

Identifying Active Normal Modes in Competitive Myers-Saito and Schmittel Cyclizations in Enyne-Allenenes From a Combined Perspective Between the Reaction Force Constant and Statistical Tools

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Table S1. Overall, activation and relative Gibbs free energies for Myers-Saito (path-a) and Schmittel (path-b) cyclization. All values are given in kcal/mol.

path-a	ΔG^\ddagger	ΔG^o	path-b	ΔG^\ddagger	ΔG^o	$\Delta\Delta G^\ddagger$	$\Delta\Delta G^o$
1a	25.87	5.46	1b	30.87	15.25	5.00	9.79
2a	28.60	10.96	2b	30.68	-26.28	2.08	-37.25
3a	28.70	11.07	3b	29.30	-30.15	0.60	-41.22
4a	28.04	10.94	4b	27.43	-33.88	-0.61	-44.82
5a	31.93	16.02	5b	34.29	15.82	2.37	-0.21
6a	29.20	1.05	6b	27.84	8.86	-1.35	7.82
7a	31.72	5.39	7b	29.41	22.82	-2.31	17.43

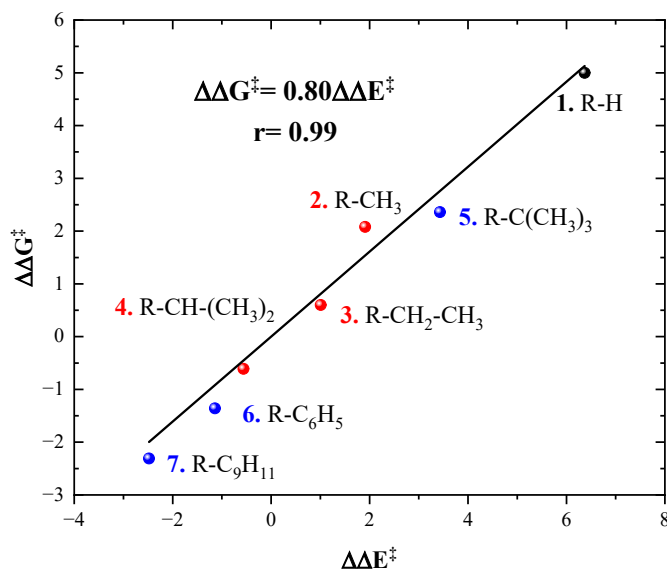


Figure S1. Linear correlation between free energy difference ($\Delta\Delta G^\ddagger$) and electronic energy difference ($\Delta\Delta E^\ddagger$), energy values in kcal/mol.

The vibrational contributions out-of-plane Bz₂ for Myers-Saito and Schmittel cyclization are considered negligible due to the marginal C₁₄-C₁₅-C₁₆-C₁₇ dihedral variation for all paths (<1° in Figure S2).

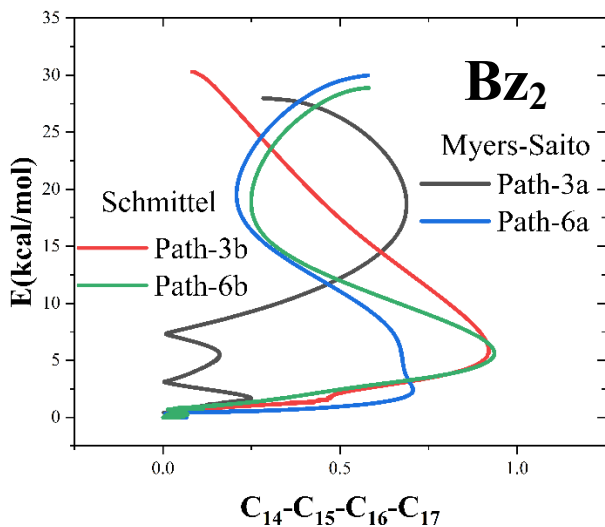


Figure S2.Comparative activation diagrams along ξ projected onto dihedral $C_{14}-C_{15}-C_{16}-C_{17}$ angle in Bz_2 substructure.

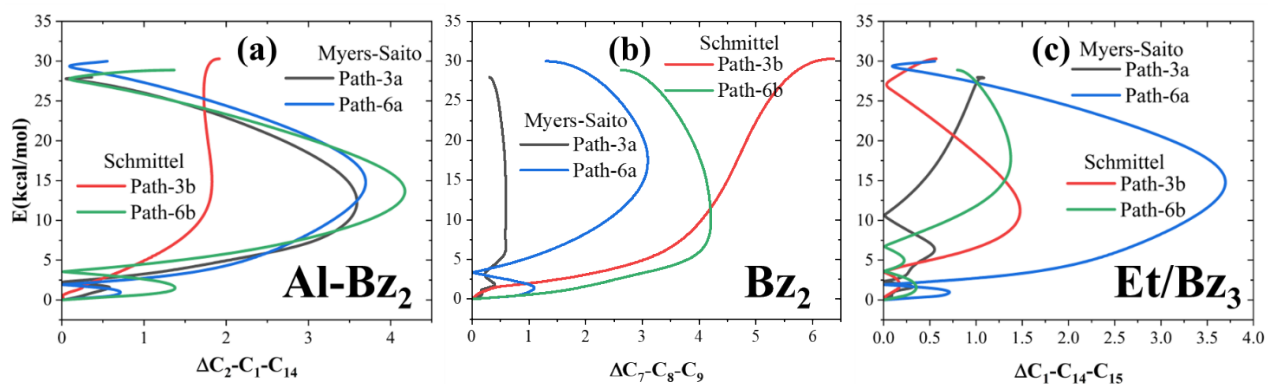


Figure S3.Comparative activation diagrams along ξ projected onto variations of $C_2-C_1-C_{14}$ (a), $C_7-C_8-C_9$ (b) and $C_1-C_{14}-C_{15}$ (c) angle.

Table S2. Validation criteria of PLS-VIP regressions in both set A and B.

Path	$\sigma^2 k_i$	σ^2 $\kappa_Y(\xi); Y = a,$	RSS	R²	$\# \kappa_Y(\xi)$ $Y = a, b$	k_i	Factors
1a	81.5 %	99.3 %	0.013	0.999	24	81	3
2a	74.4 %	96.2 %	0.072	0.998	38	90	4
3a	99.3%	96.7 %	0.013	0.999	25	99	7
4a	99.9%	99.9%	1.4×10^{-7}	0.999	21	108	17
3a	99.3%	96.7 %	0.013	0.999	25	99	7
5a	98.8 %	99.8 %	0.004	0.999	24	117	9
6a	99.9 %	99.9 %	$< 1.4 \times 10^{-7}$	0.999	13	111	13
7a	68.8%	88.6%	0.24	0.88	24	138	2
1b	91.3 %	98.6 %	0.026	0.998	21	81	4
2b	98.9%	98.0 %	0.118	0.991	49	90	13
3b	96.7%	99.9%	0.0008	0.999	48	99	7
4b	89.9%	98.5%	0.062	0.996	46	108	7
5b	98.7 %	99.9 %	0.014	0.998	14	117	8
6b	98.9%	98.0 %	1.5×10^{-5}	0.999	21	111	15
7b	98.6%	99.8%	0.004	0.998	23	138	9

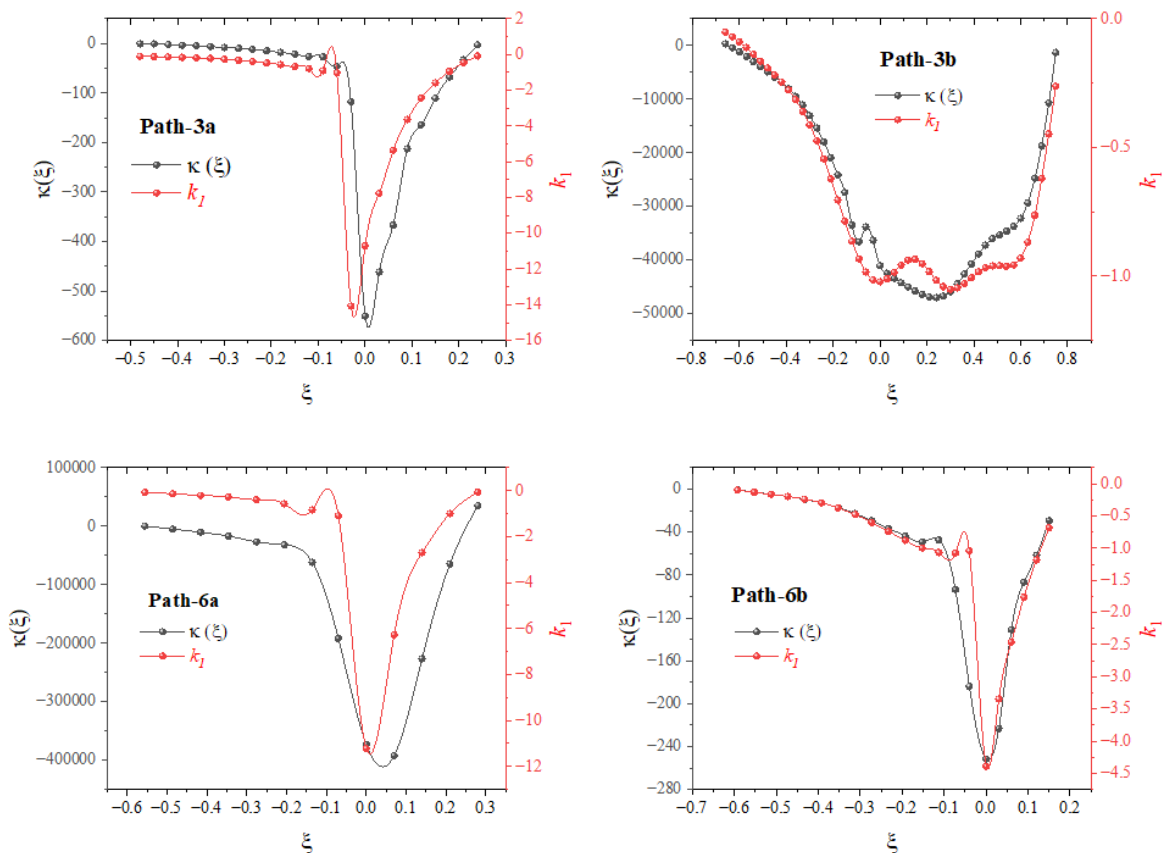


Figure S4. Reaction force constant $\kappa(\xi)$ and k_1 along the transition regions.

Table S3. PLS-VIP regressions with step size $0.03 \text{ amu}^{1/2} \text{ Bohr}$ in system **3** and system **6**.

