Mar 19, 2007
Prepared for submission as a note to J. Org. Chem.

Supporting Information for

The Rearrangement of 1,1-Diphenylethoxyl Radical is Not Concerted but Occurs Through a Bridged Intermediate

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Table S1. Calculated energies (E^{ex} (nm)) and oscillator strengths of the lowest 12 electronic excitations in the reactant, bridged and product radicals in reactions **1** and **2** calculated by B3LYP/6-311+G(d,p).

Radical	**1**	**2**
	E^{ex} / f	E^{ex} / f
	2700.97 / 0.0003	2629.30 / 0.0002
	627.87 / 0.0126	611.19 / 0.0091
	531.40 / 0.0042	530.14 / 0.0116
	501.03 / 0.0030	502.73 / 0.0056
	462.91 / 0.0369	474.23 / 0.0261
I/IV	323.28 / 0.0000	324.36 / 0.0000
	316.64 / 0.0011	312.96 / 0.0040
	310.22 / 0.0038	292.90 / 0.0007
	281.17 / 0.0049	269.55 / 0.0029
	265.49 / 0.0001	266.12 / 0.0001
	264.38 / 0.0000	265.30 / 0.0001
	262.17 / 0.0004	261.23 / 0.0020
	454.17 / 0.0009	451.08 / 0.0012
	370.24 / 0.0324	385.47 / 0.0322
	356.58 / 0.0081	348.03 / 0.0220
	336.66 / 0.0078	340.90 / 0.0561
	330.76 / 0.0337	334.48 / 0.0048
	323.86 / 0.0013	322.92 / 0.0053
II/V	316.83 / 0.0084	312.68 / 0.0007
	306.00 / 0.0561	306.39 / 0.0702
	294.07 / 0.0141	288.34 / 0.0016
	290.76 / 0.0050	285.57 / 0.0085
	270.12 / 0.0089	266.09 / 0.0022
	266.85 / 0.0051	263.76 / 0.0034
	400.64 / 0.0024	407.47 / 0.0017
	376.95 / 0.0009	387.80 / 0.0014
	369.02 / 0.0016	382.64 / 0.0002
	351.61 / 0.0005	354.96 / 0.0578
	347.08 / 0.1002	329.86 / 0.2207
III/VI	323.90 / 0.0239	324.13 / 0.0312
	323.01 / 0.0084	318.56 / 0.0014
	311.87 / 0.0005	301.48 / 0.0395
	289.15 / 0.0049	292.31 / 0.0013
	284.45 / 0.0012	285.84 / 0.0003
	282.04 / 0.0256	282.24 / 0.0210
	279.42 / 0.0013	282.08 / 0.0017

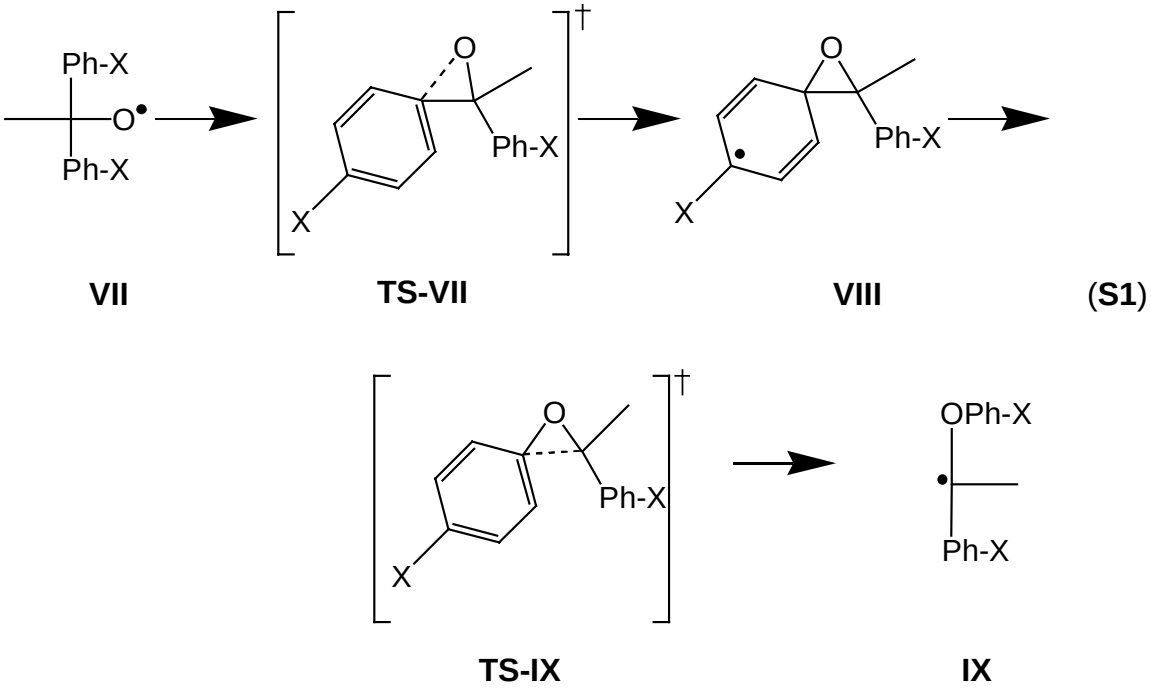

Table S2. Relative[a] zero-point corrected energies and gas phase first-order rate constants for reactions **S1** and **2** for X=H,NO_2,NH_2. All energy values are in kcal/mol and k are in s^{-1}.

Para substituent	reaction	**TS-VII/TS-IV**	**VIII/V**	**TS-IX/TS-VI**	**IX/VI**	**log k**
	S1	8.6	5.9	9.4	-15.1	6.89
X=H	**2**	9.9	7.3	10.7	-13.7	5.40
	Δ(S1-2)	-1.3	-1.4	-1.3	-1.4	1.49
	S1	8.2	3.7	6.5	-18.2	7.71
X=NO_2	**2**	9.4	5.0	7.8	-16.9	6.47
	Δ(S1-2)	-1.2	-1.4	-1.3	-1.4	1.24
	S1	7.8	6.1	11.2	-12.1	5.52
X=$N(CH_3)_2$	**2**	9.0	7.4	12.4	-10.8	4.34
	Δ(S1-2)	-1.2	-1.3	-1.2	-1.3	1.18

[a]Energies are relative to reactants.

Note that the methyl substituent lowers the energy of all of the structures relative to reactants by ca. 1.2 kcal/mol (**Δ(S1-2)**). Also note that the methyl substituent raises the rate constant by a factor of about 15-30.

Table S3. Relative[a] zero-point corrected energies for reaction **2** calculated using various methods.

method[b]/basis set	**TS-IV**	**V**	**TS-VI**	**VI**
B3LYP/6-31+G(d,p)	8.9	8.8	10.6	-15.5
MPW1K/6-31+G(d,p)	9.6	7.7	10.9	-13.5
CBS-QB3[S1,c]	3.6	3.3	5.4	-17.6
G3MP2[S2,c]	8.5	7.3	10.3	-16.9
CCSD(T) /6-311+G(d,p)[c]	9.8	8.4	11.2	-14.2
CCSD(T)/cc-PVDZ[c]	12.1	10.6	13.1	-13.1
CCSD(T)/cc-PVTZ[c]	9.0	7.5	10.4	-16.3
CCSD(T)/cc-pVDZ-TZ extrapolation[S3,c]	7.9	6.4	9.5	-17.4

[a] Energies are relative to **IV**.
[b] For all single-point energy calculations using the indicated methods, B3LYP/6-31+G(d,p) optimized structures were used.
[c] Used within an ONIOM[S4] scheme. This approximation consisted of substituting a hydrogen atom for the non-migrating phenyl ring and treating this reduced system at the indicated level of theory.

Table S4. Relative[a] zero-point corrected energies for reaction **2** calculated using various methods.

method[b]/basis set	**TS-IV**	**V**	**TS-VI**	**VI**
MPW1K/6-31+G(d,p)	9.8	7.3	10.7	-13.7
G3MP2[c]	7.6	6.2	9.6	-17.1
CCSD(T)/6-311+G(d,p)[c]	8.8	7.3	10.5	-14.5
CCSD(T)/cc-PVDZ[c]	11.1	9.5	12.5	-13.5
CCSD(T)/cc-PVTZ[c]	11.8	10.1	13.5	-12.8
CCSD(T)/basis set extrapolation[c]	12.0	10.3	13.8	-12.5

[a] Energies are relative to **IV**.
[b] For all single-point energy calculations using the indicated methods, MPW1K/6-31+G(d,p) optimized structures were used.
[c] See footnote c of Table S3.

MPW1K/6-31+G(d,p) predicts energies for reaction **2** that are in good agreement with those obtained using higher-level, wavefunction methods. On the contrary, the B3LYP/6-31+G(d,p) approach does not predict a substantial minimum for the intermediate.

We note that the relative energies for **TS-IV**, **V** and **TS-VI** obtained using CBS-QB3 are much lower than those of the other methods. Our examination of the components of the CBS-QB3 energies for these compounds revealed that the complete basis set extrapolation failed to properly converge.

Table S5. Cartesian coordinates (Å) for the MPW1K/6-31+G(d,p) optimized structures in reactions **1**, **2**, and **S1**.
a) Structure **I** (same as **VII** X=H; E^{el} = -616.341219853 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.4910	-0.1712	0.7222
6	-2.3657	0.6391	0.6918
6	-1.2660	0.2824	-0.0790
6	-1.3220	-0.8814	-0.8431
6	-2.4506	-1.6819	-0.8226
6	-3.5380	-1.3305	-0.0358
1	-4.3330	0.1084	1.3380
1	-2.3513	1.5415	1.2821
1	-0.4703	-1.1602	-1.4453
1	-2.4802	-2.5821	-1.4183
1	-4.4174	-1.9569	-0.0140
6	-0.0054	1.1485	-0.1721
6	1.2544	0.3097	-0.0046
6	2.2280	0.2991	-0.9930
6	1.4639	-0.4248	1.1585
6	3.3959	-0.4325	-0.8217
1	2.0627	0.8595	-1.9007
6	2.6283	-1.1539	1.3307
1	0.7043	-0.4406	1.9279
6	3.6005	-1.1590	0.3396
1	4.1450	-0.4335	-1.6000
1	2.7754	-1.7236	2.2366
1	4.5082	-1.7287	0.4727
8	-0.1387	1.6361	-1.4563
6	0.0131	2.3203	0.8051
1	-0.8404	2.9707	0.6352
1	0.0142	1.9752	1.8363
1	0.9200	2.8971	0.6427

b) Structure **TS-I** (same as **TS-VII** X=H; E^{el} = -616.325295884 hartree; 1 negative frequency = -533.9252)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.2625	-0.6059	-1.0196
6	-2.0393	0.0378	-1.1423
6	-1.2950	0.3506	-0.0132
6	-1.7856	0.0049	1.2418
6	-3.0028	-0.6452	1.3641
6	-3.7469	-0.9497	0.2327
1	-3.8350	-0.8416	-1.9048
1	-1.6444	0.2966	-2.1134
1	-1.2093	0.2312	2.1280
1	-3.3706	-0.9161	2.3429
1	-4.6970	-1.4541	0.3286
6	0.0133	1.0820	-0.1588
6	1.2657	0.2573	-0.1123
6	2.5312	0.8208	0.2460
6	1.2009	-1.1624	-0.2841
6	3.6358	0.0201	0.3953
1	2.6171	1.8857	0.3812
6	2.3214	-1.9387	-0.1312
1	0.2536	-1.6069	-0.5438
6	3.5493	-1.3629	0.2091
1	4.5825	0.4670	0.6607
1	2.2502	-3.0073	-0.2708
1	4.4256	-1.9817	0.3271
8	0.5626	1.0612	-1.4207
6	-0.0134	2.4386	0.5102
1	0.8887	3.0019	0.2968
1	-0.8590	3.0013	0.1206
1	-0.1350	2.3492	1.5872

c) Structure **II** (same as **VIII** X=H; E^{el} = -616.330296820 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.2535	-0.5498	-1.0244
6	-2.0291	0.0945	-1.1233
6	-1.2846	0.3670	0.0176
6	-1.7796	-0.0196	1.2593
6	-2.9991	-0.6696	1.3569
6	-3.7415	-0.9343	0.2148
1	-3.8255	-0.7524	-1.9180
1	-1.6359	0.3874	-2.0852
1	-1.2048	0.1753	2.1536
1	-3.3692	-0.9724	2.3254
1	-4.6932	-1.4390	0.2918
6	0.0175	1.0943	-0.0904
6	1.2822	0.3047	-0.3364
6	2.5825	0.8163	0.0989
6	1.1942	-1.1504	-0.4786
6	3.5952	-0.0300	0.4424
1	2.7326	1.8830	0.1222
6	2.2326	-1.9591	-0.1257
1	0.2740	-1.5622	-0.8610
6	3.4413	-1.4253	0.3578
1	4.5401	0.3812	0.7667
1	2.1281	-3.0293	-0.2291
1	4.2542	-2.0795	0.6319
8	0.6071	1.0809	-1.3587
6	0.0462	2.4128	0.6352
1	-0.0861	2.2719	1.7053
1	0.9749	2.9454	0.4651
1	-0.7722	3.0337	0.2751

d) Structure **TS-III** (same as **TS-IX** X=H; E^{el} = -616.323628533 hartree; 1 negative frequency = -640.4646)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.0984	-0.9903	-0.8898
6	-1.8916	-0.3423	-1.0911
6	-1.3121	0.4135	-0.0694
6	-1.9774	0.5024	1.1564
6	-3.1796	-0.1529	1.3555
6	-3.7465	-0.9030	0.3340
1	-3.5376	-1.5620	-1.6943
1	-1.3927	-0.3987	-2.0466
1	-1.5476	1.0799	1.9613
1	-3.6764	-0.0789	2.3117
1	-4.6862	-1.4116	0.4900
6	-0.0458	1.1150	-0.2779
6	1.3956	0.1862	-0.5636
6	2.6223	0.7728	-0.1299
6	1.2560	-1.2293	-0.4382
6	3.5480	0.0181	0.5512
1	2.8111	1.8116	-0.3471
6	2.1990	-1.9565	0.2451
1	0.3825	-1.7066	-0.8511
6	3.3428	-1.3458	0.7681
1	4.4596	0.4851	0.8948
1	2.0593	-3.0212	0.3621
1	4.0780	-1.9300	1.2995
8	0.5997	0.8862	-1.4826
6	0.1591	2.4525	0.3664
1	0.4313	2.3604	1.4167
1	0.9466	2.9977	-0.1418
1	-0.7548	3.0426	0.3052

