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Unveiling intramolecular [3+2] cycloaddition reactions of *C*,*N*-disubstituted nitrones with a molecular electron density theory perspective

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*BET study of the IM32CA reaction of nitrone **15***

The electronic rearrangement associated along the reaction path have been established by applying the Bonding evolution theory (BET) proposed by Krokoidis[1] from the conjunction of ELF topological analysis[2,3] and Thom's Catastrophe Theory[4] for several chemical reactions[5]. Herein, the BET of the IM32CA reaction of nitrone **15** has been studied, which can be divided into nine ELF topological phases (see Table S1).

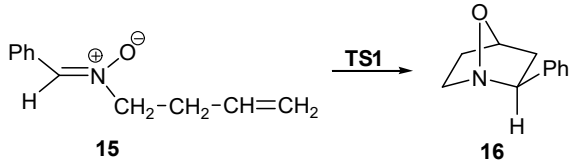
Phase I starts at **S_0-I**, d_{C3-C4} = 2.84 Å and d_{O1-C5} = 2.64 Å, which corresponds with the first structure of the IRC. ELF of **S_0-I** is similar to that of the nitrone **15** (see Table 1), showing the presence of monosynaptic basins, V(O1) and V'(O1) associated with the non bonding electron density on the O1 oxygen and the disynaptic basins, V(N2,C3), V(N2,O1) and V(C4,C5); V'(C4,C5), respectively associated with the N2-C3, N2-O1 and C4-C5 bonding regions.

Phase II starts at **S_1-I**, d_{C3-C4} = 2.43 Å and d_{O1-C5} = 2.34 Å and is associated with the creation of the monosynaptic V(N2) basin integrating 0.85 e associated with the non bonding electron density at N2 nitrogen. Note that the disynaptic V(N2,C3) experiences depopulation of 0.69 e from 3.69 e at **S_0-I** to 3.00 e at **S_1-I,** while the V(N2,O1) disynaptic basin is depopulated by 0.08 e from 1.46 e at **S_0-I** to 1.38 e at **S_1-I,** suggesting that the non-bonding electron density at N2 is created by deriving the electron density mainly from the N2-C3 bonding region. This electronic change demands the energy cost (EC) of 20.0 kcal mol^{-1}.

The short *Phase III* starts at **S_2-I**, d_{C3-C4} = 2.24 Å and d_{O1-C5} = 2.22 Å. The disynaptic V(C4,C5) and V'(C4,C5) disynaptic basins present at **S_1-I** are merged into one disynaptic basins V(C4,C5) integrating at 3.20 e, suggesting the rupture of the C4-C5 double bond by the EC of 25.2 kcal mol^{-1}.

Phase IV starts at **S_3-I**, d_{C3-C4} = 2.19 Å and d_{O1-C5} = 2.18 Å, which is characterized by the creation of a new V(C3) monosynaptic basin, integrating 0.34 e, associated with the formation of the *pseudoradical* centre at C3 carbon. The electron density for the creation of the *pseudoradical* centre mainly comes from the depopulation of the N2-C3 bonding region integrating 2.73 e at **S_2-I** to 2.42 e at **S_3-I**. In this phase, **TS1** is found. These bonding changes demand an energy cost of 26.0 kcal·mol^{-1} and the GEDT in *phase IV* is 0.04 e indicating a non-polar process consistent with the high activation energy barrier required for the formation of non-bonding electron density at N2 nitrogen, rupture of the C4-C5 bond and creation of the *pseudoradical* centre at C3.

Table S1. ELF valence basin populations, distances of the forming bonds, and relative electronic energies of the IRC structures **S_0-I** – **S_8-I** defining the nine phases characterizing the molecular mechanism of the IM32CA reaction of **15**. Distances are given in angstroms, Å, and relative energies in kcal·mol^{-1}.



15 **16**

Phases	*I*	*II*	*III*	*IV*	*V*	*VI*	*VII*	*VIII*	*IX*	
Structures	**S_0-I**	**S_1-I**	**S_2-I**	**S_3-I**	**S_4-I**	**S_5-I**	**S_6-I**	**S_7-I**	**S_8-I**	**16**
d(C3-C4)	2.840	2.426	2.243	2.193	2.091	1.959	1.943	1.791	1.750	1.550
d(O1-C5)	2.638	2.337	2.215	2.182	2.115	2.023	2.011	1.879	1.836	1.422
ΔE	0.0	20.0	25.2	26.0	26.2	22.3	21.4	9.7	5.3	-24.9
GEDT	0.005	0.004	0.028	0.040	0.071	0.121	0.128	0.194	0.212	0.291
V(O1)	2.92	2.92	2.92	2.92	2.92	2.90	2.90	2.91	2.81	2.49
V'(O1)	2.99	2.97	2.95	2.94	2.92	2.91	2.92	2.83	2.79	2.50
V''(O1)								0.07		
V(N2,C3)	3.69	3.00	2.73	2.42	2,24	2.09	2.07	1.95	1.93	1.82
V'(N2,O1)	1.46	1.38	1.31	1.29	1.25	1.20	1.19	1.13	1.13	0.97
V(C4,C5)	1.68	1.66	3.20	3.17	2.79	2.51	2.46	2.21	2.16	1.93
V'(C4,C5)	1.73	1.65								
V(N2)		0.85	1.36	1.48	1.69	1.92	1.95	2.15	2.19	2.40
V(C3)				0.28	0.44					
V(C4)					0.34					
V(C5)							0.05	0.19		
V(C3,C4)						1.16	1.20	1.50	1.56	1.84
V(O1,C5)									0.43	1.29

Phase V starts at **S_4-I**, d_{C3-C4} = 2.09 Å and d_{O1-C5} = 2.12 Å, which is characterized by the creation of a new V(C4) monosynaptic basin, integrating 0.34 e, associated with the formation of a *pseudoradical* center at the C4 carbon. The V(C4,C5) disynaptic basin experiences a depopulation of 0.38 e along *Phase V* to create this *pseudoradical* centre.

Phase VI starts at **S_5-I**, d_{C3-C4} = 1.96 Å and d_{O1-C5} = 2.02 Å, At the beginning of this phase the first more relevant change along the IRC takes place. At this structure, while the V(C3) and V(C4) monosynaptic basins present at **S_4-I** are missing, a new V(C3,C4) disynaptic basin, integrating 1.16 e, is created. This topological change indicates that the formation of the first C3-C4 single bond has begun at a C–C distance of 1.96 Å.

Phase VII starts at **S_6-I**, d_{C3-C4} = 1.94 Å and d_{O1-C5} = 2.01 Å, which is characterized by the creation of a new V(C5) monosynaptic basin, integrating 0.05 e, associated with the formation of a *pseudoradical* center at the C5 carbon. The V(C4,C5) disynaptic basin experiences a depopulation of 0.05 e along *Phase VII* to create this *pseudoradical* centre.

Phase VIII starts at **S_7-I**, d_{C3-C4} = 1.79 Å and d_{O1-C5} = 1.88 Å, which is characterized by the creation of a new V"(O1) monosynaptic basin integrating 0.07 e associated with the non-bonding electron density at O1 oxygen.

Phase IX starts at **S_8-I**, d_{C3-C4} = 1.75 Å and d_{O1-C5} = 1.84 Å, At the beginning of this phase the second relevant change along the IRC takes place. At this structure, while the V(C5) and V"(O1) monosynaptic basins present at **S_7-I** are missing, a new V(O1,C5) disynaptic basin, integrating 0.43 e, is created. This topological change indicates that the formation of the second O1-C5 single bond has begun at a C–O distance of 1.84 Å. Note that the formation of the second O1-C5 bond starts, when the first C3-C4 bond has been formed by 85%, suggesting a highly asynchronous C-C and C-O bond formation, which is not depicted from the geometrical parameters at the early TSs. The molecular geometry is finally relaxed in the isoxazolidine **16**, with the V(C3,C4) and V(O1,C5) integrating the electron density of 1.84 e and 1.29 e respectively. The electron localization domains at the selected IRC points **S_0-I** to **S_8-I** are shown in Figure S1.

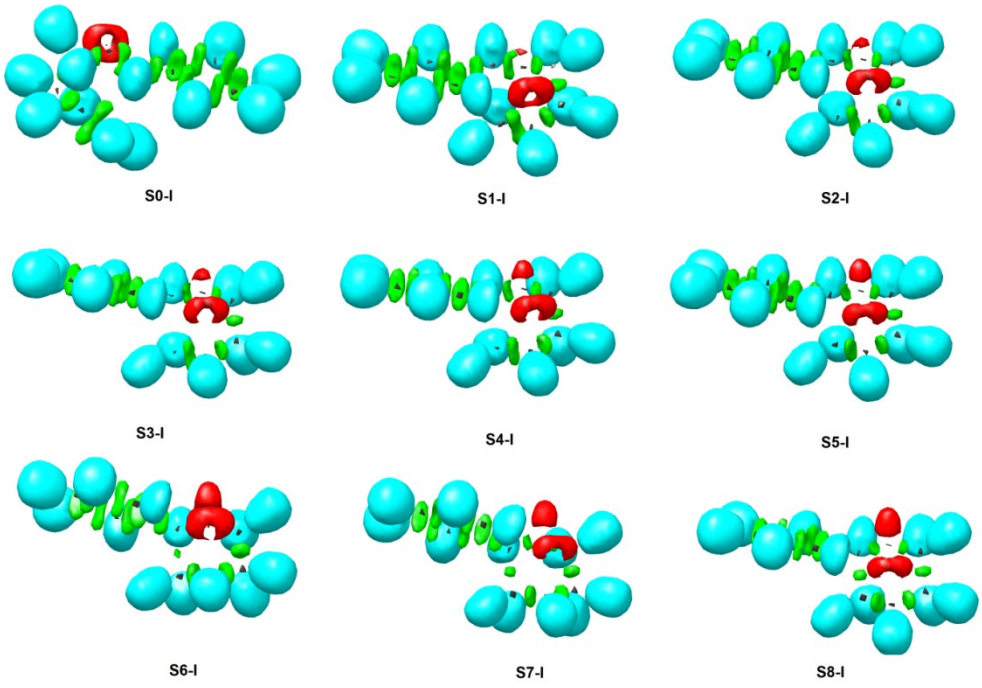


Figure S1. ELF localization domains (Isovalue = 0.84) of **S_0-I to S_8-I**

*BET study of the IM32CA reaction of nitrone **20***

Herein, the BET of the IM32CA reaction of nitrone **20** has been studied, which can be divided into six ELF topological phases (see Table S2).

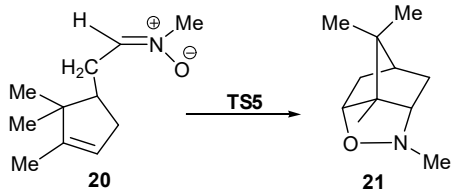
Phase I starts at **S_0-II**, d_{C3-C4} = 3.00 Å and d_{O1-C5} = 2.91 Å, which corresponds with the first structure of the IRC. ELF of **S_0-II** is similar to that of the nitrone **20** (see Table 1), showing the presence of monosynaptic basins, V(O1) and V'(O1) associated with the non bonding electron density on the O1 oxygen and the disynaptic basins, V(N2,C3), V(N2,O1) and V(C4,C5);V'(C4,C5), respectively associated with the N2-C3, N2-O1 and C4-C5 bonding regions.

Phase II starts at **S_1-II**, d_{C3-C4} = 2.27 Å and d_{O1-C5} = 2.19 Å and is associated with the creation of the monosynaptic V(N2) basin integrating 0.82 e associated with the non bonding electron density at N2 nitrogen. Note that the disynaptic V(N2,C3) experiences depopulation of 0.58 e from 3.77 e at **S_0-II** to 3.19 e at **S_1-II,** while the V(N2,O1) disynaptic basin is depopulated by 0.13 e from 1.48 e at **S_0-II** to 1.35 e at **S_1-II,** suggesting that the non-bonding electron density at N2 is created by deriving the electron density mainly from the N2-C3 bonding region. In this phase, the disynaptic V(C4,C5) and V'(C4,C5) basins present at **S_1-II** are merged into one disynaptic basins V(C4,C5) integrating at 3.38 e, suggesting the rupture of the C4-C5 double bond. These electronic changes demand the energy cost (EC) of 17.9 kcal mol^{-1}.

Phase III starts at **S_2-II**, d_{C3-C4} = 2.20 Å and d_{O1-C5} = 2.14 Å, which is characterized by the creation of a new V(C3) monosynaptic basin, integrating 0.30 e, associated with the formation of the *pseudoradical* centre at C3 carbon. The electron density for the creation of the *pseudoradical* centre mainly comes from the depopulation of the N2-C3 bonding region integrating 3.19 e at **S_1-II** to 2.72 e at **S_2-II**.

Phase IV starts at **S_3-II**, d_{C3-C4} = 2.14 Å and d_{O1-C5} = 2.10 Å, which is characterized by the creation of a new V(C4) monosynaptic basin, integrating 0.34 e, associated with the formation of a *pseudoradical* center at the C4 carbon which derives electron density from the C4-C5 bonding region. The V(C4,C5) disynaptic basin experiences a depopulation of 0.36 e from 3.35 e at **S_2-II** to 2.99 e at **S_3-II**. In this phase, the **TS5** is found and the bonding changes along the phase demand the EC of 20.2 kcal mol^{-1}. The GEDT value of 0.03 e indicates non-polar character of this 32CA reaction.

Table S2. ELF valence basin populations, distances of the forming bonds, and relative electronic energies of the IRC structures **S_0-II** – **S_5-II** defining the six phases characterizing the molecular mechanism of the intramolecular 32CA reaction of **20**. Distances are given in angstroms, Å, and relative energies in kcal·mol^{-1}.



20 **21**

Phases	*I*	*II*	*III*	*IV*	*V*	*VI*	
Structures	**S_0-II**	**S_1-II**	**S_2-II**	**S_3-II**	**S_4-II**	**S_5-II**	**21**
d(C3-C4)	3.000	2.266	2.202	2.140	1.947	1.748	1.542
d(O1-C5)	2.905	2.190	2.143	2.096	1.944	1.751	1.397
ΔE	0.0	17.9	19.4	20.2	16.8	1.56	-24.9
GEDT	0.015	0.002	0.013	0.031	0.116	0.216	0.295
V(O1)	2.89	2.88	2.89	2.89	2.87	2.75	2.53
V'(O1)	3.04	2.98	2.97	2.95	2.95	2.70	2.56
V(N2,C3)	3.77	3.19	2.72	2.53	2.20	2.00	1.85
V'(N2,O1)	1.48	1.35	1.31	1.28	1.18	1.08	0.96
V(C4,C5)	1.74	3.38	3.35	2.99	2.53	2.18	1.95
V'(C4,C5)	1.77						
V(N2)		0.82	1.10	1.31	1.79	2.11	2.34
V(C3)			0.30	0.39			
V(C4)				0.34			
V(C5)					0.10		
V(C3,C4)					1.30	1.65	1.91
V(O1,C5)						0.63	1.33

Phase V starts at **S_4-II**, d_{C3-C4} = 1.95 Å and d_{O1-C5} = 1.94 Å. At the beginning of this phase, the first relevant change along the IRC takes place. At this structure, while the V(C3) and V(C4) monosynaptic basins present at **S_3-II** are missing, a new V(C3,C4) disynaptic basin, integrating 1.30 e, is created. This topological change indicates that the formation of the first C3-C4 single bond has begun at a C–C distance of 1.95 Å. This phase is also characterized by the creation of a new V(C5) monosynaptic basin, integrating 0.10 e, associated with the formation of a *pseudoradical* center at the C5 carbon deriving electron density from the C4-C5 bonding region. The V(C4,C5) disynaptic basin experiences a depopulation of 0.46 e from **S_3-II** to **S_4-II.**

Phase VI starts at **S_5-II**, d_{C3-C4} = 1.75 Å and d_{O1-C5} = 1.75 Å. At the beginning of this phase the second relevant change along the IRC takes place. At this structure, while the

V(C5) monosynaptic basins present at **S_4-II** is missing, a new V(O1,C5) disynaptic basin, integrating 0.63 e, is created. This topological change indicates that the formation of the second O1-C5 single bond has begun at a C–C distance of 1.75 Å. Note that the formation of the second O1-C5 bond starts, when the first C3-C4 bond has been formed by 86%, suggesting a highly asynchronous C-C and C-O bond formation, which is not depicted from the geometrical parameters at the early TSs. The molecular geometry is finally relaxed in the isoxazolidine **21**, with the V(C3,C4) and V(O1,C5) integrating the electron density of 1.91 e and 1.33 e respectively.

