Supporting information

Insight of Antioxidant Properties of Non-phenolic Terpenoids Containing in Essential Oils Extracted from the Buds of *Cleistocalyxoperculatus:* A DFT study

ThiChinh Ngo[1], DuyQuang Dao[1,*], Minh Thong Nguyen[2], Pham Cam Nam [3,*]

[1]Institute of Research and Development, Duy Tan University, K7/25 QuangTrung, Danang, Viet Nam

[2]The University of Danang, Campus in Kon Tum, 704 PhanDinhPhung, Kon Tum, Viet Nam

[3]Department of Chemistry, Danang University of Science and Technology - The University of Danang, 54 Nguyen Luong Bang, Lien Chieu, Danang, Viet Nam

[*]Corresponding authors: daoduyquang@gmail.comandcamnamp@yahoo.com

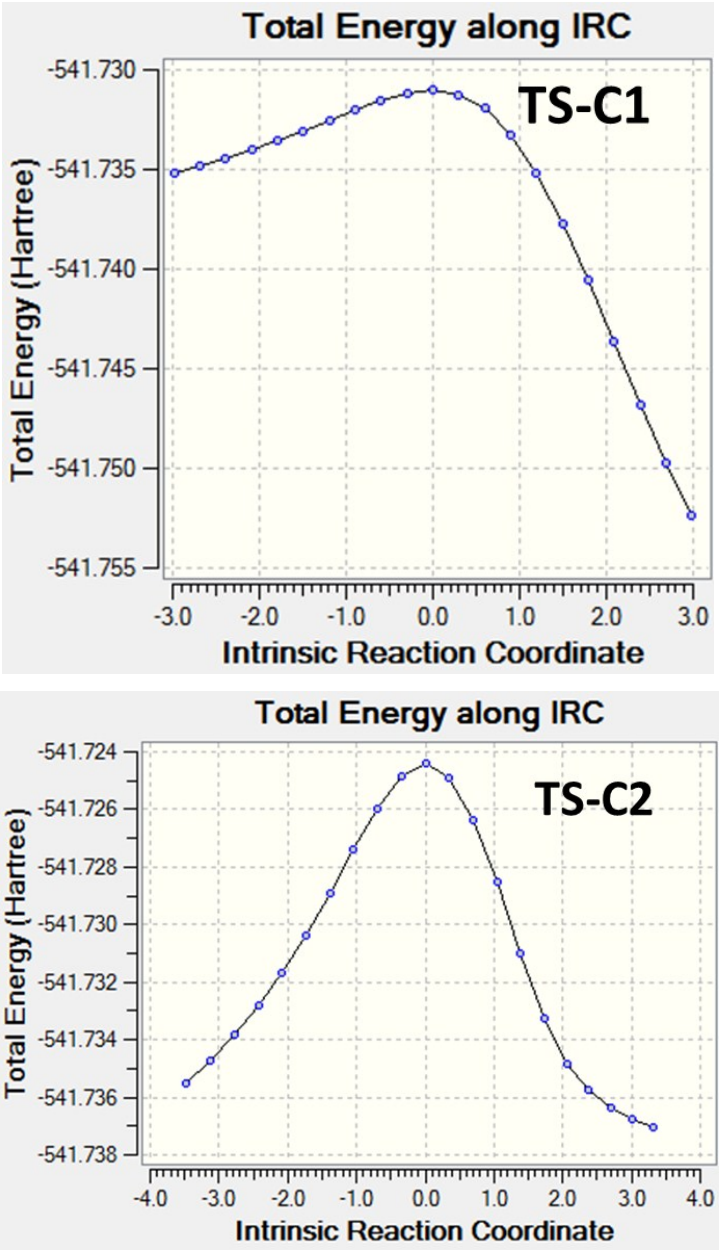
List of supporting information:

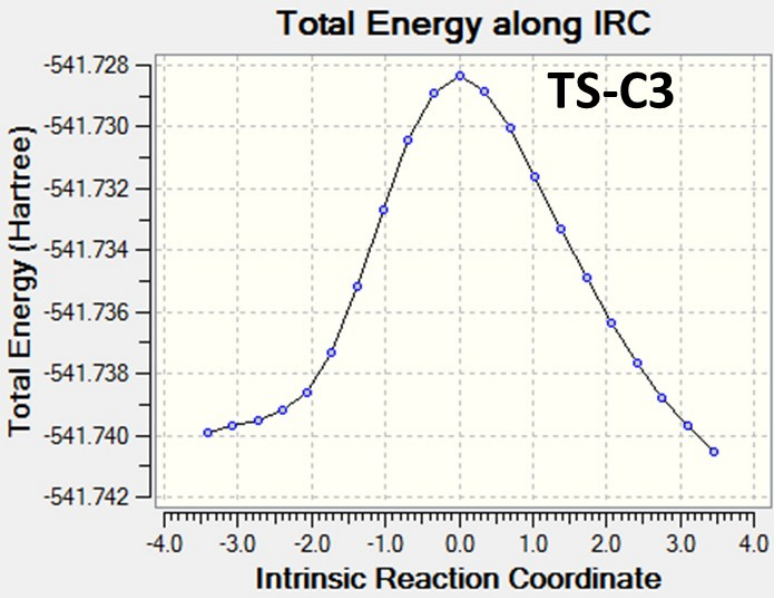
Figure S1: IRC plots for all transition states related to reaction of HOO• radical with α-terpinene at B3LYP/6-311G(d,p) level of theory in the gas phase.

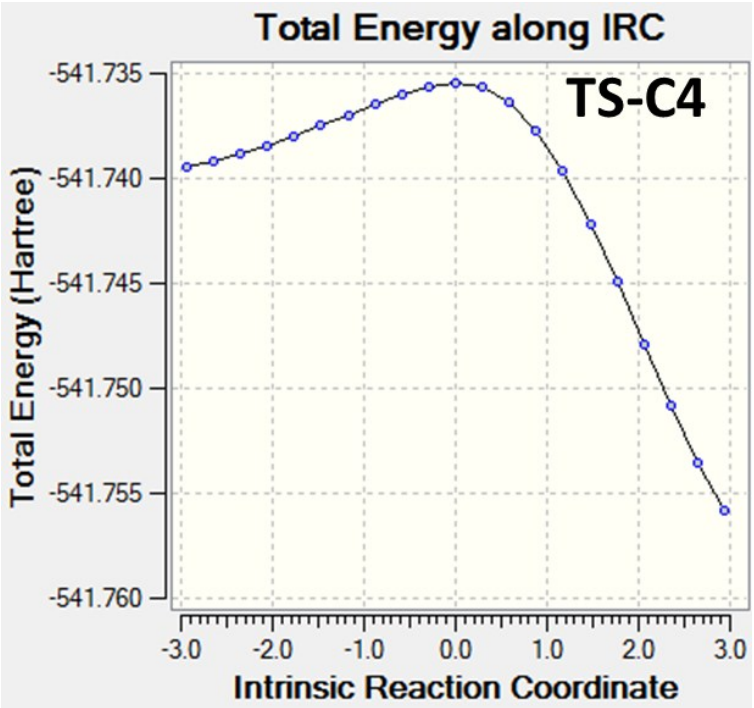
Table S1: Bond dissociation enthalpy (BDE) values of the C–H bond breaking of different compounds in the gas phase using PM6 and ROB3LYP/6-311G++G(2df,2p)//B3LYP/6-311G(d,p) methods.

Table S2:Cartesian coordinates and molecular enthalpies of all parent molecules and resulted radicals, anions optimized at B3LYP/6-311G(d,p) level of theory in the gas phase, water and ethanol.

Figure 1: IRC plots for all transition states related to reaction of HOO• radical with α-terpineneat B3LYP/6-311G(d,p) level of theory in the gas phase.




Total Energy along IRC
TS-C3
Total Energy (Hartree)
-541.728
-541.730
-541.732
-541.734
-541.736
-541.738
-541.740
-541.742
-4.0
-3.0
-2.0
-1.0
0.0
1.0
2.0
3.0
4.0
Intrinsic Reaction Coordinate


Total Energy along IRC
TS-C4
Total Energy (Hartree)
-541.735
-541.740
-541.745
-541.750
-541.755
-541.760
-3.0
-2.0
-1.0
0.0
1.0
2.0
3.0
Intrinsic Reaction Coordinate

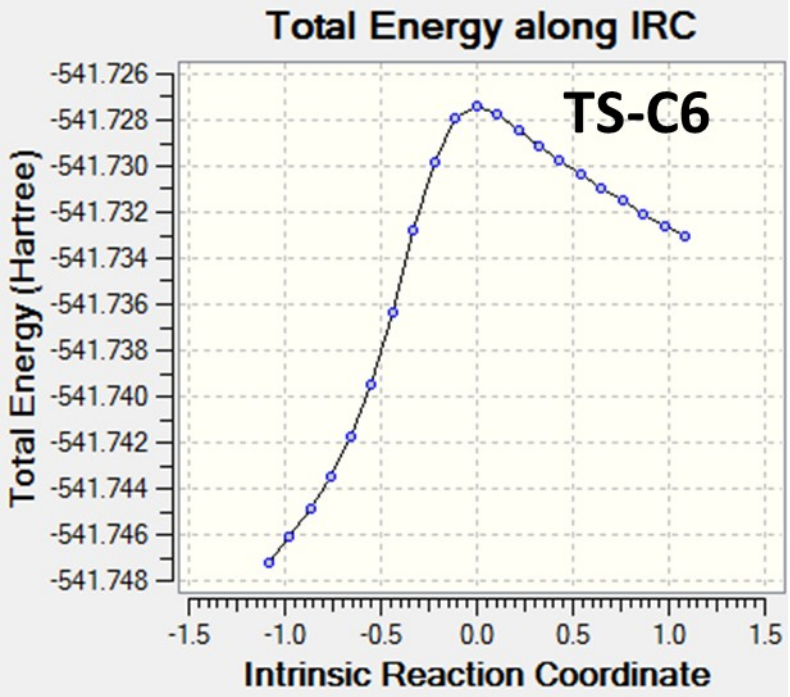


Table S1: The bond dissociation enthalpy (BDE) values of the C–H bond breaking of different compounds in the gas phase using PM6 and ROB3LYP/6-311G++G(2df,2p)//B3LYP/6-311G(d,p) methods

	Compounds	**Bond numbering**	**BDE (kcal/mol)**	
			PM6	***(RO)B3LYP/ 6-311G++G(2df,2p)***
Monoterpenes	α-Pinene	C1-H	89.5	
		C3-H	94.3	
		C4-H	**64.9**	**83.9**
		C5-H	87.5	
		C7-H	78.6	
		C8-H	68.0	
		C9-H	78.5	
		C10-H	77.9	
	Camphene	C1-H	88.3	
		C4-H	88.0	
		C5-H	74.8	97.5
		C6-H	**73.9**	**97.1**
		C7-H	77.8	
		C8-H	78.5	
		C9-H	78.8	
		C10-H	86.8	

	β-Pinene	C1-H	87.9	
		C3-H	**65.7**	**82.7**
		C4-H	71.6	
		C5-H	86.4	
		C7-H	78.5	
		C8-H	77.8	
		C9-H	78.7	
		C10-H	87.6	
	Myrcene	C1-H	85.5	
		C2-H	72.4	
		C4-H	65.4	87.6
		C5-H	**62.4**	**81.4**
		C6-H	82.8	
		C8-H	69.5	
		C9-H	69.6	
		C10-H	87.2	
	α-Terpinene	C2-H	90.9	
		C3-H	91.5	
		C5-H	58.0	74.5
		C6-H	**57.8**	**73.3**
		C7-H	**55.8**	76.9
		C8-H	78.1	
		C9-H	78.1	
		C10-H	64.6	
	Limonene	C2-H	90.4	
		C3-H	**63.0**	**83.0**
		C4-H	**62.5**	84.0
		C5-H	71.6	
		C6-H	63.9	85.1
		C8-H	87.3	
		C9-H	71.2	
		C10-H	69.4	
	γ-Terpinene	C2-H	90.5	
		C3-H	58.0	**74.9**
		C5-H	91.1	
		C6-H	**57.8**	**74.4**
		C7-H	60.1	83.6
		C8-H	78.1	
		C9-H	78.1	
		C10-H	69.5	

Sesquiterpenes	α-Copanene	C2-H	89.3	
		C4-H	94.2	
		C5-H	**64.6**	**83.1**
		C6-H	87.4	
		C7-H	85.1	
		C8-H	66.5	92.4

		C10-H	71.6	
		C9-H	69.8	
		C11-H	78.4	
		C12-H	68.3	
		C13-H	67.0	96.0
		C14-H	78.3	
		C15-H	78.2	
	Sesquithujene	C1-H	93.4	
		C3-H	99.2	
		C4-H	66.3	
		C6-H	84.6	
		C7-H	66.4	
		C8-H	72.1	
		C9-H	**62.4**	**82.1**
		C10-H	82.9	
		C12-H	68.1	
		C13-H	77.9	
		C14-H	69.2	
		C15-H	69.4	
		C2-H	65.2	91.1
		C3-H	71.6	
		C4-H	70.3	
		C5-H	70.1	
		C7-H	80.6	
		C9-H	**64.4**	**82.8**
		C10-H	71.5	
		C11-H	75.8	
		C12-H	77.8	
		C13-H	78.4	
		C14-H	78.5	
		C15-H	87.4	
	β-Cedrene			
	6-Epi-beta-cubebene	C1-H	66.3	91.1
		C2-H	72.2	
		C3-H	71.3	
		C4-H	**65.3**	90.1
		C6-H	72.8	
		C7-H	**67.9**	**85.1**
		C9-H	93.3	
		C10-H	84.1	
		C11-H	66.4	94.8
		C12-H	78.3	
		C13-H	78.1	

		C14-H	78.1	
		C15-H	88.0	
	Aromadendr-9-ene	C2-H	79.6	
		C3-H	**60.5**	**81.0**
		C4-H	66.5	
		C5-H	65.5	85.1
		C6-H	97.6	
		C8-H	**59.5**	83.8
		C9-H	72.3	
		C10-H	73.9	
		C11-H	79.2	
		C12-H	77.6	
		C13-H	77.5	
		C14-H	77.4	
		C15-H	78.4	
	γ-Muurolene	C1-H	68.4	
		C2-H	71.7	
		C3-H	65.4	84.8
		C5-H	71.4	
		C6-H	64.1	84.4
		C8-H	90.0	
		C9-H	**59.8**	**82.2**
		C10-H	62.6	84.7
		C11-H	65.2	
		C12-H	77.7	
		C13-H	77.7	
		C14-H	87.2	
		C15-H	69.8	
	γ-Amorphene	C1-H	65.3	
		C2-H	70.3	
		C3-H	64.1	
		C5-H	71.5	
		C6-H	64.2	
		C8-H	90.3	
		C9-H	**60.6**	**81.0**
		C10-H	61.7	
		C11-H	66.4	
		C12-H	78.2	
		C13-H	78.1	
		C14-H	87.4	
		C15-H	69.3	

	Cyclobazzanene	C4-H	97.6	
		C5-H	**64.1**	**82.0**
		C6-H	73.9	
		C8-H	71.9	
		C9-H	71.6	
		C10-H	72.1	
		C11-H	71.9	
		C12-H	78.2	
		C13-H	78.4	
		C14-H	68.2	
		C15-H	78.8	
	α-Cadinene	C1-H	67.6	
		C2-H	62.0	81.4
		C3-H	89.6	
		C5-H	71.3	
		C6-H	63.6	84.0
		C8-H	90.8	
		C9-H	**59.2**	**79.5**
		C10-H	59.8	81.0
		C11-H	65.3	
		C12-H	77.8	
		C13-H	77.7	
		C14-H	69.0	
		C15-H	69.5	
Diterpenes	Axinissene	C2-H	90.3	

		C3-H	63.0	82.9
		C4-H	**62.1**	83.1
		C5-H	71.5	
		C6-H	63.9	84.8
		C8-H	65.5	84.7
		C9-H	**62.6**	**82.3**
		C10-H	82.4	
		C12-H	64.5	85.7
		C13-H	62.6	86.6
		C16-H	69.4	
		C17-H	87.1	
		C18-H	69.3	
		C19-H	69.2	
		C20-H	69.5	
	Rimuene	C2-H	73.1	
		C3-H	69.0	
		C4-H	**62.5**	82.4
		C5-H	87.9	
		C8-H	71.3	
		C9-H	71.6	
		C10-H	71.1	
		C11-H	**59.3**	**80.4**
		C13-H	72.1	
		C14-H	72.2	
		C15-H	80.6	
		C16-H	85.2	
		C17-H	79.2	
		C18-H	79.0	
		C19-H	78.6	
		C20-H	78.2	
	Cembrene	C1-H	81.8	
		C2-H	73.7	
		C4-H	82.9	
		C5-H	**58.8**	73.9
		C6-H	83.6	
		C8-H	67.2	
		C9-H	64.6	
		C10-H	82.1	
		C12-H	64.8	
		C13-H	71.0	
		C14-H	**54.8**	**75.4**
		C15-H	69.2	
		C16-H	69.8	
		C17-H	69.5	

		C18-H	65.4	
		C19-H	77.9	
		C20-H	77.8	
	Kaur-16-ene	C1-H	81.0	
		C3-H	**69.5**	**84.5**
		C5-H	71.9	
		C6-H	71.7	
		C7-H	**67.0**	**92.1**
		C9-H	71.9	
		C10-H	71.1	
		C11-H	72.5	
		C13-H	**67.9**	**93.8**
		C14-H	70.9	
		C15-H	72.4	
		C16-H	76.1	
		C17-H	87.6	
		C18-H	78.8	
		C19-H	78.0	
		C20-H	77.4	
	Abieta-7,13-diene	C2-H	89.5	
		C4-H	89.1	
		C5-H	**58.5**	**75.5**
		C6-H	67.0	
		C8-H	72.2	
		C9-H	71.3	
		C10-H	72.2	
		C12-H	**59.8**	82.5
		C13-H	71.4	
		C14-H	**60.5**	80.2
		C15-H	**56.3**	**78.2**
		C16-H	78.1	
		C17-H	78.0	
		C18-H	78.8	
		C19-H	78.4	
		C20-H	77.7	

TableS2: Cartesian coordinates and molecular enthalpies of all parent molecules and resulted radicals, anions optimized at B3LYP/6-311G(d,P) level of theory in the gas phase, water and ethanol.

Name of compound	α-pinene
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)	
C	-2.19601 -1.68886 0.
C	-0.6809 -1.68886 0.
C	-0.12897 -0.27778 0.
C	-0.67863 0.52676 1.16066
C	-2.56295 0.72126 0.79131
C	-2.74656 -0.8832 1.15888
H	-0.30561 -2.23871 -0.90191
H	-2.56869 -1.25583 -0.96539
H	-2.5716 -2.74308 0.0635
H	-0.30261 1.5809 1.09867
H	-3.70296 -1.34557 1.51678
C	1.40791 -0.32448 0.08616
H	1.79516 -0.87563 -0.7452
H	1.79674 0.67216 0.06561
H	1.69966 -0.80242 0.99795
C	-1.57458 -0.68818 2.14107
H	-2.16773 -0.61933 3.02895
H	-0.91861 -1.53031 2.21477
C	-3.03795 1.52253 2.01766
H	-3.39474 2.48045 1.70147
H	-3.82768 0.99141 2.50669
H	-2.22147 1.65245 2.69691
C	-3.68881 0.77112 -0.25823
H	-4.48061 0.11459 0.03661
H	-4.06327 1.77071 -0.3324
H	-3.30482 0.4627 -1.20814
Frequency and Energyat B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.234715 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.244554
Thermal correction to Enthalpy=	0.245499
Thermal correction to Gibbs Free Frequency and Energy=	0.201035
Sum of electronic and zero-point Energies=	-390.525435
Sum of electronic and thermal Energies=	-390.515595
Sum of electronic and thermal Enthalpies=	-390.514651
Sum of electronic and thermal Free Energies=	-390.559115
Frequency and Energyat B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.234313 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.244166
Thermal correction to Enthalpy=	0.245110
Thermal correction to Gibbs Free Frequency and Energy=	0.200623
Sum of electronic and zero-point Energies=	-390.526698
Sum of electronic and thermal Energies=	-390.516845
Sum of electronic and thermal Enthalpies=	-390.515900

Sum of electronic and thermal Free Energies= -390.560387
Frequency and Energyat B3LYP/6-311G (d,p) (ethanol)
Zero-point correction= 0.234333 (Hartree/Particle) Thermal correction to Frequency and Energy= 0.244186 Thermal correction to Enthalpy= 0.245130 Thermal correction to Gibbs Free Frequency and Energy= 0.200644 Sum of electronic and zero-point Energies= -390.526631 Sum of electronic and thermal Energies= -390.516778 Sum of electronic and thermal Enthalpies= -390.515834 Sum of electronic and thermal Free Energies= -390.560320

Name of radical	α-pinene-C1-H8
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)	
C -2.19601 -1.68886 0. C -0.6809 -1.68886 0. C -0.12897 -0.27778 0. C -0.67863 0.52676 1.16066 C -2.56295 0.72126 0.79131 C -2.74656 -0.8832 1.15888 H -0.30561 -2.23871 -0.90191 H -2.5716 -2.74308 0.0635 H -0.30261 1.5809 1.09867 H -3.70296 -1.34557 1.51678 C 1.40791 -0.32448 0.08616 H 1.79516 -0.87563 -0.7452 H 1.79674 0.67216 0.06561 H 1.69966 -0.80242 0.99795 C -1.57458 -0.68818 2.14107 H -2.16773 -0.61933 3.02895 H -0.91861 -1.53031 2.21477 C -3.03795 1.52253 2.01766 H -3.39474 2.48045 1.70147 H -3.82768 0.99141 2.50669 H -2.22147 1.65245 2.69691 C -3.68881 0.77112 -0.25823 H -4.48061 0.11459 0.03661 H -4.06327 1.77071 -0.3324 H -3.30482 0.4627 -1.20814	
Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction= 0.221138 (Hartree/Particle) Thermal correction to Frequency and Energy= 0.231075 Thermal correction to Enthalpy= 0.232019 Thermal correction to Gibbs Free Frequency and Energy= 0.186607 Sum of electronic and zero-point Energies= -389.897212 Sum of electronic and thermal Energies= -389.887275 Sum of electronic and thermal Enthalpies= -389.886331 Sum of electronic and thermal Free Energies= -389.931743	
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction= 0.220730 (Hartree/Particle) Thermal correction to Frequency and Energy= 0.230680 Thermal correction to Enthalpy= 0.231624	

Thermal correction to Gibbs Free Frequency and Energy=	0.186192
Sum of electronic and zero-point Energies=	-389.898932
Sum of electronic and thermal Energies=	-389.888982
Sum of electronic and thermal Enthalpies=	-389.888038
Sum of electronic and thermal Free Energies=	-389.933470

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.220752 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.230701
Thermal correction to Enthalpy=	0.231645
Thermal correction to Gibbs Free Frequency and Energy=	0.186216
Sum of electronic and zero-point Energies=	-389.898839
Sum of electronic and thermal Energies=	-389.888890
Sum of electronic and thermal Enthalpies=	-389.887946
Sum of electronic and thermal Free Energies=	-389.933374

Name of anion	α-pinene-C1-H8-anion

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	-2.19601	-1.68886	0.
C	-0.6809	-1.68886	0.
C	-0.12897	-0.27778	0.
C	-0.67863	0.52676	1.16066
C	-2.56295	0.72126	0.79131
C	-2.74656	-0.8832	1.15888
H	-0.30561	-2.23871	-0.90191
H	-2.5716	-2.74308	0.0635
H	-0.30261	1.5809	1.09867
H	-3.70296	-1.34557	1.51678
C	1.40791	-0.32448	0.08616
H	1.79516	-0.87563	-0.7452
H	1.79674	0.67216	0.06561
H	1.69966	-0.80242	0.99795
C	-1.57458	-0.68818	2.14107
H	-2.16773	-0.61933	3.02895
H	-0.91861	-1.53031	2.21477
C	-3.03795	1.52253	2.01766
H	-3.39474	2.48045	1.70147
H	-3.82768	0.99141	2.50669
H	-2.22147	1.65245	2.69691
C	-3.68881	0.77112	-0.25823
H	-4.48061	0.11459	0.03661
H	-4.06327	1.77071	-0.3324
H	-3.30482	0.4627	-1.20814

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction=	0.216287 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.226786
Thermal correction to Enthalpy=	0.227730
Thermal correction to Gibbs Free Frequency and Energy=	0.181439
Sum of electronic and zero-point Energies=	-389.899734
Sum of electronic and thermal Energies=	-389.889236

Sum of electronic and thermal Enthalpies= -389.888291
Sum of electronic and thermal Free Energies= -389.934582
Frequency and Energy at B3LYP/6-311G (d,p) (water)
Zero-point correction= 0.216967 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.227257
Thermal correction to Enthalpy= 0.228201
Thermal correction to Gibbs Free Frequency and Energy= 0.182658
Sum of electronic and zero-point Energies= -389.974740
Sum of electronic and thermal Energies= -389.964450
Sum of electronic and thermal Enthalpies= -389.963506
Sum of electronic and thermal Free Energies= -390.009049
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)
Zero-point correction= 0.216726 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.227106
Thermal correction to Enthalpy= 0.228050
Thermal correction to Gibbs Free Frequency and Energy= 0.182212
Sum of electronic and zero-point Energies= -389.972878
Sum of electronic and thermal Energies= -389.962498
Sum of electronic and thermal Enthalpies= -389.961554
Sum of electronic and thermal Free Energies= -390.007392

Name of cationic radical	α-pinene
Cartesian Coordinates optimized at PM6	
C -2.19601 -1.68886 0.	
C -0.6809 -1.68886 0.	
C -0.12897 -0.27778 0.	
C -0.67863 0.52676 1.16066	
C -2.56295 0.72126 0.79131	
C -2.74656 -0.8832 1.15888	
H -0.30561 -2.23871 -0.90191	
H -2.56869 -1.25583 -0.96539	
H -2.5716 -2.74308 0.0635	
H -0.30261 1.5809 1.09867	
H -3.70296 -1.34557 1.51678	
C 1.40791 -0.32448 0.08616	
H 1.79516 -0.87563 -0.7452	
H 1.79674 0.67216 0.06561	
H 1.69966 -0.80242 0.99795	
C -1.57458 -0.68818 2.14107	
H -2.16773 -0.61933 3.02895	
H -0.91861 -1.53031 2.21477	
C -3.03795 1.52253 2.01766	
H -3.39474 2.48045 1.70147	
H -3.82768 0.99141 2.50669	
H -2.22147 1.65245 2.69691	
C -3.68881 0.77112 -0.25823	
H -4.48061 0.11459 0.03661	
H -4.06327 1.77071 -0.3324	

H	-3.30482	0.4627	-1.20814

Frequency and Energy at PM6(gas)

Zero-point correction=	0.212893 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.223676
Thermal correction to Enthalpy=	0.224620
Thermal correction to Gibbs Free Frequency and Energy=	0.176653
Sum of electronic and zero-point Energies=	0.509821
Sum of electronic and thermal Energies=	0.520604
Sum of electronic and thermal Enthalpies=	0.521548
Sum of electronic and thermal Free Energies=	0.473581

Name of compound	β-pinene

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	5.132	3.4296	2.5813
C	3.8427	2.7059	2.2307
C	4.1899	1.386	1.5814
C	2.8123	3.6508	1.5125
C	2.8163	2.709	3.4227
C	2.2978	4.0834	2.9121
C	1.0133	1.8875	1.8346
H	5.7532	3.5759	1.6878
H	5.7207	2.8549	3.3086
H	4.9492	4.4205	3.0189
H	3.3161	0.7349	1.4414
H	4.6419	1.5479	0.5938
H	4.9116	0.8268	2.1922
H	3.2373	4.4313	0.8579
H	3.2346	2.6583	4.4431
H	2.8216	4.9508	3.3423
H	1.2186	4.2714	3.0047
H	0.	2.2742	2.0646
H	0.8524	0.8995	1.36
C	1.7398	1.7058	3.1409
C	1.4306	0.7298	3.9926
C	1.715	2.8339	0.8434
H	0.6521	0.	3.791
H	1.9365	0.6001	4.9446
H	2.1459	2.2597	0.
H	0.9709	3.5171	0.3911

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction=	0.235401 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.245034
Thermal correction to Enthalpy=	0.245978
Thermal correction to Gibbs Free Frequency and Energy=	0.201808
Sum of electronic and zero-point Energies=	-390.520403
Sum of electronic and thermal Energies=	-390.510770
Sum of electronic and thermal Enthalpies=	-390.509826
Sum of electronic and thermal Free Energies=	-390.553996

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.235004 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.244650
Thermal correction to Enthalpy=	0.245594
Thermal correction to Gibbs Free Frequency and Energy=	0.201397
Sum of electronic and zero-point Energies=	-390.521964
Sum of electronic and thermal Energies=	-390.512318
Sum of electronic and thermal Enthalpies=	-390.511374
Sum of electronic and thermal Free Energies=	-390.555571

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.234961 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.244607
Thermal correction to Enthalpy=	0.245551
Thermal correction to Gibbs Free Frequency and Energy=	0.201362
Sum of electronic and zero-point Energies=	-390.522314
Sum of electronic and thermal Energies=	-390.512668
Sum of electronic and thermal Enthalpies=	-390.511724
Sum of electronic and thermal Free Energies=	-390.555912

Name of radical	β-pinene-C7-H18

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	5.132	3.4296	2.5813
C	3.8427	2.7059	2.2307
C	4.1899	1.386	1.5814
C	2.8123	3.6508	1.5125
C	2.8163	2.709	3.4227
C	2.2978	4.0834	2.9121
C	1.0133	1.8875	1.8346
H	5.7532	3.5759	1.6878
H	5.7207	2.8549	3.3086
H	4.9492	4.4205	3.0189
H	3.3161	0.7349	1.4414
H	4.6419	1.5479	0.5938
H	4.9116	0.8268	2.1922
H	3.2373	4.4313	0.8579
H	3.2346	2.6583	4.4431
H	2.8216	4.9508	3.3423
H	1.2186	4.2714	3.0047
H	0.8524	0.8995	1.36
C	1.7398	1.7058	3.1409
C	1.4306	0.7298	3.9926
C	1.715	2.8339	0.8434
H	0.6521	0.	3.791
H	1.9365	0.6001	4.9446
H	2.1459	2.2597	0.
H	0.9709	3.5171	0.3911