e) Structure **III** (same as **IX** X=H; E^{el} = -616.364424827 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.2091	-1.6968	0.1703
6	-1.9595	-1.1989	-0.1325
6	-1.7295	0.1949	-0.1784
6	-2.8213	1.0521	0.0876
6	-4.0654	0.5380	0.3908
6	-4.2726	-0.8376	0.4365
1	-3.3616	-2.7658	0.2005
1	-1.1400	-1.8682	-0.3402
1	-2.6848	2.1223	0.0509
1	-4.8847	1.2129	0.5912
1	-5.2483	-1.2341	0.6732
6	-0.4514	0.7154	-0.4749
6	1.7285	-0.1685	-0.3199
6	2.7752	-0.6585	-1.0875
6	1.9474	0.2648	0.9796
6	4.0491	-0.7104	-0.5484
1	2.5737	-0.9916	-2.0940
6	3.2304	0.2144	1.5039
1	1.1197	0.6239	1.5729
6	4.2853	-0.2711	0.7471
1	4.8628	-1.0925	-1.1470
1	3.4005	0.5507	2.5160
1	5.2807	-0.3097	1.1624
8	0.4897	-0.1841	-0.8874
6	-0.1264	2.1611	-0.6015
1	-0.4380	2.7283	0.2744
1	0.9430	2.3021	-0.7265
1	-0.6239	2.6005	-1.4697

f) Structure **IV** X=N(CH_3)$_2$ (E^{el} = -844.915760376 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.6067	0.8429	0.6712
6	-2.4360	1.5730	0.6647
6	-1.2763	1.0817	0.0760
6	-1.3376	-0.1579	-0.5489
6	-2.5001	-0.9017	-0.5527
6	-3.6667	-0.4252	0.0687
1	-4.4767	1.2645	1.1466
1	-2.4239	2.5496	1.1282
1	-0.4554	-0.5553	-1.0287
1	-2.4961	-1.8609	-1.0430
6	-0.0182	1.9361	0.0411
1	-0.0456	2.6030	0.9109
6	1.2711	1.1547	0.0459
6	1.9853	0.9181	-1.1179
6	1.7857	0.6516	1.2329
6	3.1640	0.1909	-1.1063
1	1.6173	1.3224	-2.0493
6	2.9589	-0.0781	1.2631
1	1.2610	0.8308	2.1623
6	3.6750	-0.3412	0.0850
1	3.6862	0.0462	-2.0377
1	3.3164	-0.4396	2.2131
8	-0.2314	2.6424	-1.1155
7	-4.8171	-1.1723	0.0936
7	4.8299	-1.0979	0.1006
6	-4.8995	-2.3679	-0.7010
1	-4.7818	-2.1714	-1.7711
1	-4.1415	-3.0911	-0.4020
1	-5.8680	-2.8310	-0.5462
6	-6.0377	-0.5744	0.5623
1	-6.3453	0.2849	-0.0417
1	-6.8309	-1.3135	0.5286
1	-5.9422	-0.2471	1.5970
6	5.4606	-1.3710	1.3634
1	5.7655	-0.4621	1.8937
1	4.7995	-1.9395	2.0153
1	6.3437	-1.9785	1.1941
6	5.6625	-1.1101	-1.0713
1	6.0373	-0.1160	-1.3391
1	6.5139	-1.7590	-0.8943

1	5.1236	-1.5120	-1.9278

g) Structure **TS-IV** X=N(CH_3)$_2$ (E^{el} = -844.899521874 hartree; 1 negative frequency = -513.2833)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.1387	-0.0204	-1.1203
6	1.9150	-0.6650	-1.1669
6	1.3134	-1.1573	-0.0184
6	1.9820	-0.9873	1.1870
6	3.2015	-0.3406	1.2530
6	3.8201	0.1516	0.0930
1	3.5634	0.3434	-2.0413
1	1.4111	-0.7980	-2.1131
1	1.5421	-1.3625	2.1017
1	3.6745	-0.2279	2.2144
6	-0.0044	-1.8515	-0.0709
1	-0.0357	-2.7273	0.5817
6	-1.2809	-1.0983	-0.1127
6	-2.4882	-1.6876	0.3784
6	-1.3420	0.2878	-0.4550
6	-3.6568	-0.9828	0.4322
1	-2.4669	-2.7225	0.6862
6	-2.5177	0.9816	-0.3959
1	-0.4362	0.7836	-0.7672
6	-3.7216	0.3716	0.0287
1	-4.5392	-1.4800	0.8007
1	-2.5088	2.0243	-0.6681
8	-0.5829	-2.0352	-1.3076
7	-4.9040	1.0646	0.0487
7	5.0557	0.7628	0.1444
6	5.5324	1.4616	-1.0174
1	6.5166	1.8679	-0.8083
1	5.6359	0.7853	-1.8646
1	4.8771	2.2867	-1.3176
6	5.5872	1.1485	1.4230
1	4.9452	1.8599	1.9540
1	5.7342	0.2802	2.0638
1	6.5587	1.6095	1.2789
6	-4.9054	2.4812	-0.2000
1	-4.4850	2.7069	-1.1789
1	-5.9284	2.8414	-0.1952
1	-4.3428	3.0409	0.5532

6	-6.0651	0.4752	0.6595
1	-6.9067	1.1499	0.5471
1	-6.3312	-0.4620	0.1726
1	-5.9243	0.2804	1.7269

h) Structure **V** X=N(CH_3)$_2$ (E^{el} = -844.902796471 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.1404	-0.1531	-1.0837
6	1.9213	-0.8070	-1.0792
6	1.2974	-1.1662	0.1075
6	1.9421	-0.8514	1.2975
6	3.1576	-0.1945	1.3106
6	3.7972	0.1639	0.1139
1	3.5813	0.1033	-2.0327
1	1.4416	-1.0523	-2.0153
1	1.4852	-1.1184	2.2412
1	3.6094	0.0335	2.2617
6	-0.0064	-1.8671	0.1223
1	-0.0796	-2.6623	0.8613
6	-1.3042	-1.2230	-0.2379
6	-2.5432	-1.7275	0.3462
6	-1.3631	0.1608	-0.6943
6	-3.6655	-0.9645	0.4273
1	-2.5510	-2.7476	0.7010
6	-2.5019	0.8970	-0.5972
1	-0.4684	0.5973	-1.1093
6	-3.7003	0.3731	-0.0451
1	-4.5477	-1.4028	0.8654
1	-2.4760	1.9154	-0.9499
8	-0.6038	-2.1662	-1.1057
7	5.0284	0.7864	0.1168
7	-4.8544	1.1223	0.0049
6	5.5292	1.3268	1.3512
1	6.5038	1.7699	1.1747
1	4.8746	2.0954	1.7765
1	5.6620	0.5433	2.0957
6	5.5179	1.3585	-1.1077
1	4.8622	2.1414	-1.5043
1	6.4967	1.7920	-0.9302
1	5.6380	0.5950	-1.8747
6	-4.7881	2.5346	-0.2615
1	-5.7889	2.9510	-0.2163

1	-4.1599	3.0719	0.4564
1	-4.4042	2.7250	-1.2618
6	-5.9683	0.6471	0.7817
1	-5.7327	0.5527	1.8468
1	-6.7952	1.3415	0.6767
1	-6.3118	-0.3203	0.4203

i) Structure **TS-VI** X=N(CH_3)$_2$ (E^{el} = -844.893327787 hartree; 1 negative frequency = -698.5580)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.0876	-0.3728	-0.9984
6	1.8928	-1.0528	-0.8723
6	1.2610	-1.1948	0.3651
6	1.8874	-0.6176	1.4734
6	3.0789	0.0653	1.3589
6	3.7211	0.2002	0.1156
1	3.5334	-0.2972	-1.9765
1	1.4424	-1.5013	-1.7452
1	1.4260	-0.7021	2.4478
1	3.5133	0.4944	2.2465
6	0.0059	-1.8874	0.5190
1	-0.2351	-2.3253	1.4798
6	-1.4758	-1.4549	-0.3002
6	-2.6780	-1.7488	0.3965
6	-1.4481	-0.2613	-1.0762
6	-3.6954	-0.8246	0.4680
1	-2.7647	-2.7016	0.8971
6	-2.4773	0.6356	-1.0050
1	-0.5962	-0.0663	-1.7079
6	-3.6199	0.4022	-0.2094
1	-4.5690	-1.0706	1.0502
1	-2.4289	1.5262	-1.6130
8	-0.5833	-2.4949	-0.5734
7	-4.6543	1.3389	-0.1875
7	4.9290	0.8516	-0.0003
6	-5.8767	0.9635	0.4674
1	-5.7772	0.8806	1.5579
1	-6.6311	1.7181	0.2582
1	-6.2393	0.0154	0.0788
6	-4.2963	2.7170	0.0555
1	-5.1137	3.3632	-0.2576
1	-4.0902	2.9086	1.1159

1	-3.4167	2.9977	-0.5115
6	5.4289	1.1656	-1.3109
1	4.7574	1.8212	-1.8756
1	6.3883	1.6630	-1.2151
1	5.5908	0.2607	-1.8949
6	5.4152	1.6242	1.1101
1	6.3756	2.0557	0.8486
1	4.7385	2.4385	1.3901
1	5.5715	0.9958	1.9858

j) Structure **VI** X=N(CH_3)$_2$ (E^{el} = -844.931850845 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.6477	-0.9749	0.4680
6	-2.3004	-0.8583	0.2100
6	-1.7623	0.3006	-0.3884
6	-2.6756	1.3255	-0.7155
6	-4.0203	1.2083	-0.4553
6	-4.5511	0.0567	0.1567
1	-4.0013	-1.8869	0.9203
1	-1.6373	-1.6702	0.4652
1	-2.3112	2.2264	-1.1895
1	-4.6674	2.0233	-0.7345
6	-0.3957	0.4500	-0.6576
1	0.0214	1.3191	-1.1442
6	1.7710	-0.3406	-0.2924
6	2.6560	-1.3250	-0.6980
6	2.2649	0.8161	0.2851
6	4.0180	-1.1520	-0.5434
1	2.2662	-2.2321	-1.1342
6	3.6311	0.9944	0.4336
1	1.5856	1.5741	0.6449
6	4.5463	0.0238	0.0099
1	4.6708	-1.9450	-0.8677
1	3.9746	1.9043	0.8967
8	0.4379	-0.5928	-0.4429
7	-5.8970	-0.0464	0.4536
7	5.9131	0.2194	0.1197
6	-6.4253	-1.3333	0.8172
1	-5.9470	-1.7093	1.7197
1	-7.4841	-1.2334	1.0331
1	-6.3043	-2.0833	0.0276

6	-6.8092	0.8905	-0.1445
1	-6.5765	1.9097	0.1587
1	-6.8064	0.8495	-1.2395
1	-7.8149	0.6756	0.2018
6	6.7796	-0.9184	-0.0294
1	7.8097	-0.5954	0.0815
1	6.5847	-1.7055	0.7083
1	6.6855	-1.3524	-1.0232
6	6.3824	1.2890	0.9577
1	6.0684	1.1841	2.0027
1	7.4669	1.3124	0.9282
1	6.0308	2.2521	0.5918

k) Structure **IV** X=NH_2 (E^{el} = -687.723665904 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.6012	0.3442	0.6686
6	-2.4405	1.0864	0.7496
6	-1.2714	0.6640	0.1248
6	-1.3058	-0.5099	-0.6198
6	-2.4620	-1.2588	-0.7087
6	-3.6292	-0.8457	-0.0627
1	-4.4967	0.6864	1.1681
1	-2.4393	2.0098	1.3114
1	-0.4109	-0.8496	-1.1196
1	-2.4669	-2.1730	-1.2857
6	-0.0207	1.5284	0.1941
1	-0.0684	2.1063	1.1245
6	1.2763	0.7603	0.1446
6	2.0117	0.6522	-1.0266
6	1.7645	0.1368	1.2864
6	3.1953	-0.0663	-1.0623
1	1.6531	1.1456	-1.9176
6	2.9431	-0.5845	1.2615
1	1.2126	0.2104	2.2141
6	3.6798	-0.6970	0.0814
1	3.7507	-0.1386	-1.9874
1	3.2986	-1.0668	2.1616
8	-0.2186	2.3460	-0.8899
7	-4.7950	-1.5699	-0.1843
7	4.8372	-1.4577	0.0390
1	-4.7013	-2.5311	-0.4482
1	-5.4959	-1.4157	0.5138
1	5.3036	-1.5860	0.9166
1	5.4751	-1.2329	-0.7004

l) Structure **TS-IV** X=NH_2 (E^{el} = -687.707711081 hartree; 1 negative frequency = -522.6400)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.1490	0.3838	1.0754
6	-1.9227	-0.2559	1.1282
6	-1.3214	-0.7451	-0.0232
6	-1.9881	-0.5869	-1.2328
6	-3.2099	0.0556	-1.2973
6	-3.8100	0.5544	-0.1400
1	-3.6056	0.7462	1.9862
1	-1.4181	-0.3908	2.0736
1	-1.5464	-0.9703	-2.1430
1	-3.7125	0.1634	-2.2485
6	-0.0017	-1.4370	0.0326
1	0.0263	-2.3247	-0.6036
6	1.2732	-0.6781	0.0459
6	2.4773	-1.2817	-0.4389
6	1.3272	0.7143	0.3685
6	3.6417	-0.5714	-0.5154
1	2.4540	-2.3248	-0.7162
6	2.5022	1.4074	0.2851
1	0.4222	1.2067	0.6876
6	3.6886	0.7849	-0.1441
1	4.5409	-1.0526	-0.8748
1	2.5209	2.4586	0.5381
8	0.5851	-1.5964	1.2675
7	4.8556	1.5050	-0.2632
1	4.9210	2.3493	0.2716
1	5.7090	0.9814	-0.2839
7	-5.0598	1.1482	-0.1922
1	-5.2867	1.7524	0.5741
1	-5.3201	1.5386	-1.0775