PLS-VIP correlations

$$\begin{aligned} \kappa_{3a}(\xi) &= 2.68k_{48} - 0.74k_{67} + 2.3k_{72} + 0.18k_1 - 0.18k_2 + 257.7k_{97} + 773.4k_{96} + 773.4k_{90} + \\ & 5.1k_{23} + 95.9 \end{aligned}$$

$$\begin{aligned} \kappa_{6a}(\xi) &= 0.24k_1 - 3.1k_{35} + 2.4k_{36} + 13.4k_{31} - 17.6k_{14} - 6.8k_{85} - 0.5k_{79} + 1.4k_{84} - 7.7k_{65} + \\ & .7k_{15} + 84.8 \end{aligned}$$

$$\begin{aligned} \kappa_{3b}(\xi) &= 3.2k_1 - 45.8k_7 - 278.4k_3 - 7.7k_{18} - 49.1k_{13} - 1.7k_{69} - 0.98k_{73} - 0.51k_{40} + 6.8k_{54} - \end{aligned}$$

$$\begin{aligned} \kappa_{6b}(\xi) &= -28.6k_{18} + 6.1k_{73} + 0.02k_1 - 9.6k_{25} - 10.2k_{72} - 1.9k_{76} + 20.3k_{37} - 13.1k_{38} - 9.1k_2 \\ & + 197.9 \end{aligned}$$

Table S4. Validation criteria of PLS-VIP regressions with step size $0.03 \text{ amu}^{1/2}$ in system 3 and 6.

Path	$\sigma^2 k_i$	σ^2 $\kappa_Y(\xi); Y = a, b$	RSS	R^2	$\# \kappa_Y(\xi)$ $Y = a, b$	k_i	Factors
3a	95.7%	98.5%	0.035	0.985	31	99	7
6a	98.9%	99.9%	$< 1.4 \times 10^{-7}$	0.999	27	111	13
3b	93.9%	99.6%	< 0.0008	0.999	48	99	7
6b	99.9%	99.9%	$< 1.5 \times 10^{-5}$	0.999	27	111	15

(a) Path-3a: The PLS-VIP model with $0.03 \text{ amu}^{1/2}$ step size shows a slight increase in the representativeness of Y ($\Delta\sigma^2\kappa_Y(\xi) = 1.8\%$) due to the higher number of transients. However, it shows a loss in the representativeness of X ($\Delta\sigma^2k_i = -3.6\%$) and a decrease in regression linearity ($R^2 = 0.985$). Most notably, there is a significant decrease in the accuracy of the regression, with the RSS error increasing by 2.7 times.

(b) Path-6a: The predictive error (RSS) and linearity (R^2) of the model do not differ significantly for either step size ($0.07 \text{ amu}^{1/2}$, $0.03 \text{ amu}^{1/2}$) despite the increase of the number of transients $\kappa_Y(\xi)$. Additionally, a marginal loss in the representativeness of X is found ($\Delta\sigma^2k_i = -1\%$), for the smaller step size.

(c) Path-3b: The number of transients $\kappa_Y(\xi)$, predictive error (RSS), and linearity (R^2) of the model do not differ significantly for either step size. However, there is a decrease in representativeness of X and Y ($\Delta\sigma^2k_i = -2.8\%$, $\Delta\sigma^2\kappa_Y(\xi) = -0.3\%$), which reduces the quality of the PLS-VIP model. This indicates that adjusting the step size to $0.03 \text{ amu}^{1/2}$ does not provide significant information to enrich the chemical space of the regressions.

(d) Path-6b: Only a marginal gain in the representativeness of X and Y is observed ($\Delta\sigma^2k_i = 1\%$, $\Delta\sigma^2\kappa_Y(\xi) = 1.9\%$), while the other validation criteria are not significantly different.

This indicates that the step size of $0.07 \text{ amu}^{1/2}$ is already sufficiently representative in describing the associated changes in the transition region.

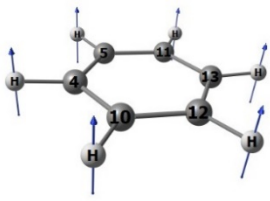
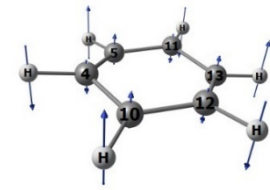
In general, it can be concluded that, although there are slight increases in the X,Y representativeness of the PLS-VIP models by tightening the step size to $0.03 \text{ amu}^{1/2}$, these changes do not always lead to significant improvements in the overall quality of the regression model. Therefore, it is considered that a step size of $0.07 \text{ amu}^{1/2}$ is able to satisfactorily describe both variables in the regression models under good statistical quality criteria.

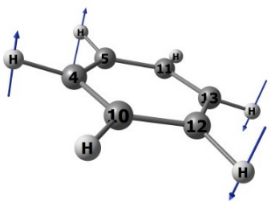
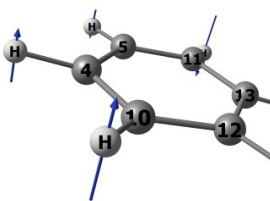
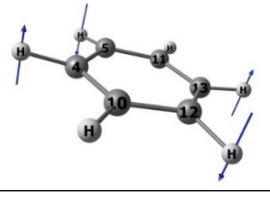
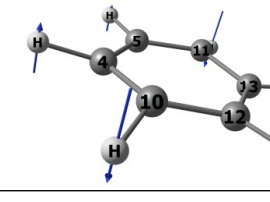
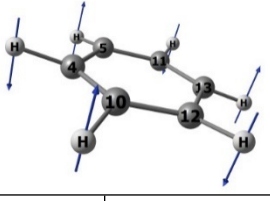
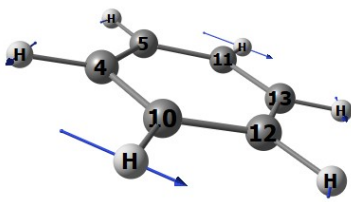
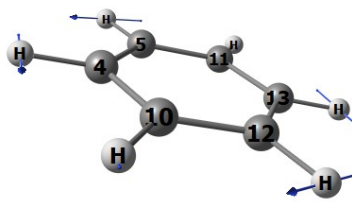
Substructure vibration characterization. The vibrational contributions of the active modes (Table 6 and 7) are associated with direct (+) and inverse (-) relationship to $\kappa(\xi)$. These contributions were analyzed based on the vibrational characteristics of the five substructures (Scheme 3) relevant to the cyclization pathways (Path-3a/3b or Path-6a/6b). Each vibrational feature of these substructures was classified according to various infrared spectroscopic assignments⁵⁸:

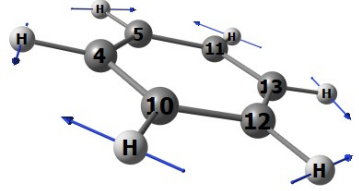
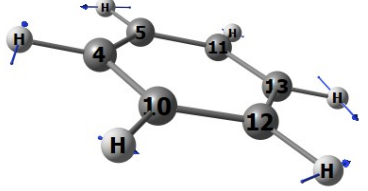
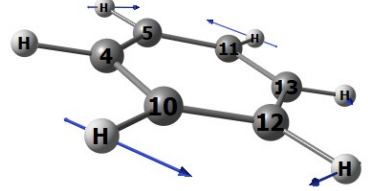
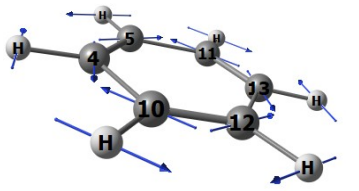
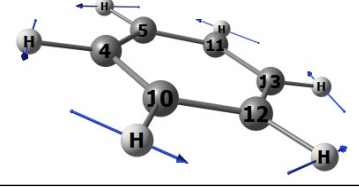
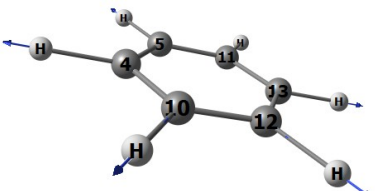
Bz₁ substructure:

Table S5. Vibrational character of Bz₁ substructure.

$\nu_{e_{2u}(I)}: 411 \text{ cm}^{-1}$	$\nu_{e_{2u}(II)}: 411 \text{ cm}^{-1}$	Description
		Double degenerate, <i>twisting</i> mode of the carbon backbone.
$\nu_{e_{2g}(I)}: 616 \text{ cm}^{-1}$	$\nu_{e_{2g}(II)}: 616 \text{ cm}^{-1}$	Description
		Double degenerate, Symmetric <i>stretching</i> of the carbon backbone
$\nu_{a_{2u}}: 690 \text{ cm}^{-1}$		Description

	<p><i>H-wagging</i> in all hydrogen.</p>
$\nu_{b_{2g}}:718 \text{ cm}^{-1}$	Description
	<p><i>H-twisting</i> and C-twisting in all the atoms</p>

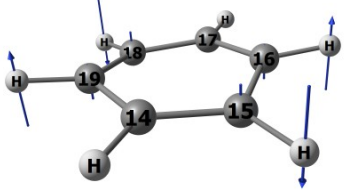
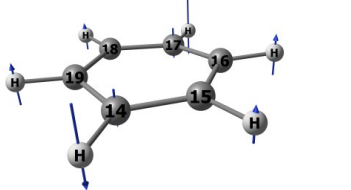
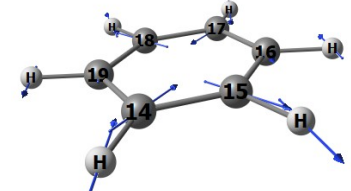
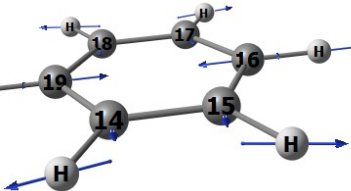
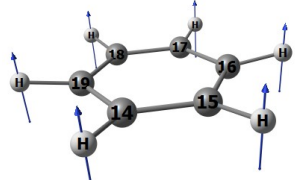
$\nu_{e_{1g}(I)}:877 \text{ cm}^{-1}$	$\nu_{e_{1g}(II)}:877 \text{ cm}^{-1}$	Description
		<p>Double degenerate, <i>H-twisting</i> mode for H-bonded to C₄-C₅, C₁₂-C₁₃ (I) and for all H-atoms (II)</p>
$\nu_{e_{2g}(I)}:1003 \text{ cm}^{-1}$	$\nu_{e_{2g}(II)}:1003 \text{ cm}^{-1}$	Description
		<p>Double degenerate, <i>H-twisting</i> mode for H-bonded to C₄-C₅, C₁₂-C₁₃ (I) and for all H-atoms (II)</p>
$\nu_{b_{2g}(I)}:1034 \text{ cm}^{-1}$		Description
		<p><i>H-twisting</i> mode for all H-atoms</p>
$\nu_{e_{1u}(I)}:1077 \text{ cm}^{-1}$	$\nu_{e_{1u}(II)}:1077 \text{ cm}^{-1}$	Description
		<p>Double degenerate, <i>H-scissoring</i> mode for all the H-atoms (I) and <i>H-scissoring</i> mode in four H-atoms.</p>
$\nu_{b_{2u}}:1175 \text{ cm}^{-1}$		Description