References

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Table with the MPWB1K/6-311G(d,p) calculated electronic energies (au), computed at 298 K in gas phase and toluene of the stationary points involved in the IM32CA reactions of nitrones **15**, **18**, **20**, **24** and **26**.

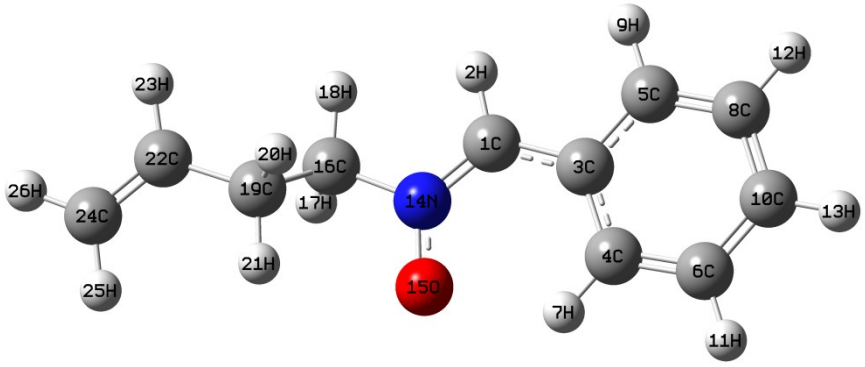
	E(Gas Phase)	E(Toluene)
15	-556.720262	-556.726939
18	-635.327011	-635.333512
20	-560.33485	-560.340302
24	-481.73552	-481.741909
26	-560.334207	-560.339869
TS1	-556.678448	-556.684362
TS2	-556.672609	-556.678224
TS3	-635.278289	-635.284086
TS4	-635.279192	-635.284155
TS5	-560.302515	-560.305957
TS6	-560.303557	-560.306490
TS7	-481.705566	-481.709178
TS8	-560.303804	-560.307202
16	-556.759889	-556.76548
17	-556.754954	-556.760572
35	-635.359606	-635.364798
36	-635.357858	-635.362965
21	-560.373376	-560.376388
22	-560.372062	-560.374669
25	-481.776448	-481.779387
27	-560.369780	-560.372710

Table with the MPWB1K/6-311G(d,p) calculated enthalpies (au), entropies (Cal $mol^{-1}K^{-1}$) and Gibbs free energies (au), computed at 298 K in toluene of the stationary points involved in the IM32CA reactions of nitrones **15**, **18**, **20**, **24** and **26**.

	H	S	G
15	-556.491914	111.574	-556.544926
18	-635.038255	127.871	-635.099011
20	-560.035255	116.542	-560.090628
24	-481.495638	103.929	-481.545018
26	-560.033486	112.406	-560.086894
TS1	-556.450807	100.453	-556.498536
TS2	-556.444705	100.227	-556.492326
TS3	-634.990267	110.718	-635.042872
TS4	-634.990473	110.207	-635.042836
TS5	-560.001779	104.637	-560.051496
TS6	-560.002763	104.589	-560.052457
TS7	-481.463925	91.925	-481.507602
TS8	-560.001817	102.752	-560.050638
16	-556.527866	100.535	-556.575633
17	-556.523201	97.298	-556.569431
35	-635.067666	108.470	-635.119203
36	-635.066176	107.677	-635.117337
21	-560.069608	104.203	-560.119118
22	-560.067733	101.915	-560.116156
25	-481.530388	88.255	-481.572321
27	-560.064008	101.150	-560.112068

MPWB1K/6-311G(d,p) gas phase computed unique imaginary frequency, and Cartesian coordinates of the stationary points involved in the IM32CA reactions of nitrones **15**, **18**, **20**, **24** and **26** in gas phase

Nitrone **15** (Gas Phase)



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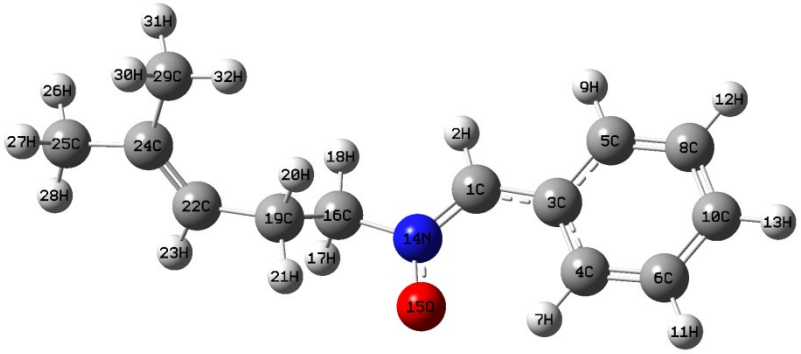
3	6	0	1.643015	-0.307456	0.082631
4	6	0	2.070319	1.017443	-0.001903
5	6	0	2.594038	-1.324863	-0.003091
6	6	0	3.411413	1.296258	-0.167595
7	1	0	1.342523	1.803636	0.063711
8	6	0	3.928415	-1.035409	-0.166771
9	1	0	2.273591	-2.353497	0.061434
10	6	0	4.343108	0.281264	-0.250087
11	1	0	3.730508	2.323735	-0.232575
12	1	0	4.647059	-1.836052	-0.229501
13	1	0	5.387981	0.511869	-0.378753
14	7	0	-0.750035	0.081102	0.375952
15	8	0	-0.716329	1.333334	0.365072
16	6	0	-2.091929	-0.485610	0.543011
17	1	0	-2.443070	-0.144150	1.511409
18	1	0	-2.023732	-1.568052	0.547407
19	6	0	-3.008381	0.021353	-0.551720
20	1	0	-2.609428	-0.300001	-1.513731
21	1	0	-2.983725	1.105174	-0.532230
22	6	0	-4.397669	-0.483936	-0.377679
23	1	0	-4.538995	-1.554548	-0.457449
24	6	0	-5.441648	0.283257	-0.131162
25	1	0	-5.341109	1.354863	-0.047481
26	1	0	-6.430255	-0.128603	-0.010685

Nitrone **18** (Gas Phase)



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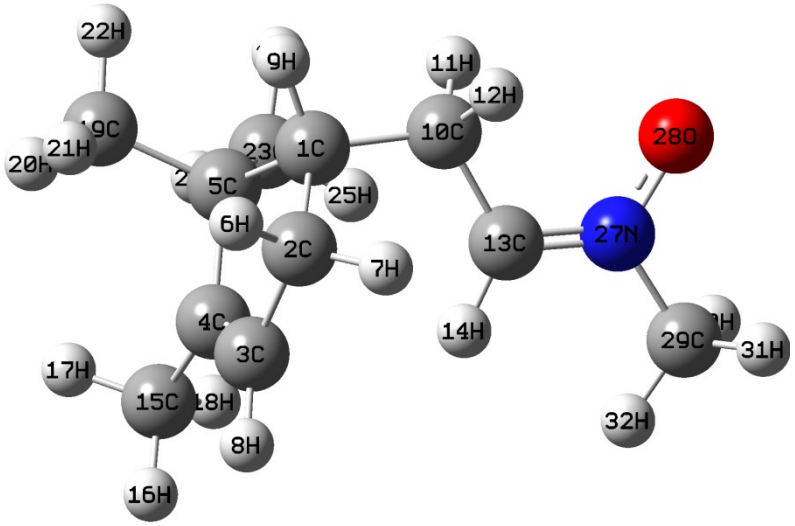
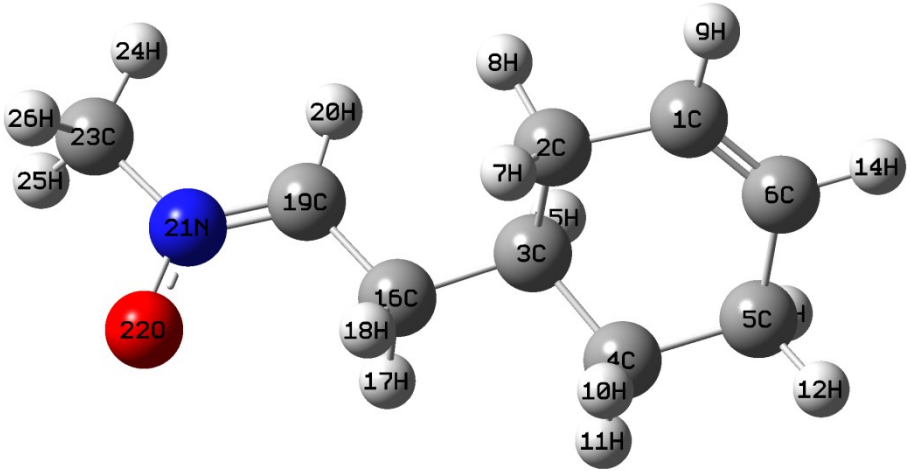
3	6	0	2.458490	0.230845	-0.222529
4	6	0	3.091599	-0.858737	0.374035
5	6	0	3.211117	1.371726	-0.501884
6	6	0	4.436661	-0.789771	0.675338
7	1	0	2.517971	-1.739105	0.590770
8	6	0	4.550723	1.430309	-0.197224
9	1	0	2.730150	2.220142	-0.964181
10	6	0	5.170501	0.345143	0.395148
11	1	0	4.915835	-1.638098	1.136429
12	1	0	5.113682	2.321640	-0.420860
13	1	0	6.220202	0.386129	0.635898
14	7	0	0.194337	-0.673375	-0.409271
15	8	0	0.416291	-1.795695	0.100145
16	6	0	-1.195105	-0.458012	-0.828510
17	1	0	-1.397889	-1.217265	-1.577729
18	1	0	-1.285655	0.522944	-1.280554
19	6	0	-2.131960	-0.618497	0.351296
20	1	0	-1.920337	0.154292	1.083747
21	1	0	-1.894485	-1.572866	0.814076
22	6	0	-3.552341	-0.595651	-0.091555
23	1	0	-3.846380	-1.429685	-0.717167
24	6	0	-4.481490	0.310726	0.184443
25	6	0	-5.870603	0.161676	-0.342338
26	1	0	-6.148124	1.020530	-0.951761
27	1	0	-6.589838	0.112837	0.473986
28	1	0	-5.977824	-0.734257	-0.944282
29	6	0	-4.268719	1.522520	1.028345
30	1	0	-4.895712	1.478224	1.917633
31	1	0	-4.566097	2.417166	0.483949
32	1	0	-3.242653	1.650115	1.349463

Nitrone **20** (Gas Phase)



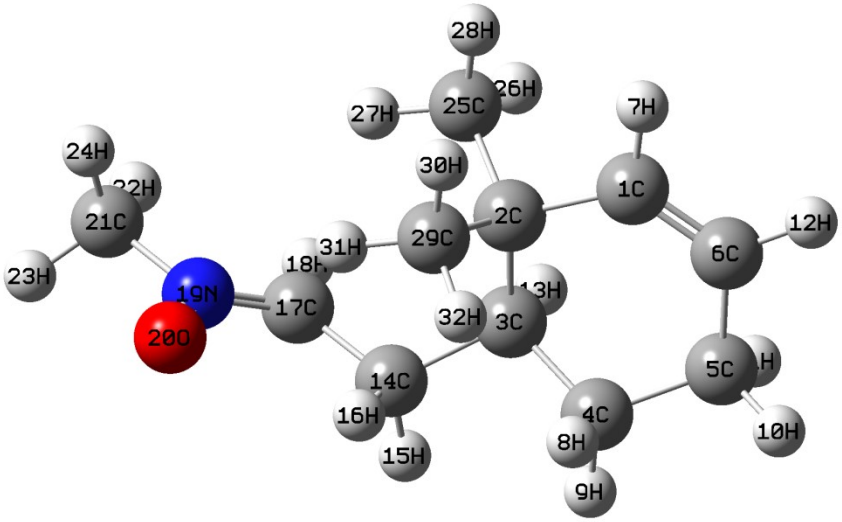
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.635669	-1.193215	0.537414
2	6	0	0.875837	-0.498572	1.884852
3	6	0	1.370920	0.854905	1.496283
4	6	0	1.701096	0.921703	0.216079
5	6	0	1.534197	-0.421796	-0.459811
6	1	0	1.617170	-1.023357	2.488685
7	1	0	-0.034406	-0.459952	2.483532
8	1	0	1.476858	1.668242	2.197839
9	1	0	0.965361	-2.228898	0.577065
10	6	0	-0.842609	-1.226201	0.187313
11	1	0	-1.015526	-1.679009	-0.789583
12	1	0	-1.366214	-1.887039	0.881425
13	6	0	-1.527663	0.081746	0.211994
14	1	0	-1.045360	1.003606	0.479027
15	6	0	2.249908	2.095090	-0.507311
16	1	0	2.387689	2.941772	0.156697
17	1	0	3.211135	1.861427	-0.962634
18	1	0	1.587966	2.399423	-1.316375
19	6	0	2.900430	-1.099694	-0.522449
20	1	0	3.611775	-0.506616	-1.092732
21	1	0	3.304139	-1.240554	0.477344
22	1	0	2.821013	-2.073672	-1.000872
23	6	0	0.972004	-0.315828	-1.865727
24	1	0	0.802074	-1.302174	-2.290460
25	1	0	0.030218	0.226232	-1.890816
26	1	0	1.675041	0.201960	-2.514316
27	7	0	-2.778647	0.118166	-0.099391
28	8	0	-3.448490	-0.891995	-0.424390
29	6	0	-3.514308	1.373446	-0.094285
30	1	0	-3.909870	1.519716	-1.091430
31	1	0	-4.339200	1.261099	0.597799
32	1	0	-2.874292	2.197088	0.194553

Nitrone **24** (Gas Phase)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.609429	1.404422	0.339984
2	6	0	1.160074	1.073149	0.468740
3	6	0	0.798730	-0.212945	-0.255711
4	6	0	1.830602	-1.275779	0.070944
5	6	0	3.204017	-0.874445	-0.426182
6	6	0	3.518939	0.541817	-0.080152
7	1	0	0.893564	0.979151	1.524708
8	1	0	0.564815	1.904545	0.091578
9	1	0	2.912351	2.408231	0.600345
10	1	0	1.861128	-1.408124	1.153159
11	1	0	1.536451	-2.231822	-0.356560
12	1	0	3.964049	-1.530482	-0.005282
13	1	0	3.266924	-1.007485	-1.508064
14	1	0	4.546695	0.861157	-0.174723
15	1	0	0.853206	-0.019437	-1.330453
16	6	0	-0.600708	-0.681345	0.084700
17	1	0	-0.798672	-1.662234	-0.353456
18	1	0	-0.707831	-0.839496	1.160366
19	6	0	-1.664405	0.242276	-0.352458
20	1	0	-1.485711	1.114092	-0.955781
21	7	0	-2.882986	-0.014444	-0.019256
22	8	0	-3.223143	-1.006224	0.668496
23	6	0	-3.973404	0.855992	-0.433113
24	1	0	-3.606074	1.689037	-1.018350
25	1	0	-4.666318	0.253910	-1.006928
26	1	0	-4.468179	1.201009	0.465764

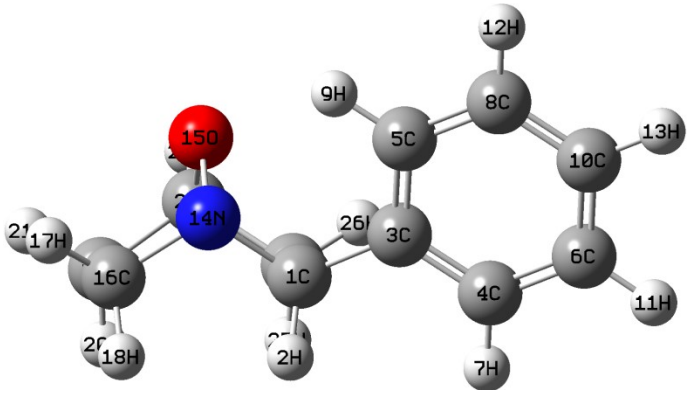
Nitrone **26** (Gas Phase)



