Supporting Information for:

Nitroxyl Radical plus Hydroxylamine Pseudo Self-Exchange Reactions: Tunneling in Hydrogen Atom Transfer

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Figures S1 – S3, the complete author lists for references 32 and 33, the optimized geometries, energies, frequencies and thermal corrections for nitroxyl radicals (RR'NO·), hydroxylamines (RR'NOH), the corresponding hydrogen bonded complexes and hydrogen atom transfer transition structures, for R=R'=Me, R=H/R'=Me, R=R'=t-butyl, R=R'=phenyl, and TEMPO, (34 pages).

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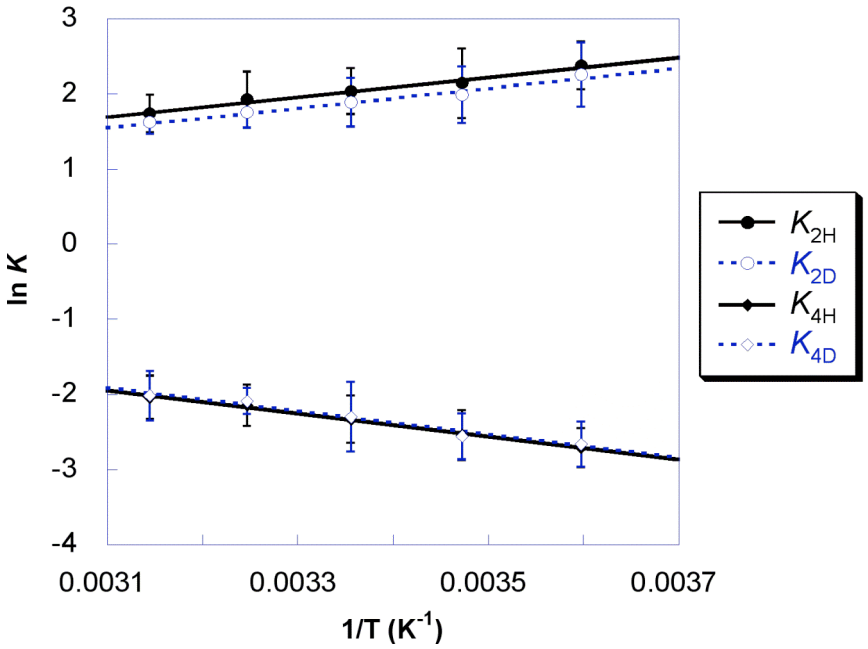


Figure S1. Van't Hoff plot for reactions 2 and 4 in CD_2Cl_2 at 278–318 K. The protio equilibrium constants are shown with filled points and solid lines (—), and the deutero ones with open points and dashed lines (---).

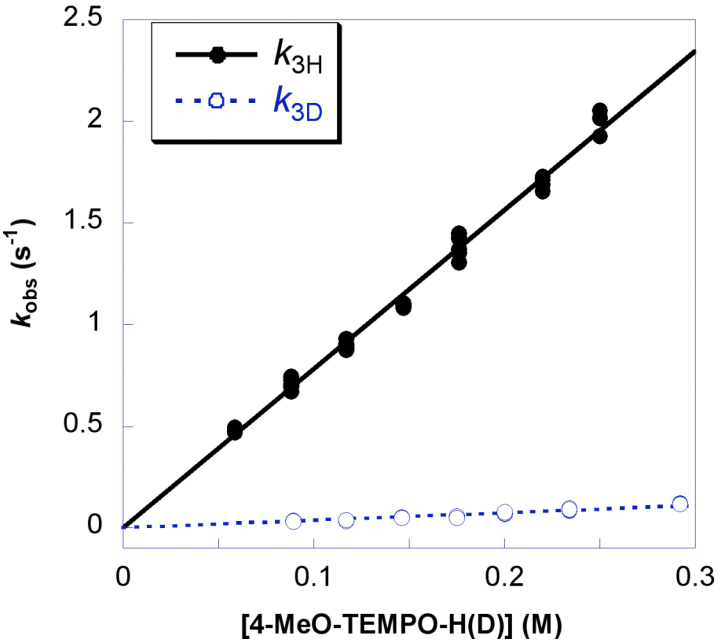


Figure S2. Plot of pseudo first order k_{obs} versus [4-MeO-TEMPO-H(D)] for reaction 3 in MeCN (k_H/k_D = 21 ± 3) at 298 K.

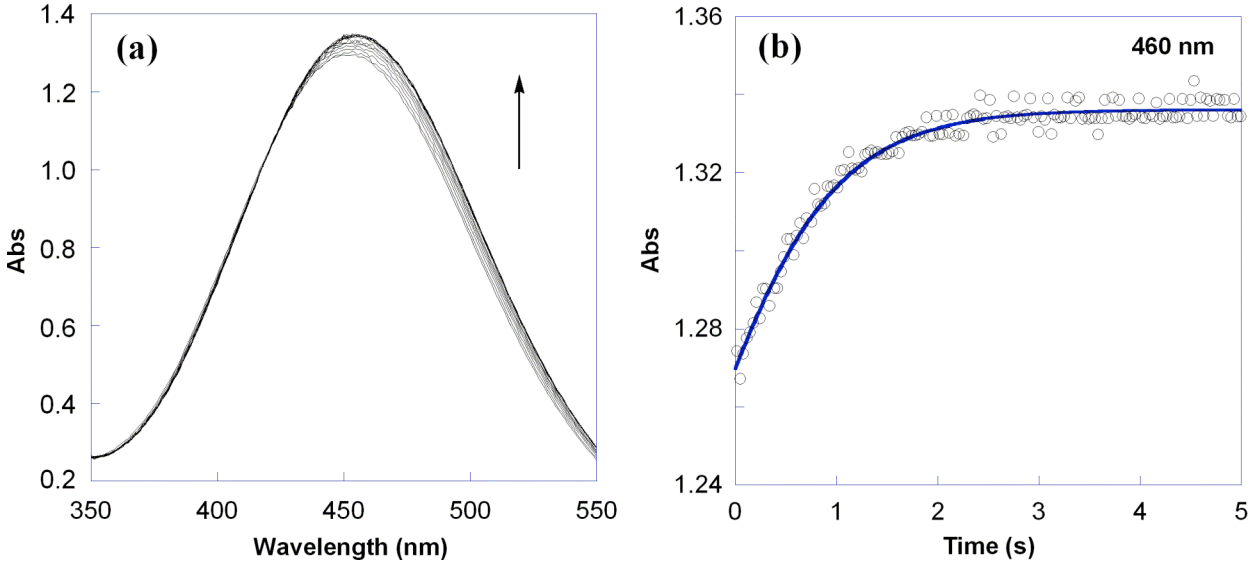
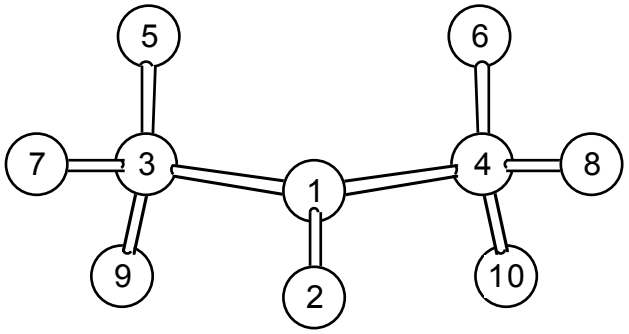


Figure S3. (a) Overlay plot of UV-vis spectra for the reaction of 139 mM $^{t}Bu_2NO^{\bullet}$ with 191 mM TEMPO-H (eq 4) in MeCN over 5 s at 298 K. (b) Absorbance at 460 nm (o) and the second order approach-to-equilibrium fit using SPECFIT (—).

Complete reference 32:
Gaussian 03, Revision D.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A., Gaussian, Inc., Wallingford CT, 2004.

Complete reference 33:
POLYRATE–version 9.5, Corchado, J. C.; Chuang, Y.-Y.; Fast, P. L.; Hu, W.-P.; Liu, Y.-P.; Lynch, G. C.; Nguyen, K. A.; Jackels, C. F.; Fernandez Ramos, A.; Ellingson, B. A.; Lynch, B. J.; Melissas, V. S.; Villà, J.; Rossi, I.; Coitiño, E. L.; Pu, J.; Albu, T. V.; Steckler, R.; Garrett, B. C.; Isaacson, A. D.; Truhlar, D. G., University of Minnesota, Minneapolis, 2007.

Dimethylnitroxyl Radical $^2A'$ UMPW1K/6-31+G(d,p) C_s Geometry	
Nuclear repulsion energy	130.801355 Hartree
UMPW1K/6-31+G(d,p) energy ($<S^2>$ = 0.7572)	0.086638 Hartree
Zero-point energy correction	0.092802 Hartree
Thermal correction to Enthalpy	0.058494 Hartree
Thermal correction to Gibbs Free Energy	-209.666559 Hartree

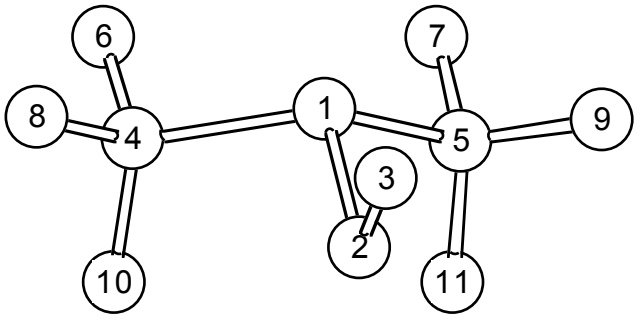


	X	Y	Z
N1	0.000000	0.116699	-0.149335
O2	0.000000	1.366277	0.042169
C3	-1.242768	-0.594647	0.025150
C4	1.242768	-0.594648	0.025150
H5	-1.222411	-1.522672	-0.540441
H6	1.222411	-1.522672	-0.540442
H7	-2.043338	0.040730	-0.335670
H8	2.043338	0.040730	-0.335669
H9	-1.415264	-0.823726	1.079210
H10	1.415263	-0.823727	1.079209

(1-2)	1.264	(1-3)	1.443	(3-5)	1.087	(3-7)	1.084	(3-9)	1.092
(2-1-3)	118.0	(3-1-4)	119.0	(1-3-5)	110.0	(1-3-7)	107.9		
(1-3-9)	110.9	(5-3-7)	109.9	(5-3-9)	109.0	(7-3-9)	109.1		
(2-1-3-5)	156.7	(2-1-3-7)	36.8	(2-1-3-9)	-82.6				
(4-1-3-5)	-49.0	(4-1-3-7)	-168.9	(4-1-3-9)	71.7				
(bond)-(plane) angle		(2-1)-(3-1-4)	22.5						

Frequencies(cm^{-1}): 145.8 166.6 290.1 413.0 531.1 873.7 1062.6 1105.4
1170.7 1192.0 1349.7 1465.8 1486.2 1508.8 1510.9 1524.1 1527.7 1597.8
3097.5 3103.1 3194.1 3196.3 3257.5 3259.1

Dimethylhydroxylamine $^1A'$ MPW1K/6-31+G(d,p) C_s Geometry	
Nuclear repulsion energy	138.862073 Hartree
UMPW1K/6-31+G(d,p) energy	-210.287997 Hartree
Zero-point energy correction	0.099435 Hartree
Thermal correction to Enthalpy	0.105539 Hartree
Thermal correction to Gibbs Free Energy	0.072374 Hartree



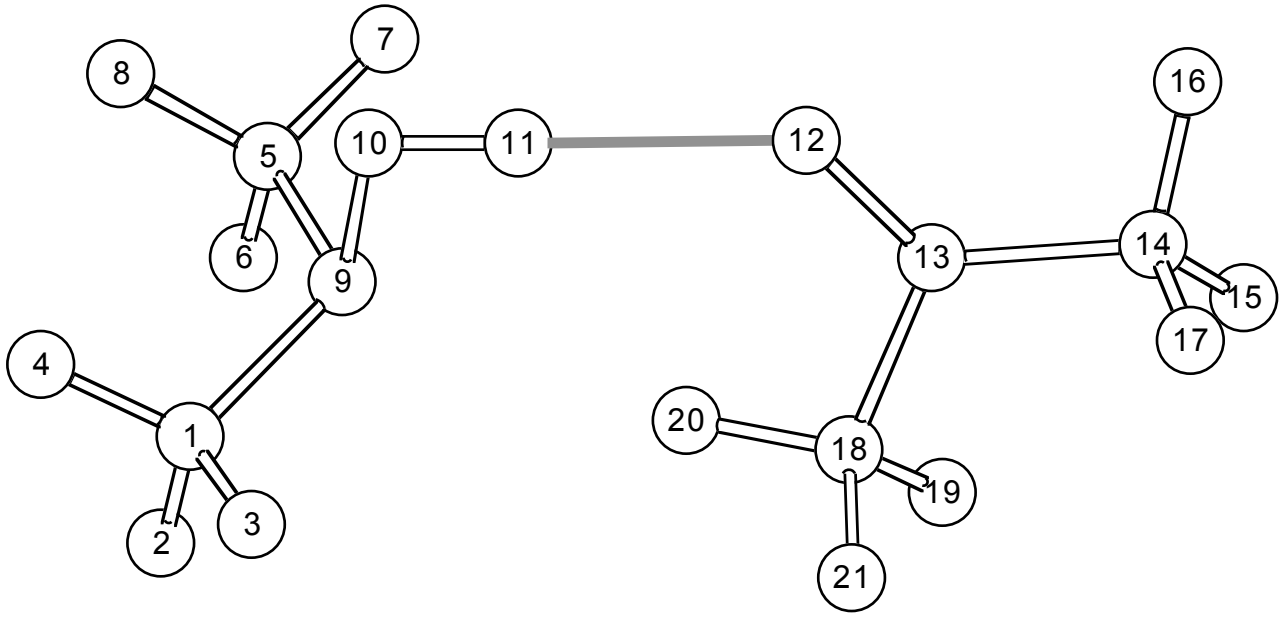
	X	Y	Z
N1	-0.312404	0.248317	0.000000
O2	0.906119	0.964734	0.000000
H3	0.635718	1.880669	0.000000
C4	-0.312404	-0.561497	1.194832
C5	-0.312404	-0.561497	-1.194832
H6	-1.231263	-1.142834	1.218235
H7	-1.231263	-1.142834	-1.218235
H8	-0.288623	0.084849	2.066871
H9	-0.288623	0.084849	-2.066871
H10	0.545388	-1.241417	1.234166
H11	0.545388	-1.241417	-1.234166

(1-4)	1.443	(2-3)	0.955	(4-6)	1.088	(4-8)	1.086	(4-10)	1.095
(4-1-5)	111.7	(1-4-6)	108.5	(1-4-8)	109.3	(1-4-10)	112.2		
(6-4-8)	108.6	(6-4-10)	109.2	(8-4-10)	108.9				
(5-1-4-6)	-63.0	(5-1-4-8)	178.7	(5-1-4-10)	57.8				
(bond)-(plane) angle		(2,1)-(4-1-5)	59.5						

Frequencies(cm^{-1}): 249.3 285.4 317.1 417.7 457.1 476.5 891.1 1058.3
1059.1 1142.6 1216.9 1276.9 1319.4 1406.2 1474.1 1498.9 1511.3 1527.9
1531.3 1553.5 3071.4 3077.2 3183.1 3187.4 3230.0 3233.1 3994.4

Dimethylhydroxylamine + Dimethylnitroxyl Radical H-bonded Complex
^{2}A UMPW1K/6-31+G(d,p) C_1 Geometry

Nuclear repulsion energy	408.999620 Hartree
UMPW1K/6-31+G(d,p) energy (<S^2> = 0.7573)	-419.966269 Hartree
Zero-point correction	0.188069 Hartree
Thermal correction to Enthalpy	0.200801 Hartree
Thermal correction to Gibbs Free Energy	0.147861 Hartree



	X	Y	Z		X	Y	Z
C1	-2.634435	0.846718	-0.802060	O12	1.442910	-0.979698	-0.413866
H2	-2.985541	1.741410	-0.291672	N13	2.064216	-0.009585	0.110967
H3	-2.074531	1.142009	-1.684553	C14	3.503063	-0.087799	0.149196
H4	-3.497695	0.251583	-1.118927	H15	3.884631	0.538207	0.951161
C5	-2.471235	-0.330296	1.268417	H16	3.778455	-1.121916	0.320690
H6	-2.812141	0.542295	1.822392	H17	3.931378	0.245650	-0.798156
H7	-1.792695	-0.900001	1.896406	C18	1.418663	1.280113	0.170447
H8	-3.332563	-0.960008	1.021291	H19	1.817210	1.847496	1.007685
N9	-1.767340	0.110117	0.086340	H20	0.349741	1.119116	0.295427
O10	-1.372246	-1.045930	-0.610351	H21	1.599255	1.837226	-0.751792
H11	-0.405296	-1.034191	-0.573361				

(1-2)	1.088	(1-3)	1.086	(1-4)	1.095	(1-9)	1.443
(5-6)	1.088	(5-7)	1.086	(5-8)	1.095	(5-9)	1.445
(9-10)	1.406	(10-11)	0.968	(11-12)	1.856	(12-13)	1.266
(13-14)	1.441	(13-18)	1.443	(14-15)	1.087	(14-16)	1.084
(14-17)	1.092	(18-19)	1.087	(18-20)	1.088	(18-21)	1.092
(2-1-3)	108.9	(2-1-4)	109.2	(2-1-9)	108.9	(3-1-4)	108.6
(3-1-9)	109.2	(4-1-9)	112.0	(6-5-7)	108.8	(6-5-8)	109.2
(6-5-9)	108.9	(7-5-8)	108.7	(7-5-9)	109.2	(8-5-9)	112.0
(1-9-5)	111.5	(1-9-10)	106.5	(5-9-10)	107.0	(9-10-11)	104.6
(10-11-12)	177.1	(11-12-13)	123.2	(12-13-14)	117.3	(12-13-18)	118.8
(14-13-18)	119.6	(13-14-15)	109.8	(13-14-16)	108.0	(13-14-17)	110.6
(15-14-16)	110.1	(15-14-17)	109.1	(16-14-17)	109.2	(13-18-19)	109.5
(13-18-20)	108.2	(13-18-21)	110.3	(19-18-20)	110.4	(19-18-21)	108.9
(20-18-21)	109.6						
(2-1-9-5)	62.3	(2-1-9-10)	178.6	(3-1-9-5)	-178.9		
(3-1-9-10)	-62.6	(4-1-9-5)	-58.6	(4-1-9-10)	57.8		
(6-5-9-1)	-62.7	(6-5-9-10)	-178.7	(7-5-9-1)	178.6		
(7-5-9-10)	62.6	(8-5-9-1)	58.2	(8-5-9-10)	-57.8		

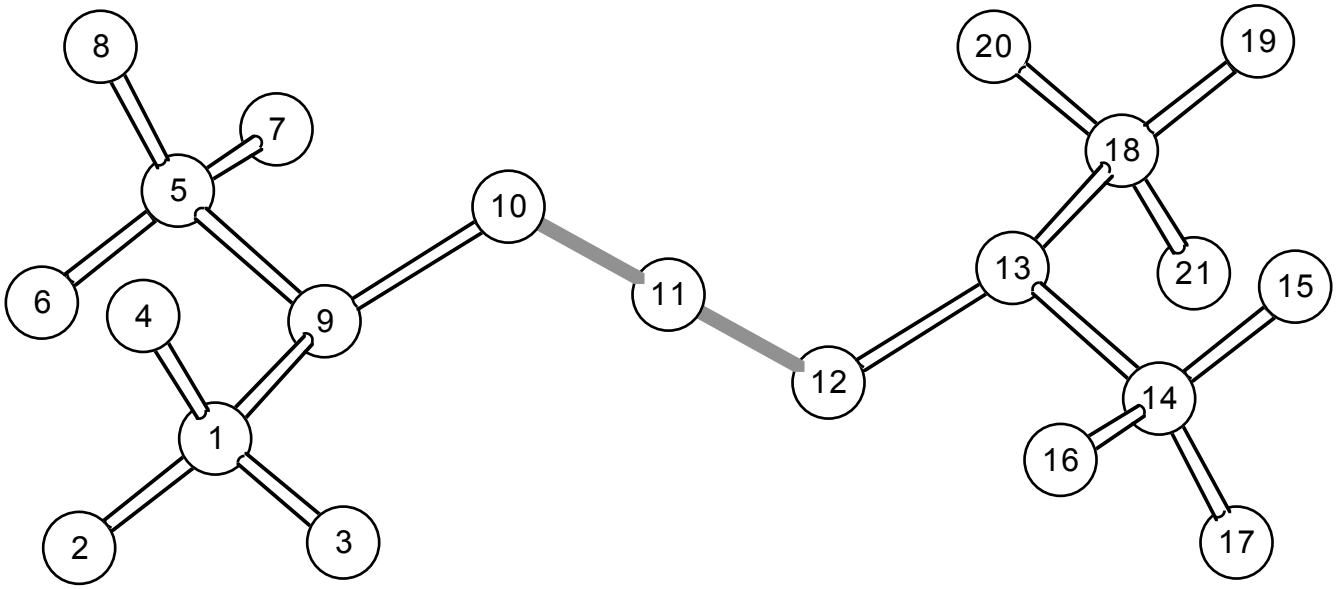
(1-9-10-11)	126.1	(5-9-10-11)	-114.6	(9-10-11-12)	38.7				
(10-11-12-13)	-43.9	(11-12-13-14)	-179.0	(11-12-13-18)	-22.1				
(12-13-14-15)	-156.1	(12-13-14-16)	-36.0	(12-13-14-17)	83.5				
(18-13-14-15)	47.2	(18-13-14-16)	167.3	(18-13-14-17)	-73.2				
(12-13-18-19)	153.4	(12-13-18-20)	33.0	(12-13-18-21)	-86.8				
(14-13-18-19)	-50.3	(14-13-18-20)	-170.7	(14-13-18-21)	69.5				
(9-10,12-13)	-5.1								
(bond)-(plane) angle		(10-9)-(1-9-5)		59.3					
(bond)-(plane) angle		(12-13)-(14-13-18)		20.6					

Frequencies(cm^{-1}):

20.8	33.3	62.2	85.2	120.6	147.0	154.5	223.1	
252.7	287.3	291.1	423.0	423.2	470.4	477.3	551.4	684.8	873.1
901.7	1057.8	1073.6	1074.4	1108.4	1140.7	1173.9	1202.1	1227.9	1287.8
1316.8	1351.4	1471.4	1472.1	1494.6	1498.8	1510.0	1510.3	1513.0	1517.2
1527.1	1531.3	1538.7	1547.4	1553.9	1609.2	3070.7	3076.2	3086.7	3106.6
3175.7	3178.4	3180.5	3201.2	3221.3	3224.5	3227.3	3261.1	3749.8	

Dimethylhydroxylamine + Dimethylnitroxyl Radical Transition Structure
$^2B_2$ UMPW1K/6-31+G(d,p) C_{2h} Geometry

Nuclear repulsion energy	410.022714 Hartree
UMPW1K/6-31+G(d,p) energy ($<S^2>$ = 0.7605)	-419.928609 Hartree
Zero-point correction	0.182002 Hartree
Thermal correction to Enthalpy	0.194085 Hartree
Thermal correction to Gibbs Free Energy	0.143384 Hartree