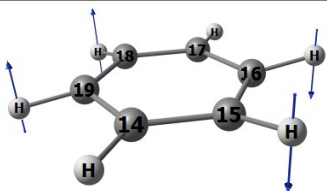
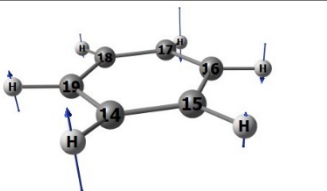
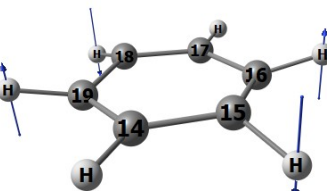
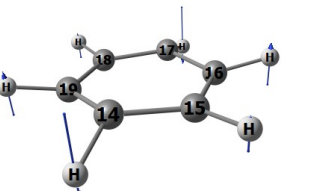
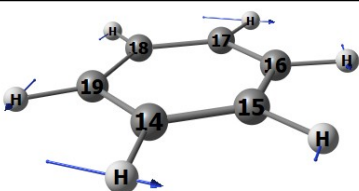
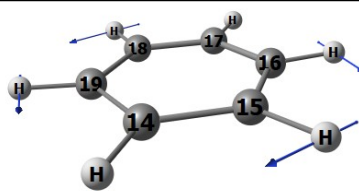
		H-scissoring mode for all the H-atoms
$\nu_{e_{2g(I)}}:1206 \text{ cm}^{-1}$	$\nu_{e_{2g(II)}}:1206 \text{ cm}^{-1}$	Description
		Double degenerate, <i>H-scissoring</i> mode for all the H-atoms.
$\nu_{b_{2u}}:1360 \text{ cm}^{-1}$		Description
		Symmetric <i>stretching</i> in the carbon backbone
$\nu_{a_{2g}}:1379 \text{ cm}^{-1}$		Description
		<i>H-rocking</i> mode in all the H-atoms
$\nu_{a_{1g}}:3231 \text{ cm}^{-1}$		Description
		symmetric <i>stretching</i> in all H-atoms.

B_Z₂ substructure:

Table S6. Vibrational character of B_Z₂ substructure.

$\nu_{e_{2u(I)}}: 411 \text{ cm}^{-1}$	$\nu_{e_{2u(II)}}: 411 \text{ cm}^{-1}$	Description
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		Double degenerate, <i>twisting</i> mode of the carbon backbone.
$\nu_{e2g(I)}:616 \text{ cm}^{-1}$	$\nu_{e2g(II)}:616 \text{ cm}^{-1}$	Description
		Double degenerate, Symmetric <i>stretching</i> of the carbon-hydrogen backbone
$\nu_{a2u}:690 \text{ cm}^{-1}$		Description
		<i>H-wagging</i> for all hydrogen atoms

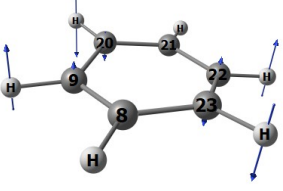
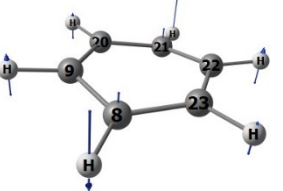
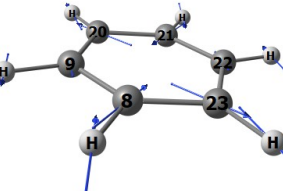
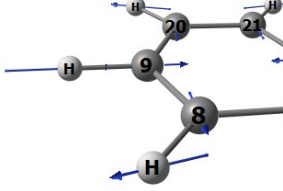
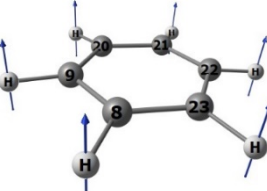
$\nu_{e1g(I)}:877 \text{ cm}^{-1}$	$\nu_{e1g(II)}:877 \text{ cm}^{-1}$	Description
		Double degenerate, <i>H-twisting</i> in four H-atoms (I) and <i>H-twisting</i> for all H-atoms (II)
$\nu_{e2g(I)}:1003 \text{ cm}^{-1}$	$\nu_{e2g(II)}:1003 \text{ cm}^{-1}$	Description
		Double degenerate, <i>H-twisting</i> in four H-atoms (I) and <i>H-twisting</i> for all H-atoms (II)
$\nu_{e1u(I)}:1077 \text{ cm}^{-1}$	$\nu_{e1u(II)}:1077 \text{ cm}^{-1}$	Description
		Double degenerate, <i>H-scissoring</i> mode for all the H-atoms (I) and <i>H-scissoring</i> mode in four H-atoms.
$\nu_{e2g(I)}:1206 \text{ cm}^{-1}$	$\nu_{e2g(II)}:1206 \text{ cm}^{-1}$	Description

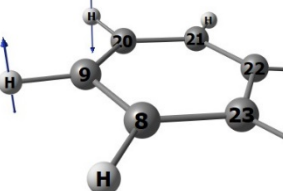
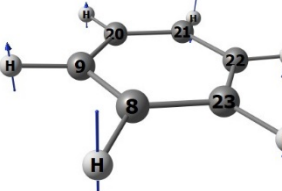
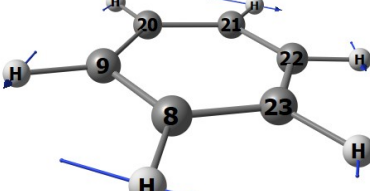
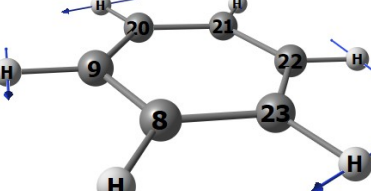
		Double degenerate, <i>H-scissoring</i> mode for all the H-atoms.
$\nu_{b_{2u}}:1360\text{ cm}^{-1}$		Description
		Symmetric <i>stretching</i> in the carbon backbone
$\nu_{a_{2g}}:1379\text{ cm}^{-1}$		Description
		<i>H-rocking</i> mode in all the H-atoms

$\nu_{e_{2g}(I)}:3208\text{ cm}^{-1}$	$\nu_{e_{2g}(II)}:3208\text{ cm}^{-1}$	Description
		Symmetric stretching among all the H atoms
$\nu_{e_{1u}(I)}:3222\text{ cm}^{-1}$	$\nu_{e_{1u}(II)}:3222\text{ cm}^{-1}$	Description
		Anti-symmetric stretching among all the H atoms

B₃ substructure:

Table S7. Vibrational character of Bz₃ substructure.

$\nu_{e_{2u}(I)}: 411 \text{ cm}^{-1}$	$\nu_{e_{2u}(II)}: 411 \text{ cm}^{-1}$	Description
		Double degenerate, <i>twisting</i> mode of the carbon backbone.
$\nu_{e_{2g}(I)}: 616 \text{ cm}^{-1}$	$\nu_{e_{2g}(II)}: 616 \text{ cm}^{-1}$	Description
		Double degenerate, symmetric <i>stretching</i> of the carbon backbone
$\nu_{a_{2u}}: 690 \text{ cm}^{-1}$		Description
		<i>H-wagging</i> for all hydrogen atoms

$\nu_{e_{2g}(I)}: 1003 \text{ cm}^{-1}$	$\nu_{e_{2g}(II)}: 1003 \text{ cm}^{-1}$	Description
		Double degenerate, <i>H-twisting</i> in four H-atoms (I) and <i>H-twisting</i> for all H-atoms (II)
$\nu_{e_{1u}(I)}: 1077 \text{ cm}^{-1}$	$\nu_{e_{1u}(II)}: 1077 \text{ cm}^{-1}$	Description
		Double degenerate, <i>H-scissoring</i> mode for all the H-atoms (I) and <i>H-scissoring</i> mode in four H-atoms.
$\nu_{e_{2g}(I)}: 1206 \text{ cm}^{-1}$	$\nu_{e_{2g}(II)}: 1206 \text{ cm}^{-1}$	Description

	Double degenerate, <i>H-scissoring</i> mode for all the H-atoms.
$\nu_{b_{2u}}:1360 \text{ cm}^{-1}$	Description
	Symmetric <i>stretching</i> in the carbon backbone
$\nu_{a_{2g}}:1379 \text{ cm}^{-1}$	Description
	<i>H-rocking</i> mode in all the H-atoms

$\nu_{a_{1g}}:3231 \text{ cm}^{-1}$	Description
	Symmetric <i>stretching</i> in all H-atoms

Al substructure:

Table S8. Vibrational character of Al substructure.

$\nu_a:379 \text{ cm}^{-1}$	$\nu_b:379 \text{ cm}^{-1}$	Description
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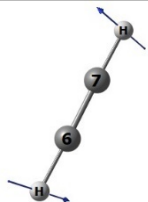
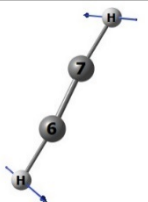
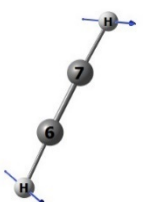
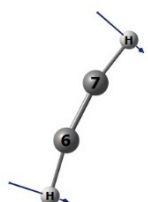
		Antisymmetric <i>bending</i> type of the three-atom group
$\nu_a: 896 \text{ cm}^{-1}$	$\nu_b: 896 \text{ cm}^{-1}$	Description
		wagging mode for the four H-atoms
$\nu_a: 1028 \text{ cm}^{-1}$	$\nu_b: 1028 \text{ cm}^{-1}$	Description
		<i>bending</i> mode of the carbon structure and antisymmetric <i>rocking</i> in the H-atoms
$\nu_b: 1442 \text{ cm}^{-1}$		Description
		<i>Scissoring</i> mode in the H-atoms.