m) Structure **V** X=NH_2 (E^{el} = -687.711239884 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.1458	0.2751	-1.0765
6	1.9216	-0.3693	-1.0726
6	1.3115	-0.7401	0.1192
6	1.9708	-0.4571	1.3107
6	3.1917	0.1901	1.3169
6	3.7990	0.5701	0.1193
1	3.6078	0.5430	-2.0167
1	1.4289	-0.6019	-2.0052
1	1.5236	-0.7458	2.2523
1	3.6873	0.3950	2.2557
6	0.0038	-1.4342	0.1374
1	-0.0647	-2.2450	0.8594
6	-1.2964	-0.7767	-0.1939
6	-2.5288	-1.2958	0.3990
6	-1.3488	0.6193	-0.6232
6	-3.6350	-0.5186	0.5378
1	-2.5388	-2.3312	0.7052
6	-2.4754	1.3633	-0.4666
1	-0.4640	1.0474	-1.0666
6	-3.6436	0.8312	0.1230
1	-4.5335	-0.9414	0.9673
1	-2.4818	2.3919	-0.8020
8	-0.6134	-1.7017	-1.0878
7	5.0470	1.1694	0.1182
1	5.2778	1.6930	-0.7042
1	5.3022	1.6473	0.9609
7	-4.7903	1.5926	0.2250
1	-5.4640	1.2952	0.9045
1	-4.6674	2.5869	0.2076

n) Structure **TS-VI** X=NH_2 (E^{el} = -687.701965168 hartree; 1 negative frequency = -706.1251)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.0909	0.2578	-1.0737
6	1.8914	-0.4248	-1.0197
6	1.3175	-0.7810	0.2041
6	2.0037	-0.4274	1.3712
6	3.2003	0.2549	1.3213
6	3.7648	0.6156	0.0946
1	3.5215	0.5073	-2.0337
1	1.3946	-0.7104	-1.9348
1	1.5880	-0.6941	2.3331
1	3.7131	0.5077	2.2390
6	0.0587	-1.4799	0.2909
1	-0.1444	-2.0809	1.1687
6	-1.4489	-0.8964	-0.3726
6	-2.6248	-1.3037	0.3198
6	-1.4369	0.4125	-0.9304
6	-3.6263	-0.4050	0.5869
1	-2.7017	-2.3304	0.6449
6	-2.4509	1.2930	-0.6533
1	-0.6021	0.7146	-1.5420
6	-3.5538	0.9188	0.1299
1	-4.5011	-0.7301	1.1334
1	-2.4110	2.2920	-1.0654
8	-0.5866	-1.8807	-0.8635
7	-4.5910	1.8084	0.3628
1	-5.1613	1.6086	1.1623
1	-4.3486	2.7792	0.3064
7	4.9905	1.2558	0.0408
1	5.1834	1.7588	-0.8039
1	5.2525	1.7683	0.8609

o) Structure **VI** X=NH_2 (E^{el} = -687.740180244 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.6237	-1.0786	-0.5523
6	2.2778	-0.9312	-0.3031
6	1.7715	0.2440	0.2958
6	2.7047	1.2528	0.6253
6	4.0467	1.0981	0.3705
6	4.5370	-0.0729	-0.2207
1	3.9821	-1.9866	-1.0181
1	1.5912	-1.7205	-0.5667
1	2.3554	2.1652	1.0881
1	4.7346	1.8921	0.6270
6	0.4079	0.4282	0.5573
1	0.0099	1.3098	1.0374
6	-1.7747	-0.3029	0.1643
6	-2.6922	-1.2560	0.5773
6	-2.2205	0.8637	-0.4350
6	-4.0453	-1.0413	0.3981
1	-2.3331	-2.1624	1.0402
6	-3.5791	1.0777	-0.6054
1	-1.5107	1.5966	-0.7875
6	-4.5135	0.1318	-0.1940
1	-4.7504	-1.7891	0.7331
1	-3.9150	1.9938	-1.0708
8	-0.4516	-0.5922	0.3382
7	5.8835	-0.2047	-0.5231
7	-5.8766	0.3716	-0.3171
1	-6.1304	1.0287	-1.0303
1	-6.4519	-0.4487	-0.3478
1	6.2128	-1.1460	-0.6242
1	6.5066	0.3560	0.0264

p) Structure **IV** X=OCH_3 (E^{el} = -806.012771169 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.5576	0.6999	-0.9130
6	2.3858	1.4236	-0.9129
6	1.2757	0.9879	-0.1907
6	1.3822	-0.1729	0.5585
6	2.5562	-0.9117	0.5705
6	3.6495	-0.4759	-0.1692
1	4.4177	1.0224	-1.4790
1	2.3253	2.3401	-1.4824
1	0.5340	-0.5192	1.1298
1	2.6034	-1.8168	1.1537
6	0.0080	1.8323	-0.1720
1	-0.0155	2.4098	-1.1030
6	-1.2687	1.0392	-0.0382
6	-1.9109	0.9026	1.1880
6	-1.8252	0.4242	-1.1475
6	-3.0704	0.1602	1.3005
1	-1.4963	1.3937	2.0554
6	-2.9884	-0.3268	-1.0518
1	-1.3454	0.5228	-2.1122
6	-3.6153	-0.4618	0.1815
1	-3.5762	0.0534	2.2479
1	-3.3924	-0.7913	-1.9367
8	0.2579	2.6580	0.8951
8	4.8296	-1.1192	-0.2309
8	-4.7492	-1.1644	0.3866
6	4.9880	-2.3014	0.5057
1	4.8633	-2.1237	1.5742
1	4.2857	-3.0695	0.1805
1	6.0001	-2.6404	0.3162
6	-5.3485	-1.7971	-0.7093
1	-5.6439	-1.0770	-1.4735
1	-4.6863	-2.5425	-1.1517
1	-6.2339	-2.2915	-0.3256

q) Structure **TS-IV** X=OCH_3 (E^{el} = -805.995516122 hartree; 1 negative frequency = -530.1619)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.1319	0.1367	-1.2890
6	-1.9021	0.7467	-1.1453
6	-1.3288	0.9061	0.1129
6	-2.0250	0.4504	1.2210
6	-3.2594	-0.1714	1.0929
6	-3.8165	-0.3309	-0.1706
1	-3.5862	0.0142	-2.2603
1	-1.3711	1.1180	-2.0092
1	-1.6035	0.5765	2.2093
1	-3.7717	-0.5170	1.9760
6	-0.0007	1.5657	0.2724
1	0.0259	2.2428	1.1288
6	1.2657	0.8157	0.0686
6	2.4637	1.2398	0.7217
6	1.3040	-0.4353	-0.6278
6	3.6248	0.5108	0.6281
1	2.4493	2.1700	1.2693
6	2.4623	-1.1495	-0.7089
1	0.4012	-0.7994	-1.0919
6	3.6398	-0.6882	-0.0924
1	4.5139	0.8723	1.1192
1	2.5012	-2.0893	-1.2382
8	0.6155	2.0453	-0.8597
8	4.7205	-1.4731	-0.2421
8	-5.0087	-0.9160	-0.4080
6	5.9305	-1.0735	0.3434
1	6.2672	-0.1163	-0.0552
1	5.8438	-1.0067	1.4281
1	6.6542	-1.8397	0.0904
6	-5.7421	-1.4014	0.6816
1	-5.1941	-2.1771	1.2181
1	-6.0061	-0.6007	1.3738
1	-6.6495	-1.8279	0.2689

r) Structure **V** X=OCH_3 (E^{el} = -805.999326075 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.0243	-0.0284	1.3042
6	-1.8319	-0.7102	1.1724
6	-1.2927	-0.9671	-0.0860
6	-1.9878	-0.5330	-1.2044
6	-3.1853	0.1586	-1.0876
6	-3.7074	0.4146	0.1748
1	-3.4517	0.1685	2.2755
1	-1.3078	-1.0638	2.0478
1	-1.5934	-0.7321	-2.1916
1	-3.6964	0.4840	-1.9791
6	-0.0159	-1.7006	-0.2427
1	-0.0090	-2.4271	-1.0518
6	1.3231	-1.1239	0.0956
6	2.5034	-1.6150	-0.6163
6	1.4432	0.2138	0.6674
6	3.6190	-0.8569	-0.7424
1	2.4619	-2.6135	-1.0252
6	2.5863	0.9515	0.5237
1	0.5995	0.6143	1.2063
6	3.6856	0.4400	-0.1826
1	4.4880	-1.2267	-1.2656
1	2.6283	1.9355	0.9633
8	0.6464	-2.1192	0.9130
8	-4.8624	1.0735	0.4021
8	4.8459	1.0955	-0.3762
6	-5.5944	1.5356	-0.6986
1	-5.0216	2.2547	-1.2856
1	-5.9099	0.7131	-1.3419
1	-6.4720	2.0263	-0.2931
6	4.9937	2.3764	0.1733
1	4.2619	3.0725	-0.2375
1	4.9050	2.3553	1.2599
1	5.9902	2.7072	-0.0965

s) Structure **TS-VI** X=OCH_3 (E^{el} = -805.991102571 hartree; 1 negative frequency = -695.4466)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-2.9589	-0.0711	1.2786
6	-1.7939	-0.7849	1.1043
6	-1.2828	-1.0260	-0.1775
6	-1.9928	-0.5283	-1.2697
6	-3.1639	0.1921	-1.1046
6	-3.6520	0.4277	0.1771
1	-3.3615	0.1086	2.2638
1	-1.2741	-1.1865	1.9611
1	-1.6229	-0.7054	-2.2700
1	-3.6832	0.5603	-1.9744
6	-0.0545	-1.7563	-0.3882
1	0.0895	-2.2732	-1.3289
6	1.4897	-1.2808	0.2573
6	2.6170	-1.6486	-0.5372
6	1.5435	-0.0374	0.9422
6	3.6272	-0.7560	-0.7645
1	2.6437	-2.6387	-0.9670
6	2.5695	0.8510	0.7013
1	0.7500	0.2218	1.6243
6	3.6095	0.5131	-0.1666
1	4.4699	-1.0170	-1.3865
1	2.5626	1.8015	1.2103
8	0.6228	-2.2886	0.6914
8	4.6512	1.3177	-0.4660
8	-4.7797	1.1158	0.4489
6	4.7041	2.5862	0.1242
1	5.6012	3.0604	-0.2577
1	3.8367	3.1889	-0.1482
1	4.7707	2.5185	1.2109
6	-5.5203	1.6321	-0.6217
1	-4.9379	2.3504	-1.2001
1	-5.8744	0.8388	-1.2811
1	-6.3735	2.1371	-0.1829

t) Structure **VI** X=OCH_3 (E^{el} = -806.030096448 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.5970	1.0917	-0.6851
6	-2.2574	0.9949	-0.4009
6	-1.7493	-0.0972	0.3421
6	-2.6704	-1.0710	0.7762
6	-4.0181	-0.9724	0.4874
6	-4.4931	0.1124	-0.2470
1	-3.9858	1.9238	-1.2521
1	-1.5750	1.7559	-0.7454
1	-2.3164	-1.9158	1.3501
1	-4.6877	-1.7407	0.8390
6	-0.3857	-0.2298	0.6409
1	0.0165	-1.0434	1.2260
6	1.7909	0.4963	0.2022
6	2.6763	1.5253	0.5007
6	2.2721	-0.7244	-0.2299
6	4.0331	1.3254	0.3725
1	2.2838	2.4737	0.8339
6	3.6432	-0.9298	-0.3524
1	1.5865	-1.5147	-0.4948
6	4.5287	0.0934	-0.0507
1	4.7340	2.1130	0.6021
1	3.9955	-1.8892	-0.6947
8	0.4603	0.7738	0.3211
8	5.8737	-0.0050	-0.1376
8	-5.7876	0.3033	-0.5812
6	6.4218	-1.2193	-0.5659
1	6.1619	-2.0354	0.1100
1	6.0966	-1.4700	-1.5767
1	7.4976	-1.0840	-0.5624
6	-6.7289	-0.6456	-0.1659
1	-6.5169	-1.6296	-0.5865
1	-6.7693	-0.7188	0.9218
1	-7.6887	-0.3012	-0.5346

u) Structure **IV** X=OH (E^{el} = -727.427598334 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.5859	0.3120	0.7142
6	-2.4264	1.0567	0.7940
6	-1.2702	0.6586	0.1287
6	-1.3077	-0.4891	-0.6518
6	-2.4647	-1.2428	-0.7417
6	-3.6058	-0.8440	-0.0570
1	-4.4816	0.6083	1.2374
1	-2.4160	1.9617	1.3846
1	-0.4215	-0.8061	-1.1806
1	-2.4788	-2.1416	-1.3434
6	-0.0202	1.5258	0.1983
1	-0.0677	2.0968	1.1324
6	1.2759	0.7545	0.1440
6	2.0176	0.6673	-1.0270
6	1.7491	0.1121	1.2796
6	3.1985	-0.0542	-1.0703
1	1.6653	1.1795	-1.9096
6	2.9274	-0.6143	1.2498
1	1.1902	0.1717	2.2038
6	3.6550	-0.6996	0.0693
1	3.7798	-0.1209	-1.9771
1	3.2814	-1.1097	2.1440
8	-0.2134	2.3550	-0.8776
8	-4.7599	-1.5405	-0.1020
8	4.8138	-1.3910	-0.0234
1	-4.6660	-2.3037	-0.6675
1	5.0348	-1.7813	0.8189

v) Structure **TS-IV** X=OH (E^{el} = -727.410223566 hartree; 1 negative frequency = -531.8692)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.1407	-0.3901	1.0888
6	1.9166	0.2530	1.1307
6	1.3221	0.7343	-0.0297
6	1.9862	0.5682	-1.2376
6	3.2086	-0.0796	-1.2939
6	3.7878	-0.5619	-0.1268
1	3.6098	-0.7603	1.9873
1	1.4086	0.3984	2.0725
1	1.5470	0.9465	-2.1507
1	3.7127	-0.2046	-2.2429
6	0.0030	1.4288	0.0171
1	-0.0270	2.3056	-0.6333
6	-1.2729	0.6674	0.0461
6	-2.4749	1.2681	-0.4450
6	-1.3217	-0.7209	0.3908
6	-3.6405	0.5516	-0.5165
1	-2.4532	2.3091	-0.7296
6	-2.4932	-1.4205	0.3110
1	-0.4166	-1.2047	0.7219
6	-3.6648	-0.7944	-0.1345
1	-4.5443	1.0265	-0.8745
1	-2.5369	-2.4651	0.5783
8	-0.5836	1.6047	1.2481
8	-4.7838	-1.5436	-0.1866
8	4.9805	-1.1987	-0.1164
1	5.3343	-1.2537	-1.0009
1	-5.5224	-1.0220	-0.4925

