

**Supporting Information for:**

**Computational Assessment of the Molecular Structure and  
Properties for High Energy Density Fuel**

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## Details of Methodology

### Computation of the enthalpy of vaporization

The enthalpy of vaporization was calculated by the SMD solvation model, with the M06-2X/6-31+G (d, p) method.

By using this model, the Gibbs free energy of solvation, which is defined as the free energy required to insert a molecule from the gas phase into the liquid phase, is computed by the following equation:

$$\Delta G_{sol} = E_{liquid}^* - \varepsilon_{0_{gas}} \quad (S1)$$

where  $\varepsilon_0$  is the electronic energy of the molecule in the gas phase, and  $E^*$  is the total energy calculated by the SMD model, consisting of the electrostatic and nonelectrostatic contributions to the energy of the molecule inside the continuum medium and is affected by the reaction field (the electric potential derived from the polarized medium and solute that mutually polarize each other), the solvent cavitation, dispersion interaction, solvent structure. More information about this model can be found in the original SMD paper<sup>1</sup>.

In order to compute the enthalpy of combustion, we need to convert  $\Delta G_{sol}$  to the enthalpy of vaporization  $\Delta H_{vap}$  (the SMD and related models can only compute the free energy of solvation). Pahima<sup>2</sup> found that the computed  $\Delta G_{sol}$  is linearly correlated to the experimental  $\Delta H_{vap}$ . To convert  $\Delta G_{sol}$  into  $\Delta H_{vap}$  without explicitly calculating  $\Delta S_{sol}$ , we employed multiple linear regression method. The entropic contribution to the solvation free energy is due to the rearrangement of the solvent<sup>3,4</sup>, induced by the solute's presence. The solvent accessible surface area (SASA) can therefore be used as a measure of the entropic effect. This can be summarized as the following expression:

$$\Delta G_{sol} + T \cdot \Delta S_{sol} = \Delta H_{sol}, \Delta S_{sol} \propto SASA \Rightarrow \Delta G_{sol} + T \cdot SASA \propto \Delta H_{sol} \quad (S2)$$

By applying multiple linear regression (MLR) method, where  $\Delta G_{sol}$  (computed as explained above) and  $T \cdot SASA$  (computed as part of the SMD model calculation, where  $T = 298.15$  K) are the variables, the  $\Delta H_{vap}$  of the hydrocarbon molecules were predicted with less than 1 kcal/mol deviation when compared with the experimental ones. The results of computed  $\Delta H_{vap}$  can be seen in the table S1, where Exp. represents experimental results, and Comp. represents computational results.

Table S1. Computed  $\Delta H_{vap}$  with M06-2X method and 6-31+G(d,p) basis set comparing with the experimental  $\Delta H_{vap}$

	<b>SASA (Å<sup>2</sup>)</b>	<b>ΔG<sub>sol</sub> (kcal/mol)</b>	<b>Exp. ΔH<sub>vap</sub> (kcal/mol)</b>	<b>Comp. ΔH<sub>vap</sub> (kcal/mol)</b>	<b>Deviation (kcal/mol)</b>
<b>Benzene</b>	112.45	-145553.1618	8.082 <sup>5</sup>	7.713	-0.4
<b>Cumene</b>	169.13	-219437.9681	10.782 <sup>6</sup>	11.213	0.4
<b>Cyclohexane</b>	134.06	-147769.2414	7.898 <sup>7</sup>	7.749	-0.1
<b>Cyclopentane</b>	115.76	-123136.9168	6.813 <sup>8</sup>	6.580	-0.2
<b>Cyclopropane</b>	82.85	-73865.1021	4.045 <sup>9</sup>	4.228	0.2
<b>Isopentane</b>	131.61	-123882.1056	6.314 <sup>10</sup>	6.562	0.2
<b>Tridecane</b>	300.47	-320898.8837	15.930 <sup>11</sup>	15.834	-0.1
<b>Undecane</b>	260.27	-271644.4815	13.517 <sup>12</sup>	13.509	0
<i>Predict</i>					
<b>1-Decene</b>	237.88	-246261.9277	—	12.316	—
<b>1,3-Butadiene</b>	97.42	-97749.0820	—	5.373	—
<b>2,3,4-Trimethylpentane</b>	176.89	-197758.7080	—	10.101	—
<b>Acenaphthene</b>	180.69	-290368.8787	—	14.723	—
<b>Acenaphthylene</b>	180.76	-289619.9637	—	14.685	—
<b>Anthracene</b>	203.65	-338149.5272	—	17.035	—
<b>Cyclobutene</b>	93.28	-97735.2829	—	5.387	—
<b>Fluoranthene</b>	214.42	-385930.8029	—	19.389	—
<b>Indane</b>	155.86	-218697.5923	—	11.223	—
<b>1-Methylnaphthalene</b>	174.96	-266480.7497	—	13.548	—
<b>Methylcyclopentane</b>	136.25	-147767.0669	—	7.741	—
<b>Tetracene</b>	248.87	-434444.0583	—	21.697	—
<b>Tetralin</b>	170.67	-243327.7367	—	12.404	—

## Computation of the enthalpy of combustion

All Gaussian<sup>13</sup> calculations with a given DFT functional for the hydrocarbons were performed using 6-31+G(d,p) basis set according to Pahima's work<sup>2</sup>.

The input file included the commands "Opt" - that instructs a geometry optimization is performed, i.e. the geometry is adjusted until a stationary point on the potential energy surface is found, and the "Freq" keyword instructs that force constants are computed, as well as the resulting vibrational frequencies. No imaginary frequencies were identified in all calculations, indicating that the molecules are at a local minimum.

The  $\Delta H_{\text{comb}}$  was calculated according to the following Gaussian white page scheme<sup>14</sup>:

$$\Delta H_{\text{comb}} = n \cdot (\varepsilon_0 + H^{\text{corr}})_{\text{CO}_2(\text{g})}^{298\text{K}} + \frac{m}{2} \cdot (\varepsilon_0 + H^{\text{corr}})_{\text{H}_2\text{O}(\text{g})}^{298\text{K}} - [(\varepsilon_0 + H^{\text{corr}})_{\text{C}_n\text{H}_m(\text{g})}^{298\text{K}} + (n + \frac{m}{4}) \cdot (\varepsilon_0 + H^{\text{corr}})_{\text{O}_2(\text{g})}^{298\text{K}}] \quad (\text{S3})$$

The equation calculates the enthalpy of combustion at 298K when all reactants and products are in the gas phase. By definition, reaction enthalpies are measured experimentally when all reactants and the products are at 298 K and 1 atm. During the oxidation reaction at room temperature, the target hydrocarbon's initial state is the liquid phase. The molecules are oxidized and vaporized at the same time, creating the products CO<sub>2</sub> and water in the gas phase.

