.761597
C	0.352763	-1.365658	0.943079
C	1.085562	-0.660065	-0.124999
C	0.369626	0.211001	-1.040418
C	-0.999012	-0.400691	-1.451608
C	0.834549	2.230861	0.693439
C	2.547495	-0.801558	-0.210439
H	-0.421348	2.170532	-1.033127
H	0.366159	3.141346	1.080549
H	1.731678	2.538540	0.146828
H	1.140934	1.638738	1.563640
H	-2.275376	1.698046	0.279833
H	-1.350831	0.957019	1.570707
H	-2.828003	-0.579960	-0.253748
H	-1.650438	-1.542814	1.746250
H	-1.375515	-2.500315	0.299514
H	0.870823	-2.296294	1.207516
H	0.563960	-0.708372	1.814848
H	3.007411	-1.183097	0.703786
H	2.724277	-1.552069	-1.004197
H	3.034192	0.114236	-0.559651
H	-1.454969	0.265479	-2.190692
H	1.007148	0.545925	-1.862095
H	-0.909717	-1.391614	-1.907294

Str-35
SCF Energy: -391.047798626
Num. Imaginary Frequencies: 0

C	0.736643	0.631783	-0.731022
C	-0.566538	1.349257	-0.570261
C	-1.754078	0.656150	-0.311561
C	-0.972827	0.838234	1.285949
C	0.056853	-0.274840	1.471845
C	0.584259	-0.706815	0.071130
C	-0.521503	-1.544436	-0.616047
C	-1.893330	-0.828048	-0.580370
C	1.940097	1.522836	-0.383436
C	1.883508	-1.510221	0.160146
H	0.798373	0.375195	-1.802208
H	1.979252	1.766401	0.683181
H	1.899090	2.462380	-0.943442
H	2.875581	1.026698	-0.647216
H	-2.419167	-0.923459	-1.537404
H	-0.594350	2.436819	-0.633183
H	-2.673871	1.237238	-0.283650
H	-0.624506	1.839488	1.554995
H	-1.934108	0.718878	1.793415
H	-0.387314	-1.131420	1.986730
H	0.874706	0.092911	2.097634
H	2.244652	-1.788885	-0.835368
H	2.676711	-0.955521	0.668350
H	1.716934	-2.435800	0.720325
H	-0.226103	-1.747875	-1.650756
H	-0.600577	-2.515799	-0.119042
H	-2.563805	-1.260655	0.169407

Str-37
SCF Energy: -391.047429366
Num. Imaginary Frequencies: 0

C	0.528363	0.829775	-0.701810
C	-0.984331	0.907065	-0.788698
C	-1.775785	0.492811	0.285559
C	-1.217735	-0.062881	1.559385
C	0.283167	-0.446739	1.477690
C	0.803966	-0.520694	0.022738
C	-0.081145	-1.513436	-0.782163
C	-1.410922	-0.813264	-1.090191
C	1.122180	2.106002	-0.079746
C	2.279014	-0.927603	-0.002101
H	0.911088	0.749696	-1.727545
H	2.211173	2.025952	-0.032434
H	0.749223	2.292939	0.931274
H	0.886284	2.982413	-0.690561
H	-1.666482	-0.645723	-2.138571
H	-1.446202	1.519240	-1.560208
H	-2.845956	0.691312	0.247891
H	-1.390912	0.727033	2.305598
H	-1.847050	-0.896251	1.891771
H	0.433943	-1.417026	1.960328
H	0.883222	0.272053	2.042012
H	2.670969	-0.939201	-1.024701
H	2.893273	-0.241517	0.588715
H	2.411894	-1.929685	0.418389
H	0.406949	-1.768062	-1.727973
H	-0.244521	-2.445707	-0.234767
H	-2.297522	-1.283690	-0.653207