w) Structure **V** X=OH (E^{el} = -727.414215452 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.1410	-0.2679	-1.0951
6	-1.9194	0.3802	-1.0792
6	-1.3100	0.7291	0.1215
6	-1.9597	0.4236	1.3107
6	-3.1805	-0.2295	1.3074
6	-3.7734	-0.5785	0.1007
1	-3.6206	-0.5344	-2.0243
1	-1.4284	0.6348	-2.0066
1	-1.5098	0.6960	2.2554
1	-3.6719	-0.4631	2.2424
6	-0.0046	1.4284	0.1491
1	0.0625	2.2298	0.8811
6	1.2977	0.7741	-0.1884
6	2.5265	1.2893	0.4171
6	1.3445	-0.6172	-0.6326
6	3.6291	0.5092	0.5627
1	2.5343	2.3229	0.7290
6	2.4706	-1.3684	-0.4713
1	0.4627	-1.0375	-1.0887
6	3.6211	-0.8297	0.1282
1	4.5330	0.8995	1.0055
1	2.4779	-2.3967	-0.8094
8	0.6148	1.7080	-1.0703
8	-4.9647	-1.2141	0.0316
8	4.7522	-1.5449	0.3081
1	4.6444	-2.4301	-0.0324
1	-5.3087	-1.3696	0.9080

x) Structure **TS-VI** X=OH (E^{el} = -727.405812596 hartree; 1 negative frequency = -697.2172)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.0842	-0.2587	-1.0924
6	-1.8870	0.4262	-1.0303
6	-1.3145	0.7687	0.1994
6	-1.9917	0.4036	1.3656
6	-3.1890	-0.2834	1.3101
6	-3.7390	-0.6208	0.0781
1	-3.5319	-0.5148	-2.0404
1	-1.3909	0.7260	-1.9410
1	-1.5735	0.6610	2.3286
1	-3.6977	-0.5567	2.2249
6	-0.0565	1.4728	0.2906
1	0.1422	2.0721	1.1704
6	1.4462	0.8887	-0.3658
6	2.6173	1.2954	0.3394
6	1.4311	-0.4182	-0.9279
6	3.6149	0.3966	0.6144
1	2.6904	2.3216	0.6664
6	2.4427	-1.3037	-0.6420
1	0.6006	-0.7165	-1.5468
6	3.5298	-0.9169	0.1444
1	4.4903	0.6923	1.1722
1	2.4023	-2.3056	-1.0486
8	0.5896	1.8765	-0.8611
8	4.5447	-1.7568	0.4536
8	-4.9062	-1.2924	-0.0400
1	4.3907	-2.6171	0.0706
1	-5.2678	-1.4832	0.8222

y) Structure **VI** X=OH (E^{el} = -727.444674445 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.6179	-1.1027	-0.5422
6	2.2729	-0.9418	-0.2998
6	1.7741	0.2449	0.2848
6	2.7061	1.2534	0.6104
6	4.0516	1.0877	0.3631
6	4.5180	-0.0913	-0.2147
1	3.9969	-2.0094	-0.9886
1	1.5808	-1.7280	-0.5572
1	2.3591	2.1716	1.0627
1	4.7467	1.8757	0.6213
6	0.4083	0.4400	0.5356
1	0.0132	1.3271	1.0077
6	-1.7760	-0.2950	0.1535
6	-2.6845	-1.2634	0.5581
6	-2.2260	0.8764	-0.4303
6	-4.0387	-1.0587	0.3867
1	-2.3143	-2.1718	1.0079
6	-3.5892	1.0836	-0.5941
1	-1.5219	1.6171	-0.7768
6	-4.4981	0.1206	-0.1872
1	-4.7554	-1.8027	0.6981
1	-3.9358	1.9996	-1.0534
8	-0.4524	-0.5792	0.3242
8	-5.8375	0.2680	-0.3232
8	5.8278	-0.3080	-0.4784
1	6.3475	0.4468	-0.2129
1	-6.0386	1.1058	-0.7329

z) Structure **IV** X=CH_3 (E^{el} = -655.657164106 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.5771	0.3184	0.7100
6	-2.4191	1.0692	0.8066
6	-1.2703	0.6825	0.1270
6	-1.3101	-0.4505	-0.6749
6	-2.4731	-1.1958	-0.7698
6	-3.6230	-0.8291	-0.0774
1	-4.4597	0.6290	1.2517
1	-2.4057	1.9638	1.4131
1	-0.4263	-0.7553	-1.2152
1	-2.4872	-2.0786	-1.3937
6	-0.0169	1.5473	0.2121
1	-0.0662	2.0997	1.1573
6	1.2754	0.7700	0.1514
6	2.0283	0.7101	-1.0105
6	1.7295	0.0947	1.2787
6	3.2082	-0.0208	-1.0451
1	1.6887	1.2428	-1.8860
6	2.9047	-0.6332	1.2387
1	1.1544	0.1322	2.1944
6	3.6672	-0.7031	0.0743
1	3.7823	-0.0561	-1.9609
1	3.2385	-1.1545	2.1256
8	-0.1986	2.4019	-0.8454
6	-4.8683	-1.6578	-0.1559
6	4.9552	-1.4689	0.0458
1	-4.9192	-2.2086	-1.0920
1	5.7505	-0.9144	0.5441
1	4.8586	-2.4261	0.5546
1	5.2782	-1.6615	-0.9743
1	-4.9011	-2.3854	0.6553
1	-5.7604	-1.0406	-0.0770

aa) Structure **TS-IV** X=CH_3 (E^{el} = -655.639960149 hartree; 1 negative frequency = -542.6494)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.1535	0.3218	-1.0825
6	1.9287	-0.3293	-1.1229
6	1.3207	-0.7504	0.0497
6	1.9629	-0.5167	1.2611
6	3.1804	0.1383	1.2959
6	3.7990	0.5678	0.1231
1	3.6153	0.6409	-2.0067
1	1.4361	-0.5225	-2.0644
1	1.5052	-0.8462	2.1843
1	3.6624	0.3165	2.2475
6	0.0060	-1.4552	0.0214
1	-0.0227	-2.3044	0.7073
6	-1.2739	-0.6962	-0.0313
6	-2.4720	-1.2812	0.4844
6	-1.3250	0.6728	-0.4327
6	-3.6310	-0.5552	0.5461
1	-2.4461	-2.3124	0.8036
6	-2.5025	1.3717	-0.3583
1	-0.4235	1.1429	-0.7928
6	-3.6827	0.7841	0.1228
1	-4.5274	-1.0199	0.9329
1	-2.5210	2.4069	-0.6698
8	-0.5736	-1.6837	-1.2013
6	-4.9659	1.5491	0.1598
1	-4.7883	2.6211	0.2024
1	-5.5626	1.3516	-0.7322
1	-5.5701	1.2703	1.0209
6	5.1318	1.2519	0.1684
1	5.3684	1.7206	-0.7836
1	5.1553	2.0218	0.9374
1	5.9277	0.5425	0.3943

ab) Structure **V** X=CH_3 (E^{el} = -655.644623525 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.1535	0.1790	-1.0756
6	1.9300	-0.4734	-1.0531
6	1.3036	-0.7475	0.1548
6	1.9316	-0.3670	1.3367
6	3.1495	0.2877	1.3068
6	3.7817	0.5759	0.0991
1	3.6306	0.3767	-2.0257
1	1.4575	-0.7880	-1.9719
1	1.4644	-0.5856	2.2873
1	3.6212	0.5763	2.2361
6	0.0020	-1.4516	0.2065
1	-0.0723	-2.2075	0.9843
6	-1.3015	-0.8206	-0.1847
6	-2.5290	-1.2972	0.4491
6	-1.3437	0.5452	-0.7004
6	-3.6159	-0.4866	0.5806
1	-2.5462	-2.3182	0.8008
6	-2.4545	1.3148	-0.5454
1	-0.4648	0.9290	-1.1939
6	-3.6201	0.8401	0.1004
1	-4.5064	-0.8715	1.0585
1	-2.4500	2.3255	-0.9308
8	-0.6074	-1.8004	-0.9980
6	5.0907	1.3047	0.0733
1	4.9452	2.3741	0.2273
1	5.7566	0.9514	0.8580
1	5.5965	1.1760	-0.8804
6	-4.8306	1.7056	0.2189
1	-5.5191	1.3266	0.9705
1	-4.5640	2.7262	0.4901
1	-5.3736	1.7570	-0.7271

ac) Structure **TS-VI** X=CH_3 (E^{el} = -655.637234164 hartree; 1 negative frequency = -685.2811)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.0932	0.1934	-1.0709
6	1.8914	-0.4910	-1.0092
6	1.3061	-0.7829	0.2240
6	1.9683	-0.3733	1.3862
6	3.1645	0.3110	1.3123
6	3.7499	0.6127	0.0820
1	3.5348	0.3995	-2.0362
1	1.4085	-0.8275	-1.9143
1	1.5367	-0.5974	2.3519
1	3.6587	0.6160	2.2245
6	0.0505	-1.4906	0.3298
1	-0.1537	-2.0523	1.2327
6	-1.4445	-0.9323	-0.3519
6	-2.6129	-1.3093	0.3707
6	-1.4244	0.3543	-0.9605
6	-3.6076	-0.3913	0.6023
1	-2.6881	-2.3223	0.7369
6	-2.4390	1.2444	-0.7107
1	-0.5911	0.6251	-1.5888
6	-3.5430	0.9110	0.0881
1	-4.4752	-0.6895	1.1750
1	-2.3930	2.2274	-1.1589
8	-0.5872	-1.9403	-0.8075
6	-4.6166	1.9117	0.3759
1	-5.5689	1.4255	0.5770
1	-4.3692	2.5164	1.2499
1	-4.7574	2.5943	-0.4598
6	5.0366	1.3762	0.0122
1	4.8735	2.4366	0.2062
1	5.7507	1.0178	0.7513
1	5.4963	1.2886	-0.9691

ad) Structure **VI** X=CH_3 (E^{el} = -655.677082826 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.6345	-1.0951	0.4878
6	-2.2809	-0.9420	0.2647
6	-1.7755	0.2593	-0.2757
6	-2.7021	1.2843	-0.5756
6	-4.0461	1.1105	-0.3432
6	-4.5473	-0.0821	0.1935
1	-3.9966	-2.0259	0.9026
1	-1.5950	-1.7401	0.5023
1	-2.3445	2.2149	-0.9941
1	-4.7319	1.9121	-0.5820
6	-0.4092	0.4606	-0.5128
1	-0.0120	1.3642	-0.9500
6	1.7762	-0.2881	-0.1504
6	2.6705	-1.2776	-0.5337
6	2.2397	0.8894	0.4119
6	4.0263	-1.0768	-0.3607
1	2.2880	-2.1907	-0.9633
6	3.6069	1.0742	0.5699
1	1.5453	1.6440	0.7479
6	4.5237	0.1049	0.1873
1	4.7148	-1.8540	-0.6626
1	3.9601	1.9945	1.0138
8	0.4521	-0.5601	-0.3208
6	5.9991	0.3174	0.3443
1	6.2090	1.1788	0.9736
1	6.4787	-0.5497	0.7948
1	6.4771	0.4892	-0.6200
6	-6.0140	-0.2516	0.4405
1	-6.5881	-0.1181	-0.4761
1	-6.2371	-1.2415	0.8309
1	-6.3815	0.4798	1.1603

ae) Structure **IV** X=H (E^{el} = -577.030895692 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.5626	-0.0789	0.6804
6	-2.4157	0.6794	0.8469
6	-1.2698	0.3858	0.1170
6	-1.2885	-0.6558	-0.8024
6	-2.4377	-1.4112	-0.9711
6	-3.5746	-1.1262	-0.2294
1	-4.4458	0.1475	1.2590
1	-2.4067	1.5020	1.5477
1	-0.3998	-0.8820	-1.3723
1	-2.4444	-2.2244	-1.6816
1	-4.4682	-1.7183	-0.3604
6	-0.0275	1.2557	0.2887
1	-0.1011	1.7352	1.2710
6	1.2731	0.4931	0.1980
6	2.0494	0.5322	-0.9512
6	1.7023	-0.2596	1.2853
6	3.2373	-0.1834	-1.0161
1	1.7206	1.1313	-1.7870
6	2.8861	-0.9748	1.2204
1	1.1036	-0.2904	2.1858
6	3.6574	-0.9392	0.0666
1	3.8366	-0.1451	-1.9140
1	3.2094	-1.5579	2.0702
1	4.5828	-1.4936	0.0159
8	-0.1951	2.1867	-0.7040

af) Structure **TS-IV** X=H (E^{el} = -577.013182521 hartree; 1 negative frequency = -546.5972)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.1866	0.6839	0.9388
6	-1.9494	0.0773	1.1016
6	-1.3245	-0.5322	0.0221
6	-1.9525	-0.5377	-1.2186
6	-3.1841	0.0739	-1.3823
6	-3.8043	0.6870	-0.3022
1	-3.6696	1.1515	1.7843
1	-1.4592	0.0619	2.0636
1	-1.4744	-1.0209	-2.0600
1	-3.6631	0.0688	-2.3504
1	-4.7673	1.1595	-0.4277
6	0.0031	-1.1943	0.1852
1	0.0507	-2.1575	-0.3265
6	1.2691	-0.4126	0.0912
6	2.4764	-1.0667	-0.3083
6	1.2859	1.0090	0.2302
6	3.6219	-0.3426	-0.5168
1	2.4677	-2.1406	-0.4186
6	2.4473	1.7082	0.0165
1	0.3741	1.5143	0.5064
6	3.6233	1.0477	-0.3546
1	4.5292	-0.8493	-0.8105
1	2.4499	2.7823	0.1287
1	4.5301	1.6096	-0.5184
8	0.5847	-1.1732	1.4266