$\Delta H_{\text{comb}}$  was calculated using the following equation, *after* the first correction to the  $\Delta H_{\text{vap}}$ .

$$\Delta H_{\text{comb}} = n \cdot (\varepsilon_0 + H^{\text{corr}})_{\text{CO}_2(\text{g})}^{298\text{K}} + \frac{m}{2} \cdot [(\varepsilon_0 + H^{\text{corr}})_{\text{H}_2\text{O}(\text{g})}^{298\text{K}} - \Delta H_{\text{vap,H}_2\text{O}}] - [(\varepsilon_0 + H^{\text{corr}})_{\text{C}_n\text{H}_m(\text{g})}^{298\text{K}} - \Delta H_{\text{vap,C}_n\text{H}_m} + (n + \frac{m}{4}) \cdot (\varepsilon_0 + H^{\text{corr}})_{\text{O}_2(\text{g})}^{298\text{K}}] \quad (\text{S4})$$

Further explanations regarding the calculation of  $\Delta H_{\text{vap}}$  appear in the last section.

Correction to the  $\Delta H_{\text{comb}}$  due to the O<sub>2</sub> overbinding effect in DFT calculations:

The second correction was added in order to account for the deviation caused by electron self interaction<sup>15</sup>.

The O<sub>2</sub> molecule's computed enthalpy is present in all the combustion energy calculations, thus causes a constant deviation from the experimental results. This problem can be overcome by using linear regression that correlates among the **computed  $\Delta H_{\text{comb}}$  (without the O<sub>2</sub> correction)**, the number of matched oxygen and the **experimental  $\Delta H_{\text{comb}}$** . There is a linear correlation among these three items because of the constant deviation caused by the O<sub>2</sub> overbinding.

Initial calculations of the enthalpy of combustion were carried out just for the **hydrocarbons which have experimental data**. For the first correction of the *enthalpy of vaporization*, we need to calculate based on the **experimental  $\Delta H_{\text{vap}}$** . Then, the second correction of the O<sub>2</sub> overbinding effect

was added. It is showed that the most accurate method is the *M06-2X/6-31+G(d,p)*. The remaining calculations were carried out using this method. The results are shown in table S2.

(Note that all calculations were performed at room temperature – 298 K)

Table S2. Computed  $\Delta H_{\text{comb}}$  using M06-2X method and 6-31+G(d,p) basis set comparing the experimental  $\Delta H_{\text{comb}}$

Molecules		Electronic and thermal Enthalpies (hartree/particle)	$\Delta H_{\text{comb}}$ after $\Delta H_{\text{vap}}$ correction, before O <sub>2</sub> correction (kcal/mol)	Exp. $\Delta H_{\text{comb}}$ (kcal/mol)	O <sub>2</sub> needed (mol)	$\Delta H_{\text{comb}}$ after O <sub>2</sub> correction (kcal/mol)	Deviation (kcal/mol)
Cyclopropane	C <sub>3</sub> H <sub>6</sub>	-117.78287	-535.224	-499.850 <sup>16</sup>	4.5	-507.977	-8.13
1,3-Butadiene	C <sub>4</sub> H <sub>6</sub>	-155.87702	-660.817	-607.160 <sup>17</sup>	5.5	-610.960	-3.80
Cyclobutene	C <sub>4</sub> H <sub>6</sub>	-155.84684	-679.804	-618.600 <sup>17</sup>	5.5	-629.947	-11.35
Isopentane	C <sub>5</sub> H <sub>12</sub>	-197.56166	-889.434	-778.850 <sup>18</sup>	8.0	-783.049	-4.20
Cyclopentane	C <sub>5</sub> H <sub>10</sub>	-196.36758	-853.482	-786.600 <sup>19</sup>	7.5	-758.402	28.20
Benzene	C <sub>6</sub> H <sub>6</sub>	-232.10170	-889.339	-756.730 <sup>18</sup>	7.5	-794.260	-37.52
Cyclohexane	C <sub>6</sub> H <sub>12</sub>	-235.65081	-1018.311	-936.500 <sup>19</sup>	9.0	-889.316	47.18
Methylcyclopentane	C <sub>6</sub> H <sub>12</sub>	-235.64505	-1021.895	-884.380 <sup>18</sup>	9.0	-892.899	-8.52
2,3,4-Trimethylpentane	C <sub>8</sub> H <sub>18</sub>	-315.37794	-1405.010	-1216.800 <sup>18</sup>	12.5	-1196.876	19.97
Cumene	C <sub>9</sub> H <sub>12</sub>	-349.93053	-1396.895	-1192.600 <sup>18</sup>	12.0	-1200.067	-7.48
Indane	C <sub>9</sub> H <sub>10</sub>	-348.74517	-1355.442	-1148.500 <sup>18</sup>	11.5	-1169.919	-21.45
Tetralin	C <sub>10</sub> H <sub>12</sub>	-388.02412	-1522.997	-1292.900 <sup>18</sup>	13.0	-1303.558	-10.63
1-Decene	C <sub>10</sub> H <sub>20</sub>	-392.72663	-1713.080	-1489.000 <sup>20</sup>	15.0	-1448.419	40.55
1-Methylnaphthalene	C <sub>11</sub> H <sub>10</sub>	-424.94075	-1602.173	-1389.600 <sup>21</sup>	13.5	-1371.429	18.16
Acenaphthylene	C <sub>12</sub> H <sub>8</sub>	-461.82817	-1699.662	-1446.500 <sup>22</sup>	14.0	-1457.612	-11.11
Acenaphthene	C <sub>12</sub> H <sub>10</sub>	-463.02947	-1731.279	-1487.000 <sup>22</sup>	14.5	-1477.923	9.08
Anthracene	C <sub>14</sub> H <sub>10</sub>	-539.22170	-1980.070	-1659.300 <sup>18</sup>	16.5	-1681.493	-22.20
Fluoranthene	C <sub>16</sub> H <sub>10</sub>	-615.40943	-2231.828	-1892.400 <sup>22</sup>	18.5	-1888.029	4.37
Tetracene	C <sub>18</sub> H <sub>12</sub>	-692.77623	-2528.866	-2107.400 <sup>18</sup>	21.0	-2128.540	-21.13
O <sub>2</sub>		-150.19732					
H <sub>2</sub> O		-76.36955					
CO <sub>2</sub>		-188.50057					

For the calculating of enthalpies, especially on enthalpies of combustion, it get much better results than the previous methods like isodesmic reaction method, but it requires adequate computational

resource since it's based on SMD model and the calculating of  $\Delta G_{\text{sol}}$  requires high-precision DFT method and basis set.