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction=	0.221298 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.230840

Thermal correction to Enthalpy= 0.231784 Thermal correction to Gibbs Free Frequency and Energy= 0.187374 Sum of electronic and zero-point Energies= -389.894299 Sum of electronic and thermal Energies= -389.884757 Sum of electronic and thermal Enthalpies= -389.883813 Sum of electronic and thermal Free Energies= -389.928223
Frequency and Energy at B3LYP/6-311G (d,p) (water)
Zero-point correction= 0.220904 (Hartree/Particle) Thermal correction to Frequency and Energy= 0.230454 Thermal correction to Enthalpy= 0.231399 Thermal correction to Gibbs Free Frequency and Energy= 0.186978 Sum of electronic and zero-point Energies= -389.896130 Sum of electronic and thermal Energies= -389.886579 Sum of electronic and thermal Enthalpies= -389.885635 Sum of electronic and thermal Free Energies= -389.930055
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)
Zero-point correction= 0.234961 (Hartree/Particle) Thermal correction to Frequency and Energy= 0.244607 Thermal correction to Enthalpy= 0.245551 Thermal correction to Gibbs Free Frequency and Energy= 0.201362 Sum of electronic and zero-point Energies= -390.522314 Sum of electronic and thermal Energies= -390.512668 Sum of electronic and thermal Enthalpies= -390.511724 Sum of electronic and thermal Free Energies= -390.555912

Name of anion	β-pinene-C7-H18-anion

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	5.132	3.4296	2.5813
C	3.8427	2.7059	2.2307
C	4.1899	1.386	1.5814
C	2.8123	3.6508	1.5125
C	2.8163	2.709	3.4227
C	2.2978	4.0834	2.9121
C	1.0133	1.8875	1.8346
H	5.7532	3.5759	1.6878
H	5.7207	2.8549	3.3086
H	4.9492	4.4205	3.0189
H	3.3161	0.7349	1.4414
H	4.6419	1.5479	0.5938
H	4.9116	0.8268	2.1922
H	3.2373	4.4313	0.8579
H	3.2346	2.6583	4.4431
H	2.8216	4.9508	3.3423
H	1.2186	4.2714	3.0047
H	0.8524	0.8995	1.36
C	1.7398	1.7058	3.1409
C	1.4306	0.7298	3.9926
C	1.715	2.8339	0.8434

H	0.6521	0.	3.791
H	1.9365	0.6001	4.9446
H	2.1459	2.2597	0.
H	0.9709	3.5171	0.3911

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction= 0.217352 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.227350
Thermal correction to Enthalpy= 0.228294
Thermal correction to Gibbs Free Frequency and Energy= 0.183623
Sum of electronic and zero-point Energies= -389.903548
Sum of electronic and thermal Energies= -389.893551
Sum of electronic and thermal Enthalpies= -389.892606
Sum of electronic and thermal Free Energies= -389.937277

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction= 0.217589 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.227641
Thermal correction to Enthalpy= 0.228585
Thermal correction to Gibbs Free Frequency and Energy= 0.183870
Sum of electronic and zero-point Energies= -389.984877
Sum of electronic and thermal Energies= -389.974825
Sum of electronic and thermal Enthalpies= -389.973881
Sum of electronic and thermal Free Energies= -390.018597

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction= 0.217614 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.227656
Thermal correction to Enthalpy= 0.228600
Thermal correction to Gibbs Free Frequency and Energy= 0.183898
Sum of electronic and zero-point Energies= -389.982169
Sum of electronic and thermal Energies= -389.972127
Sum of electronic and thermal Enthalpies= -389.971183
Sum of electronic and thermal Free Energies= -390.015885

Name of cationic radical	β-pinene		
Cartesian Coordinates optimized at PM6			
C	5.132	3.4296	2.5813
C	3.8427	2.7059	2.2307
C	4.1899	1.386	1.5814
C	2.8123	3.6508	1.5125
C	2.8163	2.709	3.4227
C	2.2978	4.0834	2.9121
C	1.0133	1.8875	1.8346
H	5.7532	3.5759	1.6878
H	5.7207	2.8549	3.3086
H	4.9492	4.4205	3.0189
H	3.3161	0.7349	1.4414
H	4.6419	1.5479	0.5938
H	4.9116	0.8268	2.1922
H	3.2373	4.4313	0.8579

H	3.2346	2.6583	4.4431
H	2.8216	4.9508	3.3423
H	1.2186	4.2714	3.0047
H	0.	2.2742	2.0646
H	0.8524	0.8995	1.36
C	1.7398	1.7058	3.1409
C	1.4306	0.7298	3.9926
C	1.715	2.8339	0.8434
H	0.6521	0.	3.791
H	1.9365	0.6001	4.9446
H	2.1459	2.2597	0.
H	0.9709	3.5171	0.3911

Frequency and Energy at PM6 (gas)

Zero-point correction= 0.212648 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.223322
Thermal correction to Enthalpy= 0.224266
Thermal correction to Gibbs Free Frequency and Energy= 0.177189
Sum of electronic and zero-point Energies= 0.528801
Sum of electronic and thermal Energies= 0.539475
Sum of electronic and thermal Enthalpies= 0.540419
Sum of electronic and thermal Free Energies= 0.493342

Name of compound	camphene

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	2.5105	2.1577	1.9983
C	1.9196	3.1794	1.0423
C	2.0927	0.7523	1.5762
C	4.072	2.2354	2.1016
C	2.1133	2.4032	3.4508
C	4.3022	1.5132	3.4494
C	4.4886	3.6774	2.456
C	0.8846	2.5158	3.9358
C	3.3959	2.4771	4.2515
C	4.0395	3.8415	3.9226
H	0.8264	3.2218	1.1333
H	2.1609	2.9328	0.
H	2.3149	4.1886	1.2418
H	2.5683	0.	2.227
H	2.3927	0.5388	0.5424
H	1.0055	0.6233	1.6471
H	4.5925	1.8141	1.223
H	3.9387	0.4674	3.4395
H	5.3509	1.5029	3.7839
H	4.0008	4.416	1.7884
H	5.5769	3.8164	2.3392
H	0.6867	2.6771	4.9909
H	0.	2.4517	3.308
H	3.2836	2.2665	5.3301
H	3.328	4.6747	4.0541
H	4.8913	4.0496	4.5934

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.236246 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.245598
Thermal correction to Enthalpy=	0.246542
Thermal correction to Gibbs Free Frequency and Energy=	0.202956
Sum of electronic and zero-point Energies=	-390.541262
Sum of electronic and thermal Energies=	-390.531910
Sum of electronic and thermal Enthalpies=	-390.530965
Sum of electronic and thermal Free Energies=	-390.574551
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.235856 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.245214
Thermal correction to Enthalpy=	0.246158
Thermal correction to Gibbs Free Frequency and Energy=	0.202570
Sum of electronic and zero-point Energies=	-390.542760
Sum of electronic and thermal Energies=	-390.533403
Sum of electronic and thermal Enthalpies=	-390.532459
Sum of electronic and thermal Free Energies=	-390.576047
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.235845 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.245194
Thermal correction to Enthalpy=	0.246138
Thermal correction to Gibbs Free Frequency and Energy=	0.202574
Sum of electronic and zero-point Energies=	-390.543063
Sum of electronic and thermal Energies=	-390.533714
Sum of electronic and thermal Enthalpies=	-390.532770
Sum of electronic and thermal Free Energies=	-390.576334

Name of radical	Camphene-C7-H20		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	2.5105	2.1577	1.9983
C	1.9196	3.1794	1.0423
C	2.0927	0.7523	1.5762
C	4.072	2.2354	2.1016
C	2.1133	2.4032	3.4508
C	4.3022	1.5132	3.4494
C	4.4886	3.6774	2.456
C	0.8846	2.5158	3.9358
C	3.3959	2.4771	4.2515
C	4.0395	3.8415	3.9226
H	0.8264	3.2218	1.1333
H	2.1609	2.9328	0.
H	2.3149	4.1886	1.2418
H	2.5683	0.	2.227
H	2.3927	0.5388	0.5424
H	1.0055	0.6233	1.6471
H	4.5925	1.8141	1.223
H	3.9387	0.4674	3.4395
H	5.3509	1.5029	3.7839

H	5.5769	3.8164	2.3392
H	0.6867	2.6771	4.9909
H	0.	2.4517	3.308
H	3.2836	2.2665	5.3301
H	3.328	4.6747	4.0541
H	4.8913	4.0496	4.5934

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction=	0.221145 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.230825
Thermal correction to Enthalpy=	0.231769
Thermal correction to Gibbs Free Frequency and Energy=	0.187037
Sum of electronic and zero-point Energies=	-389.890825
Sum of electronic and thermal Energies=	-389.881146
Sum of electronic and thermal Enthalpies=	-389.880202
Sum of electronic and thermal Free Energies=	-389.924934

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.220746 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.230428
Thermal correction to Enthalpy=	0.231373
Thermal correction to Gibbs Free Frequency and Energy=	0.186641
Sum of electronic and zero-point Energies=	-389.892556
Sum of electronic and thermal Energies=	-389.882874
Sum of electronic and thermal Enthalpies=	-389.881929
Sum of electronic and thermal Free Energies=	-389.926661

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.220781 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.230458
Thermal correction to Enthalpy=	0.231402
Thermal correction to Gibbs Free Frequency and Energy=	0.186684
Sum of electronic and zero-point Energies=	-389.892688
Sum of electronic and thermal Energies=	-389.883011
Sum of electronic and thermal Enthalpies=	-389.882067
Sum of electronic and thermal Free Energies=	-389.926786

Name of anion	Camphene-C7-H20-anion

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	2.5105	2.1577	1.9983
C	1.9196	3.1794	1.0423
C	2.0927	0.7523	1.5762
C	4.072	2.2354	2.1016
C	2.1133	2.4032	3.4508
C	4.3022	1.5132	3.4494
C	4.4886	3.6774	2.456
C	0.8846	2.5158	3.9358
C	3.3959	2.4771	4.2515
C	4.0395	3.8415	3.9226
H	0.8264	3.2218	1.1333
H	2.1609	2.9328	0.

H	2.3149	4.1886	1.2418
H	2.5683	0.	2.227
H	2.3927	0.5388	0.5424
H	1.0055	0.6233	1.6471
H	4.5925	1.8141	1.223
H	3.9387	0.4674	3.4395
H	5.3509	1.5029	3.7839
H	5.5769	3.8164	2.3392
H	0.6867	2.6771	4.9909
H	0.	2.4517	3.308
H	3.2836	2.2665	5.3301
H	3.328	4.6747	4.0541
H	4.8913	4.0496	4.5934

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction= 0.217786 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.227321
Thermal correction to Enthalpy= 0.228265
Thermal correction to Gibbs Free Frequency and Energy= 0.184415
Sum of electronic and zero-point Energies= -389.882949
Sum of electronic and thermal Energies= -389.873414
Sum of electronic and thermal Enthalpies= -389.872470
Sum of electronic and thermal Free Energies= -389.916320

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction= 0.218727 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.228254
Thermal correction to Enthalpy= 0.229198
Thermal correction to Gibbs Free Frequency and Energy= 0.185239
Sum of electronic and zero-point Energies= -389.965990
Sum of electronic and thermal Energies= -389.956463
Sum of electronic and thermal Enthalpies= -389.955518
Sum of electronic and thermal Free Energies= -389.999477

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction= 0.218662 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.228202
Thermal correction to Enthalpy= 0.229146
Thermal correction to Gibbs Free Frequency and Energy= 0.185164
Sum of electronic and zero-point Energies= -389.963197
Sum of electronic and thermal Energies= -389.953657
Sum of electronic and thermal Enthalpies= -389.952712
Sum of electronic and thermal Free Energies= -389.996695

Name of cationic radical	Camphene

Cartesian Coordinates optimized at PM6

C	2.5105	2.1577	1.9983
C	1.9196	3.1794	1.0423
C	2.0927	0.7523	1.5762
C	4.072	2.2354	2.1016
C	2.1133	2.4032	3.4508

C	4.3022	1.5132	3.4494
C	4.4886	3.6774	2.456
C	0.8846	2.5158	3.9358
C	3.3959	2.4771	4.2515
C	4.0395	3.8415	3.9226
H	0.8264	3.2218	1.1333
H	2.1609	2.9328	0.
H	2.3149	4.1886	1.2418
H	2.5683	0.	2.227
H	2.3927	0.5388	0.5424
H	1.0055	0.6233	1.6471
H	4.5925	1.8141	1.223
H	3.9387	0.4674	3.4395
H	5.3509	1.5029	3.7839
H	4.0008	4.416	1.7884
H	5.5769	3.8164	2.3392
H	0.6867	2.6771	4.9909
H	0.	2.4517	3.308
H	3.2836	2.2665	5.3301
H	3.328	4.6747	4.0541
H	4.8913	4.0496	4.5934

Frequency and Energy at PM6(gas)

Zero-point correction=	0.213315 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.223621
Thermal correction to Enthalpy=	0.224565
Thermal correction to Gibbs Free Frequency and Energy=	0.178293
Sum of electronic and zero-point Energies=	0.525098
Sum of electronic and thermal Energies=	0.535404
Sum of electronic and thermal Enthalpies=	0.536348
Sum of electronic and thermal Free Energies=	0.490076

Name of compound	Myrcene

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	3.3912	3.3839	2.0665
C	3.0714	1.9218	2.1154
C	1.8663	1.44	1.4368
C	3.8657	1.0668	2.7678
C	4.4476	3.6741	1.0075
C	0.8936	2.2401	1.0077
C	4.7589	5.1264	0.9485
C	5.9959	5.6402	0.9625
C	6.2199	7.1089	0.8799
C	7.2296	4.817	1.0546
H	2.4656	3.9663	1.8534
H	3.7435	3.7282	3.0584
H	1.7939	0.3523	1.3074
H	3.6686	0.	2.8227
H	4.7636	1.3874	3.2886
H	4.0913	3.3469	0.0102
H	5.3662	3.078	1.2119
H	0.	1.8729	0.5142

H	0.9418	3.3238	1.1284
H	3.8893	5.7939	0.882
H	6.8285	7.3579	0.
H	5.2834	7.6777	0.8072
H	6.7585	7.4691	1.7672
H	7.8229	4.9046	0.1347
H	7.8594	5.1478	1.891
H	7.0024	3.7489	1.2066

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction= 0.230851 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.243098
Thermal correction to Enthalpy= 0.244042
Thermal correction to Gibbs Free Frequency and Energy= 0.191651
Sum of electronic and zero-point Energies= -390.525103
Sum of electronic and thermal Energies= -390.512856
Sum of electronic and thermal Enthalpies= -390.511912
Sum of electronic and thermal Free Energies= -390.564303

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction= 0.230492 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.242733
Thermal correction to Enthalpy= 0.243677
Thermal correction to Gibbs Free Frequency and Energy= 0.191390
Sum of electronic and zero-point Energies= -390.527806
Sum of electronic and thermal Energies= -390.515566
Sum of electronic and thermal Enthalpies= -390.514621
Sum of electronic and thermal Free Energies= -390.566908

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction= 0.230523 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.242768
Thermal correction to Enthalpy= 0.243712
Thermal correction to Gibbs Free Frequency and Energy= 0.191348
Sum of electronic and zero-point Energies= -390.528225
Sum of electronic and thermal Energies= -390.515981
Sum of electronic and thermal Enthalpies= -390.515036
Sum of electronic and thermal Free Energies= -390.567401

Name of radical	Myrcene-C5-H16

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	3.3912	3.3839	2.0665
C	3.0714	1.9218	2.1154
C	1.8663	1.44	1.4368
C	3.8657	1.0668	2.7678
C	4.4476	3.6741	1.0075
C	0.8936	2.2401	1.0077
C	4.7589	5.1264	0.9485
C	5.9959	5.6402	0.9625
C	6.2199	7.1089	0.8799

C	7.2296	4.817	1.0546
H	2.4656	3.9663	1.8534
H	3.7435	3.7282	3.0584
H	1.7939	0.3523	1.3074
H	3.6686	0.	2.8227
H	4.7636	1.3874	3.2886
H	5.3662	3.078	1.2119
H	0.	1.8729	0.5142
H	0.9418	3.3238	1.1284
H	3.8893	5.7939	0.882
H	6.8285	7.3579	0.
H	5.2834	7.6777	0.8072
H	6.7585	7.4691	1.7672
H	7.8229	4.9046	0.1347
H	7.8594	5.1478	1.891
H	7.0024	3.7489	1.2066

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction= 0.216480 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.229092
Thermal correction to Enthalpy= 0.230036
Thermal correction to Gibbs Free Frequency and Energy= 0.174726
Sum of electronic and zero-point Energies= -389.899229
Sum of electronic and thermal Energies= -389.886617
Sum of electronic and thermal Enthalpies= -389.885673
Sum of electronic and thermal Free Energies= -389.940983

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction= 0.216430 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.228857
Thermal correction to Enthalpy= 0.229801
Thermal correction to Gibbs Free Frequency and Energy= 0.176320
Sum of electronic and zero-point Energies= -389.902093
Sum of electronic and thermal Energies= -389.889666
Sum of electronic and thermal Enthalpies= -389.888722
Sum of electronic and thermal Free Energies= -389.942203

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction= 0.216467 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.228914
Thermal correction to Enthalpy= 0.229858
Thermal correction to Gibbs Free Frequency and Energy= 0.176278
Sum of electronic and zero-point Energies= -389.902438
Sum of electronic and thermal Energies= -389.889991
Sum of electronic and thermal Enthalpies= -389.889046
Sum of electronic and thermal Free Energies= -389.942627

Name of anion	Myrcene-C5-H16-anion

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	3.3912	3.3839	2.0665

C	3.0714	1.9218	2.1154
C	1.8663	1.44	1.4368
C	3.8657	1.0668	2.7678
C	4.4476	3.6741	1.0075
C	0.8936	2.2401	1.0077
C	4.7589	5.1264	0.9485
C	5.9959	5.6402	0.9625
C	6.2199	7.1089	0.8799
C	7.2296	4.817	1.0546
H	2.4656	3.9663	1.8534
H	3.7435	3.7282	3.0584
H	1.7939	0.3523	1.3074
H	3.6686	0.	2.8227
H	4.7636	1.3874	3.2886
H	5.3662	3.078	1.2119
H	0.	1.8729	0.5142
H	0.9418	3.3238	1.1284
H	3.8893	5.7939	0.882
H	6.8285	7.3579	0.
H	5.2834	7.6777	0.8072
H	6.7585	7.4691	1.7672
H	7.8229	4.9046	0.1347
H	7.8594	5.1478	1.891
H	7.0024	3.7489	1.2066

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction= 0.212339 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.224965
Thermal correction to Enthalpy= 0.225910
Thermal correction to Gibbs Free Frequency and Energy= 0.172851
Sum of electronic and zero-point Energies= -389.909636
Sum of electronic and thermal Energies= -389.897009
Sum of electronic and thermal Enthalpies= -389.896065
Sum of electronic and thermal Free Energies= -389.949124

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction= 0.213097 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.225524
Thermal correction to Enthalpy= 0.226469
Thermal correction to Gibbs Free Frequency and Energy= 0.174527
Sum of electronic and zero-point Energies= -389.985633
Sum of electronic and thermal Energies= -389.973206
Sum of electronic and thermal Enthalpies= -389.972262
Sum of electronic and thermal Free Energies= -390.024203

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction= 0.212979 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.225516
Thermal correction to Enthalpy= 0.226460
Thermal correction to Gibbs Free Frequency and Energy= 0.173835
Sum of electronic and zero-point Energies= -389.982586
Sum of electronic and thermal Energies= -389.970049
Sum of electronic and thermal Enthalpies= -389.969105

Sum of electronic and thermal Free Energies= -390.021729

Name of cationic radical	Myrcene

Cartesian Coordinates optimized at PM6			
C	3.3912	3.3839	2.0665
C	3.0714	1.9218	2.1154
C	1.8663	1.44	1.4368
C	3.8657	1.0668	2.7678
C	4.4476	3.6741	1.0075
C	0.8936	2.2401	1.0077
C	4.7589	5.1264	0.9485
C	5.9959	5.6402	0.9625
C	6.2199	7.1089	0.8799
C	7.2296	4.817	1.0546
H	2.4656	3.9663	1.8534
H	3.7435	3.7282	3.0584
H	1.7939	0.3523	1.3074
H	3.6686	0.	2.8227
H	4.7636	1.3874	3.2886
H	4.0913	3.3469	0.0102
H	5.3662	3.078	1.2119
H	0.	1.8729	0.5142
H	0.9418	3.3238	1.1284
H	3.8893	5.7939	0.882
H	6.8285	7.3579	0.
H	5.2834	7.6777	0.8072
H	6.7585	7.4691	1.7672
H	7.8229	4.9046	0.1347
H	7.8594	5.1478	1.891
H	7.0024	3.7489	1.2066

Frequency and Energy at PM6 (gas)	
Zero-point correction=	0.207800 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.221529
Thermal correction to Enthalpy=	0.222473
Thermal correction to Gibbs Free Frequency and Energy=	0.162931
Sum of electronic and zero-point Energies=	0.533163
Sum of electronic and thermal Energies=	0.546893
Sum of electronic and thermal Enthalpies=	0.547837
Sum of electronic and thermal Free Energies=	0.488294

Name of compound	α-terpinene

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	1.2582	4.8731	4.0424
C	1.1173	3.3688	3.8659
C	0.9086	2.6893	5.2131
C	2.3187	2.7708	3.1871
C	2.0916	1.563	2.3388
C	3.559	3.2529	3.3789
C	3.1824	1.3398	1.3001
C	4.7071	2.6416	2.7429

C	4.5461	1.7254	1.7724
C	5.6929	1.08	1.0882
H	1.2177	5.3945	3.0778
H	0.4596	5.2791	4.6756
H	2.2245	5.1273	4.5092
H	0.2188	3.1754	3.2283
H	0.8097	1.6019	5.0981
H	1.7521	2.874	5.8914
H	0.	3.0563	5.7076
H	2.0172	0.6892	3.0195
H	1.1091	1.6289	1.8296
H	3.7176	4.1295	4.0246
H	3.1778	0.2783	0.9815
H	2.9689	1.9282	0.3841
H	5.7016	2.9552	3.0782
H	6.6588	1.4901	1.4115
H	5.7055	0.	1.2911
H	5.6218	1.2109	0.

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.233778 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.244659
Thermal correction to Enthalpy=	0.245603
Thermal correction to Gibbs Free Frequency and Energy=	0.197995
Sum of electronic and zero-point Energies=	-390.554110
Sum of electronic and thermal Energies=	-390.543229
Sum of electronic and thermal Enthalpies=	-390.542285
Sum of electronic and thermal Free Energies=	-390.589893

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.233407 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.244298
Thermal correction to Enthalpy=	0.245242
Thermal correction to Gibbs Free Frequency and Energy=	0.197629
Sum of electronic and zero-point Energies=	-390.556269
Sum of electronic and thermal Energies=	-390.545378
Sum of electronic and thermal Enthalpies=	-390.544434
Sum of electronic and thermal Free Energies=	-390.592047

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.233357 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.244252
Thermal correction to Enthalpy=	0.245196
Thermal correction to Gibbs Free Frequency and Energy=	0.197556
Sum of electronic and zero-point Energies=	-390.556533
Sum of electronic and thermal Energies=	-390.545638
Sum of electronic and thermal Enthalpies=	-390.544694
Sum of electronic and thermal Free Energies=	-390.592334

Name of radical	α-terpinene-C5-H18

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-2.90114	1.17792	-0.49512
C	-2.16516	-0.15394	-0.31125
C	-2.80948	-0.96862	0.83215

C	-0.66855	-0.02259	-0.10691
C	0.15123	-1.30181	-0.10623
C	-0.0235	1.13148	0.1413
C	1.59274	-1.07967	-0.58349
C	1.42422	1.17779	0.36277
C	2.22417	0.147	0.0424
C	3.71787	0.17743	0.18223
H	-2.47941	1.76054	-1.31817
H	-3.95663	0.99711	-0.71575
H	-2.85478	1.79006	0.41088
H	-2.30382	-0.73779	-1.23345
H	-2.34081	-1.94811	0.95157
H	-2.71724	-0.43219	1.78181
H	-3.87324	-1.1304	0.63549
H	-0.33077	-2.06633	-0.72379
H	-0.56596	2.06921	0.19925
H	2.19366	-1.97038	-0.37424
H	1.60975	-0.95395	-1.67805
H	1.85079	2.09468	0.76231
H	4.0681	1.13378	0.57696
H	4.07158	-0.61941	0.84738
H	4.20481	0.00845	-0.78687

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.219777 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.230755
Thermal correction to Enthalpy=	0.231700
Thermal correction to Gibbs Free Frequency and Energy=	0.182960
Sum of electronic and zero-point Energies=	-389.940226
Sum of electronic and thermal Energies=	-389.929248
Sum of electronic and thermal Enthalpies=	-389.928304
Sum of electronic and thermal Free Energies=	-389.977043

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.219458 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.230431
Thermal correction to Enthalpy=	0.231375
Thermal correction to Gibbs Free Frequency and Energy=	0.182672
Sum of electronic and zero-point Energies=	-389.943050
Sum of electronic and thermal Energies=	-389.932077
Sum of electronic and thermal Enthalpies=	-389.931133
Sum of electronic and thermal Free Energies=	-389.979836

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.219466 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.230443
Thermal correction to Enthalpy=	0.231388
Thermal correction to Gibbs Free Frequency and Energy=	0.182668
Sum of electronic and zero-point Energies=	-389.942897
Sum of electronic and thermal Energies=	-389.931921
Sum of electronic and thermal Enthalpies=	-389.930976
Sum of electronic and thermal Free Energies=	-389.979696

Name of anion	α-terpinene-C5-H18-anion

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-2.90114	1.17792	-0.49512
C	-2.16516	-0.15394	-0.31125
C	-2.80948	-0.96862	0.83215
C	-0.66855	-0.02259	-0.10691
C	0.15123	-1.30181	-0.10623
C	-0.0235	1.13148	0.1413
C	1.59274	-1.07967	-0.58349
C	1.42422	1.17779	0.36277
C	2.22417	0.147	0.0424
C	3.71787	0.17743	0.18223
H	-2.47941	1.76054	-1.31817
H	-3.95663	0.99711	-0.71575
H	-2.85478	1.79006	0.41088
H	-2.30382	-0.73779	-1.23345
H	-2.34081	-1.94811	0.95157
H	-2.71724	-0.43219	1.78181
H	-3.87324	-1.1304	0.63549
H	-0.33077	-2.06633	-0.72379
H	-0.56596	2.06921	0.19925
H	2.19366	-1.97038	-0.37424
H	1.60975	-0.95395	-1.67805
H	1.85079	2.09468	0.76231
H	4.0681	1.13378	0.57696
H	4.07158	-0.61941	0.84738
H	4.20481	0.00845	-0.78687

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.215863 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.227174
Thermal correction to Enthalpy=	0.228119
Thermal correction to Gibbs Free Frequency and Energy=	0.178607
Sum of electronic and zero-point Energies=	-389.951536
Sum of electronic and thermal Energies=	-389.940224
Sum of electronic and thermal Enthalpies=	-389.939280
Sum of electronic and thermal Free Energies=	-389.988792

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.216590 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.227770
Thermal correction to Enthalpy=	0.228714
Thermal correction to Gibbs Free Frequency and Energy=	0.179891
Sum of electronic and zero-point Energies=	-390.029482
Sum of electronic and thermal Energies=	-390.018302
Sum of electronic and thermal Enthalpies=	-390.017358
Sum of electronic and thermal Free Energies=	-390.066181

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.216583 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.227763
Thermal correction to Enthalpy=	0.228707
Thermal correction to Gibbs Free Frequency and Energy=	0.179835
Sum of electronic and zero-point Energies=	-390.026860
Sum of electronic and thermal Energies=	-390.015681

Sum of electronic and thermal Enthalpies=	-390.014736
Sum of electronic and thermal Free Energies=	-390.063609

Name of cationic radical	α-terpinene

Cartesian Coordinates optimized at PM6

C	1.2582	4.8731	4.0424
C	1.1173	3.3688	3.8659
C	0.9086	2.6893	5.2131
C	2.3187	2.7708	3.1871
C	2.0916	1.563	2.3388
C	3.559	3.2529	3.3789
C	3.1824	1.3398	1.3001
C	4.7071	2.6416	2.7429
C	4.5461	1.7254	1.7724
C	5.6929	1.08	1.0882
H	1.2177	5.3945	3.0778
H	0.4596	5.2791	4.6756
H	2.2245	5.1273	4.5092
H	0.2188	3.1754	3.2283
H	0.8097	1.6019	5.0981
H	1.7521	2.874	5.8914
H	0.	3.0563	5.7076
H	2.0172	0.6892	3.0195
H	1.1091	1.6289	1.8296
H	3.7176	4.1295	4.0246
H	3.1778	0.2783	0.9815
H	2.9689	1.9282	0.3841
H	5.7016	2.9552	3.0782
H	6.6588	1.4901	1.4115
H	5.7055	0.	1.2911
H	5.6218	1.2109	0.

Frequency and Energy at PM6 (gas)

Zero-point correction=	0.212802 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.224845
Thermal correction to Enthalpy=	0.225790
Thermal correction to Gibbs Free Frequency and Energy=	0.172805
Sum of electronic and zero-point Energies=	0.469842
Sum of electronic and thermal Energies=	0.481886
Sum of electronic and thermal Enthalpies=	0.482830
Sum of electronic and thermal Free Energies=	0.429846

Name of compound	γ-terpinene

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	1.3429	0.8441	2.6573
C	1.9644	1.9382	3.5149
C	0.9966	3.0994	3.6833
C	3.2666	2.3793	2.8994
C	4.4865	1.6594	3.3673
C	3.3205	3.3422	1.9727

C	5.736	2.0696	2.6786
C	4.5749	3.7894	1.3206
C	5.7866	3.0327	1.7518
C	7.0575	3.418	1.0847
H	1.084	1.2156	1.6569
H	2.033	0.	2.5271
H	0.4237	0.4544	3.1136
H	2.1803	1.5143	4.5271
H	0.8912	3.6645	2.7418
H	1.3466	3.8045	4.4476
H	0.	2.751	3.9818
H	4.6086	1.8196	4.459
H	4.3376	0.5672	3.232
H	2.3917	3.8509	1.6679
H	6.6435	1.5303	2.9767
H	4.4615	3.7015	0.2201
H	4.7267	4.869	1.5279
H	7.9169	2.8421	1.4523
H	7.2753	4.4822	1.2496
H	6.9898	3.2578	0.