Standard orientation:

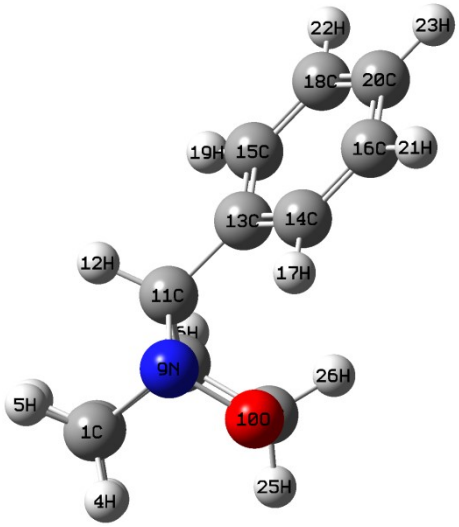
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.336891	1.210016	0.089305
2	6	0	0.884989	0.821860	0.057860
3	6	0	0.746047	-0.639876	-0.409812
4	6	0	1.839131	-1.509522	0.190888
5	6	0	3.215574	-1.070403	-0.249864
6	6	0	3.367026	0.400453	-0.078179
7	1	0	2.519172	2.266500	0.240708
8	1	0	1.774549	-1.452214	1.277638
9	1	0	1.667240	-2.549917	-0.077926
10	1	0	3.980709	-1.590192	0.324041
11	1	0	3.387140	-1.345184	-1.292699
12	1	0	4.366800	0.809872	-0.075397
13	1	0	0.884892	-0.641795	-1.494580
14	6	0	-0.601490	-1.287787	-0.089390
15	1	0	-0.552983	-2.320815	-0.438964
16	1	0	-0.761914	-1.324110	0.984172
17	6	0	-1.788249	-0.657519	-0.696575
18	1	0	-1.876271	-0.518345	-1.759767
19	7	0	-2.788995	-0.268657	0.019419
20	8	0	-2.867474	-0.348238	1.271753
21	6	0	-3.951072	0.337338	-0.615543
22	1	0	-3.840725	0.363585	-1.691910
23	1	0	-4.814459	-0.248254	-0.327248
24	1	0	-4.053210	1.336336	-0.210385
25	6	0	0.208263	1.778467	-0.920069
26	1	0	0.588896	1.638974	-1.929277
27	1	0	-0.868404	1.643547	-0.931243
28	1	0	0.403564	2.808498	-0.629302
29	6	0	0.283939	1.034384	1.442468
30	1	0	0.486546	2.047248	1.782933
31	1	0	-0.793791	0.884788	1.442561
32	1	0	0.718711	0.353518	2.170154

Isoxazolidine **16** (Gas Phase)



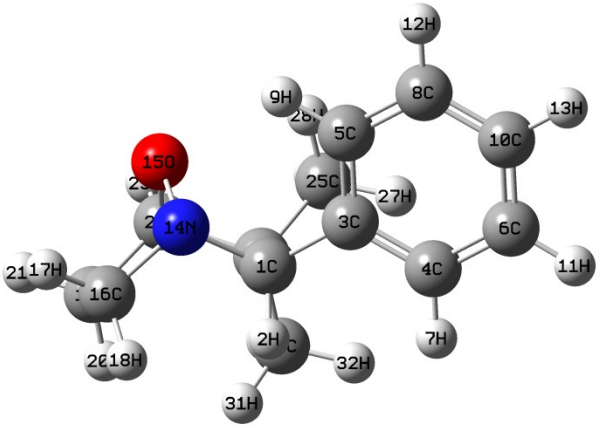
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.474749	0.501652	0.453877
2	1	0	0.587755	1.120100	1.339952
3	6	0	-0.982858	0.200126	0.260906
4	6	0	-1.899300	1.237195	0.323898
5	6	0	-1.433635	-1.079512	-0.007206
6	6	0	-3.244023	1.003625	0.121772
7	1	0	-1.556886	2.239098	0.537587
8	6	0	-2.780208	-1.313259	-0.209506
9	1	0	-0.721997	-1.885903	-0.052435
10	6	0	-3.688970	-0.276272	-0.147048
11	1	0	-3.945595	1.820129	0.179114
12	1	0	-3.120644	-2.315049	-0.416586
13	1	0	-4.738699	-0.463454	-0.304153
14	7	0	1.270404	-0.715320	0.647268
15	8	0	1.595721	-1.056547	-0.683992
16	6	0	2.588512	-0.354409	1.170247
17	1	0	3.085883	-1.265141	1.480533
18	1	0	2.475043	0.288336	2.036088
19	6	0	3.308134	0.307052	-0.017900
20	1	0	3.580912	1.341558	0.160886
21	1	0	4.199130	-0.243492	-0.297900
22	6	0	2.216538	0.164922	-1.063806
23	1	0	2.546939	0.091321	-2.090793
24	6	0	1.116456	1.167920	-0.789926
25	1	0	1.489756	2.167432	-0.594229
26	1	0	0.407446	1.210437	-1.608853

Isoxazolidine **17** (Gas Phase)



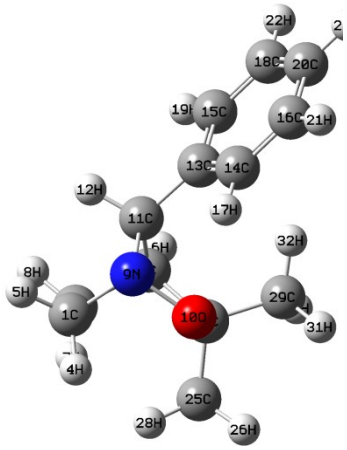
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.759398	-0.381786	-0.873398
2	6	0	1.445858	1.011527	0.504872
3	6	0	2.840969	0.952953	-0.099105
4	1	0	3.446059	-1.137573	-0.515968
5	1	0	2.910670	-0.253548	-1.940916
6	1	0	1.118357	1.978914	0.862846
7	1	0	3.617527	0.954386	0.659164
8	1	0	3.020229	1.792298	-0.764994
9	7	0	1.398823	-0.872114	-0.659651
10	8	0	1.374794	-1.279175	0.704064
11	6	0	0.628539	0.364221	-0.618243
12	1	0	0.779970	0.883568	-1.562852
13	6	0	-0.831584	0.176473	-0.356918
14	6	0	-1.399734	-1.082917	-0.279113
15	6	0	-1.637903	1.292352	-0.199969
16	6	0	-2.754315	-1.218793	-0.044936
17	1	0	-0.768260	-1.946586	-0.397632
18	6	0	-2.990850	1.155892	0.032673
19	1	0	-1.202758	2.278416	-0.265845
20	6	0	-3.552829	-0.103636	0.112039
21	1	0	-3.187711	-2.204003	0.015474
22	1	0	-3.607141	2.032350	0.150438
23	1	0	-4.609246	-0.214581	0.294651
24	6	0	1.343641	-0.102900	1.517026
25	1	0	2.178691	-0.124589	2.212536
26	1	0	0.406361	-0.081176	2.068584

Isoxazolidine **35** (Gas Phase)



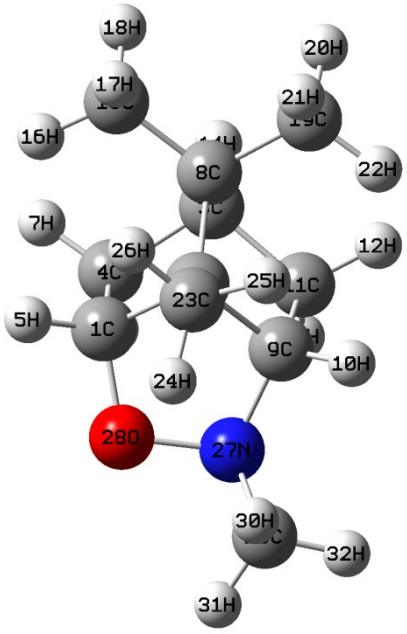
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.341458	-0.015936	-0.611427
2	1	0	-0.501930	0.311833	-1.636031
3	6	0	1.134497	-0.122191	-0.385727
4	6	0	1.979831	0.816358	-0.953122
5	6	0	1.673588	-1.117529	0.410739
6	6	0	3.340858	0.770106	-0.724749
7	1	0	1.567706	1.588732	-1.586287
8	6	0	3.034569	-1.167165	0.635971
9	1	0	1.016135	-1.853184	0.843596
10	6	0	3.872164	-0.223788	0.073010
11	1	0	3.987019	1.505072	-1.176925
12	1	0	3.444457	-1.949306	1.254485
13	1	0	4.934487	-0.266695	0.249763
14	7	0	-1.024235	-1.306722	-0.438209
15	8	0	-1.479085	-1.220684	0.898732
16	6	0	-2.297064	-1.275570	-1.157217
17	1	0	-2.701969	-2.280361	-1.166280
18	1	0	-2.131309	-0.961755	-2.181850
19	6	0	-3.175043	-0.318874	-0.335327
20	1	0	-3.502637	0.556311	-0.883318
21	1	0	-4.052483	-0.823689	0.052951
22	6	0	-2.204165	-0.002752	0.785475
23	1	0	-2.653567	0.234125	1.742108
24	6	0	-1.090710	0.954621	0.362432
25	6	0	-0.276558	1.306253	1.594724
26	1	0	-0.860388	1.950590	2.248644
27	1	0	0.637355	1.829154	1.329047
28	1	0	-0.001551	0.410718	2.142616
29	6	0	-1.530999	2.225500	-0.332860
30	1	0	-2.177290	2.821595	0.307718
31	1	0	-2.057880	2.031665	-1.263086
32	1	0	-0.660895	2.833512	-0.571074

Isoxazolidine **36** (Gas Phase)



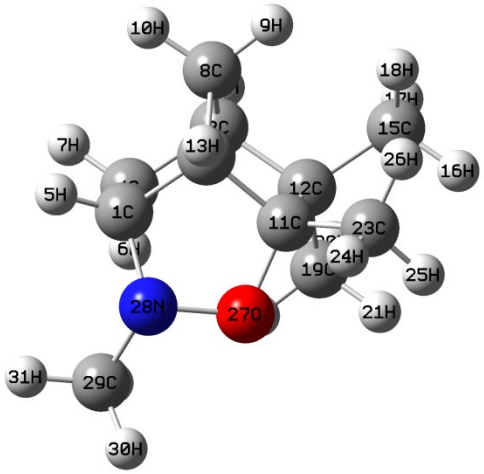
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.278343	-1.554633	-0.583478
2	6	0	-1.255874	-0.191250	1.031592
3	6	0	-2.441649	-1.134545	0.893702
4	1	0	-3.041965	-1.154049	-1.238814
5	1	0	-2.246060	-2.631794	-0.710905
6	1	0	-0.989167	0.090184	2.043064
7	1	0	-3.397784	-0.675146	1.110919
8	1	0	-2.326155	-1.984326	1.561092
9	7	0	-0.988467	-1.001764	-1.009131
10	8	0	-1.198269	0.386321	-1.197751
11	6	0	-0.229645	-1.013200	0.233629
12	1	0	-0.221066	-2.037131	0.606097
13	6	0	1.183546	-0.544710	0.102524
14	6	0	1.725066	-0.226941	-1.130259
15	6	0	1.981239	-0.462376	1.232413
16	6	0	3.040763	0.181523	-1.225700
17	1	0	1.098199	-0.291349	-2.002947
18	6	0	3.295060	-0.051694	1.136813
19	1	0	1.569143	-0.717644	2.197310
20	6	0	3.828339	0.274561	-0.095180
21	1	0	3.452267	0.431301	-2.190276
22	1	0	3.904002	0.011435	2.024065
23	1	0	4.853955	0.596525	-0.172986
24	6	0	-1.461917	0.997226	0.088044
25	6	0	-2.865520	1.568662	0.055933
26	1	0	-2.884751	2.423473	-0.613415
27	1	0	-3.174768	1.905743	1.042391
28	1	0	-3.586786	0.848874	-0.313208
29	6	0	-0.481414	2.129081	0.302605
30	1	0	-0.765324	2.705986	1.179580
31	1	0	-0.510894	2.788773	-0.559965
32	1	0	0.534664	1.780704	0.428103

Isoxazolidine **21** (Gas Phase)



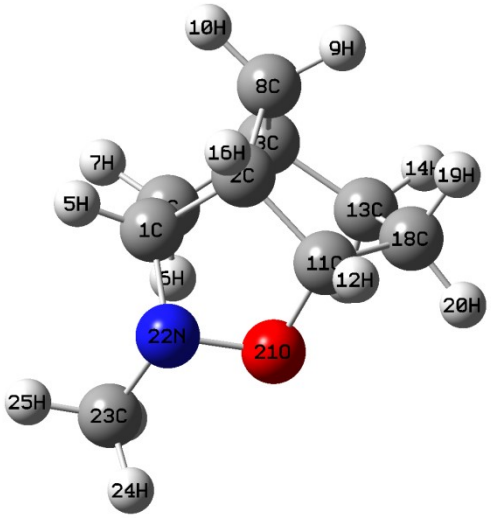
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.349410	-0.409173	-1.249044
2	6	0	0.151423	0.617546	-0.239857
3	6	0	1.082636	-1.303490	0.466259
4	6	0	0.338857	-1.713317	-0.804651
5	1	0	-0.160327	-0.153091	-2.285997
6	1	0	-0.410451	-2.476526	-0.618185
7	1	0	1.012751	-2.086588	-1.568935
8	6	0	1.553028	0.122276	0.131072
9	6	0	-0.750694	0.133419	0.912632
10	1	0	-0.979543	0.910154	1.636604
11	6	0	0.020047	-1.046174	1.520569
12	1	0	0.456877	-0.797451	2.482330
13	1	0	-0.650035	-1.887785	1.658178
14	1	0	1.865405	-1.991599	0.770603
15	6	0	2.531147	0.182210	-1.028846
16	1	0	2.148388	-0.282109	-1.931974
17	1	0	2.778356	1.213719	-1.268641
18	1	0	3.459412	-0.319723	-0.765101
19	6	0	2.157122	0.880840	1.298654
20	1	0	3.040777	0.370000	1.675094
21	1	0	2.464935	1.873985	0.979263
22	1	0	1.465112	1.008266	2.124686
23	6	0	-0.008718	2.054137	-0.652621
24	1	0	-1.016010	2.240167	-1.013740
25	1	0	0.183554	2.728717	0.178467
26	1	0	0.680091	2.306036	-1.456178
27	7	0	-1.996800	-0.332440	0.298194
28	8	0	-1.738781	-0.415405	-1.105736
29	6	0	-3.100638	0.580705	0.434264
30	1	0	-2.872287	1.593476	0.093410
31	1	0	-3.935539	0.198067	-0.141267
32	1	0	-3.392419	0.608735	1.479324

Isoxazolidine **22** (Gas Phase)



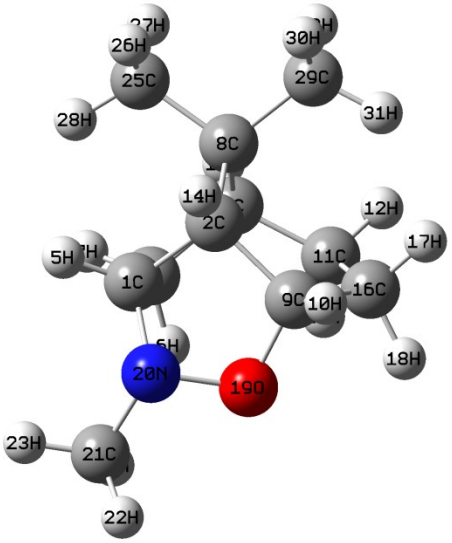
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.351903	0.878352	-0.550555
2	6	0	0.113288	0.543465	-1.363769
3	6	0	-0.767021	1.413624	0.492849
4	6	0	0.740913	1.556553	0.698705
5	1	0	2.062310	1.513111	-1.069928
6	1	0	1.093161	1.126172	1.628639
7	1	0	1.006769	2.610166	0.713427
8	6	0	-0.857791	1.649679	-1.009968
9	1	0	-1.848200	1.523262	-1.429758
10	1	0	-0.484531	2.627131	-1.306325
11	6	0	-0.338514	-0.685246	-0.551171
12	6	0	-1.186169	-0.058843	0.605344
13	1	0	0.307469	0.338821	-2.409437
14	1	0	-1.357357	2.072175	1.123267
15	6	0	-2.686385	-0.201581	0.376730
16	1	0	-2.987718	-1.242435	0.458933
17	1	0	-3.224320	0.356121	1.139919
18	1	0	-3.019669	0.157990	-0.590273
19	6	0	-0.886051	-0.687018	1.952945
20	1	0	-1.482981	-0.206247	2.725385
21	1	0	-1.145162	-1.743399	1.941704
22	1	0	0.159717	-0.620960	2.223372
23	6	0	-1.017038	-1.767693	-1.347456
24	1	0	-0.316773	-2.158920	-2.078016
25	1	0	-1.322585	-2.584350	-0.698656
26	1	0	-1.895718	-1.393168	-1.863742
27	8	0	0.847458	-1.245106	-0.005526
28	7	0	1.946768	-0.425038	-0.392661
29	6	0	2.936561	-0.572101	0.633764
30	1	0	3.289196	-1.597363	0.632107
31	1	0	3.771373	0.079087	0.393786
32	1	0	2.565800	-0.336230	1.633927