## Computation of density

We use Materials Studio 2017<sup>23,24</sup> for the Dynamics calculation. In order to get the procedure clear, the details in computing densities are given in the following part.

It is necessary to build a model at the beginning of the calculations. Minimizing the total energy and doing geometry optimization are essential in preparation for Molecular Dynamics. It is supposed to set some molecules (128 molecules recommended) through amorphous cell module. After optimizing its structure, anneal and dynamic operations are needed so that we can get a stable system eventually. Several steps are shown in table S3.

Table S3. Procedures for density simulation  
(All by Forcite module in Materials Studio)

	<b>Task</b>	<b>Ensemble</b>	<b>Forcefield</b>	<b>Thermostat</b>	<b>Other information</b>
<b>Step 1</b>	Anneal	NVT	Compass	Anderson	300K to 500K, 1fs, 200ps
<b>Step 2</b>	Dynamics	NPT	Compass	Anderson	298K, 0.001GPa, 1fs, 200ps
<b>Step 3</b>	Dynamics	NPT	Compass	Anderson	298K, 0.0001Gpa, 1fs, 200ps
<b>Step 4</b>	Dynamics	NPT	Compass	Anderson	298K, 0.0001Gpa, 1fs, 2000ps

For the details about parameters setting, we could take step 4 for example and show it as follows.

Table S4. Parameters setting during Dynamics simulation

<b>Ensemble</b>	<b>Temperature</b>	<b>Control method</b>	<b>Collision ratio</b>	<b>Pressure</b>	<b>Control method</b>
NPT	298 K	Andersen	1.0000000	0.0001 GPa	Berendsen
<b>Decay constant</b>	<b>Timestep</b>	<b>Number of steps</b>	<b>Duration</b>	<b>Initial velocities</b>	
0.1000000 ps	1.00 fs	2000000	2000 ps	Random	

By these steps, a stable system can be obtained as the total energy of system maintain in a relatively steady situation, then the computed densities can be obtained. The computed results and deviations can be seen in table S5.

Table S5. Computed densities at 1 atm compared with the experimental ones

	<b>Comp. density (g/cm<sup>3</sup>)</b>	<b>Exp. density (g/cm<sup>3</sup>)</b>	<b>T (°C)</b>	<b>T (K)</b>	<b>Deviation (g/cm<sup>3</sup>)</b>
<b>Pentane</b>	0.630	0.626 <sup>25</sup>	20.0	293.15	0.004
<b>Hexane</b>	0.660	0.664 <sup>26</sup>	25.0	298.15	-0.004
<b>Heptane</b>	0.688	0.680 <sup>27</sup>	25.0	298.15	0.008
<b>Octane</b>	0.709	0.699 <sup>28</sup>	25.0	298.15	0.010
<b>Cyclobutane</b>	0.713	0.676 <sup>29</sup>	5.0	278.15	0.037
<b>Cyclopentane</b>	0.732	0.740 <sup>30</sup>	20.0	293.15	-0.008
<b>Cyclohexane</b>	0.776	0.779 <sup>30</sup>	20.0	293.15	-0.003
<b>Cycloheptane</b>	0.798	0.811 <sup>30</sup>	25.0	298.15	-0.013
<b>Cyclooctane</b>	0.824	0.834 <sup>31</sup>	25.0	298.15	-0.010
<b>Pinane</b>	0.841	0.847 <sup>32</sup>	21.1	294.26	-0.006
<b>Trans- decahydronaphthalene</b>	0.864	0.89 <sup>33</sup>	20.0	293.15	-0.026
<b>Thujopsene</b>	0.918	0.936 <sup>34</sup>	20.0	293.15	-0.018
<b>beta-Pinene</b>	0.863	0.860 <sup>35</sup>	25.0	298.15	0.003
<b>Limonene</b>	0.851	0.861 <sup>36</sup>	25.0	298.15	-0.010
<b>Camphene</b>	0.872	0.870 <sup>33</sup>	15.0	288.15	0.002

For MD calculations on density, it's a bit time-consuming and resource-consuming, but comparing with the other approaches such as group-contribution method, MD method gets the results much more accurate and adapts to the hydrocarbons with complex structures.

### Computation of melting point

The preparing procedures are similar with those in computation of density which can be shown in

several stages:

- 1) Equilibration - perform a geometry optimization followed by 200 ps of NVT dynamics with a 0.1 ps timestep. This is followed by a temperature cycle from a high temperature (500 K recommended) to a low temperature (300 K recommended) using a short NVT and a longer NPT calculation.
- 2) Density equilibration - perform multiple restarts of an NPT calculation at the target pressure. Convergence is when the differences in block densities falls below a certain value (the density tolerance).
- 3) Production - a short NPT calculation is restarted and the densities are analyzed.
- 4) For each frame in the Amorphous Cell trajectory, the full equilibration trajectory and the density analysis are returned. A summary study table contains the densities for each frame over the production run.

After we get a stable system for the target molecule, cohesive energy density ( $e_{\text{coh}}$ ) task should be executed so as to acquire Cohesive Energy Density ( $e_{\text{coh}}$ ), Cell Volume (CV) and other parameters such as solubility parameter, inter potential energy for each frame in the Dynamics process. We can calculate the average Cohesive Energy Density ( $e_{\text{coh}}$ ) and Cell Volume (CV) in the steady period of the system. It is noted that we focus on the several nearest results (10 recommended) for the average  $e_{\text{coh}}$  and CV so as to reduce the interferences. Finally, polynomials method is employed for getting the melting point of target molecule ( $R^2$  should be more than 0.995). Since the Dynamics works at different temperatures are time-consuming and resource-consuming, we suggest to do the work with 10 K intervals so as to find the trend more distinctly. The details can be found in the following tables (table S6a to S6q).

For the error analysis, original errors from Dynamics task were calculated by 95% confidence intervals regulation. Regarding the error for every step in the calculating procedures, the errors were added in the SI. According to the propagation of uncertainty, we do the error analysis as below (take Tetralin for example):

Step 0: Use 95% confidence interval regulation to calculate the standard deviation for dynamics results  $e_{\text{coh}}$  (Cohesive Energy Density) and V (Cell volume).

Step 1: calculate deviations for  $\frac{de_{\text{coh}}}{dT}$  and  $\frac{dV}{dT}$

Take the differential over 260 K for example, computed results from 250 K and 270 K are employed



into the formulas S5 and S6:

$$f = aA - bB \quad (S5)$$

$$\sigma_f = \sqrt{a^2\sigma_A^2 + b^2\sigma_B^2 - 2ab\sigma_{AB}} \quad (S6)$$

where a and b are both  $\frac{1}{20}$ , A is the data for 270 K, B represents the data for 250 K,  $\sigma$  represents the standard error.