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction=	0.233411 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.244469
Thermal correction to Enthalpy=	0.245413
Thermal correction to Gibbs Free Frequency and Energy=	0.196821
Sum of electronic and zero-point Energies=	-390.551980
Sum of electronic and thermal Energies=	-390.540922
Sum of electronic and thermal Enthalpies=	-390.539978
Sum of electronic and thermal Free Energies=	-390.588570

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.233051 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.244114
Thermal correction to Enthalpy=	0.245059
Thermal correction to Gibbs Free Frequency and Energy=	0.196507
Sum of electronic and zero-point Energies=	-390.553973
Sum of electronic and thermal Energies=	-390.542909
Sum of electronic and thermal Enthalpies=	-390.541965
Sum of electronic and thermal Free Energies=	-390.590516

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.232969 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.244052
Thermal correction to Enthalpy=	0.244997
Thermal correction to Gibbs Free Frequency and Energy=	0.196282
Sum of electronic and zero-point Energies=	-390.554297
Sum of electronic and thermal Energies=	-390.543214
Sum of electronic and thermal Enthalpies=	-390.542270
Sum of electronic and thermal Free Energies=	-390.590985

Name of radical	γ-terpinene-C5-H18

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	1.3429	0.8441	2.6573
C	1.9644	1.9382	3.5149
C	0.9966	3.0994	3.6833
C	3.2666	2.3793	2.8994
C	4.4865	1.6594	3.3673
C	3.3205	3.3422	1.9727
C	5.736	2.0696	2.6786
C	4.5749	3.7894	1.3206
C	5.7866	3.0327	1.7518
C	7.0575	3.418	1.0847
H	1.084	1.2156	1.6569
H	2.033	0.	2.5271
H	0.4237	0.4544	3.1136
H	2.1803	1.5143	4.5271
H	0.8912	3.6645	2.7418
H	1.3466	3.8045	4.4476
H	0.	2.751	3.9818
H	4.3376	0.5672	3.232
H	2.3917	3.8509	1.6679
H	6.6435	1.5303	2.9767
H	4.4615	3.7015	0.2201
H	4.7267	4.869	1.5279
H	7.9169	2.8421	1.4523
H	7.2753	4.4822	1.2496
H	6.9898	3.2578	0.

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction=	0.219924 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.230844
Thermal correction to Enthalpy=	0.231789
Thermal correction to Gibbs Free Frequency and Energy=	0.183044
Sum of electronic and zero-point Energies=	-389.939151
Sum of electronic and thermal Energies=	-389.928231
Sum of electronic and thermal Enthalpies=	-389.927287
Sum of electronic and thermal Free Energies=	-389.976032

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.219570 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.230505
Thermal correction to Enthalpy=	0.231449
Thermal correction to Gibbs Free Frequency and Energy=	0.182623
Sum of electronic and zero-point Energies=	-389.941724
Sum of electronic and thermal Energies=	-389.930790
Sum of electronic and thermal Enthalpies=	-389.929845
Sum of electronic and thermal Free Energies=	-389.978672

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.219565 (Hartree/Particle)

Thermal correction to Frequency and Energy= 0.230499 Thermal correction to Enthalpy= 0.231443 Thermal correction to Gibbs Free Frequency and Energy= 0.182671 Sum of electronic and zero-point Energies= -389.941815 Sum of electronic and thermal Energies= -389.930881 Sum of electronic and thermal Enthalpies= -389.929937 Sum of electronic and thermal Free Energies= -389.978709

Name of anion	γ-terpinene-C5-H18-anion
Cartesian Coordinates optimzied at B3LYP/6-311G (d,p)	
C 1.3429 0.8441 2.6573 C 1.9644 1.9382 3.5149 C 0.9966 3.0994 3.6833 C 3.2666 2.3793 2.8994 C 4.4865 1.6594 3.3673 C 3.3205 3.3422 1.9727 C 5.736 2.0696 2.6786 C 4.5749 3.7894 1.3206 C 5.7866 3.0327 1.7518 C 7.0575 3.418 1.0847 H 1.084 1.2156 1.6569 H 2.033 0. 2.5271 H 0.4237 0.4544 3.1136 H 2.1803 1.5143 4.5271 H 0.8912 3.6645 2.7418 H 1.3466 3.8045 4.4476 H 0. 2.751 3.9818 H 4.3376 0.5672 3.232 H 2.3917 3.8509 1.6679 H 6.6435 1.5303 2.9767 H 4.4615 3.7015 0.2201 H 4.7267 4.869 1.5279 H 7.9169 2.8421 1.4523 H 7.2753 4.4822 1.2496 H 6.9898 3.2578 0.	
Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction= 0.215910 (Hartree/Particle) Thermal correction to Frequency and Energy= 0.227242 Thermal correction to Enthalpy= 0.228186 Thermal correction to Gibbs Free Frequency and Energy= 0.178048 Sum of electronic and zero-point Energies= -389.950376 Sum of electronic and thermal Energies= -389.939044 Sum of electronic and thermal Enthalpies= -389.938100 Sum of electronic and thermal Free Energies= -389.988238	
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction= 0.216384 (Hartree/Particle) Thermal correction to Frequency and Energy= 0.226730 Thermal correction to Enthalpy= 0.227674	

Thermal correction to Gibbs Free Frequency and Energy= 0.181256 Sum of electronic and zero-point Energies= -390.028640 Sum of electronic and thermal Energies= -390.018294 Sum of electronic and thermal Enthalpies= -390.017350 Sum of electronic and thermal Free Energies= -390.063767
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)
Zero-point correction= 0.216449 (Hartree/Particle) Thermal correction to Frequency and Energy= 0.227685 Thermal correction to Enthalpy= 0.228630 Thermal correction to Gibbs Free Frequency and Energy= 0.179044 Sum of electronic and zero-point Energies= -390.025945 Sum of electronic and thermal Energies= -390.014709 Sum of electronic and thermal Enthalpies= -390.013764 Sum of electronic and thermal Free Energies= -390.063350

Name of cationic radical	γ-terpinene
Cartesian Coordinates optimized at PM6	
C 1.3429 0.8441 2.6573 C 1.9644 1.9382 3.5149 C 0.9966 3.0994 3.6833 C 3.2666 2.3793 2.8994 C 4.4865 1.6594 3.3673 C 3.3205 3.3422 1.9727 C 5.736 2.0696 2.6786 C 4.5749 3.7894 1.3206 C 5.7866 3.0327 1.7518 C 7.0575 3.418 1.0847 H 1.084 1.2156 1.6569 H 2.033 0. 2.5271 H 0.4237 0.4544 3.1136 H 2.1803 1.5143 4.5271 H 0.8912 3.6645 2.7418 H 1.3466 3.8045 4.4476 H 0. 2.751 3.9818 H 4.6086 1.8196 4.459 H 4.3376 0.5672 3.232 H 2.3917 3.8509 1.6679 H 6.6435 1.5303 2.9767 H 4.4615 3.7015 0.2201 H 4.7267 4.869 1.5279 H 7.9169 2.8421 1.4523 H 7.2753 4.4822 1.2496 H 6.9898 3.2578 0.	
Frequency and Energy at PM6 (gas)	
Zero-point correction= 0.210957 (Hartree/Particle) Thermal correction to Frequency and Energy= 0.223160 Thermal correction to Enthalpy= 0.224105 Thermal correction to Gibbs Free Frequency and Energy= 0.170647	

Sum of electronic and zero-point Energies=	0.492514
Sum of electronic and thermal Energies=	0.504718
Sum of electronic and thermal Enthalpies=	0.505662
Sum of electronic and thermal Free Energies=	0.452204

Name of compound	Limonene		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	0	2.0085	2.985	2.9345
C	0	3.3486	3.684	3.0973
C	0	4.0413	3.8341	1.7439
C	0	2.0933	1.772	2.0673
C	0	3.1266	1.5492	1.2457
C	0	0.9466	0.8313	2.1592
C	0	4.298	2.4556	1.1317
C	0	5.3215	4.6159	1.8681
C	0	5.3908	5.8688	1.0695
C	0	6.3353	4.2231	2.6397
H	0	1.6069	2.7064	3.9291
H	0	1.2633	3.6759	2.4895
H	0	3.2045	4.6776	3.5635
H	0	3.9969	3.1146	3.7932
H	0	3.3469	4.3913	1.0655
H	0	3.1555	0.6501	0.6178
H	0	0.8806	0.3987	3.167
H	0	0.	1.3518	1.9598
H	0	1.0253	0.	1.4463
H	0	5.1642	1.9665	1.6245
H	0	4.5796	2.5678	0.0661
H	0	6.3493	6.391	1.1877
H	0	5.2585	5.6544	0.
H	0	4.5945	6.5636	1.3698
H	0	7.2588	4.7881	2.7294
H	0	6.3091	3.3125	3.2326
Frequency and Energy at B3LYP/6-311G (d,p) (gas)			
Zero-point correction=	0.233999 (Hartree/Particle)		
Thermal correction to Frequency and Energy=	0.244767		
Thermal correction to Enthalpy=	0.245712		
Thermal correction to Gibbs Free Frequency and Energy=	0.197914		
Sum of electronic and zero-point Energies=	-390.545857		
Sum of electronic and thermal Energies=	-390.535088		
Sum of electronic and thermal Enthalpies=	-390.534144		
Sum of electronic and thermal Free Energies=	-390.581942		
Frequency and Energy at B3LYP/6-311G (d,p) (water)			
Zero-point correction=	0.233593 (Hartree/Particle)		
Thermal correction to Frequency and Energy=	0.244377		
Thermal correction to Enthalpy=	0.245321		
Thermal correction to Gibbs Free Frequency and Energy=	0.197456		
Sum of electronic and zero-point Energies=	-390.547800		
Sum of electronic and thermal Energies=	-390.537016		

Sum of electronic and thermal Enthalpies=	-390.536072
Sum of electronic and thermal Free Energies=	-390.583937

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)		
Zero-point correction=	0.233576	(Hartree/Particle)
Thermal correction to Frequency and Energy=	0.244358	
Thermal correction to Enthalpy=	0.245302	
Thermal correction to Gibbs Free Frequency and Energy=	0.197467	
Sum of electronic and zero-point Energies=	-390.548252	
Sum of electronic and thermal Energies=	-390.537470	
Sum of electronic and thermal Enthalpies=	-390.536526	
Sum of electronic and thermal Free Energies=	-390.584361	

Name of radical	Limonene-C7-H20

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	1.52281	1.18183	0.41551
C	0.0601	1.30406	-0.02783
C	-0.72001	0.02	0.28327
C	2.16442	-0.12368	-0.00211
C	1.42503	-1.15515	-0.42128
C	3.66615	-0.18819	0.08847
C	-0.08167	-1.1577	-0.49218
C	-2.21979	0.09464	0.04436
C	-3.03076	-1.04416	0.61716
C	-2.8099	1.0901	-0.62242
H	2.10495	2.01635	0.00624
H	1.597	1.28355	1.50765
H	-0.40624	2.16283	0.46336
H	0.02742	1.49723	-1.1064
H	-0.58106	-0.19503	1.35337
H	1.92338	-2.07159	-0.73174
H	4.13222	0.56639	-0.55609
H	4.00617	0.02276	1.10956
H	4.04819	-1.16956	-0.20106
H	-0.4552	-2.11112	-0.10445
H	-4.10011	-0.88902	0.46239
H	-2.75967	-2.00163	0.16046
H	-2.84951	-1.14815	1.69294
H	-3.88465	1.10207	-0.7733
H	-2.25445	1.92181	-1.03878

Frequency and Energy at B3LYP/6-311G (d,p) (gas)		
Zero-point correction=	0.220112	(Hartree/Particle)
Thermal correction to Frequency and Energy=	0.230947	
Thermal correction to Enthalpy=	0.231891	
Thermal correction to Gibbs Free Frequency and Energy=	0.183320	
Sum of electronic and zero-point Energies=	-389.919534	
Sum of electronic and thermal Energies=	-389.908700	
Sum of electronic and thermal Enthalpies=	-389.907756	
Sum of electronic and thermal Free Energies=	-389.956326	

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction= 0.219815 (Hartree/Particle) Thermal correction to Frequency and Energy= 0.230635 Thermal correction to Enthalpy= 0.231579 Thermal correction to Gibbs Free Frequency and Energy= 0.183076 Sum of electronic and zero-point Energies= -389.921160 Sum of electronic and thermal Energies= -389.910340 Sum of electronic and thermal Enthalpies= -389.909396 Sum of electronic and thermal Free Energies= -389.957899
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)
Zero-point correction= 0.219831 (Hartree/Particle) Thermal correction to Frequency and Energy= 0.230652 Thermal correction to Enthalpy= 0.231596 Thermal correction to Gibbs Free Frequency and Energy= 0.183092 Sum of electronic and zero-point Energies= -389.921004 Sum of electronic and thermal Energies= -389.910183 Sum of electronic and thermal Enthalpies= -389.909239 Sum of electronic and thermal Free Energies= -389.957743

Name of anion	Limonene-C7-H20-anion
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)	
C	1.43375 -1.27389 0.11683
C	-0.04062 -1.08642 0.50386
C	-0.75526 -0.05726 -0.40876
C	2.16505 0.03657 -0.01717
C	1.43985 1.18692 -0.30284
C	3.65537 0.03514 0.12196
C	0.06684 1.20087 -0.49387
C	-2.19752 0.15462 0.0345
C	-3.19024 -0.86443 -0.46668
C	-2.56398 1.15673 0.83458
H	1.93252 -1.90696 0.86075
H	1.50329 -1.8279 -0.83317
H	-0.56121 -2.04774 0.47455
H	-0.09822 -0.71933 1.53346
H	-0.79658 -0.49889 -1.41997
H	1.98283 2.12397 -0.4031
H	3.96475 -0.31781 1.11496
H	4.12381 -0.64494 -0.60272
H	4.07906 1.03033 -0.03045
H	-0.43299 2.123 -0.76685
H	-4.18708 -0.69046 -0.05756
H	-3.25844 -0.8344 -1.56039
H	-2.88727 -1.88288 -0.19966
H	-3.59237 1.27115 1.16046
H	-1.85145 1.88986 1.19512
Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction= 0.215697 (Hartree/Particle) Thermal correction to Frequency and Energy= 0.226775 Thermal correction to Enthalpy= 0.227719	

Thermal correction to Gibbs Free Frequency and Energy= 0.179442
Sum of electronic and zero-point Energies= -389.923252
Sum of electronic and thermal Energies= -389.912174
Sum of electronic and thermal Enthalpies= -389.911229
Sum of electronic and thermal Free Energies= -389.959507
Frequency and Energy at B3LYP/6-311G (d,p) (water)
Zero-point correction= 0.216242 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.227313
Thermal correction to Enthalpy= 0.228257
Thermal correction to Gibbs Free Frequency and Energy= 0.179798
Sum of electronic and zero-point Energies= -389.999150
Sum of electronic and thermal Energies= -389.988078
Sum of electronic and thermal Enthalpies= -389.987134
Sum of electronic and thermal Free Energies= -390.035593
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)
Zero-point correction= 0.216140 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.227243
Thermal correction to Enthalpy= 0.228187
Thermal correction to Gibbs Free Frequency and Energy= 0.179546
Sum of electronic and zero-point Energies= -389.996627
Sum of electronic and thermal Energies= -389.985524
Sum of electronic and thermal Enthalpies= -389.984580
Sum of electronic and thermal Free Energies= -390.033221

Name of cationic radical	Limonene
Cartesian Coordinates optimized at PM6	

C	0	2.0085	2.985	2.9345
C	0	3.3486	3.684	3.0973
C	0	4.0413	3.8341	1.7439
C	0	2.0933	1.772	2.0673
C	0	3.1266	1.5492	1.2457
C	0	0.9466	0.8313	2.1592
C	0	4.298	2.4556	1.1317
C	0	5.3215	4.6159	1.8681
C	0	5.3908	5.8688	1.0695
C	0	6.3353	4.2231	2.6397
H	0	1.6069	2.7064	3.9291
H	0	1.2633	3.6759	2.4895
H	0	3.2045	4.6776	3.5635
H	0	3.9969	3.1146	3.7932
H	0	3.3469	4.3913	1.0655
H	0	3.1555	0.6501	0.6178
H	0	0.8806	0.3987	3.167
H	0	0.	1.3518	1.9598
H	0	1.0253	0.	1.4463
H	0	5.1642	1.9665	1.6245
H	0	4.5796	2.5678	0.0661
H	0	6.3493	6.391	1.1877
H	0	5.2585	5.6544	0.

H	0	4.5945	6.5636	1.3698
H	0	7.2588	4.7881	2.7294
H	0	6.3091	3.3125	3.2326

Frequency and Energy at PM6 (gas)

Zero-point correction= 0.211922 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.223699
Thermal correction to Enthalpy= 0.224644
Thermal correction to Gibbs Free Frequency and Energy= 0.172729
Sum of electronic and zero-point Energies= 0.500291
Sum of electronic and thermal Energies= 0.512068
Sum of electronic and thermal Enthalpies= 0.513012
Sum of electronic and thermal Free Energies= 0.461097

Name of compound	Axinissene

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	4.19532	0.46152	-1.21681
C	3.70072	0.95765	0.15716
C	3.2513	-0.24082	1.02001
C	4.24341	-1.36391	0.98868
C	5.19641	-1.4874	0.05337
C	5.39736	-0.47784	-1.04746
C	2.59122	1.97878	-0.00123
C	2.75551	3.24029	0.40776
C	6.15664	-2.63713	0.04214
C	1.30807	1.52437	-0.6488
C	0.15487	1.46393	0.36913
C	-1.08974	0.92506	-0.26756
C	-1.64111	-0.26933	-0.00428
C	-2.90704	-0.7068	-0.70175
C	-4.14931	-0.247	0.07944
C	-5.42814	-0.67054	-0.57574
C	-6.64679	-0.35894	-0.10555
C	-7.894	-0.81096	-0.80232
C	-1.07908	-1.25471	0.97172
C	-6.85631	0.45388	1.13493
H	4.46985	1.32078	-1.85519
H	3.37805	-0.06844	-1.74302
H	4.56834	1.43988	0.67783
H	2.27042	-0.62516	0.66688
H	3.08845	0.09786	2.06201
H	4.12321	-2.09731	1.78241
H	6.30954	0.11366	-0.8225
H	5.60189	-0.99262	-2.00695
H	1.99669	4.00033	0.30713
H	3.65509	3.60879	0.87361
H	6.07143	-3.26657	0.93701
H	5.98133	-3.28649	-0.82651
H	7.19746	-2.29186	-0.01017
H	1.04189	2.21196	-1.47715
H	1.43043	0.52976	-1.12451

H	0.45968	0.84929	1.2429
H	-0.04326	2.47698	0.77609
H	-1.54273	1.59667	-0.99718
H	-2.94264	-0.30135	-1.73298
H	-2.92227	-1.80837	-0.82026
H	-4.10702	-0.64723	1.11454
H	-4.127	0.85858	0.18793
H	-5.31724	-1.26363	-1.48148
H	-7.68771	-1.40178	-1.70346
H	-8.51131	-1.43396	-0.14098
H	-8.5057	0.04756	-1.11134
H	-0.29011	-0.81638	1.6007
H	-1.85553	-1.64391	1.64318
H	-0.63605	-2.11317	0.44844
H	-6.39695	1.44789	1.03858
H	-7.91588	0.6086	1.36931
H	-6.39807	-0.03111	2.00821

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction= 0.469288 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.493160
Thermal correction to Enthalpy= 0.494104
Thermal correction to Gibbs Free Frequency and Energy= 0.411994
Sum of electronic and zero-point Energies= -781.089225
Sum of electronic and thermal Energies= -781.065354
Sum of electronic and thermal Enthalpies= -781.064410
Sum of electronic and thermal Free Energies= -781.146520

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction= 0.468624 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.492459
Thermal correction to Enthalpy= 0.493403
Thermal correction to Gibbs Free Frequency and Energy= 0.411807
Sum of electronic and zero-point Energies= -781.093925
Sum of electronic and thermal Energies= -781.070090
Sum of electronic and thermal Enthalpies= -781.069146
Sum of electronic and thermal Free Energies= -781.150743

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction= 0.468584 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.492456
Thermal correction to Enthalpy= 0.493400
Thermal correction to Gibbs Free Frequency and Energy= 0.411386
Sum of electronic and zero-point Energies= -781.093676
Sum of electronic and thermal Energies= -781.069804
Sum of electronic and thermal Enthalpies= -781.068860
Sum of electronic and thermal Free Energies= -781.150874

Name of radical	Axinissene-C2-H23

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	2.53658	0.77883	-0.65627
C	3.24175	-0.53829	-0.71173

C	4.74087	-0.50451	-0.70783
C	5.3574	0.80499	-0.31498
C	4.65439	1.82929	0.18779
C	3.16477	1.72644	0.37813
C	2.54895	-1.76985	-0.81842
C	3.19669	-2.98345	-0.90974
C	5.28463	3.12126	0.59968
C	1.03547	-1.78407	-0.82738
C	0.48469	-1.84505	0.60791
C	-1.00935	-1.74326	0.62437
C	-1.71991	-0.90467	1.39361
C	-3.22899	-0.8973	1.34042
C	-3.73444	0.07868	0.26483
C	-5.22986	0.12378	0.18847
C	-5.91037	0.8673	-0.69877
C	-7.40848	0.87431	-0.72897
C	-1.11136	0.06953	2.35313
C	-5.23812	1.7371	-1.71619
H	1.45542	0.66445	-0.43828
H	2.5946	1.24291	-1.66646
H	5.10261	-0.78865	-1.72328
H	5.13116	-1.2902	-0.01939
H	6.43358	0.85849	-0.45834
H	2.95979	1.35273	1.40322
H	2.6832	2.7203	0.31216
H	2.66409	-3.91478	-0.98558
H	4.26517	-3.09142	-0.9079
H	6.38097	3.08733	0.56067
H	4.96382	3.94221	-0.05652
H	5.00672	3.39296	1.62676
H	0.63361	-0.89219	-1.34851
H	0.66212	-2.64842	-1.41177
H	0.794	-2.7978	1.08724
H	0.95203	-1.04369	1.22046
H	-1.51243	-2.43152	-0.05569
H	-3.61556	-1.91543	1.13274
H	-3.64906	-0.62153	2.32794
H	-3.33808	1.09564	0.46958
H	-3.31295	-0.21115	-0.72144
H	-5.75531	-0.49618	0.91242
H	-7.8525	0.22155	0.03293
H	-7.80163	1.88559	-0.55784
H	-7.7844	0.53553	-1.70398
H	-0.03084	0.19638	2.18806
H	-1.57518	1.0608	2.2692
H	-1.24384	-0.26906	3.38976
H	-4.5957	1.14278	-2.38129
H	-5.94943	2.27743	-2.35156
H	-4.59779	2.48869	-1.23376

Frequency and Energy at B3LYP/6-311G (d,p) (gas)
Zero-point correction= 0.455560 (Hartree/Particle)

Thermal correction to Frequency and Energy= 0.479418
Thermal correction to Enthalpy= 0.480362
Thermal correction to Gibbs Free Frequency and Energy= 0.397439
Sum of electronic and zero-point Energies= -780.462110
Sum of electronic and thermal Energies= -780.438252
Sum of electronic and thermal Enthalpies= -780.437308
Sum of electronic and thermal Free Energies= -780.520230
Frequency and Energy at B3LYP/6-311G (d,p) (water)
Zero-point correction= 0.454735 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.478662
Thermal correction to Enthalpy= 0.479606
Thermal correction to Gibbs Free Frequency and Energy= 0.396224
Sum of electronic and zero-point Energies= -780.467194
Sum of electronic and thermal Energies= -780.443267
Sum of electronic and thermal Enthalpies= -780.442323
Sum of electronic and thermal Free Energies= -780.525705
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)
Zero-point correction= 0.454791 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.478708
Thermal correction to Enthalpy= 0.479652
Thermal correction to Gibbs Free Frequency and Energy= 0.396375
Sum of electronic and zero-point Energies= -780.466899
Sum of electronic and thermal Energies= -780.442982
Sum of electronic and thermal Enthalpies= -780.442038
Sum of electronic and thermal Free Energies= -780.525314

Name of anion	Axinissene-C2-H23-anion
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)	
C	2.53658 0.77883 -0.65627
C	3.24175 -0.53829 -0.71173
C	4.74087 -0.50451 -0.70783
C	5.3574 0.80499 -0.31498
C	4.65439 1.82929 0.18779
C	3.16477 1.72644 0.37813
C	2.54895 -1.76985 -0.81842
C	3.19669 -2.98345 -0.90974
C	5.28463 3.12126 0.59968
C	1.03547 -1.78407 -0.82738
C	0.48469 -1.84505 0.60791
C	-1.00935 -1.74326 0.62437
C	-1.71991 -0.90467 1.39361
C	-3.22899 -0.8973 1.34042
C	-3.73444 0.07868 0.26483
C	-5.22986 0.12378 0.18847
C	-5.91037 0.8673 -0.69877
C	-7.40848 0.87431 -0.72897
C	-1.11136 0.06953 2.35313
C	-5.23812 1.7371 -1.71619
H	1.45542 0.66445 -0.43828

H	2.5946	1.24291	-1.66646
H	5.10261	-0.78865	-1.72328
H	5.13116	-1.2902	-0.01939
H	6.43358	0.85849	-0.45834
H	2.95979	1.35273	1.40322
H	2.6832	2.7203	0.31216
H	2.66409	-3.91478	-0.98558
H	4.26517	-3.09142	-0.9079
H	6.38097	3.08733	0.56067
H	4.96382	3.94221	-0.05652
H	5.00672	3.39296	1.62676
H	0.63361	-0.89219	-1.34851
H	0.66212	-2.64842	-1.41177
H	0.794	-2.7978	1.08724
H	0.95203	-1.04369	1.22046
H	-1.51243	-2.43152	-0.05569
H	-3.61556	-1.91543	1.13274
H	-3.64906	-0.62153	2.32794
H	-3.33808	1.09564	0.46958
H	-3.31295	-0.21115	-0.72144
H	-5.75531	-0.49618	0.91242
H	-7.8525	0.22155	0.03293
H	-7.80163	1.88559	-0.55784
H	-7.7844	0.53553	-1.70398
H	-0.03084	0.19638	2.18806
H	-1.57518	1.0608	2.2692
H	-1.24384	-0.26906	3.38976
H	-4.5957	1.14278	-2.38129
H	-5.94943	2.27743	-2.35156
H	-4.59779	2.48869	-1.23376

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction= 0.451626 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.475584
Thermal correction to Enthalpy= 0.476528
Thermal correction to Gibbs Free Frequency and Energy= 0.394816
Sum of electronic and zero-point Energies= -780.477860
Sum of electronic and thermal Energies= -780.453902
Sum of electronic and thermal Enthalpies= -780.452958
Sum of electronic and thermal Free Energies= -780.534670

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction= 0.451397 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.475534
Thermal correction to Enthalpy= 0.476478
Thermal correction to Gibbs Free Frequency and Energy= 0.394350
Sum of electronic and zero-point Energies= -780.555679
Sum of electronic and thermal Energies= -780.531542
Sum of electronic and thermal Enthalpies= -780.530598
Sum of electronic and thermal Free Energies= -780.612726

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.451543 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.475620
Thermal correction to Enthalpy=	0.476564
Thermal correction to Gibbs Free Frequency and Energy=	0.394741
Sum of electronic and zero-point Energies=	-780.552765
Sum of electronic and thermal Energies=	-780.528688
Sum of electronic and thermal Enthalpies=	-780.527744
Sum of electronic and thermal Free Energies=	-780.609567

Name of cationic radical	Axinissene

Cartesian Coordinates optimized at PM6

C	0	-2.14324	-2.40931	0.25897
C	0	-3.29159	-1.40388	0.25897
C	0	-4.18416	-1.57689	-0.97275
C	0	-4.47208	-3.01472	-1.29368
C	0	-3.798	-4.03711	-0.74645
C	0	-2.66248	-3.84887	0.21713
C	0	-2.72529	-0.01812	0.25897
C	0	-3.54423	1.03871	0.25897
C	0	-4.19709	-5.4323	-1.11414
C	0	-1.24204	0.18432	0.25897
C	0	-0.93247	1.67553	0.25897
C	0	0.55078	1.87797	0.25897
C	0	1.05655	3.11562	0.25897
C	0	2.5398	3.31806	0.25897
C	0	3.23767	1.96436	0.25897
C	0	4.72091	2.1668	0.25897
C	0	5.53986	1.10997	0.25897
C	0	7.0231	1.31241	0.25897
C	0	0.13961	4.29893	0.25897
C	0	4.97355	-0.27579	0.25897
H	0	-1.53946	-2.2691	1.18339
H	0	-1.52302	-2.23354	-0.64834
H	0	-3.91018	-1.57776	1.16775
H	0	-3.67407	-1.1144	-1.84721
H	0	-5.15733	-1.08509	-0.74947
H	0	-5.27407	-3.24068	-2.01183
H	0	-3.01278	-4.12848	1.23589
H	0	-1.82395	-4.49458	-0.12739
H	0	-3.12811	2.05697	0.25897
H	0	-4.63413	0.88996	0.25897
H	0	-5.04722	-5.39865	-1.83172
H	0	-3.33383	-5.95221	-1.58663
H	0	-4.50679	-5.98307	-0.19789
H	0	-0.8041	-0.28495	1.16823
H	0	-0.80366	-0.28542	-0.64984
H	0	-1.37042	2.14481	-0.65029
H	0	-1.37085	2.14527	1.16778
H	0	1.22455	1.00848	0.25897
H	0	2.83597	3.88754	-0.65029