Isoxazolidine **25** (Gas Phase)



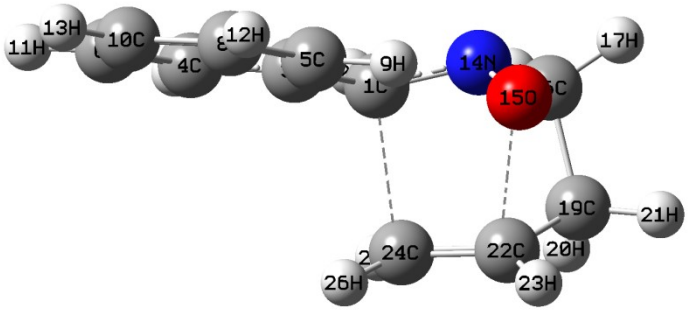
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.796226	-0.907339	0.546553
2	6	0	-0.329237	-0.221348	1.307970
3	6	0	-1.363961	-0.986054	-0.634926
4	6	0	0.102141	-1.423387	-0.729737
5	1	0	1.279230	-1.698191	1.111253
6	1	0	0.573816	-1.040734	-1.629755
7	1	0	0.161968	-2.508001	-0.766851
8	6	0	-1.581977	-0.952415	0.870956
9	1	0	-2.505005	-0.461908	1.167740
10	1	0	-1.593935	-1.956913	1.289298
11	6	0	-0.241049	1.198968	0.700147
12	1	0	-0.112450	1.943333	1.484065
13	6	0	-1.616597	0.411103	-1.216876
14	1	0	-2.629226	0.467718	-1.609712
15	1	0	-0.943787	0.576779	-2.053876
16	1	0	-0.164496	-0.200796	2.378581
17	1	0	-2.007587	-1.703780	-1.134934
18	6	0	-1.420886	1.511232	-0.182160
19	1	0	-2.303535	1.608499	0.446946
20	1	0	-1.273007	2.473098	-0.665128
21	8	0	0.899660	1.197408	-0.136482
22	7	0	1.736608	0.181501	0.390567
23	6	0	2.802333	-0.000425	-0.549366
24	1	0	3.407955	0.898729	-0.565283
25	1	0	3.418015	-0.825298	-0.205096
26	1	0	2.456550	-0.204316	-1.564723

Isoxazolidine **27** (Gas Phase)



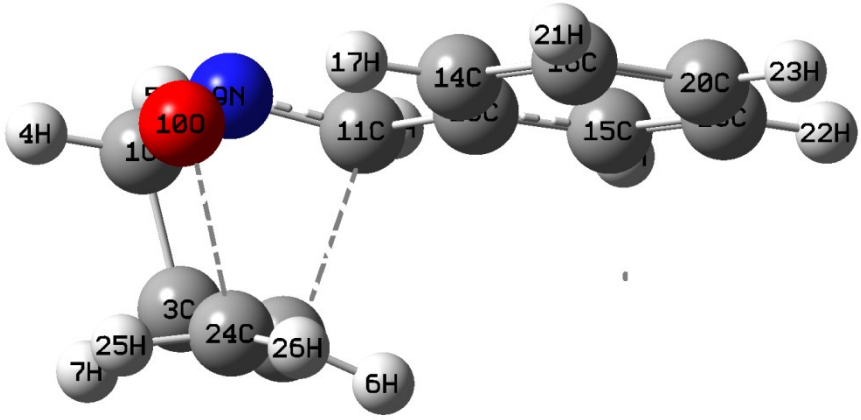
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.834056	-1.055932	-0.175854
2	6	0	0.217660	-0.312347	-0.986126
3	6	0	0.966925	-0.071687	1.191515
4	6	0	-0.377638	-0.812164	1.278237
5	1	0	-0.918337	-2.106890	-0.429820
6	1	0	-1.109655	-0.215282	1.813192
7	1	0	-0.271258	-1.750310	1.814137
8	6	0	1.501100	-0.496215	-0.179455
9	6	0	-0.393321	1.111236	-0.942764
10	1	0	-0.483975	1.510027	-1.951586
11	6	0	0.808363	1.447899	1.264552
12	1	0	1.765199	1.891219	1.532739
13	1	0	0.126761	1.683254	2.077727
14	1	0	0.292191	-0.670122	-2.008226
15	1	0	1.632082	-0.388041	1.993078
16	6	0	0.313219	2.088510	-0.035856
17	1	0	1.128809	2.554291	-0.579111
18	1	0	-0.392086	2.886138	0.179883
19	8	0	-1.690460	0.966147	-0.387102
20	7	0	-2.045076	-0.388937	-0.593808
21	6	0	-3.221794	-0.625478	0.189844
22	1	0	-4.034825	-0.036438	-0.219269
23	1	0	-3.478914	-1.676262	0.102621
24	1	0	-3.100354	-0.366601	1.243779
25	6	0	1.888464	-1.970654	-0.168927
26	1	0	2.104531	-2.315811	-1.177957
27	1	0	2.784751	-2.115227	0.430138
28	1	0	1.113846	-2.609884	0.241557
29	6	0	2.719831	0.263068	-0.670648
30	1	0	3.002138	-0.085562	-1.661805
31	1	0	2.582754	1.333844	-0.725205
32	1	0	3.563027	0.073621	-0.009504

TS1 (Gas Phase)



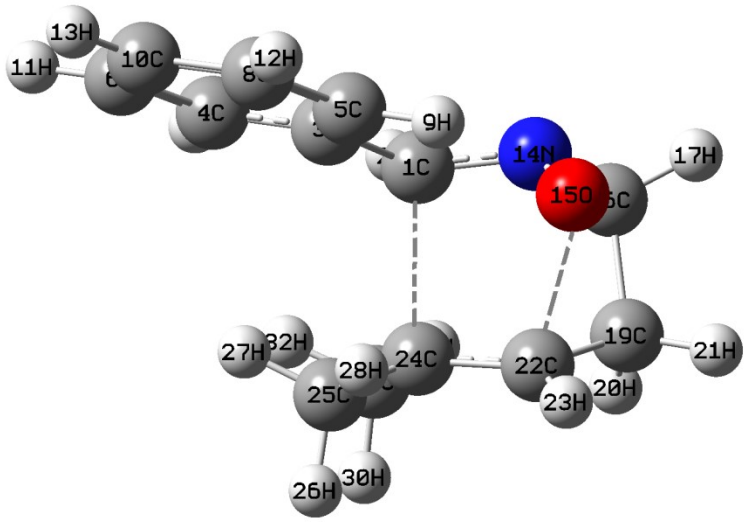
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.412572	-0.601752	-0.542981
2	1	0	0.544350	-1.589294	-0.959456
3	6	0	-0.979496	-0.237469	-0.278282
4	6	0	-1.910852	-1.269765	-0.275187
5	6	0	-1.416298	1.061623	-0.040805
6	6	0	-3.244878	-1.021213	-0.036887
7	1	0	-1.581421	-2.279677	-0.467073
8	6	0	-2.755899	1.304822	0.181783
9	1	0	-0.697518	1.860349	-0.037136
10	6	0	-3.673065	0.271850	0.191320
11	1	0	-3.950915	-1.835493	-0.037992
12	1	0	-3.085872	2.316180	0.355759
13	1	0	-4.716012	0.473044	0.373788
14	7	0	1.340723	0.272922	-0.952461
15	8	0	1.409118	1.371301	-0.288829
16	6	0	2.670831	-0.246494	-1.102201
17	1	0	3.217785	0.403067	-1.772509
18	1	0	2.647225	-1.252364	-1.507520
19	6	0	3.299778	-0.168221	0.338825
20	1	0	3.736502	-1.135935	0.571420
21	1	0	4.085336	0.576334	0.349591
22	6	0	2.214366	0.166980	1.290529
23	1	0	2.261338	1.057458	1.888636
24	6	0	1.221060	-0.770657	1.424336
25	1	0	1.455720	-1.804990	1.219001
26	1	0	0.396775	-0.607775	2.098657

TS2 (Gas Phase)



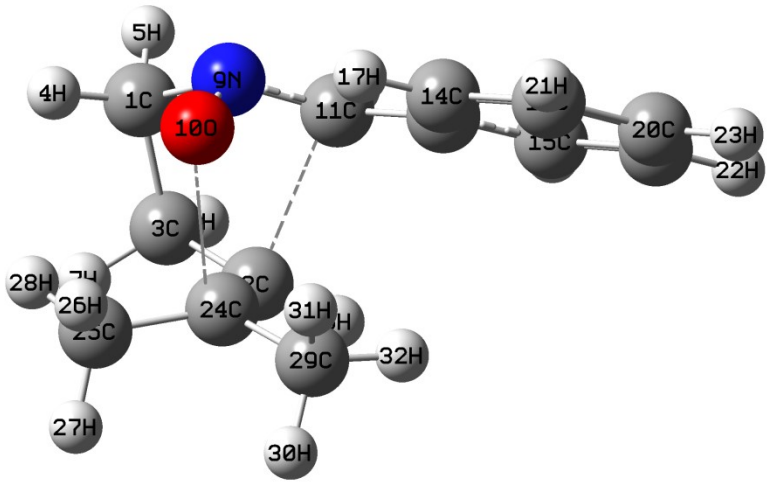
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.757081	-0.296367	-0.944405
2	6	0	-1.631981	-0.488902	1.236853
3	6	0	-2.880568	-0.871155	0.504575
4	1	0	-3.465659	0.493136	-1.149906
5	1	0	-2.854982	-1.072631	-1.696229
6	1	0	-1.004267	-1.228837	1.702816
7	1	0	-3.760906	-0.455666	0.987419
8	1	0	-3.006745	-1.948607	0.463200
9	7	0	-1.434256	0.298046	-1.014397
10	8	0	-1.395879	1.464844	-0.470184
11	6	0	-0.508422	-0.566813	-0.591894
12	1	0	-0.703187	-1.586446	-0.892161
13	6	0	0.889510	-0.257967	-0.331876
14	6	0	1.420847	1.026240	-0.259812
15	6	0	1.740430	-1.342602	-0.138608
16	6	0	2.765646	1.202332	-0.004438
17	1	0	0.773404	1.868377	-0.413063
18	6	0	3.078082	-1.159734	0.130363
19	1	0	1.341139	-2.343409	-0.203196
20	6	0	3.597498	0.118879	0.198161
21	1	0	3.165929	2.202295	0.039709
22	1	0	3.717752	-2.014040	0.279884
23	1	0	4.644493	0.269603	0.404325
24	6	0	-1.494589	0.850280	1.505869
25	1	0	-2.353719	1.497750	1.530712
26	1	0	-0.602654	1.228239	1.980021

TS3 (Gas Phase)



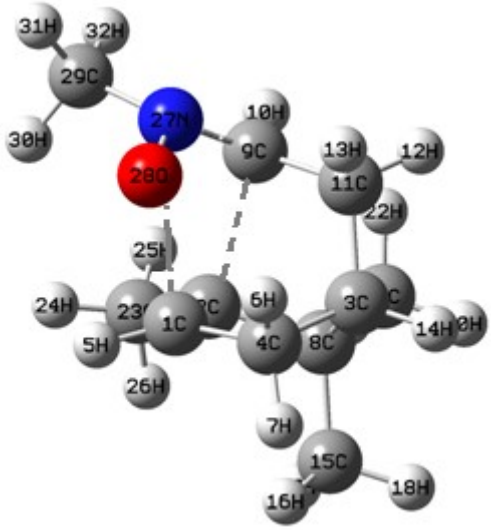
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.294625	-0.256106	-0.874890
2	1	0	-0.481481	0.231619	-1.820659
3	6	0	1.107753	-0.271059	-0.475851
4	6	0	1.961110	0.606727	-1.137338
5	6	0	1.629694	-1.083567	0.525902
6	6	0	3.298180	0.679825	-0.810184
7	1	0	1.567548	1.231923	-1.924728
8	6	0	2.971975	-1.017940	0.835895
9	1	0	0.971941	-1.755452	1.045291
10	6	0	3.809469	-0.136591	0.179574
11	1	0	3.942267	1.366596	-1.334668
12	1	0	3.367181	-1.659510	1.606787
13	1	0	4.855041	-0.087393	0.436235
14	7	0	-1.145057	-1.264602	-0.620168
15	8	0	-1.172803	-1.645486	0.611920
16	6	0	-2.500335	-1.059400	-1.053770
17	1	0	-2.977301	-2.023466	-1.173536
18	1	0	-2.520327	-0.525244	-1.998590
19	6	0	-3.179741	-0.278228	0.124529
20	1	0	-3.761038	0.540795	-0.290350
21	1	0	-3.853788	-0.940020	0.652783
22	6	0	-2.101086	0.190380	1.023401
23	1	0	-2.114432	-0.087885	2.061984
24	6	0	-1.180269	1.111570	0.545250
25	6	0	-0.139266	1.606587	1.502631
26	1	0	-0.521398	2.450123	2.077530
27	1	0	0.751882	1.945866	0.980544
28	1	0	0.160598	0.823275	2.191324
29	6	0	-1.557236	2.123866	-0.507859
30	1	0	-2.043587	2.983991	-0.047380
31	1	0	-2.228332	1.727009	-1.263508
32	1	0	-0.670687	2.497497	-1.016993

TS4 (Gas Phase)



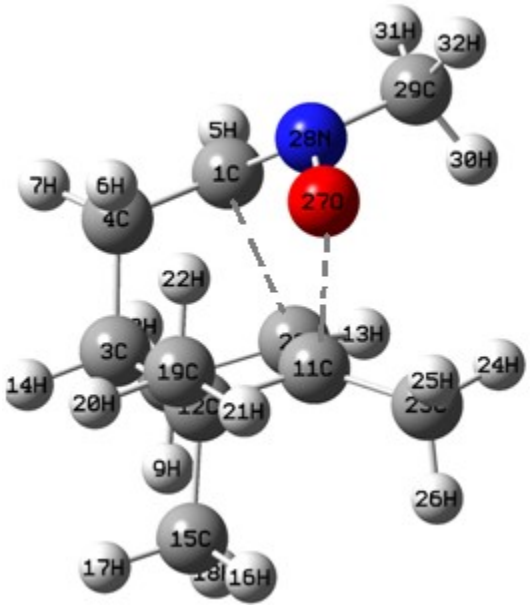
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.324131	-1.534480	0.668311
2	6	0	1.456797	-0.156635	-1.170073
3	6	0	2.520444	-1.150887	-0.832488
4	1	0	3.074798	-1.105423	1.318171
5	1	0	2.299202	-2.610081	0.808940
6	1	0	0.813110	-0.309886	-2.020835
7	1	0	3.523494	-0.763261	-0.986283
8	1	0	2.420427	-2.037216	-1.451951
9	7	0	1.056579	-0.943907	1.059404
10	8	0	1.176828	0.305121	1.369316
11	6	0	0.116712	-1.206428	0.148450
12	1	0	0.190264	-2.194686	-0.283969
13	6	0	-1.216092	-0.621996	0.138263
14	6	0	-1.656611	0.333662	1.047632
15	6	0	-2.099400	-1.074965	-0.836759
16	6	0	-2.946792	0.816381	0.969203
17	1	0	-0.976420	0.689125	1.799629
18	6	0	-3.380110	-0.576039	-0.921223
19	1	0	-1.771478	-1.828308	-1.537026
20	6	0	-3.809412	0.375069	-0.015428
21	1	0	-3.279246	1.551301	1.684375
22	1	0	-4.047142	-0.935254	-1.687768
23	1	0	-4.812062	0.765924	-0.073593
24	6	0	1.505197	1.085600	-0.559929
25	6	0	2.771079	1.696815	-0.047275
26	1	0	2.560618	2.356320	0.788232
27	1	0	3.232613	2.291045	-0.837471
28	1	0	3.486359	0.958226	0.292569
29	6	0	0.420373	2.070464	-0.837262
30	1	0	0.805268	2.900441	-1.429067
31	1	0	0.046841	2.479871	0.098331
32	1	0	-0.415231	1.618873	-1.361179