	X	Y	Z		X	Y	Z
C1	0.000000	2.780659	1.223811	O12	-0.682560	-0.952277	0.000000
H2	-0.753498	3.564007	1.221718	N13	0.088101	-2.029816	0.000000
H3	-0.184292	2.110154	2.056821	C14	0.000000	-2.780659	1.223811
H4	0.989454	3.234132	1.347576	H15	0.753498	-3.564007	1.221718
C5	0.000000	2.780659	-1.223811	H16	0.184292	-2.110154	2.056821
H6	-0.753498	3.564007	-1.221718	H17	-0.989454	-3.234132	1.347576
H7	-0.184292	2.110154	-2.056821	C18	0.000000	-2.780659	-1.223811
H8	0.989454	3.234132	-1.347576	H19	0.753498	-3.564007	-1.221718
N9	-0.088101	2.029816	0.000000	H20	0.184292	-2.110154	-2.056821
O10	0.682560	0.952277	0.000000	H21	-0.989454	-3.234132	-1.347576
H11	0.000000	0.000000	0.000000				

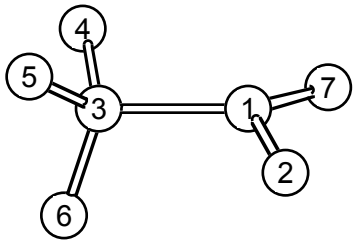
(1-2)	1.087	(1-3)	1.085	(1-4)	1.095	(1-9)	1.438	(9-10)	1.325	
(10-11)	1.172									

(2-1-3)	109.2	(2-1-4)	109.1	(2-1-9)	109.4	(3-1-4)	108.8				
(3-1-9)	108.7	(4-1-9)	111.6	(1-9-5)	116.6	(1-9-10)	112.9				
(9-10-11)	108.8										
(2-1-9-5)	55.0	(2-1-9-10)	-171.9	(3-1-9-5)	174.1						
(3-1-9-10)	-52.7	(4-1-9-5)	-65.9	(4-1-9-10)	67.2						
(1-9-10-11)	112.6										
(bond)-(plane) angle		(10-9)-(1-9-5)	42.3								

Frequencies(cm^{-1}): -2715.4 18.7 44.5 59.7 87.2 166.6 210.1 210.5
215.1 225.4 329.0 389.8 424.4 435.4 503.1 503.6 722.6 896.0
909.2 1017.8 1069.7 1070.6 1127.7 1128.0 1157.5 1168.1 1204.3 1206.2
1347.7 1348.0 1406.1 1422.5 1470.0 1471.6 1491.3 1495.1 1509.2 1509.4
1524.2 1525.5 1528.0 1528.7 1548.7 1549.1 1718.1 3067.9 3067.9 3068.0
3075.1 3185.5 3185.7 3188.5 3188.7 3240.8 3240.8 3243.4 3243.5

Methylnitroxyl Radical ^2A UMPW1K/6-31+G(d,p) C_1 Geometry

Nuclear repulsion energy	77.236334 Hartree
UMPW1K/6-31+G(d,p) energy ($<S^2>$ = 0.7569)	-170.358632 Hartree
Zero-point energy correction	0.057519 Hartree
Thermal correction to Enthalpy	0.062573 Hartree
Thermal correction to Gibbs Free Energy	0.031707 Hartree



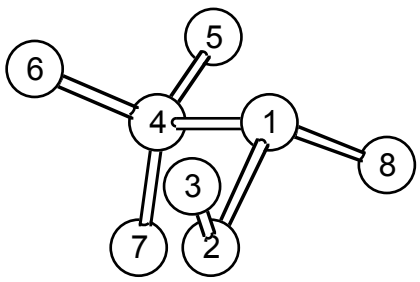
	X	Y	Z
N1	-0.176583	0.423749	-0.054887
O2	-1.207831	-0.299469	0.014678
C3	1.131949	-0.168668	0.009456
H4	1.875097	0.576628	-0.260643
H5	1.173427	-0.993893	-0.694962
H6	1.345671	-0.546716	1.009728
H7	-0.287162	1.405502	0.155925

(1-2)	1.261	(1-3)	1.438	(1-7)	1.010	(3-4)	1.087	(3-5)	1.086		
(3-6)	1.090										
(2-1-3)	120.4	(2-1-7)	117.1	(3-1-7)	119.4	(1-3-4)	109.2				
(1-3-5)	108.6	(1-3-6)	111.2	(4-3-5)	109.5	(4-3-6)	109.4				
(5-3-6)	108.9										
(2-1-3-4)	169.0	(2-1-3-5)	49.6	(2-1-3-6)	-70.2						
(7-1-3-4)	-31.6	(7-1-3-5)	-150.9	(7-1-3-6)	89.2						
(bond)-(plane) angle		(2-1)-(3-1-7)	17.6								

Frequencies(cm^{-1}): 151.0 370.3 528.8 1020.5 1142.4 1231.0 1471.5 1505.4
1513.2 1533.1 1605.1 3113.5 3202.2 3241.4 3618.7

Methylhydroxylamine ^1A MPW1K/6-31+G(d,p) C_1 Geometry

Nuclear repulsion energy	83.231875 Hartree
UMPW1K/6-31+G(d,p) energy	-170.982727 Hartree
Zero-point energy correction	0.071264 Hartree
Thermal correction to Enthalpy	0.076267 Hartree
Thermal correction to Gibbs Free Energy	0.046168 Hartree



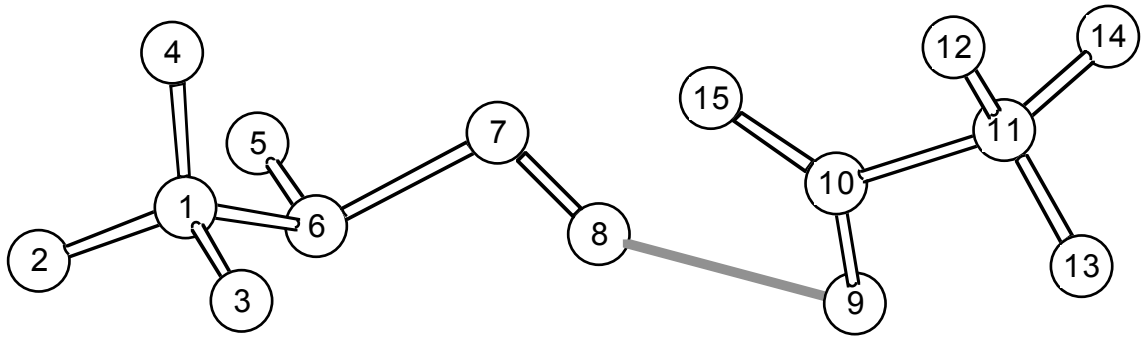
	X	Y	Z
N1	-0.052374	0.553516	-0.150725
O2	-1.150083	-0.286082	0.128047
H3	-1.685557	-0.235822	-0.660601
C4	1.153224	-0.224884	0.004760
H5	2.000876	0.453741	-0.070200
H6	1.221810	-0.948841	-0.802612
H7	1.199535	-0.757128	0.957714
H8	-0.088727	1.251393	0.577839

(1-2)	1.410	(1-4)	1.443	(1-8)	1.010	(2-3)	0.955	(4-5)	1.088
(4-6)	1.087	(4-7)	1.092						
(2-1-4)	107.9	(2-1-8)	103.9	(4-1-8)	109.0	(1-2-3)	104.0		
(1-4-5)	107.9	(1-4-6)	109.4	(1-4-7)	113.1	(5-4-6)	108.4		
(5-4-7)	109.3	(6-4-7)	108.7						
(4-1-2-3)	-123.6	(8-1-2-3)	120.7	(2-1-4-5)	-172.1				
(2-1-4-6)	70.3	(2-1-4-7)	-51.0	(8-1-4-5)	-59.8				
(8-1-4-6)	-177.5	(8-1-4-7)	61.2						
(bond)-(plane) angle		(2-1)-(4-1-8)		61.7					

Frequencies(cm^{-1}): 270.3 361.4 457.5 925.3 1002.3 1154.3 1191.9 1263.8
1415.2 1485.8 1515.7 1541.5 1566.1 3095.2 3184.4 3220.6 3632.0 3997.9

Methylhydroxylamine + Methylnitroxyl Radical H-bonded Complex
^{2}A UMPW1K/6-31+G(d,p) C_1 Geometry

Nuclear repulsion energy	247.045913 Hartree
UMPW1K/6-31+G(d,p) energy ($<S^2>$ = 0.7570)	-341.351990 Hartree
Zero-point correction	0.130910 Hartree
Thermal correction to Enthalpy	0.141306 Hartree
Thermal correction to Gibbs Free Energy	0.094136 Hartree



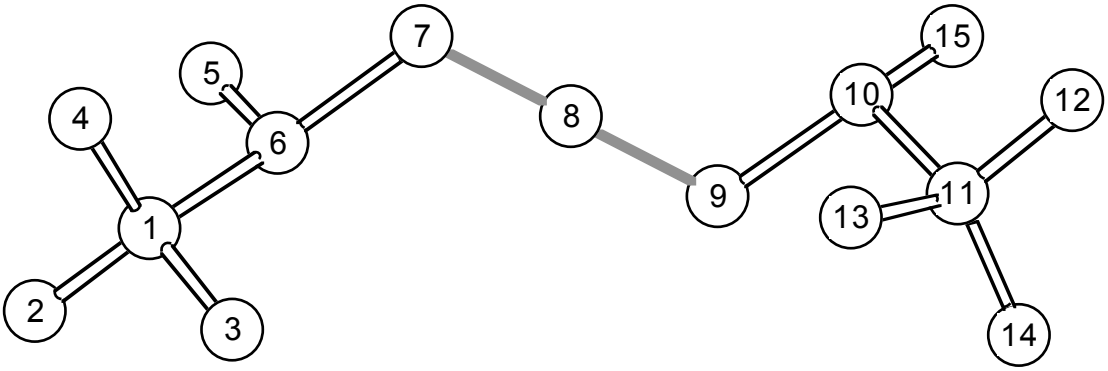
	X	Y	Z		X	Y	Z
C1	-2.702925	0.870337	0.291331	O9	1.435199	-0.965749	0.525162
H2	-3.737693	0.847948	0.628363	N10	1.669114	0.176757	0.036896
H3	-2.093100	1.275696	1.094692	C11	3.022894	0.612120	-0.160527
H4	-2.624101	1.528613	-0.578563	H12	3.023021	1.670590	-0.404207
H5	-2.897285	-0.873253	-0.693113	H13	3.581014	0.448977	0.756636
N6	-2.294484	-0.485255	0.017551	H14	3.498370	0.055013	-0.968084
O7	-1.026930	-0.450180	-0.591276	H15	0.898878	0.625370	-0.445199
H8	-0.457493	-0.986780	-0.027567				

(1-2)	1.089	(1-3)	1.087	(1-4)	1.094	(1-6)	1.442	(5-6)	1.009
(6-7)	1.407	(7-8)	0.964	(8-9)	1.972	(9-10)	1.264	(10-11)	1.436
(10-15)	1.013	(11-12)	1.086	(11-13)	1.086	(11-14)	1.090		
(2-1-3)	108.2	(2-1-4)	109.1	(2-1-6)	108.0	(3-1-4)	108.8		
(3-1-6)	109.4	(4-1-6)	113.2	(1-6-5)	109.0	(1-6-7)	108.3		
(5-6-7)	104.1	(6-7-8)	105.4	(7-8-9)	136.4	(8-9-10)	94.5		
(9-10-11)	120.1	(9-10-15)	116.3	(11-10-15)	121.1	(10-11-12)	109.1		
(10-11-13)	108.8	(10-11-14)	111.0	(12-11-13)	109.6	(12-11-14)	109.4		
(13-11-14)	108.9								
(2-1-6-5)	59.4	(2-1-6-7)	172.0	(3-1-6-5)	176.9				
(3-1-6-7)	-70.5	(4-1-6-5)	-61.5	(4-1-6-7)	51.1				
(1-6-7-8)	122.8	(5-6-7-8)	-121.3	(6-7-8-9)	-146.1				
(7-8-9-10)	10.0	(8-9-10-11)	-164.3	(8-9-10-15)	-1.9				
(9-10-11-12)	-169.3	(9-10-11-13)	-49.8	(9-10-11-14)	70.1				
(15-10-11-12)	29.1	(15-10-11-13)	148.7	(15-10-11-14)	-91.4				
(bond)-(plane) angle		(7-6)-(1-6-5)		61.2					

(bond)-(plane) angle	(9-10)-(11-10-15)	15.9							
Frequencies(cm^{-1}):	28.6	56.2	69.0	82.9	135.7	166.3	193.9	289.0	
	447.7	475.2	547.3	689.0	926.8	1004.0	1027.3	1141.6	1172.7	1195.1
	1232.5	1266.1	1462.3	1477.2	1484.6	1510.7	1514.1	1517.2	1535.6	1545.8
	1568.2	1612.2	3083.2	3116.4	3177.5	3205.1	3216.5	3243.2	3587.8	3632.6

Methylhydroxylamine + Methylnitroxyl Radical Transition Structure
^{2}B UMPW1K/6-31+G(d,p) C_2 Geometry

Nuclear repulsion energy	252.296032 Hartree
UMPW1K/6-31+G(d,p) energy (<S^2> = 0.7609)	-341.314519 Hartree
Zero-point correction	0.125143 Hartree
Thermal correction to Enthalpy	0.134611 Hartree
Thermal correction to Gibbs Free Energy	0.090596 Hartree

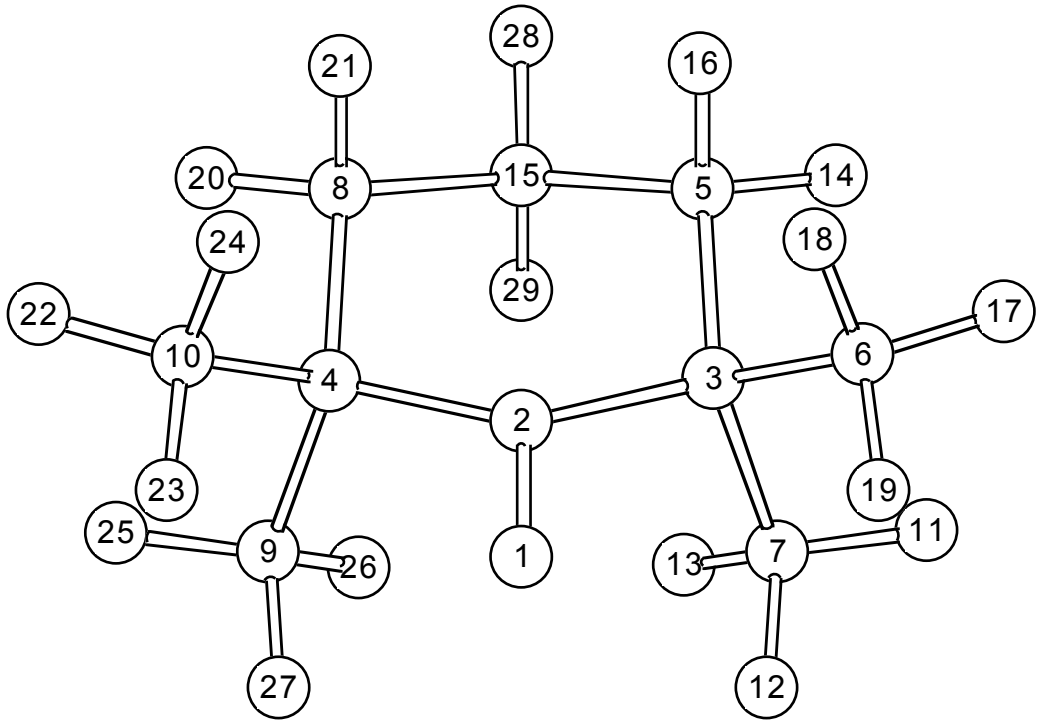


	X	Y	Z		X	Y	Z
C1	-0.051842	2.784553	-0.794427	O9	0.699723	-0.936707	0.457025
H2	0.592533	3.656659	-0.715210	N10	-0.051842	-2.024840	0.420163
H3	0.289546	2.171327	-1.623903	C11	0.051842	-2.784553	-0.794427
H4	-1.076416	3.106982	-0.996188	H12	-0.592533	-3.656659	-0.715210
H5	-0.032981	2.555729	1.273211	H13	-0.289546	-2.171327	-1.623903
N6	0.051842	2.024840	0.420163	H14	1.076416	-3.106982	-0.996188
O7	-0.699723	0.936707	0.457025	H15	0.032981	-2.555729	1.273211
H8	0.000000	0.000000	0.462626				

(1-2)	1.087	(1-3)	1.087	(1-4)	1.093	(1-6)	1.436	(5-6)	1.008
(6-7)	1.323	(7-8)	1.169						
(2-1-3)	108.8	(2-1-4)	109.4	(2-1-6)	108.7	(3-1-4)	108.7		
(3-1-6)	108.9	(4-1-6)	112.3	(1-6-5)	115.5	(1-6-7)	114.7		
(5-6-7)	111.2	(6-7-8)	108.6	(7-8-9)	179.5				
(2-1-6-5)	48.0	(2-1-6-7)	179.4	(3-1-6-5)	166.4				
(3-1-6-7)	-62.3	(4-1-6-5)	-73.2	(4-1-6-7)	58.2				
(1-6-7-8)	113.1	(5-6-7-8)	-113.5	(6-7-8-9)	-88.4				
(bond)-(plane) angle		(7-6)-(1-6-5)	43.0						
Frequencies(cm^{-1}):	-2652.4	24.8	77.3	79.9	130.6	195.3	240.6	273.6	
	429.5	467.2	700.0	751.7	776.1	995.8	1022.1	1030.3	1166.7	1168.9
	1238.5	1238.7	1358.4	1363.3	1481.7	1484.5	1512.4	1513.2	1531.4	1531.9
	1561.6	1567.2	1710.9	3089.7	3092.1	3186.4	3186.7	3229.1	3229.2	3646.5

2,2,6,6-Tetramethyl-piperidin-1-oxyl Radical (TEMPO)
^{2}A′ UMPW1K/6-31+G(d,p) C_s Geometry

Nuclear repulsion energy	721.579792 Hartree
UMPW1K/6-31+G(d,p) energy ($<S^2>$ = 0.7571)	-483.640242 Hartree
Zero-point correction	0.269673 Hartree
Thermal correction to Enthalpy	0.282283 Hartree
Thermal correction to Gibbs Free Energy	0.233322 Hartree



	X	Y	Z		X	Y	Z
O1	-1.995583	0.069855	0.000000	H16	1.390334	1.588813	1.228705
N2	-0.737579	0.201408	0.000000	H17	-0.326188	0.821241	3.286201
C3	-0.072780	0.025100	1.311094	H18	-0.850433	1.918392	2.003974
C4	-0.072780	0.025100	-1.311094	H19	-1.850173	0.533332	2.433319
C5	1.377127	0.496748	1.232278	H20	1.882836	0.180710	-2.144755
C6	-0.827317	0.877868	2.321269	H21	1.390334	1.588813	-1.228705
C7	-0.159326	-1.441837	1.731134	H22	-0.326188	0.821241	-3.286201
C8	1.377127	0.496748	-1.232278	H23	-1.850173	0.533332	-2.433319
C9	-0.159326	-1.441837	-1.731134	H24	-0.850433	1.918392	-2.003974
C10	-0.827317	0.877868	-2.321269	H25	0.177091	-1.549218	-2.761131
H11	0.177091	-1.549218	2.761131	H26	0.454824	-2.089155	-1.110311
H12	-1.190411	-1.780631	1.667432	H27	-1.190411	-1.780631	-1.667432
H13	0.454824	-2.089155	1.110311	H28	3.130251	0.371887	0.000000
H14	1.882836	0.180710	2.144755	H29	2.175008	-1.087613	0.000000
C15	2.105707	0.000917	0.000000				

(1-2)	1.265	(2-3)	1.481	(3-5)	1.527	(3-6)	1.522	(3-7)	1.528
(5-14)	1.090	(5-15)	1.515	(5-16)	1.092	(6-17)	1.089	(6-18)	1.088
(6-19)	1.085	(7-11)	1.089	(7-12)	1.087	(7-13)	1.087	(15-28)	1.090
(15-29)	1.091								
(1-2-3)	115.7	(3-2-4)	124.6	(2-3-5)	110.1	(2-3-6)	107.4		
(2-3-7)	109.4	(5-3-6)	109.4	(5-3-7)	111.4	(6-3-7)	109.1		
(3-5-14)	107.9	(3-5-15)	113.4	(3-5-16)	108.7	(14-5-15)	111.3		
(14-5-16)	106.7	(15-5-16)	108.6	(3-6-17)	109.3	(3-6-18)	110.7		
(3-6-19)	111.0	(17-6-18)	108.5	(17-6-19)	109.0	(18-6-19)	108.3		
(3-7-11)	109.7	(3-7-12)	109.7	(3-7-13)	112.5	(11-7-12)	108.5		

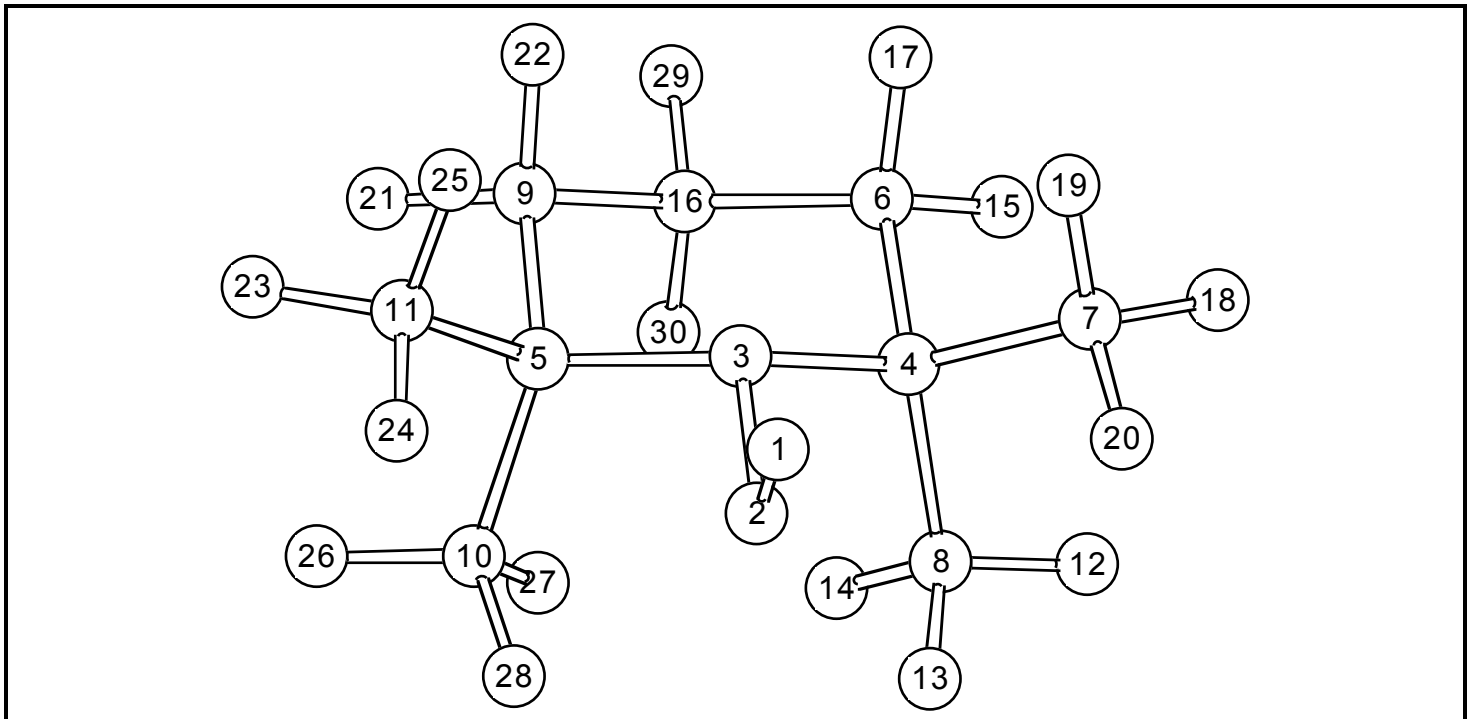
(11-7-13)	107.9	(12-7-13)	108.5	(5-15-8)	108.9	(5-15-28)	109.9
(5-15-29)	110.9	(28-15-29)	106.3				
(1-2-3-5)	-168.0	(1-2-3-6)	-49.0	(1-2-3-7)	69.3		
(4-2-3-5)	35.3	(4-2-3-6)	154.3	(4-2-3-7)	-87.5		
(2-3-5-14)	-169.4	(2-3-5-15)	-45.7	(2-3-5-16)	75.2		
(6-3-5-14)	72.8	(6-3-5-15)	-163.4	(6-3-5-16)	-42.5		
(7-3-5-14)	-47.9	(7-3-5-15)	75.9	(7-3-5-16)	-163.2		
(2-3-6-17)	-176.5	(2-3-6-18)	-57.0	(2-3-6-19)	63.3		
(5-3-6-17)	-57.0	(5-3-6-18)	62.5	(5-3-6-19)	-177.3		
(7-3-6-17)	65.1	(7-3-6-18)	-175.4	(7-3-6-19)	-55.2		
(2-3-7-11)	-170.6	(2-3-7-12)	-51.5	(2-3-7-13)	69.3		
(5-3-7-11)	67.4	(5-3-7-12)	-173.5	(5-3-7-13)	-52.7		
(6-3-7-11)	-53.5	(6-3-7-12)	65.7	(6-3-7-13)	-173.5		
(3-5-15-8)	59.4	(3-5-15-28)	179.8	(3-5-15-29)	-62.9		
(14-5-15-8)	-178.7	(14-5-15-28)	-58.2	(14-5-15-29)	59.0		
(16-5-15-8)	-61.6	(16-5-15-28)	58.9	(16-5-15-29)	176.1		
(bond)-(plane) angle		(1-2)-(3-2-4)	20.8				