H	0	2.83626	3.8881	1.16778
H	0	2.94149	1.39488	1.16823
H	0	2.9412	1.39432	-0.64984
H	0	5.13703	3.18506	0.25897
H	0	7.24934	2.40218	0.25897
H	0	7.46105	0.84313	1.16823
H	0	7.46148	0.84267	-0.64984
H	0	-0.91728	3.94997	0.25897
H	0	0.32704	4.91284	1.16823
H	0	0.32722	4.91344	-0.64984
H	0	3.86182	-0.22282	0.25897
H	0	5.31865	-0.81702	-0.65029
H	0	5.31899	-0.81755	1.16778

Frequency and Energy at PM6 (gas)

Zero-point correction= 0.429512 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.454841
Thermal correction to Enthalpy= 0.455786
Thermal correction to Gibbs Free Frequency and Energy= 0.366652
Sum of electronic and zero-point Energies= 0.698631
Sum of electronic and thermal Energies= 0.723961
Sum of electronic and thermal Enthalpies= 0.724905
Sum of electronic and thermal Free Energies= 0.635771

Name of compound	Rimuene

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	-0.50014	0.7347	0.90458
C	-1.07475	-0.68684	1.1836
C	0.75312	0.64218	-0.0252
C	-1.6081	1.58121	0.22195
C	-1.63351	-1.34324	-0.09216
C	1.70255	-0.48064	0.34331
C	-2.74048	-0.48762	-0.75753
C	-0.00023	-1.58146	1.8297
C	-2.17157	0.92371	-1.04115
C	3.04505	-0.51984	-0.39551
C	1.46979	2.00289	-0.12471
C	-0.15185	1.39715	2.25293
C	1.33423	-1.47874	1.15964
C	3.66791	0.89177	-0.54873
C	2.66931	1.92564	-1.07142
C	-3.15763	-1.14809	-2.089
C	4.0844	-1.38836	0.34811
C	2.78682	-1.1407	-1.78599
C	-3.97409	-0.44346	0.13004
C	-4.92874	0.48209	0.06844
H	-1.91789	-0.57717	1.90965
H	0.37287	0.38573	-1.05405
H	-1.21347	2.58393	-0.02704

H	-2.43118	1.75096	0.94372
H	-0.80965	-1.51172	-0.81222
H	-2.02405	-2.34913	0.14527
H	-0.33859	-2.63698	1.82827
H	0.11278	-1.30994	2.90064
H	-2.95437	1.56811	-1.48136
H	-1.37467	0.84749	-1.80774
H	1.81487	2.32663	0.87618
H	0.75657	2.77476	-0.47037
H	0.74482	0.94222	2.6904
H	0.04574	2.46762	2.14335
H	-0.96483	1.29164	2.97745
H	2.00158	-2.30806	1.39169
H	4.54403	0.83837	-1.22035
H	4.05706	1.22414	0.43349
H	2.34054	1.66335	-2.09475
H	3.15576	2.91548	-1.15323
H	-3.56239	-2.15242	-1.92653
H	-3.93375	-0.56326	-2.5943
H	-2.31149	-1.24126	-2.77618
H	5.05595	-1.36301	-0.15484
H	3.77515	-2.4379	0.39564
H	4.23214	-1.0399	1.37552
H	3.71629	-1.25493	-2.35111
H	2.11261	-0.51702	-2.38175
H	2.32767	-2.13062	-1.69714
H	-4.04705	-1.27244	0.837
H	-5.80312	0.47068	0.70153
H	-4.91253	1.32051	-0.61216

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction=	0.476533 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.496248
Thermal correction to Enthalpy=	0.497192
Thermal correction to Gibbs Free Frequency and Energy=	0.431498
Sum of electronic and zero-point Energies=	-781.108364
Sum of electronic and thermal Energies=	-781.088649
Sum of electronic and thermal Enthalpies=	-781.087704
Sum of electronic and thermal Free Energies=	-781.153398

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.475730 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.495468
Thermal correction to Enthalpy=	0.496412
Thermal correction to Gibbs Free Frequency and Energy=	0.430685
Sum of electronic and zero-point Energies=	-781.111210
Sum of electronic and thermal Energies=	-781.091472
Sum of electronic and thermal Enthalpies=	-781.090528
Sum of electronic and thermal Free Energies=	-781.156255

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.475770 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.495508

Thermal correction to Enthalpy=	0.496453
Thermal correction to Gibbs Free Frequency and Energy=	0.430723
Sum of electronic and zero-point Energies=	-781.111051
Sum of electronic and thermal Energies=	-781.091313
Sum of electronic and thermal Enthalpies=	-781.090368
Sum of electronic and thermal Free Energies=	-781.156098

Name of radical	Rimuene-C3-H22		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	0.49679	0.10593	1.25728
C	1.04049	1.34587	0.479
C	-0.82606	-0.37044	0.67599
C	1.60837	-0.97638	1.25311
C	1.52458	0.96587	-0.93345
C	-1.69254	0.53798	0.04329
C	2.62314	-0.12409	-0.91863
C	-0.0478	2.43261	0.3761
C	2.06842	-1.35186	-0.15764
C	-3.03652	0.09309	-0.54727
C	-1.21381	-1.79282	0.92907
C	0.22513	0.49649	2.73044
C	-1.34094	1.87945	-0.10864
C	-3.4845	-1.28459	0.00295
C	-2.33258	-2.28847	0.00759
C	2.95793	-0.52657	-2.37062
C	-4.14457	1.11039	-0.19746
C	-2.87659	0.01471	-2.0801
C	3.89871	0.4174	-0.29388
C	4.87858	-0.32827	0.21186
H	1.90507	1.75966	1.05056
H	1.26449	-1.88107	1.7877
H	2.47596	-0.6013	1.83255
H	0.65957	0.60275	-1.525
H	1.88803	1.8662	-1.45942
H	0.29551	3.25386	-0.28365
H	-0.20563	2.90166	1.37153
H	2.83301	-2.14779	-0.1056
H	1.21953	-1.77761	-0.72787
H	-1.53772	-1.87607	1.99042
H	-0.33839	-2.46808	0.83365
H	-0.60197	1.212	2.80217
H	-0.05168	-0.37705	3.32826
H	1.10278	0.95342	3.19575
H	-2.01032	2.58106	-0.59139
H	-4.32892	-1.67082	-0.59546
H	-3.8724	-1.16312	1.03274
H	-1.94251	-2.42788	-1.01944
H	-2.68779	-3.28129	0.33909
H	3.34401	0.32403	-2.94164
H	3.72231	-1.31042	-2.39744
H	2.07609	-0.90404	-2.89724

H	-5.12684	0.75894	-0.52676
H	-3.97172	2.07985	-0.67646
H	-4.19361	1.28463	0.88242
H	-3.80827	-0.28694	-2.5663
H	-2.10325	-0.71076	-2.35565
H	-2.57946	0.98046	-2.50106
H	3.97853	1.50617	-0.31033
H	5.78211	0.08915	0.62986
H	4.85614	-1.4073	0.25002

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction= 0.462380 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.482402
Thermal correction to Enthalpy= 0.483346
Thermal correction to Gibbs Free Frequency and Energy= 0.415929
Sum of electronic and zero-point Energies= -780.486261
Sum of electronic and thermal Energies= -780.466239
Sum of electronic and thermal Enthalpies= -780.465294
Sum of electronic and thermal Free Energies= -780.532711

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction= 0.461598 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.481641
Thermal correction to Enthalpy= 0.482585
Thermal correction to Gibbs Free Frequency and Energy= 0.415116
Sum of electronic and zero-point Energies= -780.489101
Sum of electronic and thermal Energies= -780.469057
Sum of electronic and thermal Enthalpies= -780.468113
Sum of electronic and thermal Free Energies= -780.535582

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction= 0.461646 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.481687
Thermal correction to Enthalpy= 0.482631
Thermal correction to Gibbs Free Frequency and Energy= 0.415176
Sum of electronic and zero-point Energies= -780.488935
Sum of electronic and thermal Energies= -780.468894
Sum of electronic and thermal Enthalpies= -780.467950
Sum of electronic and thermal Free Energies= -780.535404

Name of anion	Rimuene-C3-H22-anion

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	0.49679	0.10593	1.25728
C	1.04049	1.34587	0.479
C	-0.82606	-0.37044	0.67599
C	1.60837	-0.97638	1.25311
C	1.52458	0.96587	-0.93345
C	-1.69254	0.53798	0.04329
C	2.62314	-0.12409	-0.91863
C	-0.0478	2.43261	0.3761
C	2.06842	-1.35186	-0.15764
C	-3.03652	0.09309	-0.54727

C	-1.21381	-1.79282	0.92907
C	0.22513	0.49649	2.73044
C	-1.34094	1.87945	-0.10864
C	-3.4845	-1.28459	0.00295
C	-2.33258	-2.28847	0.00759
C	2.95793	-0.52657	-2.37062
C	-4.14457	1.11039	-0.19746
C	-2.87659	0.01471	-2.0801
C	3.89871	0.4174	-0.29388
C	4.87858	-0.32827	0.21186
H	1.90507	1.75966	1.05056
H	1.26449	-1.88107	1.7877
H	2.47596	-0.6013	1.83255
H	0.65957	0.60275	-1.525
H	1.88803	1.8662	-1.45942
H	0.29551	3.25386	-0.28365
H	-0.20563	2.90166	1.37153
H	2.83301	-2.14779	-0.1056
H	1.21953	-1.77761	-0.72787
H	-1.53772	-1.87607	1.99042
H	-0.33839	-2.46808	0.83365
H	-0.60197	1.212	2.80217
H	-0.05168	-0.37705	3.32826
H	1.10278	0.95342	3.19575
H	-2.01032	2.58106	-0.59139
H	-4.32892	-1.67082	-0.59546
H	-3.8724	-1.16312	1.03274
H	-1.94251	-2.42788	-1.01944
H	-2.68779	-3.28129	0.33909
H	3.34401	0.32403	-2.94164
H	3.72231	-1.31042	-2.39744
H	2.07609	-0.90404	-2.89724
H	-5.12684	0.75894	-0.52676
H	-3.97172	2.07985	-0.67646
H	-4.19361	1.28463	0.88242
H	-3.80827	-0.28694	-2.5663
H	-2.10325	-0.71076	-2.35565
H	-2.57946	0.98046	-2.50106
H	3.97853	1.50617	-0.31033
H	5.78211	0.08915	0.62986
H	4.85614	-1.4073	0.25002

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction= 0.458256 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.478437
Thermal correction to Enthalpy= 0.479381
Thermal correction to Gibbs Free Frequency and Energy= 0.412495
Sum of electronic and zero-point Energies= -780.500081
Sum of electronic and thermal Energies= -780.479899
Sum of electronic and thermal Enthalpies= -780.478955
Sum of electronic and thermal Free Energies= -780.545841

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.458030 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.478165
Thermal correction to Enthalpy=	0.479109
Thermal correction to Gibbs Free Frequency and Energy=	0.412632
Sum of electronic and zero-point Energies=	-780.564573
Sum of electronic and thermal Energies=	-780.544438
Sum of electronic and thermal Enthalpies=	-780.543494
Sum of electronic and thermal Free Energies=	-780.609971

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.458136 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.478237
Thermal correction to Enthalpy=	0.479181
Thermal correction to Gibbs Free Frequency and Energy=	0.412847
Sum of electronic and zero-point Energies=	-780.562253
Sum of electronic and thermal Energies=	-780.542152
Sum of electronic and thermal Enthalpies=	-780.541208
Sum of electronic and thermal Free Energies=	-780.607543

Name of cationic radical	Rimuene

Cartesian Coordinates optimized at PM6

C	0	-0.467	-0.8457	-0.8491
C	0	-1.045	0.5483	-1.2274
C	0	0.8183	-0.6732	0.0629
C	0	-1.5769	-1.657	-0.121
C	0	-1.6429	1.2844	-0.0049
C	0	1.7386	0.4928	-0.3336
C	0	-2.7424	0.472	0.7157
C	0	0.0135	1.4117	-1.93
C	0	-2.2086	-0.9308	1.0712
C	0	3.0636	0.6254	0.4491
C	0	1.62	-1.9884	0.1887
C	0	-0.1331	-1.6152	-2.1553
C	0	1.3506	1.3926	-1.2585
C	0	3.7541	-0.7526	0.5902
C	0	2.8294	-1.8484	1.1024
C	0	-3.1527	1.2021	2.0055
C	0	4.098	1.5693	-0.2126
C	0	2.7522	1.2096	1.846
C	0	-3.972	0.3612	-0.1547
C	0	-5.0978	-0.2584	0.2157
H	0	-1.8573	0.408	-1.9534
H	0	0.4744	-0.425	1.0738
H	0	-1.1876	-2.6222	0.222
H	0	-2.373	-1.9016	-0.8374
H	0	-0.847	1.5314	0.7092
H	0	-2.0535	2.2493	-0.3335
H	0	-0.3402	2.4485	-1.9869
H	0	0.1447	1.0804	-2.9671
H	0	-2.9998	-1.5664	1.4888
H	0	-1.4654	-0.846	1.8735

H	0	1.98	-2.317	-0.7934
H	0	0.9838	-2.7884	0.5811
H	0	0.7471	-1.208	-2.6628
H	0	0.0578	-2.6762	-1.9593
H	0	-0.9707	-1.5738	-2.8615
H	0	1.9982	2.2177	-1.5362
H	0	4.6175	-0.6768	1.2638
H	0	4.1531	-1.0639	-0.3854
H	0	2.5078	-1.6401	2.1286
H	0	3.3749	-2.7988	1.132
H	0	-3.5983	2.1807	1.7891
H	0	-3.8724	0.629	2.601
H	0	-2.2809	1.3775	2.6472
H	0	5.0473	1.5577	0.3364
H	0	3.755	2.6101	-0.2252
H	0	4.313	1.2666	-1.244
H	0	3.6655	1.3039	2.4451
H	0	2.0523	0.5912	2.4164
H	0	2.3077	2.2089	1.7644
H	0	-3.9643	0.8358	-1.1329
H	0	-5.9489	-0.2863	-0.4567
H	0	-5.2057	-0.7475	1.1767

Frequency and Energy at PM6 (gas)	
Zero-point correction=	0.436662 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.457934
Thermal correction to Enthalpy=	0.458878
Thermal correction to Gibbs Free Frequency and Energy=	0.387368
Sum of electronic and zero-point Energies=	0.668634
Sum of electronic and thermal Energies=	0.689905
Sum of electronic and thermal Enthalpies=	0.690850
Sum of electronic and thermal Free Energies=	0.619339

Name of compound	Cembrene

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	2.08429	-0.95566	-0.40877
C	3.29275	-1.37198	0.48617
C	0.80309	-1.65854	0.09
C	-0.21448	-1.89407	-1.03655
C	1.98117	0.54426	-0.50897
C	4.62533	-1.03443	-0.19566
C	3.22066	-0.73692	1.87862
C	-1.46251	-2.57679	-0.53938
C	0.85467	1.2617	-0.44387
C	-2.68937	-2.03649	-0.60192
C	-3.02858	-0.69323	-1.17265
C	-1.2649	-3.94978	0.03495
C	-3.69339	0.23586	-0.13851
C	0.7928	2.72939	-0.56163
C	-2.65886	0.94783	0.70038
C	-1.13411	2.9277	1.05972
C	-0.1066	3.47213	0.10859

C	-2.1966	2.15323	0.33478
C	1.78173	3.37713	-1.48725
C	-2.20257	0.2079	1.91749
H	2.2991	-1.32764	-1.44712
H	3.24877	-2.48464	0.60871
H	0.33446	-1.06423	0.89909
H	1.0691	-2.62999	0.55073
H	0.24084	-2.50502	-1.84185
H	-0.47058	-0.92041	-1.51344
H	2.94836	1.03256	-0.65876
H	4.74592	0.04523	-0.34048
H	5.47361	-1.37583	0.40759
H	4.70815	-1.51041	-1.17796
H	3.25991	0.35763	1.82664
H	4.05147	-1.0658	2.51082
H	2.28859	-0.99936	2.38996
H	-3.55413	-2.58447	-0.22556
H	-0.11986	0.78407	-0.28539
H	-2.12571	-0.1953	-1.59137
H	-3.71571	-0.83513	-2.03284
H	-0.53803	-4.53201	-0.54562
H	-2.19416	-4.53226	0.06379
H	-0.88814	-3.88968	1.06524
H	-4.38361	-0.34155	0.5073
H	-4.33415	0.96998	-0.66643
H	-0.63635	2.2976	1.8319
H	-1.61281	3.75687	1.62306
H	-0.13443	4.55358	-0.01253
H	-2.56951	2.64879	-0.56154
H	1.84378	2.83758	-2.44173
H	2.78649	3.38168	-1.04387
H	1.52387	4.4175	-1.71959
H	-2.00039	-0.84831	1.68235
H	-2.96983	0.23063	2.70183
H	-1.28221	0.63293	2.34384

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.471005 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.493925
Thermal correction to Enthalpy=	0.494869
Thermal correction to Gibbs Free Frequency and Energy=	0.420171
Sum of electronic and zero-point Energies=	-781.083591
Sum of electronic and thermal Energies=	-781.060671
Sum of electronic and thermal Enthalpies=	-781.059727
Sum of electronic and thermal Free Energies=	-781.134425

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.470060 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.493108
Thermal correction to Enthalpy=	0.494052
Thermal correction to Gibbs Free Frequency and Energy=	0.418672
Sum of electronic and zero-point Energies=	-781.087570
Sum of electronic and thermal Energies=	-781.064522

Sum of electronic and thermal Enthalpies= -781.063578
Sum of electronic and thermal Free Energies= -781.138959
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)
Zero-point correction= 0.470094 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.493149
Thermal correction to Enthalpy= 0.494093
Thermal correction to Gibbs Free Frequency and Energy= 0.418606
Sum of electronic and zero-point Energies= -781.087350
Sum of electronic and thermal Energies= -781.064295
Sum of electronic and thermal Enthalpies= -781.063351
Sum of electronic and thermal Free Energies= -781.138839

Name of radical	Cembrene-C16-H43
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)	
C	2.41483 -0.61322 -0.50487
C	3.87714 -0.77657 0.01599
C	1.4755 -1.56495 0.26782
C	0.31683 -2.06903 -0.60458
C	1.99572 0.83009 -0.47467
C	4.88436 -0.16791 -0.96862
C	4.05706 -0.17799 1.41479
C	-0.82629 -2.64359 0.1918
C	0.79847 1.3039 -0.03446
C	-2.11465 -2.39913 -0.09636
C	-2.59899 -1.56153 -1.24016
C	-0.45844 -3.54844 1.32996
C	-3.81948 -0.70148 -0.87847
C	0.44772 2.69481 0.05505
C	-3.52615 0.53851 -0.07814
C	-2.05162 2.46354 0.43293
C	-0.83432 3.15129 0.40988
C	-2.33761 1.21608 -0.18806
C	1.51645 3.72472 -0.15315
C	-4.64296 0.98859 0.80631
H	2.41525 -0.92464 -1.58464
H	4.08688 -1.87523 0.07779
H	1.0801 -1.05208 1.16729
H	2.04668 -2.43158 0.65267
H	0.68482 -2.84072 -1.31153
H	-0.05301 -1.23581 -1.24555
H	2.75737 1.51197 -0.85565
H	4.7461 0.91394 -1.07529
H	5.91327 -0.33013 -0.62939
H	4.7933 -0.61179 -1.96515
H	3.86956 0.90219 1.41976
H	5.07269 -0.33789 1.79006
H	3.36175 -0.62493 2.13338
H	-2.91001 -2.83415 0.50867
H	0.0331 0.6003 0.31909
H	-1.78184 -0.91091 -1.63009

H	-2.86658	-2.23623	-2.08164
H	0.34508	-4.24159	1.05037
H	-1.3043	-4.15593	1.67533
H	-0.10701	-2.96647	2.1935
H	-4.56188	-1.33139	-0.34528
H	-4.32625	-0.38228	-1.81637
H	-2.88824	2.96744	0.92894
H	-0.89398	4.20496	0.71389
H	-1.55185	0.78875	-0.82349
H	1.88755	3.69393	-1.18737
H	2.37266	3.55133	0.51301
H	1.16624	4.74786	0.02999
H	-4.69736	0.35703	1.70534
H	-5.6165	0.93275	0.30324
H	-4.51501	2.02519	1.15122

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.457668 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.480478
Thermal correction to Enthalpy=	0.481422
Thermal correction to Gibbs Free Frequency and Energy=	0.406134
Sum of electronic and zero-point Energies=	-780.471259
Sum of electronic and thermal Energies=	-780.448449
Sum of electronic and thermal Enthalpies=	-780.447505
Sum of electronic and thermal Free Energies=	-780.522793

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.457137 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.479927
Thermal correction to Enthalpy=	0.480871
Thermal correction to Gibbs Free Frequency and Energy=	0.405856
Sum of electronic and zero-point Energies=	-780.476088
Sum of electronic and thermal Energies=	-780.453297
Sum of electronic and thermal Enthalpies=	-780.452353
Sum of electronic and thermal Free Energies=	-780.527368

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.457159 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.479953
Thermal correction to Enthalpy=	0.480897
Thermal correction to Gibbs Free Frequency and Energy=	0.405859
Sum of electronic and zero-point Energies=	-780.475806
Sum of electronic and thermal Energies=	-780.453013
Sum of electronic and thermal Enthalpies=	-780.452068
Sum of electronic and thermal Free Energies=	-780.527106

Name of anion	Cembrene-C16-H43-anion

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	2.45892	-0.67307	-0.48048
C	3.86779	-0.79928	0.19041
C	1.43282	-1.60712	0.18888
C	0.27498	-2.02686	-0.74165

C	2.01748	0.76734	-0.59261
C	4.96978	-0.09121	-0.61083
C	3.87997	-0.34207	1.65566
C	-0.87849	-2.7048	-0.02946
C	0.88941	1.31872	-0.08345
C	-2.16978	-2.42692	-0.25055
C	-2.79836	-1.48678	-1.24466
C	-0.50194	-3.79012	0.95367
C	-3.9035	-0.59466	-0.64408
C	0.54765	2.71785	-0.10489
C	-3.50633	0.63675	0.14641
C	-1.92349	2.54036	0.485
C	-0.70066	3.19672	0.3101
C	-2.31312	1.27148	-0.03692
C	1.60031	3.71992	-0.51024
C	-4.58586	1.13454	1.06879
H	2.60656	-1.03892	-1.50964
H	4.10022	-1.87221	0.17402
H	1.02941	-1.1369	1.09075
H	1.95695	-2.50553	0.52882
H	0.68108	-2.717	-1.49553
H	-0.08042	-1.15555	-1.29343
H	2.69832	1.40869	-1.14515
H	4.86826	0.99699	-0.56965
H	5.95527	-0.33946	-0.2062
H	4.95738	-0.39205	-1.66322
H	3.63342	0.72031	1.73976
H	4.87031	-0.49197	2.09573
H	3.16203	-0.89825	2.26346
H	-2.89942	-2.99978	0.32284
H	0.18858	0.67728	0.43821
H	-2.05525	-0.88528	-1.77106
H	-3.27516	-2.10029	-2.02132
H	0.12323	-4.55311	0.47343
H	-1.3876	-4.28541	1.35588
H	0.076	-3.3971	1.79604
H	-4.54684	-1.22217	-0.01322
H	-4.56041	-0.25503	-1.45946
H	-2.6902	3.12505	0.98359
H	-0.73198	4.26421	0.52254
H	-1.6071	0.80393	-0.71209
H	1.83469	3.63849	-1.57884
H	2.53912	3.56553	0.03222
H	1.26195	4.74199	-0.33084
H	-4.78939	0.39052	1.84868
H	-5.52764	1.2767	0.52413
H	-4.33697	2.07154	1.56497

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction= 0.454618 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.477362
Thermal correction to Enthalpy= 0.478306

Thermal correction to Gibbs Free Frequency and Energy=	0.404164
Sum of electronic and zero-point Energies=	-780.508925
Sum of electronic and thermal Energies=	-780.486181
Sum of electronic and thermal Enthalpies=	-780.485236
Sum of electronic and thermal Free Energies=	-780.559379
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.454618 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.477362
Thermal correction to Enthalpy=	0.478306
Thermal correction to Gibbs Free Frequency and Energy=	0.404164
Sum of electronic and zero-point Energies=	-780.508925
Sum of electronic and thermal Energies=	-780.486181
Sum of electronic and thermal Enthalpies=	-780.485236
Sum of electronic and thermal Free Energies=	-780.559379
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.454670 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.477455
Thermal correction to Enthalpy=	0.478399
Thermal correction to Gibbs Free Frequency and Energy=	0.403988
Sum of electronic and zero-point Energies=	-780.574666
Sum of electronic and thermal Energies=	-780.551881
Sum of electronic and thermal Enthalpies=	-780.550937
Sum of electronic and thermal Free Energies=	-780.625348

Name of cationic radical	Cembrene		
Cartesian Coordinates optimized at PM6			
C	0	-2.1112	1.3223	-0.3894
C	0	-3.2334	1.5719	0.6235
C	0	-0.7914	1.9457	0.1205
C	0	0.3131	1.9814	-0.9517
C	0	-2.0842	-0.1545	-0.7302
C	0	-4.5843	1.1954	0.0237
C	0	-2.9744	0.7902	1.9074
C	0	1.6395	2.502	-0.4328
C	0	-1.2489	-1.0765	-0.2227
C	0	2.817	1.8507	-0.5204
C	0	3.1163	0.5206	-1.1551
C	0	1.6038	3.8767	0.1886
C	0	3.6482	-0.525	-0.1642
C	0	-1.2074	-2.4965	-0.5621
C	0	2.5623	-1.1575	0.6849
C	0	0.8268	-3.0255	0.917
C	0	-0.2821	-3.3394	-0.0553
C	0	1.9593	-2.2864	0.2605
C	0	-2.2353	-3.0281	-1.5296
C	0	2.2663	-0.4675	1.9874
H	0	-2.3622	1.8539	-1.3186
H	0	-3.2657	2.6417	0.8672
H	0	-0.4106	1.4208	1.0025
H	0	-0.9991	2.9749	0.4405
H	0	-0.0107	2.6308	-1.7752

H	0	0.4255	0.9853	-1.3838
H	0	-2.8158	-0.4547	-1.4774
H	0	-4.7	0.1166	-0.1223
H	0	-5.392	1.5125	0.6935
H	0	-4.745	1.6942	-0.938
H	0	-3.0368	-0.2938	1.7739
H	0	-3.7418	1.0484	2.6477
H	0	-2.0139	1.0335	2.3683
H	0	-0.5309	-0.7484	0.5212
H	0	3.6989	2.3434	-0.1109
H	0	2.2656	0.1154	-1.7099
H	0	3.8964	0.6998	-1.9067
H	0	1.0999	4.5826	-0.4799
H	0	2.6067	4.273	0.3815
H	0	1.0709	3.855	1.1442
H	0	4.4284	-0.0958	0.4772
H	0	4.1538	-1.3103	-0.7429
H	0	0.4089	-2.4989	1.7794
H	0	1.2178	-3.9737	1.3064
H	0	-0.3129	-4.3829	-0.368
H	0	2.2982	-2.717	-0.682
H	0	-2.1389	-2.5401	-2.5055
H	0	-3.2487	-2.863	-1.1476
H	0	-2.1286	-4.1056	-1.6977
H	0	1.7219	0.4644	1.8186
H	0	3.1992	-0.2307	2.5105
H	0	1.6773	-1.0792	2.6744

Frequency and Energy at PM6 (gas)

Zero-point correction= 0.432040 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.456723
Thermal correction to Enthalpy= 0.457667
Thermal correction to Gibbs Free Frequency and Energy= 0.375284
Sum of electronic and zero-point Energies= 0.688202
Sum of electronic and thermal Energies= 0.712885
Sum of electronic and thermal Enthalpies= 0.713829
Sum of electronic and thermal Free Energies= 0.631445

Name of compound	Kaur-16-ene

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	-1.3861	-0.85024	-0.43502
C	-0.69486	0.53889	-0.62098
C	0.69209	0.68755	0.09972
C	1.57447	-0.51605	-0.36489
C	-0.41688	-2.0127	-0.69542
C	-2.58366	-0.87988	-1.4384
C	0.90994	-1.83947	0.05109
C	-3.58207	0.06511	-0.73117
C	3.08574	-0.448	0.01637
C	-1.66842	1.68408	-0.25976
C	-2.1216	-0.99583	0.93243

C	1.36648	1.99646	-0.39956
C	-3.06967	1.51352	-0.87518
C	-3.47874	-0.36741	0.72605
C	0.52096	0.77323	1.62238
C	3.66052	0.93008	-0.40936
C	2.81803	2.11177	0.07624
C	3.84457	-1.53228	-0.7904
C	3.35801	-0.69977	1.50781
C	-4.42373	-0.22214	1.6502
H	-0.48178	0.62453	-1.71824
H	1.5633	-0.47958	-1.48845
H	-0.2215	-2.09431	-1.78273
H	-0.88755	-2.97196	-0.41003
H	-2.31134	-0.53859	-2.44498
H	-2.99661	-1.89368	-1.54776
H	1.57787	-2.69357	-0.17238
H	0.74254	-1.86272	1.14387
H	-4.60964	-0.0301	-1.12976
H	-1.24233	2.65015	-0.58768
H	-1.76799	1.75447	0.84169
H	-2.22461	-2.05737	1.21686
H	-1.55944	-0.51402	1.75489
H	1.33594	2.03613	-1.50442
H	0.79113	2.87362	-0.05082
H	-3.7744	2.21046	-0.38526
H	-3.05238	1.78987	-1.94518
H	-0.02424	1.67656	1.91465
H	-0.03597	-0.08975	2.01506
H	1.4944	0.79718	2.13467
H	4.6959	1.03073	-0.03566
H	3.73689	0.96882	-1.51312
H	3.25702	3.05834	-0.29295
H	2.85239	2.17499	1.18097
H	3.71136	-1.40656	-1.86861
H	4.91855	-1.50097	-0.58523
H	3.49181	-2.53715	-0.53318
H	2.85992	0.05413	2.13612
H	2.9944	-1.68129	1.82519
H	4.42801	-0.65725	1.73197
H	-4.30963	-0.54106	2.67304
H	-5.38263	0.22852	1.45469