TS5 (Gas Phase)



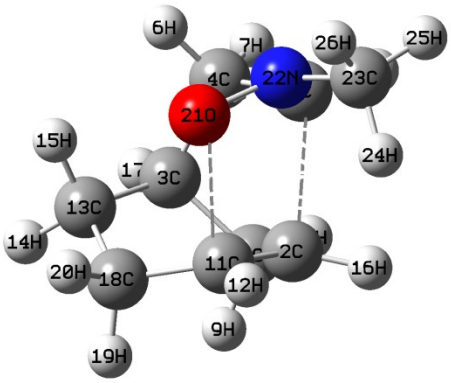
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.141633	-0.368809	-1.382489
2	6	0	0.289771	0.642253	-0.536957
3	6	0	1.060988	-1.293192	0.384555
4	6	0	0.534541	-1.648531	-1.004607
5	1	0	-0.613172	-0.211290	-2.335821
6	1	0	-0.164073	-2.479190	-0.990675
7	1	0	1.347114	-1.902160	-1.684805
8	6	0	1.537706	0.147834	0.195212
9	6	0	-0.948211	0.015086	1.046467
10	1	0	-0.987301	0.813564	1.772826
11	6	0	-0.119298	-1.205441	1.348345
12	1	0	0.232131	-1.154890	2.375276
13	1	0	-0.757176	-2.079592	1.251263
14	1	0	1.827589	-1.974955	0.744058
15	6	0	2.766886	0.246579	-0.701175
16	1	0	2.614164	-0.227697	-1.664145
17	1	0	3.016037	1.289434	-0.885701
18	1	0	3.630117	-0.212175	-0.222677
19	6	0	1.863486	0.895406	1.475605
20	1	0	2.745636	0.469627	1.948759
21	1	0	2.087217	1.936115	1.249624
22	1	0	1.061277	0.885324	2.204067
23	6	0	0.103825	2.100159	-0.811894
24	1	0	-0.661557	2.267895	-1.564085
25	1	0	-0.174693	2.661553	0.077862
26	1	0	1.027558	2.541585	-1.187042
27	7	0	-2.069553	-0.156730	0.357656
28	8	0	-1.965609	-0.978734	-0.618314
29	6	0	-2.999688	0.925019	0.161219
30	1	0	-2.707365	1.493575	-0.719647
31	1	0	-3.983359	0.504077	-0.005350
32	1	0	-3.018631	1.568009	1.033449

TS6 (Gas Phase)



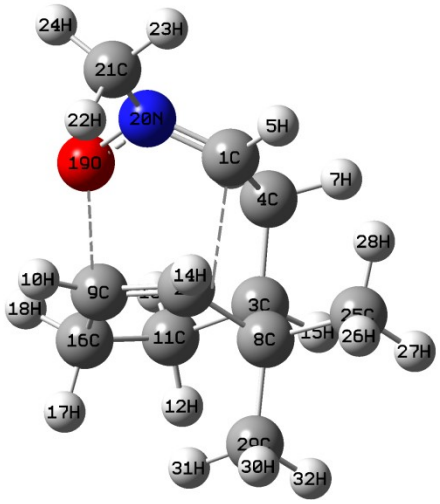
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.433479	-1.127132	0.057616
2	6	0	-0.164909	-0.244283	-1.383743
3	6	0	1.041497	-1.377453	0.163237
4	6	0	-0.285936	-1.695347	0.850644
5	1	0	-2.088475	-1.799138	-0.476967
6	1	0	-0.336066	-1.292532	1.856687
7	1	0	-0.400767	-2.774460	0.913857
8	6	0	0.686788	-1.485365	-1.309347
9	1	0	1.554056	-1.441620	-1.964137
10	1	0	0.149170	-2.403068	-1.540499
11	6	0	0.333876	0.736538	-0.542735
12	6	0	1.428285	0.105540	0.300527
13	1	0	-0.762982	-0.003706	-2.250866
14	1	0	1.835963	-2.038878	0.499706
15	6	0	2.775256	0.360524	-0.379781
16	1	0	3.056154	1.404418	-0.266491
17	1	0	3.553287	-0.241870	0.084440
18	1	0	2.758713	0.139715	-1.442492
19	6	0	1.541925	0.602326	1.728673
20	1	0	2.354302	0.083873	2.235316
21	1	0	1.780398	1.663687	1.737382
22	1	0	0.624614	0.472437	2.284665
23	6	0	0.292593	2.201769	-0.790911
24	1	0	-0.591750	2.475518	-1.357364
25	1	0	0.280112	2.759438	0.139379
26	1	0	1.166370	2.513168	-1.364952
27	8	0	-1.159225	0.847659	0.955197
28	7	0	-1.991431	-0.009795	0.486986
29	6	0	-3.130794	0.540822	-0.199822
30	1	0	-2.791320	1.059500	-1.096284
31	1	0	-3.825184	-0.247240	-0.467358
32	1	0	-3.613387	1.250412	0.459358

TS7 (Gas Phase)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.932800	1.127485	0.031460
2	6	0	0.202202	-0.087654	1.394318
3	6	0	1.573032	0.922696	-0.289963
4	6	0	0.267396	1.574062	-0.747315
5	1	0	-1.472853	1.860836	0.611198
6	1	0	0.082353	1.358346	-1.796913
7	1	0	0.352228	2.652841	-0.638670
8	6	0	1.429487	0.755083	1.214273
9	1	0	2.314214	0.274478	1.635472
10	1	0	1.323720	1.722407	1.700475
11	6	0	0.186438	-1.279369	0.708764
12	1	0	-0.474924	-2.074882	1.009499
13	6	0	1.836419	-0.429320	-0.960860
14	1	0	2.901439	-0.533001	-1.156666
15	1	0	1.330323	-0.450078	-1.920260
16	1	0	-0.412839	0.033453	2.273465
17	1	0	2.393148	1.595337	-0.530576
18	6	0	1.368556	-1.620243	-0.128429
19	1	0	2.175334	-1.934192	0.539289
20	1	0	1.150384	-2.465537	-0.772605
21	8	0	-1.046423	-0.842031	-0.949361
22	7	0	-1.678330	0.144035	-0.441856
23	6	0	-2.913859	-0.198950	0.212957
24	1	0	-2.683359	-0.817718	1.081579
25	1	0	-3.443657	0.694679	0.520154
26	1	0	-3.517040	-0.771707	-0.478784

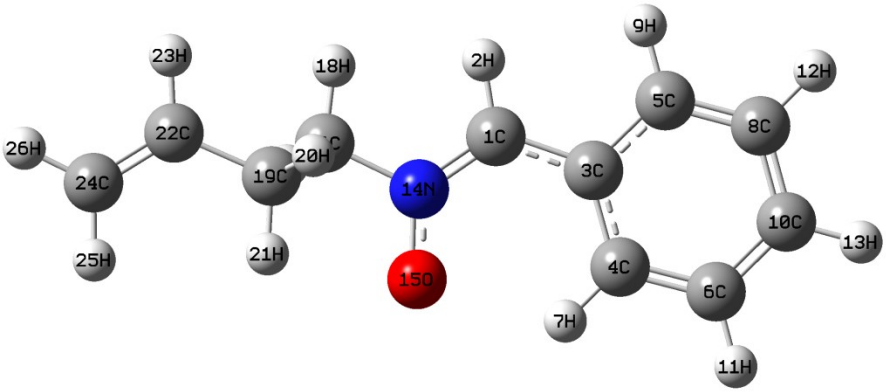
TS8 (Gas Phase)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.081377	-1.022504	0.513663
2	6	0	0.176686	-0.278682	-1.056657
3	6	0	1.146400	0.049600	1.085475
4	6	0	-0.141309	-0.598318	1.602571
5	1	0	-1.251715	-2.075939	0.351413
6	1	0	-0.679039	0.098277	2.239906
7	1	0	0.103803	-1.473612	2.198827
8	6	0	1.434479	-0.582488	-0.276721
9	6	0	-0.281769	1.019839	-1.087930
10	1	0	-0.927678	1.334591	-1.891566
11	6	0	1.043624	1.572190	0.978310
12	1	0	2.043963	1.991129	1.062521
13	1	0	0.487762	1.935600	1.837771
14	1	0	-0.094691	-0.945009	-1.865117
15	1	0	1.953926	-0.179531	1.781082
16	6	0	0.391129	2.093237	-0.306316
17	1	0	1.139014	2.572910	-0.939168
18	1	0	-0.339754	2.858943	-0.068897
19	8	0	-1.890384	1.000992	0.241261
20	7	0	-2.123999	-0.253968	0.248341
21	6	0	-3.124447	-0.692075	-0.689297
22	1	0	-2.756440	-0.502030	-1.698486
23	1	0	-3.332046	-1.747327	-0.558675
24	1	0	-4.022668	-0.111827	-0.524660
25	6	0	1.667975	-2.079988	-0.154174
26	1	0	1.806814	-2.520401	-1.139156
27	1	0	2.567627	-2.276114	0.425515
28	1	0	0.846079	-2.601562	0.325084
29	6	0	2.676941	0.011398	-0.927894
30	1	0	2.852266	-0.453045	-1.895172
31	1	0	2.588858	1.079672	-1.086834
32	1	0	3.554986	-0.168129	-0.309039

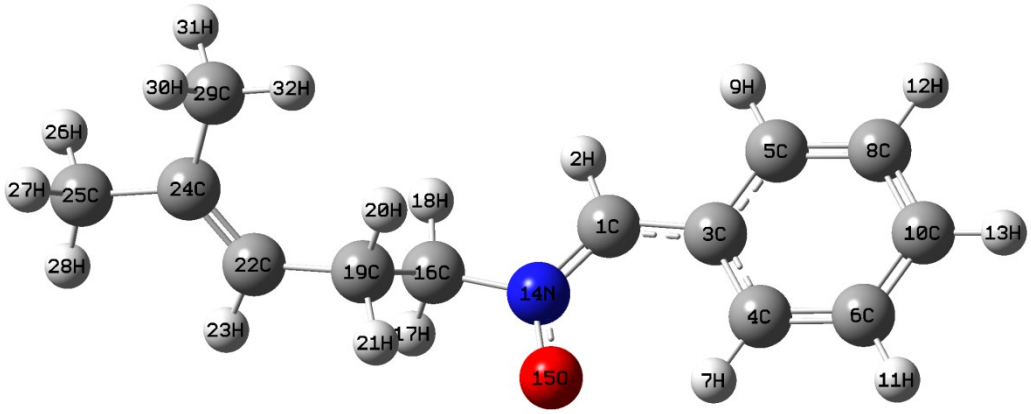
MPWB1K/6-311G(d,p) computed unique imaginary frequency, and Cartesian coordinates of the stationary points involved in the IM32CA reactions of nitrones **15**, **18**, **20**, **24** and **26** in toluene

Nitrone **15** (Toluene)



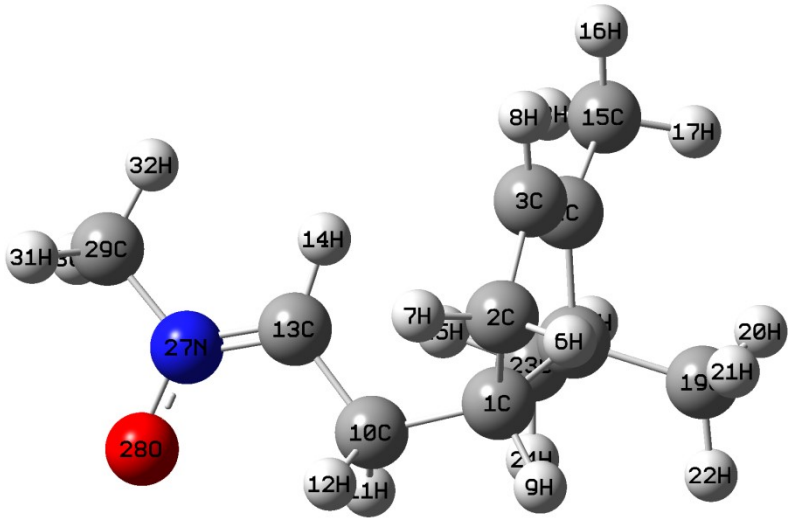
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.263977	-0.692751	0.267226
2	1	0	0.034240	-1.743482	0.308224
3	6	0	1.639576	-0.300034	0.087360
4	6	0	2.080784	1.019801	-0.007979
5	6	0	2.579163	-1.328602	0.002191
6	6	0	3.423954	1.284422	-0.184369
7	1	0	1.363216	1.815669	0.056897
8	6	0	3.916074	-1.053960	-0.171773
9	1	0	2.247414	-2.354066	0.075033
10	6	0	4.344377	0.258235	-0.266342
11	1	0	3.753659	2.309160	-0.258066
12	1	0	4.626549	-1.863385	-0.234102
13	1	0	5.391875	0.477227	-0.403373
14	7	0	-0.750923	0.101959	0.394211
15	8	0	-0.709515	1.358544	0.382235
16	6	0	-2.094152	-0.459585	0.564293
17	1	0	-2.450906	-0.098035	1.523778
18	1	0	-2.024659	-1.541618	0.591928
19	6	0	-3.004120	0.019846	-0.548336
20	1	0	-2.591785	-0.315470	-1.500301
21	1	0	-2.996548	1.104485	-0.549467
22	6	0	-4.388811	-0.500602	-0.379855
23	1	0	-4.512668	-1.575895	-0.433887
24	6	0	-5.446601	0.258806	-0.167969
25	1	0	-5.361596	1.334013	-0.109858
26	1	0	-6.431534	-0.164119	-0.050845

Nitrone **18** (Toluene)



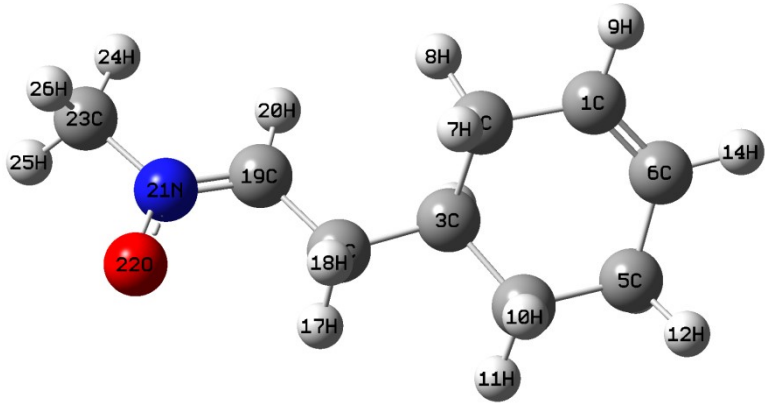
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.054684	0.243169	-0.582898
2	1	0	0.665317	1.133050	-1.046569
3	6	0	2.450923	0.219613	-0.225779
4	6	0	3.103430	-0.856170	0.374777
5	6	0	3.184013	1.372562	-0.510100
6	6	0	4.447677	-0.764518	0.675742
7	1	0	2.547578	-1.746185	0.597354
8	6	0	4.523128	1.455018	-0.205276
9	1	0	2.687814	2.211485	-0.975764
10	6	0	5.161964	0.382487	0.391193
11	1	0	4.941364	-1.603971	1.140375
12	1	0	5.071092	2.356095	-0.432391
13	1	0	6.211906	0.442470	0.631971
14	7	0	0.193543	-0.708255	-0.407050
15	8	0	0.426237	-1.829574	0.111370
16	6	0	-1.197774	-0.503020	-0.823862
17	1	0	-1.407721	-1.284601	-1.548167
18	1	0	-1.285442	0.463804	-1.306095
19	6	0	-2.129522	-0.618969	0.365533
20	1	0	-1.907476	0.174619	1.072340
21	1	0	-1.902363	-1.561296	0.858111
22	6	0	-3.551931	-0.596682	-0.072534
23	1	0	-3.854047	-1.444147	-0.677206
24	6	0	-4.471822	0.324984	0.184973
25	6	0	-5.864108	0.176053	-0.333865
26	1	0	-6.134432	1.022036	-0.964302
27	1	0	-6.581219	0.156525	0.485629
28	1	0	-5.981877	-0.734183	-0.912148
29	6	0	-4.245576	1.556314	0.996592
30	1	0	-4.880946	1.547016	1.881050
31	1	0	-4.524582	2.439684	0.424512
32	1	0	-3.220174	1.676929	1.322713