Str-40
SCF Energy: -391.062901752
Num. Imaginary Frequencies: 0

C	0.162726	1.502946	0.203728
C	1.461761	0.994846	-0.480723
C	1.757226	-0.405366	0.115273
C	1.173384	-1.528011	-0.761821
C	-0.353716	-1.365728	-0.942837
C	-1.086051	-0.659366	0.125026
C	-0.369715	0.211288	1.040418
C	0.998552	-0.401459	1.451599
C	-0.832810	2.231308	-0.693722
C	-2.548122	-0.799792	0.210293
H	0.422515	2.170358	1.033272
H	-0.363560	3.141327	-1.080934
H	-1.729778	2.539871	-0.147340
H	-1.139502	1.639181	-1.563813
H	2.276757	1.696506	-0.279189
H	1.351972	0.956452	-1.570413
H	2.827558	-0.581717	0.253994
H	1.649260	-1.542896	-1.746631
H	1.374522	-2.501066	-0.300222
H	-0.872075	-2.296600	-1.206116
H	-0.565138	-0.709313	-1.815184
H	-2.725906	-1.550345	1.003760
H	-3.034114	0.116359	0.559624
H	-3.008124	-1.180672	-0.704185
H	-1.007003	0.546698	1.862078
H	0.908439	-1.392381	1.907069
H	1.454769	0.264235	2.190826

Str-41
SCF Energy: -391.041526546
Num. Imaginary Frequencies: 0

C	-0.756351	0.992393	0.313599
C	0.620573	1.301795	0.789596
C	1.899636	0.319320	-0.378673
C	1.410502	-0.846412	-1.238035
C	-0.129965	-0.986934	-1.217998
C	-0.743502	-0.579318	0.147766
C	0.260973	-0.991170	1.257114
C	1.294961	0.132552	1.201465
C	-1.328068	1.874647	-0.800580
C	-2.139908	-1.180191	0.323474
H	-1.338224	1.200416	1.236456
H	-2.349202	1.567943	-1.039466
H	-0.737308	1.818499	-1.719236
H	-1.364891	2.922214	-0.487208
H	1.019444	2.309008	0.898190
H	1.663734	1.272969	-0.885521
H	2.972395	0.383110	-0.187721
H	1.777511	-0.696804	-2.258324
H	1.880496	-1.761569	-0.867419
H	-0.384241	-2.031588	-1.421102
H	-0.585107	-0.403407	-2.023836
H	-2.595523	-0.867891	1.269483
H	-2.807287	-0.878109	-0.490010
H	-2.092914	-2.273414	0.317941
H	-0.202316	-0.967901	2.251447
H	0.686578	-1.987439	1.117469
H	2.123737	0.173872	1.902499

Str-43
SCF Energy: -391.039554254
Num. Imaginary Frequencies: 0

C	0.445179	0.949781	-0.615069
C	-1.014073	0.622661	-1.002437
C	-1.903409	0.339848	0.396840
C	-1.278306	-0.637420	1.399478
C	0.264561	-0.566132	1.438185
C	0.893640	-0.403213	0.034719
C	0.196083	-1.419498	-0.933491
C	-1.028880	-0.747126	-1.364833
C	0.662363	2.241760	0.173117
C	2.411229	-0.585846	0.082391
H	0.991977	1.053093	-1.564459
H	0.328416	3.105265	-0.410612
H	1.727554	2.384158	0.376156
H	0.140326	2.264250	1.132996
H	-1.605831	1.329930	-1.584352
H	-1.897951	1.368946	0.770850
H	-2.928687	0.083308	0.126162
H	-1.693798	-0.419386	2.388307
H	-1.595408	-1.659841	1.163928
H	0.652335	-1.475263	1.909684
H	0.592545	0.266492	2.068206
H	2.865605	-0.435153	-0.902984
H	2.866262	0.128594	0.774996
H	2.676554	-1.589768	0.429023
H	0.783387	-1.475308	-1.877743
H	0.073265	-2.455069	-0.598476
H	-1.866881	-1.243135	-1.855086