Frequencies(cm^{-1}):

83.0	124.6	203.2	212.2	242.7	262.9	274.9	292.4
298.6	314.8	324.2	338.3	388.6	415.0	415.4	463.4	482.1	557.7
572.9	593.1	668.0	825.1	840.8	890.6	920.3	965.2	970.7	970.7
997.0	1019.1	1035.9	1037.1	1091.8	1108.7	1113.6	1139.5	1208.9	1245.7
1268.5	1281.0	1300.2	1319.1	1343.5	1362.0	1408.6	1425.6	1428.1	1437.9
1438.8	1449.5	1452.7	1505.4	1511.8	1518.0	1522.6	1526.3	1529.9	1532.6
1534.8	1540.6	1547.1	1547.5	1559.1	3112.9	3113.8	3125.7	3125.8	3128.6
3130.1	3132.3	3167.8	3168.5	3178.1	3207.9	3210.6	3211.8	3214.8	3226.4
3230.7	3243.4	3243.7							

2,2,6,6-Tetramethyl-piperidin-1-hydroxyloxylamine (TEMPOH)
^{1}A′ MPW1K/6-31+G(d,p) C_s Geometry

Nuclear repulsion energy	738.601062 Hartree
MPW1K/6-31+G(d,p) energy	-484.255451 Hartree
Zero-point correction	0.281964 Hartree
Thermal correction to Enthalpy	0.294706 Hartree
Thermal correction to Gibbs Free Energy	0.246599 Hartree



	X	Y	Z		X	Y	Z
H1	-2.509802	0.812791	0.000000	C16	2.145223	-0.012932	0.000000
O2	-2.004144	0.003174	0.000000	H17	1.447394	1.560596	1.262886
N3	-0.662174	0.437352	0.000000	H18	-0.245618	0.688693	3.322276
C4	-0.050850	0.033174	1.276220	H19	-0.766434	1.884121	2.129296
C5	-0.050850	0.033174	-1.276220	H20	-1.786577	0.485360	2.496837
C6	1.413690	0.469465	1.237050	H21	1.900913	0.113853	-2.145508
C7	-0.760314	0.822813	2.371959	H22	1.447394	1.560596	-1.262886
C8	-0.177406	-1.456427	1.605414	H23	-0.245618	0.688693	-3.322276
C9	1.413690	0.469465	-1.237050	H24	-1.786577	0.485360	-2.496837
C10	-0.177406	-1.456427	-1.605414	H25	-0.766434	1.884121	-2.129296
C11	-0.760314	0.822813	-2.371959	H26	0.058033	-1.616202	-2.656811
H12	0.058033	-1.616202	2.656811	H27	0.494639	-2.080014	-1.024198
H13	-1.196016	-1.794394	1.432856	H28	-1.196016	-1.794394	-1.432856
H14	0.494639	-2.080014	1.024198	H29	3.167233	0.366251	0.000000
H15	1.900913	0.113853	2.145508	H30	2.225506	-1.100643	0.000000

(1-2)	0.955	(2-3)	1.410	(3-4)	1.472	(4-6)	1.529
(4-7)	1.526	(4-8)	1.531	(6-15)	1.090	(6-16)	1.516
(6-17)	1.092	(7-18)	1.089	(7-19)	1.089	(7-20)	1.088
(8-12)	1.089	(8-13)	1.087	(8-14)	1.086	(16-29)	1.090

(1-2-3)	104.1	(2-3-4)	108.1	(4-3-5)	120.3	(3-4-6)	107.3
(3-4-7)	106.7	(3-4-8)	114.8	(6-4-7)	108.4	(6-4-8)	111.3
(7-4-8)	108.1	(4-6-15)	108.3	(4-6-16)	113.1	(4-6-17)	108.3
(15-6-16)	111.1	(15-6-17)	107.0	(16-6-17)	108.8	(4-7-18)	110.1
(4-7-19)	110.3	(4-7-20)	111.1	(18-7-19)	108.5	(18-7-20)	107.9
(19-7-20)	108.8	(4-8-12)	109.4	(4-8-13)	110.2	(4-8-14)	113.1
(12-8-13)	108.1	(12-8-14)	107.4	(13-8-14)	108.5	(6-16-9)	109.4
(6-16-29)	110.0	(6-16-30)	110.7	(29-16-30)	106.1		

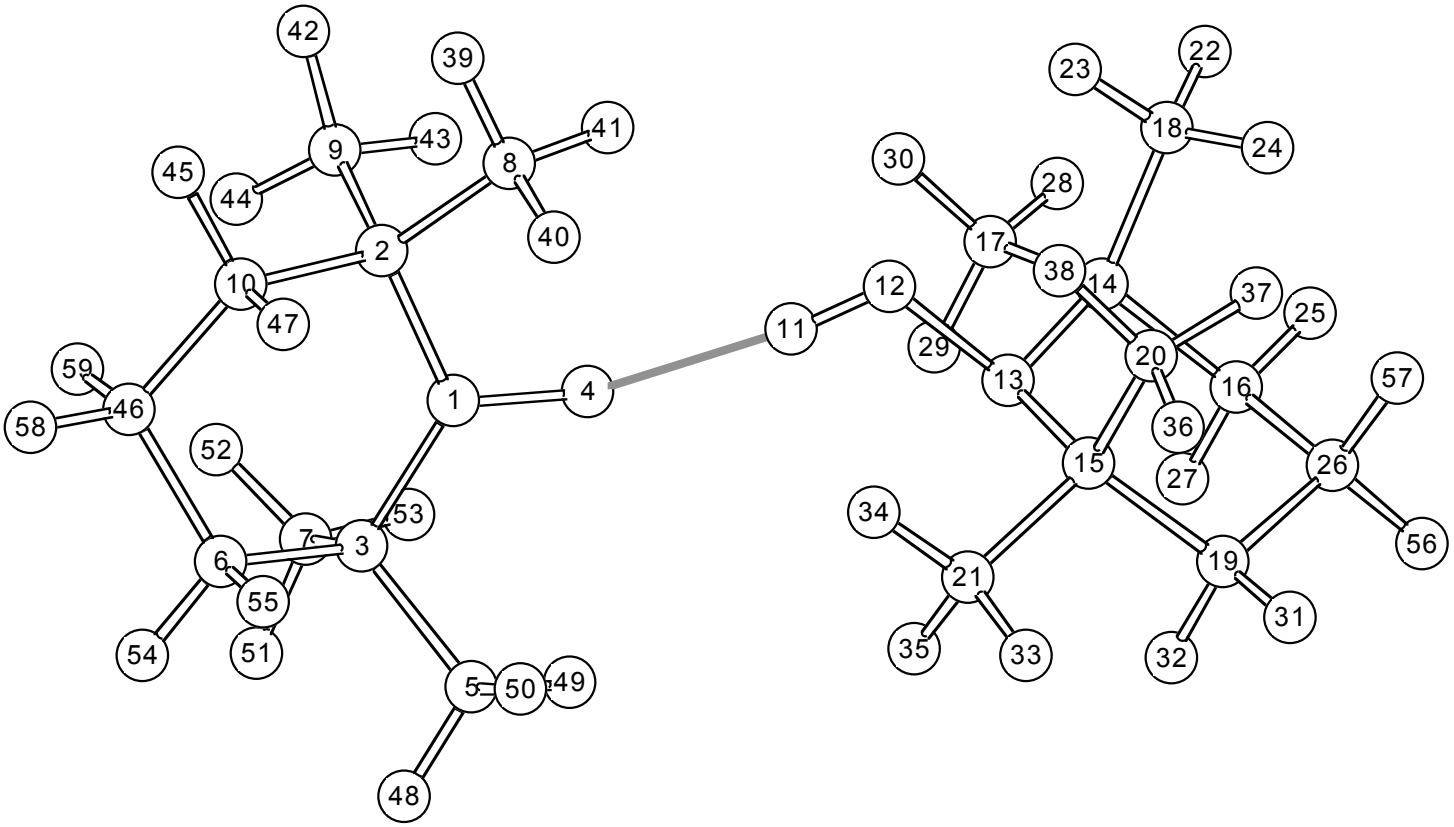
(1-2-3-4)	114.2	(2-3-4-6)	178.1	(2-3-4-7)	-65.9		
(2-3-4-8)	53.9	(5-3-4-6)	53.4	(5-3-4-7)	169.5		
(5-3-4-8)	-70.8	(3-4-6-15)	-176.0	(3-4-6-16)	-52.3		
(3-4-6-17)	68.3	(7-4-6-15)	69.1	(7-4-6-16)	-167.3		
(7-4-6-17)	-46.6	(8-4-6-15)	-49.6	(8-4-6-16)	74.0		
(8-4-6-17)	-165.3	(3-4-7-18)	-170.9	(3-4-7-19)	-51.2		

(3-4-7-20)	69.6	(6-4-7-18)	-55.6	(6-4-7-19)	64.1
(6-4-7-20)	-175.1	(8-4-7-18)	65.2	(8-4-7-19)	-175.2
(8-4-7-20)	-54.3	(3-4-8-12)	-165.2	(3-4-8-13)	-46.5
(3-4-8-14)	75.1	(6-4-8-12)	72.7	(6-4-8-13)	-168.6
(6-4-8-14)	-46.9	(7-4-8-12)	-46.2	(7-4-8-13)	72.5
(7-4-8-14)	-165.9	(4-6-16-9)	56.4	(4-6-16-29)	177.2
(4-6-16-30)	-65.8	(15-6-16-9)	178.4	(15-6-16-29)	-60.7
(15-6-16-30)	56.2	(17-6-16-9)	-64.1	(17-6-16-29)	56.8
(17-6-16-30)	173.8				
(bond)-(plane) angle		(2-3)-(4-3-5)	51.4		

Frequencies(cm^{-1}):	125.4	142.5	185.5	243.6	261.9	271.5	282.6	295.9	
296.4	312.3	332.7	363.7	365.5	392.2	411.1	429.6	471.0	483.0
537.9	593.1	604.4	700.2	812.7	834.3	885.6	916.7	958.2	963.8
964.6	992.2	1012.6	1026.1	1026.9	1075.0	1106.7	1107.6	1117.8	1136.4
1211.8	1254.5	1275.2	1275.9	1300.9	1326.1	1354.0	1361.8	1387.6	1408.9
1424.9	1426.3	1433.0	1436.4	1444.5	1452.4	1506.0	1514.2	1515.2	1524.7
1527.6	1535.1	1535.9	1540.7	1550.3	1553.4	1561.3	3113.0	3113.0	3119.5
3120.1	3125.1	3130.6	3134.2	3162.9	3166.5	3176.0	3202.8	3204.2	3208.3
3213.7	3216.4	3217.0	3232.3	3242.6	3992.7				

TEMPOH + TEMPO H-Bonded Complexe
^{2}A UMPW1K/6-31+G(d,p) C_1 Geometry

Nuclear repulsion energy	2098.110482 Hartree
UMPW1K/6-31+G(d,p) energy (<S^2> = 0.7571)	-967.903789 Hartree
Zero-point correction	0.552736 Hartree
Thermal correction to Enthalpy	0.579266 Hartree
Thermal correction to Gibbs Free Energy	0.494855 Hartree



	X	Y	Z		X	Y	Z
N1	-2.380214	0.033447	0.119788	H31	4.554232	2.362429	-0.832845
C2	-2.948446	-1.123319	-0.611768	H32	3.610616	2.325667	0.646369
C3	-3.178586	1.116575	0.740855	H33	2.266979	2.832398	-1.762448
O4	-1.219697	-0.124611	0.598487	H34	1.049080	1.557158	-1.794228
C5	-2.296913	2.356040	0.797813	H35	1.401042	2.396543	-0.280686
C6	-4.412751	1.409595	-0.108432	H36	3.588310	1.169051	-2.909011
C7	-3.561911	0.707071	2.162277	H37	4.345556	-0.175527	-2.077330
C8	-1.897793	-1.610754	-1.599054	H38	2.663074	-0.297189	-2.589215
C9	-3.260458	-2.241381	0.382270	H39	-2.331599	-2.393099	-2.219473
C10	-4.197391	-0.691996	-1.377098	H40	-1.568913	-0.801504	-2.247320
H11	0.489141	-0.431956	-0.160174	H41	-1.027986	-2.016248	-1.092770
O12	1.304987	-0.677448	-0.609830	H42	-3.519880	-3.148365	-0.161054
N13	2.320255	0.018608	0.067468	H43	-2.385220	-2.445242	0.993984
C14	3.169057	-0.960383	0.762271	H44	-4.091108	-1.996029	1.038905
C15	2.920798	0.980952	-0.867090	H45	-4.691676	-1.592651	-1.740876
C16	4.292403	-0.188091	1.453761	C46	-5.144125	0.162181	-0.559493
C17	2.300352	-1.609292	1.835494	H47	-3.889154	-0.126211	-2.258852
C18	3.729680	-2.071448	-0.130445	H48	-2.878949	3.190783	1.184478
C19	4.052256	1.696707	-0.129486	H49	-1.438974	2.195851	1.442496
C20	3.415453	0.374491	-2.183772	H50	-1.935184	2.617781	-0.194298
C21	1.839238	2.005236	-1.196779	H51	-4.001677	1.557893	2.679828
H22	4.107522	-2.882621	0.491090	H52	-4.284086	-0.104948	2.181390

H23	2.942999	-2.469546	-0.766271	H53	-2.674636	0.393375	2.706431
H24	4.547399	-1.738855	-0.762737	H54	-5.065854	2.065095	0.467471
H25	4.970995	-0.907096	1.914550	H55	-4.104435	1.972309	-0.992078
C26	5.037140	0.743305	0.517855	H56	5.791435	1.304048	1.070650
H27	3.854695	0.401646	2.261957	H57	5.577226	0.174963	-0.240575
H28	2.913123	-2.231264	2.487212	H58	-6.009319	0.436951	-1.161892
H29	1.812349	-0.845304	2.437563	H59	-5.531230	-0.393610	0.295374
H30	1.533497	-2.237512	1.389247				

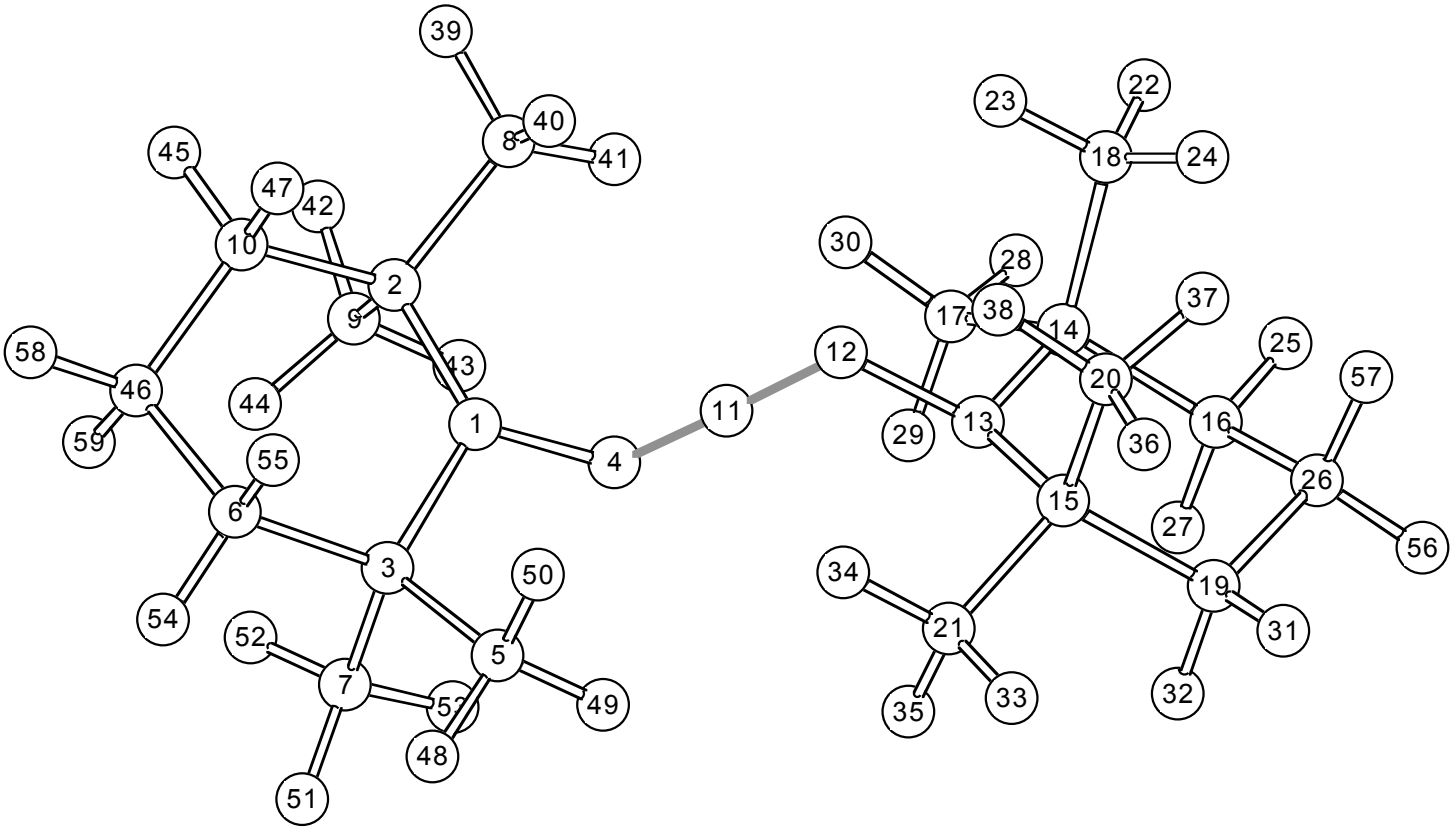
(1-2)	1.482	(1-3)	1.482	(1-4)	1.265	(2-8)	1.522
(2-9)	1.528	(2-10)	1.527	(3-5)	1.522	(3-6)	1.527
(3-7)	1.528	(4-11)	1.895	(5-48)	1.089	(5-49)	1.085
(5-50)	1.088	(6-46)	1.515	(6-54)	1.090	(6-55)	1.092
(7-51)	1.089	(7-52)	1.087	(7-53)	1.087	(8-39)	1.089
(8-40)	1.088	(8-41)	1.085	(9-42)	1.089	(9-43)	1.087
(9-44)	1.087	(10-45)	1.090	(10-46)	1.515	(10-47)	1.092
(11-12)	0.963	(12-13)	1.405	(13-14)	1.470	(13-15)	1.470
(14-16)	1.529	(14-17)	1.526	(14-18)	1.532	(15-19)	1.529
(15-20)	1.532	(15-21)	1.526	(16-25)	1.091	(16-26)	1.516
(16-27)	1.092	(17-28)	1.090	(17-29)	1.088	(17-30)	1.087
(18-22)	1.090	(18-23)	1.087	(18-24)	1.086	(19-26)	1.516
(19-31)	1.091	(19-32)	1.092	(20-36)	1.090	(20-37)	1.086
(20-38)	1.087	(21-33)	1.090	(21-34)	1.087	(21-35)	1.088
(26-56)	1.090	(26-57)	1.091	(46-58)	1.089	(46-59)	1.091
(2-1-3)	124.8	(2-1-4)	116.2	(3-1-4)	115.3	(1-2-8)	107.8
(1-2-9)	109.2	(1-2-10)	109.9	(8-2-9)	109.2	(8-2-10)	109.3
(9-2-10)	111.4	(1-3-5)	107.4	(1-3-6)	110.0	(1-3-7)	109.2
(5-3-6)	109.4	(5-3-7)	109.2	(6-3-7)	111.5	(1-4-11)	134.1
(3-5-48)	109.1	(3-5-49)	111.1	(3-5-50)	110.8	(48-5-49)	109.0
(48-5-50)	108.5	(49-5-50)	108.3	(3-6-46)	113.5	(3-6-54)	107.8
(3-6-55)	108.7	(46-6-54)	111.3	(46-6-55)	108.6	(54-6-55)	106.7
(3-7-51)	109.5	(3-7-52)	112.5	(3-7-53)	109.8	(51-7-52)	107.9
(51-7-53)	108.5	(52-7-53)	108.5	(2-8-39)	109.0	(2-8-40)	110.9
(2-8-41)	111.7	(39-8-40)	108.4	(39-8-41)	108.5	(40-8-41)	108.3
(2-9-42)	109.5	(2-9-43)	109.8	(2-9-44)	112.6	(42-9-43)	108.4
(42-9-44)	107.9	(43-9-44)	108.5	(2-10-45)	107.7	(2-10-46)	113.6
(2-10-47)	108.7	(45-10-46)	111.3	(45-10-47)	106.7	(46-10-47)	108.7
(4-11-12)	172.7	(11-12-13)	105.1	(12-13-14)	108.4	(12-13-15)	108.2
(14-13-15)	120.0	(13-14-16)	107.6	(13-14-17)	106.7	(13-14-18)	114.8
(16-14-17)	108.4	(16-14-18)	111.2	(17-14-18)	108.1	(13-15-19)	107.6
(13-15-20)	114.8	(13-15-21)	106.7	(19-15-20)	111.2	(19-15-21)	108.3
(20-15-21)	108.0	(14-16-25)	108.4	(14-16-26)	113.1	(14-16-27)	108.2
(25-16-26)	111.1	(25-16-27)	107.0	(26-16-27)	108.8	(14-17-28)	110.1
(14-17-29)	110.2	(14-17-30)	111.0	(28-17-29)	108.8	(28-17-30)	108.2
(29-17-30)	108.4	(14-18-22)	109.5	(14-18-23)	110.0	(14-18-24)	113.1
(22-18-23)	108.2	(22-18-24)	107.4	(23-18-24)	108.5	(15-19-26)	113.1
(15-19-31)	108.4	(15-19-32)	108.2	(26-19-31)	111.1	(26-19-32)	108.8
(31-19-32)	107.0	(15-20-36)	109.6	(15-20-37)	113.1	(15-20-38)	110.0
(36-20-37)	107.4	(36-20-38)	108.2	(37-20-38)	108.4	(15-21-33)	110.1
(15-21-34)	110.9	(15-21-35)	110.2	(33-21-34)	108.2	(33-21-35)	108.8
(34-21-35)	108.5	(16-26-19)	109.3	(16-26-56)	110.0	(16-26-57)	110.6
(19-26-56)	110.0	(19-26-57)	110.6	(56-26-57)	106.1	(6-46-10)	108.9
(6-46-58)	109.9	(6-46-59)	111.0	(10-46-58)	109.9	(10-46-59)	110.9
(58-46-59)	106.3						
(3-1-2-8)	154.1	(3-1-2-9)	-87.4	(3-1-2-10)	35.1		
(4-1-2-8)	-48.8	(4-1-2-9)	69.6	(4-1-2-10)	-167.8		
(2-1-3-5)	-154.2	(2-1-3-6)	-35.2	(2-1-3-7)	87.5		
(4-1-3-5)	48.6	(4-1-3-6)	167.6	(4-1-3-7)	-69.7		
(2-1-4-11)	63.7	(3-1-4-11)	-137.0	(1-2-8-39)	-174.1		