ag) Structure **V** X=H (E^{el} = -577.017962675 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.1709	0.5857	-0.9856
6	1.9345	-0.0346	-1.0836
6	1.3145	-0.5399	0.0528
6	1.9513	-0.4273	1.2850
6	3.1834	0.1972	1.3820
6	3.7964	0.7070	0.2458
1	3.6483	0.9710	-1.8747
1	1.4440	-0.1428	-2.0394
1	1.4785	-0.8277	2.1712
1	3.6674	0.2838	2.3436
1	4.7591	1.1906	0.3205
6	-0.0038	-1.2099	-0.0288
1	-0.0937	-2.1080	0.5765
6	-1.2957	-0.4784	-0.2652
6	-2.5261	-1.0538	0.2760
6	-1.3001	0.9660	-0.4827
6	-3.5839	-0.2630	0.6110
1	-2.5662	-2.1270	0.3905
6	-2.3825	1.7184	-0.1346
1	-0.4199	1.4173	-0.9122
6	-3.5332	1.1312	0.4237
1	-4.4792	-0.7133	1.0144
1	-2.3580	2.7863	-0.2955
1	-4.3798	1.7447	0.6896
8	-0.6319	-1.2834	-1.2699

ah) Structure **TS-VI** X=H (E^{el} = -577.011265816 hartree; 1 negative frequency = -674.3955)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.1165	0.7481	-0.9227
6	1.8977	0.1064	-1.0602
6	1.3327	-0.5719	0.0230
6	2.0215	-0.5952	1.2399
6	3.2362	0.0507	1.3720
6	3.7890	0.7277	0.2915
1	3.5480	1.2617	-1.7694
1	1.3824	0.1033	-2.0088
1	1.5952	-1.1219	2.0823
1	3.7562	0.0263	2.3182
1	4.7391	1.2301	0.3947
6	0.0587	-1.2495	-0.0832
1	-0.1380	-2.0870	0.5744
6	-1.4315	-0.4613	-0.4728
6	-2.5870	-1.0523	0.1184
6	-1.3833	0.9572	-0.5953
6	-3.5471	-0.2575	0.6957
1	-2.6746	-2.1285	0.1113
6	-2.3616	1.7246	-0.0106
1	-0.5565	1.4106	-1.1177
6	-3.4411	1.1355	0.6540
1	-4.4049	-0.7168	1.1646
1	-2.3005	2.8006	-0.0826
1	-4.2033	1.7521	1.1044
8	-0.6185	-1.2631	-1.2837

ai) Structure **VI** X=H (E^{el} = -577.051888393 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.5811	-1.2248	0.5878
6	-2.2373	-1.0195	0.3532
6	-1.7868	0.2010	-0.1974
6	-2.7480	1.1929	-0.4975
6	-4.0862	0.9720	-0.2552
6	-4.5164	-0.2372	0.2888
1	-3.9090	-2.1637	1.0096
1	-1.5155	-1.7861	0.5878
1	-2.4233	2.1323	-0.9226
1	-4.8054	1.7426	-0.4910
1	-5.5659	-0.4064	0.4761
6	-0.4296	0.4515	-0.4447
1	-0.0690	1.3681	-0.8863
6	1.7837	-0.2177	-0.0913
6	2.7062	-1.1779	-0.4822
6	2.2016	0.9800	0.4697
6	4.0571	-0.9300	-0.3181
1	2.3489	-2.1009	-0.9119
6	3.5605	1.2169	0.6216
1	1.4774	1.7058	0.8059
6	4.4923	0.2699	0.2294
1	4.7743	-1.6768	-0.6248
1	3.8871	2.1477	1.0612
1	5.5473	0.4608	0.3529
8	0.4696	-0.5357	-0.2551

aj) Structure **IV** X=COOH (E^{el} = -954.064526893 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.5471	0.7400	0.7840
6	-2.3878	1.4902	0.8240
6	-1.2729	1.0924	0.0942
6	-1.3340	-0.0477	-0.6977
6	-2.4951	-0.7986	-0.7432
6	-3.6026	-0.4070	0.0002
1	-4.4190	1.0264	1.3516
1	-2.3448	2.3873	1.4241
1	-0.4698	-0.3539	-1.2672
1	-2.5457	-1.6875	-1.3516
6	-0.0121	1.9518	0.1192
1	-0.0522	2.5604	1.0291
6	1.2679	1.1503	0.1081
6	2.0475	1.0660	-1.0366
6	1.6733	0.4938	1.2665
6	3.2180	0.3239	-1.0299
1	1.7357	1.5899	-1.9270
6	2.8382	-0.2467	1.2777
1	1.0708	0.5603	2.1619
6	3.6153	-0.3355	0.1265
1	3.8259	0.2581	-1.9183
1	3.1657	-0.7624	2.1673
8	-0.1803	2.7492	-0.9831
6	4.8548	-1.1361	0.1867
8	5.2428	-1.7214	1.1637
8	5.5278	-1.1575	-0.9674
1	6.3092	-1.6969	-0.8269
6	-4.8647	-1.1781	-0.0099
8	-5.8464	-0.8838	0.6190
8	-4.8182	-2.2551	-0.7974
1	-5.6744	-2.6853	-0.7394

ak) Structure **TS-IV** X=COOH (E^{el} = -954.048067719 hartree; 1 negative frequency = -565.4759)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.1641	0.0667	-1.0944
6	-1.9461	0.7249	-1.1327
6	-1.3085	1.0811	0.0480
6	-1.9014	0.7819	1.2713
6	-3.1123	0.1200	1.3134
6	-3.7480	-0.2401	0.1290
1	-3.6649	-0.2075	-2.0093
1	-1.4821	0.9761	-2.0744
1	-1.4119	1.0674	2.1919
1	-3.5852	-0.1242	2.2522
6	-0.0011	1.8014	0.0152
1	0.0321	2.6272	0.7284
6	1.2819	1.0394	-0.0593
6	2.4774	1.6269	0.4514
6	1.3258	-0.3109	-0.5142
6	3.6417	0.9083	0.4915
1	2.4475	2.6521	0.7876
6	2.4998	-1.0130	-0.4657
1	0.4239	-0.7657	-0.8915
6	3.6673	-0.4181	0.0338
1	4.5449	1.3544	0.8759
1	2.5488	-2.0366	-0.8035
8	0.5500	2.0727	-1.2063
6	-5.0448	-0.9413	0.2245
8	-5.5935	-1.2238	1.2572
8	-5.5711	-1.2441	-0.9654
1	-6.4034	-1.6923	-0.7992
6	4.8974	-1.2274	0.0608
8	4.9702	-2.3683	-0.3166
8	5.9523	-0.5709	0.5532
1	6.6975	-1.1753	0.5288

al) Structure **V** X=COOH (E^{el} = -954.055337438 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.1337	0.2301	-1.0341
6	-1.9315	0.9154	-1.0031
6	-1.2645	1.1018	0.2023
6	-1.8174	0.6047	1.3801
6	-3.0131	-0.0845	1.3507
6	-3.6755	-0.2755	0.1420
1	-3.6564	0.0893	-1.9669
1	-1.5058	1.3216	-1.9080
1	-1.3065	0.7564	2.3203
1	-3.4527	-0.4812	2.2528
6	0.0177	1.8381	0.2576
1	0.1087	2.5337	1.0868
6	1.3241	1.2650	-0.2314
6	2.5542	1.7219	0.4124
6	1.3616	-0.0646	-0.8336
6	3.6314	0.9054	0.5233
1	2.5725	2.7315	0.7949
6	2.4591	-0.8557	-0.7072
1	0.4885	-0.4070	-1.3657
6	3.6059	-0.4011	-0.0171
1	4.5347	1.2370	1.0116
1	2.4677	-1.8424	-1.1424
8	0.5807	2.2768	-0.9358
6	-4.9539	-1.0149	0.1614
8	-5.4658	-1.4668	1.1519
8	-5.5087	-1.1436	-1.0472
1	-6.3267	-1.6321	-0.9307
6	4.8013	-1.2337	0.1382
8	5.8041	-0.8881	0.7125
8	4.6859	-2.4430	-0.4232
1	5.5127	-2.9045	-0.2671

am) Structure **TS-VI** X=COOH (E^{el} = -954.049190374 hartree; 1 negative frequency = -661.2515)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.0636	0.1903	-1.0232
6	-1.8828	0.9046	-0.9750
6	-1.2609	1.1563	0.2518
6	-1.8534	0.6817	1.4282
6	-3.0286	-0.0351	1.3774
6	-3.6400	-0.2877	0.1509
1	-3.5486	0.0044	-1.9684
1	-1.4424	1.2948	-1.8797
1	-1.3815	0.8772	2.3804
1	-3.4939	-0.4098	2.2760
6	-0.0245	1.8977	0.3364
1	0.2014	2.4281	1.2525
6	1.4571	1.3856	-0.4006
6	2.6273	1.7680	0.3199
6	1.4322	0.1127	-1.0388
6	3.6366	0.8659	0.5139
1	2.6862	2.7721	0.7120
6	2.4573	-0.7722	-0.8334
1	0.5876	-0.1503	-1.6547
6	3.5614	-0.4199	-0.0425
1	4.5178	1.1316	1.0773
1	2.4275	-1.7467	-1.2944
8	0.5693	2.3884	-0.8033
6	-4.8983	-1.0573	0.1485
8	-5.4399	-1.4840	1.1350
8	-5.4006	-1.2471	-1.0755
1	-6.2104	-1.7516	-0.9716
6	4.6763	-1.3430	0.1981
8	5.6501	-1.0838	0.8599
8	4.5194	-2.5331	-0.3938
1	5.2938	-3.0568	-0.1771

an) Structure **VI** X=COOH (E^{el} = -954.089757629 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.6500	-1.0186	0.3383
6	-2.2975	-0.8790	0.1346
6	-1.7695	0.3368	-0.3592
6	-2.6660	1.3972	-0.6367
6	-4.0134	1.2463	-0.4282
6	-4.5226	0.0383	0.0608
1	-4.0476	-1.9475	0.7155
1	-1.6256	-1.6943	0.3508
1	-2.2799	2.3319	-1.0171
1	-4.7027	2.0499	-0.6369
6	-0.4008	0.5194	-0.5741
1	0.0171	1.4331	-0.9681
6	1.7666	-0.2938	-0.2267
6	2.6167	-1.3280	-0.5970
6	2.2656	0.8806	0.3225
6	3.9780	-1.1806	-0.4301
1	2.1943	-2.2279	-1.0156
6	3.6320	1.0190	0.4797
1	1.5971	1.6621	0.6475
6	4.4952	-0.0026	0.1041
1	4.6473	-1.9754	-0.7186
1	4.0480	1.9184	0.9072
8	0.4390	-0.5184	-0.4005
6	5.9415	0.2038	0.2971
8	6.4358	1.2026	0.7517
8	6.6801	-0.8424	-0.0865
1	7.5977	-0.6130	0.0765
6	-5.9734	-0.0709	0.2654
8	-6.7663	0.8094	0.0442
8	-6.3573	-1.2654	0.7320
1	-7.3113	-1.2320	0.8295

ao) Structure **IV** X=CHO (E^{el} = -803.599673275 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.5715	0.4391	0.6235
6	-2.4253	1.1995	0.7337
6	-1.2646	0.8198	0.0633
6	-1.2651	-0.3116	-0.7421
6	-2.4169	-1.0712	-0.8562
6	-3.5693	-0.7027	-0.1736
1	-4.4781	0.7100	1.1432
1	-2.4232	2.0924	1.3418
1	-0.3667	-0.6013	-1.2655
1	-2.4206	-1.9559	-1.4781
6	-0.0193	1.6959	0.1697
1	-0.1109	2.2789	1.0926
6	1.2731	0.9145	0.1969
6	2.1016	0.8664	-0.9193
6	1.6390	0.2424	1.3577
6	3.2800	0.1439	-0.8790
1	1.8155	1.4056	-1.8093
6	2.8171	-0.4804	1.3985
1	0.9989	0.2825	2.2283
6	3.6423	-0.5347	0.2800
1	3.9366	0.0962	-1.7350
1	3.1013	-1.0040	2.3012
8	-0.1503	2.5205	-0.9172
6	4.8957	-1.3053	0.3354
8	5.6698	-1.4130	-0.5798
1	5.0971	-1.8008	1.3002
6	-4.7869	-1.5246	-0.3004
8	-5.8240	-1.2887	0.2614
1	-4.6933	-2.4008	-0.9632

ap) Structure **TS-IV** X=CHO (E^{el} = -803.584165330 hartree; 1 negative frequency = -569.1363)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.2225	-0.1224	-0.9443
6	-1.9984	0.5103	-1.0511
6	-1.3149	0.9066	0.0947
6	-1.8702	0.6754	1.3482
6	-3.0924	0.0369	1.4551
6	-3.7729	-0.3653	0.3107
1	-3.7709	-0.4339	-1.8207
1	-1.5592	0.7135	-2.0161
1	-1.3454	0.9936	2.2382
1	-3.5246	-0.1480	2.4292
6	0.0060	1.5956	-0.0133
1	0.0813	2.4491	0.6631
6	1.2685	0.7993	-0.0881
6	2.4926	1.3807	0.3624
6	1.2659	-0.5652	-0.4953
6	3.6379	0.6385	0.3984
1	2.4922	2.4188	0.6587
6	2.4287	-1.2907	-0.4539
1	0.3431	-1.0110	-0.8307
6	3.6227	-0.7078	-0.0090
1	4.5707	1.0623	0.7381
1	2.4262	-2.3274	-0.7612
8	0.5176	1.8053	-1.2629
6	4.8511	-1.5050	0.0321
8	5.9177	-1.0848	0.4085
1	4.7483	-2.5475	-0.3098
6	-5.0755	-1.0408	0.4377
8	-5.7341	-1.4288	-0.4917
1	-5.4310	-1.1794	1.4728

aq) Structure **V** X=CHO (E^{el} = -803.592206106 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.1297	0.0702	-0.9342
6	1.9349	-0.6207	-0.9839
6	1.2624	-0.9407	0.1939
6	1.8033	-0.5715	1.4214
6	2.9965	0.1258	1.4691
6	3.6646	0.4503	0.2935
1	3.6684	0.3223	-1.8354
1	1.5143	-0.9316	-1.9282
1	1.2882	-0.8274	2.3364
1	3.4151	0.4186	2.4224
6	-0.0124	-1.6913	0.1606
1	-0.1000	-2.4739	0.9087
6	-1.3213	-1.0836	-0.2759
6	-2.5492	-1.6265	0.3038
6	-1.3720	0.3053	-0.7303
6	-3.6381	-0.8380	0.4921
1	-2.5553	-2.6727	0.5710
6	-2.4766	1.0612	-0.5272
1	-0.4986	0.7118	-1.2153
6	-3.6285	0.5202	0.0999
1	-4.5344	-1.2517	0.9339
1	-2.5120	2.0922	-0.8452
8	-0.5627	-2.0050	-1.0774
6	4.9375	1.1877	0.3579
8	5.5862	1.5096	-0.6032
1	5.2801	1.4405	1.3755
6	-4.8054	1.3471	0.3128
8	-4.8807	2.5151	0.0011
1	-5.6596	0.8414	0.7910