Str-45
SCF Energy: -391.044878967
Num. Imaginary Frequencies: 0

C	-1.038434	-0.764860	-0.296023
C	0.170141	-1.769348	-0.145786
C	1.967920	-0.002466	-0.086245
C	1.521670	0.464277	1.296355
C	0.089037	1.061534	1.178381
C	-0.485765	0.689021	-0.211805
C	0.735525	0.702501	-1.129020
C	1.406880	-1.143319	-0.681566
C	-2.176378	-1.125416	0.658622
C	-1.533550	1.709523	-0.697958
H	-1.408478	-0.889046	-1.322546
H	-2.507036	-2.153997	0.485011
H	-3.042146	-0.476741	0.499063
H	-1.878185	-1.047188	1.708710
H	-0.049824	-2.709542	-0.654340
H	0.321369	-1.980159	0.920551
H	2.946818	0.306772	-0.446315
H	1.556026	-0.386179	1.985862
H	2.230771	1.203248	1.674302
H	0.147464	2.151725	1.252962
H	-0.558195	0.729913	1.992815
H	-1.926266	1.447932	-1.685672
H	-2.375955	1.748048	-0.002031
H	-1.108729	2.716178	-0.752788
H	0.571036	0.299663	-2.133908
H	1.257366	1.656166	-1.256049
H	1.881691	-1.545487	-1.575356

Str-46
SCF Energy: -391.046773284
Num. Imaginary Frequencies: 0

C	0.922104	0.761859	-0.475598
C	-0.302855	1.695697	-0.269348
C	-1.777328	-0.331553	-0.739561
C	-1.578443	-0.193847	1.152949
C	-0.145343	-0.699867	1.324240
C	0.551508	-0.699875	-0.069577
C	-0.573066	-1.173158	-1.026876
C	-1.627315	0.974470	-0.273997
C	2.154146	1.346869	0.226973
C	1.753889	-1.646590	-0.116862
H	1.144114	0.731093	-1.550394
H	2.305252	2.385537	-0.084449
H	3.063780	0.797876	-0.025764
H	2.047364	1.345958	1.317861
H	-0.358556	2.450591	-1.064027
H	-0.217348	2.265996	0.664004
H	-2.776587	-0.707341	-0.949036
H	-1.886634	0.642967	1.785210
H	-2.368309	-0.942132	1.253731
H	-0.175152	-1.716096	1.728178
H	0.400354	-0.081306	2.040747
H	1.439469	-2.683541	0.040250
H	2.261684	-1.591951	-1.085507
H	2.485683	-1.402922	0.657643
H	-0.290397	-1.043254	-2.080271
H	-0.813465	-2.232985	-0.890336
H	-2.525025	1.577476	-0.151909

Str-48
SCF Energy: -391.033590949
Num. Imaginary Frequencies: 0

C	0.971781	1.095945	-0.344387
C	-3.463858	0.012585	0.047441
C	-1.098003	-0.574533	-0.566054
C	-0.215240	-1.640764	0.106126
C	0.859724	-0.971258	1.091883
C	1.614449	-0.110721	0.189488
C	-0.204306	0.480709	-1.255165
C	-2.165179	-0.022669	0.355569
C	0.471747	2.126849	0.691370
C	2.920482	-0.547397	-0.326515
H	1.652892	1.600915	-1.036618
H	1.320951	2.575047	1.214754
H	-0.210741	1.710347	1.431222
H	-0.055191	2.924294	0.161770
H	-4.198859	0.408672	0.740809
H	-3.839867	-0.352140	-0.905851
H	-1.624171	-1.084211	-1.385457
H	-0.793260	-2.332534	0.725352
H	0.315496	-2.236095	-0.644486
H	1.465927	-1.756336	1.547355
H	0.306096	-0.420494	1.854600
H	3.658484	-0.039931	0.325962
H	3.099393	-1.620219	-0.223911
H	3.125270	-0.190074	-1.339687
H	-0.782135	1.343324	-1.600159
H	0.265783	0.030329	-2.136393
H	-1.855653	0.346620	1.332203