(1-2-8-40)	-54.9	(1-2-8-41)	66.0	(9-2-8-39)	67.4
(9-2-8-40)	-173.4	(9-2-8-41)	-52.4	(10-2-8-39)	-54.7
(10-2-8-40)	64.5	(10-2-8-41)	-174.6	(1-2-9-42)	-170.6
(1-2-9-43)	-51.7	(1-2-9-44)	69.4	(8-2-9-42)	-53.0
(8-2-9-43)	65.9	(8-2-9-44)	-173.0	(10-2-9-42)	67.8
(10-2-9-43)	-173.3	(10-2-9-44)	-52.2	(1-2-10-45)	-169.3
(1-2-10-46)	-45.6	(1-2-10-47)	75.5	(8-2-10-45)	72.6
(8-2-10-46)	-163.7	(8-2-10-47)	-42.6	(9-2-10-45)	-48.1
(9-2-10-46)	75.6	(9-2-10-47)	-163.3	(1-3-5-48)	176.0
(1-3-5-49)	-63.8	(1-3-5-50)	56.6	(6-3-5-48)	56.6
(6-3-5-49)	176.7	(6-3-5-50)	-62.8	(7-3-5-48)	-65.7
(7-3-5-49)	54.5	(7-3-5-50)	174.9	(1-3-6-46)	45.6
(1-3-6-54)	169.3	(1-3-6-55)	-75.4	(5-3-6-46)	163.4
(5-3-6-54)	-72.9	(5-3-6-55)	42.4	(7-3-6-46)	-75.7
(7-3-6-54)	48.0	(7-3-6-55)	163.3	(1-3-7-51)	170.6
(1-3-7-52)	-69.4	(1-3-7-53)	51.6	(5-3-7-51)	53.5
(5-3-7-52)	173.4	(5-3-7-53)	-65.6	(6-3-7-51)	-67.6
(6-3-7-52)	52.4	(6-3-7-53)	173.4	(1-4-11-12)	-49.9
(3-6-46-10)	-59.4	(3-6-46-58)	-179.8	(3-6-46-59)	63.0
(54-6-46-10)	178.8	(54-6-46-58)	58.4	(54-6-46-59)	-58.8
(55-6-46-10)	61.6	(55-6-46-58)	-58.8	(55-6-46-59)	-176.0
(2-10-46-6)	59.4	(2-10-46-58)	179.9	(2-10-46-59)	-62.9
(45-10-46-6)	-178.8	(45-10-46-58)	-58.4	(45-10-46-59)	58.9
(47-10-46-6)	-61.6	(47-10-46-58)	58.8	(47-10-46-59)	176.0
(4-11-12-13)	-169.1	(11-12-13-14)	112.9	(11-12-13-15)	-115.5
(12-13-14-16)	178.2	(12-13-14-17)	-65.7	(12-13-14-18)	53.9
(15-13-14-16)	53.2	(15-13-14-17)	169.3	(15-13-14-18)	-71.1
(12-13-15-19)	-178.2	(12-13-15-20)	-53.9	(12-13-15-21)	65.7
(14-13-15-19)	-53.2	(14-13-15-20)	71.2	(14-13-15-21)	-169.2
(13-14-16-25)	-176.0	(13-14-16-26)	-52.4	(13-14-16-27)	68.2
(17-14-16-25)	69.0	(17-14-16-26)	-167.3	(17-14-16-27)	-46.7
(18-14-16-25)	-49.6	(18-14-16-26)	74.1	(18-14-16-27)	-165.3
(13-14-17-28)	-171.1	(13-14-17-29)	-51.1	(13-14-17-30)	69.1
(16-14-17-28)	-55.6	(16-14-17-29)	64.4	(16-14-17-30)	-175.4
(18-14-17-28)	65.0	(18-14-17-29)	-175.0	(18-14-17-30)	-54.8
(13-14-18-22)	-164.7	(13-14-18-23)	-45.9	(13-14-18-24)	75.5
(16-14-18-22)	73.0	(16-14-18-23)	-168.3	(16-14-18-24)	-46.8
(17-14-18-22)	-45.8	(17-14-18-23)	72.9	(17-14-18-24)	-165.6
(13-15-19-26)	52.3	(13-15-19-31)	175.9	(13-15-19-32)	-68.3
(20-15-19-26)	-74.2	(20-15-19-31)	49.5	(20-15-19-32)	165.2
(21-15-19-26)	167.3	(21-15-19-31)	-69.1	(21-15-19-32)	46.7
(13-15-20-36)	164.7	(13-15-20-37)	-75.5	(13-15-20-38)	45.9
(19-15-20-36)	-72.9	(19-15-20-37)	46.9	(19-15-20-38)	168.3
(21-15-20-36)	45.8	(21-15-20-37)	165.6	(21-15-20-38)	-73.0
(13-15-21-33)	171.2	(13-15-21-34)	-69.0	(13-15-21-35)	51.2
(19-15-21-33)	55.6	(19-15-21-34)	175.4	(19-15-21-35)	-64.4
(20-15-21-33)	-64.9	(20-15-21-34)	54.9	(20-15-21-35)	175.1
(14-16-26-19)	56.2	(14-16-26-56)	177.2	(14-16-26-57)	-65.9
(25-16-26-19)	178.4	(25-16-26-56)	-60.7	(25-16-26-57)	56.3
(27-16-26-19)	-64.1	(27-16-26-56)	56.9	(27-16-26-57)	173.8
(15-19-26-16)	-56.2	(15-19-26-56)	-177.1	(15-19-26-57)	65.9
(31-19-26-16)	-178.3	(31-19-26-56)	60.7	(31-19-26-57)	-56.2
(32-19-26-16)	64.1	(32-19-26-56)	-56.8	(32-19-26-57)	-173.8
(bond)-(plane) angle		(4-1)-(2-1-3)	20.5		
(bond)-(plane) angle		(12-13)-(14-13-15)	51.1		

Frequencies(cm^{-1}):	7.5	11.5	18.4	29.1	39.7	57.6	98.2	123.6	
	142.9	151.0	189.9	210.8	213.2	245.1	257.1	259.8	264.4	268.7
	280.6	286.8	292.2	295.9	296.6	299.8	313.6	314.1	323.7	337.6
	343.3	367.4	367.5	390.3	411.4	413.0	415.1	429.2	463.0	472.5
	481.7	483.5	534.9	556.9	577.7	592.6	594.6	607.9	668.2	676.1
	704.7	812.6	825.3	835.7	840.2	885.3	890.6	915.9	920.6	958.4
	963.4	964.3	965.0	970.7	972.1	992.0	998.0	1012.0	1019.8	1025.7
	1026.6	1035.7	1037.2	1079.3	1092.6	1106.1	1108.9	1109.5	1110.7	1134.2
	1135.5	1139.2	1208.3	1212.3	1244.1	1255.2	1269.0	1274.7	1276.1	1280.9
	1299.6	1299.7	1317.6	1326.9	1340.2	1354.8	1362.0	1362.7	1408.2	1409.0
	1422.0	1423.7	1426.5	1429.5	1431.2	1434.7	1439.0	1440.8	1442.2	1444.6
	1451.5	1454.4	1465.5	1505.0	1506.5	1512.5	1513.6	1514.0	1518.2	1522.9
	1523.3	1527.1	1527.8	1532.2	1533.2	1534.5	1535.1	1538.0	1538.8	1543.1
	1546.9	1548.3	1549.7	1553.1	1560.6	1561.7	3110.2	3110.7	3114.7	3115.6
	3118.4	3119.3	3121.8	3127.6	3127.7	3127.9	3130.6	3131.2	3132.3	3134.2
	3158.4	3162.6	3170.1	3170.9	3172.5	3180.0	3200.8	3202.7	3205.4	3210.8
	3210.8	3213.2	3214.5	3217.4	3219.8	3221.1	3228.2	3230.6	3232.7	3240.2
	3244.9	3245.3	3830.8							

TEMPOH + TEMPO H-Transfer Transition Structure
^{2}A UMPW1K/6-31+G(d,p) C_1 Geometry

Nuclear repulsion energy	2158.721460 Hartree
UMPW1K/6-31+G(d,p) energy ($<S^2>$ = 0.7608)	-967.869274 Hartree
Zero-point correction	0.547159 Hartree
Thermal correction to Enthalpy	0.572788 Hartree
Thermal correction to Gibbs Free Energy	0.494434 Hartree



	X	Y	Z		X	Y	Z
N1	-0.033899	2.073567	-0.029139	H31	0.167630	-4.614533	-2.245268
C2	-0.338847	2.754660	1.240966	H32	1.547670	-3.677994	-1.706595
C3	0.351238	2.801012	-1.250055	H33	-0.305874	-2.403886	-3.361057
O4	0.674348	0.965382	0.139887	H34	-0.804828	-1.018301	-2.387210

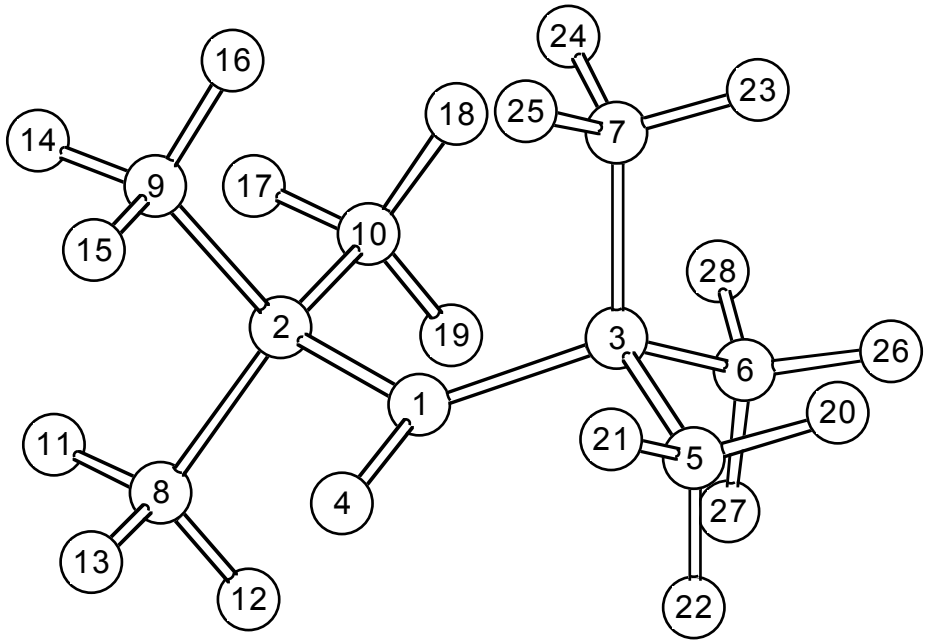
C5	0.128846	1.866081	-2.430830	H35	0.893814	-1.494633	-2.433742
C6	-0.552495	4.020866	-1.415676	H36	-2.130510	-3.554510	-2.209394
C7	1.828144	3.204982	-1.223130	H37	-2.032353	-4.001298	-0.513093
C8	-1.138411	1.784221	2.102060	H38	-2.438606	-2.344647	-0.960575
C9	0.935007	3.141753	1.996671	H39	-1.487783	2.295691	2.997813
C10	-1.209452	3.977554	0.958065	H40	-1.999462	1.406281	1.555417
H11	0.000000	0.000000	0.115303	H41	-0.531220	0.938069	2.406667
O12	-0.674348	-0.965382	0.139887	H42	0.682317	3.439719	3.013347
N13	0.033899	-2.073567	-0.029139	H43	1.605927	2.287734	2.044849
C14	0.338847	-2.754660	1.240966	H44	1.463320	3.969173	1.531323
C15	-0.351238	-2.801012	-1.250055	H45	-1.311869	4.539252	1.886921
C16	1.209452	-3.977554	0.958065	C46	-0.674348	4.852563	-0.156016
C17	1.138411	-1.784221	2.102060	H47	-2.209407	3.634660	0.684081
C18	-0.935007	-3.141753	1.996671	H48	0.305874	2.403886	-3.361057
C19	0.552495	-4.020866	-1.415676	H49	0.804828	1.018301	-2.387210
C20	-1.828144	-3.204982	-1.223130	H50	-0.893814	1.494633	-2.433742
C21	-0.128846	-1.866081	-2.430830	H51	2.130510	3.554510	-2.209394
H22	-0.682317	-3.439719	3.013347	H52	2.032353	4.001298	-0.513093
H23	-1.605927	-2.287734	2.044849	H53	2.438606	2.344647	-0.960575
H24	-1.463320	-3.969173	1.531323	H54	-0.167630	4.614533	-2.245268
H25	1.311869	-4.539252	1.886921	H55	-1.547670	3.677994	-1.706595
C26	0.674348	-4.852563	-0.156016	H56	1.347633	-5.692474	-0.326859
H27	2.209407	-3.634660	0.684081	H57	-0.288875	-5.284559	0.118275
H28	1.487783	-2.295691	2.997813	H58	-1.347633	5.692474	-0.326859
H29	1.999462	-1.406281	1.555417	H59	0.288875	5.284559	0.118275
H30	0.531220	-0.938069	2.406667				

(1-2)	1.473	(1-3)	1.472	(1-4)	1.326	(2-8)	1.524	(2-9)	1.531
(2-10)	1.528	(3-5)	1.522	(3-6)	1.527	(3-7)	1.531	(4-11)	1.178
(5-48)	1.089	(5-49)	1.085	(5-50)	1.088	(6-46)	1.514	(6-54)	1.090
(6-55)	1.092	(7-51)	1.089	(7-52)	1.086	(7-53)	1.087	(8-39)	1.089
(8-40)	1.088	(8-41)	1.085	(9-42)	1.089	(9-43)	1.087	(9-44)	1.086
(10-45)	1.090	(10-46)	1.514	(10-47)	1.092	(26-56)	1.090	(26-57)	1.091
(2-1-3)	122.7	(2-1-4)	112.8	(3-1-4)	112.3	(1-2-8)	107.5		
(1-2-9)	111.7	(1-2-10)	109.2	(8-2-9)	108.6	(8-2-10)	108.4		
(9-2-10)	111.3	(1-3-5)	107.5	(1-3-6)	109.3	(1-3-7)	111.6		
(5-3-6)	108.7	(5-3-7)	108.5	(6-3-7)	111.2	(1-4-11)	112.1		
(3-5-48)	109.6	(3-5-49)	111.0	(3-5-50)	110.4	(48-5-49)	108.6		
(48-5-50)	108.6	(49-5-50)	108.6	(3-6-46)	113.3	(3-6-54)	108.0		
(3-6-55)	108.5	(46-6-54)	111.2	(46-6-55)	108.7	(54-6-55)	106.9		
(3-7-51)	109.7	(3-7-52)	112.7	(3-7-53)	109.7	(51-7-52)	107.7		
(51-7-53)	108.5	(52-7-53)	108.5	(2-8-39)	109.5	(2-8-40)	110.6		
(2-8-41)	111.2	(39-8-40)	108.8	(39-8-41)	108.4	(40-8-41)	108.2		
(2-9-42)	109.7	(2-9-43)	109.7	(2-9-44)	112.7	(42-9-43)	108.5		
(42-9-44)	107.7	(43-9-44)	108.5	(2-10-45)	107.9	(2-10-46)	113.4		
(2-10-47)	108.5	(45-10-46)	111.2	(45-10-47)	106.8	(46-10-47)	108.7		
(4-11-12)	177.6	(16-26-19)	108.8	(16-26-56)	110.0	(16-26-57)	110.8		
(19-26-56)	110.0	(19-26-57)	110.8	(56-26-57)	106.2				
(3-1-2-8)	160.8	(3-1-2-9)	-80.2	(3-1-2-10)	43.4				
(4-1-2-8)	-59.9	(4-1-2-9)	59.1	(4-1-2-10)	-177.3				
(2-1-3-5)	-161.2	(2-1-3-6)	-43.4	(2-1-3-7)	80.0				
(4-1-3-5)	59.3	(4-1-3-6)	177.1	(4-1-3-7)	-59.5				
(2-1-4-11)	98.9	(3-1-4-11)	-117.4	(1-2-8-39)	-173.0				
(1-2-8-40)	-53.0	(1-2-8-41)	67.3	(9-2-8-39)	65.9				
(9-2-8-40)	-174.1	(9-2-8-41)	-53.8	(10-2-8-39)	-55.1				
(10-2-8-40)	64.9	(10-2-8-41)	-174.8	(1-2-9-42)	-167.7				

(1-2-9-43)	-48.7	(1-2-9-44)	72.3	(8-2-9-42)	-49.3
(8-2-9-43)	69.8	(8-2-9-44)	-169.3	(10-2-9-42)	70.0
(10-2-9-43)	-171.0	(10-2-9-44)	-50.0	(1-2-10-45)	-172.5
(1-2-10-46)	-48.8	(1-2-10-47)	72.1	(8-2-10-45)	70.6
(8-2-10-46)	-165.7	(8-2-10-47)	-44.8	(9-2-10-45)	-48.7
(9-2-10-46)	75.0	(9-2-10-47)	-164.1	(1-3-5-48)	174.2
(1-3-5-49)	-65.9	(1-3-5-50)	54.6	(6-3-5-48)	56.1
(6-3-5-49)	176.0	(6-3-5-50)	-63.5	(7-3-5-48)	-65.0
(7-3-5-49)	55.0	(7-3-5-50)	175.4	(1-3-6-46)	48.9
(1-3-6-54)	172.6	(1-3-6-55)	-72.0	(5-3-6-46)	166.0
(5-3-6-54)	-70.4	(5-3-6-55)	45.1	(7-3-6-46)	-74.7
(7-3-6-54)	48.9	(7-3-6-55)	164.4	(1-3-7-51)	168.5
(1-3-7-52)	-71.5	(1-3-7-53)	49.5	(5-3-7-51)	50.3
(5-3-7-52)	170.3	(5-3-7-53)	-68.8	(6-3-7-51)	-69.2
(6-3-7-52)	50.8	(6-3-7-53)	171.8	(1-4-11-12)	-98.4
(3-6-46-10)	-58.0	(3-6-46-58)	-178.7	(3-6-46-59)	64.1
(54-6-46-10)	-179.9	(54-6-46-58)	59.5	(54-6-46-59)	-57.7
(55-6-46-10)	62.7	(55-6-46-58)	-57.9	(55-6-46-59)	-175.1
(2-10-46-6)	58.0	(2-10-46-58)	178.7	(2-10-46-59)	-64.1
(45-10-46-6)	179.9	(45-10-46-58)	-59.4	(45-10-46-59)	57.8
(47-10-46-6)	-62.7	(47-10-46-58)	57.9	(47-10-46-59)	175.1
(bond)-(plane) angle		(4-1)-(2-1-3)	37.0		
(bond)-(plane) angle		(12-13)-(14-13-15)	37.0		

Frequencies(cm^{-1}):	-3138.9	14.7	26.8	48.1	58.1	70.0	107.1	113.6	
134.6	135.1	188.9	201.4	201.6	237.3	245.7	251.3	261.7	263.5
277.9	280.3	296.7	297.4	298.3	298.7	313.5	313.7	324.3	332.6
347.8	348.8	371.5	375.7	415.7	420.3	421.9	424.9	467.1	471.6
483.4	485.4	534.1	545.7	552.5	591.5	596.5	604.7	681.8	697.4
732.6	817.6	818.4	838.8	849.9	888.0	888.2	918.2	918.7	961.2
962.0	965.4	965.7	967.1	967.9	994.9	995.2	1016.8	1017.3	1029.4
1029.8	1033.2	1034.8	1088.2	1088.6	1095.6	1108.5	1109.1	1115.2	1116.3
1137.1	1137.8	1210.6	1210.9	1241.5	1244.4	1264.4	1271.1	1276.6	1277.7
1299.5	1299.5	1303.1	1303.1	1346.5	1347.3	1360.0	1361.1	1368.4	1370.6
1408.8	1408.9	1423.3	1423.9	1424.2	1425.1	1435.3	1435.5	1440.4	1440.7
1444.5	1446.8	1451.4	1452.8	1504.7	1504.9	1512.2	1512.4	1515.4	1515.7
1522.4	1522.6	1523.6	1527.5	1528.8	1531.7	1532.3	1536.6	1537.4	1539.5
1542.7	1547.7	1547.7	1550.1	1556.0	1561.9	1711.9	3112.8	3112.9	3113.4
3113.5	3124.7	3125.0	3125.3	3125.7	3126.8	3127.4	3129.7	3130.3	3131.0
3132.9	3164.1	3164.5	3166.7	3166.7	3176.4	3176.4	3206.2	3206.6	3208.9
3209.3	3211.9	3212.0	3214.0	3214.3	3229.1	3229.2	3236.3	3236.4	3241.4
3242.9	3243.1	3244.7							

Di-t-Butylhydroxylamine + Di-t-butylnitroxyl Radical Transition Structure $^2B_2$ UMPW1K/6-31+G(d,p) C_{2h} Geometry	
Nuclear repulsion energy	625.815492 Hartree
UMPW1K/6-31+G(d,p) energy ($<S^2>$ = 0.7574)	-445.522224 Hartree
Zero-point correction	0.260563 Hartree
Thermal correction to Enthalpy	0.273779 Hartree
Thermal correction to Gibbs Free Energy	0.223461 Hartree