Then the results and deviations for  $\frac{de_{coh}}{dT}$  and  $\frac{dV}{dT}$  can be obtained.

Step 2: calculate deviations for  $\frac{de_{coh}}{dT} \times \frac{dV}{dT}$

Use the formulas S7 and S8,

$$f = CD \quad (S7)$$

$$\sigma_f \approx |f| \sqrt{\left(\frac{\sigma_C}{C}\right)^2 + \left(\frac{\sigma_D}{D}\right)^2 + 2\frac{\sigma_{CD}}{CD}} \quad (S8)$$

where C and D are  $\frac{de_{coh}}{dT}$  and  $\frac{dV}{dT}$  respectively.

Eventually, we can get the final results and deviations for  $\frac{de_{coh}}{dT} \times \frac{dV}{dT}$ .

As for the melting point calculating part, it's more time-consuming than density calculation part since it's based on the stable or balanced systems and we need to calculate the dynamical parameters in 10 K intervals. Also, few usual or weird hydrocarbons with too complex structures which are tough to optimize though via QC method may not adapt to this method, because for these usual hydrocarbons (not natural origin), there exist weird structures such as the caged hydrocarbons with complex ways of carbon linking, which it is hard to get an optimized structure with very low energies, thus further calculation may not come to convergence easily.

All the details are in the tables from S6a to S6q.

Table S6a. Details about melting point for cyclohexane ( $T_M = 279.62 \text{ K}^{37}$ )

Temp (K)	$e_{coh}$ ( $10^8 \text{ J/m}^3$ )	CV ( $10^4 \text{ A}^3$ )	$de_{coh}/dT$ ( $10^8 \text{ J}/(\text{m}^3 \cdot \text{T})$ )	$dCV/dT$ ( $10^4 \text{ A}^3/\text{T}$ )	$(de_{coh}/dT) \times (dCV/dT)$ ( $10^{22} \text{ J/T}^2$ )
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<b>250</b>	3.265± 0.003	2.178± 0.001			
<b>260</b>	3.217± 0.002	2.194± 0.003	-0.01335± 0.00025	0.00390± 0.000158	-0.000052065± 0.000002325
<b>270</b>	2.998± 0.004	2.256± 0.003	-0.01290± 0.000269	0.00358± 0.00018	-0.000046440± 0.000002520
<b>280</b>	2.959± 0.005	2.266± 0.002	-0.00720± 0.00025	0.00215± 0.00025	-0.000015480± 0.000001879
<b>290</b>	2.854± 0.003	2.299± 0.004	-0.01030± 0.00032	0.00330± 0.000269	-0.000033990± 0.000002968
<b>300</b>	2.753± 0.004	2.332± 0.005			

Table S6b. Details about melting point for cis-Decalin ( $T_M = 230.3 \text{ K}^{38}$ )

<b>Temp (K)</b>	<b><math>\epsilon_{\text{coh}}</math> (<math>10^8 \text{ J/m}^3</math>)</b>	<b>CV (<math>10^4 \text{ A}^3</math>)</b>	<b><math>d\epsilon_{\text{coh}}/dT</math> (<math>10^8 \text{ J}/(\text{m}^3 \cdot \text{T})</math>)</b>	<b><math>d\text{CV}/dT</math> (<math>10^4 \text{ A}^3/\text{T}</math>)</b>	<b><math>(d\epsilon_{\text{coh}}/dT) \times (d\text{CV}/dT)</math> (<math>10^{-22} \text{ J/T}^2</math>)</b>
<b>210</b>	3.609± 0.004	3.049± 0.002			
<b>220</b>	3.527± 0.003	3.136± 0.004	-0.00560± 0.00032	0.00460± 0.00018	-0.000025760± 0.000001786
<b>230</b>	3.497± 0.005	3.141± 0.003	-0.00695± 0.00018	0.00210± 0.000224	-0.000014595± 0.000001600
<b>240</b>	3.388± 0.002	3.178± 0.002	-0.00755± 0.00032	0.00255± 0.00025	-0.000019253± 0.000002056
<b>250</b>	3.346± 0.004	3.192± 0.004	-0.00785± 0.00018	0.00275± 0.000141	-0.000021588± 0.000001216
<b>260</b>	3.231± 0.003	3.233± 0.002	-0.01010± 0.000361	0.00365± 0.000224	-0.000036865± 0.000002614
<b>270</b>	3.144± 0.006	3.265± 0.002			

Table S6c. Details about melting point for Heptane ( $T_M = 182.60 \text{ K}^{39}$ )

<b>Temp (K)</b>	<b><math>\epsilon_{\text{coh}}</math> (<math>10^8 \text{ J/m}^3</math>)</b>	<b>CV (<math>10^4 \text{ A}^3</math>)</b>	<b><math>d\epsilon_{\text{coh}}/dT</math> (<math>10^8 \text{ J}/(\text{m}^3 \cdot \text{T})</math>)</b>	<b><math>d\text{CV}/dT</math> (<math>10^4 \text{ A}^3/\text{T}</math>)</b>	<b><math>(d\epsilon_{\text{coh}}/dT) \times (d\text{CV}/dT)</math> (<math>10^{-22} \text{ J/T}^2</math>)</b>
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<b>160</b>	3.638± 0.005	2.634± 0.003			
<b>170</b>	3.563± 0.002	2.656± 0.004	-0.01165± 0.00018	0.00325± 0.000255	-0.000037863± 0.000003027
<b>180</b>	3.405± 0.001	2.699± 0.002	-0.01145± 0.000206	0.00330± 0.00018	-0.000037785± 0.000002173
<b>190</b>	3.334± 0.003	2.722± 0.001	-0.00985± 0.000141	0.00300± 0.000158	-0.000029550± 0.000001614
<b>200</b>	3.208± 0.003	2.759± 0.002	-0.01035± 0.000158	0.00315± 0.00018	-0.000032603± 0.000001931
<b>210</b>	3.127± 0.002	2.785± 0.003	-0.01135± 0.00018	0.00380± 0.000292	-0.000043130± 0.000003379
<b>220</b>	2.981± 0.005	2.835± 0.003			

Table S6d. Details about melting point for Methane ( $T_M = 90.58 \text{ K}^{40}$ )