$\nu_b: 3177 \text{ cm}^{-1}$	Description
	C-H antisymmetric <i>stretching</i>

Ac substructure:

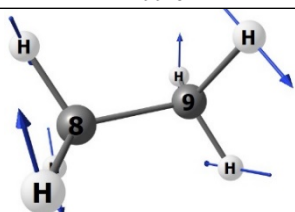
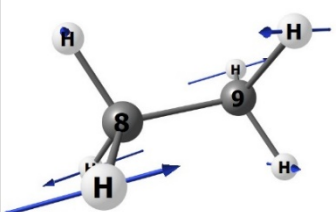
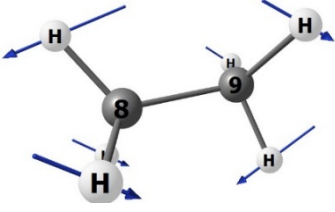
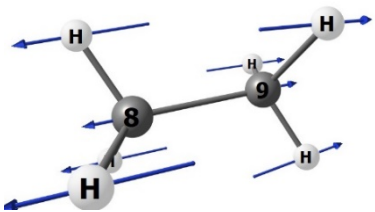
Table S9. Vibrational character of Ac substructure.

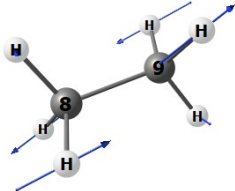
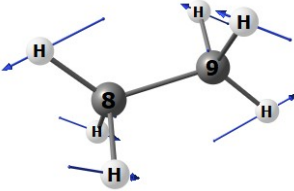
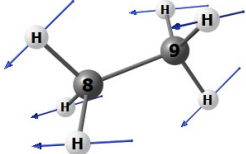
$\nu_{\pi_g(I)}: 671 \text{ cm}^{-1}$	$\nu_{\pi_g(II)}: 671 \text{ cm}^{-1}$	Description
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		Double degenerated, <i>c</i> -twisting mode
$\nu_{\pi_u(I)}:799 \text{ cm}^{-1}$	$\nu_{\pi_u(II)}:799 \text{ cm}^{-1}$	Description
		<i>H</i> -wagging mode

Et substructure:

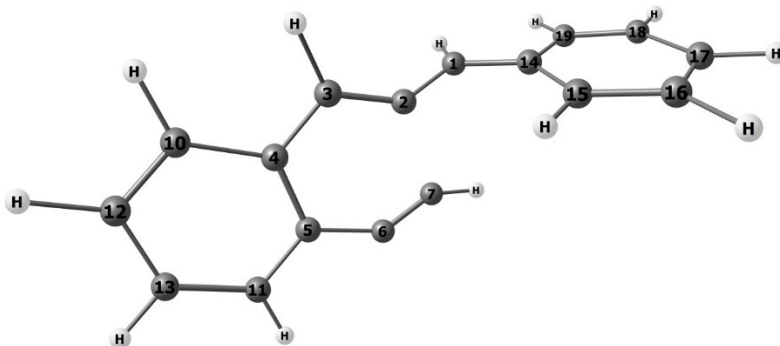
Table S10. Vibrational character of Et substructure

$\nu_{a_{1u}}:299 \text{ cm}^{-1}$		Description
		<i>rocking</i> mode for all H-atoms
$\nu_{eu(I)}:819 \text{ cm}^{-1}$	$\nu_{eu(II)}:819 \text{ cm}^{-1}$	Description
		<i>scissoring</i> mode in the H-atoms
$\nu_{a_{1g}}:1030 \text{ cm}^{-1}$		Description
		<i>stretching</i> mode on the two C-atoms

$\nu_{e g(I)}:1225 \text{ cm}^{-1}$	$\nu_{e g(II)}:1225 \text{ cm}^{-1}$	Description
		<i>twisting</i> mode on the two C-atoms and <i>scissoring</i> mode in the H-atoms
$\nu_{a 2u}:1417 \text{ cm}^{-1}$		Description
		<i>scissoring</i> mode on the H-atoms

Cartesian coordinates of Transition States:

TS1a:

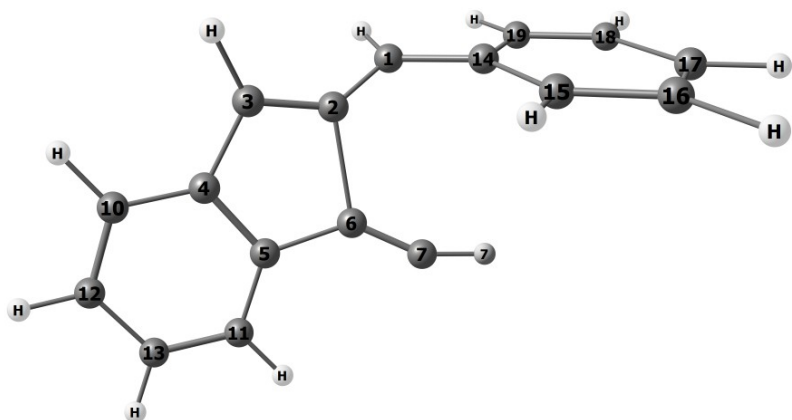


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C	2.847716000000	0.074290000000	0.638501000000
C	2.361856000000	-0.054050000000	-0.714911000000
C	0.981186000000	0.102615000000	-1.014214000000
H	-0.259240000000	0.370115000000	2.307631000000
C	3.262094000000	-0.216723000000	-1.786890000000
C	2.815949000000	-0.210892000000	-3.095898000000
C	1.454448000000	-0.016042000000	-3.381657000000
C	0.547819000000	0.151489000000	-2.350120000000
H	-0.508907000000	0.298221000000	-2.551286000000
H	1.113471000000	0.000434000000	-4.412354000000
H	3.524458000000	-0.348613000000	-3.907386000000
H	4.318874000000	-0.356400000000	-1.571573000000
C	2.231183000000	0.024071000000	3.110768000000
H	2.615228000000	-0.931410000000	3.470487000000

H	3.924755000000	0.188813000000	0.752943000000
C	1.702456000000	0.928775000000	4.117941000000
C	1.683523000000	0.529785000000	5.467307000000
C	1.205524000000	2.205095000000	3.792947000000
C	1.193371000000	1.374020000000	6.455889000000
H	2.061700000000	-0.455082000000	5.732166000000
C	0.712829000000	3.046507000000	4.784600000000
H	1.223163000000	2.536170000000	2.757674000000
C	0.703313000000	2.636760000000	6.118492000000
H	1.189356000000	1.047291000000	7.491831000000
H	0.336994000000	4.029598000000	4.515575000000
H	0.317571000000	3.297279000000	6.889357000000

TS1b:

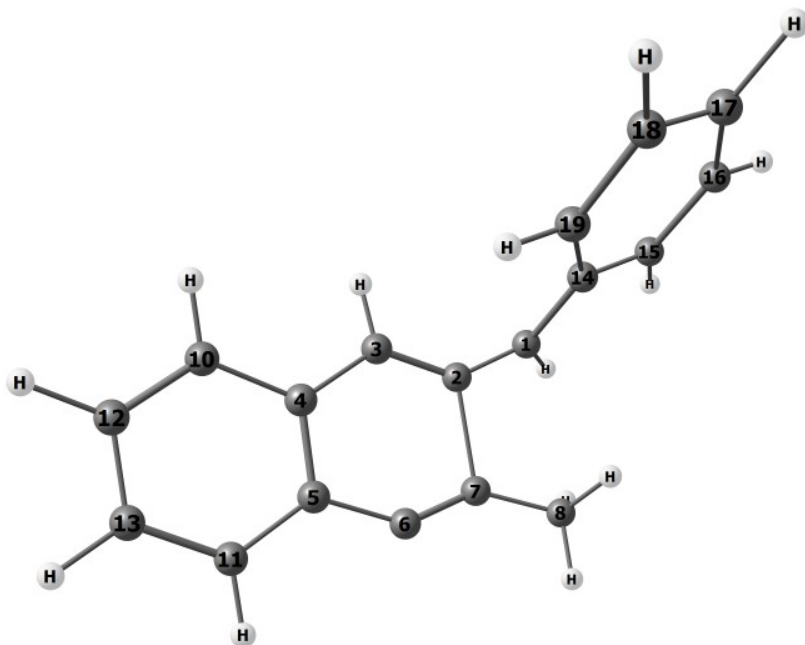


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C	1.042335000000	-0.304348000000	3.619255000000
C	-0.407741000000	-0.218631000000	3.638977000000
C	-0.915823000000	-0.018846000000	2.344828000000
H	0.660485000000	0.126925000000	-0.906564000000
C	-2.285118000000	0.100655000000	2.128192000000
C	-3.149370000000	0.008080000000	3.219029000000
C	-2.647726000000	-0.194089000000	4.509226000000
C	-1.276734000000	-0.312234000000	4.726852000000
H	-2.664924000000	0.248362000000	1.121546000000
H	-4.221451000000	0.084121000000	3.063247000000
H	-3.334357000000	-0.261469000000	5.348147000000
H	-0.885613000000	-0.461398000000	5.729809000000
C	2.811999000000	0.396323000000	1.928883000000
H	3.316967000000	1.198302000000	2.467451000000

H	1.621833000000	-0.644506000000	4.473150000000
C	3.349550000000	0.036372000000	0.644992000000
C	4.348728000000	0.839650000000	0.050280000000
C	2.892004000000	-1.091869000000	-0.064835000000
C	4.853103000000	0.538047000000	-1.203240000000
H	4.711685000000	1.711385000000	0.590107000000
C	3.406301000000	-1.393503000000	-1.325981000000
H	2.168549000000	-1.754107000000	0.400300000000
C	4.378857000000	-0.580802000000	-1.900736000000
H	5.616178000000	1.171117000000	-1.646819000000
H	3.050676000000	-2.273598000000	-1.854603000000
H	4.778248000000	-0.818164000000	-2.882562000000

TS2a:

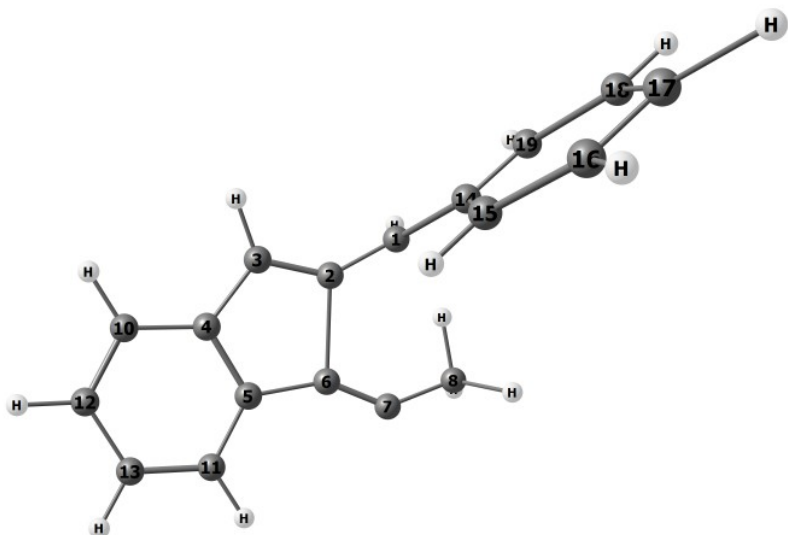


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C	2.611782000000	0.097063000000	0.746558000000
C	2.252884000000	0.165741000000	-0.645128000000
C	0.902701000000	-0.030851000000	-1.040953000000
C	3.234637000000	0.297482000000	-1.649085000000
C	2.893869000000	0.214454000000	-2.985621000000
C	1.561491000000	-0.027593000000	-3.365910000000
C	0.577369000000	-0.158201000000	-2.404054000000
H	-0.457437000000	-0.335144000000	-2.680897000000
H	1.305451000000	-0.106603000000	-4.418214000000
H	3.660114000000	0.327961000000	-3.746793000000
H	4.268336000000	0.468762000000	-1.357278000000