	X	Y	Z		X	Y	Z
N1	0.002211	-0.522345	-0.188039	H15	-1.767530	-1.230067	1.617555
C2	-1.335483	0.111728	-0.011964	H16	-1.216815	0.362707	2.149160
C3	1.341637	0.109149	-0.012134	H17	-2.383209	1.951185	-0.136695
O4	-0.034163	-1.786924	-0.115320	H18	-0.731252	2.180053	0.386805
C5	2.383083	-0.983940	-0.219226	H19	-1.087651	1.836426	-1.313009
C6	1.592282	1.193613	-1.058919	H20	3.370986	-0.536456	-0.127786
C7	1.496718	0.667252	1.401188	H21	2.284533	-1.776496	0.514068
C8	-2.270643	-0.569718	-1.006992	H22	2.292200	-1.430250	-1.205867
C9	-1.817558	-0.164316	1.411281	H23	2.509327	1.046362	1.530877
C10	-1.361734	1.607022	-0.286744	H24	0.812914	1.486662	1.606071
H11	-3.272057	-0.155007	-0.907249	H25	1.331362	-0.114781	2.139202
H12	-1.930486	-0.404930	-2.027789	H26	2.649589	1.451772	-1.048390
H13	-2.310093	-1.638566	-0.827588	H27	1.348368	0.828370	-2.054548
H14	-2.849958	0.163292	1.522209	H28	1.037790	2.106792	-0.877129

(1-2)	1.491	(1-3)	1.491	(1-4)	1.267	(2-8)	1.526	(2-9)	1.528
(2-10)	1.521	(3-5)	1.524	(3-6)	1.528	(3-7)	1.527	(5-20)	1.088
(5-21)	1.084	(5-22)	1.087	(6-26)	1.088	(6-27)	1.088	(6-28)	1.084
(7-23)	1.089	(7-24)	1.087	(7-25)	1.088	(8-11)	1.088	(8-12)	1.089
(8-13)	1.085	(9-14)	1.089	(9-15)	1.087	(9-16)	1.088	(10-17)	1.088
(10-18)	1.086	(10-19)	1.087						

(2-1-3)	127.7	(2-1-4)	113.1	(3-1-4)	116.2	(1-2-8)	106.4
(1-2-9)	108.4	(1-2-10)	114.4	(8-2-9)	109.5	(8-2-10)	108.1
(9-2-10)	109.9	(1-3-5)	107.1	(1-3-6)	111.5	(1-3-7)	110.8
(5-3-6)	107.7	(5-3-7)	108.6	(6-3-7)	111.0	(3-5-20)	108.3
(3-5-21)	111.7	(3-5-22)	111.2	(20-5-21)	109.0	(20-5-22)	108.7
(21-5-22)	107.8	(3-6-26)	108.7	(3-6-27)	110.6	(3-6-28)	113.5
(26-6-27)	107.8	(26-6-28)	107.2	(27-6-28)	108.8	(3-7-23)	109.4

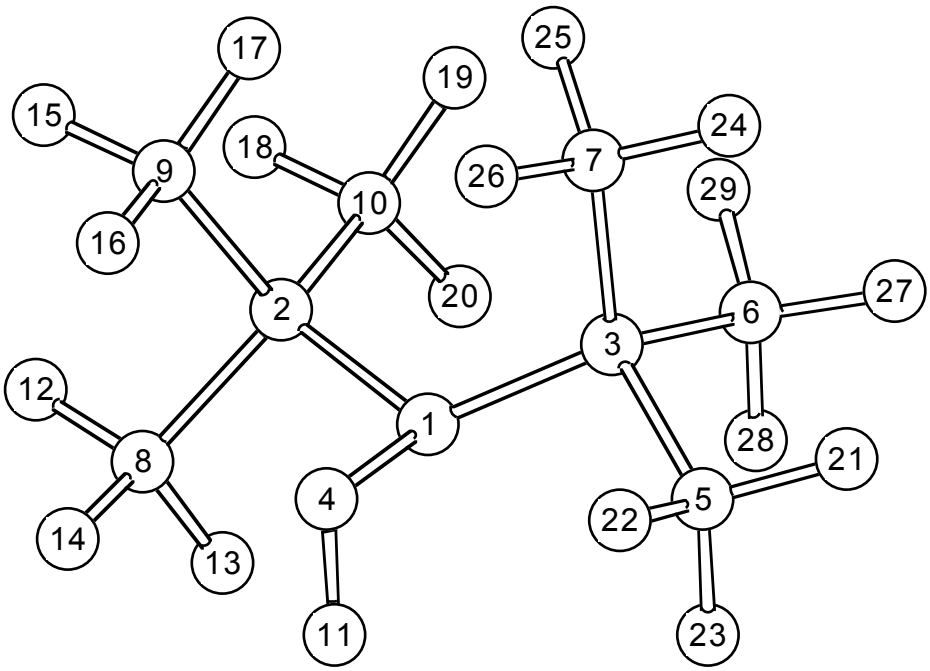
(3-7-24)	112.7	(3-7-25)	110.5	(23-7-24)	107.5	(23-7-25)	108.1
(24-7-25)	108.6	(2-8-11)	109.5	(2-8-12)	110.6	(2-8-13)	110.8
(11-8-12)	108.4	(11-8-13)	109.1	(12-8-13)	108.4	(2-9-14)	109.9
(2-9-15)	109.8	(2-9-16)	111.7	(14-9-15)	108.6	(14-9-16)	108.0
(15-9-16)	108.7	(2-10-17)	107.6	(2-10-18)	113.4	(2-10-19)	112.0
(17-10-18)	107.0	(17-10-19)	107.5	(18-10-19)	109.1		
(3-1-2-8)	148.0	(3-1-2-9)	-94.3	(3-1-2-10)	28.7		
(4-1-2-8)	-52.5	(4-1-2-9)	65.1	(4-1-2-10)	-171.8		
(2-1-3-5)	176.3	(2-1-3-6)	-66.1	(2-1-3-7)	58.1		
(4-1-3-5)	17.4	(4-1-3-6)	135.0	(4-1-3-7)	-100.8		
(1-2-8-11)	178.9	(1-2-8-12)	-61.6	(1-2-8-13)	58.6		
(9-2-8-11)	61.9	(9-2-8-12)	-178.6	(9-2-8-13)	-58.4		
(10-2-8-11)	-57.8	(10-2-8-12)	61.6	(10-2-8-13)	-178.1		
(1-2-9-14)	-171.9	(1-2-9-15)	-52.5	(1-2-9-16)	68.3		
(8-2-9-14)	-56.2	(8-2-9-15)	63.3	(8-2-9-16)	-176.0		
(10-2-9-14)	62.4	(10-2-9-15)	-178.2	(10-2-9-16)	-57.4		
(1-2-10-17)	179.4	(1-2-10-18)	-62.4	(1-2-10-19)	61.6		
(8-2-10-17)	61.1	(8-2-10-18)	179.2	(8-2-10-19)	-56.8		
(9-2-10-17)	-58.3	(9-2-10-18)	59.8	(9-2-10-19)	-176.2		
(1-3-5-20)	178.1	(1-3-5-21)	-61.7	(1-3-5-22)	58.8		
(6-3-5-20)	58.1	(6-3-5-21)	178.2	(6-3-5-22)	-61.3		
(7-3-5-20)	-62.2	(7-3-5-21)	57.9	(7-3-5-22)	178.5		
(1-3-6-26)	-166.4	(1-3-6-27)	-48.2	(1-3-6-28)	74.4		
(5-3-6-26)	-49.2	(5-3-6-27)	69.1	(5-3-6-28)	-168.4		
(7-3-6-26)	69.5	(7-3-6-27)	-172.2	(7-3-6-28)	-49.7		
(1-3-7-23)	175.2	(1-3-7-24)	-65.3	(1-3-7-25)	56.4		
(5-3-7-23)	57.9	(5-3-7-24)	177.4	(5-3-7-25)	-61.0		
(6-3-7-23)	-60.3	(6-3-7-24)	59.2	(6-3-7-25)	-179.1		
(bond)-(plane) angle		(4-1)-(2-1-3)	18.8				

Frequencies(cm^{-1}):	56.8	85.2	184.2	201.4	228.9	262.1	266.0	273.7	
293.1	306.2	322.8	334.6	358.2	375.1	396.2	420.2	428.9	447.6
553.6	558.5	563.9	667.1	830.7	874.8	959.4	960.3	965.3	968.6
983.9	988.0	1043.2	1068.2	1073.4	1081.0	1113.4	1269.2	1277.7	1285.1
1292.0	1314.3	1323.0	1429.7	1433.8	1438.0	1442.1	1463.7	1468.8	1506.4
1508.4	1516.5	1520.6	1522.9	1528.3	1529.7	1535.5	1536.5	1548.1	1551.4
1562.3	1570.6	3125.2	3126.3	3129.2	3132.5	3137.2	3140.1	3206.3	3207.8
3209.4	3209.9	3215.1	3222.6	3223.1	3231.6	3236.3	3249.7	3250.6	3251.7

Di-t-butylhydroxylamine

^{1}A MPW1K/6-31+G(d,p) C_1 Geometry

Nuclear repulsion energy	641.599066 Hartree
UMPW1K/6-31+G(d,p) energy	-446.135689 Hartree
Zero-point correction	0.273057 Hartree
Thermal correction to Enthalpy	0.286327 Hartree
Thermal correction to Gibbs Free Energy	0.236965 Hartree



	X	Y	Z		X	Y	Z
N1	0.002846	-0.419237	-0.436265	H16	-1.594128	-1.207922	1.643075
C2	-1.310370	0.140932	-0.031270	H17	-1.105070	0.415236	2.131715
C3	1.313726	0.135374	-0.016326	H18	-2.428405	1.948354	-0.154153
O4	-0.035980	-1.771939	-0.019767	H19	-0.803875	2.212997	0.434952
C5	2.375215	-0.862315	-0.485710	H20	-1.083291	1.901182	-1.286714
C6	1.597799	1.437360	-0.764335	H21	3.363174	-0.427141	-0.349369
C7	1.475669	0.339071	1.488367	H22	2.333810	-1.790437	0.075001
C8	-2.334807	-0.529664	-0.948358	H23	2.249151	-1.083157	-1.545289
C9	-1.699675	-0.150264	1.420673	H24	2.514642	0.571776	1.719441
C10	-1.391738	1.640329	-0.277161	H25	0.869661	1.163613	1.856754
H11	0.039616	-2.266000	-0.833054	H26	1.204614	-0.564729	2.029644
H12	-3.330013	-0.132257	-0.755626	H27	2.651441	1.684970	-0.647650
H13	-2.084396	-0.345557	-1.991605	H28	1.394104	1.316542	-1.826435
H14	-2.366989	-1.602811	-0.780202	H29	1.031104	2.284247	-0.397107
H15	-2.742145	0.126334	1.573326				

(1-2)	1.484	(1-3)	1.484	(1-4)	1.416	(2-8)	1.530	(2-9)	1.531	
(2-10)	1.522	(3-5)	1.531	(3-6)	1.528	(3-7)	1.527	(4-11)	0.955	
(5-21)	1.088	(5-22)	1.085	(5-23)	1.090	(6-27)	1.089	(6-28)	1.088	
(6-29)	1.083	(7-24)	1.090	(7-25)	1.088	(7-26)	1.088	(8-12)	1.089	
(8-13)	1.089	(8-14)	1.087	(9-15)	1.089	(9-16)	1.086	(9-17)	1.086	
(10-18)	1.088	(10-19)	1.087	(10-20)	1.087					
(2-1-3)	124.3	(2-1-4)	104.8	(3-1-4)	107.3	(1-2-8)	105.3			
(1-2-9)	114.3	(1-2-10)	112.0	(8-2-9)	108.4	(8-2-10)	107.4			
(9-2-10)	109.1	(1-3-5)	106.4	(1-3-6)	110.1	(1-3-7)	115.0			
(5-3-6)	106.0	(5-3-7)	108.4	(6-3-7)	110.4	(1-4-11)	104.0			
(3-5-21)	109.3	(3-5-22)	111.9	(3-5-23)	110.5	(21-5-22)	108.2			
(21-5-23)	107.9	(22-5-23)	108.9	(3-6-27)	108.7	(3-6-28)	110.4			

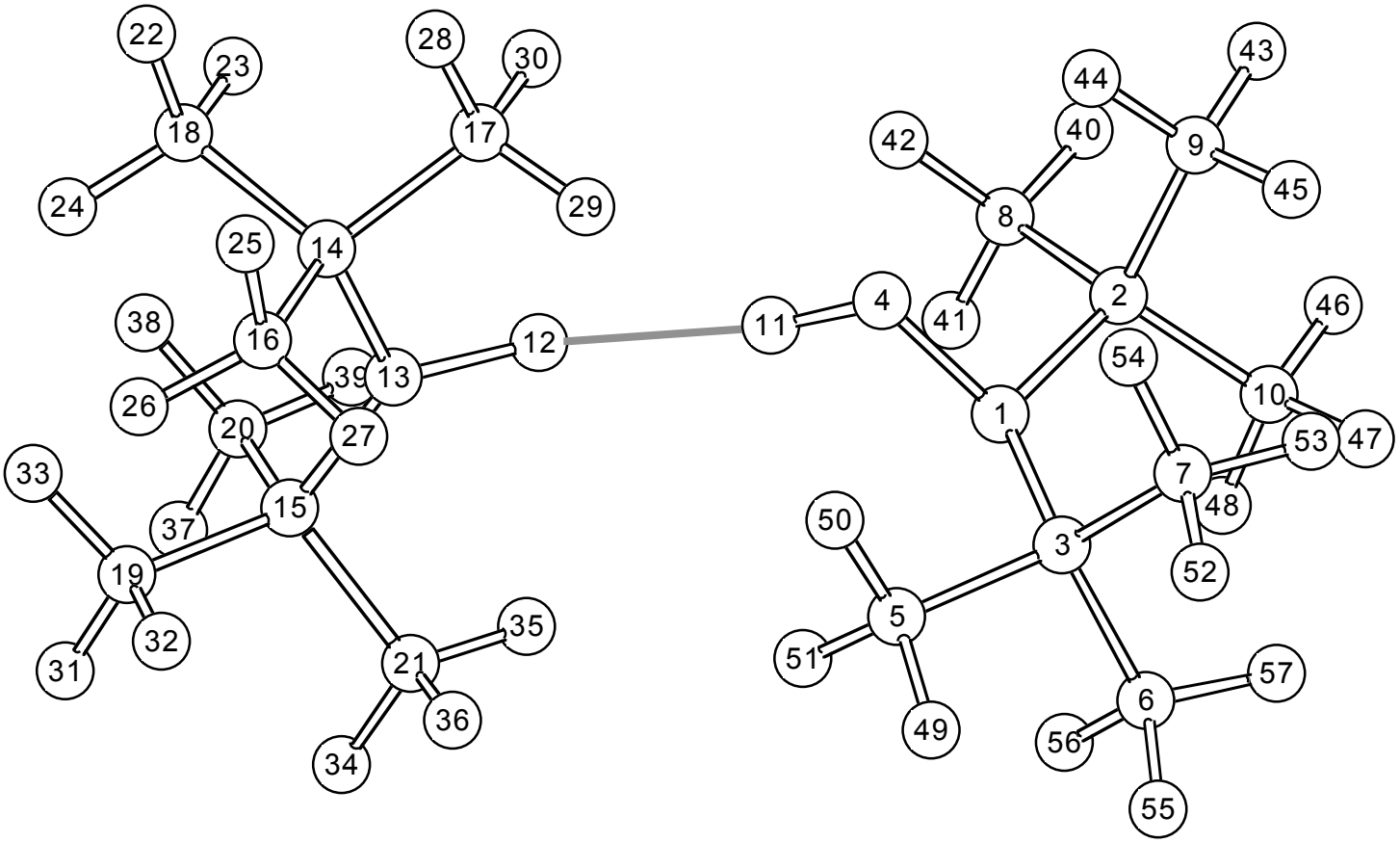
(3-6-29)	113.8	(27-6-28)	108.1	(27-6-29)	107.0	(28-6-29)	108.6
(3-7-24)	109.8	(3-7-25)	112.1	(3-7-26)	110.7	(24-7-25)	107.3
(24-7-26)	108.0	(25-7-26)	108.8	(2-8-12)	110.2	(2-8-13)	110.3
(2-8-14)	111.1	(12-8-13)	108.6	(12-8-14)	107.8	(13-8-14)	108.8
(2-9-15)	109.1	(2-9-16)	110.8	(2-9-17)	112.5	(15-9-16)	108.2
(15-9-17)	107.5	(16-9-17)	108.7	(2-10-18)	108.2	(2-10-19)	112.6
(2-10-20)	111.8	(18-10-19)	107.0	(18-10-20)	107.9	(19-10-20)	109.2
(3-1-2-8)	167.0	(3-1-2-9)	-74.2	(3-1-2-10)	50.5		
(4-1-2-8)	-69.4	(4-1-2-9)	49.4	(4-1-2-10)	174.2		
(2-1-3-5)	171.8	(2-1-3-6)	-73.7	(2-1-3-7)	51.8		
(4-1-3-5)	49.3	(4-1-3-6)	163.8	(4-1-3-7)	-70.7		
(2-1-4-11)	117.7	(3-1-4-11)	-108.4	(1-2-8-12)	-176.9		
(1-2-8-13)	-57.0	(1-2-8-14)	63.7	(9-2-8-12)	60.4		
(9-2-8-13)	-179.7	(9-2-8-14)	-59.1	(10-2-8-12)	-57.3		
(10-2-8-13)	62.5	(10-2-8-14)	-176.8	(1-2-9-15)	-169.3		
(1-2-9-16)	-50.3	(1-2-9-17)	71.5	(8-2-9-15)	-52.3		
(8-2-9-16)	66.7	(8-2-9-17)	-171.4	(10-2-9-15)	64.4		
(10-2-9-16)	-176.6	(10-2-9-17)	-54.8	(1-2-10-18)	168.6		
(1-2-10-19)	-73.3	(1-2-10-20)	50.0	(8-2-10-18)	53.5		
(8-2-10-19)	171.5	(8-2-10-20)	-65.1	(9-2-10-18)	-63.7		
(9-2-10-19)	54.3	(9-2-10-20)	177.6	(1-3-5-21)	170.7		
(1-3-5-22)	-69.5	(1-3-5-23)	52.1	(6-3-5-21)	53.5		
(6-3-5-22)	173.3	(6-3-5-23)	-65.1	(7-3-5-21)	-65.1		
(7-3-5-22)	54.7	(7-3-5-23)	176.3	(1-3-6-27)	-165.2		
(1-3-6-28)	-46.8	(1-3-6-29)	75.7	(5-3-6-27)	-50.5		
(5-3-6-28)	68.0	(5-3-6-29)	-169.6	(7-3-6-27)	66.7		
(7-3-6-28)	-174.8	(7-3-6-29)	-52.4	(1-3-7-24)	169.7		
(1-3-7-25)	-71.1	(1-3-7-26)	50.5	(5-3-7-24)	50.8		
(5-3-7-25)	170.0	(5-3-7-26)	-68.3	(6-3-7-24)	-64.9		
(6-3-7-25)	54.2	(6-3-7-26)	175.9				
(bond)-(plane) angle		(4-1)-(2-1-3)	53.6				

Frequencies(cm^{-1}):

62.4	107.4	208.8	215.5	236.5	262.6	289.0	292.4	299.9	313.5
329.1	344.7	371.3	382.5	387.0	412.7	431.4	440.3	452.9	541.9
558.1	606.0	696.7	819.2	874.9	950.3	955.2	961.5	966.5	978.6
980.7	1038.1	1045.8	1066.8	1075.6	1098.9	1107.9	1278.1	1281.1	1290.5
1299.2	1313.1	1331.2	1383.3	1427.3	1432.0	1433.1	1437.2	1457.5	1466.8
1508.1	1513.7	1517.1	1527.1	1530.7	1532.4	1539.4	1543.7	1550.7	1556.6
1564.5	1576.9	3120.0	3122.1	3123.8	3129.0	3134.5	3136.5	3197.7	3201.9
3204.1	3208.6	3211.0	3215.1	3220.7	3223.5	3227.2	3236.5	3244.0	3257.0
3991.1									

Di-t-Butylhydroxylamine + Di-t-butylnitroxyl Radical H-Bonded Complex
^{2}A UMPW1K/6-31+G(d,p) C_1 Geometry

Nuclear repulsion energy	1851.664989 Hartree
UMPW1K/6-31+G(d,p) energy ($<S^2>$ = 0.7575)	-891.665954 Hartree
Zero-point correction	0.534679 Hartree
Thermal correction to Enthalpy	0.562345 Hartree
Thermal correction to Gibbs Free Energy	0.474967 Hartree



	X	Y	Z		X	Y	Z
N1	2.297407	0.099746	0.128371	H30	-1.381528	-2.537091	-0.211045
C2	3.191240	-0.751801	0.949936	H31	-4.782837	2.346641	0.601516
C3	2.770568	0.984365	-0.962212	H32	-4.084058	1.935536	-0.953022
O4	1.349082	-0.785225	-0.425771	H33	-5.091918	0.768822	-0.082892
C5	1.517887	1.504430	-1.670963	H34	-2.625023	3.081551	1.369298
C6	3.468349	2.215371	-0.383362	H35	-1.246731	1.975488	1.444609
C7	3.663717	0.309122	-2.002055	H36	-1.819096	2.568803	-0.114212
C8	2.335927	-1.207388	2.133721	H37	-3.900143	1.451550	2.745677
C9	3.715422	-1.996818	0.227943	H38	-4.233410	-0.176263	2.164417
C10	4.370407	0.026463	1.515698	H39	-2.607432	0.248496	2.712523
H11	0.509729	-0.539909	-0.021756	H40	2.931229	-1.809141	2.819276
O12	-1.240919	-0.280807	0.662730	H41	1.949220	-0.344243	2.672221
N13	-2.358246	-0.038761	0.115543	H42	1.495054	-1.808336	1.799311
C14	-2.908985	-1.098815	-0.780681	H43	4.190946	-2.658289	0.951447
C15	-3.100073	1.071450	0.782451	H44	2.898548	-2.536483	-0.241817
C16	-3.407027	-0.505177	-2.097300	H45	4.455282	-1.757027	-0.530180
C17	-1.774476	-2.062508	-1.103614	H46	4.863055	-0.596119	2.260636
C18	-4.016946	-1.876175	-0.072833	H47	5.114355	0.267114	0.760818
C19	-4.334240	1.538638	0.027113	H48	4.049698	0.942914	2.005518
C20	-3.486163	0.613496	2.187730	H49	1.799424	2.290659	-2.369435
C21	-2.130569	2.246106	0.877482	H50	1.015150	0.717667	-2.223632

H22	-4.350599	-2.688095	-0.716855	H51	0.819720	1.921361	-0.946982
H23	-3.646639	-2.310695	0.853185	H52	3.808895	0.973789	-2.853500
H24	-4.884408	-1.263012	0.154281	H53	4.648117	0.072313	-1.604345
H25	-3.577125	-1.316628	-2.802168	H54	3.202440	-0.607360	-2.363639
H26	-4.339783	0.037945	-2.001324	H55	3.571113	2.962940	-1.168432
H27	-2.657880	0.156750	-2.526894	H56	2.870824	2.644801	0.418440
H28	-2.164560	-2.833131	-1.765411	H57	4.463412	2.015880	-0.004340
H29	-0.952688	-1.562378	-1.608679				