ar) Structure **TS-VI** X=CHO (E^{el} = -803.585697975 hartree; 1 negative frequency = -669.3700)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	2.9916	-0.0652	-1.2200
6	1.8158	-0.7757	-1.0767
6	1.2748	-0.9777	0.1966
6	1.9413	-0.4597	1.3171
6	3.1095	0.2512	1.1674
6	3.6433	0.4560	-0.1060
1	3.4151	0.0833	-2.2042
1	1.3188	-1.1992	-1.9359
1	1.5275	-0.6199	2.3026
1	3.6317	0.6588	2.0199
6	0.0475	-1.7112	0.3888
1	-0.1235	-2.1998	1.3395
6	-1.4821	-1.2261	-0.2786
6	-2.6041	-1.5775	0.5270
6	-1.4938	0.0214	-0.9699
6	-3.6010	-0.6629	0.7398
1	-2.6377	-2.5644	0.9630
6	-2.5033	0.9130	-0.7435
1	-0.6858	0.2536	-1.6447
6	-3.5630	0.5972	0.1258
1	-4.4412	-0.9215	1.3698
1	-2.5173	1.8721	-1.2388
8	-0.6183	-2.2456	-0.6891
6	4.8933	1.2102	-0.2774
8	5.5268	1.6911	0.6271
1	5.2356	1.3175	-1.3203
6	-4.6391	1.5559	0.3593
8	-4.6925	2.6564	-0.1365
1	-5.4353	1.2111	1.0398

as) Structure **VI** X=CHO (E^{el} = -803.625831075 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.6527	-0.9911	0.2918
6	-2.3038	-0.8287	0.1097
6	-1.7820	0.4220	-0.3091
6	-2.6839	1.4902	-0.5334
6	-4.0326	1.3114	-0.3456
6	-4.5367	0.0737	0.0679
1	-4.0615	-1.9381	0.6109
1	-1.6234	-1.6474	0.2832
1	-2.3021	2.4482	-0.8559
1	-4.7147	2.1325	-0.5192
6	-0.4152	0.6277	-0.5002
1	-0.0013	1.5679	-0.8319
6	1.7551	-0.1848	-0.1740
6	2.6226	-1.1821	-0.6117
6	2.2300	0.9493	0.4695
6	3.9767	-1.0339	-0.4154
1	2.2122	-2.0506	-1.1027
6	3.5955	1.0859	0.6555
1	1.5469	1.6954	0.8433
6	4.4756	0.1062	0.2159
1	4.6729	-1.7886	-0.7488
1	3.9786	1.9625	1.1598
8	0.4332	-0.4103	-0.3839
6	5.9200	0.2726	0.4255
8	6.7549	-0.5231	0.0793
1	6.2131	1.2044	0.9384
6	-5.9757	-0.1000	0.2627
8	-6.4995	-1.1282	0.6181
1	-6.5868	0.7956	0.0597

at) Structure **IV** X=CF_3 (E^{el} = -1250.93109739 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.5668	0.8958	0.7709
6	-2.4005	1.6317	0.8514
6	-1.2687	1.2316	0.1493
6	-1.3220	0.1034	-0.6562
6	-2.4901	-0.6369	-0.7412
6	-3.6079	-0.2405	-0.0264
1	-4.4426	1.2041	1.3214
1	-2.3674	2.5227	1.4611
1	-0.4484	-0.2063	-1.2092
1	-2.5302	-1.5165	-1.3638
6	-0.0046	2.0835	0.2204
1	-0.0360	2.6322	1.1682
6	1.2749	1.2846	0.1463
6	2.0480	1.2799	-1.0042
6	1.6872	0.5463	1.2507
6	3.2190	0.5383	-1.0571
1	1.7318	1.8629	-1.8554
6	2.8515	-0.1955	1.2034
1	1.0903	0.5452	2.1523
6	3.6173	-0.2000	0.0441
1	3.8173	0.5348	-1.9548
1	3.1641	-0.7720	2.0606
8	-0.1783	2.9534	-0.8249
6	-4.8706	-1.0440	-0.0747
6	4.9003	-0.9688	0.0183
9	5.3183	-1.2110	-1.2241
9	4.7858	-2.1471	0.6363
9	5.8853	-0.3077	0.6378
9	-4.8571	-1.9498	-1.0507
9	-5.9408	-0.2686	-0.2646
9	-5.0754	-1.7036	1.0707

au) Structure **TS-IV** X=CF_3 (E^{el} = -1250.91348857 hartree; 1 negative frequency = -561.2753)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.1420	0.2664	-1.1290
6	-1.9333	0.9444	-1.1001
6	-1.3092	1.2076	0.1104
6	-1.9069	0.7942	1.2963
6	-3.1079	0.1111	1.2722
6	-3.7241	-0.1532	0.0558
1	-3.6269	0.0623	-2.0708
1	-1.4673	1.2800	-2.0141
1	-1.4293	1.0029	2.2433
1	-3.5651	-0.2180	2.1927
6	-0.0119	1.9450	0.1496
1	0.0060	2.7124	0.9253
6	1.2826	1.2146	0.0117
6	2.4702	1.7704	0.5773
6	1.3479	-0.0952	-0.5477
6	3.6434	1.0659	0.5589
1	2.4287	2.7636	0.9974
6	2.5338	-0.7847	-0.5569
1	0.4546	-0.5315	-0.9649
6	3.6860	-0.2136	-0.0098
1	4.5394	1.4960	0.9788
1	2.5790	-1.7727	-0.9873
8	0.5486	2.3157	-1.0426
6	4.9636	-0.9879	0.0287
6	-5.0478	-0.8507	0.0416
9	5.0008	-1.9426	-0.8999
9	5.1388	-1.5897	1.2119
9	6.0255	-0.2026	-0.1610
9	-5.3044	-1.4199	-1.1363
9	-5.1138	-1.8086	0.9695
9	-6.0551	-0.0062	0.2922

av) Structure **V** X=CF_3 (E^{el} = -1250.91934711 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.1236	0.4132	-1.0769
6	-1.9220	1.1001	-1.0024
6	-1.2761	1.2502	0.2171
6	-1.8506	0.7162	1.3676
6	-3.0450	0.0269	1.2965
6	-3.6812	-0.1251	0.0706
1	-3.6278	0.3045	-2.0241
1	-1.4837	1.5348	-1.8878
1	-1.3597	0.8396	2.3225
1	-3.4865	-0.3875	2.1901
6	0.0045	1.9860	0.3162
1	0.0787	2.6604	1.1646
6	1.3178	1.4270	-0.1659
6	2.5396	1.8695	0.5016
6	1.3693	0.1155	-0.8056
6	3.6304	1.0592	0.5866
1	2.5492	2.8640	0.9213
6	2.4762	-0.6664	-0.7015
1	0.5014	-0.2228	-1.3484
6	3.6130	-0.2214	0.0051
1	4.5186	1.4003	1.0948
1	2.4898	-1.6406	-1.1664
8	0.5841	2.4587	-0.8566
6	-4.9611	-0.8974	0.0102
6	4.8213	-1.0933	0.0522
9	-4.7562	-2.2066	0.1955
9	-5.5795	-0.7618	-1.1620
9	-5.8180	-0.5100	0.9592
9	5.4883	-1.0837	-1.1094
9	4.5024	-2.3682	0.2937
9	5.6822	-0.7122	0.9961

aw) Structure **TS-VI** X=CF_3 (E^{el} = -1250.91339274 hartree; 1 negative frequency = -662.0426)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.0501	0.4253	-1.0472
6	-1.8734	1.1448	-0.9414
6	-1.2571	1.3110	0.3000
6	-1.8512	0.7478	1.4346
6	-3.0218	0.0280	1.3279
6	-3.6227	-0.1363	0.0839
1	-3.5286	0.3091	-2.0069
1	-1.4357	1.6037	-1.8146
1	-1.3872	0.8770	2.4017
1	-3.4746	-0.4036	2.2075
6	-0.0238	2.0532	0.4424
1	0.1891	2.5284	1.3914
6	1.4582	1.6027	-0.3225
6	2.6287	1.9429	0.4166
6	1.4469	0.3783	-1.0509
6	3.6493	1.0362	0.5477
1	2.6852	2.9188	0.8742
6	2.4810	-0.5092	-0.9081
1	0.6078	0.1515	-1.6879
6	3.5800	-0.2011	-0.0979
1	4.5234	1.2902	1.1267
1	2.4582	-1.4460	-1.4434
8	0.5671	2.6264	-0.6611
6	4.6657	-1.2081	0.0787
6	-4.8759	-0.9459	-0.0140
9	-5.4759	-0.8098	-1.1959
9	-5.7625	-0.6012	0.9244
9	-4.6350	-2.2517	0.1539
9	4.3471	-2.1310	0.9970
9	4.9184	-1.8731	-1.0519
9	5.8103	-0.6508	0.4773

ax) Structure **VI** X=CF_3 (E^{el} = -1250.95446513 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.6491	-0.9974	0.3423
6	-2.2957	-0.8693	0.1252
6	-1.7638	0.3340	-0.3892
6	-2.6554	1.3935	-0.6719
6	-4.0052	1.2554	-0.4498
6	-4.5112	0.0601	0.0600
1	-4.0446	-1.9190	0.7406
1	-1.6290	-1.6864	0.3502
1	-2.2693	2.3225	-1.0656
1	-4.6744	2.0740	-0.6647
6	-0.3923	0.5047	-0.6149
1	0.0308	1.4081	-1.0267
6	1.7666	-0.3245	-0.2612
6	2.6143	-1.3583	-0.6379
6	2.2708	0.8390	0.2992
6	3.9752	-1.2186	-0.4635
1	2.1916	-2.2546	-1.0637
6	3.6403	0.9721	0.4640
1	1.6062	1.6209	0.6311
6	4.4926	-0.0500	0.0836
1	4.6381	-2.0193	-0.7536
1	4.0394	1.8712	0.9065
8	0.4376	-0.5419	-0.4383
6	5.9725	0.1025	0.2221
6	-5.9823	-0.1051	0.2488
9	6.5530	0.4075	-0.9453
9	6.3012	1.0685	1.0803
9	6.5502	-1.0236	0.6488
9	-6.5833	1.0510	0.5412
9	-6.2695	-0.9621	1.2310
9	-6.5797	-0.5759	-0.8548

ay) Structure **IV** X=CN (E^{el} = -761.437434225 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.5560	0.4730	0.7746
6	-2.3962	1.2193	0.8547
6	-1.2678	0.8445	0.1347
6	-1.3142	-0.2714	-0.6919
6	-2.4709	-1.0228	-0.7819
6	-3.5935	-0.6529	-0.0453
1	-4.4305	0.7547	1.3400
1	-2.3670	2.0985	1.4812
1	-0.4414	-0.5608	-1.2570
1	-2.5099	-1.8936	-1.4174
6	-0.0114	1.7071	0.2078
1	-0.0530	2.2634	1.1506
6	1.2736	0.9154	0.1495
6	2.0566	0.9109	-0.9961
6	1.6811	0.1882	1.2630
6	3.2313	0.1792	-1.0369
1	1.7441	1.4893	-1.8518
6	2.8500	-0.5460	1.2334
1	1.0779	0.1917	2.1602
6	3.6298	-0.5530	0.0774
1	3.8426	0.1754	-1.9260
1	3.1660	-1.1117	2.0960
8	-0.1843	2.5654	-0.8468
6	4.8427	-1.3090	0.0398
7	5.8192	-1.9191	0.0097
6	-4.7901	-1.4312	-0.1304
7	-5.7540	-2.0577	-0.1977

az) Structure **TS-IV** X=CN (E^{el} = -761.421518941 hartree; 1 negative frequency = -567.4169)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.1622	-0.0753	-1.1131
6	-1.9450	0.5829	-1.1067
6	-1.3152	0.8776	0.0950
6	-1.9164	0.5166	1.2963
6	-3.1275	-0.1471	1.3009
6	-3.7541	-0.4452	0.0915
1	-3.6579	-0.3016	-2.0443
1	-1.4758	0.8822	-2.0315
1	-1.4350	0.7542	2.2345
1	-3.5944	-0.4328	2.2306
6	-0.0076	1.5993	0.1053
1	0.0175	2.3960	0.8511
6	1.2748	0.8400	0.0140
6	2.4669	1.4066	0.5546
6	1.3225	-0.4887	-0.4983
6	3.6324	0.6921	0.5669
1	2.4354	2.4152	0.9369
6	2.4952	-1.1940	-0.4808
1	0.4233	-0.9294	-0.8981
6	3.6620	-0.6162	0.0497
1	4.5342	1.1221	0.9736
1	2.5317	-2.2005	-0.8672
8	0.5509	1.9200	-1.1007
6	4.8754	-1.3567	0.0678
7	5.8605	-1.9569	0.0843
6	-5.0104	-1.1278	0.0902
7	-6.0219	-1.6788	0.0898

ba) Structure **V** X=CN (E^{el} = -761.429110241 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.1444	-0.0712	-1.0630
6	1.9372	-0.7416	-0.9901
6	1.2823	-0.8763	0.2288
6	1.8545	-0.3428	1.3800
6	3.0565	0.3336	1.3159
6	3.7054	0.4724	0.0898
1	3.6579	0.0300	-2.0065
1	1.4980	-1.1764	-1.8750
1	1.3551	-0.4539	2.3318
1	3.4985	0.7530	2.2062
6	-0.0073	-1.5960	0.3239
1	-0.0951	-2.2648	1.1752
6	-1.3099	-1.0252	-0.1716
6	-2.5410	-1.4500	0.4936
6	-1.3410	0.2843	-0.8189
6	-3.6147	-0.6271	0.5809
1	-2.5661	-2.4454	0.9107
6	-2.4296	1.0870	-0.7184
1	-0.4694	0.6031	-1.3677
6	-3.5809	0.6637	-0.0065
1	-4.5120	-0.9503	1.0855
1	-2.4338	2.0584	-1.1881
8	-0.5864	-2.0665	-0.8503
6	4.9520	1.1683	0.0177
7	5.9560	1.7298	-0.0406
6	-4.7044	1.5164	0.0951
7	-5.6223	2.2136	0.1817