Str-50
SCF Energy: -391.037536704
Num. Imaginary Frequencies: 0

C	-1.502335	0.713523	0.368826
C	-0.011445	1.058657	0.608388
C	2.159892	-0.376833	0.872466
C	2.669981	-0.362965	-0.546619
C	3.257956	0.681258	-1.140593
C	-1.498865	-0.690461	-0.071675
C	-0.179490	-1.283638	0.139986
C	0.622110	-0.285779	1.016236
C	-2.388063	1.727608	-0.364941
C	-2.645575	-1.386195	-0.663600
H	-1.949290	0.538272	1.382475
H	-2.355498	2.684831	0.159753
H	-3.433404	1.412071	-0.417275
H	-2.018299	1.888233	-1.382411
H	0.109483	1.837529	1.364248
H	0.429822	1.424348	-0.326953
H	2.594686	0.457757	1.433985
H	2.584222	-1.295681	-1.106879
H	2.498400	-1.293554	1.371226
H	3.627679	0.620978	-2.159674
H	3.417734	1.622251	-0.618429
H	-2.691955	-1.064676	-1.720313
H	-2.554629	-2.473056	-0.643116
H	-3.594871	-1.055464	-0.228286
H	-0.184299	-2.345481	0.407645
H	0.245399	-1.239488	-0.892620
H	0.369835	-0.489925	2.065772

Str-54
SCF Energy: -391.065786367
Num. Imaginary Frequencies: 0

C	0.815672	-0.935077	-0.505823
C	1.112382	0.407679	-1.213335
C	0.113237	1.491110	-0.736706
C	0.477031	0.592702	1.584118
C	-0.117079	-0.618659	0.822212
C	-1.318985	-0.356458	0.070762
C	-1.295018	0.874192	-0.753698
C	0.454787	1.876116	0.715651
C	2.046391	-1.729446	-0.048086
C	-2.457430	-1.292688	0.040353
H	0.248626	-1.588467	-1.180481
H	2.653913	-1.166015	0.664838
H	2.665006	-1.937248	-0.927724
H	1.770208	-2.687151	0.401047
H	1.055806	0.273344	-2.297922
H	2.131523	0.736222	-0.984538
H	0.144168	2.367963	-1.387832
H	1.493585	0.327055	1.883683
H	-0.282656	2.590446	1.096879
H	-0.091064	0.722558	2.509697
H	-0.174399	-1.519309	1.436444
H	-2.142005	-2.331240	0.182189
H	-3.069996	-1.050253	0.927456
H	-3.091575	-1.187249	-0.841794
H	-1.677952	0.648943	-1.759499
H	-2.043929	1.564236	-0.323854
H	1.424816	2.379349	0.748721

Str-57
SCF Energy: -391.065786343
Num. Imaginary Frequencies: 0

C	0.815406	-0.935171	-0.505678
C	1.112394	0.407434	-1.213368
C	0.455009	1.876284	0.715295
C	0.477235	0.593092	1.584154
C	-0.117035	-0.618400	0.822435
C	-1.318968	-0.356291	0.070884
C	-1.295036	0.874273	-0.753693
C	0.113324	1.490983	-0.736944
C	2.045945	-1.729942	-0.048091
C	-2.457257	-1.292672	0.040425
H	0.248095	-1.588475	-1.180222
H	2.653679	-1.166708	0.664810
H	2.664420	-1.937868	-0.927793
H	1.769503	-2.687598	0.401025
H	1.055944	0.272954	-2.297941
H	2.131519	0.735936	-0.984485
H	1.425031	2.379532	0.748175
H	1.493805	0.327439	1.883771
H	-0.282370	2.590751	1.096401
H	-0.090840	0.723253	2.509694
H	-0.174477	-1.518955	1.436789
H	-3.068906	-1.051248	0.928484
H	-3.092262	-1.186392	-0.840991
H	-2.141649	-2.331347	0.180974
H	-1.678233	0.648985	-1.759383
H	-2.043665	1.564467	-0.323603
H	0.144306	2.367724	-1.388210