(1-2)	1.483	(1-3)	1.482	(1-4)	1.411	(2-8)	1.530
(2-9)	1.532	(2-10)	1.522	(3-5)	1.530	(3-6)	1.529
(3-7)	1.528	(4-11)	0.963	(5-49)	1.089	(5-50)	1.085
(5-51)	1.089	(6-55)	1.089	(6-56)	1.088	(6-57)	1.083
(7-52)	1.090	(7-53)	1.088	(7-54)	1.088	(8-40)	1.089
(8-41)	1.088	(8-42)	1.086	(9-43)	1.090	(9-44)	1.086
(9-45)	1.086	(10-46)	1.089	(10-47)	1.087	(10-48)	1.088
(11-12)	1.897	(12-13)	1.267	(13-14)	1.493	(13-15)	1.493
(14-16)	1.528	(14-17)	1.523	(14-18)	1.527	(15-19)	1.521
(15-20)	1.528	(15-21)	1.526	(16-25)	1.088	(16-26)	1.084
(16-27)	1.088	(17-28)	1.088	(17-29)	1.087	(17-30)	1.085
(18-22)	1.089	(18-23)	1.088	(18-24)	1.086	(19-31)	1.088
(19-32)	1.087	(19-33)	1.086	(20-37)	1.089	(20-38)	1.087
(20-39)	1.087	(21-34)	1.088	(21-35)	1.084	(21-36)	1.088

(2-1-3)	123.9	(2-1-4)	105.2	(3-1-4)	107.5	(1-2-8)	105.2
(1-2-9)	114.3	(1-2-10)	112.3	(8-2-9)	108.3	(8-2-10)	107.3
(9-2-10)	109.0	(1-3-5)	106.4	(1-3-6)	110.4	(1-3-7)	115.1
(5-3-6)	106.0	(5-3-7)	108.3	(6-3-7)	110.3	(1-4-11)	105.1
(3-5-49)	109.3	(3-5-50)	111.6	(3-5-51)	110.3	(49-5-50)	108.5
(49-5-51)	108.4	(50-5-51)	108.6	(3-6-55)	108.8	(3-6-56)	110.2
(3-6-57)	113.8	(55-6-56)	108.2	(55-6-57)	107.0	(56-6-57)	108.6
(3-7-52)	109.9	(3-7-53)	112.1	(3-7-54)	110.5	(52-7-53)	107.3
(52-7-54)	108.1	(53-7-54)	108.8	(2-8-40)	110.2	(2-8-41)	110.2
(2-8-42)	111.1	(40-8-41)	108.7	(40-8-42)	108.1	(41-8-42)	108.4
(2-9-43)	109.3	(2-9-44)	110.5	(2-9-45)	112.5	(43-9-44)	108.3
(43-9-45)	107.5	(44-9-45)	108.7	(2-10-46)	108.2	(2-10-47)	112.7
(2-10-48)	111.7	(46-10-47)	107.0	(46-10-48)	107.9	(47-10-48)	109.2
(4-11-12)	171.9	(11-12-13)	133.1	(12-13-14)	116.7	(12-13-15)	112.8
(14-13-15)	127.8	(13-14-16)	111.2	(13-14-17)	107.6	(13-14-18)	110.5
(16-14-17)	107.8	(16-14-18)	111.1	(17-14-18)	108.5	(13-15-19)	114.2
(13-15-20)	108.3	(13-15-21)	106.5	(19-15-20)	110.1	(19-15-21)	108.1
(20-15-21)	109.5	(14-16-25)	108.6	(14-16-26)	113.5	(14-16-27)	110.6
(25-16-26)	107.3	(25-16-27)	107.8	(26-16-27)	108.8	(14-17-28)	108.1
(14-17-29)	111.8	(14-17-30)	111.9	(28-17-29)	108.3	(28-17-30)	108.7
(29-17-30)	108.1	(14-18-22)	109.1	(14-18-23)	110.5	(14-18-24)	112.9
(22-18-23)	108.1	(22-18-24)	107.5	(23-18-24)	108.6	(15-19-31)	107.5
(15-19-32)	111.9	(15-19-33)	113.5	(31-19-32)	107.4	(31-19-33)	107.0
(32-19-33)	109.2	(15-20-37)	109.7	(15-20-38)	111.8	(15-20-39)	109.9
(37-20-38)	108.0	(37-20-39)	108.6	(38-20-39)	108.8	(15-21-34)	109.3
(15-21-35)	111.0	(15-21-36)	110.7	(34-21-35)	109.0	(34-21-36)	108.3
(35-21-36)	108.5						

(3-1-2-8)	166.7	(3-1-2-9)	-74.6	(3-1-2-10)	50.3
(4-1-2-8)	-69.4	(4-1-2-9)	49.3	(4-1-2-10)	174.2
(2-1-3-5)	171.6	(2-1-3-6)	-73.8	(2-1-3-7)	51.7
(4-1-3-5)	48.7	(4-1-3-6)	163.3	(4-1-3-7)	-71.2
(2-1-4-11)	113.4	(3-1-4-11)	-112.8	(1-2-8-40)	-177.5
(1-2-8-41)	-57.5	(1-2-8-42)	62.6	(9-2-8-40)	59.8
(9-2-8-41)	179.8	(9-2-8-42)	-60.0	(10-2-8-40)	-57.8
(10-2-8-41)	62.3	(10-2-8-42)	-177.6	(1-2-9-43)	-168.8

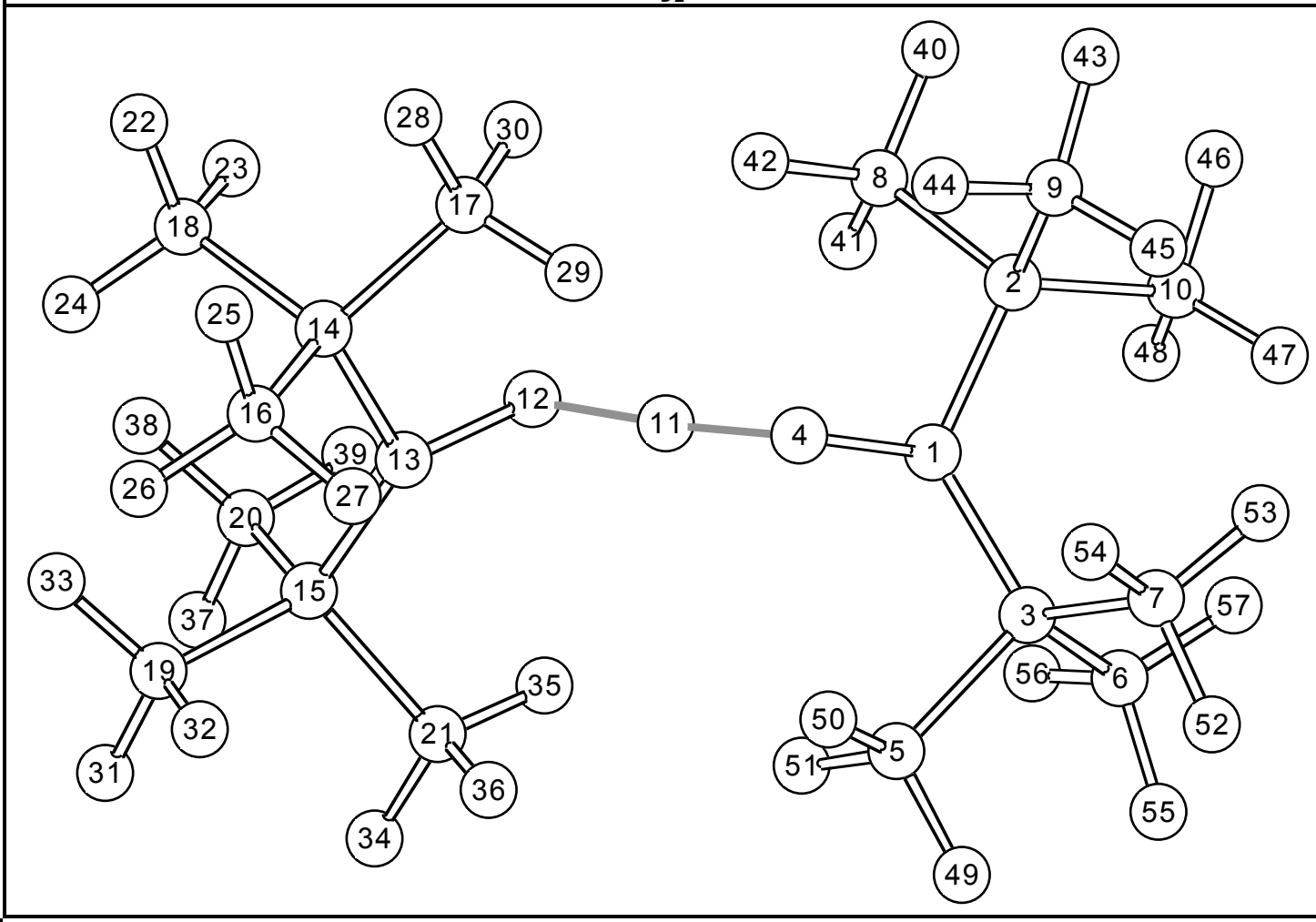
(1-2-9-44)	-49.7	(1-2-9-45)	72.0	(8-2-9-43)	-51.8
(8-2-9-44)	67.3	(8-2-9-45)	-171.1	(10-2-9-43)	64.7
(10-2-9-44)	-176.3	(10-2-9-45)	-54.6	(1-2-10-46)	168.6
(1-2-10-47)	-73.3	(1-2-10-48)	50.0	(8-2-10-46)	53.5
(8-2-10-47)	171.5	(8-2-10-48)	-65.2	(9-2-10-46)	-63.6
(9-2-10-47)	54.5	(9-2-10-48)	177.8	(1-3-5-49)	170.3
(1-3-5-50)	-69.7	(1-3-5-51)	51.2	(6-3-5-49)	52.9
(6-3-5-50)	172.9	(6-3-5-51)	-66.3	(7-3-5-49)	-65.5
(7-3-5-50)	54.6	(7-3-5-51)	175.4	(1-3-6-55)	-165.3
(1-3-6-56)	-46.8	(1-3-6-57)	75.5	(5-3-6-55)	-50.5
(5-3-6-56)	68.0	(5-3-6-57)	-169.7	(7-3-6-55)	66.5
(7-3-6-56)	-175.0	(7-3-6-57)	-52.7	(1-3-7-52)	169.5
(1-3-7-53)	-71.3	(1-3-7-54)	50.3	(5-3-7-52)	50.6
(5-3-7-53)	169.9	(5-3-7-54)	-68.6	(6-3-7-52)	-64.9
(6-3-7-53)	54.3	(6-3-7-54)	175.9	(1-4-11-12)	-170.2
(4-11-12-13)	-66.5	(11-12-13-14)	64.6	(11-12-13-15)	-132.7
(12-13-14-16)	-133.3	(12-13-14-17)	-15.5	(12-13-14-18)	102.8
(15-13-14-16)	67.0	(15-13-14-17)	-175.1	(15-13-14-18)	-56.9
(12-13-15-19)	170.7	(12-13-15-20)	-66.2	(12-13-15-21)	51.5
(14-13-15-19)	-29.0	(14-13-15-20)	94.1	(14-13-15-21)	-148.2
(13-14-16-25)	166.8	(13-14-16-26)	-74.0	(13-14-16-27)	48.7
(17-14-16-25)	49.1	(17-14-16-26)	168.3	(17-14-16-27)	-69.0
(18-14-16-25)	-69.6	(18-14-16-26)	49.6	(18-14-16-27)	172.3
(13-14-17-28)	-179.4	(13-14-17-29)	-60.3	(13-14-17-30)	61.0
(16-14-17-28)	-59.4	(16-14-17-29)	59.7	(16-14-17-30)	-179.0
(18-14-17-28)	61.0	(18-14-17-29)	-179.9	(18-14-17-30)	-58.6
(13-14-18-22)	-175.8	(13-14-18-23)	-57.1	(13-14-18-24)	64.8
(16-14-18-22)	60.2	(16-14-18-23)	178.9	(16-14-18-24)	-59.2
(17-14-18-22)	-58.2	(17-14-18-23)	60.5	(17-14-18-24)	-177.6
(13-15-19-31)	-179.6	(13-15-19-32)	-61.9	(13-15-19-33)	62.3
(20-15-19-31)	58.3	(20-15-19-32)	176.1	(20-15-19-33)	-59.8
(21-15-19-31)	-61.3	(21-15-19-32)	56.5	(21-15-19-33)	-179.4
(13-15-20-37)	171.9	(13-15-20-38)	-68.4	(13-15-20-39)	52.6
(19-15-20-37)	-62.6	(19-15-20-38)	57.1	(19-15-20-39)	178.1
(21-15-20-37)	56.1	(21-15-20-38)	175.8	(21-15-20-39)	-63.2
(13-15-21-34)	-179.4	(13-15-21-35)	-59.1	(13-15-21-36)	61.4
(19-15-21-34)	57.5	(19-15-21-35)	177.7	(19-15-21-36)	-61.7
(20-15-21-34)	-62.5	(20-15-21-35)	57.7	(20-15-21-36)	178.3
(bond)-(plane) angle		(4-1)-(2-1-3)	53.2		
(bond)-(plane) angle		(12-13)-(14-13-15)	18.1		

Frequencies(cm^{-1}):								
4.8	13.1	19.8	26.3	43.1	47.8	61.8	84.3	
88.4	139.4	191.1	205.0	205.7	214.6	231.8	245.9	259.9	261.9
268.5	277.1	281.0	292.3	294.8	303.9	313.5	318.9	329.2	330.3
338.6	343.7	355.9	372.2	374.8	384.0	394.6	397.3	420.6	427.3
427.9	439.6	445.1	450.9	541.6	554.2	558.9	562.3	563.6	609.3
666.8	691.0	700.8	818.6	831.0	874.0	875.2	949.1	953.7	959.3
960.4	961.8	965.0	966.4	969.5	976.7	979.5	984.7	988.5	1038.7
1040.9	1055.2	1065.8	1068.4	1074.1	1074.6	1081.7	1102.6	1111.5	1117.3
1266.5	1274.8	1276.5	1281.4	1284.4	1290.5	1292.0	1299.2	1313.0	1313.8
1324.0	1330.4	1424.3	1428.2	1430.1	1431.3	1434.6	1434.9	1439.5	1443.3
1447.8	1454.7	1464.8	1467.5	1471.0	1506.2	1506.8	1511.1	1511.5	1516.9
1521.0	1521.4	1525.4	1526.7	1528.7	1529.6	1530.4	1534.5	1536.7	1537.6
1538.6	1541.8	1548.9	1549.7	1552.8	1556.0	1563.0	1564.3	1570.4	1575.7
3116.9	3120.9	3124.0	3126.0	3128.1	3128.8	3131.1	3131.6	3134.1	3134.8
3139.2	3142.1	3193.4	3200.5	3202.0	3205.2	3208.9	3209.3	3210.4	3211.3

3212.0 3212.9 3217.5 3218.5 3224.0 3224.6 3227.1 3228.2 3233.3 3236.6
3239.8 3241.1 3249.6 3250.9 3254.0 3254.2 3829.8

Di-t-Butylhydroxylamine + Di-t-butylnitroxyl Radical Transition Structure
^{2}A UMPW1K/6-31+G(d,p) C_1 Geometry

Nuclear repulsion energy	1903.958628 Hartree
UMPW1K/6-31+G(d,p) energy ($<S^2>$ = 0.7572)	-891.629802 Hartree
Zero-point correction	0.529503 Hartree
Thermal correction to Enthalpy	0.556068 Hartree
Thermal correction to Gibbs Free Energy	0.474890 Hartree



	X	Y	Z		X	Y	Z
N1	2.075972	0.059000	0.066169	H30	-1.223156	-2.571340	0.059483
C2	2.727692	-1.168087	0.588628	H31	-4.357160	2.570970	0.191465
C3	2.770972	1.220075	-0.544594	H32	-3.747488	1.849288	-1.290026
O4	0.965504	-0.262316	-0.588947	H33	-4.787764	0.921922	-0.197170
C5	1.700182	2.167710	-1.075600	H34	-2.196751	3.283341	0.859848
C6	3.571139	2.000535	0.498637	H35	-0.864143	2.144445	1.065337
C7	3.668075	0.810130	-1.713861	H36	-1.434261	2.550570	-0.556625
C8	1.766411	-1.758287	1.620072	H37	-3.459510	1.932655	2.446720
C9	2.948573	-2.193783	-0.525811	H38	-3.933322	0.274204	2.109429
C10	4.046895	-0.897667	1.295892	H39	-2.264027	0.637814	2.557033
H11	-0.009063	-0.210620	0.072834	H40	2.195714	-2.663343	2.046801
O12	-1.004551	-0.257684	0.701897	H41	1.585424	-1.047435	2.423803
N13	-2.070457	0.039209	-0.033535	H42	0.811700	-2.010529	1.170604
C14	-2.742511	-1.160759	-0.595816	H43	3.273904	-3.138550	-0.092722
C15	-2.749007	1.226841	0.536901	H44	2.022148	-2.362625	-1.066908
C16	-3.387652	-0.837637	-1.943739	H45	3.709851	-1.871594	-1.231389

C17	-1.665545	-2.208788	-0.862191	H46	4.395012	-1.837827	1.719412
C18	-3.769421	-1.768339	0.361007	H47	4.824913	-0.543515	0.625462
C19	-3.981825	1.648528	-0.247591	H48	3.930844	-0.191036	2.113610
C20	-3.127550	0.995105	2.002828	H49	2.188800	3.055028	-1.473565
C21	-1.743214	2.373132	0.471258	H50	1.109790	1.709622	-1.860959
H22	-4.138882	-2.706697	-0.051056	H51	1.029342	2.475760	-0.278658
H23	-3.312695	-1.979404	1.325573	H52	4.063793	1.701038	-2.200250
H24	-4.628487	-1.120382	0.515740	H53	4.515991	0.209097	-1.395065
H25	-3.673553	-1.769334	-2.428852	H54	3.098242	0.246654	-2.449667
H26	-4.282362	-0.232016	-1.864432	H55	3.847509	2.965315	0.076841
H27	-2.676408	-0.325660	-2.588554	H56	2.964932	2.181723	1.383876
H28	-2.122547	-3.050148	-1.379354	H57	4.489149	1.511204	0.800794
H29	-0.871009	-1.808317	-1.487580				

(1-2)	1.484	(1-3)	1.485	(1-4)	1.329	(2-8)	1.528
(2-9)	1.531	(2-10)	1.521	(3-5)	1.525	(3-6)	1.529
(3-7)	1.530	(4-11)	1.179	(5-49)	1.088	(5-50)	1.084
(5-51)	1.086	(6-55)	1.089	(6-56)	1.088	(6-57)	1.083
(7-52)	1.089	(7-53)	1.087	(7-54)	1.088	(8-40)	1.089
(8-41)	1.088	(8-42)	1.085	(9-43)	1.089	(9-44)	1.086
(9-45)	1.087	(10-46)	1.088	(10-47)	1.086	(10-48)	1.087
(11-12)	1.179	(12-13)	1.329	(13-14)	1.486	(13-15)	1.482
(14-16)	1.529	(14-17)	1.526	(14-18)	1.529	(15-19)	1.521
(15-20)	1.532	(15-21)	1.526	(16-25)	1.089	(16-26)	1.083
(16-27)	1.088	(17-28)	1.088	(17-29)	1.088	(17-30)	1.085
(18-22)	1.089	(18-23)	1.088	(18-24)	1.087	(19-31)	1.088
(19-32)	1.087	(19-33)	1.086	(20-37)	1.089	(20-38)	1.086
(20-39)	1.086	(21-34)	1.089	(21-35)	1.085	(21-36)	1.088
(2-1-3)	125.9	(2-1-4)	109.9	(3-1-4)	112.2	(1-2-8)	106.3
(1-2-9)	111.2	(1-2-10)	113.4	(8-2-9)	108.9	(8-2-10)	107.5
(9-2-10)	109.4	(1-3-5)	107.5	(1-3-6)	111.3	(1-3-7)	112.3
(5-3-6)	106.7	(5-3-7)	108.2	(6-3-7)	110.6	(1-4-11)	113.8
(3-5-49)	108.6	(3-5-50)	111.8	(3-5-51)	110.8	(49-5-50)	108.9
(49-5-51)	108.3	(50-5-51)	108.4	(3-6-55)	108.7	(3-6-56)	110.4
(3-6-57)	113.8	(55-6-56)	108.0	(55-6-57)	107.1	(56-6-57)	108.7
(3-7-52)	109.6	(3-7-53)	112.4	(3-7-54)	110.4	(52-7-53)	107.4
(52-7-54)	108.2	(53-7-54)	108.7	(2-8-40)	109.7	(2-8-41)	110.5
(2-8-42)	111.3	(40-8-41)	108.6	(40-8-42)	108.4	(41-8-42)	108.2
(2-9-43)	109.6	(2-9-44)	110.1	(2-9-45)	112.0	(43-9-44)	108.5
(43-9-45)	107.8	(44-9-45)	108.7	(2-10-46)	107.7	(2-10-47)	113.1
(2-10-48)	111.9	(46-10-47)	107.0	(46-10-48)	107.6	(47-10-48)	109.2
(4-11-12)	174.8	(11-12-13)	111.9	(12-13-14)	113.1	(12-13-15)	109.5
(14-13-15)	125.9	(13-14-16)	110.7	(13-14-17)	107.5	(13-14-18)	112.8
(16-14-17)	106.8	(16-14-18)	110.6	(17-14-18)	108.1	(13-15-19)	113.3
(13-15-20)	111.1	(13-15-21)	106.5	(19-15-20)	109.6	(19-15-21)	107.7
(20-15-21)	108.5	(14-16-25)	108.8	(14-16-26)	113.7	(14-16-27)	110.2
(25-16-26)	107.1	(25-16-27)	108.1	(26-16-27)	108.7	(14-17-28)	108.5
(14-17-29)	111.3	(14-17-30)	111.7	(28-17-29)	108.6	(28-17-30)	108.5
(29-17-30)	108.3	(14-18-22)	109.5	(14-18-23)	110.5	(14-18-24)	112.5
(22-18-23)	108.1	(22-18-24)	107.4	(23-18-24)	108.7	(15-19-31)	107.8
(15-19-32)	111.8	(15-19-33)	113.1	(31-19-32)	107.7	(31-19-33)	107.0
(32-19-33)	109.1	(15-20-37)	109.6	(15-20-38)	112.2	(15-20-39)	110.0
(37-20-38)	107.8	(37-20-39)	108.5	(38-20-39)	108.7	(15-21-34)	109.8
(15-21-35)	110.6	(15-21-36)	110.5	(34-21-35)	108.6	(34-21-36)	108.6
(35-21-36)	108.8						
(3-1-2-8)	155.8	(3-1-2-9)	-85.9	(3-1-2-10)	37.9		
(4-1-2-8)	-65.0	(4-1-2-9)	53.4	(4-1-2-10)	177.2		
(2-1-3-5)	173.7	(2-1-3-6)	-69.8	(2-1-3-7)	54.8		