bb) Structure **TS-VI** X=CN (E^{el} = -761.422299275 hartree; 1 negative frequency = -674.2525)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.0782	-0.0192	-1.0593
6	1.8923	-0.7177	-0.9652
6	1.2858	-0.9177	0.2791
6	1.9010	-0.4071	1.4278
6	3.0825	0.2956	1.3380
6	3.6775	0.4958	0.0905
1	3.5515	0.1266	-2.0179
1	1.4362	-1.1362	-1.8490
1	1.4431	-0.5620	2.3939
1	3.5532	0.6917	2.2241
6	0.0428	-1.6403	0.4069
1	-0.1777	-2.1367	1.3431
6	-1.4446	-1.1357	-0.3335
6	-2.6116	-1.4812	0.4090
6	-1.4142	0.1139	-1.0159
6	-3.6122	-0.5654	0.5853
1	-2.6795	-2.4713	0.8334
6	-2.4253	1.0172	-0.8316
1	-0.5765	0.3471	-1.6526
6	-3.5270	0.7029	-0.0161
1	-4.4848	-0.8186	1.1671
1	-2.3908	1.9752	-1.3267
8	-0.5720	-2.1599	-0.7089
6	4.9033	1.2210	-0.0072
7	5.8924	1.8069	-0.0860
6	-4.5690	1.6503	0.1708
7	-5.4145	2.4201	0.3267

bc) Structure **VI** X=CN (E^{el} = -761.462738527 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.6299	-1.0677	-0.4217
6	2.2822	-0.9147	-0.2061
6	1.7700	0.3003	0.3074
6	2.6793	1.3471	0.5917
6	4.0243	1.1894	0.3729
6	4.5166	-0.0208	-0.1364
1	4.0156	-1.9961	-0.8138
1	1.6018	-1.7211	-0.4279
1	2.3074	2.2810	0.9873
1	4.7110	1.9922	0.5918
6	0.4054	0.4928	0.5346
1	-0.0019	1.4048	0.9435
6	-1.7685	-0.2992	0.1841
6	-2.6295	-1.3226	0.5590
6	-2.2560	0.8774	-0.3681
6	-3.9886	-1.1634	0.3940
1	-2.2184	-2.2263	0.9802
6	-3.6209	1.0346	-0.5264
1	-1.5805	1.6513	-0.6964
6	-4.4941	0.0204	-0.1450
1	-4.6661	-1.9503	0.6863
1	-4.0118	1.9427	-0.9582
8	-0.4436	-0.5370	0.3555
6	-5.9025	0.1886	-0.3109
7	-7.0387	0.3241	-0.4441
6	5.9122	-0.1847	-0.3630
7	7.0434	-0.3166	-0.5464

bd) Structure **IV** X=NO_2 (E^{el} = -985.870430523 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.5469	0.6744	0.7979
6	-2.3858	1.4217	0.8616
6	-1.2699	1.0517	0.1194
6	-1.3253	-0.0602	-0.7129
6	-2.4817	-0.8147	-0.7902
6	-3.5711	-0.4339	-0.0291
1	-4.4218	0.9341	1.3706
1	-2.3474	2.2971	1.4926
1	-0.4612	-0.3443	-1.2935
1	-2.5498	-1.6837	-1.4235
6	-0.0125	1.9138	0.1756
1	-0.0526	2.4870	1.1081
6	1.2700	1.1165	0.1332
6	2.0612	1.1022	-1.0073
6	1.6645	0.3974	1.2575
6	3.2350	0.3675	-1.0345
1	1.7570	1.6747	-1.8696
6	2.8317	-0.3406	1.2459
1	1.0534	0.4101	2.1491
6	3.5985	-0.3432	0.0931
1	3.8661	0.3416	-1.9076
1	3.1558	-0.9059	2.1040
8	-0.1799	2.7567	-0.8923
7	4.8319	-1.1172	0.0715
8	5.1271	-1.7257	1.0739
8	5.4830	-1.1039	-0.9471
7	-4.7916	-1.2289	-0.1012
8	-5.7268	-0.8769	0.5787
8	-4.7894	-2.1882	-0.8360

be) Structure **TS-IV** X=NO_2 (E^{el} = -985.853727787 hartree; 1 negative frequency = -573.6945)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.1558	0.0659	-1.1252
6	-1.9398	0.7273	-1.1413
6	-1.3072	1.0578	0.0502
6	-1.9006	0.7317	1.2660
6	-3.1105	0.0658	1.2977
6	-3.7176	-0.2561	0.0959
1	-3.6697	-0.1978	-2.0349
1	-1.4754	1.0004	-2.0764
1	-1.4150	0.9981	2.1939
1	-3.5884	-0.2017	2.2255
6	-0.0025	1.7841	0.0349
1	0.0238	2.6019	0.7570
6	1.2836	1.0250	-0.0387
6	2.4734	1.6121	0.4853
6	1.3319	-0.3177	-0.5131
6	3.6413	0.9001	0.5236
1	2.4399	2.6324	0.8346
6	2.5057	-1.0229	-0.4722
1	0.4346	-0.7704	-0.9032
6	3.6474	-0.4108	0.0443
1	4.5512	1.3245	0.9141
1	2.5653	-2.0396	-0.8234
8	0.5540	2.0684	-1.1800
7	4.8835	-1.1646	0.0905
8	4.8644	-2.2973	-0.3358
8	5.8573	-0.6139	0.5533
7	-4.9961	-0.9539	0.1208
8	-5.4686	-1.2156	1.2025
8	-5.5039	-1.2282	-0.9414

bf) Structure **V** X=NO_2 (E^{el} = -985.861584371 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.1316	0.2480	-1.0572
6	-1.9282	0.9273	-0.9974
6	-1.2630	1.0694	0.2158
6	-1.8171	0.5364	1.3768
6	-3.0154	-0.1487	1.3301
6	-3.6524	-0.2824	0.1086
1	-3.6691	0.1289	-1.9835
1	-1.5020	1.3630	-1.8880
1	-1.3076	0.6547	2.3222
1	-3.4609	-0.5748	2.2137
6	0.0206	1.8005	0.2960
1	0.1155	2.4679	1.1473
6	1.3264	1.2367	-0.2148
6	2.5558	1.6698	0.4461
6	1.3551	-0.0748	-0.8561
6	3.6291	0.8455	0.5464
1	2.5812	2.6697	0.8519
6	2.4416	-0.8816	-0.7457
1	0.4853	-0.3943	-1.4070
6	3.5687	-0.4354	-0.0323
1	4.5340	1.1513	1.0448
1	2.4664	-1.8581	-1.2002
8	0.5862	2.2710	-0.8821
7	-4.9181	-1.0003	0.0512
8	-5.3567	-1.4426	1.0874
8	-5.4501	-1.1092	-1.0290
7	4.7077	-1.3034	0.0823
8	5.6699	-0.8909	0.6961
8	4.6372	-2.3968	-0.4393

bg) Structure **TS-VI** X=NO_2 (E^{el} = -985.855858653 hartree; 1 negative frequency = -649.6796)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.0640	0.2020	-1.0517
6	-1.8817	0.9098	-0.9762
6	-1.2615	1.1197	0.2598
6	-1.8542	0.6125	1.4219
6	-3.0324	-0.0996	1.3551
6	-3.6194	-0.2969	0.1150
1	-3.5648	0.0361	-1.9913
1	-1.4407	1.3270	-1.8681
1	-1.3832	0.7769	2.3799
1	-3.5029	-0.5018	2.2369
6	-0.0233	1.8564	0.3671
1	0.2010	2.3636	1.2966
6	1.4555	1.3536	-0.3769
6	2.6240	1.7146	0.3581
6	1.4249	0.0958	-1.0463
6	3.6307	0.8069	0.5399
1	2.6879	2.7095	0.7712
6	2.4407	-0.8016	-0.8594
1	0.5846	-0.1472	-1.6757
6	3.5260	-0.4530	-0.0529
1	4.5123	1.0493	1.1100
1	2.4284	-1.7686	-1.3345
8	0.5750	2.3700	-0.7586
7	4.5892	-1.4059	0.1396
8	5.5240	-1.0726	0.8367
8	4.4844	-2.4843	-0.4046
7	-4.8630	-1.0445	0.0376
8	-5.3329	-1.4568	1.0732
8	-5.3504	-1.2080	-1.0575

bh) Structure **VI** X=NO_2 (E^{el} = -985.896899626 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.6386	-1.0494	-0.3655
6	2.2887	-0.9001	-0.1600
6	1.7689	0.3163	0.3432
6	2.6687	1.3714	0.6293
6	4.0168	1.2214	0.4223
6	4.4917	0.0104	-0.0737
1	4.0515	-1.9681	-0.7482
1	1.6136	-1.7107	-0.3824
1	2.2880	2.3049	1.0167
1	4.7133	2.0153	0.6353
6	0.4018	0.5043	0.5596
1	-0.0116	1.4176	0.9593
6	-1.7681	-0.3031	0.2153
6	-2.6133	-1.3442	0.5807
6	-2.2703	0.8771	-0.3187
6	-3.9752	-1.2014	0.4254
1	-2.1879	-2.2479	0.9871
6	-3.6372	1.0216	-0.4691
1	-1.6057	1.6625	-0.6410
6	-4.4703	-0.0151	-0.0928
1	-4.6581	-1.9870	0.7034
1	-4.0615	1.9209	-0.8845
8	-0.4407	-0.5280	0.3779
7	-5.9044	0.1409	-0.2524
8	-6.3076	1.1907	-0.6986
8	-6.6074	-0.7887	0.0713
7	5.9104	-0.1498	-0.2914
8	6.6295	0.7904	-0.0304
8	6.2978	-1.2144	-0.7220

bi) Structure **VII** X=H see a)

bj) Structure **TS-VII** X=H see b)

bk) Structure **VIII** X=H see c)

bl) Structure **TS-IX** X=H see d)

bm) Structure **IX** X=H see e)

bn) Structure **VII** X=NO_2 (E^{el} = -1025.18154347 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	3.4436	0.4656	-0.8428
6	2.3080	1.2565	-0.8325
6	1.2673	0.9825	0.0468
6	1.3844	-0.0823	0.9388
6	2.5177	-0.8720	0.9491
6	3.5291	-0.5843	0.0511
1	4.2559	0.6535	-1.5253
1	2.2426	2.0806	-1.5239
1	0.5787	-0.2976	1.6238
1	2.6263	-1.6986	1.6315
6	0.0005	1.8402	0.1148
6	-1.2474	0.9688	0.0525
6	-2.1794	1.0116	1.0808
6	-1.4813	0.1509	-1.0502
6	-3.3357	0.2520	1.0151
1	-1.9934	1.6393	1.9381
6	-2.6292	-0.6127	-1.1315
1	-0.7556	0.0971	-1.8488
6	-3.5416	-0.5472	-0.0925
1	-4.0705	0.2715	1.8031
1	-2.8255	-1.2541	-1.9747
8	0.1522	2.4440	1.3463
7	-4.7542	-1.3487	-0.1699
8	-4.9086	-2.0354	-1.1534
8	-5.5320	-1.2782	0.7532
7	4.7262	-1.4161	0.0462
8	5.5908	-1.1449	-0.7538
8	4.7775	-2.3237	0.8424
6	-0.0697	2.9299	-0.9520
1	0.7804	3.6004	-0.8645
1	-0.1025	2.5019	-1.9508
1	-0.9777	3.5084	-0.8042

bo) Structure **TS-VII** X= NO_2 (E^{el} = -1025.16657789 hartree; 1 negative frequency = -557.3822)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.2157	0.0431	-1.1430
6	-2.0165	0.7336	-1.1870
6	-1.2768	0.9340	-0.0287
6	-1.7418	0.4300	1.1829
6	-2.9329	-0.2680	1.2417
6	-3.6529	-0.4462	0.0731
1	-3.8078	-0.1207	-2.0283
1	-1.6411	1.1179	-2.1228
1	-1.1679	0.5713	2.0869
1	-3.3086	-0.6729	2.1669
6	0.0025	1.7267	-0.0928
6	1.2827	0.9352	-0.1206
6	2.5219	1.5057	0.2980
6	1.2654	-0.4479	-0.4744
6	3.6581	0.7433	0.3596
1	2.5683	2.5489	0.5588
6	2.4062	-1.2030	-0.4135
1	0.3385	-0.8925	-0.7979
6	3.5928	-0.6034	0.0052
1	4.5993	1.1612	0.6759
1	2.4050	-2.2474	-0.6775
8	0.5352	1.8747	-1.3482
7	4.7965	-1.4053	0.0768
8	4.7117	-2.5711	-0.2378
8	5.8116	-0.8592	0.4475
7	-4.9112	-1.1774	0.1279
8	-5.2713	-1.5901	1.2061
8	-5.5171	-1.3260	-0.9076
6	-0.0673	2.9908	0.7365
1	-0.9512	3.5527	0.4433
1	-0.1437	2.7690	1.7980
1	0.7984	3.6200	0.5615

bp) Structure **VIII** X= NO_2 (E^{el} = -1025.17465638 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.1960	0.1887	-1.0770
6	-2.0077	0.8973	-1.0777
6	-1.2296	0.9699	0.0727
6	-1.6500	0.3205	1.2307
6	-2.8307	-0.3971	1.2437
6	-3.5868	-0.4482	0.0859
1	-3.8170	0.1238	-1.9554
1	-1.6730	1.3984	-1.9727
1	-1.0484	0.3625	2.1263
1	-3.1703	-0.9140	2.1260
6	0.0317	1.7701	0.0703
6	1.3144	1.1099	-0.4088
6	2.6079	1.5756	0.0902
6	1.2644	-0.2855	-0.8476
6	3.6454	0.7186	0.2720
1	2.7307	2.6244	0.3021
6	2.3139	-1.1254	-0.6585
1	0.3586	-0.6375	-1.3137
6	3.4944	-0.6359	-0.0726
1	4.5939	1.0564	0.6554
1	2.2695	-2.1590	-0.9591
8	0.5577	2.0493	-1.1911
7	-4.8344	-1.1991	0.0935
8	-5.1535	-1.7419	1.1257
8	-5.4729	-1.2323	-0.9326
7	4.5957	-1.5339	0.1335
8	5.6078	-1.0802	0.6270
8	4.4468	-2.6927	-0.1949
6	0.0591	2.8933	1.0711
1	-0.8199	3.5187	0.9273
1	0.0387	2.5130	2.0893
1	0.9381	3.5147	0.9475