Nitrone **20** (Toluene)



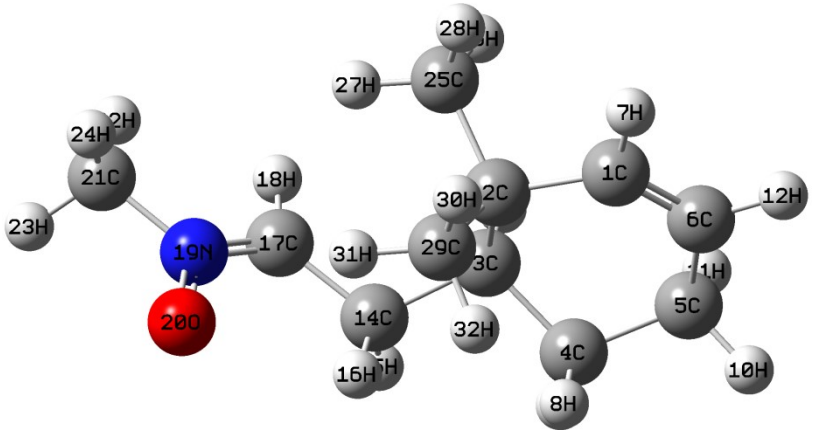
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.638361	-1.195970	0.536252
2	6	0	0.873955	-0.500931	1.884245
3	6	0	1.363460	0.855394	1.497096
4	6	0	1.695525	0.923479	0.217132
5	6	0	1.535532	-0.420833	-0.459147
6	1	0	1.617453	-1.023326	2.487812
7	1	0	-0.036618	-0.467035	2.483442
8	1	0	1.464136	1.669512	2.200081
9	1	0	0.969409	-2.231745	0.575639
10	6	0	-0.839605	-1.233002	0.183760
11	1	0	-1.008187	-1.685353	-0.794245
12	1	0	-1.361084	-1.894390	0.879256
13	6	0	-1.527505	0.073001	0.208559
14	1	0	-1.041982	0.993369	0.476262
15	6	0	2.240565	2.098958	-0.505939
16	1	0	2.374157	2.946090	0.158492
17	1	0	3.203000	1.868865	-0.960789
18	1	0	1.578172	2.400939	-1.315645
19	6	0	2.904290	-1.093835	-0.519145
20	1	0	3.614605	-0.497028	-1.086894
21	1	0	3.305345	-1.234611	0.481847
22	1	0	2.829110	-2.067651	-0.998779
23	6	0	0.976242	-0.316673	-1.866497
24	1	0	0.808231	-1.303710	-2.290800
25	1	0	0.034494	0.225714	-1.895067
26	1	0	1.680183	0.201855	-2.513453
27	7	0	-2.776523	0.118816	-0.099695
28	8	0	-3.455688	-0.892423	-0.426806
29	6	0	-3.504566	1.378213	-0.091145
30	1	0	-3.899376	1.531758	-1.087818
31	1	0	-4.329191	1.271579	0.602620
32	1	0	-2.858217	2.196039	0.199327

Nitrone **24** (Toluene)



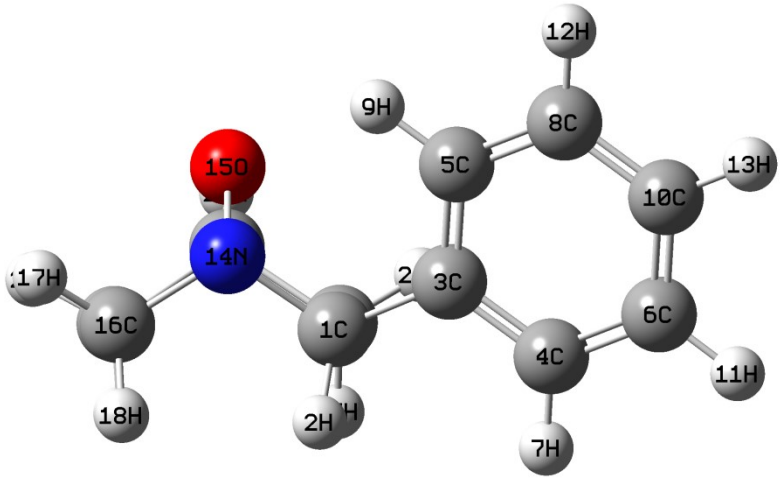
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.604120	1.406156	0.345751
2	6	0	1.155035	1.070457	0.469896
3	6	0	0.799492	-0.214429	-0.259394
4	6	0	1.832718	-1.276139	0.066527
5	6	0	3.206290	-0.869673	-0.426085
6	6	0	3.517258	0.546621	-0.074968
7	1	0	0.886554	0.972642	1.525304
8	1	0	0.558342	1.901365	0.093230
9	1	0	2.903385	2.411043	0.610544
10	1	0	1.860727	-1.411968	1.148698
11	1	0	1.542232	-2.231488	-0.365609
12	1	0	3.967382	-1.525071	-0.005538
13	1	0	3.271877	-0.999318	-1.508431
14	1	0	4.545708	0.868416	-0.166019
15	1	0	0.853371	-0.018338	-1.334211
16	6	0	-0.598887	-0.687691	0.079105
17	1	0	-0.791053	-1.669526	-0.360403
18	1	0	-0.706558	-0.843698	1.155110
19	6	0	-1.665240	0.231019	-0.361659
20	1	0	-1.486432	1.093757	-0.980284
21	7	0	-2.881555	-0.012574	-0.019311
22	8	0	-3.223988	-0.998264	0.688130
23	6	0	-3.969982	0.856563	-0.439039
24	1	0	-3.600001	1.678523	-1.037860
25	1	0	-4.669421	0.251355	-1.002096
26	1	0	-4.458146	1.219138	0.456900

Nitrone **26** (Toluene)



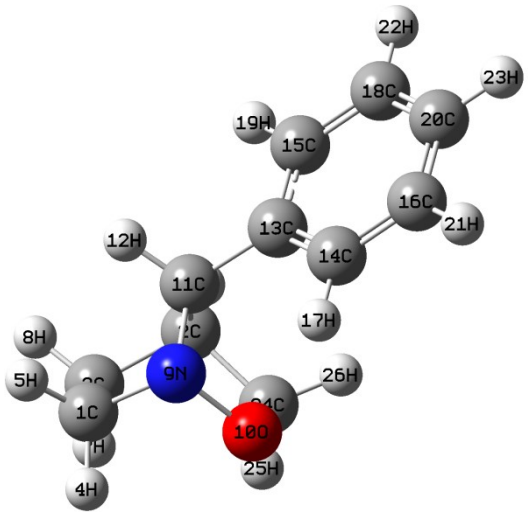
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.341525	1.207767	0.099594
2	6	0	0.888680	0.822314	0.064099
3	6	0	0.746396	-0.635144	-0.415712
4	6	0	1.836776	-1.512673	0.178448
5	6	0	3.214671	-1.072873	-0.257224
6	6	0	3.369999	0.396410	-0.073769
7	1	0	2.525803	2.263703	0.259358
8	1	0	1.771378	-1.465430	1.265961
9	1	0	1.662454	-2.550072	-0.100517
10	1	0	3.978451	-1.598897	0.313181
11	1	0	3.386729	-1.339663	-1.302237
12	1	0	4.371983	0.803230	-0.067442
13	1	0	0.883512	-0.629953	-1.500932
14	6	0	-0.602467	-1.282047	-0.098842
15	1	0	-0.560486	-2.309839	-0.464831
16	1	0	-0.758598	-1.333621	0.974614
17	6	0	-1.785498	-0.637864	-0.697879
18	1	0	-1.862611	-0.474510	-1.759792
19	7	0	-2.793886	-0.269549	0.014556
20	8	0	-2.885803	-0.385652	1.269055
21	6	0	-3.948297	0.353989	-0.616220
22	1	0	-3.822754	0.410706	-1.689621
23	1	0	-4.816085	-0.239861	-0.358447
24	1	0	-4.056745	1.341838	-0.185332
25	6	0	0.212884	1.789791	-0.903760
26	1	0	0.587772	1.655169	-1.915790
27	1	0	-0.864760	1.661676	-0.912009
28	1	0	0.415277	2.816521	-0.605990
29	6	0	0.288421	1.023415	1.450686
30	1	0	0.491984	2.033073	1.800185
31	1	0	-0.789736	0.875505	1.447235
32	1	0	0.721508	0.333977	2.171538

Isoxazolidine **16** (Toluene)



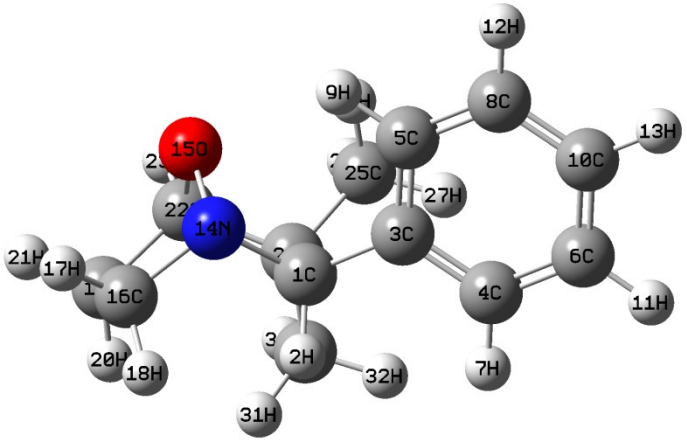
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.473921	0.527105	-0.408767
2	1	0	-0.588525	1.218041	-1.240279
3	6	0	0.984005	0.213947	-0.245398
4	6	0	1.905510	1.247433	-0.303339
5	6	0	1.432238	-1.071652	0.000312
6	6	0	3.251400	1.004550	-0.115653
7	1	0	1.565191	2.254164	-0.500495
8	6	0	2.779850	-1.315892	0.185830
9	1	0	0.718686	-1.877472	0.040799
10	6	0	3.693335	-0.281604	0.130397
11	1	0	3.956792	1.819363	-0.167991
12	1	0	3.117331	-2.323347	0.374139
13	1	0	4.744591	-0.475803	0.274472
14	7	0	-1.274321	-0.669803	-0.700608
15	8	0	-1.614491	-1.110786	0.598847
16	6	0	-2.588234	-0.258479	-1.200840
17	1	0	-3.094260	-1.140808	-1.573911
18	1	0	-2.464807	0.441050	-2.020040
19	6	0	-3.303773	0.325856	0.028699
20	1	0	-3.553837	1.376273	-0.074902
21	1	0	-4.208067	-0.225577	0.261059
22	6	0	-2.225838	0.087236	1.070079
23	1	0	-2.568171	-0.063678	2.085582
24	6	0	-1.108794	1.090929	0.886513
25	1	0	-1.460851	2.111365	0.779923
26	1	0	-0.402563	1.044764	1.708127

Isoxazolidine **17** (Toluene)



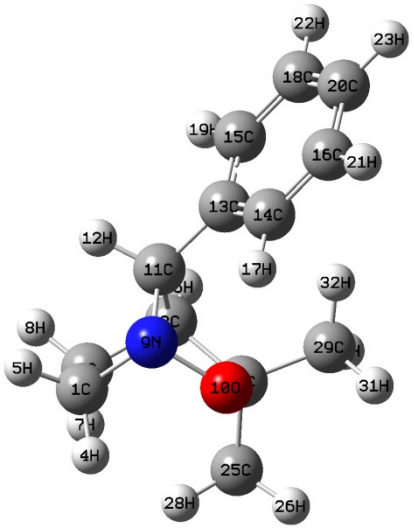
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.759577	-0.365841	-0.886102
2	6	0	1.444307	1.005593	0.513769
3	6	0	2.840663	0.954391	-0.088789
4	1	0	3.457990	-1.123070	-0.553951
5	1	0	2.893610	-0.214792	-1.953155
6	1	0	1.112804	1.969927	0.878526
7	1	0	3.613680	0.937989	0.673109
8	1	0	3.025522	1.804472	-0.739117
9	7	0	1.402713	-0.868414	-0.667620
10	8	0	1.386878	-1.286797	0.694751
11	6	0	0.627481	0.365621	-0.613569
12	1	0	0.776858	0.895070	-1.553884
13	6	0	-0.832591	0.174874	-0.353158
14	6	0	-1.404205	-1.083480	-0.277098
15	6	0	-1.638136	1.292343	-0.197058
16	6	0	-2.760157	-1.217997	-0.045922
17	1	0	-0.777712	-1.951819	-0.396495
18	6	0	-2.992224	1.157715	0.033275
19	1	0	-1.200767	2.278481	-0.261362
20	6	0	-3.557433	-0.101273	0.110626
21	1	0	-3.195472	-2.203771	0.012034
22	1	0	-3.607606	2.036246	0.150783
23	1	0	-4.615557	-0.210613	0.290951
24	6	0	1.347608	-0.115514	1.518256
25	1	0	2.183332	-0.137981	2.212863
26	1	0	0.409960	-0.105456	2.069649

Isoxazolidine **35** (Toluene)



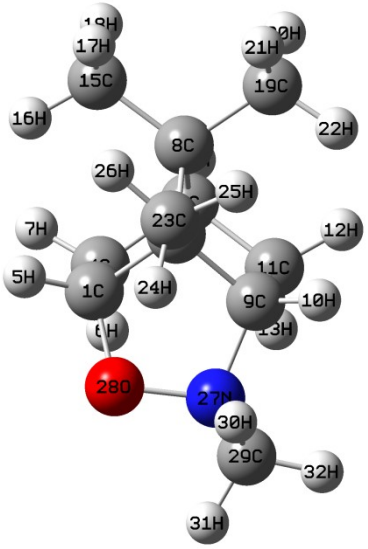
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.341579	-0.017139	-0.610971
2	1	0	-0.500632	0.314225	-1.634958
3	6	0	1.134399	-0.124926	-0.385057
4	6	0	1.979011	0.809851	-0.961006
5	6	0	1.676303	-1.113296	0.419269
6	6	0	3.340980	0.766270	-0.734089
7	1	0	1.565846	1.577918	-1.600015
8	6	0	3.038293	-1.161147	0.642549
9	1	0	1.023217	-1.846678	0.864233
10	6	0	3.874914	-0.221541	0.070512
11	1	0	3.986231	1.499360	-1.193252
12	1	0	3.449570	-1.938767	1.267809
13	1	0	4.938650	-0.262518	0.246123
14	7	0	-1.028960	-1.307520	-0.444450
15	8	0	-1.484413	-1.225883	0.894088
16	6	0	-2.302679	-1.264396	-1.165026
17	1	0	-2.712882	-2.267338	-1.183975
18	1	0	-2.133423	-0.941607	-2.186414
19	6	0	-3.177121	-0.311524	-0.335892
20	1	0	-3.504038	0.567082	-0.878795
21	1	0	-4.055023	-0.817655	0.050234
22	6	0	-2.206299	-0.002802	0.786071
23	1	0	-2.655827	0.231523	1.744361
24	6	0	-1.088773	0.950899	0.366866
25	6	0	-0.274243	1.296912	1.600560
26	1	0	-0.857840	1.940100	2.255668
27	1	0	0.640246	1.819737	1.336229
28	1	0	-0.000663	0.399703	2.146732
29	6	0	-1.525020	2.225627	-0.323845
30	1	0	-2.168597	2.821138	0.319986
31	1	0	-2.053393	2.036027	-1.253972
32	1	0	-0.652539	2.830732	-0.561189