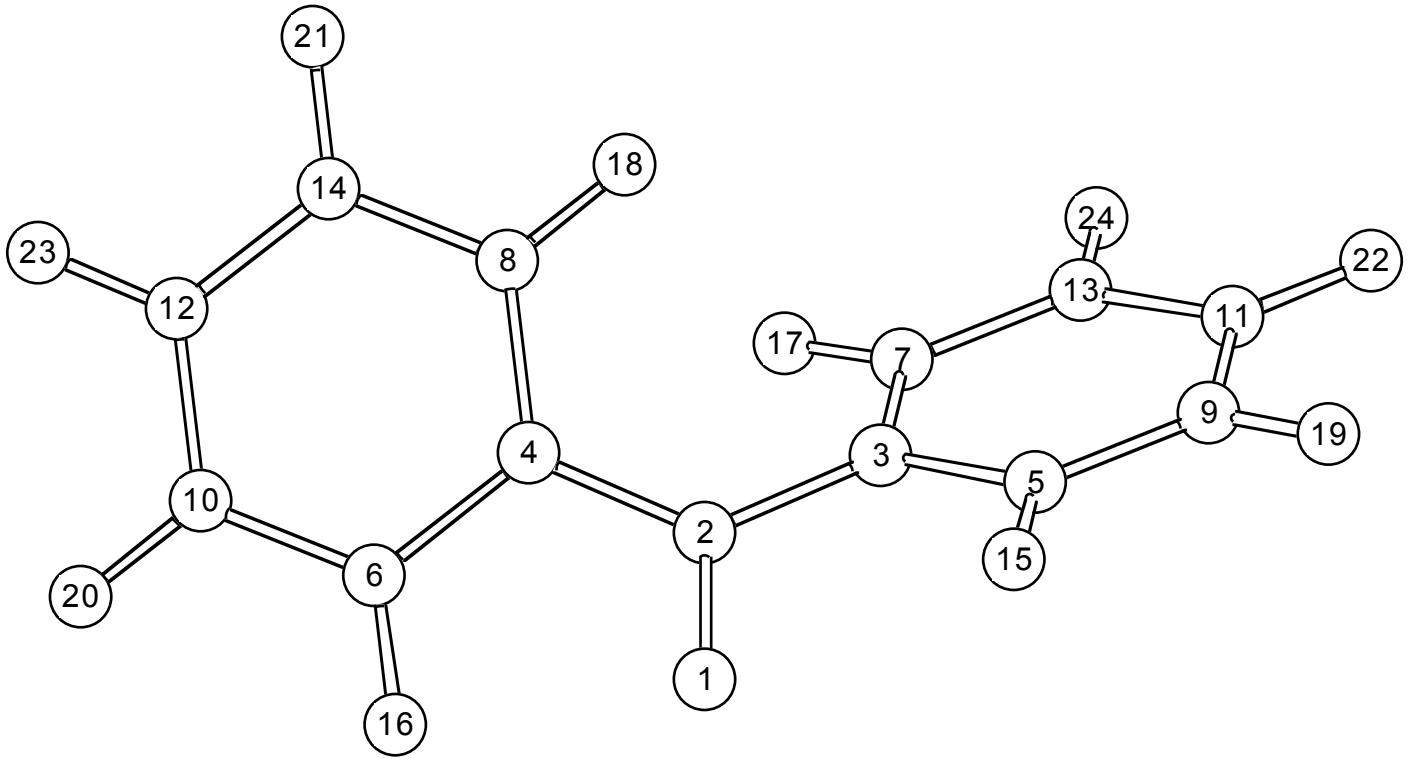
(4-1-3-5)	35.2	(4-1-3-6)	151.8	(4-1-3-7)	-83.6
(2-1-4-11)	94.3	(3-1-4-11)	-120.6	(1-2-8-40)	-179.6
(1-2-8-41)	-59.8	(1-2-8-42)	60.4	(9-2-8-40)	60.6
(9-2-8-41)	-179.7	(9-2-8-42)	-59.5	(10-2-8-40)	-57.9
(10-2-8-41)	61.9	(10-2-8-42)	-177.9	(1-2-9-43)	-170.8
(1-2-9-44)	-51.5	(1-2-9-45)	69.6	(8-2-9-43)	-54.0
(8-2-9-44)	65.3	(8-2-9-45)	-173.6	(10-2-9-43)	63.2
(10-2-9-44)	-177.5	(10-2-9-45)	-56.5	(1-2-10-46)	174.8
(1-2-10-47)	-67.1	(1-2-10-48)	56.7	(8-2-10-46)	57.6
(8-2-10-47)	175.7	(8-2-10-48)	-60.5	(9-2-10-46)	-60.4
(9-2-10-47)	57.6	(9-2-10-48)	-178.6	(1-3-5-49)	176.6
(1-3-5-50)	-63.2	(1-3-5-51)	57.8	(6-3-5-49)	57.1
(6-3-5-50)	177.3	(6-3-5-51)	-61.7	(7-3-5-49)	-61.9
(7-3-5-50)	58.3	(7-3-5-51)	179.3	(1-3-6-55)	-165.6
(1-3-6-56)	-47.3	(1-3-6-57)	75.2	(5-3-6-55)	-48.6
(5-3-6-56)	69.7	(5-3-6-57)	-167.8	(7-3-6-55)	68.8
(7-3-6-56)	-172.9	(7-3-6-57)	-50.4	(1-3-7-52)	173.5
(1-3-7-53)	-67.1	(1-3-7-54)	54.4	(5-3-7-52)	55.0
(5-3-7-53)	174.4	(5-3-7-54)	-64.0	(6-3-7-52)	-61.5
(6-3-7-53)	57.9	(6-3-7-54)	179.4	(1-4-11-12)	-128.0
(4-11-12-13)	-83.4	(11-12-13-14)	94.4	(11-12-13-15)	-119.9
(12-13-14-16)	-148.7	(12-13-14-17)	-32.3	(12-13-14-18)	86.7
(15-13-14-16)	72.3	(15-13-14-17)	-171.4	(15-13-14-18)	-52.3
(12-13-15-19)	179.6	(12-13-15-20)	-56.5	(12-13-15-21)	61.5
(14-13-15-19)	-40.2	(14-13-15-20)	83.7	(14-13-15-21)	-158.3
(13-14-16-25)	167.5	(13-14-16-26)	-73.2	(13-14-16-27)	49.2
(17-14-16-25)	50.7	(17-14-16-26)	170.0	(17-14-16-27)	-67.6
(18-14-16-25)	-66.6	(18-14-16-26)	52.7	(18-14-16-27)	175.0
(13-14-17-28)	-173.6	(13-14-17-29)	-54.2	(13-14-17-30)	66.9
(16-14-17-28)	-54.7	(16-14-17-29)	64.7	(16-14-17-30)	-174.2
(18-14-17-28)	64.3	(18-14-17-29)	-176.3	(18-14-17-30)	-55.1
(13-14-18-22)	-173.2	(13-14-18-23)	-54.3	(13-14-18-24)	67.5
(16-14-18-22)	62.2	(16-14-18-23)	-178.9	(16-14-18-24)	-57.2
(17-14-18-22)	-54.4	(17-14-18-23)	64.5	(17-14-18-24)	-173.8
(13-15-19-31)	-175.1	(13-15-19-32)	-56.9	(13-15-19-33)	66.8
(20-15-19-31)	60.2	(20-15-19-32)	178.4	(20-15-19-33)	-57.9
(21-15-19-31)	-57.7	(21-15-19-32)	60.6	(21-15-19-33)	-175.8
(13-15-20-37)	170.0	(13-15-20-38)	-70.4	(13-15-20-39)	50.8
(19-15-20-37)	-64.1	(19-15-20-38)	55.6	(19-15-20-39)	176.7
(21-15-20-37)	53.2	(21-15-20-38)	172.9	(21-15-20-39)	-65.9
(13-15-21-34)	178.8	(13-15-21-35)	-61.5	(13-15-21-36)	59.0
(19-15-21-34)	57.0	(19-15-21-35)	176.8	(19-15-21-36)	-62.7
(20-15-21-34)	-61.5	(20-15-21-35)	58.2	(20-15-21-36)	178.7
(bond)-(plane) angle		(4-1)-(2-1-3)	37.9		
(bond)-(plane) angle		(12-13)-(14-13-15)	37.1		

Frequencies(cm^{-1}):	-3238.1	11.4	27.9	38.5	63.4	65.1	86.1	92.1	
	109.8	113.6	175.8	198.5	208.8	218.6	222.9	242.4	263.2	268.7
	272.2	277.1	291.8	293.2	299.4	304.4	310.9	313.9	326.3	334.4
	335.5	340.1	369.6	372.9	379.7	388.0	395.0	400.7	421.2	423.2
	433.6	438.4	440.9	445.9	516.9	552.9	554.5	557.4	578.5	597.9
	679.1	682.8	728.7	824.7	826.2	874.1	878.7	952.7	953.9	954.8
	955.4	964.3	964.8	966.7	967.3	979.6	983.0	985.2	986.3	1042.9
	1044.9	1067.4	1068.2	1073.2	1073.8	1077.4	1080.4	1107.7	1109.9	1160.4
	1261.7	1266.2	1275.7	1277.9	1281.5	1284.6	1288.9	1295.7	1297.8	1298.6
	1310.1	1312.8	1364.3	1369.2	1425.6	1425.7	1429.7	1430.1	1435.1	1436.1

1441.6	1442.5	1460.6	1460.9	1468.4	1468.7	1506.4	1507.5	1508.8	1510.9
1519.2	1519.5	1522.6	1525.2	1525.6	1527.1	1527.8	1532.9	1535.9	1537.5
1538.6	1541.8	1547.2	1549.5	1552.7	1553.0	1562.0	1564.9	1571.3	1573.7
1693.1	3121.3	3121.5	3126.3	3126.7	3129.4	3129.7	3130.9	3132.4	3134.7
3135.5	3137.7	3141.0	3201.6	3201.8	3206.5	3207.0	3208.0	3208.6	3210.1
3210.7	3214.7	3215.5	3218.1	3221.4	3221.5	3224.4	3231.0	3231.6	3237.9
3238.1	3240.3	3243.4	3245.7	3254.4	3255.2	3257.2			

Diphenylnitroxyl Radical
^{2}B UMPW1K/6-31+G(d,p) C_2 Geometry

Nuclear repulsion energy	806.316437 Hartree
UMPW1K/6-31+G(d,p) energy (<S^2> = 0.7831)	-593.059542 Hartree
Zero-point correction	0.196104 Hartree
Thermal correction to Enthalpy	0.207610 Hartree
Thermal correction to Gibbs Free Energy	0.158664 Hartree



	X	Y	Z		X	Y	Z
O1	0.000000	0.000000	2.255414	C13	0.632898	2.655096	-1.509824
N2	0.000000	0.000000	0.990804	C14	-0.632898	-2.655096	-1.509824
C3	0.000000	1.244097	0.322570	H15	-1.042829	2.182266	1.927273
C4	0.000000	-1.244097	0.322570	H16	1.042829	-2.182266	1.927273
C5	-0.589367	2.330268	0.960696	H17	1.116380	0.572664	-1.385386
C6	0.589367	-2.330268	0.960696	H18	-1.116380	-0.572664	-1.385386
C7	0.624490	1.406789	-0.910255	H19	-1.038443	4.411138	0.843809
C8	-0.624490	-1.406789	-0.910255	H20	1.038443	-4.411138	0.843809
C9	-0.573846	3.570940	0.349721	H21	-1.124770	-2.780813	-2.462810
C10	0.573846	-3.570940	0.349721	H22	0.041227	4.709963	-1.360859
C11	0.031475	3.739507	-0.888158	H23	-0.041227	-4.709963	-1.360859
C12	-0.031475	-3.739507	-0.888158	H24	1.124770	2.780813	-2.462810

(1-2)	1.265	(2-3)	1.412	(3-5)	1.391	(3-7)	1.392	(5-9)	1.383
(5-15)	1.078	(7-13)	1.385	(7-17)	1.079	(9-11)	1.388	(9-19)	1.080
(11-13)	1.387	(11-22)	1.080	(13-24)	1.080				
(1-2-3)	118.2	(3-2-4)	123.5	(2-3-5)	118.1	(2-3-7)	121.5		
(5-3-7)	120.4	(3-5-9)	119.5	(3-5-15)	118.8	(9-5-15)	121.6		

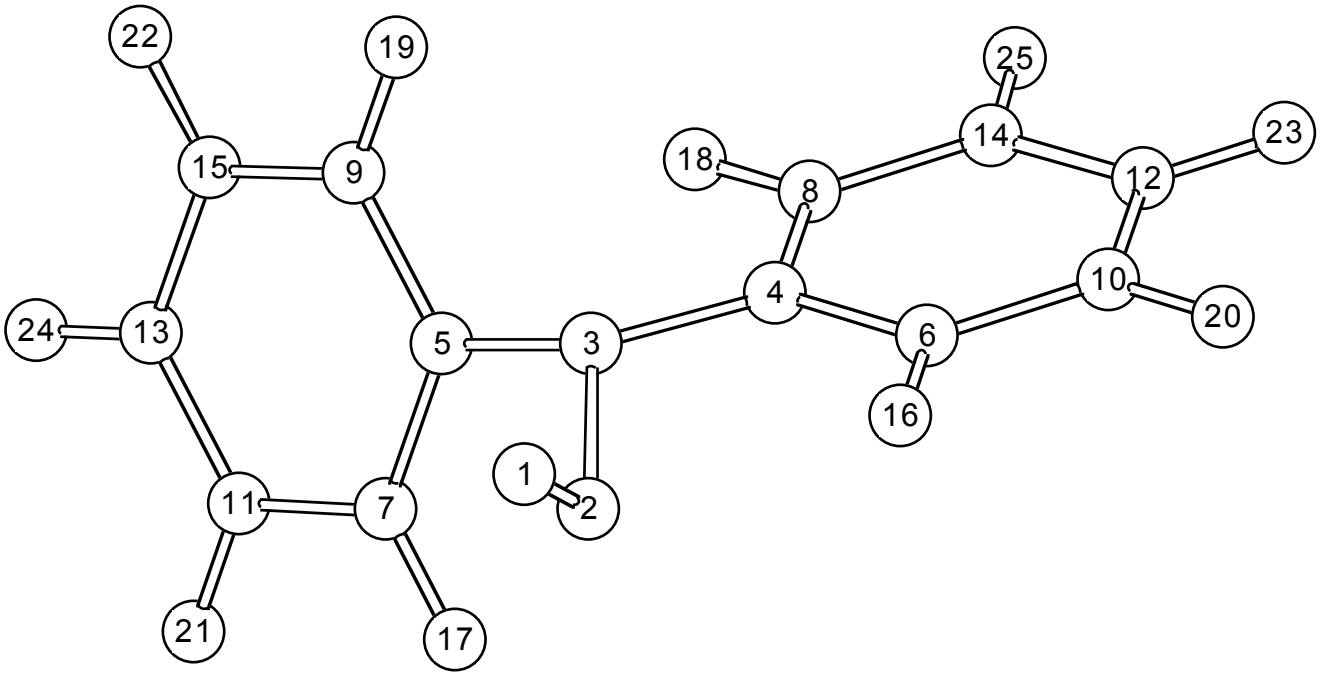
(3-7-13)	119.5	(3-7-17)	120.3	(13-7-17)	120.2	(5-9-11)	120.5				
(5-9-19)	119.4	(11-9-19)	120.1	(9-11-13)	119.6	(9-11-22)	120.2				
(13-11-22)	120.2	(7-13-11)	120.5	(7-13-24)	119.3	(11-13-24)	120.1				
(1-2-3-5)	-28.7	(1-2-3-7)	148.2	(4-2-3-5)	151.3						
(4-2-3-7)	-31.8	(2-3-5-9)	178.2	(2-3-5-15)	-1.4						
(7-3-5-9)	1.2	(7-3-5-15)	-178.3	(2-3-7-13)	-178.1						
(2-3-7-17)	0.6	(5-3-7-13)	-1.2	(5-3-7-17)	177.5						
(3-5-9-11)	-0.4	(3-5-9-19)	179.6	(15-5-9-11)	179.2						
(15-5-9-19)	-0.9	(3-7-13-11)	0.3	(3-7-13-24)	179.5						
(17-7-13-11)	-178.4	(17-7-13-24)	0.8	(5-9-11-13)	-0.5						
(5-9-11-22)	180.0	(19-9-11-13)	179.6	(19-9-11-22)	0.1						
(9-11-13-7)	0.5	(9-11-13-24)	-178.7	(22-11-13-7)	180.0						
(22-11-13-24)	0.8										
(bond)-(plane) angle		(1-2)-(3-2-4)		0.0							

Frequencies(cm^{-1}):	37.1	68.5	101.9	136.7	240.9	249.9	316.6	385.7	
425.4	434.6	438.6	477.0	559.8	597.6	639.7	640.2	660.4	720.9
725.0	761.8	794.6	802.2	877.8	886.1	956.3	968.8	975.4	1024.2
1029.2	1039.5	1040.2	1041.1	1042.1	1081.9	1083.9	1137.0	1140.7	1201.8
1208.0	1209.4	1222.3	1239.0	1346.5	1375.5	1382.4	1398.4	1403.3	1507.9
1532.8	1560.6	1572.3	1575.5	1700.0	1706.8	1710.3	1714.1	3276.5	3276.7
3285.8	3286.1	3297.9	3298.8	3305.5	3307.3	3319.5	3319.7		

Diphenylhydroxylamine

^{1}A MPW1K/6-31+G(d,p) C_1 Geometry

Nuclear repulsion energy	822.737431 Hartree
UMPW1K/6-31+G(d,p) energy	-593.674253 Hartree
Zero-point correction	0.208269 Hartree
Thermal correction to Enthalpy	0.220244 Hartree
Thermal correction to Gibbs Free Energy	0.169583 Hartree



	X	Y	Z		X	Y	Z
H1	-0.081603	2.760105	-0.953060	C14	2.420687	-1.760323	0.361635
O2	0.097643	2.275139	-0.148192	C15	-2.968271	-1.164674	-0.834932
N3	0.046676	0.936435	-0.534540	H16	2.448423	2.010996	-0.372841
C4	1.231250	0.259469	-0.188705	H17	-1.520701	1.488591	1.557985
C5	-1.213872	0.360523	-0.229444	H18	0.302512	-1.654955	0.114723

C6	2.441597	0.951643	-0.179524	H19	-1.181304	-0.846992	-1.988889
C7	-1.931044	0.741006	0.897879	H20	4.548565	0.839233	0.103066
C8	1.229302	-1.104862	0.095329	H21	-3.724794	0.468354	2.024134
C9	-1.739864	-0.581802	-1.103512	H22	-3.370827	-1.899703	-1.516106
C10	3.621805	0.284163	0.096751	H23	4.549504	-1.592546	0.576213
C11	-3.167498	0.168369	1.148915	H24	-4.649798	-1.234789	0.492472
C12	3.625551	-1.076740	0.363681	H25	2.397469	-2.817977	0.580139
C13	-3.687197	-0.789518	0.290173				

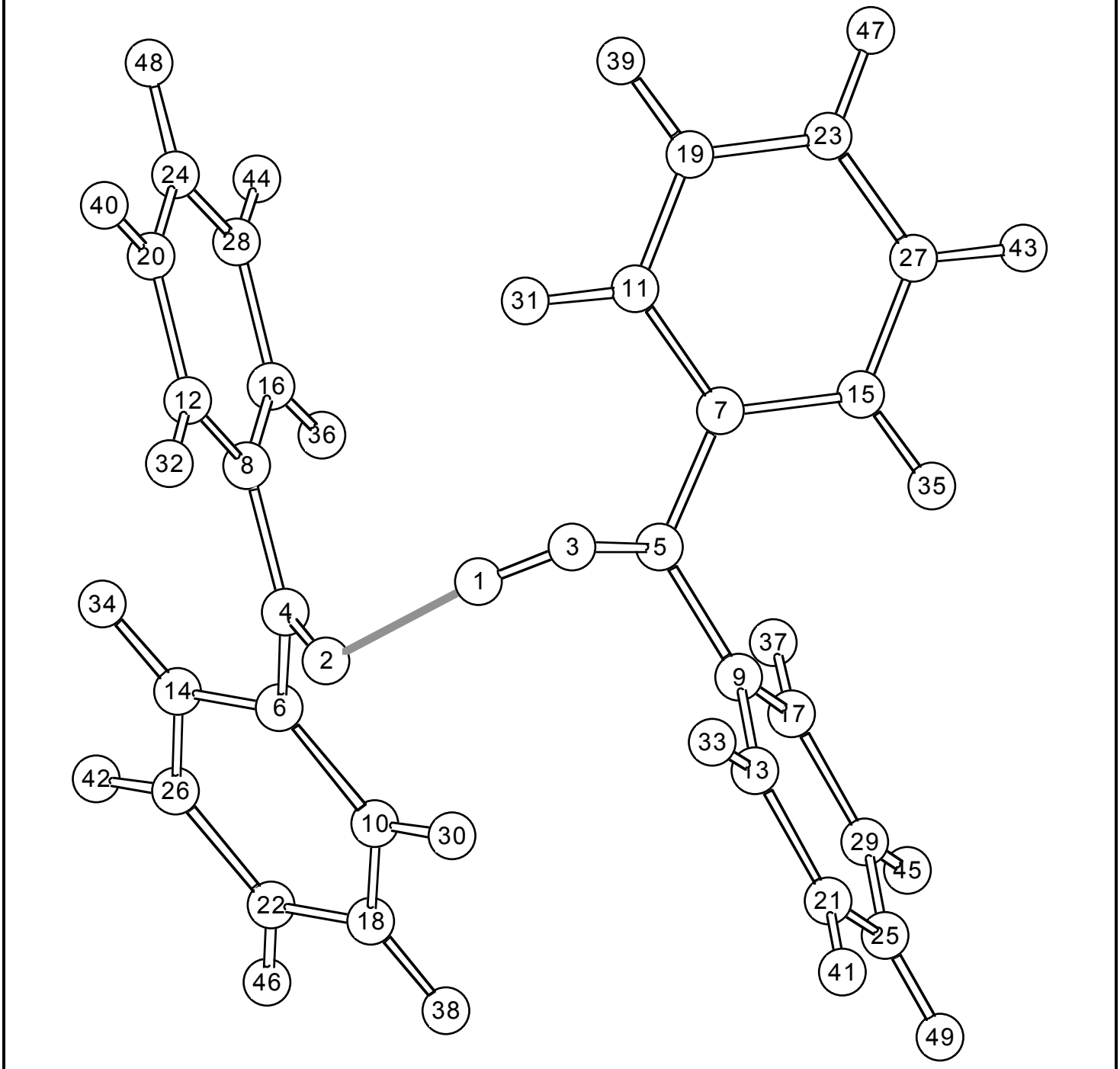
(1-2)	0.957	(2-3)	1.394	(3-4)	1.408	(3-5)	1.419
(4-6)	1.394	(4-8)	1.394	(5-7)	1.389	(5-9)	1.389
(6-10)	1.384	(6-16)	1.077	(7-11)	1.386	(7-17)	1.078
(8-14)	1.386	(8-18)	1.078	(9-15)	1.386	(9-19)	1.080
(10-12)	1.387	(10-20)	1.080	(11-13)	1.387	(11-21)	1.080
(12-14)	1.385	(12-23)	1.079	(13-15)	1.387	(13-24)	1.080
(14-25)	1.080	(15-22)	1.080				

(1-2-3)	104.3	(2-3-4)	111.3	(2-3-5)	111.3	(4-3-5)	120.0
(3-4-6)	119.6	(3-4-8)	121.3	(6-4-8)	119.1	(3-5-7)	121.5
(3-5-9)	118.5	(7-5-9)	120.1	(4-6-10)	120.1	(4-6-16)	119.5
(10-6-16)	120.3	(5-7-11)	119.6	(5-7-17)	119.3	(11-7-17)	121.0
(4-8-14)	120.1	(4-8-18)	120.3	(14-8-18)	119.6	(5-9-15)	119.9
(5-9-19)	119.1	(15-9-19)	120.9	(6-10-12)	120.9	(6-10-20)	119.0
(12-10-20)	120.1	(7-11-13)	120.5	(7-11-21)	119.5	(13-11-21)	120.0
(10-12-14)	118.8	(10-12-23)	120.6	(14-12-23)	120.6	(11-13-15)	119.6
(11-13-24)	120.2	(15-13-24)	120.2	(8-14-12)	121.0	(8-14-25)	118.9
(12-14-25)	120.1	(9-15-13)	120.2	(9-15-22)	119.6	(13-15-22)	120.2