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction= 0.479594 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.497997
Thermal correction to Enthalpy= 0.498941
Thermal correction to Gibbs Free Frequency and Energy= 0.436358
Sum of electronic and zero-point Energies= -781.112406
Sum of electronic and thermal Energies= -781.094004
Sum of electronic and thermal Enthalpies= -781.093060
Sum of electronic and thermal Free Energies= -781.155643

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.478815 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.497229
Thermal correction to Enthalpy=	0.498174
Thermal correction to Gibbs Free Frequency and Energy=	0.435597
Sum of electronic and zero-point Energies=	-781.114914
Sum of electronic and thermal Energies=	-781.096500
Sum of electronic and thermal Enthalpies=	-781.095555
Sum of electronic and thermal Free Energies=	-781.158132
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.478857 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.497271
Thermal correction to Enthalpy=	0.498215
Thermal correction to Gibbs Free Frequency and Energy=	0.435638
Sum of electronic and zero-point Energies=	-781.114779
Sum of electronic and thermal Energies=	-781.096365
Sum of electronic and thermal Enthalpies=	-781.095421
Sum of electronic and thermal Free Energies=	-781.157998

Name of radical	Kaur-16-ene-C11-H32

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-1.4082	-0.85072	-0.37811
C	-0.69444	0.53524	-0.54282
C	0.70403	0.68647	0.17789
C	1.58538	-0.52482	-0.2999
C	-0.42695	-2.00484	-0.62914
C	-2.5755	-0.8987	-1.39837
C	0.92089	-1.85959	0.08181
C	-3.59284	0.0731	-0.78249
C	3.12597	-0.45459	-0.01309
C	-1.68371	1.68857	-0.25567
C	-2.20724	-0.97497	0.95769
C	1.36646	1.99921	-0.32129
C	-3.04609	1.50857	-0.95057
C	-3.56949	-0.34517	0.67882
C	0.56341	0.77421	1.71596
C	3.65035	0.92307	-0.48866
C	2.85207	2.11595	0.03913
C	3.84776	-1.52617	-0.86198
C	3.51703	-0.70239	1.45872
C	-4.56832	-0.21183	1.54931
H	-0.44797	0.59478	-1.61269
H	1.53218	-0.47153	-1.39828
H	-0.23316	-2.05897	-1.70857
H	-0.90777	-2.9513	-0.35567
H	-2.263	-0.61419	-2.40737
H	-2.98428	-1.91499	-1.44554
H	1.55776	-2.70018	-0.20454
H	0.78881	-1.93535	1.16538
H	-4.59305	-0.00095	-1.217

H	-1.25155	2.64277	-0.56551
H	-1.85953	1.76908	0.82065
H	-1.72049	-0.51807	1.81811
H	1.27019	2.04811	-1.41398
H	0.82799	2.86411	0.07747
H	-3.75995	2.23262	-0.54472
H	-2.95329	1.7169	-2.02321
H	-0.23202	1.46842	1.99384
H	0.34258	-0.18541	2.18344
H	1.47485	1.1507	2.17841
H	4.70745	1.01895	-0.21423
H	3.61321	0.94186	-1.58598
H	3.25397	3.04184	-0.38664
H	2.97806	2.2087	1.1228
H	3.54562	-1.47052	-1.91257
H	4.93032	-1.36994	-0.81648
H	3.65176	-2.5403	-0.50594
H	3.1886	0.08987	2.13035
H	3.10381	-1.64474	1.82833
H	4.60683	-0.76863	1.54125
H	-4.47464	-0.53565	2.58175
H	-5.51857	0.22546	1.25815

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction= 0.465622 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.484106
Thermal correction to Enthalpy= 0.485050
Thermal correction to Gibbs Free Frequency and Energy= 0.421712
Sum of electronic and zero-point Energies= -780.483705
Sum of electronic and thermal Energies= -780.465220
Sum of electronic and thermal Enthalpies= -780.464276
Sum of electronic and thermal Free Energies= -780.527614

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction= 0.464920 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.483405
Thermal correction to Enthalpy= 0.484349
Thermal correction to Gibbs Free Frequency and Energy= 0.421051
Sum of electronic and zero-point Energies= -780.486295
Sum of electronic and thermal Energies= -780.467809
Sum of electronic and thermal Enthalpies= -780.466865
Sum of electronic and thermal Free Energies= -780.530164

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction= 0.464959 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.483444
Thermal correction to Enthalpy= 0.484389
Thermal correction to Gibbs Free Frequency and Energy= 0.421087
Sum of electronic and zero-point Energies= -780.486150
Sum of electronic and thermal Energies= -780.467665
Sum of electronic and thermal Enthalpies= -780.466721
Sum of electronic and thermal Free Energies= -780.530022

Name of anion	Kaur-16-ene-C11-H32-anion

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	-1.42072	-0.8617	-0.39621
C	-0.70644	0.53378	-0.58465
C	0.6758	0.68454	0.15703
C	1.56667	-0.52696	-0.30552
C	-0.44398	-2.02455	-0.62209
C	-2.60214	-0.90289	-1.40454
C	0.90695	-1.86337	0.08006
C	-3.61449	0.03853	-0.73428
C	3.1048	-0.4518	-0.00209
C	-1.7029	1.68693	-0.30583
C	-2.20516	-0.91519	0.90062
C	1.34556	1.99998	-0.32332
C	-3.10228	1.48362	-0.92335
C	-3.49506	-0.40088	0.72899
C	0.49424	0.76316	1.69008
C	3.63151	0.93065	-0.46042
C	2.8231	2.11684	0.0664
C	3.83933	-1.5154	-0.84994
C	3.48176	-0.70769	1.47216
C	-4.48349	-0.27798	1.67641
H	-0.4542	0.57529	-1.654
H	1.52425	-0.48031	-1.40483
H	-0.25967	-2.10613	-1.70144
H	-0.9267	-2.96111	-0.32113
H	-2.31038	-0.58344	-2.40981
H	-2.99599	-1.9225	-1.46722
H	1.5473	-2.702	-0.20419
H	0.78183	-1.93509	1.16462
H	-4.63259	-0.06204	-1.11908
H	-1.29113	2.63179	-0.6686
H	-1.83227	1.80068	0.77231
H	-1.81302	-1.27253	1.84507
H	1.2709	2.05376	-1.41767
H	0.7961	2.86146	0.06741
H	-3.79805	2.19938	-0.47349
H	-3.07827	1.69961	-1.99802
H	-0.26202	1.50456	1.95296
H	0.18848	-0.18322	2.13524
H	1.41325	1.07015	2.18709
H	4.68467	1.02708	-0.17177
H	3.61025	0.95889	-1.558
H	3.23175	3.04806	-0.34054
H	2.92782	2.1973	1.15328
H	3.55136	-1.45315	-1.90404
H	4.9209	-1.35829	-0.79069
H	3.64214	-2.53289	-0.5046
H	3.14681	0.08027	2.14561
H	3.06719	-1.65209	1.83416
H	4.57052	-0.77325	1.56556

H	-4.32541	-0.60383	2.69837
H	-5.45421	0.13591	1.43049

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.461871 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.480714
Thermal correction to Enthalpy=	0.481659
Thermal correction to Gibbs Free Frequency and Energy=	0.418228
Sum of electronic and zero-point Energies=	-780.500865
Sum of electronic and thermal Energies=	-780.482022
Sum of electronic and thermal Enthalpies=	-780.481078
Sum of electronic and thermal Free Energies=	-780.544508

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.461925 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.480767
Thermal correction to Enthalpy=	0.481711
Thermal correction to Gibbs Free Frequency and Energy=	0.418536
Sum of electronic and zero-point Energies=	-780.576509
Sum of electronic and thermal Energies=	-780.557666
Sum of electronic and thermal Enthalpies=	-780.556722
Sum of electronic and thermal Free Energies=	-780.619898

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.461919 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.480795
Thermal correction to Enthalpy=	0.481739
Thermal correction to Gibbs Free Frequency and Energy=	0.418364
Sum of electronic and zero-point Energies=	-780.573846
Sum of electronic and thermal Energies=	-780.554971
Sum of electronic and thermal Enthalpies=	-780.554027
Sum of electronic and thermal Free Energies=	-780.617402

Name of cationic radical	Kaur-16-ene		
Cartesian Coordinates optimized at PM6			
C	0	1.7632	0.7543	-0.019
C	0	1.0599	-0.5607	0.5396
C	0	-0.5039	-0.674	0.2253
C	0	-0.7563	-0.4354	-1.3336
C	0	1.5234	0.8378	-1.5553
C	0	3.2826	0.7355	0.3271
C	0	0.0169	0.7974	-1.9135
C	0	3.2083	1.0164	1.8472
C	0	-2.2524	-0.616	-1.8545
C	0	1.5209	-0.9815	1.9918
C	0	1.4427	2.1099	0.6907
C	0	-1.0173	-2.1393	0.5087
C	0	2.795	-0.2935	2.5754
C	0	2.2019	2.0621	1.9159

C	0	-1.303	0.3108	1.1656
C	0	-2.7625	-2.034	-1.4004
C	0	-2.4791	-2.4371	0.0683
C	0	-2.3351	-0.6076	-3.4243
C	0	-3.2444	0.5025	-1.373
C	0	1.9933	2.8882	2.9511
H	0	1.5196	-1.3507	-0.069
H	0	-0.2194	-1.2542	-1.8316
H	0	2.0285	0.0015	-2.05
H	0	1.9692	1.7418	-1.9808
H	0	3.7747	-0.2106	0.0832
H	0	3.8566	1.5158	-0.1895
H	0	-0.0092	0.7929	-3.0055
H	0	-0.4462	1.7313	-1.595
H	0	4.1759	1.3719	2.2158
H	0	1.6848	-2.0645	2.0231
H	0	0.7287	-0.8359	2.7235
H	0	1.7951	2.9727	0.1145
H	0	0.3894	2.3036	0.853
H	0	-0.3797	-2.8648	-0.0075
H	0	-0.9362	-2.3869	1.5702
H	0	2.6652	-0.0939	3.6435
H	0	3.6387	-0.9868	2.5083
H	0	-0.769	0.6233	2.0599
H	0	-1.5698	1.2362	0.6642
H	0	-2.2327	-0.0869	1.5674
H	0	-3.8392	-2.1289	-1.5775
H	0	-2.2939	-2.8117	-2.012
H	0	-2.6777	-3.506	0.1912
H	0	-3.1951	-1.9393	0.7235
H	0	-1.64	-1.3208	-3.8724
H	0	-3.3341	-0.8739	-3.781
H	0	-2.1183	0.3744	-3.8484
H	0	-3.6254	0.3231	-0.3684
H	0	-2.7825	1.4903	-1.3822
H	0	-4.1376	0.5892	-1.9961
H	0	1.2852	3.5841	2.9173
H	0	2.5403	2.8275	3.7752

Frequency and Energy at PM6 (gas)

Zero-point correction= 0.439829 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.458962
Thermal correction to Enthalpy= 0.459906
Thermal correction to Gibbs Free Frequency and Energy= 0.395287
Sum of electronic and zero-point Energies= 0.675553
Sum of electronic and thermal Energies= 0.694686
Sum of electronic and thermal Enthalpies= 0.695630
Sum of electronic and thermal Free Energies= 0.631012

Name of compound	Abieta-7,13-diene

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	1.1298	0.646	-0.2869
C	1.9519	-0.5798	0.2604
C	3.5183	-0.4439	0.2893
C	-0.3685	0.4255	0.1847
C	1.6745	1.955	0.3401
C	3.9094	0.934	0.876
C	1.4397	-1.898	-0.3617
C	3.1873	2.1045	0.2219
C	1.1811	0.7758	-1.8294
C	-0.8876	-0.9784	-0.1122
C	-1.3608	1.4812	-0.3468
C	-0.0583	-2.0056	-0.3673
C	4.1084	-1.5231	1.2356
C	4.2155	-0.6446	-1.0707
C	-2.7722	1.2555	0.2054
C	-2.3276	-1.1798	-0.0817
C	-3.2107	-0.1811	0.0908
C	-4.6871	-0.4324	0.1777
C	-5.2201	0.0178	1.5337
C	-5.4229	0.2714	-0.9588
H	1.6754	-0.6382	1.3276
H	-0.3776	0.5172	1.2827
H	1.4089	1.9908	1.4051
H	1.2029	2.8303	-0.122
H	4.9927	1.0895	0.7929
H	3.6828	0.951	1.951
H	1.8292	-2.7493	0.207
H	1.7891	-2.0143	-1.3926
H	3.4858	2.2067	-0.8263
H	3.4924	3.0334	0.7187
H	2.1945	0.8706	-2.2132
H	0.7179	-0.074	-2.339
H	0.6583	1.6771	-2.168
H	-1.4145	1.442	-1.4419
H	-1.0385	2.4922	-0.0765
H	-0.4611	-2.9922	-0.5858
H	3.6386	-1.4878	2.225
H	3.9736	-2.533	0.8348
H	5.1851	-1.3742	1.3803
H	5.3058	-0.6459	-0.9461
H	3.9535	-1.6026	-1.529
H	3.9999	0.1467	-1.7869
H	-3.4413	1.9318	-0.3339
H	-2.7964	1.553	1.261
H	-2.6872	-2.2009	-0.185
H	-4.8846	-1.5084	0.083
H	-5.1568	1.1032	1.6678
H	-4.6717	-0.4587	2.3542
H	-6.2749	-0.2603	1.6377
H	-4.9665	0.0497	-1.9299
H	-5.4588	1.3585	-0.8347

H	-6.4625	-0.0742	-0.9997

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.476133 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.496461
Thermal correction to Enthalpy=	0.497405
Thermal correction to Gibbs Free Frequency and Energy=	0.429657
Sum of electronic and zero-point Energies=	-781.125258
Sum of electronic and thermal Energies=	-781.104931
Sum of electronic and thermal Enthalpies=	-781.103986
Sum of electronic and thermal Free Energies=	-781.171734
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.475352 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.495690
Thermal correction to Enthalpy=	0.496634
Thermal correction to Gibbs Free Frequency and Energy=	0.428905
Sum of electronic and zero-point Energies=	-781.128306
Sum of electronic and thermal Energies=	-781.107969
Sum of electronic and thermal Enthalpies=	-781.107025
Sum of electronic and thermal Free Energies=	-781.174754
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.475395 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.495732
Thermal correction to Enthalpy=	0.496676
Thermal correction to Gibbs Free Frequency and Energy=	0.428945
Sum of electronic and zero-point Energies=	-781.128133
Sum of electronic and thermal Energies=	-781.107796
Sum of electronic and thermal Enthalpies=	-781.106852
Sum of electronic and thermal Free Energies=	-781.174583

Name of radical	Abieta-7,13-diene-C7-H27

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-1.09814	0.59583	0.17388
C	-1.96759	-0.5761	-0.39827
C	-3.50702	-0.44359	-0.18593
C	0.35398	0.36634	-0.38082
C	-1.65146	1.9357	-0.36951
C	-3.96849	0.95822	-0.66701
C	-1.4064	-1.8923	0.0461
C	-3.14488	2.10188	-0.06965
C	-1.06775	0.62377	1.70793
C	0.87267	-1.00636	-0.01932
C	1.3463	1.45486	0.07215
C	-0.05409	-2.0703	0.1831
C	-4.21794	-1.49703	-1.0707
C	-3.93713	-0.67735	1.27013
C	2.76077	1.16634	-0.45207
C	2.27363	-1.22511	0.07908
C	3.20116	-0.22667	-0.11777
C	4.68128	-0.5122	-0.01172

C	5.42232	-0.08078	-1.28481
C	5.26801	0.17149	1.23181
H	-1.82168	-0.54202	-1.51721
H	0.29958	0.39835	-1.50161
H	-1.48432	1.99621	-1.46132
H	-1.08933	2.78071	0.06945
H	-5.03677	1.09964	-0.42015
H	-3.9084	1.0045	-1.77134
H	-2.10328	-2.70275	0.22431
H	-3.30741	2.15535	1.02446
H	-3.50105	3.06815	-0.47499
H	-2.07667	0.74974	2.12699
H	-0.66182	-0.31065	2.11377
H	-0.44721	1.44212	2.08509
H	1.36836	1.50208	1.17927
H	1.01154	2.44816	-0.27593
H	0.33988	-3.04708	0.46304
H	-3.94153	-1.39958	-2.12451
H	-3.96442	-2.51615	-0.76126
H	-5.30589	-1.40069	-1.00547
H	-5.0244	-0.6375	1.38017
H	-3.60068	-1.65171	1.63814
H	-3.50727	0.08437	1.9384
H	3.46949	1.9122	-0.04106
H	2.79303	1.29375	-1.55517
H	2.60985	-2.2342	0.32125
H	4.82911	-1.61834	0.10634
H	5.40882	1.0057	-1.419
H	4.96854	-0.52946	-2.17561
H	6.47172	-0.39221	-1.25308
H	4.72474	-0.12581	2.13621
H	5.21153	1.263	1.16139
H	6.32051	-0.09572	1.36988

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.462679 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.482934
Thermal correction to Enthalpy=	0.483878
Thermal correction to Gibbs Free Frequency and Energy=	0.415594
Sum of electronic and zero-point Energies=	-780.508407
Sum of electronic and thermal Energies=	-780.488151
Sum of electronic and thermal Enthalpies=	-780.487207
Sum of electronic and thermal Free Energies=	-780.555492

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.461948 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.482219
Thermal correction to Enthalpy=	0.483164
Thermal correction to Gibbs Free Frequency and Energy=	0.414876
Sum of electronic and zero-point Energies=	-780.511696
Sum of electronic and thermal Energies=	-780.491425
Sum of electronic and thermal Enthalpies=	-780.490481

Sum of electronic and thermal Free Energies= -780.558769
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)
Zero-point correction= 0.461993 (Hartree/Particle) Thermal correction to Frequency and Energy= 0.482260 Thermal correction to Enthalpy= 0.483205 Thermal correction to Gibbs Free Frequency and Energy= 0.414928 Sum of electronic and zero-point Energies= -780.511503 Sum of electronic and thermal Energies= -780.491235 Sum of electronic and thermal Enthalpies= -780.490291 Sum of electronic and thermal Free Energies= -780.558567

Name of anion	Abieta-7,13-diene-C7-H27-anion
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)	
Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction= 0.458642 (Hartree/Particle) Thermal correction to Frequency and Energy= 0.479188 Thermal correction to Enthalpy= 0.480132 Thermal correction to Gibbs Free Frequency and Energy= 0.411886 Sum of electronic and zero-point Energies= -780.532116 Sum of electronic and thermal Energies= -780.511570 Sum of electronic and thermal Enthalpies= -780.510626 Sum of electronic and thermal Free Energies= -780.578873	
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction= 0.458276 (Hartree/Particle) Thermal correction to Frequency and Energy= 0.478879 Thermal correction to Enthalpy= 0.479823 Thermal correction to Gibbs Free Frequency and Energy= 0.411429 Sum of electronic and zero-point Energies= -780.598276 Sum of electronic and thermal Energies= -780.577674 Sum of electronic and thermal Enthalpies= -780.576730 Sum of electronic and thermal Free Energies= -780.645124	
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction= 0.458346 (Hartree/Particle) Thermal correction to Frequency and Energy= 0.478927 Thermal correction to Enthalpy= 0.479871 Thermal correction to Gibbs Free Frequency and Energy= 0.411600 Sum of electronic and zero-point Energies= -780.595881 Sum of electronic and thermal Energies= -780.575300 Sum of electronic and thermal Enthalpies= -780.574356 Sum of electronic and thermal Free Energies= -780.642627	

Name of cationic radical	Abieta-7,13-diene
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)	
C -1.1 0.60624 0.23379 C -1.94292 -0.57748 -0.34276	

C	-3.49339	-0.41691	-0.26333
C	0.37152	0.38035	-0.2659
C	-1.61516	1.94156	-0.36255
C	-3.89837	0.97445	-0.81914
C	-1.46346	-1.91027	0.26548
C	-3.12275	2.12039	-0.166
C	-1.13174	0.67367	1.76732
C	0.8668	-1.02344	0.0231
C	1.36109	1.41757	0.29899
C	0.02648	-2.05099	0.23626
C	-4.14732	-1.48719	-1.17204
C	-4.05657	-0.59586	1.15648
C	2.76666	1.20056	-0.27926
C	2.32205	-1.22863	0.00744
C	3.2107	-0.22804	-0.12687
C	4.70309	-0.50423	-0.13906
C	5.36011	0.05885	-1.40582
C	5.36005	0.05931	1.12818
H	-1.70405	-0.61335	-1.43921
H	0.36793	0.4854	-1.38332
H	-1.37884	1.98381	-1.44289
H	-1.07535	2.79041	0.09634
H	-4.98394	1.1286	-0.68023
H	-3.73124	0.99592	-1.91307
H	-1.9295	-2.75588	-0.28021
H	-1.81209	-2.00155	1.31607
H	-3.3629	2.1785	0.91291
H	-3.4452	3.08602	-0.59965
H	-2.16466	0.65787	2.14571
H	-0.60464	-0.1781	2.21258
H	-0.66122	1.58595	2.14431
H	1.40326	1.3346	1.40265
H	1.01376	2.44208	0.07571
H	0.39198	-3.05918	0.4176
H	-3.79003	-1.41917	-2.20368
H	-3.92952	-2.49976	-0.81752
H	-5.23579	-1.37842	-1.1927
H	-5.13762	-0.43183	1.18209
H	-3.86735	-1.60209	1.54282
H	-3.59532	0.11664	1.858
H	3.48288	1.88753	0.21302
H	2.78308	1.46683	-1.35686
H	2.65116	-2.26232	0.1161
H	4.86346	-1.61494	-0.14055
H	5.33803	1.15332	-1.42857
H	4.85187	-0.30126	-2.30749
H	6.40997	-0.24633	-1.47238
H	4.87643	-0.33374	2.03005
H	5.29323	1.15185	1.17154
H	6.42104	-0.20696	1.17482

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.437455 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.458857
Thermal correction to Enthalpy=	0.459801
Thermal correction to Gibbs Free Frequency and Energy=	0.387797
Sum of electronic and zero-point Energies=	0.635373
Sum of electronic and thermal Energies=	0.656775
Sum of electronic and thermal Enthalpies=	0.657719
Sum of electronic and thermal Free Energies=	0.585715

Name of compound	α-copanene

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-1.0246	-1.2509	0.2996
C	0.2109	0.4838	0.2294
C	0.4675	-0.9824	0.7082
C	-1.2518	0.2392	0.7298
C	0.4027	0.6963	-1.3157
C	-1.1842	-1.4402	-1.2504
C	-0.4422	-0.3693	-2.106
C	0.6853	-0.985	2.2672
C	-1.3313	0.4127	2.2083
C	-1.8072	-2.3906	1.0296
C	1.911	0.8267	-1.7534
C	-0.3642	-0.2016	2.9357
C	-2.4112	1.1813	2.7919
C	2.6944	1.9556	-1.0156
C	2.1242	1.0329	-3.2842
H	0.6975	1.2775	0.8035
H	1.2261	-1.55	0.1626
H	-2.0165	0.7819	0.1643
H	-0.0484	1.674	-1.5182
H	-0.8186	-2.4376	-1.5152
H	-2.2467	-1.4217	-1.511
H	-1.1732	0.1548	-2.7309
H	0.1719	-0.9311	-2.8093
H	1.665	-0.5627	2.5019
H	0.6715	-2.0151	2.6299
H	-2.8148	-2.499	0.6252
H	-1.279	-3.337	0.9053
H	-1.9317	-2.2344	2.0999
H	2.4087	-0.114	-1.4996
H	-0.3505	-0.1462	3.9281
H	-3.3695	0.7739	2.464
H	-2.3411	2.2192	2.4621
H	-2.4082	1.1747	3.8843
H	3.7347	2.0045	-1.3431
H	2.233	2.9284	-1.2
H	2.7442	1.7985	0.0611
H	3.186	1.1024	-3.5303
H	1.6309	1.9449	-3.6247

H	1.7493	0.2056	-3.8844

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.355240 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.370258
Thermal correction to Enthalpy=	0.371202
Thermal correction to Gibbs Free Frequency and Energy=	0.314738
Sum of electronic and zero-point Energies=	-585.814409
Sum of electronic and thermal Energies=	-585.799391
Sum of electronic and thermal Enthalpies=	-585.798447
Sum of electronic and thermal Free Energies=	-585.854912

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.354487 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.369539
Thermal correction to Enthalpy=	0.370484
Thermal correction to Gibbs Free Frequency and Energy=	0.313943
Sum of electronic and zero-point Energies=	-585.816233
Sum of electronic and thermal Energies=	-585.801181
Sum of electronic and thermal Enthalpies=	-585.800236
Sum of electronic and thermal Free Energies=	-585.856777

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.354527 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.369578
Thermal correction to Enthalpy=	0.370522
Thermal correction to Gibbs Free Frequency and Energy=	0.313984
Sum of electronic and zero-point Energies=	-585.816134
Sum of electronic and thermal Energies=	-585.801084
Sum of electronic and thermal Enthalpies=	-585.800139
Sum of electronic and thermal Free Energies=	-585.856678

Name of radical	α-copanene-C8-H24

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-1.0246	-1.2509	0.2996
C	0.2109	0.4838	0.2294
C	0.4675	-0.9824	0.7082
C	-1.2518	0.2392	0.7298
C	0.4027	0.6963	-1.3157
C	-1.1842	-1.4402	-1.2504
C	-0.4422	-0.3693	-2.106
C	0.6853	-0.985	2.2672
C	-1.3313	0.4127	2.2083
C	-1.8072	-2.3906	1.0296
C	1.911	0.8267	-1.7534
C	-0.3642	-0.2016	2.9357
C	-2.4112	1.1813	2.7919
C	2.6944	1.9556	-1.0156
C	2.1242	1.0329	-3.2842
H	0.6975	1.2775	0.8035

H	1.2261	-1.55	0.1626
H	-2.0165	0.7819	0.1643
H	-0.0484	1.674	-1.5182
H	-0.8186	-2.4376	-1.5152
H	-2.2467	-1.4217	-1.511
H	-1.1732	0.1548	-2.7309
H	0.1719	-0.9311	-2.8093
H	0.6715	-2.0151	2.6299
H	-2.8148	-2.499	0.6252
H	-1.279	-3.337	0.9053
H	-1.9317	-2.2344	2.0999
H	2.4087	-0.114	-1.4996
H	-0.3505	-0.1462	3.9281
H	-3.3695	0.7739	2.464
H	-2.3411	2.2192	2.4621
H	-2.4082	1.1747	3.8843
H	3.7347	2.0045	-1.3431
H	2.233	2.9284	-1.2
H	2.7442	1.7985	0.0611
H	3.186	1.1024	-3.5303
H	1.6309	1.9449	-3.6247
H	1.7493	0.2056	-3.8844

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction=	0.341708 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.356799
Thermal correction to Enthalpy=	0.357743
Thermal correction to Gibbs Free Frequency and Energy=	0.300387
Sum of electronic and zero-point Energies=	-585.187311
Sum of electronic and thermal Energies=	-585.172220
Sum of electronic and thermal Enthalpies=	-585.171276
Sum of electronic and thermal Free Energies=	-585.228632

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.341024 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.356145
Thermal correction to Enthalpy=	0.357089
Thermal correction to Gibbs Free Frequency and Energy=	0.299674
Sum of electronic and zero-point Energies=	-585.189481
Sum of electronic and thermal Energies=	-585.174359
Sum of electronic and thermal Enthalpies=	-585.173415
Sum of electronic and thermal Free Energies=	-585.230830

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.341061 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.356180
Thermal correction to Enthalpy=	0.357124
Thermal correction to Gibbs Free Frequency and Energy=	0.299711
Sum of electronic and zero-point Energies=	-585.189362
Sum of electronic and thermal Energies=	-585.174243
Sum of electronic and thermal Enthalpies=	-585.173299
Sum of electronic and thermal Free Energies=	-585.230712

Name of anion	α-copanene-C8-H24-anion

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	-1.0246	-1.2509	0.2996
C	0.2109	0.4838	0.2294
C	0.4675	-0.9824	0.7082
C	-1.2518	0.2392	0.7298
C	0.4027	0.6963	-1.3157
C	-1.1842	-1.4402	-1.2504
C	-0.4422	-0.3693	-2.106
C	0.6853	-0.985	2.2672
C	-1.3313	0.4127	2.2083
C	-1.8072	-2.3906	1.0296
C	1.911	0.8267	-1.7534
C	-0.3642	-0.2016	2.9357
C	-2.4112	1.1813	2.7919
C	2.6944	1.9556	-1.0156
C	2.1242	1.0329	-3.2842
H	0.6975	1.2775	0.8035
H	1.2261	-1.55	0.1626
H	-2.0165	0.7819	0.1643
H	-0.0484	1.674	-1.5182
H	-0.8186	-2.4376	-1.5152
H	-2.2467	-1.4217	-1.511
H	-1.1732	0.1548	-2.7309
H	0.1719	-0.9311	-2.8093
H	0.6715	-2.0151	2.6299
H	-2.8148	-2.499	0.6252
H	-1.279	-3.337	0.9053
H	-1.9317	-2.2344	2.0999
H	2.4087	-0.114	-1.4996
H	-0.3505	-0.1462	3.9281
H	-3.3695	0.7739	2.464
H	-2.3411	2.2192	2.4621
H	-2.4082	1.1747	3.8843
H	3.7347	2.0045	-1.3431
H	2.233	2.9284	-1.2
H	2.7442	1.7985	0.0611
H	3.186	1.1024	-3.5303
H	1.6309	1.9449	-3.6247
H	1.7493	0.2056	-3.8844

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction=	0.336909 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.352452
Thermal correction to Enthalpy=	0.353396
Thermal correction to Gibbs Free Frequency and Energy=	0.295660
Sum of electronic and zero-point Energies=	-585.191776
Sum of electronic and thermal Energies=	-585.176233
Sum of electronic and thermal Enthalpies=	-585.175288
Sum of electronic and thermal Free Energies=	-585.233024