C	1.848719000000	0.059205000000	3.157370000000
H	1.471814000000	-0.764890000000	3.763906000000
H	3.676419000000	0.049551000000	0.974158000000
C	2.246578000000	1.257246000000	3.884522000000
C	2.285183000000	1.225212000000	5.290834000000
C	2.607906000000	2.453050000000	3.235997000000
C	2.690882000000	2.336220000000	6.021098000000
H	2.001913000000	0.310509000000	5.806960000000
C	3.008248000000	3.563054000000	3.969884000000
H	2.559859000000	2.504682000000	2.151548000000
C	3.055055000000	3.512203000000	5.364628000000
H	2.719864000000	2.286538000000	7.105953000000
H	3.279606000000	4.478167000000	3.450997000000
H	3.365692000000	4.383100000000	5.934029000000
C	-0.943698000000	-0.092513000000	2.454609000000
H	-0.847973000000	-0.986608000000	3.079461000000
H	-0.720076000000	0.779536000000	3.076695000000
H	-1.971540000000	-0.027583000000	2.090729000000

TS2b:

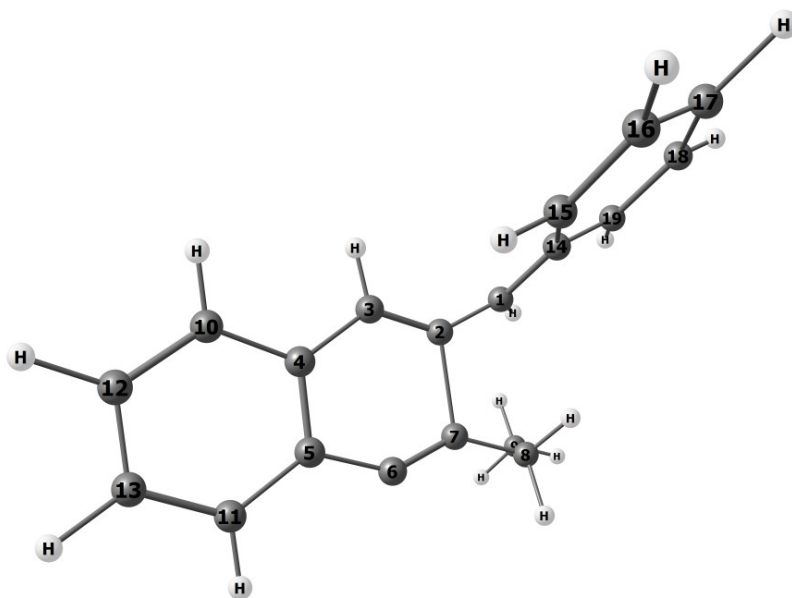


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C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.262131000000
C	1.763790000000	0.000000000000	1.914606000000
C	1.501057000000	0.011719000000	3.226951000000
C	0.093849000000	0.038240000000	3.621043000000
C	-0.750223000000	0.020425000000	2.499266000000
C	-2.135442000000	0.034746000000	2.645290000000
C	-2.673075000000	0.063223000000	3.931308000000
C	-1.836284000000	0.079562000000	5.051578000000
C	-0.449902000000	0.066991000000	4.903502000000
H	-2.776190000000	0.022151000000	1.768809000000
H	-3.750852000000	0.072215000000	4.063494000000
H	-2.270855000000	0.102717000000	6.046782000000
H	0.199047000000	0.079901000000	5.775241000000
C	2.831310000000	-0.076441000000	1.035233000000

H	3.400599000000	0.828599000000	0.822634000000
H	2.300639000000	-0.023933000000	3.963059000000
C	3.451208000000	-1.356930000000	0.662042000000
C	4.702946000000	-1.375013000000	0.026750000000
C	2.808757000000	-2.580637000000	0.909851000000
C	5.301501000000	-2.577319000000	-0.334186000000
H	5.208789000000	-0.433499000000	-0.176744000000
C	3.408877000000	-3.781740000000	0.544417000000
H	1.834069000000	-2.581294000000	1.392496000000
C	4.657235000000	-3.788371000000	-0.077960000000
H	6.274222000000	-2.569831000000	-0.818370000000
H	2.897459000000	-4.719077000000	0.745288000000
H	5.123050000000	-4.727133000000	-0.362650000000
C	0.923712000000	0.040292000000	-1.063989000000
H	1.927481000000	0.080688000000	-0.417618000000
H	0.984694000000	-0.861697000000	-1.679085000000
H	0.899881000000	0.944870000000	-1.676612000000

TS3a:

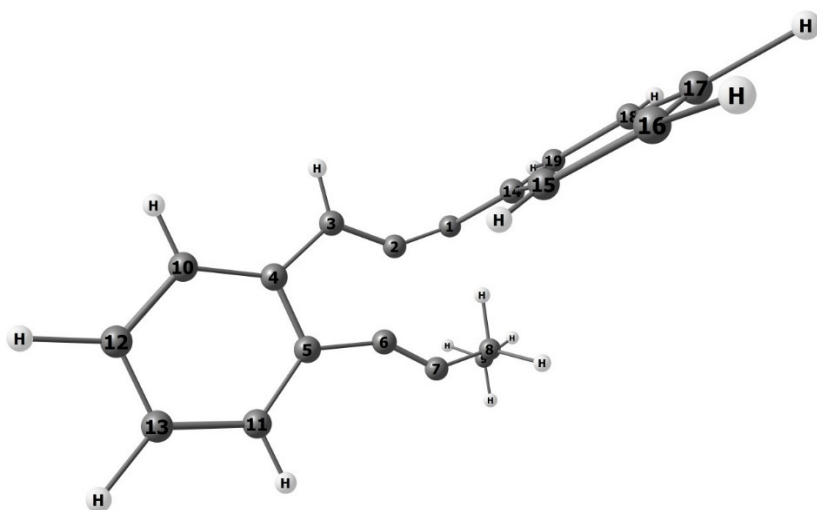


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C	1.856206000000	1.322715000000	0.632638000000
C	0.677167000000	1.709444000000	0.382961000000
C	-0.062873000000	0.370093000000	-0.695342000000
C	0.789175000000	-0.660196000000	-0.904725000000
C	2.122331000000	-0.811016000000	-0.384974000000
C	2.724495000000	0.246272000000	0.348683000000
C	2.902369000000	-1.945393000000	-0.690712000000
C	4.227556000000	-2.016747000000	-0.305594000000
C	4.827253000000	-0.943703000000	0.378138000000
C	4.086973000000	0.180287000000	0.693882000000
H	4.533135000000	1.011882000000	1.230698000000
H	5.873412000000	-1.000922000000	0.663478000000
H	4.812060000000	-2.901099000000	-0.541423000000
H	2.443872000000	-2.769156000000	-1.233058000000
C	-1.389396000000	0.609992000000	-0.891462000000

H	-1.694942000000	1.516420000000	-1.413488000000
H	0.456836000000	-1.413020000000	-1.619287000000
C	-2.465652000000	-0.193517000000	-0.325476000000
C	-3.800060000000	0.135800000000	-0.628793000000
C	-2.227562000000	-1.305114000000	0.504464000000
C	-4.853987000000	-0.630901000000	-0.145844000000
H	-4.001668000000	0.997265000000	-1.261784000000
C	-3.284168000000	-2.066535000000	0.988681000000
H	-1.205519000000	-1.558023000000	0.773369000000
C	-4.602262000000	-1.738081000000	0.664948000000
H	-5.875772000000	-0.363524000000	-0.400286000000
H	-3.079184000000	-2.919880000000	1.629167000000
H	-5.424943000000	-2.335769000000	1.046067000000
C	-0.281903000000	2.790194000000	0.746537000000
H	-1.273311000000	2.353142000000	0.905318000000
H	0.050627000000	3.217507000000	1.697869000000
C	-0.339320000000	3.889741000000	-0.319966000000
H	-1.062792000000	4.660074000000	-0.035679000000
H	0.642082000000	4.358263000000	-0.434689000000
H	-0.631952000000	3.486832000000	-1.294532000000

TS3b:

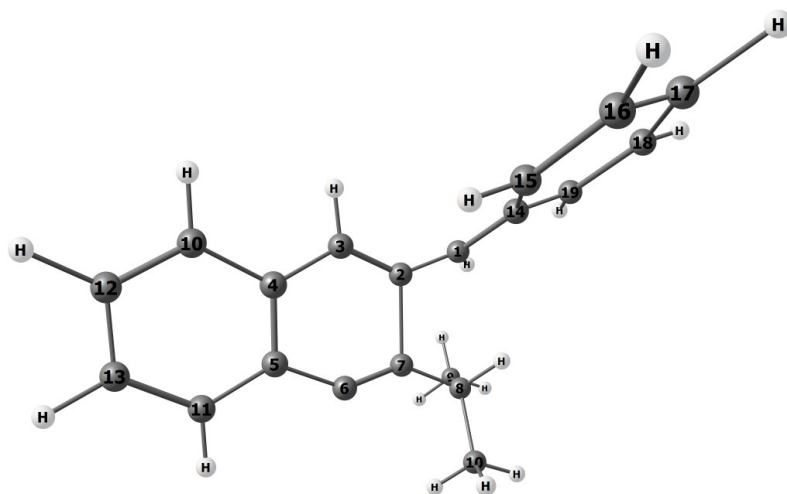


0 1

C	0.183184000000	-0.289405000000	0.094063000000
C	0.031223000000	-0.184266000000	1.340591000000
C	1.723515000000	0.137207000000	2.172042000000
C	1.307650000000	0.215672000000	3.440025000000
C	-0.124246000000	0.057824000000	3.687715000000
C	-0.834180000000	-0.175932000000	2.498497000000
C	-2.215604000000	-0.358401000000	2.515232000000
C	-2.884739000000	-0.308557000000	3.737350000000
C	-2.181489000000	-0.078025000000	4.923663000000
C	-0.799435000000	0.106223000000	4.905617000000
H	-2.752426000000	-0.536824000000	1.588462000000
H	-3.960817000000	-0.450686000000	3.767058000000
H	-2.717135000000	-0.042108000000	5.867734000000
H	-0.253777000000	0.285555000000	5.828271000000
C	2.868103000000	0.146108000000	1.397609000000
H	3.307978000000	1.106149000000	1.125501000000