bq) Structure **TS-IX** X= NO_2 (E^{el} = -1025.16907343 hartree; 1 negative frequency = -609.8892)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.0510	-0.0394	-1.1220
6	-1.8813	0.6938	-1.1422
6	-1.2376	1.0418	0.0490
6	-1.7948	0.6379	1.2664
6	-2.9586	-0.1027	1.2975
6	-3.5707	-0.4312	0.0996
1	-3.5668	-0.3051	-2.0301
1	-1.4656	1.0234	-2.0814
1	-1.3112	0.8953	2.1959
1	-3.3966	-0.4289	2.2263
6	-0.0132	1.8397	0.0272
6	1.4206	1.1321	-0.6595
6	2.6580	1.5837	-0.1092
6	1.3101	-0.2421	-1.0327
6	3.6408	0.6877	0.2138
1	2.8122	2.6391	0.0414
6	2.2995	-1.1278	-0.7064
1	0.4247	-0.5785	-1.5458
6	3.4484	-0.6669	-0.0602
1	4.5724	1.0095	0.6492
1	2.2179	-2.1737	-0.9524
8	0.5473	2.0756	-1.2136
7	4.4847	-1.6047	0.2835
8	5.4776	-1.1722	0.8304
8	4.3024	-2.7720	0.0092
7	-4.8002	-1.2059	0.1267
8	-5.2396	-1.5204	1.2090
8	-5.3073	-1.4876	-0.9348
6	0.2116	2.8623	1.0981
1	-0.7163	3.3947	1.3027
1	0.5534	2.4108	2.0274
1	0.9510	3.5866	0.7767

br) Structure **IX** X= NO_2 (E^{el} = -1025.21020888 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.3312	-1.1893	-0.3124
6	-2.0588	-0.7253	-0.5395
6	-1.7275	0.6313	-0.3048
6	-2.7450	1.4961	0.1659
6	-4.0173	1.0315	0.3948
6	-4.3014	-0.3083	0.1541
1	-3.5939	-2.2196	-0.4873
1	-1.2978	-1.3961	-0.9032
1	-2.5273	2.5366	0.3483
1	-4.7984	1.6813	0.7533
6	-0.4252	1.1131	-0.5281
6	1.7040	0.1021	-0.6525
6	2.6583	-0.3344	-1.5639
6	2.0339	0.3247	0.6791
6	3.9555	-0.5419	-1.1452
1	2.3673	-0.5027	-2.5886
6	3.3350	0.1225	1.0976
1	1.2765	0.6370	1.3812
6	4.2788	-0.3053	0.1813
1	4.7191	-0.8775	-1.8273
1	3.6245	0.2827	2.1232
8	0.4411	0.2452	-1.1229
7	5.6444	-0.5147	0.6233
8	5.8986	-0.2896	1.7848
8	6.4458	-0.9008	-0.1968
7	-5.6395	-0.7966	0.3933
8	-6.4632	-0.0058	0.8004
8	-5.8596	-1.9677	0.1730
6	0.0010	2.5286	-0.3657
1	1.0588	2.6407	-0.5805
1	-0.5478	3.1753	-1.0527
1	-0.1777	2.8979	0.6432

bs) Structure **VII** X= $N(CH_3)_2$ (E^{el} = -884.225984396 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.5730	0.6677	0.6579
6	-2.4271	1.4375	0.6216
6	-1.2767	1.0017	-0.0276
6	-1.3393	-0.2231	-0.6893
6	-2.4771	-1.0009	-0.6707
6	-3.6274	-0.5814	0.0186
1	-4.4312	1.0490	1.1858
1	-2.4409	2.3928	1.1222
1	-0.4700	-0.5767	-1.2233
1	-2.4671	-1.9407	-1.1973
6	-0.0103	1.8503	-0.1362
6	1.2488	1.0015	-0.0758
6	2.1449	0.9753	-1.1321
6	1.5665	0.2553	1.0523
6	3.3138	0.2333	-1.0750
1	1.9223	1.5439	-2.0228
6	2.7269	-0.4915	1.1270
1	0.8888	0.2413	1.8954
6	3.6311	-0.5312	0.0544
1	3.9760	0.2551	-1.9248
1	2.9213	-1.0509	2.0271
8	-0.2244	2.3736	-1.3930
7	-4.7539	-1.3620	0.0703
7	4.7744	-1.3050	0.1062
6	-4.8397	-2.5330	-0.7600
1	-4.7847	-2.2979	-1.8274
1	-4.0441	-3.2389	-0.5250
1	-5.7831	-3.0336	-0.5711
6	-5.9693	-0.8128	0.6078
1	-6.3256	0.0540	0.0427
1	-6.7427	-1.5730	0.5860
1	-5.8379	-0.5122	1.6466
6	5.1966	-1.8300	1.3762
1	5.4035	-1.0476	2.1149
1	4.4449	-2.4992	1.7918
1	6.1012	-2.4127	1.2358
6	5.7858	-1.1065	-0.8956
1	6.1923	-0.0889	-0.8967
1	6.6019	-1.7993	-0.7177
1	5.3954	-1.3171	-1.8899

6	0.0654	2.9784	0.8887
1	-0.7769	3.6558	0.7778
1	0.0899	2.5905	1.9047
1	0.9784	3.5442	0.7200

bt) Structure **TS-VII** X=N(CH_3)$_2$ (E^{el} = -884.211613515 hartree; 1 negative frequency = -503.0735)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.2062	0.0913	-1.1346
6	-2.0008	0.7706	-1.1806
6	-1.2807	1.0502	-0.0293
6	-1.8048	0.6111	1.1800
6	-3.0036	-0.0752	1.2440
6	-3.7474	-0.3398	0.0841
1	-3.7218	-0.1021	-2.0608
1	-1.5968	1.0846	-2.1318
1	-1.2641	0.7895	2.0995
1	-3.3567	-0.4050	2.2071
6	0.0128	1.8134	-0.1047
6	1.2787	1.0257	-0.1411
6	2.5413	1.5644	0.2652
6	1.2625	-0.3788	-0.4221
6	3.6713	0.7956	0.3053
1	2.6118	2.6068	0.5274
6	2.3987	-1.1349	-0.3802
1	0.3220	-0.8379	-0.6817
6	3.6504	-0.5762	-0.0321
1	4.5932	1.2621	0.6122
1	2.3203	-2.1854	-0.6084
8	0.5628	1.9146	-1.3691
7	4.7937	-1.3320	-0.0243
7	-4.9649	-0.9887	0.1437
6	-5.5491	-1.4728	-1.0773
1	-6.5015	-1.9420	-0.8531
1	-5.7478	-0.6534	-1.7661
1	-4.9173	-2.2055	-1.5916
6	-5.3369	-1.6507	1.3641
1	-4.6342	-2.4402	1.6533
1	-5.4081	-0.9414	2.1872
1	-6.3181	-2.0974	1.2403
6	4.7073	-2.7568	-0.2001
1	4.2370	-3.0061	-1.1501

1	5.7083	-3.1742	-0.2139
1	4.1444	-3.2456	0.6007
6	6.0096	-0.7791	0.5087
1	6.8094	-1.5026	0.3938
1	6.3020	0.1192	-0.0334
1	5.9263	-0.5280	1.5703
6	-0.0386	3.1100	0.6735
1	-0.1831	2.9323	1.7371
1	0.8641	3.6944	0.5288
1	-0.8798	3.6983	0.3126

bu) Structure **VIII** X= $N(CH_3)_2$ (E^{el} = -884.214990654 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.2150	0.2143	-1.0780
6	-2.0165	0.9059	-1.0913
6	-1.2577	1.0666	0.0593
6	-1.7382	0.4949	1.2311
6	-2.9308	-0.2039	1.2611
6	-3.7126	-0.3491	0.1052
1	-3.7613	0.1172	-2.0016
1	-1.6513	1.3241	-2.0177
1	-1.1667	0.5783	2.1452
1	-3.2486	-0.6386	2.1944
6	0.0203	1.8396	0.0351
6	1.2965	1.1447	-0.3438
6	2.6013	1.6186	0.1137
6	1.2716	-0.2719	-0.7065
6	3.6780	0.7922	0.2151
1	2.7155	2.6630	0.3528
6	2.3658	-1.0695	-0.5946
1	0.3412	-0.6804	-1.0672
6	3.6134	-0.5818	-0.1253
1	4.6078	1.2164	0.5589
1	2.2653	-2.1058	-0.8743
8	0.5719	2.0404	-1.2401
7	-4.9236	-1.0103	0.1354
7	4.7202	-1.3973	-0.0434
6	-5.2530	-1.8001	1.2904
1	-6.2355	-2.2393	1.1512
1	-4.5375	-2.6097	1.4715
1	-5.3006	-1.1820	2.1857

6	-5.5541	-1.3562	-1.1092
1	-4.9420	-2.0229	-1.7267
1	-6.4967	-1.8527	-0.9032
1	-5.7798	-0.4651	-1.6927
6	4.5539	-2.8204	-0.1747
1	5.5267	-3.2974	-0.1187
1	3.9168	-3.2464	0.6073
1	4.1250	-3.0752	-1.1418
6	5.8847	-0.9301	0.6605
1	5.6852	-0.7213	1.7167
1	6.6604	-1.6865	0.6038
1	6.2820	-0.0262	0.2026
6	0.0265	3.0434	0.9402
1	-0.1075	2.7502	1.9792
1	0.9477	3.6091	0.8543
1	-0.8004	3.6969	0.6672

bv) Structure **TS-IX** X= $N(CH_3)_2$ (E^{el} = -884.205728121 hartree; 1 negative frequency = -653.1122)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.0971	0.2194	-1.0747
6	-1.9177	0.9359	-1.0213
6	-1.2359	1.1449	0.1786
6	-1.7940	0.5801	1.3274
6	-2.9685	-0.1429	1.2875
6	-3.6652	-0.3327	0.0831
1	-3.5788	0.0968	-2.0308
1	-1.5119	1.3555	-1.9296
1	-1.2936	0.6868	2.2786
1	-3.3415	-0.5647	2.2062
6	0.0105	1.9063	0.2172
6	1.4359	1.2586	-0.5852
6	2.7185	1.6396	-0.1081
6	1.3059	-0.0791	-1.0655
6	3.7085	0.7017	0.0915
1	2.9116	2.6796	0.1020
6	2.3041	-0.9912	-0.8733
1	0.3935	-0.3690	-1.5612
6	3.5245	-0.6445	-0.2523
1	4.6485	1.0343	0.5022
1	2.1672	-1.9932	-1.2502
8	0.5486	2.2504	-1.0176

7	4.5203	-1.6085	-0.0892
7	-4.8580	-1.0207	0.0435
6	5.8059	-1.1623	0.3718
1	5.7955	-0.8134	1.4130
1	6.5082	-1.9893	0.3034
1	6.1771	-0.3591	-0.2594
6	4.1292	-2.8704	0.4950
1	4.8978	-3.6140	0.2950
1	3.9919	-2.7972	1.5810
1	3.2019	-3.2294	0.0645
6	-5.4027	-1.3966	-1.2327
1	-4.7389	-2.0578	-1.8002
1	-6.3450	-1.9115	-1.0782
1	-5.6103	-0.5187	-1.8425
6	-5.2647	-1.7769	1.1963
1	-6.2261	-2.2385	0.9968
1	-4.5530	-2.5667	1.4598
1	-5.3911	-1.1300	2.0632
6	0.2380	2.8863	1.3205
1	-0.0628	2.4783	2.2808
1	1.2800	3.1803	1.3923
1	-0.3567	3.7841	1.1383

bw) Structure **IX** X= $N(CH_3)_2$ (E^{el} = -884.244289509 hartree; 0 negative frequencies)

Atomic number	X coordinate	Y coordinate	Z coordinate
6	-3.2678	-1.0391	-0.5528
6	-2.0197	-0.4772	-0.6867
6	-1.7097	0.7880	-0.1421
6	-2.7595	1.4531	0.5269
6	-4.0087	0.8895	0.6619
6	-4.3015	-0.3823	0.1398
1	-3.4403	-2.0058	-0.9969
1	-1.2530	-1.0106	-1.2264
1	-2.5948	2.4369	0.9401
1	-4.7680	1.4533	1.1786
6	-0.4226	1.3500	-0.2664
6	1.7014	0.4176	-0.6674
6	2.7160	0.3491	-1.6058
6	1.9870	0.1329	0.6565
6	4.0019	0.0080	-1.2276
1	2.4881	0.5573	-2.6403

6	3.2761	-0.1986	1.0394
1	1.1959	0.1581	1.3918
6	4.3225	-0.2582	0.1108
1	4.7595	-0.0424	-1.9918
1	3.4543	-0.4183	2.0789
8	0.4406	0.7053	-1.1111
7	-5.5416	-0.9663	0.3113
7	5.6208	-0.5504	0.4997
6	-5.8721	-2.1269	-0.4707
1	-5.1840	-2.9444	-0.2636
1	-6.8658	-2.4667	-0.1972
1	-5.8593	-1.9333	-1.5491
6	-6.6336	-0.1487	0.7649
1	-6.4233	0.2725	1.7464
1	-6.8629	0.6756	0.0803
1	-7.5208	-0.7656	0.8644
6	6.5710	-0.9085	-0.5181
1	7.5315	-1.1044	-0.0523
1	6.2761	-1.7981	-1.0868
1	6.7171	-0.0894	-1.2199
6	5.8276	-1.1147	1.8057
1	5.3093	-2.0702	1.9478
1	6.8899	-1.2772	1.9570
1	5.4950	-0.4286	2.5826
6	-0.0226	2.6995	0.2100
1	-0.4113	2.9086	1.2044
1	1.0604	2.7826	0.2529
1	-0.3871	3.4842	-0.4597

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