<b>Temp (K)</b>	<b><math>e_{\text{coh}}</math> (<math>10^8 \text{ J/m}^3</math>)</b>	<b>CV (<math>10^4 \text{ A}^3</math>)</b>	<b><math>de_{\text{coh}}/dT</math> (<math>10^8 \text{ J}/(\text{m}^3 \cdot \text{T})</math>)</b>	<b><math>dCV/dT</math> (<math>10^4 \text{ A}^3/\text{T}</math>)</b>	<b><math>(de_{\text{coh}}/dT) \times (dCV/dT)</math> (<math>10^{-22} \text{ J/T}^2</math>)</b>
<b>70</b>	2.919± 0.004	0.673± 0.004			
<b>80</b>	2.507± 0.005	0.719± 0.002	-0.03000± 0.000224	0.00350± 0.000283	-0.000105000± 0.000008521
<b>90</b>	2.319± 0.002	0.743± 0.004	-0.01700± 0.000292	0.00230± 0.00018	-0.000039100± 0.000003137
<b>100</b>	2.167± 0.003	0.765± 0.003	-0.01495± 0.000224	0.00235±0.0 00224	-0.000035133± 0.000003384
<b>110</b>	2.020± 0.004	0.790± 0.002	-0.01500± 0.000212	0.00260± 0.000212	-0.000039000± 0.000003229
<b>120</b>	1.867± 0.003	0.817± 0.003			

Table S6e. Details about melting point for  $\alpha$ -Pinene ( $T_M = 218.15 \text{ K}^{35}$ )

<b>Temp (K)</b>	<b><math>e_{\text{coh}}</math> (<math>10^8 \text{ J/m}^3</math>)</b>	<b>CV (<math>10^4 \text{ A}^3</math>)</b>	<b><math>de_{\text{coh}}/dT</math> (<math>10^8 \text{ J}/(\text{m}^3 \cdot \text{T})</math>)</b>	<b><math>dCV/dT</math> (<math>10^4 \text{ A}^3/\text{T}</math>)</b>	<b><math>(de_{\text{coh}}/dT) \times (dCV/dT)</math> (<math>10^{-22} \text{ J/T}^2</math>)</b>
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<b>170</b>	3.595± 0.004	2.998± 0.003			
<b>180</b>	3.480± 0.005	3.035± 0.004	-0.00880± 0.000224	0.00270± 0.00018	-0.000023760± 0.000001697
<b>190</b>	3.419± 0.002	3.052± 0.002	-0.00730± 0.000292	0.00235± 0.00025	-0.000017155± 0.000001949
<b>200</b>	3.334± 0.003	3.082± 0.003	-0.00805± 0.000224	0.00290± 0.000141	-0.000023345± 0.000001310
<b>210</b>	3.258± 0.004	3.110± 0.002	-0.00630± 0.000212	0.00230± 0.000212	-0.000014490± 0.000001423
<b>220</b>	3.208± 0.003	3.128± 0.003	-0.00860± 0.00032	0.00305± 0.000224	-0.000026230± 0.000002157
<b>230</b>	3.086± 0.005	3.171± 0.004			

Table S6f. Details about melting point for Isopentane ( $T_M = 113.25 \text{ K}^{32}$ )

<b>Temp (K)</b>	<b><math>\epsilon_{\text{coh}}</math> (<math>10^8 \text{ J/m}^3</math>)</b>	<b>CV (<math>10^4 \text{ A}^3</math>)</b>	<b><math>d\epsilon_{\text{coh}}/dT</math> (<math>10^8 \text{ J}/(\text{m}^3 \cdot \text{T})</math>)</b>	<b><math>dCV/dT</math> (<math>10^4 \text{ A}^3/\text{T}</math>)</b>	<b><math>(d\epsilon_{\text{coh}}/dT) \times (dCV/dT)</math> (<math>10^{-22} \text{ J/T}^2</math>)</b>
<b>100</b>	3.790± 0.001	1.870± 0.002			
<b>110</b>	3.708± 0.002	1.891± 0.002	-0.00815± 0.000141	0.00190± 0.000224	-0.000015485± 0.000001842
<b>120</b>	3.627± 0.001	1.908± 0.001	-0.01205± 0.000144	0.00250± 0.000224	-0.000030125± 0.000002718
<b>130</b>	3.467± 0.002	1.941± 0.004	-0.01425± 0.000206	0.00300± 0.000158	-0.000042750± 0.000002336
<b>140</b>	3.342± 0.004	1.968± 0.003	-0.01050± 0.00018	0.00235± 0.000224	-0.000024675± 0.000002386
<b>150</b>	3.257± 0.003	1.988± 0.002	-0.00840± 0.000224	0.00200± 0.00025	-0.000016800± 0.000002147
<b>160</b>	3.174± 0.002	2.008± 0.004			

Table S6g. Details about melting point for Methylcyclohexane ( $T_M = 147.15 \text{ K}^{30}$ )

<b>Temp (K)</b>	<b><math>\epsilon_{\text{coh}}</math> (<math>10^8 \text{ J/m}^3</math>)</b>	<b>CV (<math>10^4 \text{ A}^3</math>)</b>	<b><math>d\epsilon_{\text{coh}}/dT</math> (<math>10^8 \text{ J}/(\text{m}^3 \cdot \text{T})</math>)</b>	<b><math>dCV/dT</math> (<math>10^4 \text{ A}^3/\text{T}</math>)</b>	<b><math>(d\epsilon_{\text{coh}}/dT) \times (dCV/dT)</math> (<math>10^{-22} \text{ J/T}^2</math>)</b>
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<b>130</b>	4.080± 0.003	2.275± 0.002			
<b>140</b>	3.978± 0.002	2.297± 0.003	-0.00955± 0.00018	0.00205± 0.000112	-0.000019578± 0.000001130
<b>150</b>	3.889± 0.002	2.316± 0.001	-0.00785± 0.00018	0.00170± 0.00018	-0.000013345± 0.000001448
<b>160</b>	3.821± 0.003	2.331± 0.002	-0.00880± 0.00018	0.00205± 0.000158	-0.000018040± 0.000001440
<b>170</b>	3.713± 0.003	2.357± 0.003	-0.01130± 0.00018	0.00270± 0.000141	-0.000030510± 0.000001671
<b>180</b>	3.595± 0.002	2.385± 0.002	-0.01180± 0.00018	0.00285± 0.00025	-0.000033630± 0.000002994
<b>190</b>	3.477± 0.002	2.414± 0.004			

Table S6h. Details about melting point for Tetralin ( $T_M = 242.54 \text{ K}^{30}$ )