H	2.010960000000	0.371368000000	4.254799000000
C	3.718312000000	-1.044560000000	1.235292000000
C	5.021402000000	-0.914938000000	0.729966000000
C	3.250828000000	-2.328041000000	1.559951000000
C	5.837839000000	-2.029832000000	0.569462000000
H	5.394206000000	0.073391000000	0.469684000000
C	4.068813000000	-3.441727000000	1.395009000000
H	2.239655000000	-2.444558000000	1.942773000000
C	5.365895000000	-3.300332000000	0.900869000000
H	6.846410000000	-1.906882000000	0.184758000000
H	3.690229000000	-4.427014000000	1.652273000000
H	6.001843000000	-4.171164000000	0.773484000000
C	1.201697000000	-0.191533000000	-0.879655000000
H	2.100884000000	-0.005683000000	-0.110730000000
H	1.445563000000	-1.140663000000	-1.369792000000
C	1.156041000000	0.987494000000	-1.849044000000
H	0.973259000000	1.919641000000	-1.307201000000
H	2.107408000000	1.071730000000	-2.381579000000
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TS4a:

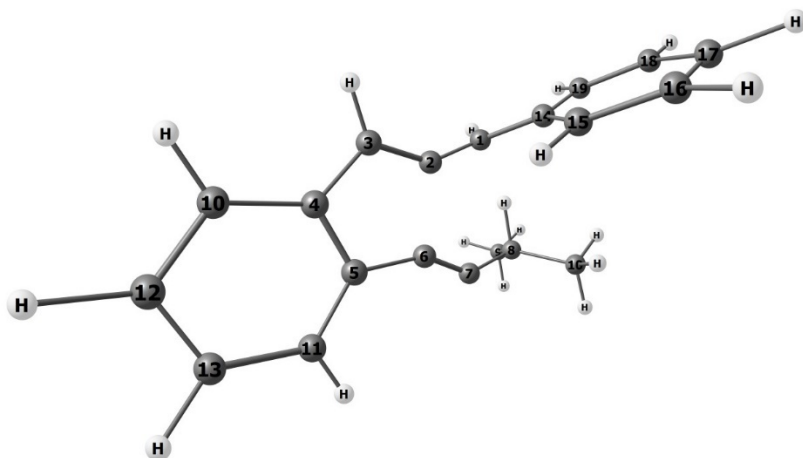


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C	2.587063000000	0.083911000000	0.767650000000
C	2.235345000000	0.171900000000	-0.624390000000
C	0.879815000000	0.031389000000	-1.024815000000
C	3.223816000000	0.276616000000	-1.625034000000
C	2.883257000000	0.220019000000	-2.962972000000
C	1.543274000000	0.033418000000	-3.347931000000
C	0.552435000000	-0.069134000000	-2.389625000000
H	-0.487772000000	-0.202561000000	-2.670630000000
H	1.286652000000	-0.024096000000	-4.401502000000
H	3.654788000000	0.312425000000	-3.721690000000
H	4.262447000000	0.405812000000	-1.328986000000
C	1.850995000000	0.082984000000	3.177119000000
H	1.468565000000	-0.718383000000	3.808763000000

H	3.649806000000	0.010026000000	0.997196000000
C	2.296027000000	1.282129000000	3.873873000000
C	2.372535000000	1.269285000000	5.279395000000
C	2.667005000000	2.460417000000	3.198755000000
C	2.825697000000	2.379518000000	5.981952000000
H	2.081250000000	0.369109000000	5.816228000000
C	3.115778000000	3.569629000000	3.905194000000
H	2.587827000000	2.499839000000	2.115717000000
C	3.200898000000	3.536779000000	5.298624000000
H	2.883506000000	2.344204000000	7.066242000000
H	3.394345000000	4.470637000000	3.365867000000
H	3.549096000000	4.407347000000	5.846547000000
C	-1.014248000000	-0.071482000000	2.451415000000
H	-0.580700000000	0.544486000000	3.248551000000
C	-1.227436000000	-1.496670000000	2.980931000000
H	-1.888765000000	-1.481408000000	3.853809000000
H	-1.690376000000	-2.115097000000	2.204605000000
H	-0.285421000000	-1.972734000000	3.269620000000
C	-2.346724000000	0.549056000000	2.020245000000
H	-2.819737000000	-0.054354000000	1.239558000000
H	-3.025544000000	0.598718000000	2.878456000000
H	-2.201010000000	1.559804000000	1.629330000000

TS4b:

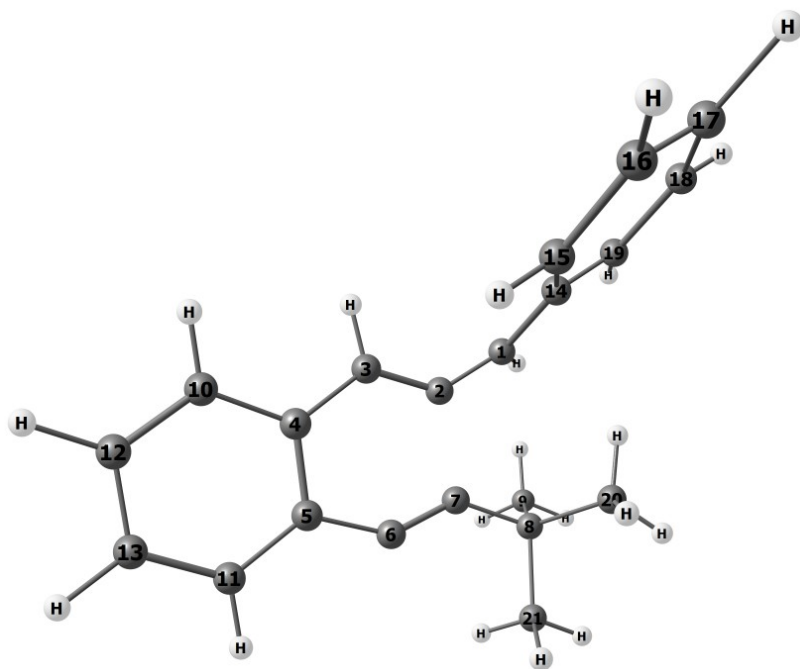


0 1

C	0.114248000000	-0.230339000000	0.072150000000
C	-0.019183000000	-0.141014000000	1.321083000000
C	1.711466000000	0.153102000000	2.138890000000
C	1.309641000000	0.229449000000	3.410152000000
C	-0.122103000000	0.095870000000	3.675366000000
C	-0.857033000000	-0.123565000000	2.498404000000
C	-2.240590000000	-0.287838000000	2.542480000000
C	-2.885682000000	-0.235303000000	3.777056000000
C	-2.157270000000	-0.017672000000	4.950306000000
C	-0.773767000000	0.148897000000	4.905656000000
H	-2.796606000000	-0.456846000000	1.625156000000
H	-3.962753000000	-0.364893000000	3.826659000000
H	-2.674267000000	0.022003000000	5.904744000000
H	-0.208590000000	0.318439000000	5.818531000000
C	2.829288000000	0.140558000000	1.330665000000
H	3.296901000000	1.088316000000	1.061755000000

H	2.024801000000	0.358675000000	4.219640000000
C	3.618027000000	-1.082566000000	1.099755000000
C	4.862341000000	-1.009024000000	0.454603000000
C	3.141820000000	-2.343705000000	1.490995000000
C	5.611454000000	-2.156903000000	0.217365000000
H	5.241624000000	-0.038668000000	0.140524000000
C	3.892063000000	-3.490636000000	1.250337000000
H	2.174989000000	-2.417495000000	1.983766000000
C	5.129667000000	-3.405516000000	0.612210000000
H	6.575493000000	-2.076720000000	-0.277490000000
H	3.506958000000	-4.457576000000	1.562344000000
H	5.712640000000	-4.302167000000	0.423918000000
C	1.119368000000	-0.135835000000	-0.922104000000
H	2.008315000000	0.059401000000	-0.142880000000
C	1.058631000000	1.097379000000	-1.823532000000
H	2.013873000000	1.221025000000	-2.344125000000
H	0.272424000000	0.984068000000	-2.576864000000
H	0.854101000000	2.000366000000	-1.241858000000
C	1.476872000000	-1.418915000000	-1.670309000000
H	0.732741000000	-1.629695000000	-2.445488000000
H	2.453499000000	-1.303808000000	-2.152115000000
H	1.528561000000	-2.272425000000	-0.989233000000

TS5a:

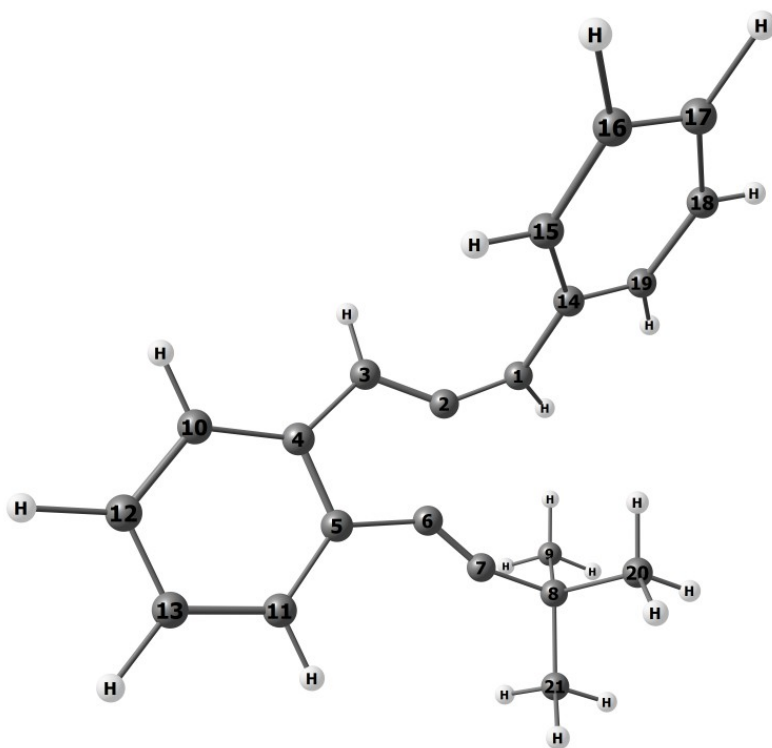


0 1

C	0.026630000000	-0.046781000000	0.048540000000
C	0.048208000000	-0.059757000000	1.315645000000
C	1.897180000000	-0.034273000000	1.734160000000
C	2.676655000000	0.037724000000	0.627424000000
C	2.259837000000	0.108680000000	-0.745299000000
C	0.884863000000	-0.024433000000	-1.070330000000
C	3.197057000000	0.171940000000	-1.797374000000
C	2.786407000000	0.079371000000	-3.113358000000
C	1.426440000000	-0.105887000000	-3.422868000000
C	0.485624000000	-0.167906000000	-2.412008000000
H	-0.569091000000	-0.298521000000	-2.634320000000
H	1.114959000000	-0.193572000000	-4.459421000000
H	3.518140000000	0.140440000000	-3.913648000000