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.337086 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.352576
Thermal correction to Enthalpy=	0.353521
Thermal correction to Gibbs Free Frequency and Energy=	0.295967
Sum of electronic and zero-point Energies=	-585.264389
Sum of electronic and thermal Energies=	-585.248898
Sum of electronic and thermal Enthalpies=	-585.247954
Sum of electronic and thermal Free Energies=	-585.305507

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.337133 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.352598
Thermal correction to Enthalpy=	0.353542
Thermal correction to Gibbs Free Frequency and Energy=	0.296093
Sum of electronic and zero-point Energies=	-585.261915
Sum of electronic and thermal Energies=	-585.246450
Sum of electronic and thermal Enthalpies=	-585.245506
Sum of electronic and thermal Free Energies=	-585.302955

Name of cationic radical	α-copanene

Cartesian Coordinates optimized at PM6			
C	-1.0246	-1.2509	0.2996
C	0.2109	0.4838	0.2294
C	0.4675	-0.9824	0.7082
C	-1.2518	0.2392	0.7298
C	0.4027	0.6963	-1.3157
C	-1.1842	-1.4402	-1.2504
C	-0.4422	-0.3693	-2.106
C	0.6853	-0.985	2.2672
C	-1.3313	0.4127	2.2083
C	-1.8072	-2.3906	1.0296
C	1.911	0.8267	-1.7534
C	-0.3642	-0.2016	2.9357
C	-2.4112	1.1813	2.7919
C	2.6944	1.9556	-1.0156
C	2.1242	1.0329	-3.2842
H	0.6975	1.2775	0.8035
H	1.2261	-1.55	0.1626
H	-2.0165	0.7819	0.1643
H	-0.0484	1.674	-1.5182
H	-0.8186	-2.4376	-1.5152
H	-2.2467	-1.4217	-1.511
H	-1.1732	0.1548	-2.7309
H	0.1719	-0.9311	-2.8093
H	1.665	-0.5627	2.5019
H	0.6715	-2.0151	2.6299
H	-2.8148	-2.499	0.6252
H	-1.279	-3.337	0.9053
H	-1.9317	-2.2344	2.0999

H	2.4087	-0.114	-1.4996
H	-0.3505	-0.1462	3.9281
H	-3.3695	0.7739	2.464
H	-2.3411	2.2192	2.4621
H	-2.4082	1.1747	3.8843
H	3.7347	2.0045	-1.3431
H	2.233	2.9284	-1.2
H	2.7442	1.7985	0.0611
H	3.186	1.1024	-3.5303
H	1.6309	1.9449	-3.6247
H	1.7493	0.2056	-3.8844

Frequency and Energy at PM6 (gas)

Zero-point correction= 0.325239 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.341356
Thermal correction to Enthalpy= 0.342300
Thermal correction to Gibbs Free Frequency and Energy= 0.281835
Sum of electronic and zero-point Energies= 0.590982
Sum of electronic and thermal Energies= 0.607098
Sum of electronic and thermal Enthalpies= 0.608043
Sum of electronic and thermal Free Energies= 0.547578

Name of compound	Sesquithujene

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	6.3391	-2.5497	-0.1321
C	7.6256	-3.3437	0.0582
C	6.2989	-4.0305	0.196
C	5.864	-1.5682	0.9321
C	8.2951	-3.3037	-1.2566
C	6.3028	-2.1238	-1.6039
C	7.5953	-2.6357	-2.195
C	4.3319	-1.4211	0.8319
C	6.5973	-0.2273	0.8185
C	9.5969	-3.9883	-1.4758
C	3.6983	-0.5361	1.9187
C	2.7126	0.4472	1.345
C	1.9888	1.3379	2.0503
C	1.0318	2.2592	1.3474
C	2.0938	1.4773	3.5411
H	8.227	-3.1602	0.9381
H	5.9827	-4.7236	-0.5767
H	5.9912	-4.3325	1.1904
H	6.1001	-1.9854	1.9202
H	6.2528	-1.0391	-1.7252
H	5.4431	-2.5727	-2.1135
H	3.8818	-2.4184	0.9166
H	4.0763	-1.0655	-0.1735
H	6.5436	0.3261	1.7611
H	6.168	0.4058	0.035
H	7.6622	-0.3702	0.6024
H	7.891	-2.4981	-3.2225

H	10.2164	-3.4406	-2.1935
H	9.4315	-4.9991	-1.8636
H	10.1592	-4.0686	-0.5402
H	4.4579	0.0068	2.4898
H	3.1771	-1.1802	2.6375
H	2.5726	0.4316	0.2664
H	1.5382	3.1902	1.0726
H	0.1773	2.5059	1.986
H	0.6317	1.8041	0.4345
H	1.4697	2.2952	3.9143
H	3.1249	1.6912	3.8393
H	1.7687	0.5571	4.0363

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction=	0.350662 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.367946
Thermal correction to Enthalpy=	0.368890
Thermal correction to Gibbs Free Frequency and Energy=	0.304680
Sum of electronic and zero-point Energies=	-585.803260
Sum of electronic and thermal Energies=	-585.785976
Sum of electronic and thermal Enthalpies=	-585.785032
Sum of electronic and thermal Free Energies=	-585.849242

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.349938 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.367269
Thermal correction to Enthalpy=	0.368213
Thermal correction to Gibbs Free Frequency and Energy=	0.303511
Sum of electronic and zero-point Energies=	-585.806435
Sum of electronic and thermal Energies=	-585.789104
Sum of electronic and thermal Enthalpies=	-585.788159
Sum of electronic and thermal Free Energies=	-585.852862

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.349978 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.367307
Thermal correction to Enthalpy=	0.368251
Thermal correction to Gibbs Free Frequency and Energy=	0.303556
Sum of electronic and zero-point Energies=	-585.806251
Sum of electronic and thermal Energies=	-585.788921
Sum of electronic and thermal Enthalpies=	-585.787977
Sum of electronic and thermal Free Energies=	-585.852672

Name of radical	Sesquithujene-C11-H31

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	6.3391	-2.5497	-0.1321
C	7.6256	-3.3437	0.0582
C	6.2989	-4.0305	0.196
C	5.864	-1.5682	0.9321
C	8.2951	-3.3037	-1.2566

C	6.3028	-2.1238	-1.6039
C	7.5953	-2.6357	-2.195
C	4.3319	-1.4211	0.8319
C	6.5973	-0.2273	0.8185
C	9.5969	-3.9883	-1.4758
C	3.6983	-0.5361	1.9187
C	2.7126	0.4472	1.345
C	1.9888	1.3379	2.0503
C	1.0318	2.2592	1.3474
C	2.0938	1.4773	3.5411
H	8.227	-3.1602	0.9381
H	5.9827	-4.7236	-0.5767
H	5.9912	-4.3325	1.1904
H	6.1001	-1.9854	1.9202
H	6.2528	-1.0391	-1.7252
H	5.4431	-2.5727	-2.1135
H	3.8818	-2.4184	0.9166
H	4.0763	-1.0655	-0.1735
H	6.5436	0.3261	1.7611
H	6.168	0.4058	0.035
H	7.6622	-0.3702	0.6024
H	7.891	-2.4981	-3.2225
H	10.2164	-3.4406	-2.1935
H	9.4315	-4.9991	-1.8636
H	10.1592	-4.0686	-0.5402
H	3.1771	-1.1802	2.6375
H	2.5726	0.4316	0.2664
H	1.5382	3.1902	1.0726
H	0.1773	2.5059	1.986
H	0.6317	1.8041	0.4345
H	1.4697	2.2952	3.9143
H	3.1249	1.6912	3.8393
H	1.7687	0.5571	4.0363

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.336764 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.354189
Thermal correction to Enthalpy=	0.355133
Thermal correction to Gibbs Free Frequency and Energy=	0.290080
Sum of electronic and zero-point Energies=	-585.178480
Sum of electronic and thermal Energies=	-585.161054
Sum of electronic and thermal Enthalpies=	-585.160110
Sum of electronic and thermal Free Energies=	-585.225163

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.336029 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.353504
Thermal correction to Enthalpy=	0.354449
Thermal correction to Gibbs Free Frequency and Energy=	0.289170
Sum of electronic and zero-point Energies=	-585.182051
Sum of electronic and thermal Energies=	-585.164575
Sum of electronic and thermal Enthalpies=	-585.163631

Sum of electronic and thermal Free Energies= -585.228909

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)
Zero-point correction= 0.336146 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.353589
Thermal correction to Enthalpy= 0.354533
Thermal correction to Gibbs Free Frequency and Energy= 0.289476
Sum of electronic and zero-point Energies= -585.181801
Sum of electronic and thermal Energies= -585.164359
Sum of electronic and thermal Enthalpies= -585.163415
Sum of electronic and thermal Free Energies= -585.228472

Name of anion	Sesquithujene-C11-H31-anion

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	6.3391	-2.5497	-0.1321
C	7.6256	-3.3437	0.0582
C	6.2989	-4.0305	0.196
C	5.864	-1.5682	0.9321
C	8.2951	-3.3037	-1.2566
C	6.3028	-2.1238	-1.6039
C	7.5953	-2.6357	-2.195
C	4.3319	-1.4211	0.8319
C	6.5973	-0.2273	0.8185
C	9.5969	-3.9883	-1.4758
C	3.6983	-0.5361	1.9187
C	2.7126	0.4472	1.345
C	1.9888	1.3379	2.0503
C	1.0318	2.2592	1.3474
C	2.0938	1.4773	3.5411
H	8.227	-3.1602	0.9381
H	5.9827	-4.7236	-0.5767
H	5.9912	-4.3325	1.1904
H	6.1001	-1.9854	1.9202
H	6.2528	-1.0391	-1.7252
H	5.4431	-2.5727	-2.1135
H	3.8818	-2.4184	0.9166
H	4.0763	-1.0655	-0.1735
H	6.5436	0.3261	1.7611
H	6.168	0.4058	0.035
H	7.6622	-0.3702	0.6024
H	7.891	-2.4981	-3.2225
H	10.2164	-3.4406	-2.1935
H	9.4315	-4.9991	-1.8636
H	10.1592	-4.0686	-0.5402
H	3.1771	-1.1802	2.6375
H	2.5726	0.4316	0.2664
H	1.5382	3.1902	1.0726
H	0.1773	2.5059	1.986
H	0.6317	1.8041	0.4345

H	1.4697	2.2952	3.9143
H	3.1249	1.6912	3.8393
H	1.7687	0.5571	4.0363

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction=	0.332245 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.349736
Thermal correction to Enthalpy=	0.350680
Thermal correction to Gibbs Free Frequency and Energy=	0.286396
Sum of electronic and zero-point Energies=	-585.186053
Sum of electronic and thermal Energies=	-585.168562
Sum of electronic and thermal Enthalpies=	-585.167618
Sum of electronic and thermal Free Energies=	-585.231901

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.332320 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.349920
Thermal correction to Enthalpy=	0.350864
Thermal correction to Gibbs Free Frequency and Energy=	0.286245
Sum of electronic and zero-point Energies=	-585.261178
Sum of electronic and thermal Energies=	-585.243578
Sum of electronic and thermal Enthalpies=	-585.242634
Sum of electronic and thermal Free Energies=	-585.307253

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.332240 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.349889
Thermal correction to Enthalpy=	0.350833
Thermal correction to Gibbs Free Frequency and Energy=	0.285787
Sum of electronic and zero-point Energies=	-585.258688
Sum of electronic and thermal Energies=	-585.241039
Sum of electronic and thermal Enthalpies=	-585.240095
Sum of electronic and thermal Free Energies=	-585.305141

Name of cationic radical	Sesquithujene

Cartesian Coordinates optimized at PM6

C	6.3391	-2.5497	-0.1321
C	7.6256	-3.3437	0.0582
C	6.2989	-4.0305	0.196
C	5.864	-1.5682	0.9321
C	8.2951	-3.3037	-1.2566
C	6.3028	-2.1238	-1.6039
C	7.5953	-2.6357	-2.195
C	4.3319	-1.4211	0.8319
C	6.5973	-0.2273	0.8185
C	9.5969	-3.9883	-1.4758
C	3.6983	-0.5361	1.9187
C	2.7126	0.4472	1.345
C	1.9888	1.3379	2.0503
C	1.0318	2.2592	1.3474
C	2.0938	1.4773	3.5411

H	8.227	-3.1602	0.9381
H	5.9827	-4.7236	-0.5767
H	5.9912	-4.3325	1.1904
H	6.1001	-1.9854	1.9202
H	6.2528	-1.0391	-1.7252
H	5.4431	-2.5727	-2.1135
H	3.8818	-2.4184	0.9166
H	4.0763	-1.0655	-0.1735
H	6.5436	0.3261	1.7611
H	6.168	0.4058	0.035
H	7.6622	-0.3702	0.6024
H	7.891	-2.4981	-3.2225
H	10.2164	-3.4406	-2.1935
H	9.4315	-4.9991	-1.8636
H	10.1592	-4.0686	-0.5402
H	4.4579	0.0068	2.4898
H	3.1771	-1.1802	2.6375
H	2.5726	0.4316	0.2664
H	1.5382	3.1902	1.0726
H	0.1773	2.5059	1.986
H	0.6317	1.8041	0.4345
H	1.4697	2.2952	3.9143
H	3.1249	1.6912	3.8393
H	1.7687	0.5571	4.0363

Frequency and Energy at PM6 (gas)

Zero-point correction=	0.319846 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.338734
Thermal correction to Enthalpy=	0.339678
Thermal correction to Gibbs Free Frequency and Energy=	0.267775
Sum of electronic and zero-point Energies=	0.613422
Sum of electronic and thermal Energies=	0.632310
Sum of electronic and thermal Enthalpies=	0.633254
Sum of electronic and thermal Free Energies=	0.561351

Name of compound	β-cedrene

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	-0.8539	-0.5105	0.1493
C	0.6662	-0.661	-0.1847
C	1.215	0.7627	-0.6023
C	-0.0172	1.6933	-0.2866
C	-1.2108	0.7739	-0.6629
C	-1.5333	-1.8343	-0.3366
C	0.7701	-1.885	-1.1491
C	-1.1684	-0.134	1.6464
C	-0.6661	-2.2755	-1.5394
C	-0.1823	2.1442	1.1192
C	-0.4377	1.138	2.1562
C	2.5192	1.1522	0.1783
C	1.6184	0.9005	-2.1171
C	-1.6444	-2.9837	0.7104
C	-0.0863	3.4399	1.469

H	1.1678	-0.984	0.7346
H	-0.0354	2.5588	-0.959
H	-2.1815	1.2115	-0.406
H	-1.2663	0.5983	-1.7408
H	-2.5533	-1.6316	-0.679
H	1.2431	-2.7307	-0.6407
H	1.3604	-1.7306	-2.0509
H	-2.249	0.0146	1.7477
H	-0.9075	-0.9436	2.3301
H	-0.9711	-1.7418	-2.4439
H	-0.7405	-3.3428	-1.7696
H	0.5223	0.8389	2.5821
H	-1.0165	1.5353	2.9972
H	3.3277	0.4492	-0.0347
H	2.8619	2.1563	-0.0816
H	2.3934	1.1385	1.2589
H	1.8807	1.9291	-2.3748
H	0.8196	0.6021	-2.7963
H	2.4894	0.289	-2.3642
H	-2.0325	-3.8984	0.26
H	-0.6721	-3.2095	1.1542
H	-2.3331	-2.7149	1.5128
H	-0.188	3.7354	2.4122
H	0.0918	4.1504	0.8018

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.357403 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.371454
Thermal correction to Enthalpy=	0.372398
Thermal correction to Gibbs Free Frequency and Energy=	0.318962
Sum of electronic and zero-point Energies=	-585.829945
Sum of electronic and thermal Energies=	-585.815894
Sum of electronic and thermal Enthalpies=	-585.814950
Sum of electronic and thermal Free Energies=	-585.868386

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.356810 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.370862
Thermal correction to Enthalpy=	0.371807
Thermal correction to Gibbs Free Frequency and Energy=	0.318391
Sum of electronic and zero-point Energies=	-585.832262
Sum of electronic and thermal Energies=	-585.818210
Sum of electronic and thermal Enthalpies=	-585.817265
Sum of electronic and thermal Free Energies=	-585.870681

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.356840 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.370894
Thermal correction to Enthalpy=	0.371838
Thermal correction to Gibbs Free Frequency and Energy=	0.318418
Sum of electronic and zero-point Energies=	-585.832137
Sum of electronic and thermal Energies=	-585.818083

Sum of electronic and thermal Enthalpies= -585.817139
Sum of electronic and thermal Free Energies= -585.870559

Name of radical	β-cedrene-C11-H27
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)	
C	-0.8539 -0.5105 0.1493
C	0.6662 -0.661 -0.1847
C	1.215 0.7627 -0.6023
C	-0.0172 1.6933 -0.2866
C	-1.2108 0.7739 -0.6629
C	-1.5333 -1.8343 -0.3366
C	0.7701 -1.885 -1.1491
C	-1.1684 -0.134 1.6464
C	-0.6661 -2.2755 -1.5394
C	-0.1823 2.1442 1.1192
C	-0.4377 1.138 2.1562
C	2.5192 1.1522 0.1783
C	1.6184 0.9005 -2.1171
C	-1.6444 -2.9837 0.7104
C	-0.0863 3.4399 1.469
H	1.1678 -0.984 0.7346
H	-0.0354 2.5588 -0.959
H	-2.1815 1.2115 -0.406
H	-1.2663 0.5983 -1.7408
H	-2.5533 -1.6316 -0.679
H	1.2431 -2.7307 -0.6407
H	1.3604 -1.7306 -2.0509
H	-2.249 0.0146 1.7477
H	-0.9075 -0.9436 2.3301
H	-0.9711 -1.7418 -2.4439
H	-0.7405 -3.3428 -1.7696
H	-1.0165 1.5353 2.9972
H	3.3277 0.4492 -0.0347
H	2.8619 2.1563 -0.0816
H	2.3934 1.1385 1.2589
H	1.8807 1.9291 -2.3748
H	0.8196 0.6021 -2.7963
H	2.4894 0.289 -2.3642
H	-2.0325 -3.8984 0.26
H	-0.6721 -3.2095 1.1542
H	-2.3331 -2.7149 1.5128
H	-0.188 3.7354 2.4122
H	0.0918 4.1504 0.8018
Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction= 0.343265 (Hartree/Particle)	
Thermal correction to Frequency and Energy= 0.357308	
Thermal correction to Enthalpy= 0.358252	
Thermal correction to Gibbs Free Frequency and Energy= 0.304192	
Sum of electronic and zero-point Energies= -585.203949	
Sum of electronic and thermal Energies= -585.189906	
Sum of electronic and thermal Enthalpies= -585.188962	

Sum of electronic and thermal Free Energies= -585.243022
Frequency and Energy at B3LYP/6-311G (d,p) (water)
Zero-point correction= 0.342665 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.356728
Thermal correction to Enthalpy= 0.357672
Thermal correction to Gibbs Free Frequency and Energy= 0.303579
Sum of electronic and zero-point Energies= -585.206271
Sum of electronic and thermal Energies= -585.192208
Sum of electronic and thermal Enthalpies= -585.191264
Sum of electronic and thermal Free Energies= -585.245357
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)
Zero-point correction= 0.342702 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.356762
Thermal correction to Enthalpy= 0.357707
Thermal correction to Gibbs Free Frequency and Energy= 0.303620
Sum of electronic and zero-point Energies= -585.206141
Sum of electronic and thermal Energies= -585.192080
Sum of electronic and thermal Enthalpies= -585.191136
Sum of electronic and thermal Free Energies= -585.245223

Name of anion	β-cedrene-C11-H27-anion

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-0.8539	-0.5105	0.1493
C	0.6662	-0.661	-0.1847
C	1.215	0.7627	-0.6023
C	-0.0172	1.6933	-0.2866
C	-1.2108	0.7739	-0.6629
C	-1.5333	-1.8343	-0.3366
C	0.7701	-1.885	-1.1491
C	-1.1684	-0.134	1.6464
C	-0.6661	-2.2755	-1.5394
C	-0.1823	2.1442	1.1192
C	-0.4377	1.138	2.1562
C	2.5192	1.1522	0.1783
C	1.6184	0.9005	-2.1171
C	-1.6444	-2.9837	0.7104
C	-0.0863	3.4399	1.469
H	1.1678	-0.984	0.7346
H	-0.0354	2.5588	-0.959
H	-2.1815	1.2115	-0.406
H	-1.2663	0.5983	-1.7408
H	-2.5533	-1.6316	-0.679
H	1.2431	-2.7307	-0.6407
H	1.3604	-1.7306	-2.0509
H	-2.249	0.0146	1.7477
H	-0.9075	-0.9436	2.3301
H	-0.9711	-1.7418	-2.4439
H	-0.7405	-3.3428	-1.7696

H	-1.0165	1.5353	2.9972
H	3.3277	0.4492	-0.0347
H	2.8619	2.1563	-0.0816
H	2.3934	1.1385	1.2589
H	1.8807	1.9291	-2.3748
H	0.8196	0.6021	-2.7963
H	2.4894	0.289	-2.3642
H	-2.0325	-3.8984	0.26
H	-0.6721	-3.2095	1.1542
H	-2.3331	-2.7149	1.5128
H	-0.188	3.7354	2.4122
H	0.0918	4.1504	0.8018

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction= 0.339421 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.353857
Thermal correction to Enthalpy= 0.354801
Thermal correction to Gibbs Free Frequency and Energy= 0.300709
Sum of electronic and zero-point Energies= -585.214966
Sum of electronic and thermal Energies= -585.200530
Sum of electronic and thermal Enthalpies= -585.199586
Sum of electronic and thermal Free Energies= -585.253677

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction= 0.339645 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.354061
Thermal correction to Enthalpy= 0.355005
Thermal correction to Gibbs Free Frequency and Energy= 0.301072
Sum of electronic and zero-point Energies= -585.292400
Sum of electronic and thermal Energies= -585.277984
Sum of electronic and thermal Enthalpies= -585.277040
Sum of electronic and thermal Free Energies= -585.330973

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction= 0.339667 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.354081
Thermal correction to Enthalpy= 0.355025
Thermal correction to Gibbs Free Frequency and Energy= 0.301107
Sum of electronic and zero-point Energies= -585.289711
Sum of electronic and thermal Energies= -585.275297
Sum of electronic and thermal Enthalpies= -585.274352
Sum of electronic and thermal Free Energies= -585.328270

Name of cationic radical	β-cedrene

Cartesian Coordinates optimized at PM6

C	-0.8539	-0.5105	0.1493
C	0.6662	-0.661	-0.1847
C	1.215	0.7627	-0.6023
C	-0.0172	1.6933	-0.2866
C	-1.2108	0.7739	-0.6629
C	-1.5333	-1.8343	-0.3366

C	0.7701	-1.885	-1.1491
C	-1.1684	-0.134	1.6464
C	-0.6661	-2.2755	-1.5394
C	-0.1823	2.1442	1.1192
C	-0.4377	1.138	2.1562
C	2.5192	1.1522	0.1783
C	1.6184	0.9005	-2.1171
C	-1.6444	-2.9837	0.7104
C	-0.0863	3.4399	1.469
H	1.1678	-0.984	0.7346
H	-0.0354	2.5588	-0.959
H	-2.1815	1.2115	-0.406
H	-1.2663	0.5983	-1.7408
H	-2.5533	-1.6316	-0.679
H	1.2431	-2.7307	-0.6407
H	1.3604	-1.7306	-2.0509
H	-2.249	0.0146	1.7477
H	-0.9075	-0.9436	2.3301
H	-0.9711	-1.7418	-2.4439
H	-0.7405	-3.3428	-1.7696
H	0.5223	0.8389	2.5821
H	-1.0165	1.5353	2.9972
H	3.3277	0.4492	-0.0347
H	2.8619	2.1563	-0.0816
H	2.3934	1.1385	1.2589
H	1.8807	1.9291	-2.3748
H	0.8196	0.6021	-2.7963
H	2.4894	0.289	-2.3642
H	-2.0325	-3.8984	0.26
H	-0.6721	-3.2095	1.1542
H	-2.3331	-2.7149	1.5128
H	-0.188	3.7354	2.4122
H	0.0918	4.1504	0.8018

Frequency and Energy at PM6 (gas)

Zero-point correction= 0.325779 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.341142
Thermal correction to Enthalpy= 0.342086
Thermal correction to Gibbs Free Frequency and Energy= 0.284535
Sum of electronic and zero-point Energies= 0.586350
Sum of electronic and thermal Energies= 0.601713
Sum of electronic and thermal Enthalpies= 0.602657
Sum of electronic and thermal Free Energies= 0.545105

Name of compound	6-Epi-beta-cubebene

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	-1.0038	0.5784	-0.4843
C	0.2024	-0.339	-0.6323
C	-0.7284	-0.5262	0.5287
C	-0.8111	2.043	-0.1284
C	1.6001	0.1805	-0.4288

C	-2.2813	0.2152	-1.2198
C	-1.8421	-1.481	0.4331
C	-2.9616	-0.8726	-0.3738
C	0.6535	2.4975	-0.2318
C	1.6337	1.4921	0.3639
C	2.4843	-0.8766	0.2304
C	-1.4169	2.3879	1.2347
C	-1.8729	-2.7259	0.9229
C	2.4183	-2.1901	-0.545
C	3.9258	-0.3833	0.3305
H	0.1592	-1.0451	-1.4564
H	-0.3933	-0.2763	1.5253
H	-1.3611	2.6415	-0.8675
H	1.9982	0.3956	-1.4312
H	-2.0405	-0.1679	-2.2187
H	-2.9551	1.0688	-1.3493
H	-3.4842	-1.5971	-1.0057
H	-3.6867	-0.4117	0.3073
H	0.7819	3.4734	0.2513
H	0.9046	2.6436	-1.2909
H	2.6318	1.9413	0.3189
H	1.4057	1.3248	1.4229
H	2.1271	-1.0803	1.2485
H	-0.8759	1.9131	2.0586
H	-1.3933	3.4698	1.4037
H	-2.4616	2.0636	1.2905
H	-1.0311	-3.1274	1.4767
H	-2.7378	-3.3645	0.7799
H	2.6517	-2.0435	-1.6052
H	3.1412	-2.9098	-0.1443
H	1.4354	-2.665	-0.4671
H	4.3031	-0.0417	-0.6393
H	4.5848	-1.1874	0.6772
H	4.0297	0.4326	1.0518

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction= 0.355293 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.370522
Thermal correction to Enthalpy= 0.371466
Thermal correction to Gibbs Free Frequency and Energy= 0.314013
Sum of electronic and zero-point Energies= -585.814210
Sum of electronic and thermal Energies= -585.798981
Sum of electronic and thermal Enthalpies= -585.798037
Sum of electronic and thermal Free Energies= -585.855491

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction= 0.354655 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.369892
Thermal correction to Enthalpy= 0.370836
Thermal correction to Gibbs Free Frequency and Energy= 0.313413
Sum of electronic and zero-point Energies= -585.817059
Sum of electronic and thermal Energies= -585.801822
Sum of electronic and thermal Enthalpies= -585.800878

Sum of electronic and thermal Free Energies= -585.858301
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)
Zero-point correction= 0.354692 (Hartree/Particle) Thermal correction to Frequency and Energy= 0.369928 Thermal correction to Enthalpy= 0.370872 Thermal correction to Gibbs Free Frequency and Energy= 0.313457 Sum of electronic and zero-point Energies= -585.816900 Sum of electronic and thermal Energies= -585.801664 Sum of electronic and thermal Enthalpies= -585.800720 Sum of electronic and thermal Free Energies= -585.858135

Name of radical	6-Epi-beta-cubebene-C8-H22

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-1.15905	0.51703	-0.45723
C	0.09876	-0.33092	-0.65948
C	-0.79183	-0.59652	0.55487
C	-1.08551	2.00386	-0.16234
C	1.48163	0.27867	-0.47902
C	-2.41491	0.03361	-1.20501
C	-1.81563	-1.68302	0.39803
C	-2.73189	-1.30805	-0.61745
C	0.35406	2.54336	-0.30502
C	1.40412	1.60748	0.30125
C	2.44378	-0.72371	0.21956
C	-1.6689	2.31464	1.22196
C	-1.84407	-2.83396	1.13638
C	2.46745	-2.07513	-0.50741
C	3.8684	-0.15596	0.29596
H	0.07931	-1.07308	-1.46859
H	-0.42843	-0.39428	1.55623
H	-1.71127	2.53896	-0.92401
H	1.88393	0.49952	-1.49943
H	-2.2389	-0.02797	-2.29449
H	-3.2621	0.73148	-1.06326
H	-3.56864	-1.88862	-0.94649
H	0.42541	3.54088	0.16719
H	0.57545	2.69981	-1.37876
H	2.39278	2.10364	0.29483
H	1.16665	1.41333	1.36429
H	2.07291	-0.89438	1.26036
H	-1.03172	1.9242	2.02341
H	-1.77567	3.39205	1.37947
H	-2.65727	1.85673	1.34527
H	-1.11067	-3.05449	1.89189
H	-2.59925	-3.58868	1.00636
H	2.72333	-1.96387	-1.56569
H	3.20472	-2.75134	-0.06177
H	1.49408	-2.57676	-0.44978
H	4.27128	0.05859	-0.69949
H	4.54991	-0.86623	0.77661
H	3.90577	0.77217	0.87551

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.341071 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.356288
Thermal correction to Enthalpy=	0.357232
Thermal correction to Gibbs Free Frequency and Energy=	0.299412
Sum of electronic and zero-point Energies=	-585.184518
Sum of electronic and thermal Energies=	-585.169301
Sum of electronic and thermal Enthalpies=	-585.168357
Sum of electronic and thermal Free Energies=	-585.226177
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.340459 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.355690
Thermal correction to Enthalpy=	0.356634
Thermal correction to Gibbs Free Frequency and Energy=	0.298818
Sum of electronic and zero-point Energies=	-585.187237
Sum of electronic and thermal Energies=	-585.172006
Sum of electronic and thermal Enthalpies=	-585.171062
Sum of electronic and thermal Free Energies=	-585.228879
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.340496 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.355725
Thermal correction to Enthalpy=	0.356669
Thermal correction to Gibbs Free Frequency and Energy=	0.298852
Sum of electronic and zero-point Energies=	-585.187085
Sum of electronic and thermal Energies=	-585.171855
Sum of electronic and thermal Enthalpies=	-585.170911
Sum of electronic and thermal Free Energies=	-585.228728