<b>Temp (K)</b>	<b><math>\epsilon_{\text{coh}}</math> (<math>10^8 \text{ J/m}^3</math>)</b>	<b>CV (<math>10^4 \text{ A}^3</math>)</b>	<b><math>d\epsilon_{\text{coh}}/dT</math> (<math>10^8 \text{ J}/(\text{m}^3 \cdot \text{T})</math>)</b>	<b><math>dCV/dT</math> (<math>10^4 \text{ A}^3/\text{T}</math>)</b>	<b><math>(d\epsilon_{\text{coh}}/dT) \times (dCV/dT)</math> (<math>10^{-22} \text{ J/T}^2</math>)</b>
<b>210</b>	4.584± 0.004	2.707± 0.002			
<b>220</b>	4.436± 0.003	2.739± 0.003	-0.01380± 0.000224	0.00310± 0.000141	-0.000042780± 0.000002071
<b>230</b>	4.308± 0.002	2.769± 0.002	-0.01170± 0.000212	0.00280± 0.000180	-0.000032760± 0.000002191
<b>240</b>	4.202± 0.003	2.795± 0.002	-0.00800± 0.000141	0.00205± 0.000141	-0.000016400± 0.000001168
<b>250</b>	4.148± 0.002	2.810± 0.002	-0.00865± 0.00025	0.00215± 0.00018	-0.000018598± 0.000001649
<b>260</b>	4.029± 0.004	2.838± 0.003	-0.00895± 0.000141	0.00225± 0.00018	-0.000020137± 0.000001645
<b>270</b>	3.969± 0.002	2.855± 0.003			

Table S6i. Details about melting point for Bicyclohexyl ( $T_M = 277.15 \text{ K}^{33}$ )

<b>Temp (K)</b>	<b><math>\epsilon_{\text{coh}}</math> (<math>10^8 \text{ J/m}^3</math>)</b>	<b>CV (<math>10^4 \text{ A}^3</math>)</b>	<b><math>d\epsilon_{\text{coh}}/dT</math> (<math>10^8 \text{ J}/(\text{m}^3 \cdot \text{T})</math>)</b>	<b><math>dCV/dT</math> (<math>10^4 \text{ A}^3/\text{T}</math>)</b>	<b><math>(d\epsilon_{\text{coh}}/dT) \times (dCV/dT)</math> (<math>10^{-22} \text{ J/T}^2</math>)</b>
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<b>240</b>	3.389± 0.003	3.845± 0.003			
<b>250</b>	3.333± 0.003	3.869± 0.005	0.00705± 0.00018	-0.0031± 0.000212	-0.000021855± 0.000001597
<b>260</b>	3.248± 0.002	3.907± 0.003	0.0075± 0.00018	-0.0034± 0.00032	-0.000025500± 0.000002478
<b>270</b>	3.183± 0.002	3.937± 0.004	0.00665± 0.00018	-0.003± 0.00025	-0.000019950± 0.000001748
<b>280</b>	3.115± 0.003	3.967± 0.004	0.0078± 0.000141	-0.00365± 0.00025	-0.000028470± 0.000002017
<b>290</b>	3.027± 0.002	4.010± 0.003	0.0075± 0.000212	-0.00365± 0.000283	-0.000027375± 0.000002258
<b>300</b>	2.965± 0.003	4.040± 0.004			

Table S6j. Details about melting point for 1-Butene ( $T_M = 87.82K^{32}$ )

<b>Temp (K)</b>	<b><math>\epsilon_{coh}</math> (<math>10^8J/m^3</math>)</b>	<b>CV (<math>10^4A^3</math>)</b>	<b><math>d\epsilon_{coh}/dT</math> (<math>10^8J/(m^3 \cdot T)</math>)</b>	<b><math>dCV/dT</math> (<math>10^4A^3/T</math>)</b>	<b><math>(d\epsilon_{coh}/dT) \times (dCV/dT)</math> (<math>10^{-22}J/T^2</math>)</b>
<b>60</b>	4.708± 0.002	1.412± 0.001			
<b>70</b>	4.644± 0.003	1.420± 0.002	0.00765± 0.000141	-0.00095± 0.000112	-0.000007268± 0.000000866
<b>80</b>	4.555± 0.002	1.431± 0.002	0.01200± 0.00025	-0.00145± 0.000112	-0.000017400± 0.000001390
<b>90</b>	4.404± 0.004	1.449± 0.001	0.01125± 0.000269	-0.00145± 0.00018	-0.000016312± 0.000002065
<b>100</b>	4.330± 0.005	1.460± 0.003	0.01605± 0.00025	-0.0022± 0.000112	-0.000035310± 0.000001877
<b>110</b>	4.083± 0.003	1.493± 0.002	0.0177± 0.000292	-0.0024± 0.000212	-0.000042480± 0.000003819
<b>120</b>	3.976± 0.003	1.508± 0.003			

Table S6k. Details about melting point for Cycloheptane ( $T_M = 261.15K^{30}$ )

<b>Temp (K)</b>	<b><math>\epsilon_{coh}</math> (<math>10^8J/m^3</math>)</b>	<b>CV (<math>10^4A^3</math>)</b>	<b><math>d\epsilon_{coh}/dT</math> (<math>10^8J/(m^3 \cdot T)</math>)</b>	<b><math>dCV/dT</math> (<math>10^4A^3/T</math>)</b>	<b><math>(d\epsilon_{coh}/dT) \times (dCV/dT)</math> (<math>10^{-22}J/T^2</math>)</b>
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<b>240</b>	3.413± 0.004	2.458± 0.003			
<b>250</b>	3.312± 0.003	2.488± 0.005	0.0102± 0.000283	-0.00295± 0.00018	-0.000030090± 0.000002019
<b>260</b>	3.209± 0.004	2.517± 0.002	0.00935± 0.00018	-0.00275± 0.000292	-0.000025713± 0.000002771
<b>270</b>	3.125± 0.002	2.543± 0.003	0.0086± 0.00025	-0.0027± 0.00018	-0.000023220± 0.000001691
<b>280</b>	3.037± 0.003	2.571± 0.003	0.00965± 0.000224	-0.00315± 0.00025	-0.000030397± 0.000002513
<b>290</b>	2.932± 0.004	2.606± 0.004	0.007± 0.000212	-0.0024± 0.00025	-0.000016800± 0.000001823
<b>300</b>	2.897± 0.003	2.619± 0.004			

Table S6l. Details about melting point for Cyclohexene ( $T_M = 169.82\text{K}^{32}$ )