Isoxazolidine **36** (Toluene)



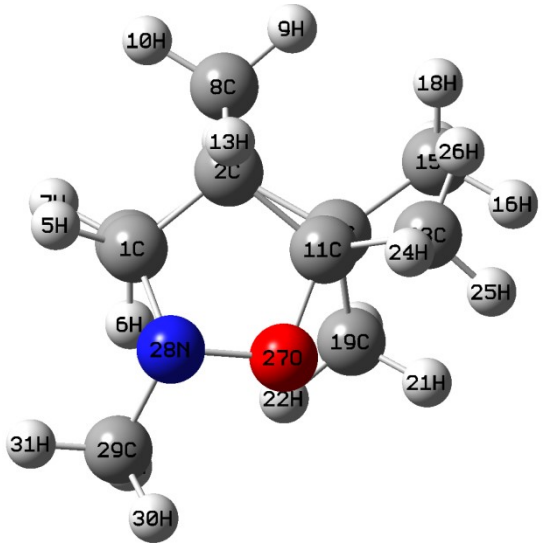
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.283485	-1.558114	-0.570967
2	6	0	-1.252652	-0.184221	1.030020
3	6	0	-2.439151	-1.127874	0.903178
4	1	0	-3.050833	-1.161870	-1.225326
5	1	0	-2.251560	-2.636448	-0.690465
6	1	0	-0.981950	0.102386	2.039776
7	1	0	-3.394833	-0.667819	1.121399
8	1	0	-2.319296	-1.973549	1.574964
9	7	0	-0.993569	-1.008557	-1.007287
10	8	0	-1.204405	0.379922	-1.204358
11	6	0	-0.230267	-1.012256	0.234178
12	1	0	-0.221684	-2.034702	0.613207
13	6	0	1.183483	-0.545484	0.100451
14	6	0	1.733163	-0.239128	-1.131797
15	6	0	1.975641	-0.452068	1.234356
16	6	0	3.049803	0.169564	-1.224194
17	1	0	1.116043	-0.310943	-2.011697
18	6	0	3.290221	-0.041526	1.142382
19	1	0	1.557798	-0.698252	2.200169
20	6	0	3.831215	0.274104	-0.089825
21	1	0	3.466477	0.410833	-2.190064
22	1	0	3.894253	0.030382	2.033764
23	1	0	4.858078	0.596708	-0.164787
24	6	0	-1.462279	0.998991	0.081268
25	6	0	-2.865628	1.570413	0.053036
26	1	0	-2.888668	2.424664	-0.617323
27	1	0	-3.169420	1.908981	1.040669
28	1	0	-3.588575	0.848967	-0.309732
29	6	0	-0.479832	2.130971	0.284776
30	1	0	-0.748100	2.698898	1.172472
31	1	0	-0.527673	2.799669	-0.570355
32	1	0	0.538781	1.782387	0.388036

Isoxazolidine **21** (Toluene)



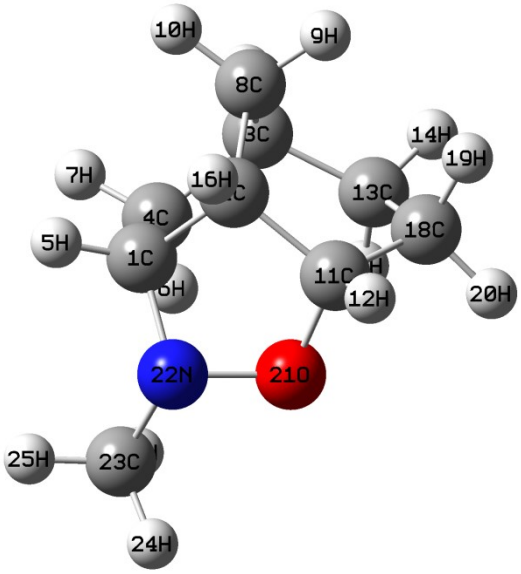
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.348102	-0.423543	-1.245548
2	6	0	0.147610	0.613365	-0.245106
3	6	0	1.088496	-1.298323	0.475406
4	6	0	0.346601	-1.720863	-0.792129
5	1	0	-0.161574	-0.175090	-2.285744
6	1	0	-0.397479	-2.488215	-0.598860
7	1	0	1.021585	-2.095582	-1.554934
8	6	0	1.551541	0.127235	0.129588
9	6	0	-0.751153	0.135377	0.912772
10	1	0	-0.979515	0.916162	1.633034
11	6	0	0.024089	-1.038026	1.527246
12	1	0	0.459231	-0.779607	2.487260
13	1	0	-0.641142	-1.882873	1.671798
14	1	0	1.875248	-1.980662	0.784719
15	6	0	2.529836	0.183935	-1.030332
16	1	0	2.152418	-0.293754	-1.928868
17	1	0	2.767027	1.215339	-1.280715
18	1	0	3.462463	-0.306202	-0.759628
19	6	0	2.150860	0.897290	1.292200
20	1	0	3.034549	0.391033	1.674862
21	1	0	2.457460	1.888214	0.964648
22	1	0	1.456348	1.030427	2.115372
23	6	0	-0.015845	2.046404	-0.669252
24	1	0	-1.023796	2.229822	-1.029881
25	1	0	0.177597	2.727297	0.156372
26	1	0	0.671453	2.292065	-1.476016
27	7	0	-2.000238	-0.333861	0.304365
28	8	0	-1.740070	-0.437193	-1.099583
29	6	0	-3.095739	0.593205	0.426929
30	1	0	-2.857054	1.597643	0.070454
31	1	0	-3.936888	0.210975	-0.140409
32	1	0	-3.384863	0.641258	1.472006

Isoxazolidine **22** (Toluene)



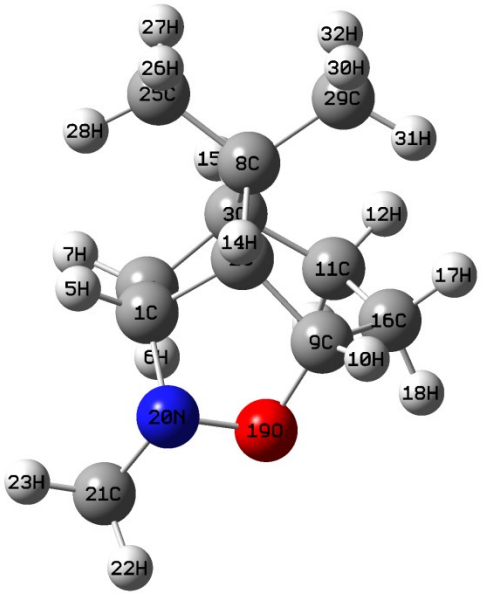
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.350556	0.873074	-0.560796
2	6	0	0.107914	0.539440	-1.368305
3	6	0	-0.759572	1.416701	0.492417
4	6	0	0.748842	1.561778	0.686750
5	1	0	2.061641	1.503550	-1.086044
6	1	0	1.108032	1.142561	1.619163
7	1	0	1.015034	2.615514	0.687782
8	6	0	-0.861018	1.646543	-1.010860
9	1	0	-1.854214	1.515877	-1.423464
10	1	0	-0.490872	2.623352	-1.313561
11	6	0	-0.344688	-0.686152	-0.553888
12	6	0	-1.175717	-0.056000	0.613742
13	1	0	0.295519	0.333833	-2.416037
14	1	0	-1.346814	2.077374	1.124634
15	6	0	-2.679271	-0.197406	0.407260
16	1	0	-2.980906	-1.238240	0.490297
17	1	0	-3.204179	0.358645	1.180747
18	1	0	-3.026424	0.166831	-0.553203
19	6	0	-0.857134	-0.681694	1.957968
20	1	0	-1.438821	-0.195203	2.738518
21	1	0	-1.122525	-1.736773	1.954072
22	1	0	0.193264	-0.619573	2.211594
23	6	0	-1.043903	-1.758052	-1.346521
24	1	0	-0.357550	-2.152513	-2.088852
25	1	0	-1.352315	-2.574887	-0.699020
26	1	0	-1.923819	-1.370802	-1.850917
27	8	0	0.845055	-1.261291	-0.029145
28	7	0	1.945836	-0.431651	-0.398618
29	6	0	2.924150	-0.572961	0.641290
30	1	0	3.291050	-1.593579	0.640674
31	1	0	3.753736	0.090134	0.415698
32	1	0	2.537922	-0.345822	1.637056

Isoxazolidine **25** (Toluene)



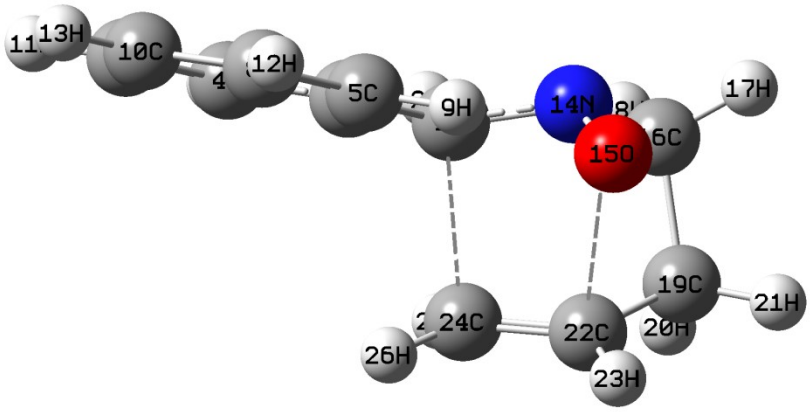
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.795549	-0.904207	0.551465
2	6	0	-0.330918	-0.216104	1.308969
3	6	0	-1.362192	-0.989797	-0.633207
4	6	0	0.104390	-1.425830	-0.723757
5	1	0	1.278334	-1.693592	1.119788
6	1	0	0.576280	-1.047938	-1.625796
7	1	0	0.165658	-2.510641	-0.754401
8	6	0	-1.582392	-0.950046	0.872335
9	1	0	-2.506083	-0.458598	1.166194
10	1	0	-1.593188	-1.952988	1.294715
11	6	0	-0.245172	1.202182	0.698204
12	1	0	-0.123581	1.949874	1.480945
13	6	0	-1.614015	0.404795	-1.221373
14	1	0	-2.625990	0.459814	-1.616515
15	1	0	-0.939523	0.567042	-2.058157
16	1	0	-0.168627	-0.192143	2.380707
17	1	0	-2.004645	-1.710562	-1.131584
18	6	0	-1.421593	1.508985	-0.190404
19	1	0	-2.305838	1.606615	0.436516
20	1	0	-1.274890	2.470153	-0.676080
21	8	0	0.903490	1.204109	-0.132556
22	7	0	1.738857	0.183727	0.392892
23	6	0	2.798845	-0.005410	-0.554127
24	1	0	3.412523	0.888584	-0.573925
25	1	0	3.409891	-0.835498	-0.214105
26	1	0	2.444759	-0.206501	-1.566721

Isoxazolidine **27** (Toluene)



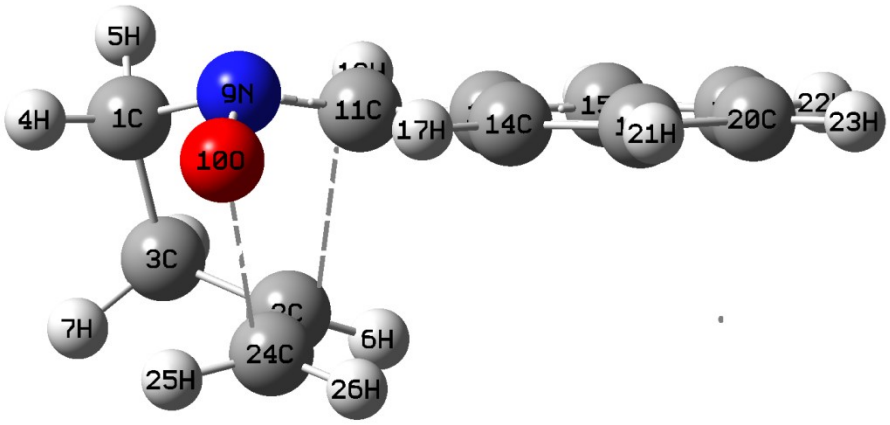
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.833863	-1.055473	-0.181112
2	6	0	0.218985	-0.309742	-0.988045
3	6	0	0.964550	-0.075259	1.192630
4	6	0	-0.378490	-0.818750	1.274473
5	1	0	-0.920409	-2.105991	-0.438795
6	1	0	-1.111206	-0.227310	1.814685
7	1	0	-0.269959	-1.760690	1.803442
8	6	0	1.500950	-0.495167	-0.178863
9	6	0	-0.390092	1.114213	-0.942848
10	1	0	-0.477659	1.516019	-1.951432
11	6	0	0.802271	1.443824	1.270159
12	1	0	1.756137	1.888507	1.547073
13	1	0	0.113629	1.674780	2.079049
14	1	0	0.297039	-0.664640	-2.011711
15	1	0	1.629442	-0.392921	1.994601
16	6	0	0.316448	2.087714	-0.032109
17	1	0	1.137111	2.548355	-0.572082
18	1	0	-0.384499	2.890635	0.180434
19	8	0	-1.691879	0.969340	-0.391686
20	7	0	-2.046604	-0.387222	-0.596592
21	6	0	-3.219882	-0.625402	0.193729
22	1	0	-4.037023	-0.037350	-0.209433
23	1	0	-3.476147	-1.676474	0.107306
24	1	0	-3.092219	-0.368036	1.246945
25	6	0	1.889142	-1.969437	-0.172612
26	1	0	2.108261	-2.310239	-1.182546
27	1	0	2.783892	-2.114968	0.428616
28	1	0	1.113711	-2.610771	0.233280
29	6	0	2.720264	0.266049	-0.665698
30	1	0	3.003458	-0.079194	-1.657862
31	1	0	2.583737	1.337150	-0.716346
32	1	0	3.562261	0.073543	-0.003814

TS1 (Toluene)



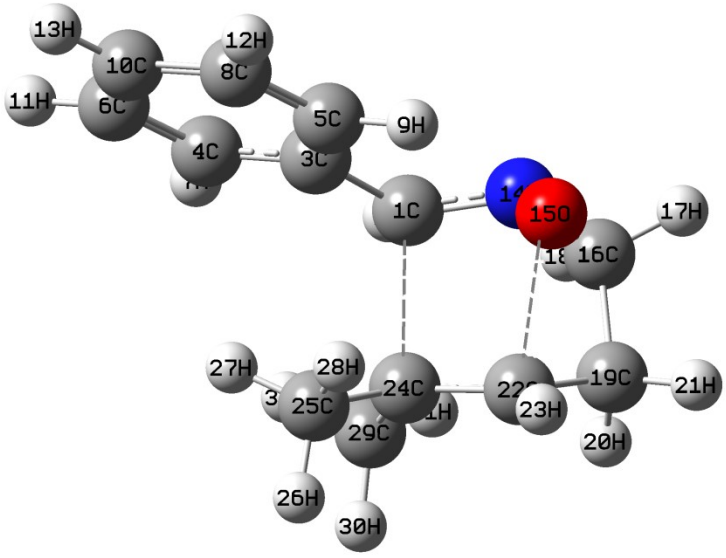
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.416613	-0.591607	-0.536534
2	1	0	0.548305	-1.579747	-0.954220
3	6	0	-0.978104	-0.231265	-0.274042
4	6	0	-1.904963	-1.268113	-0.281543
5	6	0	-1.422372	1.063934	-0.029160
6	6	0	-3.241708	-1.026651	-0.047236
7	1	0	-1.569672	-2.275960	-0.479319
8	6	0	-2.764337	1.300932	0.189824
9	1	0	-0.709089	1.867599	-0.016625
10	6	0	-3.677226	0.263382	0.188078
11	1	0	-3.944765	-1.844960	-0.056976
12	1	0	-3.099347	2.310818	0.369809
13	1	0	-4.722953	0.458913	0.367586
14	7	0	1.342652	0.283619	-0.952669
15	8	0	1.412932	1.385041	-0.288271
16	6	0	2.670444	-0.240268	-1.104378
17	1	0	3.223567	0.413267	-1.766355
18	1	0	2.642204	-1.241910	-1.519560
19	6	0	3.300273	-0.181777	0.338339
20	1	0	3.724887	-1.158091	0.557877
21	1	0	4.095391	0.552845	0.356319
22	6	0	2.220856	0.152910	1.294748
23	1	0	2.274379	1.039318	1.900674
24	6	0	1.214404	-0.773488	1.415119
25	1	0	1.439457	-1.809214	1.204453
26	1	0	0.392337	-0.606478	2.091898