Name of anion	6-Epi-beta-cubebene-C8-H22-anion
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)	
Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.337381 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.353025
Thermal correction to Enthalpy=	0.353969
Thermal correction to Gibbs Free Frequency and Energy=	0.296098
Sum of electronic and zero-point Energies=	-585.196485
Sum of electronic and thermal Energies=	-585.180841
Sum of electronic and thermal Enthalpies=	-585.179897
Sum of electronic and thermal Free Energies=	-585.237769
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.337391 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.353164
Thermal correction to Enthalpy=	0.354108
Thermal correction to Gibbs Free Frequency and Energy=	0.296133
Sum of electronic and zero-point Energies=	-585.278207
Sum of electronic and thermal Energies=	-585.262434
Sum of electronic and thermal Enthalpies=	-585.261490
Sum of electronic and thermal Free Energies=	-585.319465

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.337533 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.353238
Thermal correction to Enthalpy=	0.354183
Thermal correction to Gibbs Free Frequency and Energy=	0.296397
Sum of electronic and zero-point Energies=	-585.275203
Sum of electronic and thermal Energies=	-585.259497
Sum of electronic and thermal Enthalpies=	-585.258553
Sum of electronic and thermal Free Energies=	-585.316339

Name of cationic radical	6-Epi-beta-cubebene

Cartesian Coordinates optimized at PM6 (d,p)

C	0	-1.0038	0.5784	-0.4843
C	0	0.2024	-0.339	-0.6323
C	0	-0.7284	-0.5262	0.5287
C	0	-0.8111	2.043	-0.1284
C	0	1.6001	0.1805	-0.4288
C	0	-2.2813	0.2152	-1.2198
C	0	-1.8421	-1.481	0.4331
C	0	-2.9616	-0.8726	-0.3738
C	0	0.6535	2.4975	-0.2318
C	0	1.6337	1.4921	0.3639
C	0	2.4843	-0.8766	0.2304
C	0	-1.4169	2.3879	1.2347
C	0	-1.8729	-2.7259	0.9229
C	0	2.4183	-2.1901	-0.545
C	0	3.9258	-0.3833	0.3305
H	0	0.1592	-1.0451	-1.4564
H	0	-0.3933	-0.2763	1.5253
H	0	-1.3611	2.6415	-0.8675
H	0	1.9982	0.3956	-1.4312
H	0	-2.0405	-0.1679	-2.2187
H	0	-2.9551	1.0688	-1.3493
H	0	-3.4842	-1.5971	-1.0057
H	0	-3.6867	-0.4117	0.3073
H	0	0.7819	3.4734	0.2513
H	0	0.9046	2.6436	-1.2909
H	0	2.6318	1.9413	0.3189
H	0	1.4057	1.3248	1.4229
H	0	2.1271	-1.0803	1.2485
H	0	-0.8759	1.9131	2.0586
H	0	-1.3933	3.4698	1.4037
H	0	-2.4616	2.0636	1.2905
H	0	-1.0311	-3.1274	1.4767
H	0	-2.7378	-3.3645	0.7799
H	0	2.6517	-2.0435	-1.6052
H	0	3.1412	-2.9098	-0.1443
H	0	1.4354	-2.665	-0.4671
H	0	4.3031	-0.0417	-0.6393
H	0	4.5848	-1.1874	0.6772
H	0	4.0297	0.4326	1.0518

Frequency and Energy at PM6 (gas)	
Zero-point correction=	0.323768 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.340294
Thermal correction to Enthalpy=	0.341238
Thermal correction to Gibbs Free Frequency and Energy=	0.279618
Sum of electronic and zero-point Energies=	0.588979
Sum of electronic and thermal Energies=	0.605505
Sum of electronic and thermal Enthalpies=	0.606450
Sum of electronic and thermal Free Energies=	0.544829

Name of compound	Aromadendr-9-ene		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	4.2599	-5.2064	0.4174
C	3.4887	-4.1619	1.2037
C	4.8613	-3.803	0.6793
C	5.133	-2.809	-0.4302
C	6.6278	-2.3473	-0.558
C	6.5164	-1.0589	-1.3874
C	5.1502	-0.5497	-1.0536
C	4.3479	-1.5092	-0.536
C	2.8261	-1.4413	-0.4476
C	2.1915	-2.08	0.8081
C	2.2096	-3.6007	0.7216
C	3.8062	-5.6087	-0.9759
C	4.684	-6.3806	1.2711
C	7.4054	-2.0432	0.7361
C	2.247	-0.025	-0.6245
H	4.9212	-3.312	-1.3766
H	5.5891	-3.7348	1.473
H	3.4462	-4.2864	2.2829
H	3.6068	-4.7668	-1.6434
H	2.8735	-6.182	-0.9183
H	4.5642	-6.2352	-1.464
H	5.3995	-6.0793	2.0399
H	5.14	-7.1722	0.6685
H	3.8087	-6.803	1.7774
H	1.4163	-3.9987	1.3662
H	1.946	-3.936	-0.2851
H	7.2062	-3.0966	-1.1171
H	6.5423	-1.2616	-2.4627
H	7.3059	-0.3319	-1.1673
H	6.8994	-2.3675	1.6431
H	7.5857	-0.9714	0.8607
H	8.3871	-2.5368	0.7211
H	4.8078	0.412	-1.4055
H	2.4588	-2.0182	-1.3146
H	1.1333	-1.7879	0.8672
H	2.6723	-1.7145	1.726
H	1.2643	0.08	-0.1522
H	2.1026	0.1895	-1.6897
H	2.8972	0.742	-0.1907

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.355407 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.370659
Thermal correction to Enthalpy=	0.371603
Thermal correction to Gibbs Free Frequency and Energy=	0.315030
Sum of electronic and zero-point Energies=	-585.813227
Sum of electronic and thermal Energies=	-585.797975
Sum of electronic and thermal Enthalpies=	-585.797031
Sum of electronic and thermal Free Energies=	-585.853604

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.354722 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.369995
Thermal correction to Enthalpy=	0.370940
Thermal correction to Gibbs Free Frequency and Energy=	0.314330
Sum of electronic and zero-point Energies=	-585.815427
Sum of electronic and thermal Energies=	-585.800153
Sum of electronic and thermal Enthalpies=	-585.799209
Sum of electronic and thermal Free Energies=	-585.855819

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.354761 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.370032
Thermal correction to Enthalpy=	0.370976
Thermal correction to Gibbs Free Frequency and Energy=	0.314373
Sum of electronic and zero-point Energies=	-585.815300
Sum of electronic and thermal Energies=	-585.800028
Sum of electronic and thermal Enthalpies=	-585.799084
Sum of electronic and thermal Free Energies=	-585.855687

Name of radical	Aromadendr-9-ene-C4-H16

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-2.15845	-0.77001	-0.10327
C	-0.93318	-1.48846	-0.64399
C	-0.9136	0.01948	-0.48394
C	0.04242	0.67559	0.50964
C	-0.01176	2.2353	0.50294
C	1.0494	2.63566	-0.55168
C	2.01294	1.47213	-0.50821
C	1.49211	0.40053	0.10258
C	2.16884	-0.91646	0.41326
C	1.48147	-2.16089	-0.20701
C	0.00223	-2.36535	0.16885
C	-2.57967	-0.92141	1.34765
C	-3.34646	-0.65682	-1.04597
C	-1.38498	2.87952	0.31962
C	3.66258	-0.91794	0.06016
H	-0.99633	0.5697	-1.4178
H	-1.0344	-1.83345	-1.67117
H	-1.74092	-1.01063	2.03807

H	-3.20319	-1.81371	1.47129
H	-3.175	-0.05789	1.66364
H	-3.02331	-0.54179	-2.08401
H	-3.96926	0.20799	-0.79105
H	-3.97928	-1.54987	-0.98907
H	-0.26486	-3.41457	-0.00123
H	-0.11952	-2.19738	1.24299
H	0.38291	2.55361	1.47524
H	1.52448	3.59355	-0.31391
H	0.60369	2.75201	-1.55012
H	-2.07988	2.56885	1.10567
H	-1.83101	2.6191	-0.64379
H	-1.30376	3.97019	0.3627
H	3.01002	1.52732	-0.93002
H	2.08774	-1.04366	1.50446
H	2.05348	-3.03689	0.11902
H	1.57834	-2.11755	-1.29926
H	4.12847	-1.85516	0.37622
H	4.19078	-0.09633	0.55037
H	3.81368	-0.81809	-1.01918

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.341074 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.356738
Thermal correction to Enthalpy=	0.357682
Thermal correction to Gibbs Free Frequency and Energy=	0.298392
Sum of electronic and zero-point Energies=	-585.189894
Sum of electronic and thermal Energies=	-585.174230
Sum of electronic and thermal Enthalpies=	-585.173286
Sum of electronic and thermal Free Energies=	-585.232576
Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.340411 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.356093
Thermal correction to Enthalpy=	0.357037
Thermal correction to Gibbs Free Frequency and Energy=	0.297729
Sum of electronic and zero-point Energies=	-585.192010
Sum of electronic and thermal Energies=	-585.176328
Sum of electronic and thermal Enthalpies=	-585.175384
Sum of electronic and thermal Free Energies=	-585.234692
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.340444 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.356126
Thermal correction to Enthalpy=	0.357071
Thermal correction to Gibbs Free Frequency and Energy=	0.297754
Sum of electronic and zero-point Energies=	-585.191891
Sum of electronic and thermal Energies=	-585.176209
Sum of electronic and thermal Enthalpies=	-585.175265
Sum of electronic and thermal Free Energies=	-585.234581

Name of anion	Aromadendr-9-ene-C4-H16-anion
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)	
C	-2.15844 -0.76996 -0.10335

C	-0.93312	-1.48841	-0.6439
C	-0.91352	0.01947	-0.48391
C	0.04249	0.6756	0.50966
C	-0.01179	2.23525	0.50292
C	1.04933	2.63555	-0.55173
C	2.01287	1.47207	-0.5082
C	1.49216	0.40055	0.10265
C	2.16893	-0.91641	0.41331
C	1.4815	-2.16083	-0.20687
C	0.00226	-2.36522	0.16905
C	-2.57989	-0.92145	1.34748
C	-3.34632	-0.65678	-1.04618
C	-1.38514	2.87925	0.31981
C	3.66261	-0.9178	0.05999
H	-0.99591	0.5696	-1.41784
H	-1.03418	-1.83345	-1.67106
H	-1.74122	-1.01006	2.03808
H	-3.20283	-1.81414	1.47114
H	-3.17582	-0.05828	1.66328
H	-3.02304	-0.54196	-2.08421
H	-3.969	0.20818	-0.79151
H	-3.97925	-1.54974	-0.98929
H	-0.26493	-3.41445	-0.00079
H	-0.11958	-2.19707	1.24317
H	0.38306	2.55359	1.47515
H	1.52439	3.59346	-0.31394
H	0.60373	2.75186	-1.55022
H	-2.07979	2.56871	1.10612
H	-1.83153	2.61849	-0.64334
H	-1.30415	3.96995	0.36257
H	3.00988	1.52727	-0.93012
H	2.08808	-1.04352	1.50456
H	2.05349	-3.03689	0.11909
H	1.57831	-2.1174	-1.29909
H	4.12865	-1.85508	0.37567
H	4.19079	-0.09629	0.55037
H	3.81345	-0.81769	-1.01934

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.337171 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.352753
Thermal correction to Enthalpy=	0.353698
Thermal correction to Gibbs Free Frequency and Energy=	0.296051
Sum of electronic and zero-point Energies=	-585.193127
Sum of electronic and thermal Energies=	-585.177544
Sum of electronic and thermal Enthalpies=	-585.176600
Sum of electronic and thermal Free Energies=	-585.234246

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.337674 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.353259
Thermal correction to Enthalpy=	0.354203
Thermal correction to Gibbs Free Frequency and Energy=	0.296170

Sum of electronic and zero-point Energies=	-585.265048
Sum of electronic and thermal Energies=	-585.249463
Sum of electronic and thermal Enthalpies=	-585.248518
Sum of electronic and thermal Free Energies=	-585.306551

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.337599 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.353237
Thermal correction to Enthalpy=	0.354181
Thermal correction to Gibbs Free Frequency and Energy=	0.295643
Sum of electronic and zero-point Energies=	-585.262562
Sum of electronic and thermal Energies=	-585.246924
Sum of electronic and thermal Enthalpies=	-585.245980
Sum of electronic and thermal Free Energies=	-585.304518

Name of cationic radical	Aromadendr-9-ene

Cartesian Coordinates optimized at PM6				
C	0	4.2599	-5.2064	0.4174
C	0	3.4887	-4.1619	1.2037
C	0	4.8613	-3.803	0.6793
C	0	5.133	-2.809	-0.4302
C	0	6.6278	-2.3473	-0.558
C	0	6.5164	-1.0589	-1.3874
C	0	5.1502	-0.5497	-1.0536
C	0	4.3479	-1.5092	-0.536
C	0	2.8261	-1.4413	-0.4476
C	0	2.1915	-2.08	0.8081
C	0	2.2096	-3.6007	0.7216
C	0	3.8062	-5.6087	-0.9759
C	0	4.684	-6.3806	1.2711
C	0	7.4054	-2.0432	0.7361
C	0	2.247	-0.025	-0.6245
H	0	3.4462	-4.2864	2.2829
H	0	5.5891	-3.7348	1.473
H	0	4.9212	-3.312	-1.3766
H	0	7.2062	-3.0966	-1.1171
H	0	6.5423	-1.2616	-2.4627
H	0	7.3059	-0.3319	-1.1673
H	0	4.8078	0.412	-1.4055
H	0	2.4588	-2.0182	-1.3146
H	0	1.1333	-1.7879	0.8672
H	0	2.6723	-1.7145	1.726
H	0	1.4163	-3.9987	1.3662
H	0	1.946	-3.936	-0.2851
H	0	3.6068	-4.7668	-1.6434
H	0	2.8735	-6.182	-0.9183
H	0	4.5642	-6.2352	-1.464
H	0	5.3995	-6.0793	2.0399
H	0	5.14	-7.1722	0.6685
H	0	3.8087	-6.803	1.7774
H	0	6.8994	-2.3675	1.6431
H	0	7.5857	-0.9714	0.8607

H	0	8.3871	-2.5368	0.7211
H	0	1.2643	0.08	-0.1522
H	0	2.1026	0.1895	-1.6897
H	0	2.8972	0.742	-0.1907

Frequency and Energy at PM6 (gas)

Zero-point correction= 0.324839 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.341197
Thermal correction to Enthalpy= 0.342141
Thermal correction to Gibbs Free Frequency and Energy= 0.281528
Sum of electronic and zero-point Energies= 0.594957
Sum of electronic and thermal Energies= 0.611315
Sum of electronic and thermal Enthalpies= 0.612259
Sum of electronic and thermal Free Energies= 0.551646

Name of compound	γ-Muurolene

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	0.1014	-0.1754	0.6095
C	-1.054	-0.5288	-0.3716
C	0.7034	1.2333	0.3506
C	-2.1036	0.5964	-0.4178
C	-1.7515	-1.8457	-0.0059
C	1.661	1.2066	-0.8514
C	-0.3756	2.2809	0.1799
C	-1.4858	1.9437	-0.7755
C	1.1838	-1.2328	0.5844
C	2.8169	0.2313	-0.6136
C	2.4042	-1.0584	0.0478
C	-2.3946	-1.739	1.3722
C	-2.789	-2.2069	-1.0628
C	-0.3622	3.4331	0.8678
C	3.4455	-2.1383	0.0865
H	-0.2849	-0.1323	1.6344
H	-0.6292	-0.637	-1.3798
H	1.3061	1.4971	1.2336
H	-2.6083	0.7211	0.5457
H	-2.8762	0.3906	-1.1652
H	-1.0194	-2.6608	0.0108
H	2.0705	2.2067	-1.0414
H	1.128	0.9135	-1.7647
H	-2.2684	2.7121	-0.7651
H	-1.0914	1.9148	-1.7983
H	0.9488	-2.1812	1.0613
H	3.5699	0.7165	0.0202
H	3.2972	0.0203	-1.5766
H	-3.2239	-1.0285	1.4188
H	-2.8291	-2.7126	1.6339
H	-1.6848	-1.5129	2.1702
H	-3.6866	-1.5832	-1.0117
H	-3.1226	-3.2408	-0.9155
H	-2.3724	-2.1418	-2.0734
H	0.436	3.6653	1.5649

H	-1.1477	4.1716	0.7477
H	3.0881	-3.0403	0.5942
H	4.3359	-1.7874	0.6181
H	3.7363	-2.4216	-0.9303

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction= 0.355630 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.371088
Thermal correction to Enthalpy= 0.372032
Thermal correction to Gibbs Free Frequency and Energy= 0.314119
Sum of electronic and zero-point Energies= -585.832678
Sum of electronic and thermal Energies= -585.817220
Sum of electronic and thermal Enthalpies= -585.816276
Sum of electronic and thermal Free Energies= -585.874189

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction= 0.355004 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.370482
Thermal correction to Enthalpy= 0.371426
Thermal correction to Gibbs Free Frequency and Energy= 0.313434
Sum of electronic and zero-point Energies= -585.835496
Sum of electronic and thermal Energies= -585.820019
Sum of electronic and thermal Enthalpies= -585.819074
Sum of electronic and thermal Free Energies= -585.877066

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction= 0.355038 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.370515
Thermal correction to Enthalpy= 0.371459
Thermal correction to Gibbs Free Frequency and Energy= 0.313471
Sum of electronic and zero-point Energies= -585.835345
Sum of electronic and thermal Energies= -585.819868
Sum of electronic and thermal Enthalpies= -585.818924
Sum of electronic and thermal Free Energies= -585.876912

Name of radical	γ-Muurolene-C1-H16

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	0.1014	-0.1754	0.6095
C	-1.054	-0.5288	-0.3716
C	0.7034	1.2333	0.3506
C	-2.1036	0.5964	-0.4178
C	-1.7515	-1.8457	-0.0059
C	1.661	1.2066	-0.8514
C	-0.3756	2.2809	0.1799
C	-1.4858	1.9437	-0.7755
C	1.1838	-1.2328	0.5844
C	2.8169	0.2313	-0.6136
C	2.4042	-1.0584	0.0478
C	-2.3946	-1.739	1.3722
C	-2.789	-2.2069	-1.0628

C	-0.3622	3.4331	0.8678
C	3.4455	-2.1383	0.0865
H	-0.6292	-0.637	-1.3798
H	1.3061	1.4971	1.2336
H	-2.6083	0.7211	0.5457
H	-2.8762	0.3906	-1.1652
H	-1.0194	-2.6608	0.0108
H	2.0705	2.2067	-1.0414
H	1.128	0.9135	-1.7647
H	-2.2684	2.7121	-0.7651
H	-1.0914	1.9148	-1.7983
H	0.9488	-2.1812	1.0613
H	3.5699	0.7165	0.0202
H	3.2972	0.0203	-1.5766
H	-3.2239	-1.0285	1.4188
H	-2.8291	-2.7126	1.6339
H	-1.6848	-1.5129	2.1702
H	-3.6866	-1.5832	-1.0117
H	-3.1226	-3.2408	-0.9155
H	-2.3724	-2.1418	-2.0734
H	0.436	3.6653	1.5649
H	-1.1477	4.1716	0.7477
H	3.0881	-3.0403	0.5942
H	4.3359	-1.7874	0.6181
H	3.7363	-2.4216	-0.9303

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction= 0.341502 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.357172
Thermal correction to Enthalpy= 0.358116
Thermal correction to Gibbs Free Frequency and Energy= 0.298515
Sum of electronic and zero-point Energies= -585.207104
Sum of electronic and thermal Energies= -585.191434
Sum of electronic and thermal Enthalpies= -585.190490
Sum of electronic and thermal Free Energies= -585.250091

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction= 0.340950 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.356611
Thermal correction to Enthalpy= 0.357555
Thermal correction to Gibbs Free Frequency and Energy= 0.298059
Sum of electronic and zero-point Energies= -585.209922
Sum of electronic and thermal Energies= -585.194261
Sum of electronic and thermal Enthalpies= -585.193317
Sum of electronic and thermal Free Energies= -585.252813

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction= 0.340938 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.356623
Thermal correction to Enthalpy= 0.357567
Thermal correction to Gibbs Free Frequency and Energy= 0.297928
Sum of electronic and zero-point Energies= -585.209823

Sum of electronic and thermal Energies=	-585.194138
Sum of electronic and thermal Enthalpies=	-585.193194
Sum of electronic and thermal Free Energies=	-585.252833

Name of anion	γ-Muurolene-C1-H16-anion		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	0.1014	-0.1754	0.6095
C	-1.054	-0.5288	-0.3716
C	0.7034	1.2333	0.3506
C	-2.1036	0.5964	-0.4178
C	-1.7515	-1.8457	-0.0059
C	1.661	1.2066	-0.8514
C	-0.3756	2.2809	0.1799
C	-1.4858	1.9437	-0.7755
C	1.1838	-1.2328	0.5844
C	2.8169	0.2313	-0.6136
C	2.4042	-1.0584	0.0478
C	-2.3946	-1.739	1.3722
C	-2.789	-2.2069	-1.0628
C	-0.3622	3.4331	0.8678
C	3.4455	-2.1383	0.0865
H	-0.6292	-0.637	-1.3798
H	1.3061	1.4971	1.2336
H	-2.6083	0.7211	0.5457
H	-2.8762	0.3906	-1.1652
H	-1.0194	-2.6608	0.0108
H	2.0705	2.2067	-1.0414
H	1.128	0.9135	-1.7647
H	-2.2684	2.7121	-0.7651
H	-1.0914	1.9148	-1.7983
H	0.9488	-2.1812	1.0613
H	3.5699	0.7165	0.0202
H	3.2972	0.0203	-1.5766
H	-3.2239	-1.0285	1.4188
H	-2.8291	-2.7126	1.6339
H	-1.6848	-1.5129	2.1702
H	-3.6866	-1.5832	-1.0117
H	-3.1226	-3.2408	-0.9155
H	-2.3724	-2.1418	-2.0734
H	0.436	3.6653	1.5649
H	-1.1477	4.1716	0.7477
H	3.0881	-3.0403	0.5942
H	4.3359	-1.7874	0.6181
H	3.7363	-2.4216	-0.9303
Frequency and Energy at B3LYP/6-311G (d,p) (gas)			
Zero-point correction=	0.336939 (Hartree/Particle)		
Thermal correction to Frequency and Energy=	0.352753		
Thermal correction to Enthalpy=	0.353697		
Thermal correction to Gibbs Free Frequency and Energy=	0.294353		
Sum of electronic and zero-point Energies=	-585.213196		
Sum of electronic and thermal Energies=	-585.197382		

Sum of electronic and thermal Enthalpies= -585.196438
Sum of electronic and thermal Free Energies= -585.255782
Frequency and Energy at B3LYP/6-311G (d,p) (water)
Zero-point correction= 0.337367 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.353066
Thermal correction to Enthalpy= 0.354010
Thermal correction to Gibbs Free Frequency and Energy= 0.295352
Sum of electronic and zero-point Energies= -585.281583
Sum of electronic and thermal Energies= -585.265884
Sum of electronic and thermal Enthalpies= -585.264939
Sum of electronic and thermal Free Energies= -585.323598
Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)
Zero-point correction= 0.337451 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.353104
Thermal correction to Enthalpy= 0.354049
Thermal correction to Gibbs Free Frequency and Energy= 0.295651
Sum of electronic and zero-point Energies= -585.279124
Sum of electronic and thermal Energies= -585.263470
Sum of electronic and thermal Enthalpies= -585.262526
Sum of electronic and thermal Free Energies= -585.320924

Name of cationic radical	γ-Muurolene

Cartesian Coordinates optimized at PM6				
C	0	0.1014	-0.1754	0.6095
C	0	-1.054	-0.5288	-0.3716
C	0	0.7034	1.2333	0.3506
C	0	-2.1036	0.5964	-0.4178
C	0	-1.7515	-1.8457	-0.0059
C	0	1.661	1.2066	-0.8514
C	0	-0.3756	2.2809	0.1799
C	0	-1.4858	1.9437	-0.7755
C	0	1.1838	-1.2328	0.5844
C	0	2.8169	0.2313	-0.6136
C	0	2.4042	-1.0584	0.0478
C	0	-2.3946	-1.739	1.3722
C	0	-2.789	-2.2069	-1.0628
C	0	-0.3622	3.4331	0.8678
C	0	3.4455	-2.1383	0.0865
H	0	-0.2849	-0.1323	1.6344
H	0	-0.6292	-0.637	-1.3798
H	0	1.3061	1.4971	1.2336
H	0	-2.6083	0.7211	0.5457
H	0	-2.8762	0.3906	-1.1652
H	0	-1.0194	-2.6608	0.0108
H	0	2.0705	2.2067	-1.0414
H	0	1.128	0.9135	-1.7647
H	0	-2.2684	2.7121	-0.7651
H	0	-1.0914	1.9148	-1.7983

H	0	0.9488	-2.1812	1.0613
H	0	3.5699	0.7165	0.0202
H	0	3.2972	0.0203	-1.5766
H	0	-3.2239	-1.0285	1.4188
H	0	-2.8291	-2.7126	1.6339
H	0	-1.6848	-1.5129	2.1702
H	0	-3.6866	-1.5832	-1.0117
H	0	-3.1226	-3.2408	-0.9155
H	0	-2.3724	-2.1418	-2.0734
H	0	0.436	3.6653	1.5649
H	0	-1.1477	4.1716	0.7477
H	0	3.0881	-3.0403	0.5942
H	0	4.3359	-1.7874	0.6181
H	0	3.7363	-2.4216	-0.9303

Frequency and Energy at PM6 (gas)

Zero-point correction=	0.324975 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.341660
Thermal correction to Enthalpy=	0.342604
Thermal correction to Gibbs Free Frequency and Energy=	0.279821
Sum of electronic and zero-point Energies=	0.584822
Sum of electronic and thermal Energies=	0.601507
Sum of electronic and thermal Enthalpies=	0.602451
Sum of electronic and thermal Free Energies=	0.539668

Name of compound	γ-Amorphene

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	-0.17061	-0.27108	0.74873
C	-1.41815	0.38664	0.09942
C	0.87391	0.83987	1.04382
C	-1.06649	0.95273	-1.29211
C	-2.62523	-0.58779	0.03051
C	2.24858	0.21398	1.35123
C	0.96939	1.8583	-0.07643
C	0.38587	1.44801	-1.4001
C	0.37786	-1.40838	-0.06925
C	2.74943	-0.67621	0.20739
C	1.68279	-1.61247	-0.29496
C	-3.02254	-1.07073	1.43332
C	-3.8374	0.07048	-0.64385
C	1.54932	3.04771	0.10812
C	2.18222	-2.78273	-1.08586
H	-0.47767	-0.70988	1.73653
H	-1.71396	1.24604	0.75202
H	0.53213	1.38287	1.96291
H	-1.75702	1.7843	-1.52732
H	-1.23355	0.18147	-2.06819
H	-2.32506	-1.47874	-0.57605
H	2.17127	-0.38551	2.27898
H	2.98743	1.01139	1.55648
H	0.44035	2.27409	-2.13449
H	1.02035	0.63264	-1.81322

H	-0.38029	-2.08488	-0.46062
H	3.64035	-1.24327	0.54055
H	3.09256	-0.04168	-0.63744
H	-3.36004	-0.24273	2.06547
H	-3.83875	-1.79884	1.38453
H	-2.18132	-1.555	1.94437
H	-4.1098	1.01201	-0.15511
H	-4.71522	-0.58366	-0.60215
H	-3.6483	0.28866	-1.69952
H	1.9862	3.36183	1.04133
H	1.6299	3.79821	-0.66042
H	1.37076	-3.34638	-1.56315
H	2.72836	-3.48608	-0.44244
H	2.86767	-2.46678	-1.8829

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction=	0.355451 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.370914
Thermal correction to Enthalpy=	0.371858
Thermal correction to Gibbs Free Frequency and Energy=	0.313831
Sum of electronic and zero-point Energies=	-585.825441
Sum of electronic and thermal Energies=	-585.809978
Sum of electronic and thermal Enthalpies=	-585.809034
Sum of electronic and thermal Free Energies=	-585.867061

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.354838 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.370300
Thermal correction to Enthalpy=	0.371244
Thermal correction to Gibbs Free Frequency and Energy=	0.313291
Sum of electronic and zero-point Energies=	-585.827985
Sum of electronic and thermal Energies=	-585.812523
Sum of electronic and thermal Enthalpies=	-585.811579
Sum of electronic and thermal Free Energies=	-585.869532

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.354869 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.370331
Thermal correction to Enthalpy=	0.371275
Thermal correction to Gibbs Free Frequency and Energy=	0.313320
Sum of electronic and zero-point Energies=	-585.827849
Sum of electronic and thermal Energies=	-585.812387
Sum of electronic and thermal Enthalpies=	-585.811443
Sum of electronic and thermal Free Energies=	-585.869399

Name of radical	γ-Amorphene-C1-H16

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	0.10788	-0.18842	-0.26817
C	1.49293	0.36612	-0.07098
C	-0.84797	0.84869	-0.81
C	1.40373	1.38147	1.10178
C	2.59677	-0.69997	0.15146

C	-2.25302	0.27878	-1.09098
C	-0.85759	2.04431	0.13058
C	-0.02576	1.88491	1.37688
C	-0.32502	-1.44177	0.15331
C	-2.71791	-0.72285	-0.02623
C	-1.67834	-1.76812	0.23519
C	2.75457	-1.57092	-1.10355
C	3.94401	-0.04747	0.49348
C	-1.54322	3.15838	-0.13463
C	-2.14214	-3.12346	0.63232
H	1.77367	0.93841	-0.99375
H	-0.43835	1.20795	-1.79448
H	2.06209	2.24091	0.87885
H	1.79486	0.92204	2.02919
H	2.29536	-1.35361	1.00689
H	-2.23601	-0.22707	-2.07697
H	-2.98725	1.10135	-1.17732
H	0.02457	2.83246	1.94679
H	-0.54833	1.1598	2.04001
H	0.41358	-2.18647	0.45304
H	-3.6791	-1.1769	-0.33443
H	-2.92537	-0.18798	0.9265
H	3.13938	-0.9931	-1.9506
H	3.44995	-2.39758	-0.92765
H	1.79819	-2.00477	-1.41851
H	4.241	0.68818	-0.26149
H	4.74083	-0.79759	0.5474
H	3.91652	0.46415	1.46058
H	-2.15127	3.29161	-1.0144
H	-1.5491	4.02324	0.50817
H	-1.32483	-3.7663	0.98367
H	-2.61441	-3.63739	-0.2181
H	-2.88696	-3.07622	1.4387