<b>Temp (K)</b>	<b><math>\epsilon_{\text{coh}}</math> (<math>10^8\text{J}/\text{m}^3</math>)</b>	<b>CV (<math>10^4\text{A}^3</math>)</b>	<b><math>d\epsilon_{\text{coh}}/dT</math> (<math>10^8\text{J}/(\text{m}^3\cdot\text{T})</math>)</b>	<b><math>d\text{CV}/dT</math> (<math>10^4\text{A}^3/\text{T}</math>)</b>	<b><math>(d\epsilon_{\text{coh}}/dT) \times (d\text{CV}/dT)</math> (<math>10^{-22}\text{J}/\text{T}^2</math>)</b>
<b>140</b>	4.722± 0.003	1.845± 0.002			
<b>150</b>	4.581± 0.001	1.867± 0.002	0.01355± 0.00018	-0.00205± 0.000112	-0.000027778± 0.000001559
<b>160</b>	4.451± 0.002	1.886± 0.001	0.01135± 0.000112	-0.0018± 0.00018	-0.000020430± 0.000002056
<b>170</b>	4.354± 0.002	1.903± 0.003	0.0107± 0.000224	-0.0018± 0.000206	-0.000019260± 0.000002242
<b>180</b>	4.237± 0.004	1.922± 0.004	0.01075± 0.00018	-0.0019± 0.00018	-0.000020425± 0.000001968
<b>190</b>	4.139± 0.003	1.941± 0.002	0.0107± 0.000224	-0.00195± 0.000224	-0.000020865± 0.000002432
<b>200</b>	4.023± 0.002	1.961± 0.002			

Table S6m. Details about melting point for Cyclopentane ( $T_M = 179.75\text{K}^{41}$ )

<b>Temp (K)</b>	<b><math>\epsilon_{\text{coh}}</math> (<math>10^8\text{J}/\text{m}^3</math>)</b>	<b>CV (<math>10^4\text{A}^3</math>)</b>	<b><math>d\epsilon_{\text{coh}}/dT</math> (<math>10^8\text{J}/(\text{m}^3\cdot\text{T})</math>)</b>	<b><math>d\text{CV}/dT</math> (<math>10^4\text{A}^3/\text{T}</math>)</b>	<b><math>(d\epsilon_{\text{coh}}/dT) \times (d\text{CV}/dT)</math> (<math>10^{-22}\text{J}/\text{T}^2</math>)</b>
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<b>160</b>	3.950± 0.003	1.724± 0.003			
<b>170</b>	3.848± 0.003	1.742± 0.002	0.01285± 0.00018	-0.00235± 0.000158	-0.000030198± 0.000002075
<b>180</b>	3.693± 0.002	1.771± 0.001	0.00925± 0.000212	-0.00175± 0.000112	-0.000016188± 0.000001099
<b>190</b>	3.663± 0.003	1.777± 0.001	0.00605± 0.000141	-0.00115± 0.000112	-0.000006958± 0.000000696
<b>200</b>	3.572± 0.002	1.794± 0.002	0.01400± 0.000158	-0.00285± 0.000158	-0.000039900± 0.000002259
<b>210</b>	3.383± 0.001	1.834± 0.003	0.01485± 0.00018	-0.00320± 0.000141	-0.000047520± 0.000002178
<b>220</b>	3.275± 0.003	1.858± 0.002			

Table S6n. Details about melting point for Dimethylpentane ( $T_M = 153.25K^{32}$ )

<b>Temp (K)</b>	<b><math>\epsilon_{coh}</math> (<math>10^8J/m^3</math>)</b>	<b>CV (<math>10^4A^3</math>)</b>	<b><math>d\epsilon_{coh}/dT</math> (<math>10^8J/(m^3 \cdot T)</math>)</b>	<b><math>dCV/dT</math> (<math>10^4A^3/T</math>)</b>	<b><math>(d\epsilon_{coh}/dT) \times (dCV/dT)</math> (<math>10^{-22}J/T^2</math>)</b>
<b>120</b>	3.512± 0.003	2.546± 0.003			
<b>130</b>	3.530± 0.003	2.540± 0.004	0.00635± 0.00018	-0.0018± 0.000158	-0.000011430± 0.000001055
<b>140</b>	3.385± 0.002	2.582± 0.001	0.01020± 0.000212	-0.0029± 0.000224	-0.000029580± 0.000002362
<b>150</b>	3.326± 0.003	2.598± 0.002	0.00910± 0.000141	-0.0027± 0.000158	-0.000024570± 0.000001489
<b>160</b>	3.203± 0.002	2.636± 0.003	0.01005± 0.00025	-0.00305± 0.00018	-0.000030653± 0.000001966
<b>170</b>	3.125± 0.004	2.659± 0.003	0.0095± 0.00018	-0.00305± 0.00025	-0.000028975± 0.000002438
<b>180</b>	3.013± 0.003	2.697± 0.004			

Table S6o. Details about melting point for Ethylcyclohexane ( $T_M = 162.04K^{30}$ )

<b>Temp (K)</b>	<b><math>\epsilon_{coh}</math> (<math>10^8J/m^3</math>)</b>	<b>CV (<math>10^4A^3</math>)</b>	<b><math>d\epsilon_{coh}/dT</math> (<math>10^8J/(m^3 \cdot T)</math>)</b>	<b><math>dCV/dT</math> (<math>10^4A^3/T</math>)</b>	<b><math>(d\epsilon_{coh}/dT) \times (dCV/dT)</math> (<math>10^{-22}J/T^2</math>)</b>
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<b>130</b>	4.008± 0.002	2.601± 0.002			
<b>140</b>	3.991± 0.003	2.605± 0.004	0.00580± 0.000112	-0.00145± 0.000112	-0.000008410± 0.000000668
<b>150</b>	3.892± 0.001	2.630± 0.001	0.00825± 0.000212	-0.00205± 0.000224	-0.000016913± 0.000001895
<b>160</b>	3.826± 0.003	2.646± 0.002	0.00810± 0.000112	-0.00205± 0.000071	-0.000016605± 0.000000617
<b>170</b>	3.730± 0.002	2.671± 0.001	0.00995± 0.000212	-0.00270± 0.000141	-0.000026865± 0.000001519
<b>180</b>	3.627± 0.003	2.700± 0.002	0.00955± 0.000141	-0.0027± 0.000071	-0.000025785± 0.000000776
<b>190</b>	3.539± 0.002	2.725± 0.001			

Table S6p. Details about melting point for Isopropylcyclohexane ( $T_M = 183.71\text{K}^{30}$ )