Str-59
SCF Energy: -391.025787309
Num. Imaginary Frequencies: 0

C	-3.088824	0.503856	-0.234396
C	-2.587226	-0.440624	0.643965
C	-0.594174	-1.259404	-0.802182
C	0.926151	-1.104970	-0.460641
C	1.281326	0.297509	0.071948
C	2.777569	0.471656	0.242730
C	3.357576	0.276613	1.437365
C	-1.457450	-1.220504	0.382036
C	-4.280266	1.327911	0.011771
C	3.559728	0.869260	-0.984673
H	-2.576472	0.662845	-1.182511
H	-4.757250	1.133832	0.973171
H	-5.003833	1.172792	-0.804077
H	-4.009772	2.392675	-0.065670
H	-3.099339	-0.591614	1.590999
H	-0.705431	-2.281873	-1.206216
H	-0.891550	-0.558385	-1.585509
H	1.214927	-1.866838	0.271153
H	1.476590	-1.324389	-1.380254
H	0.775872	0.455402	1.034457
H	0.898236	1.057955	-0.622944
H	3.403784	0.168353	-1.814357
H	3.243430	1.857861	-1.341906
H	4.631855	0.910676	-0.780411
H	2.779939	0.013552	2.319997
H	4.428769	0.388989	1.574305
H	-1.176222	-1.919654	1.172241

Str-61
SCF Energy: -391.063625475
Num. Imaginary Frequencies: 0

C	-0.630349	-0.633616	-0.231346
C	0.600235	-0.942547	-1.121882
C	1.773359	-0.309149	-0.365695
C	1.544855	-0.779507	1.090818
C	0.012132	-0.915160	1.262957
C	-0.839090	0.787693	-0.010992
C	0.302724	1.739658	-0.014629
C	1.669708	1.218503	-0.504180
C	-1.864442	-1.490421	-0.515177
C	-2.176058	1.341803	0.295365
H	0.476401	-0.559814	-2.140370
H	-2.307775	-1.228801	-1.481447
H	-2.638012	-1.401271	0.251654
H	-1.569661	-2.541814	-0.562439
H	1.810271	1.496050	-1.554318
H	0.702350	-2.030241	-1.188346
H	2.740241	-0.642307	-0.752205
H	2.011177	-1.755533	1.253482
H	1.980719	-0.093753	1.822983
H	-0.400402	-0.286794	2.058914
H	-0.325790	-1.934822	1.471435
H	-2.720916	1.379343	-0.663844
H	-2.769442	0.685416	0.937550
H	-2.137606	2.351995	0.705885
H	-0.031552	2.637482	-0.557002
H	0.357107	2.105731	1.026833
H	2.464446	1.715587	0.059799

Str-62
SCF Energy: -391.043417760
Num. Imaginary Frequencies: 0

C	-2.879253	0.000052	-0.039436
C	-1.549034	-0.000108	0.113988
C	-0.555418	-0.000906	-1.026378
C	0.342446	-1.257061	-1.037264
C	1.357158	-1.268285	0.130124
C	2.041117	0.000379	0.403804
C	1.356968	1.268519	0.128204
C	0.342265	1.255347	-1.039190
C	-3.887267	0.000876	1.070093
C	3.386078	0.000922	0.990607
H	-3.283963	-0.000447	-1.053245
H	-4.539794	-0.877630	1.001424
H	-4.539603	0.879415	1.000307
H	-3.413262	0.001451	2.056151
H	-0.261919	2.163874	-0.979817
H	-1.152972	0.000354	1.134083
H	-1.124578	-0.001651	-1.963243
H	-0.261595	-2.165584	-0.976520
H	0.904813	-1.307993	-1.977147
H	2.069367	-2.100205	0.091185
H	0.802665	-1.427972	1.082855
H	3.613241	0.909227	1.554803
H	3.613325	-0.906493	1.556205
H	4.067839	0.000237	0.116228
H	0.802428	1.429628	1.080658
H	2.069064	2.100464	0.087940
H	0.904582	1.304906	-1.979182