TS2 (Toluene)



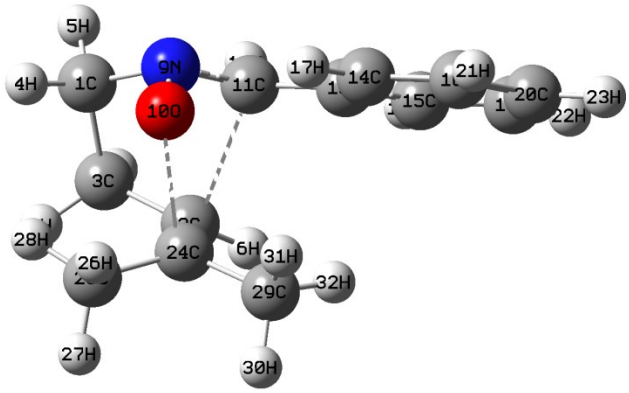
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.759073	-0.283907	-0.948797
2	6	0	-1.627157	-0.508520	1.223871
3	6	0	-2.879697	-0.879317	0.490761
4	1	0	-3.471791	0.505144	-1.143657
5	1	0	-2.853332	-1.050498	-1.711018
6	1	0	-0.998331	-1.257375	1.676745
7	1	0	-3.757583	-0.469533	0.983076
8	1	0	-3.006133	-1.955991	0.433176
9	7	0	-1.436400	0.315189	-1.011824
10	8	0	-1.398946	1.478390	-0.453667
11	6	0	-0.511943	-0.553671	-0.591900
12	1	0	-0.705682	-1.571311	-0.903432
13	6	0	0.887923	-0.249106	-0.330748
14	6	0	1.425878	1.031982	-0.250617
15	6	0	1.734053	-1.339707	-0.147149
16	6	0	2.772928	1.200372	0.001551
17	1	0	0.784101	1.880568	-0.394536
18	6	0	3.073964	-1.165169	0.119494
19	1	0	1.329072	-2.338841	-0.217963
20	6	0	3.600351	0.110854	0.194210
21	1	0	3.178426	2.199201	0.051642
22	1	0	3.710302	-2.024652	0.261662
23	1	0	4.649861	0.255314	0.398172
24	6	0	-1.493404	0.824470	1.524706
25	1	0	-2.354480	1.469373	1.561469
26	1	0	-0.601012	1.195466	2.004484

TS3 (Toluene)



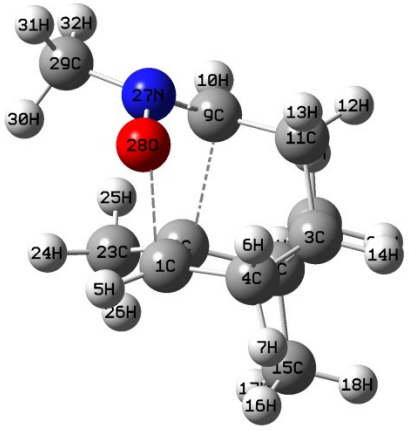
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.298378	-0.250335	-0.867809
2	1	0	-0.483132	0.242334	-1.812209
3	6	0	1.106156	-0.269143	-0.471447
4	6	0	1.958560	0.607052	-1.137010
5	6	0	1.631343	-1.080399	0.529850
6	6	0	3.297484	0.678671	-0.814696
7	1	0	1.563743	1.232089	-1.925022
8	6	0	2.975194	-1.016754	0.835759
9	1	0	0.976338	-1.751327	1.054376
10	6	0	3.811772	-0.137253	0.174687
11	1	0	3.940973	1.364792	-1.343099
12	1	0	3.372261	-1.658191	1.607414
13	1	0	4.859458	-0.089015	0.427779
14	7	0	-1.147369	-1.264990	-0.626617
15	8	0	-1.174128	-1.659956	0.604317
16	6	0	-2.502563	-1.051176	-1.057449
17	1	0	-2.985589	-2.011892	-1.183806
18	1	0	-2.520252	-0.510304	-1.998500
19	6	0	-3.180456	-0.275058	0.125645
20	1	0	-3.760863	0.545400	-0.288139
21	1	0	-3.855741	-0.938142	0.651267
22	6	0	-2.102786	0.191362	1.024888
23	1	0	-2.115312	-0.088608	2.064208
24	6	0	-1.176575	1.107300	0.545742
25	6	0	-0.136904	1.601280	1.505796
26	1	0	-0.521038	2.444312	2.080057
27	1	0	0.754672	1.941192	0.984930
28	1	0	0.161591	0.817633	2.194853
29	6	0	-1.554292	2.124652	-0.503061
30	1	0	-2.038829	2.982485	-0.036647
31	1	0	-2.226887	1.731497	-1.259023
32	1	0	-0.668103	2.499129	-1.012024

TS4 (Toluene)



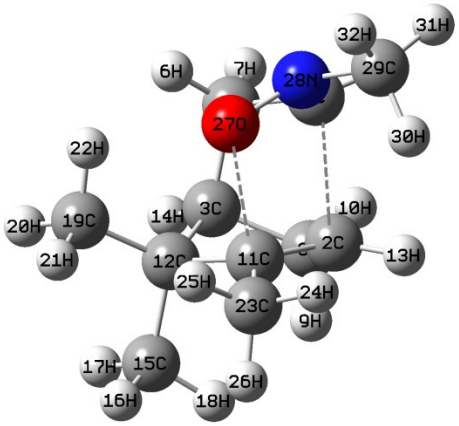
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.329337	-1.535367	0.661628
2	6	0	1.449841	-0.153458	-1.166590
3	6	0	2.519102	-1.145466	-0.837459
4	1	0	3.083240	-1.109392	1.310379
5	1	0	2.305520	-2.611862	0.796289
6	1	0	0.802601	-0.307749	-2.015595
7	1	0	3.520420	-0.754261	-0.994117
8	1	0	2.418138	-2.030051	-1.459268
9	7	0	1.060999	-0.948892	1.061171
10	8	0	1.180277	0.300187	1.382447
11	6	0	0.122562	-1.202590	0.145375
12	1	0	0.196932	-2.188099	-0.295779
13	6	0	-1.212291	-0.620682	0.138134
14	6	0	-1.660216	0.324729	1.054764
15	6	0	-2.090115	-1.067922	-0.845089
16	6	0	-2.952352	0.803914	0.976418
17	1	0	-0.986068	0.677402	1.814116
18	6	0	-3.372774	-0.572534	-0.929855
19	1	0	-1.756130	-1.814081	-1.551664
20	6	0	-3.809592	0.368611	-0.016263
21	1	0	-3.290361	1.531654	1.698030
22	1	0	-4.036026	-0.927198	-1.703394
23	1	0	-4.814543	0.756736	-0.074738
24	6	0	1.499973	1.090386	-0.560328
25	6	0	2.766637	1.702176	-0.051355
26	1	0	2.558241	2.367351	0.780509
27	1	0	3.227451	2.293024	-0.844717
28	1	0	3.481627	0.963953	0.289906
29	6	0	0.411764	2.072945	-0.831056
30	1	0	0.793156	2.907215	-1.419334
31	1	0	0.038517	2.476858	0.107212
32	1	0	-0.423183	1.620788	-1.355555

TS5 (Toluene)



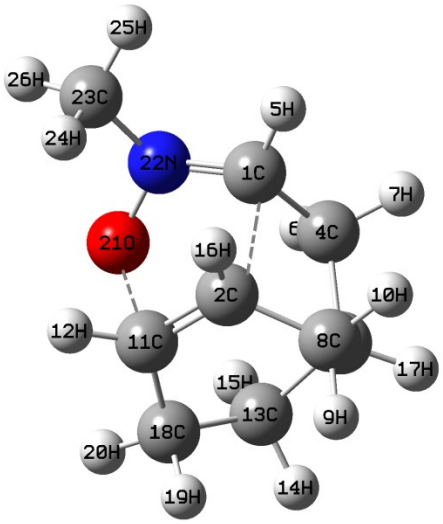
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.140443	-0.374559	-1.381732
2	6	0	0.285179	0.639051	-0.536011
3	6	0	1.065565	-1.292397	0.387524
4	6	0	0.539450	-1.651221	-1.000752
5	1	0	-0.613171	-0.219076	-2.335930
6	1	0	-0.154853	-2.485896	-0.985452
7	1	0	1.352542	-1.902512	-1.681549
8	6	0	1.537179	0.149663	0.194462
9	6	0	-0.943891	0.016290	1.041301
10	1	0	-0.978048	0.819403	1.763672
11	6	0	-0.115593	-1.203425	1.349849
12	1	0	0.234364	-1.147431	2.377109
13	1	0	-0.751855	-2.079386	1.256413
14	1	0	1.834232	-1.971642	0.748968
15	6	0	2.763603	0.251415	-0.705294
16	1	0	2.611261	-0.226051	-1.666922
17	1	0	3.008067	1.294971	-0.892393
18	1	0	3.629192	-0.202966	-0.226824
19	6	0	1.863640	0.900654	1.472609
20	1	0	2.748476	0.477845	1.943498
21	1	0	2.083594	1.941605	1.243698
22	1	0	1.063552	0.889336	2.203383
23	6	0	0.096038	2.096130	-0.814429
24	1	0	-0.662557	2.260599	-1.574213
25	1	0	-0.193084	2.656658	0.072335
26	1	0	1.022460	2.539605	-1.180273
27	7	0	-2.071939	-0.158164	0.362506
28	8	0	-1.973932	-0.987115	-0.612689
29	6	0	-2.993275	0.930204	0.159133
30	1	0	-2.702068	1.484631	-0.731150
31	1	0	-3.983683	0.519054	0.006555
32	1	0	-2.998111	1.584481	1.023090

TS6 (Toluene)



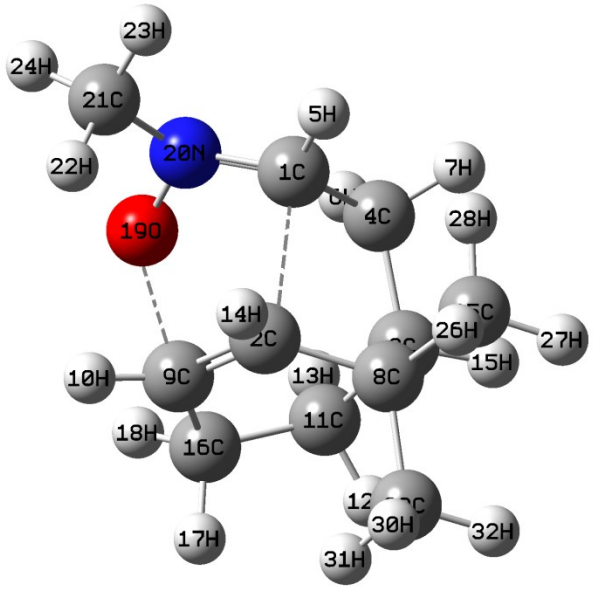
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.428489	-1.124355	0.057997
2	6	0	-0.171220	-0.245782	-1.377797
3	6	0	1.044311	-1.377262	0.163486
4	6	0	-0.282311	-1.693269	0.853429
5	1	0	-2.077712	-1.798203	-0.483314
6	1	0	-0.331616	-1.290146	1.859557
7	1	0	-0.398686	-2.772326	0.916324
8	6	0	0.683557	-1.485905	-1.307671
9	1	0	1.547270	-1.439617	-1.967235
10	1	0	0.145502	-2.404044	-1.535970
11	6	0	0.333758	0.736013	-0.541884
12	6	0	1.430878	0.106044	0.297554
13	1	0	-0.774913	-0.006032	-2.242194
14	1	0	1.839903	-2.039139	0.498292
15	6	0	2.775392	0.361907	-0.387697
16	1	0	3.054398	1.406903	-0.278388
17	1	0	3.555576	-0.238157	0.076081
18	1	0	2.755927	0.137542	-1.449659
19	6	0	1.549436	0.604241	1.724551
20	1	0	2.365848	0.088814	2.227846
21	1	0	1.783530	1.666758	1.731960
22	1	0	0.634801	0.468714	2.283789
23	6	0	0.288394	2.200605	-0.791326
24	1	0	-0.602182	2.472157	-1.349063
25	1	0	0.286257	2.760580	0.137879
26	1	0	1.156425	2.512096	-1.374357
27	8	0	-1.166550	0.848416	0.968367
28	7	0	-1.995285	-0.012368	0.491756
29	6	0	-3.127752	0.537834	-0.207724
30	1	0	-2.777386	1.066191	-1.094324
31	1	0	-3.812709	-0.252254	-0.492889
32	1	0	-3.626569	1.238984	0.448929

TS7 (Toluene)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.928218	1.121596	0.026791
2	6	0	0.192489	-0.083425	1.387877
3	6	0	1.576686	0.923389	-0.287202
4	6	0	0.271146	1.567291	-0.754551
5	1	0	-1.461728	1.856626	0.612245
6	1	0	0.089563	1.343743	-1.803305
7	1	0	0.351336	2.647105	-0.652409
8	6	0	1.421469	0.759841	1.216347
9	1	0	2.303176	0.281460	1.646834
10	1	0	1.309421	1.728723	1.698209
11	6	0	0.184699	-1.278784	0.707517
12	1	0	-0.478409	-2.074734	1.006263
13	6	0	1.848248	-0.430180	-0.951274
14	1	0	2.915311	-0.533635	-1.136709
15	1	0	1.351737	-0.452782	-1.916051
16	1	0	-0.430777	0.039376	2.262042
17	1	0	2.396698	1.598112	-0.524337
18	6	0	1.373776	-1.619350	-0.119845
19	1	0	2.175652	-1.929110	0.556128
20	1	0	1.164565	-2.468620	-0.762499
21	8	0	-1.055195	-0.846180	-0.960098
22	7	0	-1.682530	0.144977	-0.448158
23	6	0	-2.912183	-0.194507	0.220247
24	1	0	-2.674394	-0.815322	1.085603
25	1	0	-3.433639	0.701345	0.534894
26	1	0	-3.527913	-0.762917	-0.464455

TS8 (Toluene)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.078318	-1.013709	0.517211
2	6	0	0.170170	-0.283778	-1.050273
3	6	0	1.150708	0.054146	1.085427
4	6	0	-0.139635	-0.584995	1.606339
5	1	0	-1.243362	-2.069116	0.357372
6	1	0	-0.675164	0.117752	2.238996
7	1	0	0.101058	-1.457862	2.208176
8	6	0	1.431778	-0.585927	-0.274444
9	6	0	-0.282136	1.017111	-1.089562
10	1	0	-0.929985	1.329694	-1.893540
11	6	0	1.052959	1.576347	0.970079
12	1	0	2.054997	1.992868	1.047488
13	1	0	0.501685	1.945990	1.830282
14	1	0	-0.107235	-0.953965	-1.854518
15	1	0	1.958848	-0.174758	1.781057
16	6	0	0.396872	2.091771	-0.315140
17	1	0	1.144211	2.565573	-0.953433
18	1	0	-0.329432	2.863171	-0.080149
19	8	0	-1.900101	1.006348	0.242999
20	7	0	-2.127623	-0.252892	0.253263
21	6	0	-3.118286	-0.699522	-0.691206
22	1	0	-2.745720	-0.504774	-1.697939
23	1	0	-3.315036	-1.757084	-0.562880
24	1	0	-4.024909	-0.130317	-0.532196
25	6	0	1.663112	-2.083269	-0.145093
26	1	0	1.791146	-2.529665	-1.128976
27	1	0	2.568306	-2.276939	0.426805
28	1	0	0.845395	-2.600448	0.345835
29	6	0	2.672400	0.001355	-0.935088
30	1	0	2.842640	-0.470205	-1.900020
31	1	0	2.586550	1.068999	-1.100137
32	1	0	3.552426	-0.176633	-0.318562