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction=	0.341509 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.357176
Thermal correction to Enthalpy=	0.358120
Thermal correction to Gibbs Free Frequency and Energy=	0.298922
Sum of electronic and zero-point Energies=	-585.201573
Sum of electronic and thermal Energies=	-585.185906
Sum of electronic and thermal Enthalpies=	-585.184962
Sum of electronic and thermal Free Energies=	-585.244160

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.340731 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.356467
Thermal correction to Enthalpy=	0.357411
Thermal correction to Gibbs Free Frequency and Energy=	0.298029
Sum of electronic and zero-point Energies=	-585.204365
Sum of electronic and thermal Energies=	-585.188628
Sum of electronic and thermal Enthalpies=	-585.187684
Sum of electronic and thermal Free Energies=	-585.247067

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)
Zero-point correction= 0.340908 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.356600
Thermal correction to Enthalpy= 0.357544
Thermal correction to Gibbs Free Frequency and Energy= 0.298276
Sum of electronic and zero-point Energies= -585.204114
Sum of electronic and thermal Energies= -585.188421
Sum of electronic and thermal Enthalpies= -585.187477
Sum of electronic and thermal Free Energies= -585.246745

Name of anion	γ-Amorphene-C1-H16-anion

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	0.10788	-0.18842	-0.26817
C	1.49293	0.36612	-0.07098
C	-0.84797	0.84869	-0.81
C	1.40373	1.38147	1.10178
C	2.59677	-0.69997	0.15146
C	-2.25302	0.27878	-1.09098
C	-0.85759	2.04431	0.13058
C	-0.02576	1.88491	1.37688
C	-0.32502	-1.44177	0.15331
C	-2.71791	-0.72285	-0.02623
C	-1.67834	-1.76812	0.23519
C	2.75457	-1.57092	-1.10355
C	3.94401	-0.04747	0.49348
C	-1.54322	3.15838	-0.13463
C	-2.14214	-3.12346	0.63232
H	1.77367	0.93841	-0.99375
H	-0.43835	1.20795	-1.79448
H	2.06209	2.24091	0.87885
H	1.79486	0.92204	2.02919
H	2.29536	-1.35361	1.00689
H	-2.23601	-0.22707	-2.07697
H	-2.98725	1.10135	-1.17732
H	0.02457	2.83246	1.94679
H	-0.54833	1.1598	2.04001
H	0.41358	-2.18647	0.45304
H	-3.6791	-1.1769	-0.33443
H	-2.92537	-0.18798	0.9265
H	3.13938	-0.9931	-1.9506
H	3.44995	-2.39758	-0.92765
H	1.79819	-2.00477	-1.41851
H	4.241	0.68818	-0.26149
H	4.74083	-0.79759	0.5474
H	3.91652	0.46415	1.46058
H	-2.15127	3.29161	-1.0144
H	-1.5491	4.02324	0.50817
H	-1.32483	-3.7663	0.98367

H	-2.61441	-3.63739	-0.2181
H	-2.88696	-3.07622	1.4387

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.336864 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.352697
Thermal correction to Enthalpy=	0.353641
Thermal correction to Gibbs Free Frequency and Energy=	0.294595
Sum of electronic and zero-point Energies=	-585.210272
Sum of electronic and thermal Energies=	-585.194439
Sum of electronic and thermal Enthalpies=	-585.193494
Sum of electronic and thermal Free Energies=	-585.252541

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.336982 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.352761
Thermal correction to Enthalpy=	0.353706
Thermal correction to Gibbs Free Frequency and Energy=	0.295056
Sum of electronic and zero-point Energies=	-585.278205
Sum of electronic and thermal Energies=	-585.262425
Sum of electronic and thermal Enthalpies=	-585.261481
Sum of electronic and thermal Free Energies=	-585.320130

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.337069 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.352809
Thermal correction to Enthalpy=	0.353753
Thermal correction to Gibbs Free Frequency and Energy=	0.295303
Sum of electronic and zero-point Energies=	-585.275856
Sum of electronic and thermal Energies=	-585.260117
Sum of electronic and thermal Enthalpies=	-585.259173
Sum of electronic and thermal Free Energies=	-585.317622

Name of cationic radical	γ-Amorphene		
Cartesian Coordinates optimized at PM6			
C	0.2049	-0.3196	-0.739
C	1.4738	0.3011	-0.0998
C	-0.8303	0.8135	-1.013
C	1.1812	0.9529	1.2656
C	2.651	-0.6715	0.003
C	-2.2268	0.2279	-1.2696
C	-0.8309	1.8925	0.0628
C	-0.2316	1.5315	1.3944
C	-0.3658	-1.4815	0.0486
C	-2.7155	-0.6643	-0.129
C	-1.6683	-1.6361	0.3439
C	2.9109	-1.338	-1.3447
C	3.8997	0.053	0.497
C	-1.2898	3.1297	-0.1846
C	-2.1625	-2.7912	1.1643
H	0.456	-0.7238	-1.7277
H	1.7879	1.1133	-0.7748

H	0	-0.5114	1.3069	-1.9441
H	0	1.901	1.765	1.4319
H	0	1.3324	0.2374	2.0838
H	0	2.4318	-1.4618	0.7313
H	0	-2.1905	-0.3674	-2.1924
H	0	-2.9602	1.0232	-1.4505
H	0	-0.2036	2.3925	2.0737
H	0	-0.8822	0.7969	1.8836
H	0	0.3337	-2.242	0.3847
H	0	-3.5979	-1.213	-0.4801
H	0	-3.0401	-0.0494	0.719
H	0	2.9879	-0.6019	-2.1522
H	0	3.8532	-1.8975	-1.3204
H	0	2.1345	-2.0639	-1.603
H	0	4.1466	0.9082	-0.1415
H	0	4.7631	-0.6219	0.4943
H	0	3.7864	0.4121	1.5244
H	0	-1.6985	3.3938	-1.1543
H	0	-1.2679	3.9039	0.5749
H	0	-1.3478	-3.4458	1.4911
H	0	-2.8648	-3.3974	0.5832
H	0	-2.6757	-2.4263	2.06

Frequency and Energy at PM6 (gas)

Zero-point correction=	0.325042 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.341645
Thermal correction to Enthalpy=	0.342589
Thermal correction to Gibbs Free Frequency and Energy=	0.280079
Sum of electronic and zero-point Energies=	0.585560
Sum of electronic and thermal Energies=	0.602163
Sum of electronic and thermal Enthalpies=	0.603107
Sum of electronic and thermal Free Energies=	0.540597

Name of compound	Cyclobazzanene

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	1.9145	-0.3882	1.3377
C	3.3987	-0.1973	1.0085
C	3.7352	-0.8555	-0.3476
C	1.1321	-0.9096	0.0978
C	1.6306	-2.3683	-0.2751
C	3.2042	-2.3213	-0.3903
C	3.7708	-3.2336	0.7148
C	2.5755	-3.9182	1.2685
C	1.4227	-3.4607	0.7638
C	-0.37	-0.7979	0.3961
C	5.243	-0.7999	-0.6146
C	1.4871	0.0536	-1.0731
C	2.9764	-0.0531	-1.4328
C	1.041	-2.8761	-1.6144
C	0.103	-4.0981	1.0504
H	1.8044	-1.0774	2.1834

H	1.5033	0.5706	1.6803
H	3.6218	0.8775	0.9614
H	4.0154	-0.5854	1.8261
H	3.5076	-2.7582	-1.3538
H	5.5939	0.2356	-0.6884
H	5.8116	-1.2821	0.1873
H	5.4966	-1.3039	-1.5539
H	3.3952	0.9554	-1.5419
H	3.0903	-0.5366	-2.4112
H	-0.6813	0.2527	0.4432
H	-0.9848	-1.2783	-0.3692
H	-0.6186	-1.2355	1.3677
H	0.8723	-0.141	-1.9594
H	1.2652	1.0896	-0.7822
H	1.4457	-2.3334	-2.4744
H	1.2769	-3.9349	-1.7802
H	-0.048	-2.7804	-1.6465
H	4.4631	-3.9656	0.2859
H	4.3003	-2.7038	1.5096
H	2.6475	-4.7311	1.9769
H	0.114	-4.6264	2.0095
H	-0.7109	-3.3747	1.0856
H	-0.1366	-4.8296	0.271

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction=	0.356680 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.371194
Thermal correction to Enthalpy=	0.372139
Thermal correction to Gibbs Free Frequency and Energy=	0.317676
Sum of electronic and zero-point Energies=	-585.838252
Sum of electronic and thermal Energies=	-585.823738
Sum of electronic and thermal Enthalpies=	-585.822794
Sum of electronic and thermal Free Energies=	-585.877256

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.356034 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.370566
Thermal correction to Enthalpy=	0.371510
Thermal correction to Gibbs Free Frequency and Energy=	0.317001
Sum of electronic and zero-point Energies=	-585.840072
Sum of electronic and thermal Energies=	-585.825541
Sum of electronic and thermal Enthalpies=	-585.824597
Sum of electronic and thermal Free Energies=	-585.879105

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.356073 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.370603
Thermal correction to Enthalpy=	0.371547
Thermal correction to Gibbs Free Frequency and Energy=	0.317044
Sum of electronic and zero-point Energies=	-585.839968
Sum of electronic and thermal Energies=	-585.825438
Sum of electronic and thermal Enthalpies=	-585.824494
Sum of electronic and thermal Free Energies=	-585.878997

Name of radical	Cyclobazzanene-C7-H34

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	1.9145	-0.3882	1.3377
C	3.3987	-0.1973	1.0085
C	3.7352	-0.8555	-0.3476
C	1.1321	-0.9096	0.0978
C	1.6306	-2.3683	-0.2751
C	3.2042	-2.3213	-0.3903
C	3.7708	-3.2336	0.7148
C	2.5755	-3.9182	1.2685
C	1.4227	-3.4607	0.7638
C	-0.37	-0.7979	0.3961
C	5.243	-0.7999	-0.6146
C	1.4871	0.0536	-1.0731
C	2.9764	-0.0531	-1.4328
C	1.041	-2.8761	-1.6144
C	0.103	-4.0981	1.0504
H	1.8044	-1.0774	2.1834
H	1.5033	0.5706	1.6803
H	3.6218	0.8775	0.9614
H	4.0154	-0.5854	1.8261
H	3.5076	-2.7582	-1.3538
H	5.5939	0.2356	-0.6884
H	5.8116	-1.2821	0.1873
H	5.4966	-1.3039	-1.5539
H	3.3952	0.9554	-1.5419
H	3.0903	-0.5366	-2.4112
H	-0.6813	0.2527	0.4432
H	-0.9848	-1.2783	-0.3692
H	-0.6186	-1.2355	1.3677
H	0.8723	-0.141	-1.9594
H	1.2652	1.0896	-0.7822
H	1.4457	-2.3334	-2.4744
H	1.2769	-3.9349	-1.7802
H	-0.048	-2.7804	-1.6465
H	4.3003	-2.7038	1.5096
H	2.6475	-4.7311	1.9769
H	0.114	-4.6264	2.0095
H	-0.7109	-3.3747	1.0856
H	-0.1366	-4.8296	0.271

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction=	0.342957 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.357497
Thermal correction to Enthalpy=	0.358441
Thermal correction to Gibbs Free Frequency and Energy=	0.303055
Sum of electronic and zero-point Energies=	-585.213274
Sum of electronic and thermal Energies=	-585.198733
Sum of electronic and thermal Enthalpies=	-585.197789
Sum of electronic and thermal Free Energies=	-585.253176

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction=	0.342157 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.356783
Thermal correction to Enthalpy=	0.357727
Thermal correction to Gibbs Free Frequency and Energy=	0.302260
Sum of electronic and zero-point Energies=	-585.215523
Sum of electronic and thermal Energies=	-585.200897
Sum of electronic and thermal Enthalpies=	-585.199953
Sum of electronic and thermal Free Energies=	-585.255421

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction=	0.342410 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.356957
Thermal correction to Enthalpy=	0.357901
Thermal correction to Gibbs Free Frequency and Energy=	0.302525
Sum of electronic and zero-point Energies=	-585.215196
Sum of electronic and thermal Energies=	-585.200648
Sum of electronic and thermal Enthalpies=	-585.199704
Sum of electronic and thermal Free Energies=	-585.255081

Name of anion	Cyclobazzanene-C7-H34-anion

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	1.9145	-0.3882	1.3377
C	3.3987	-0.1973	1.0085
C	3.7352	-0.8555	-0.3476
C	1.1321	-0.9096	0.0978
C	1.6306	-2.3683	-0.2751
C	3.2042	-2.3213	-0.3903
C	3.7708	-3.2336	0.7148
C	2.5755	-3.9182	1.2685
C	1.4227	-3.4607	0.7638
C	-0.37	-0.7979	0.3961
C	5.243	-0.7999	-0.6146
C	1.4871	0.0536	-1.0731
C	2.9764	-0.0531	-1.4328
C	1.041	-2.8761	-1.6144
C	0.103	-4.0981	1.0504
H	1.8044	-1.0774	2.1834
H	1.5033	0.5706	1.6803
H	3.6218	0.8775	0.9614
H	4.0154	-0.5854	1.8261
H	3.5076	-2.7582	-1.3538
H	5.5939	0.2356	-0.6884
H	5.8116	-1.2821	0.1873
H	5.4966	-1.3039	-1.5539
H	3.3952	0.9554	-1.5419
H	3.0903	-0.5366	-2.4112
H	-0.6813	0.2527	0.4432
H	-0.9848	-1.2783	-0.3692
H	-0.6186	-1.2355	1.3677
H	0.8723	-0.141	-1.9594
H	1.2652	1.0896	-0.7822
H	1.4457	-2.3334	-2.4744

H	1.2769	-3.9349	-1.7802
H	-0.048	-2.7804	-1.6465
H	4.3003	-2.7038	1.5096
H	2.6475	-4.7311	1.9769
H	0.114	-4.6264	2.0095
H	-0.7109	-3.3747	1.0856
H	-0.1366	-4.8296	0.271

Frequency and Energy at B3LYP/6-311G (d,p) (gas)		
Zero-point correction=	0.337982	(Hartree/Particle)
Thermal correction to Frequency and Energy=	0.352927	
Thermal correction to Enthalpy=	0.353872	
Thermal correction to Gibbs Free Frequency and Energy=	0.298494	
Sum of electronic and zero-point Energies=	-585.215360	
Sum of electronic and thermal Energies=	-585.200415	
Sum of electronic and thermal Enthalpies=	-585.199470	
Sum of electronic and thermal Free Energies=	-585.254848	

Frequency and Energy at B3LYP/6-311G (d,p) (water)		
Zero-point correction=	0.338339	(Hartree/Particle)
Thermal correction to Frequency and Energy=	0.353168	
Thermal correction to Enthalpy=	0.354112	
Thermal correction to Gibbs Free Frequency and Energy=	0.299355	
Sum of electronic and zero-point Energies=	-585.285702	
Sum of electronic and thermal Energies=	-585.270873	
Sum of electronic and thermal Enthalpies=	-585.269929	
Sum of electronic and thermal Free Energies=	-585.324687	

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)		
Zero-point correction=	0.338372	(Hartree/Particle)
Thermal correction to Frequency and Energy=	0.353186	
Thermal correction to Enthalpy=	0.354130	
Thermal correction to Gibbs Free Frequency and Energy=	0.299452	
Sum of electronic and zero-point Energies=	-585.283348	
Sum of electronic and thermal Energies=	-585.268534	
Sum of electronic and thermal Enthalpies=	-585.267590	
Sum of electronic and thermal Free Energies=	-585.322268	

Name of cationic radical	Cyclobazzanene

Cartesian Coordinates optimized at PM6				
C	0	1.9145	-0.3882	1.3377
C	0	3.3987	-0.1973	1.0085
C	0	3.7352	-0.8555	-0.3476
C	0	1.1321	-0.9096	0.0978
C	0	1.6306	-2.3683	-0.2751
C	0	3.2042	-2.3213	-0.3903
C	0	3.7708	-3.2336	0.7148
C	0	2.5755	-3.9182	1.2685
C	0	1.4227	-3.4607	0.7638
C	0	-0.37	-0.7979	0.3961
C	0	5.243	-0.7999	-0.6146
C	0	1.4871	0.0536	-1.0731
C	0	2.9764	-0.0531	-1.4328
C	0	1.041	-2.8761	-1.6144

C	0	0.103	-4.0981	1.0504
H	0	1.8044	-1.0774	2.1834
H	0	1.5033	0.5706	1.6803
H	0	3.6218	0.8775	0.9614
H	0	4.0154	-0.5854	1.8261
H	0	3.5076	-2.7582	-1.3538
H	0	4.4631	-3.9656	0.2859
H	0	4.3003	-2.7038	1.5096
H	0	2.6475	-4.7311	1.9769
H	0	-0.6813	0.2527	0.4432
H	0	-0.9848	-1.2783	-0.3692
H	0	-0.6186	-1.2355	1.3677
H	0	5.5939	0.2356	-0.6884
H	0	5.8116	-1.2821	0.1873
H	0	5.4966	-1.3039	-1.5539
H	0	0.8723	-0.141	-1.9594
H	0	1.2652	1.0896	-0.7822
H	0	3.3952	0.9554	-1.5419
H	0	3.0903	-0.5366	-2.4112
H	0	1.4457	-2.3334	-2.4744
H	0	1.2769	-3.9349	-1.7802
H	0	-0.048	-2.7804	-1.6465
H	0	0.114	-4.6264	2.0095
H	0	-0.7109	-3.3747	1.0856
H	0	-0.1366	-4.8296	0.271

Frequency and Energy at PM6 (gas)

Zero-point correction=	0.325337 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.340721
Thermal correction to Enthalpy=	0.341665
Thermal correction to Gibbs Free Frequency and Energy=	0.284292
Sum of electronic and zero-point Energies=	0.561398
Sum of electronic and thermal Energies=	0.576782
Sum of electronic and thermal Enthalpies=	0.577726
Sum of electronic and thermal Free Energies=	0.520354

Name of compound	α-Cadiene

Cartesian Coordinates optimized at B3LYP/6-311G (d,p)

C	-0.0493	-0.2559	0.2381
C	1.3503	-0.2786	-0.426
C	-0.8162	1.0123	-0.2498
C	-2.2026	1.0239	0.4163
C	2.143	0.9685	0.0204
C	2.1777	-1.528	-0.1073
C	-0.0009	2.2805	-0.0585
C	-0.8845	-1.4989	0.0332
C	-3.0199	-0.2036	-0.0052
C	1.3373	2.2318	0.0637
C	-2.2243	-1.4811	-0.0805
C	3.4965	-1.5021	-0.8731
C	2.4259	-1.633	1.394

C	-0.7143	3.6026	-0.0835
C	-3.0189	-2.7383	-0.2818
H	0.0858	-0.1584	1.325
H	1.208	-0.2303	-1.5158
H	-0.9806	0.9284	-1.3357
H	-2.7735	1.919	0.1449
H	-2.0926	1.0392	1.5087
H	2.9729	1.1398	-0.6755
H	2.5771	0.87	1.0176
H	1.6459	-2.4243	-0.4419
H	-0.3882	-2.4633	0.0289
H	-3.4588	-0.0157	-0.9934
H	-3.8532	-0.3238	0.6973
H	1.9004	3.1531	0.1914
H	4.1876	-0.7387	-0.502
H	4.0075	-2.4663	-0.7705
H	3.3323	-1.3318	-1.9424
H	3.1401	-0.9005	1.7786
H	2.8737	-2.6123	1.6074
H	1.5122	-1.5881	1.9907
H	-0.0177	4.4479	-0.0937
H	-1.3509	3.7143	0.7997
H	-1.3358	3.6825	-0.9814
H	-2.3815	-3.6269	-0.3385
H	-3.5909	-2.6793	-1.2134
H	-3.7186	-2.8823	0.5477

Frequency and Energy at B3LYP/6-311G (d,p) (gas)

Zero-point correction= 0.354820 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.370562
Thermal correction to Enthalpy= 0.371506
Thermal correction to Gibbs Free Frequency and Energy= 0.313208
Sum of electronic and zero-point Energies= -585.835195
Sum of electronic and thermal Energies= -585.819453
Sum of electronic and thermal Enthalpies= -585.818508
Sum of electronic and thermal Free Energies= -585.876806

Frequency and Energy at B3LYP/6-311G (d,p) (water)

Zero-point correction= 0.354143 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.369915
Thermal correction to Enthalpy= 0.370859
Thermal correction to Gibbs Free Frequency and Energy= 0.312490
Sum of electronic and zero-point Energies= -585.837879
Sum of electronic and thermal Energies= -585.822108
Sum of electronic and thermal Enthalpies= -585.821164
Sum of electronic and thermal Free Energies= -585.879533

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)

Zero-point correction= 0.354181 (Hartree/Particle)
Thermal correction to Frequency and Energy= 0.369951
Thermal correction to Enthalpy= 0.370895
Thermal correction to Gibbs Free Frequency and Energy= 0.312529
Sum of electronic and zero-point Energies= -585.837733

Sum of electronic and thermal Energies=	-585.821963
Sum of electronic and thermal Enthalpies=	-585.821019
Sum of electronic and thermal Free Energies=	-585.879385

Name of radical	α-Cadiene-C1-H16		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-0.0493	-0.2559	0.2381
C	1.3503	-0.2786	-0.426
C	-0.8162	1.0123	-0.2498
C	-2.2026	1.0239	0.4163
C	2.143	0.9685	0.0204
C	2.1777	-1.528	-0.1073
C	-0.0009	2.2805	-0.0585
C	-0.8845	-1.4989	0.0332
C	-3.0199	-0.2036	-0.0052
C	1.3373	2.2318	0.0637
C	-2.2243	-1.4811	-0.0805
C	3.4965	-1.5021	-0.8731
C	2.4259	-1.633	1.394
C	-0.7143	3.6026	-0.0835
C	-3.0189	-2.7383	-0.2818
H	1.208	-0.2303	-1.5158
H	-0.9806	0.9284	-1.3357
H	-2.7735	1.919	0.1449
H	-2.0926	1.0392	1.5087
H	2.9729	1.1398	-0.6755
H	2.5771	0.87	1.0176
H	1.6459	-2.4243	-0.4419
H	-0.3882	-2.4633	0.0289
H	-3.4588	-0.0157	-0.9934
H	-3.8532	-0.3238	0.6973
H	1.9004	3.1531	0.1914
H	4.1876	-0.7387	-0.502
H	4.0075	-2.4663	-0.7705
H	3.3323	-1.3318	-1.9424
H	3.1401	-0.9005	1.7786
H	2.8737	-2.6123	1.6074
H	1.5122	-1.5881	1.9907
H	-0.0177	4.4479	-0.0937
H	-1.3509	3.7143	0.7997
H	-1.3358	3.6825	-0.9814
H	-2.3815	-3.6269	-0.3385
H	-3.5909	-2.6793	-1.2134
H	-3.7186	-2.8823	0.5477

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.341168 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.357084
Thermal correction to Enthalpy=	0.358029
Thermal correction to Gibbs Free Frequency and Energy=	0.298481
Sum of electronic and zero-point Energies=	-585.214473

Sum of electronic and thermal Energies=	-585.198557
Sum of electronic and thermal Enthalpies=	-585.197613
Sum of electronic and thermal Free Energies=	-585.257161

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.340541 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.356478
Thermal correction to Enthalpy=	0.357422
Thermal correction to Gibbs Free Frequency and Energy=	0.297851
Sum of electronic and zero-point Energies=	-585.217242
Sum of electronic and thermal Energies=	-585.201305
Sum of electronic and thermal Enthalpies=	-585.200361
Sum of electronic and thermal Free Energies=	-585.259932

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.340634 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.356534
Thermal correction to Enthalpy=	0.357478
Thermal correction to Gibbs Free Frequency and Energy=	0.298088
Sum of electronic and zero-point Energies=	-585.217008
Sum of electronic and thermal Energies=	-585.201107
Sum of electronic and thermal Enthalpies=	-585.200163
Sum of electronic and thermal Free Energies=	-585.259554

Name of anion	α-Cadiene-C1-H16-anion		
Cartesian Coordinates optimized at B3LYP/6-311G (d,p)			
C	-0.0493	-0.2559	0.2381
C	1.3503	-0.2786	-0.426
C	-0.8162	1.0123	-0.2498
C	-2.2026	1.0239	0.4163
C	2.143	0.9685	0.0204
C	2.1777	-1.528	-0.1073
C	-0.0009	2.2805	-0.0585
C	-0.8845	-1.4989	0.0332
C	-3.0199	-0.2036	-0.0052
C	1.3373	2.2318	0.0637
C	-2.2243	-1.4811	-0.0805
C	3.4965	-1.5021	-0.8731
C	2.4259	-1.633	1.394
C	-0.7143	3.6026	-0.0835
C	-3.0189	-2.7383	-0.2818
H	1.208	-0.2303	-1.5158
H	-0.9806	0.9284	-1.3357
H	-2.7735	1.919	0.1449
H	-2.0926	1.0392	1.5087
H	2.9729	1.1398	-0.6755
H	2.5771	0.87	1.0176
H	1.6459	-2.4243	-0.4419
H	-0.3882	-2.4633	0.0289
H	-3.4588	-0.0157	-0.9934

H	-3.8532	-0.3238	0.6973
H	1.9004	3.1531	0.1914
H	4.1876	-0.7387	-0.502
H	4.0075	-2.4663	-0.7705
H	3.3323	-1.3318	-1.9424
H	3.1401	-0.9005	1.7786
H	2.8737	-2.6123	1.6074
H	1.5122	-1.5881	1.9907
H	-0.0177	4.4479	-0.0937
H	-1.3509	3.7143	0.7997
H	-1.3358	3.6825	-0.9814
H	-2.3815	-3.6269	-0.3385
H	-3.5909	-2.6793	-1.2134
H	-3.7186	-2.8823	0.5477

Frequency and Energy at B3LYP/6-311G (d,p) (gas)	
Zero-point correction=	0.336318 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.352408
Thermal correction to Enthalpy=	0.353353
Thermal correction to Gibbs Free Frequency and Energy=	0.294144
Sum of electronic and zero-point Energies=	-585.220311
Sum of electronic and thermal Energies=	-585.204221
Sum of electronic and thermal Enthalpies=	-585.203277
Sum of electronic and thermal Free Energies=	-585.262485

Frequency and Energy at B3LYP/6-311G (d,p) (water)	
Zero-point correction=	0.336379 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.352538
Thermal correction to Enthalpy=	0.353482
Thermal correction to Gibbs Free Frequency and Energy=	0.293964
Sum of electronic and zero-point Energies=	-585.290380
Sum of electronic and thermal Energies=	-585.274221
Sum of electronic and thermal Enthalpies=	-585.273277
Sum of electronic and thermal Free Energies=	-585.332796

Frequency and Energy at B3LYP/6-311G (d,p) (ethanol)	
Zero-point correction=	0.336388 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.352542
Thermal correction to Enthalpy=	0.353486
Thermal correction to Gibbs Free Frequency and Energy=	0.294013
Sum of electronic and zero-point Energies=	-585.287932
Sum of electronic and thermal Energies=	-585.271778
Sum of electronic and thermal Enthalpies=	-585.270834
Sum of electronic and thermal Free Energies=	-585.330308

Name of cationic radical	α-Cadiene

Cartesian Coordinates optimized at PM6				
C	0	-0.0493	-0.2559	0.2381
C	0	1.3503	-0.2786	-0.426
C	0	-0.8162	1.0123	-0.2498
C	0	-2.2026	1.0239	0.4163
C	0	2.143	0.9685	0.0204
C	0	2.1777	-1.528	-0.1073
C	0	-0.0009	2.2805	-0.0585

C	0	-0.8845	-1.4989	0.0332
C	0	-3.0199	-0.2036	-0.0052
C	0	1.3373	2.2318	0.0637
C	0	-2.2243	-1.4811	-0.0805
C	0	3.4965	-1.5021	-0.8731
C	0	2.4259	-1.633	1.394
C	0	-0.7143	3.6026	-0.0835
C	0	-3.0189	-2.7383	-0.2818
H	0	0.0858	-0.1584	1.325
H	0	1.208	-0.2303	-1.5158
H	0	-0.9806	0.9284	-1.3357
H	0	-2.7735	1.919	0.1449
H	0	-2.0926	1.0392	1.5087
H	0	2.9729	1.1398	-0.6755
H	0	2.5771	0.87	1.0176
H	0	1.6459	-2.4243	-0.4419
H	0	-0.3882	-2.4633	0.0289
H	0	-3.4588	-0.0157	-0.9934
H	0	-3.8532	-0.3238	0.6973
H	0	1.9004	3.1531	0.1914
H	0	4.1876	-0.7387	-0.502
H	0	4.0075	-2.4663	-0.7705
H	0	3.3323	-1.3318	-1.9424
H	0	3.1401	-0.9005	1.7786
H	0	2.8737	-2.6123	1.6074
H	0	1.5122	-1.5881	1.9907
H	0	-0.0177	4.4479	-0.0937
H	0	-1.3509	3.7143	0.7997
H	0	-1.3358	3.6825	-0.9814
H	0	-2.3815	-3.6269	-0.3385
H	0	-3.5909	-2.6793	-1.2134
H	0	-3.7186	-2.8823	0.5477

Frequency and Energy at PM6 (gas)

Zero-point correction=	0.323705 (Hartree/Particle)
Thermal correction to Frequency and Energy=	0.340849
Thermal correction to Enthalpy=	0.341793
Thermal correction to Gibbs Free Frequency and Energy=	0.277794
Sum of electronic and zero-point Energies=	0.574149
Sum of electronic and thermal Energies=	0.591293
Sum of electronic and thermal Enthalpies=	0.592238
Sum of electronic and thermal Free Energies=	0.528238