H	4.250895000000	0.297725000000	-1.559383000000
C	2.141646000000	0.115394000000	3.065172000000
H	1.791774000000	-0.638948000000	3.766691000000
H	3.747112000000	-0.069710000000	0.802924000000
C	2.775977000000	1.287193000000	3.658495000000
C	3.049534000000	1.289986000000	5.038682000000
C	3.133331000000	2.422707000000	2.908086000000
C	3.682373000000	2.371331000000	5.641401000000
H	2.768968000000	0.424264000000	5.634894000000
C	3.762121000000	3.503581000000	3.514692000000
H	2.899105000000	2.454080000000	1.847517000000
C	4.044255000000	3.484390000000	4.882088000000
H	3.891948000000	2.347507000000	6.707115000000
H	4.027868000000	4.372181000000	2.918714000000
H	4.534264000000	4.331672000000	5.352337000000
C	-0.957541000000	0.012457000000	2.441257000000
C	-0.983040000000	-1.312091000000	3.219913000000
H	-1.742317000000	-1.256799000000	4.008645000000
H	-1.234759000000	-2.143872000000	2.554311000000
H	-0.023547000000	-1.534197000000	3.692909000000
C	-2.336657000000	0.206739000000	1.781075000000
H	-2.551208000000	-0.605369000000	1.080703000000
H	-3.113264000000	0.221946000000	2.554738000000
H	-2.370992000000	1.152016000000	1.230866000000
C	-0.722427000000	1.198086000000	3.389585000000
H	0.137162000000	1.056716000000	4.046008000000
H	-0.572617000000	2.125638000000	2.826605000000
H	-1.608052000000	1.319559000000	4.023954000000

TS5b:



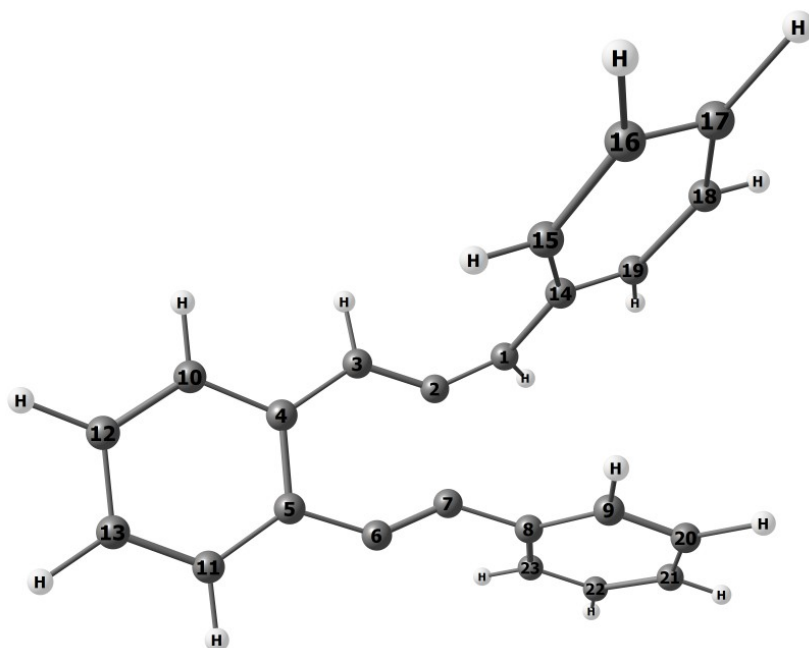
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C	0.142768000000	0.056532000000	0.096623000000
C	0.015175000000	0.119229000000	1.348490000000
C	1.477940000000	0.448992000000	2.507305000000
C	0.830631000000	0.590401000000	3.685324000000
C	-0.571096000000	0.218019000000	3.675607000000
C	-1.023367000000	-0.033745000000	2.368101000000
C	-2.349092000000	-0.389703000000	2.132836000000
C	-3.227891000000	-0.478679000000	3.211446000000
C	-2.782810000000	-0.224356000000	4.513241000000
C	-1.456955000000	0.128080000000	4.751609000000
H	-2.687382000000	-0.577515000000	1.117721000000
H	-4.268184000000	-0.737363000000	3.037247000000

H	-3.478658000000	-0.299444000000	5.343915000000
H	-1.109220000000	0.320745000000	5.763252000000
C	2.746163000000	0.400495000000	2.013597000000
H	2.935186000000	0.860517000000	1.044004000000
H	1.298016000000	1.084096000000	4.535109000000
C	3.869557000000	-0.304785000000	2.608209000000
C	5.127056000000	-0.229585000000	1.978846000000
C	3.763641000000	-1.064310000000	3.789307000000
C	6.238604000000	-0.867293000000	2.516808000000
H	5.223281000000	0.347335000000	1.061273000000
C	4.875409000000	-1.705494000000	4.320183000000
H	2.796879000000	-1.156998000000	4.275918000000
C	6.119705000000	-1.608639000000	3.692408000000
H	7.200078000000	-0.787722000000	2.017278000000
H	4.772775000000	-2.289944000000	5.230414000000
H	6.985794000000	-2.109934000000	4.114114000000
C	0.772421000000	-0.017756000000	-1.230924000000
C	-0.288101000000	-0.397419000000	-2.282006000000
H	0.182528000000	-0.470960000000	-3.269637000000
H	-0.744045000000	-1.363470000000	-2.043744000000
H	-1.079549000000	0.357220000000	-2.327185000000
C	1.878405000000	-1.090479000000	-1.212706000000
H	1.453443000000	-2.076249000000	-0.999609000000
H	2.371483000000	-1.127759000000	-2.191391000000
H	2.634398000000	-0.877623000000	-0.450924000000
C	1.364141000000	1.357885000000	-1.591117000000
H	0.586042000000	2.127260000000	-1.591221000000
H	2.140914000000	1.657537000000	-0.881080000000

H 1.810085000000 1.311274000000 -2.591301000000

TS6a:

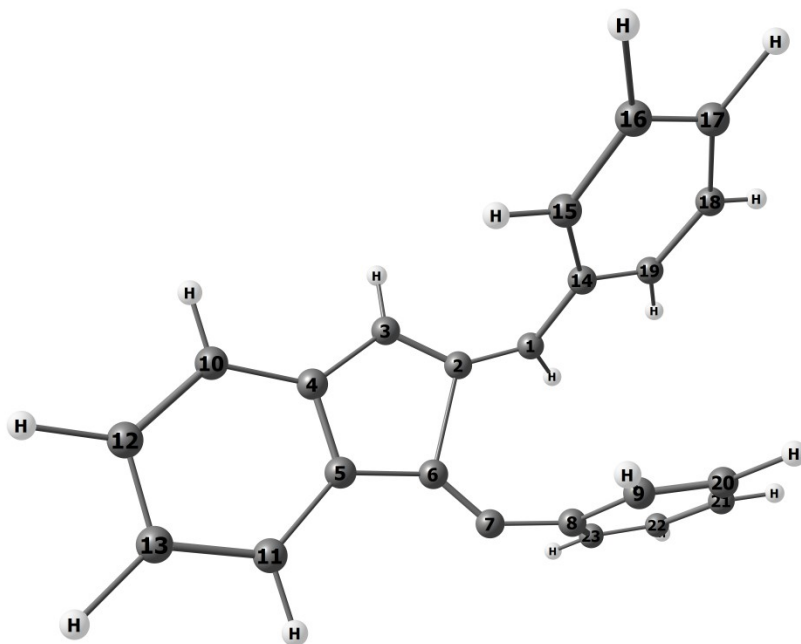


0 1

C	-0.006038000000	-0.028215000000	-0.023810000000
C	0.049545000000	0.006697000000	1.240555000000
C	1.906716000000	0.039979000000	1.662032000000
C	2.676725000000	0.056539000000	0.552315000000
C	2.239223000000	0.101732000000	-0.820610000000
C	0.860769000000	-0.025838000000	-1.140444000000
C	3.170759000000	0.134617000000	-1.878130000000
C	2.754991000000	0.026871000000	-3.192344000000
C	1.392808000000	-0.143496000000	-3.495184000000
C	0.455933000000	-0.179649000000	-2.478808000000
H	-0.601121000000	-0.300003000000	-2.694772000000
H	1.076051000000	-0.242242000000	-4.528945000000
H	3.485789000000	0.063619000000	-3.994762000000

H	4.227160000000	0.248431000000	-1.646301000000
C	2.057366000000	0.179651000000	3.005971000000
H	1.601818000000	-0.562969000000	3.660933000000
H	3.745601000000	-0.086047000000	0.712934000000
C	2.637584000000	1.341837000000	3.666636000000
C	2.665393000000	1.383100000000	5.072597000000
C	3.175600000000	2.430966000000	2.956203000000
C	3.231821000000	2.460377000000	5.744890000000
H	2.237910000000	0.554701000000	5.632875000000
C	3.737026000000	3.507793000000	3.631750000000
H	3.139212000000	2.428094000000	1.870132000000
C	3.772061000000	3.528410000000	5.027907000000
H	3.248474000000	2.469415000000	6.830991000000
H	4.146412000000	4.340452000000	3.066796000000
H	4.211331000000	4.372331000000	5.551266000000
C	-0.832799000000	0.108130000000	2.404813000000
C	-1.783845000000	-0.895164000000	2.623017000000
C	-0.760347000000	1.192680000000	3.287087000000
C	-2.646175000000	-0.817841000000	3.714482000000
H	-1.836361000000	-1.731458000000	1.932472000000
C	-1.627236000000	1.267823000000	4.373627000000
H	-0.031303000000	1.978502000000	3.113246000000
C	-2.568618000000	0.261582000000	4.592854000000
H	-3.377974000000	-1.603459000000	3.878151000000
H	-1.568380000000	2.117032000000	5.048102000000
H	-3.240986000000	0.321151000000	5.443690000000

TS6b:

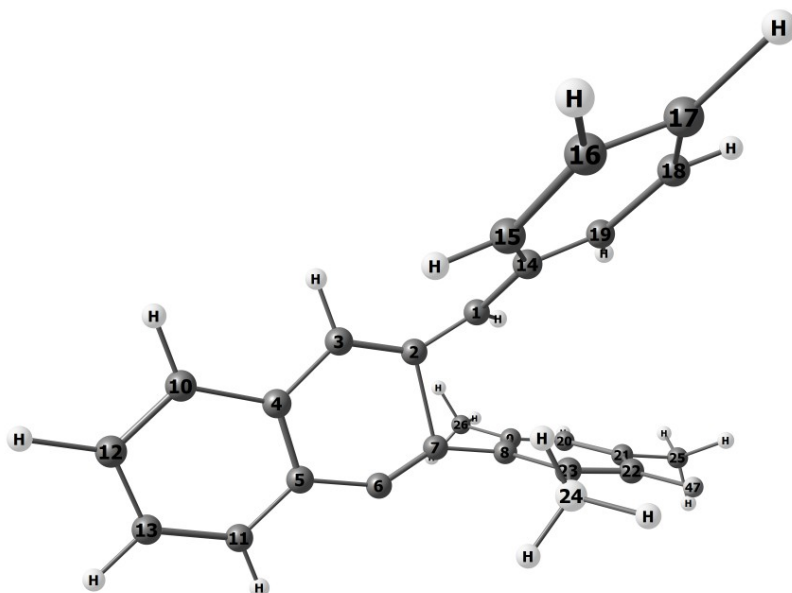


0 1

C	-0.199965000000	-0.236452000000	0.037806000000
C	-0.203997000000	-0.091408000000	1.299488000000
C	1.428005000000	0.119685000000	2.140103000000
C	1.030819000000	0.309491000000	3.417169000000
C	-0.383683000000	0.098932000000	3.663803000000
C	-1.078004000000	-0.120043000000	2.460125000000
C	-2.453809000000	-0.348064000000	2.459240000000
C	-3.136149000000	-0.332319000000	3.673073000000
C	-2.450230000000	-0.108151000000	4.874166000000
C	-1.075916000000	0.110276000000	4.877612000000
H	-2.975512000000	-0.514941000000	1.521761000000
H	-4.210921000000	-0.486391000000	3.687885000000
H	-2.998440000000	-0.102650000000	5.811738000000

H	-0.544367000000	0.277520000000	5.810615000000
C	2.573125000000	-0.029545000000	1.412448000000
H	2.671029000000	0.522570000000	0.477863000000
H	1.701545000000	0.720142000000	4.168655000000
C	3.690236000000	-0.899802000000	1.753768000000
C	4.820931000000	-0.908836000000	0.915663000000
C	3.691552000000	-1.734266000000	2.886361000000
C	5.920633000000	-1.706844000000	1.208271000000
H	4.823163000000	-0.279199000000	0.028506000000
C	4.791080000000	-2.534619000000	3.172820000000
H	2.817860000000	-1.755269000000	3.531827000000
C	5.911930000000	-2.524096000000	2.339564000000
H	6.786119000000	-1.694423000000	0.551873000000
H	4.774294000000	-3.174568000000	4.050453000000
H	6.769142000000	-3.150120000000	2.568571000000
C	0.701510000000	-0.540793000000	-1.002549000000
C	0.886437000000	0.296382000000	-2.126764000000
C	1.551099000000	-1.659072000000	-0.833246000000
C	1.900200000000	0.030718000000	-3.031375000000
H	0.233567000000	1.154230000000	-2.256133000000
C	2.554354000000	-1.926894000000	-1.763369000000
H	1.402562000000	-2.308846000000	0.023421000000
C	2.737766000000	-1.081287000000	-2.853042000000
H	2.046343000000	0.685364000000	-3.885527000000
H	3.200386000000	-2.788824000000	-1.624580000000
H	3.525461000000	-1.284355000000	-3.572764000000

TS7a:



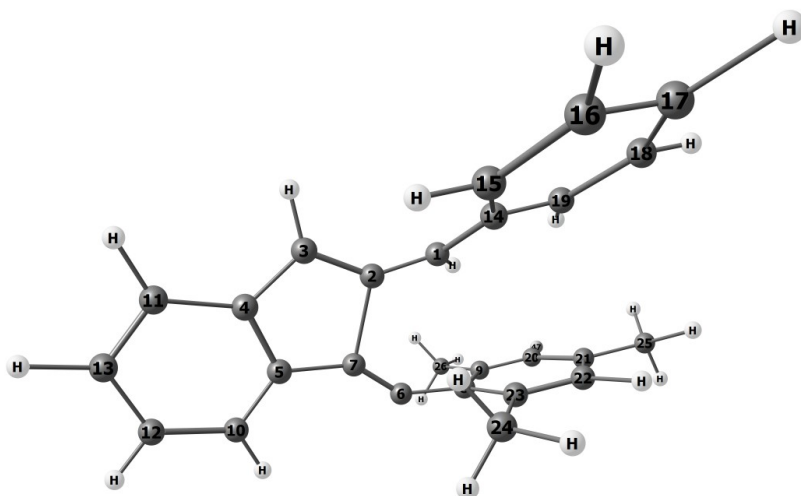
0 1

C	-0.048533000000	0.106665000000	0.004424000000
C	-0.068974000000	0.078207000000	1.272151000000
C	1.742222000000	0.020783000000	1.815107000000
C	2.596449000000	0.014550000000	0.768165000000
C	2.260577000000	0.119531000000	-0.629999000000
C	0.902483000000	0.095224000000	-1.045745000000
C	3.264476000000	0.126672000000	-1.619616000000
C	2.936214000000	0.093542000000	-2.962473000000
C	1.590560000000	0.027298000000	-3.362672000000
C	0.584540000000	0.018426000000	-2.413450000000
H	-0.460414000000	-0.023719000000	-2.704966000000
H	1.340789000000	-0.012924000000	-4.418519000000
H	3.722462000000	0.109130000000	-3.711403000000
H	4.307091000000	0.162426000000	-1.312219000000

C	1.792657000000	0.159190000000	3.170186000000
H	1.230712000000	-0.542356000000	3.786858000000
H	3.643131000000	-0.183957000000	1.000993000000
C	2.359569000000	1.300633000000	3.873883000000
C	2.174367000000	1.402054000000	5.265225000000
C	3.091822000000	2.312399000000	3.223526000000
C	2.714944000000	2.462538000000	5.983235000000
H	1.595383000000	0.636012000000	5.775970000000
C	3.628644000000	3.371893000000	3.944180000000
H	3.225201000000	2.264283000000	2.145973000000
C	3.446362000000	3.453022000000	5.326799000000
H	2.561547000000	2.520227000000	7.057047000000
H	4.189873000000	4.143727000000	3.425097000000
H	3.866622000000	4.283812000000	5.885641000000
C	-0.972171000000	0.203597000000	2.418042000000
C	-1.505450000000	-0.954480000000	3.003833000000
C	-1.241543000000	1.476134000000	2.949790000000
C	-2.321831000000	-0.818488000000	4.128119000000
C	-2.060742000000	1.566223000000	4.074565000000
C	-2.611254000000	0.431876000000	4.676087000000
C	-1.184327000000	-2.313727000000	2.437929000000
H	-1.527139000000	-2.398078000000	1.401445000000
H	-0.102251000000	-2.492069000000	2.427327000000
H	-1.657805000000	-3.103453000000	3.027036000000
C	-3.518447000000	0.562557000000	5.873829000000
H	-4.539218000000	0.812758000000	5.562574000000
H	-3.564203000000	-0.371321000000	6.441224000000
H	-3.175933000000	1.355342000000	6.545716000000

C	-0.657477000000	2.708932000000	2.312812000000
H	-0.960426000000	3.608544000000	2.854787000000
H	0.437891000000	2.667205000000	2.304446000000
H	-0.984155000000	2.799906000000	1.271092000000
H	-2.272876000000	2.548315000000	4.494155000000
H	-2.738662000000	-1.712665000000	4.588520000000

TS7b



0 1

C	0.024269000000	-0.075162000000	0.016093000000
C	0.019360000000	-0.046552000000	1.284738000000
C	1.701763000000	0.029231000000	2.094037000000
C	1.340567000000	0.011493000000	3.391088000000
C	-0.079853000000	-0.172082000000	3.654262000000
C	-0.822295000000	-0.180601000000	2.460389000000
C	-2.207336000000	-0.335638000000	2.481221000000
C	-2.850228000000	-0.463069000000	3.711166000000
C	-2.115921000000	-0.449274000000	4.902689000000
C	-0.730752000000	-0.302794000000	4.881959000000
H	-2.766858000000	-0.341735000000	1.550571000000
H	-3.930548000000	-0.567622000000	3.745001000000
H	-2.632224000000	-0.551930000000	5.852720000000
H	-0.161547000000	-0.296037000000	5.807798000000
C	2.821354000000	0.039855000000	1.302399000000
H	2.907771000000	0.820296000000	0.545221000000

H	2.050186000000	0.241384000000	4.182855000000
C	3.873409000000	-0.958812000000	1.298024000000
C	4.934076000000	-0.827408000000	0.378782000000
C	3.875704000000	-2.071010000000	2.162664000000
C	5.956625000000	-1.766174000000	0.328233000000
H	4.936519000000	0.021544000000	-0.301726000000
C	4.898771000000	-3.009702000000	2.105364000000
H	3.061829000000	-2.192305000000	2.872957000000
C	5.944128000000	-2.864888000000	1.190022000000
H	6.765604000000	-1.644330000000	-0.386905000000
H	4.881875000000	-3.862826000000	2.777834000000
H	6.741835000000	-3.600641000000	1.150429000000
C	0.943787000000	-0.245885000000	-1.034938000000
C	1.326966000000	0.852426000000	-1.852111000000
C	1.622966000000	-1.489708000000	-1.139987000000
C	2.393554000000	0.694492000000	-2.723631000000
C	2.677105000000	-1.598390000000	-2.045799000000
C	3.086626000000	-0.522470000000	-2.831500000000
C	0.616718000000	2.170635000000	-1.710126000000
H	-0.465771000000	2.045330000000	-1.816268000000
H	0.789731000000	2.599484000000	-0.715832000000
H	0.964353000000	2.886596000000	-2.459287000000
C	4.236593000000	-0.660482000000	-3.794492000000
H	3.872982000000	-0.778320000000	-4.822090000000
H	4.877563000000	0.226800000000	-3.774711000000
H	4.849932000000	-1.533317000000	-3.554019000000
C	1.222926000000	-2.666273000000	-0.293081000000
H	1.427425000000	-2.476183000000	0.767462000000

H	0.150528000000	-2.870402000000	-0.380172000000
H	1.778261000000	-3.559707000000	-0.589632000000
H	2.707106000000	1.539470000000	-3.334801000000
H	3.213426000000	-2.542817000000	-2.116259000000