<b>Temp (K)</b>	<b><math>\epsilon_{\text{coh}}</math> (<math>10^8\text{J}/\text{m}^3</math>)</b>	<b>CV (<math>10^4\text{A}^3</math>)</b>	<b><math>d\epsilon_{\text{coh}}/dT</math> (<math>10^8\text{J}/(\text{m}^3\cdot\text{T})</math>)</b>	<b><math>d\text{CV}/dT</math> (<math>10^4\text{A}^3/\text{T}</math>)</b>	<b><math>(d\epsilon_{\text{coh}}/dT) \times (d\text{CV}/dT)</math> (<math>10^{-22}\text{J}/\text{T}^2</math>)</b>
<b>150</b>	3.797± 0.003	2.924± 0.002			
<b>160</b>	3.709± 0.003	2.949± 0.004	0.01010± 0.00018	-0.00295± 0.000141	-0.000029795± 0.000001524
<b>170</b>	3.595± 0.002	2.983± 0.002	0.0090± 0.000212	-0.0027± 0.00025	-0.000024300± 0.000002322
<b>180</b>	3.529± 0.003	3.003± 0.003	0.00780± 0.000141	-0.00245± 0.000141	-0.000019110± 0.000001156
<b>190</b>	3.439± 0.002	3.032± 0.002	0.00860± 0.000212	-0.0028± 0.000158	-0.000024080± 0.000001484
<b>200</b>	3.357± 0.003	3.059± 0.001	0.00830± 0.000141	-0.00280± 0.000224	-0.000023240± 0.000001898
<b>210</b>	3.273± 0.002	3.088± 0.004			

Table S6q. Details about melting point for 1-Octene ( $T_M = 171.48\text{K}^{30}$ )

<b>Temp (K)</b>	<b><math>\epsilon_{\text{coh}}</math> (<math>10^8\text{J}/\text{m}^3</math>)</b>	<b>CV (<math>10^4\text{A}^3</math>)</b>	<b><math>d\epsilon_{\text{coh}}/dT</math> (<math>10^8\text{J}/(\text{m}^3\cdot\text{T})</math>)</b>	<b><math>d\text{CV}/dT</math> (<math>10^4\text{A}^3/\text{T}</math>)</b>	<b><math>(d\epsilon_{\text{coh}}/dT) \times (d\text{CV}/dT)</math> (<math>10^{-22}\text{J}/\text{T}^2</math>)</b>
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<b>150</b>	3.894± 0.004	2.825± 0.002			
<b>160</b>	3.823± 0.002	2.846± 0.003	0.00950± 0.00025	-0.00255± 0.000141	-0.000024225± 0.000001487
<b>170</b>	3.704± 0.003	2.876± 0.002	0.00975± 0.000141	-0.0024± 0.000212	-0.000023400± 0.000002096
<b>180</b>	3.628± 0.002	2.894± 0.003	0.00895± 0.000212	-0.00280± 0.000141	-0.000025060± 0.000001398
<b>190</b>	3.525± 0.003	2.932± 0.002	0.01285± 0.000141	-0.00420± 0.00018	-0.000053970± 0.000002392
<b>200</b>	3.371± 0.002	2.978± 0.002	0.00995± 0.00018	-0.00345± 0.000224	-0.000034328± 0.000002310
<b>210</b>	3.326± 0.002	3.001± 0.004			

### **Evaluations of olefin saturation treatment: cyclopropanation vs. hydrogenation**

In terms of olefin saturation treatment methods, cyclopropanation and hydrogenation are both

available in this field. Through the protocol we proposed in the paper, it is obvious that cyclopropanation products exceed hydrogenation towards both the density and volumetric net heat of combustion sides. See details in table S7.

Table S7. Computed densities and  $\text{NHOG}_V$  through cyclopropanation and hydrogenation

Molecules		Electronic and thermal Enthalpies (hartree/particle)	Predicted $\Delta H_{\text{vap}}$ (kcal/mol)	$\Delta H_{\text{comb}}$ after correction (kcal/mol)	$\text{NHOC}_G$ (MJ/kg)	Density (g/cm <sup>3</sup> )	$\text{NHOC}_V$ (MJ/L)
<b>a. <math>\beta</math>-Caryophyllen</b>	$\text{C}_{15}\text{H}_{24}$						
<b>Cyclopropanation</b>	$\text{C}_{17}\text{H}_{28}$	-663.992	20.664	-2373.967	-42.832	0.908	-38.892
<b>Hydrogenation</b>	$\text{C}_{15}\text{H}_{28}$	-587.893	18.316	-2112.443	-42.511	0.866	-36.815
<b>b. Norbornadiene</b>	$\text{C}_7\text{H}_8$						
<b>Cyclopropanation</b>	$\text{C}_9\text{H}_{12}$	-349.811	11.273	-1274.127	-44.444	0.913	-40.578
<b>Hydrogenation</b>	$\text{C}_7\text{H}_{12}$	-273.722	8.945	-1006.165	-43.871	0.848	-37.203
<b>c. <math>\beta</math>-Pinene</b>	$\text{C}_{10}\text{H}_{16}$						
<b>Cyclopropanation</b>	$\text{C}_{11}\text{H}_{18}$	-429.575	13.624	-1558.720	-43.497	0.866	-37.669
<b>Hydrogenation</b>	$\text{C}_{10}\text{H}_{18}$	-391.522	12.481	-1429.784	-43.369	0.841	-36.473
<b>d. <math>\alpha</math>-Pinene</b>	$\text{C}_{10}\text{H}_{16}$						
<b>Cyclopropanation</b>	$\text{C}_{11}\text{H}_{18}$	-429.567	13.656	-1563.857	-43.641	0.863	-37.662
<b>Hydrogenation</b>	$\text{C}_{10}\text{H}_{18}$	-391.522	12.459	-1429.805	-43.369	0.841	-36.473
<b>e. GermacreneC</b>	$\text{C}_{15}\text{H}_{24}$						
<b>Cyclopropanation</b>	$\text{C}_{18}\text{H}_{30}$	-703.262	21.837	-2513.493	-42.769	0.903	-38.620
<b>Hydrogenation</b>	$\text{C}_{15}\text{H}_{30}$	-589.094	18.35	-2132.772	-42.512	0.863	-36.688
<b>f. <math>\beta</math>-Macrocarpene</b>	$\text{C}_{15}\text{H}_{24}$						
<b>Cyclopropanation</b>	$\text{C}_{17}\text{H}_{28}$	-664.036	20.664	-2346.455	-42.336	0.904	-38.272
<b>Hydrogenation</b>	$\text{C}_{15}\text{H}_{28}$	-587.93	18.316	-2089.434	-42.048	0.875	-36.792
<b>g. Aristolochene</b>	$\text{C}_{15}\text{H}_{24}$						
<b>Cyclopropanation</b>	$\text{C}_{17}\text{H}_{28}$	-664.034	20.704	-2347.918	-42.362	0.914	-38.719
<b>Hydrogenation</b>	$\text{C}_{15}\text{H}_{28}$	-587.933	18.367	-2087.431	-42.008	0.89	-37.387

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