(1-2-3-4)	125.1	(1-2-3-5)	-98.3	(2-3-4-6)	-31.7		
(2-3-4-8)	150.8	(5-3-4-6)	-164.1	(5-3-4-8)	18.4		
(2-3-5-7)	-34.1	(2-3-5-9)	144.5	(4-3-5-7)	98.3		
(4-3-5-9)	-83.1	(3-4-6-10)	-176.9	(3-4-6-16)	4.1		
(8-4-6-10)	0.6	(8-4-6-16)	-178.4	(3-4-8-14)	176.5		
(3-4-8-18)	-3.9	(6-4-8-14)	-1.0	(6-4-8-18)	178.7		
(3-5-7-11)	179.0	(3-5-7-17)	-0.2	(9-5-7-11)	0.5		
(9-5-7-17)	-178.7	(3-5-9-15)	179.9	(3-5-9-19)	-0.2		
(7-5-9-15)	-1.4	(7-5-9-19)	178.4	(4-6-10-12)	0.2		
(4-6-10-20)	-179.7	(16-6-10-12)	179.2	(16-6-10-20)	-0.8		
(5-7-11-13)	0.6	(5-7-11-21)	-179.8	(17-7-11-13)	179.8		
(17-7-11-21)	-0.6	(4-8-14-12)	0.6	(4-8-14-25)	180.0		
(18-8-14-12)	-179.0	(18-8-14-25)	0.3	(5-9-15-13)	1.3		
(5-9-15-22)	-179.8	(19-9-15-13)	-178.5	(19-9-15-22)	0.4		
(6-10-12-14)	-0.6	(6-10-12-23)	179.9	(20-10-12-14)	179.4		
(20-10-12-23)	-0.2	(7-11-13-15)	-0.7	(7-11-13-24)	179.8		
(21-11-13-15)	179.7	(21-11-13-24)	0.2	(10-12-14-8)	0.2		
(10-12-14-25)	-179.2	(23-12-14-8)	179.7	(23-12-14-25)	0.4		
(11-13-15-9)	-0.3	(11-13-15-22)	-179.2	(24-13-15-9)	179.2		
(24-13-15-22)	0.3						
(bond)-(plane) angle		(2-3)-(4-3-5)		43.5			

Frequencies(cm^{-1}):	18.5	45.7	84.6	149.8	233.2	245.1	315.7	371.6	
381.8	428.3	431.7	466.8	479.6	559.4	591.9	638.4	642.2	644.0
725.4	734.2	756.2	792.2	811.9	869.6	887.9	939.8	946.0	974.5
1017.3	1028.2	1033.4	1035.4	1043.1	1043.5	1080.7	1089.5	1106.3	1133.2
1151.9	1207.6	1207.7	1221.2	1235.4	1285.7	1352.3	1378.4	1386.3	1395.0
1401.7	1433.3	1531.9	1537.8	1578.4	1582.4	1703.1	1707.4	1718.0	1728.5
3271.2	3272.3	3279.1	3280.8	3291.1	3297.5	3299.7	3309.3	3311.7	3323.1

Diphenylhydroxylamine + Diphenylnitroxyl Radical Transition Structure ^{2}A UMPW1K/6-31+G(d,p) C_1 Geometry	
Nuclear repulsion energy	2482.179704 Hartree
UMPW1K/6-31+G(d,p) energy (<S^2> = 0.7888)	-1186.745154 Hartree
Zero-point correction	0.405488 Hartree
Thermal correction to Enthalpy	0.429997 Hartree
Thermal correction to Gibbs Free Energy	0.344302 Hartree



	X	Y	Z		X	Y	Z
H1	0.389498	0.228301	1.911034	C26	-3.879594	-2.697277	-1.373385
O2	-1.193562	-0.632825	1.807809	C27	3.464567	2.624335	-1.726748
O3	1.288535	0.587314	1.849200	C28	-2.941179	2.666899	-0.955219
N4	-1.940859	-0.426087	0.804403	C29	3.082935	-2.772054	-0.922461
N5	1.689962	0.301780	0.555804	H30	-0.487639	-2.555013	0.457013
C6	-2.309978	-1.533209	0.012623	H31	0.512304	2.627114	0.732623

C7	2.072655	1.454491	-0.145651	H32	-2.368267	1.372179	2.630499
C8	-2.370465	0.894078	0.550532	H33	2.848063	-1.062277	2.519342
C9	2.376273	-0.918175	0.443392	H34	-4.234021	-0.754563	-0.543777
C10	-1.430813	-2.608626	-0.062012	H35	3.761174	0.588922	-1.154334
C11	1.333425	2.624553	0.034929	H36	-2.388094	0.695941	-1.587649
C12	-2.538749	1.748877	1.634750	H37	1.982782	-1.086181	-1.656303
C13	2.925442	-1.543331	1.558419	H38	-1.096307	-4.550549	-0.871753
C14	-3.541431	-1.576530	-0.634625	H39	1.076489	4.666174	-0.507831
C15	3.153813	1.469998	-1.024913	H40	-3.057118	3.722339	2.254813
C16	-2.561507	1.351982	-0.749261	H41	3.974035	-3.247355	2.297203
C17	2.442801	-1.551867	-0.797642	H42	-4.838184	-2.735912	-1.868593
C18	-1.782875	-3.720082	-0.805517	H43	4.308666	2.614994	-2.401077
C19	1.661459	3.771301	-0.663913	H44	-3.076254	3.026933	-1.963922
C20	-2.919185	3.060184	1.413302	H45	3.130174	-3.248044	-1.891202
C21	3.550520	-2.773533	1.423564	H46	-3.272671	-4.640065	-2.043873
C22	-3.003389	-3.769248	-1.465469	H47	2.974253	4.679490	-2.102797
C23	2.723823	3.782272	-1.557265	H48	-3.421389	4.547698	-0.047077
C24	-3.125854	3.523118	0.120959	H49	4.132923	-4.348943	0.088291
C25	3.641651	-3.392647	0.186921				

(1-2)	1.805	(1-3)	0.970	(2-4)	1.268	(3-5)	1.384
(4-6)	1.410	(4-8)	1.411	(5-7)	1.403	(5-9)	1.404
(6-10)	1.391	(6-14)	1.392	(7-11)	1.396	(7-15)	1.394
(8-12)	1.391	(8-16)	1.391	(9-13)	1.391	(9-17)	1.395
(10-18)	1.383	(10-30)	1.078	(11-19)	1.382	(11-31)	1.078
(12-20)	1.383	(12-32)	1.078	(13-21)	1.386	(13-33)	1.077
(14-26)	1.384	(14-34)	1.079	(15-27)	1.386	(15-35)	1.078
(16-28)	1.384	(16-36)	1.079	(17-29)	1.384	(17-37)	1.080
(18-22)	1.388	(18-38)	1.080	(19-23)	1.388	(19-39)	1.080
(20-24)	1.388	(20-40)	1.080	(21-25)	1.386	(21-41)	1.080
(22-26)	1.388	(22-46)	1.080	(23-27)	1.385	(23-47)	1.080
(24-28)	1.388	(24-48)	1.080	(25-29)	1.389	(25-49)	1.080
(26-42)	1.080	(27-43)	1.080	(28-44)	1.080	(29-45)	1.080

(2-1-3)	170.3	(1-2-4)	119.0	(1-3-5)	104.6	(2-4-6)	118.1
(2-4-8)	118.3	(6-4-8)	123.6	(3-5-7)	112.1	(3-5-9)	113.3
(7-5-9)	122.7	(4-6-10)	118.1	(4-6-14)	121.1	(10-6-14)	120.7
(5-7-11)	118.7	(5-7-15)	122.4	(11-7-15)	118.9	(4-8-12)	118.1
(4-8-16)	121.2	(12-8-16)	120.6	(5-9-13)	121.3	(5-9-17)	119.3
(13-9-17)	119.3	(6-10-18)	119.3	(6-10-30)	119.3	(18-10-30)	121.4
(7-11-19)	120.3	(7-11-31)	119.3	(19-11-31)	120.4	(8-12-20)	119.4
(8-12-32)	119.1	(20-12-32)	121.5	(9-13-21)	119.9	(9-13-33)	119.1
(21-13-33)	121.0	(6-14-26)	119.3	(6-14-34)	120.3	(26-14-34)	120.3
(7-15-27)	120.2	(7-15-35)	120.2	(27-15-35)	119.6	(8-16-28)	119.3
(8-16-36)	120.3	(28-16-36)	120.4	(9-17-29)	120.2	(9-17-37)	119.4
(29-17-37)	120.4	(10-18-22)	120.5	(10-18-38)	119.3	(22-18-38)	120.2
(11-19-23)	120.9	(11-19-39)	119.0	(23-19-39)	120.1	(12-20-24)	120.4
(12-20-40)	119.5	(24-20-40)	120.1	(13-21-25)	120.8	(13-21-41)	119.2
(25-21-41)	120.0	(18-22-26)	119.7	(18-22-46)	120.2	(26-22-46)	120.1
(19-23-27)	118.8	(19-23-47)	120.6	(27-23-47)	120.6	(20-24-28)	119.8
(20-24-48)	120.1	(28-24-48)	120.1	(21-25-29)	119.1	(21-25-49)	120.5
(29-25-49)	120.4	(14-26-22)	120.4	(14-26-42)	119.4	(22-26-42)	120.2
(15-27-23)	121.0	(15-27-43)	118.9	(23-27-43)	120.1	(16-28-24)	120.5
(16-28-44)	119.4	(24-28-44)	120.1	(17-29-25)	120.5	(17-29-45)	119.3
(25-29-45)	120.1						

(3-1-2-4)	-73.4	(2-1-3-5)	26.4	(1-2-4-6)	121.9		
(1-2-4-8)	-58.8	(1-3-5-7)	123.4	(1-3-5-9)	-92.4		
(2-4-6-10)	-29.4	(2-4-6-14)	148.1	(8-4-6-10)	151.4		
(8-4-6-14)	-31.1	(2-4-8-12)	-30.5	(2-4-8-16)	146.5		

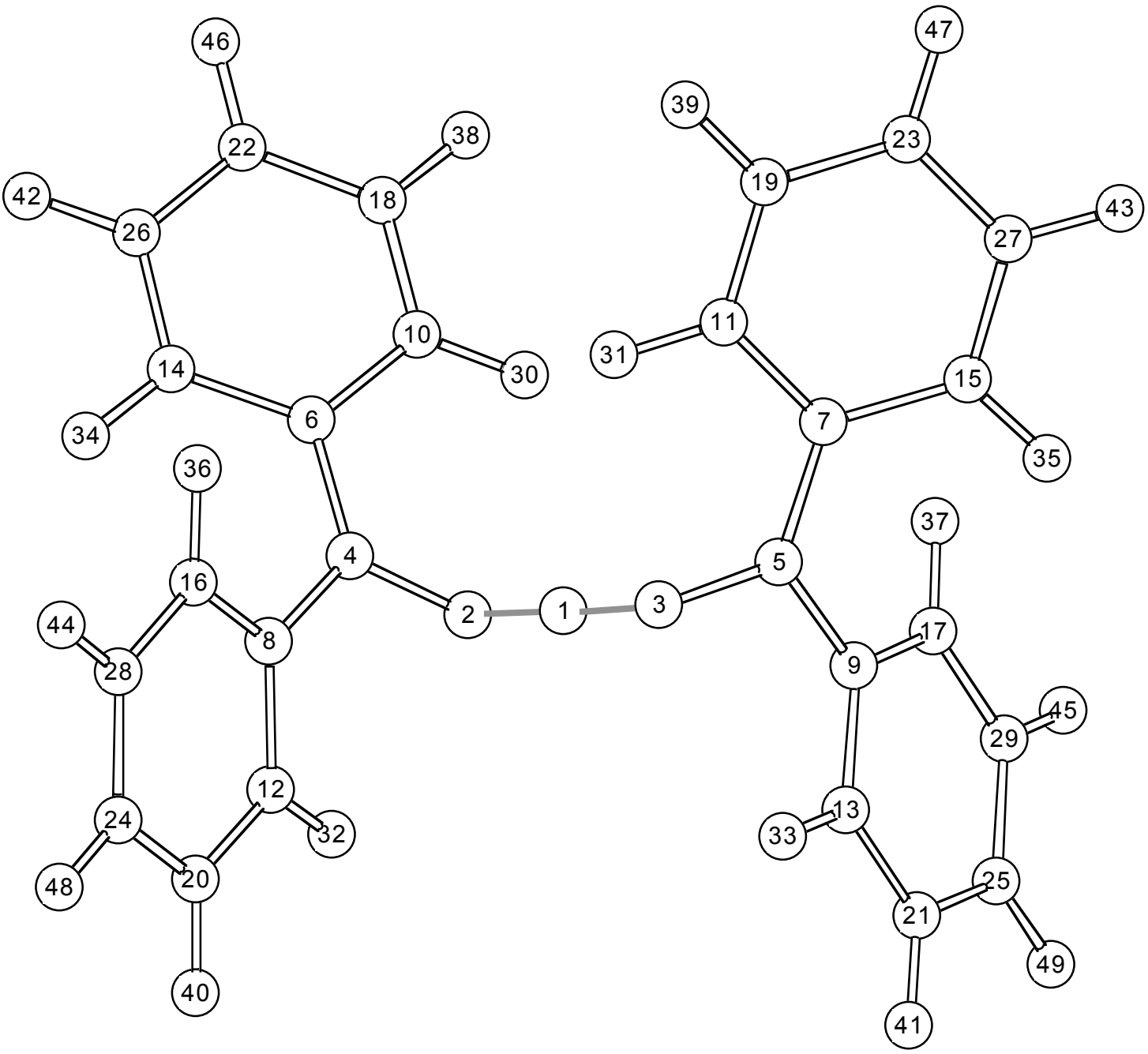
(6-4-8-12)	148.7	(6-4-8-16)	-34.3	(3-5-7-11)	-39.4
(3-5-7-15)	141.3	(9-5-7-11)	-179.7	(9-5-7-15)	1.0
(3-5-9-13)	-17.8	(3-5-9-17)	158.5	(7-5-9-13)	122.1
(7-5-9-17)	-61.6	(4-6-10-18)	178.5	(4-6-10-30)	-1.9
(14-6-10-18)	1.0	(14-6-10-30)	-179.3	(4-6-14-26)	-178.3
(4-6-14-34)	0.4	(10-6-14-26)	-0.9	(10-6-14-34)	177.8
(5-7-11-19)	-178.4	(5-7-11-31)	2.2	(15-7-11-19)	0.9
(15-7-11-31)	-178.4	(5-7-15-27)	177.9	(5-7-15-35)	-2.9
(11-7-15-27)	-1.4	(11-7-15-35)	177.8	(4-8-12-20)	178.0
(4-8-12-32)	-1.9	(16-8-12-20)	1.0	(16-8-12-32)	-179.0
(4-8-16-28)	-177.9	(4-8-16-36)	0.4	(12-8-16-28)	-0.9
(12-8-16-36)	177.4	(5-9-13-21)	177.4	(5-9-13-33)	-2.0
(17-9-13-21)	1.1	(17-9-13-33)	-178.4	(5-9-17-29)	-178.2
(5-9-17-37)	1.2	(13-9-17-29)	-1.8	(13-9-17-37)	177.6
(6-10-18-22)	-0.4	(6-10-18-38)	179.4	(30-10-18-22)	179.9
(30-10-18-38)	-0.3	(7-11-19-23)	0.2	(7-11-19-39)	-179.9
(31-11-19-23)	179.5	(31-11-19-39)	-0.6	(8-12-20-24)	-0.3
(8-12-20-40)	179.5	(32-12-20-24)	179.7	(32-12-20-40)	-0.5
(9-13-21-25)	0.2	(9-13-21-41)	179.9	(33-13-21-25)	179.6
(33-13-21-41)	-0.7	(6-14-26-22)	0.2	(6-14-26-42)	179.5
(34-14-26-22)	-178.5	(34-14-26-42)	0.8	(7-15-27-23)	0.8
(7-15-27-43)	179.8	(35-15-27-23)	-178.4	(35-15-27-43)	0.6
(8-16-28-24)	0.2	(8-16-28-44)	179.2	(36-16-28-24)	-178.1
(36-16-28-44)	0.9	(9-17-29-25)	1.3	(9-17-29-45)	-179.7
(37-17-29-25)	-178.1	(37-17-29-45)	0.9	(10-18-22-26)	-0.3
(10-18-22-46)	180.0	(38-18-22-26)	179.9	(38-18-22-46)	0.3
(11-19-23-27)	-0.8	(11-19-23-47)	179.8	(39-19-23-27)	179.3
(39-19-23-47)	-0.1	(12-20-24-28)	-0.4	(12-20-24-48)	-179.9
(40-20-24-28)	179.7	(40-20-24-48)	0.2	(13-21-25-29)	-0.8
(13-21-25-49)	179.8	(41-21-25-29)	179.6	(41-21-25-49)	0.1
(18-22-26-14)	0.4	(18-22-26-42)	-178.9	(46-22-26-14)	-179.9
(46-22-26-42)	0.8	(19-23-27-15)	0.3	(19-23-27-43)	-178.7
(47-23-27-15)	179.7	(47-23-27-43)	0.7	(20-24-28-16)	0.5
(20-24-28-44)	-178.5	(48-24-28-16)	180.0	(48-24-28-44)	1.0
(21-25-29-17)	0.0	(21-25-29-45)	-179.0	(49-25-29-17)	179.5
(49-25-29-45)	0.5				
(bond)-(plane) angle		(2-4)-(6-4-8)	0.7		
(bond)-(plane) angle		(3-5)-(7-5-9)	36.3		

Frequencies(cm^{-1}):									
6.2	11.7	12.9	22.5	25.3	33.9	45.6	64.3	69.5	90.0
101.8	102.8	165.1	205.9	240.0	245.3	249.1	251.3	316.3	317.6
372.4	392.3	424.3	427.1	432.2	433.7	438.9	441.5	474.7	484.1
544.7	563.8	589.1	598.7	638.7	639.0	640.3	641.1	643.8	659.4
716.2	719.5	722.3	730.3	734.2	756.3	762.2	790.8	795.6	803.0
803.2	869.4	877.7	883.8	887.6	939.2	953.2	958.9	963.5	970.8
977.3	1016.6	1025.5	1026.0	1029.5	1030.9	1035.7	1037.4	1038.8	1039.3
1040.2	1043.4	1043.9	1080.9	1082.9	1083.2	1088.7	1121.4	1136.8	1138.5
1142.1	1157.3	1199.9	1205.4	1206.2	1208.8	1209.7	1222.7	1224.1	1234.4
1238.7	1308.3	1345.6	1355.4	1376.2	1383.1	1387.6	1393.6	1396.6	1399.1
1403.3	1409.1	1503.0	1528.3	1533.0	1540.0	1542.7	1560.2	1569.6	1570.9
1579.1	1582.7	1697.5	1698.9	1703.8	1705.1	1709.1	1709.6	1715.9	1727.8
3268.2	3268.7	3276.4	3277.1	3278.5	3279.4	3288.8	3289.3	3290.1	3294.8
3298.0	3299.2	3300.2	3306.5	3308.0	3309.0	3316.5	3316.8	3321.0	3322.2
3684.5									

Diphenylhydroxylamine + Diphenylnitroxyl Radical Transition Structure

^{2}B UMPW1K/6-31+G(d,p) C_2 Geometry

Nuclear repulsion energy	2441.883207 Hartree
UMPW1K/6-31+G(d,p) energy ($<S^2>$ = 0.7814)	-1186.721926 Hartree
Zero-point correction	0.400245 Hartree
Thermal correction to Enthalpy	0.423917 Hartree
Thermal correction to Gibbs Free Energy	0.342677 Hartree



	X	Y	Z		X	Y	Z
H1	0.000000	0.000000	0.777960	C26	-0.335792	4.117030	-2.712853
O2	-0.665990	0.976864	0.765120	C27	0.335792	-4.117030	-2.712853
O3	0.665990	-0.976864	0.765120	C28	2.956922	3.766112	1.651653
N4	0.005333	2.009440	0.293732	C29	-2.956922	-3.766112	1.651653
N5	-0.005333	-2.009440	0.293732	H30	-1.214359	0.569954	-1.509883
C6	-0.293644	2.431969	-0.993259	H31	1.214359	-0.569954	-1.509883
C7	0.293644	-2.431969	-0.993259	H32	-0.321383	2.151520	2.867809
C8	0.893244	2.628824	1.179473	H33	0.321383	-2.151520	2.867809

C9	-0.893244	-2.628824	1.179473	H34	0.446275	4.441567	-0.755179
C10	-0.951962	1.553706	-1.858652	H35	-0.446275	-4.441567	-0.755179
C11	0.951962	-1.553706	-1.858652	H36	2.351558	3.155214	-0.307572
C12	0.595020	2.615543	2.541256	H37	-2.351558	-3.155214	-0.307572
C13	-0.595020	-2.615543	2.541256	H38	-1.775578	1.264599	-3.798887
C14	-0.005333	3.731022	-1.427888	H39	1.775578	-1.264599	-3.798887
C15	0.005333	-3.731022	-1.427888	H40	1.229785	3.182392	4.494538
C16	2.090186	3.192132	0.738247	H41	-1.229785	-3.182392	4.494538
C17	-2.090186	-3.192132	0.738247	H42	-0.113263	5.125069	-3.030451
C18	-1.273720	1.958749	-3.141054	H43	0.113263	-5.125069	-3.030451
C19	1.273720	-1.958749	-3.141054	H44	3.885149	4.193291	1.302174
C20	1.472561	3.189287	3.442275	H45	-3.885149	-4.193291	1.302174
C21	-1.472561	-3.189287	3.442275	H46	-1.217156	3.545816	-4.585807
C22	-0.962696	3.235821	-3.583808	H47	1.217156	-3.545816	-4.585807
C23	0.962696	-3.235821	-3.583808	H48	3.335027	4.220482	3.713120
C24	2.653414	3.773744	3.005287	H49	-3.335027	-4.220482	3.713120
C25	-2.653414	-3.773744	3.005287				

(1-2)	1.182	(2-4)	1.319	(4-6)	1.387	(4-8)	1.399
(6-10)	1.398	(6-14)	1.400	(8-12)	1.394	(8-16)	1.395
(10-18)	1.383	(10-30)	1.076	(12-20)	1.382	(12-32)	1.078
(14-26)	1.382	(14-34)	1.078	(16-28)	1.384	(16-36)	1.079
(18-22)	1.387	(18-38)	1.080	(20-24)	1.388	(20-40)	1.080
(22-26)	1.389	(22-46)	1.079	(24-28)	1.387	(24-48)	1.079
(26-42)	1.080	(28-44)	1.080				

(2-1-3)	178.8	(1-2-4)	111.3	(2-4-6)	117.4	(2-4-8)	116.3
(6-4-8)	126.1	(4-6-10)	119.0	(4-6-14)	121.8	(10-6-14)	119.2
(4-8-12)	118.6	(4-8-16)	121.6	(12-8-16)	119.8	(6-10-18)	120.0
(6-10-30)	119.2	(18-10-30)	120.8	(8-12-20)	119.8	(8-12-32)	118.8
(20-12-32)	121.4	(6-14-26)	119.9	(6-14-34)	120.3	(26-14-34)	119.8
(8-16-28)	119.8	(8-16-36)	120.1	(28-16-36)	120.2	(10-18-22)	120.9
(10-18-38)	119.0	(22-18-38)	120.1	(12-20-24)	120.6	(12-20-40)	119.3
(24-20-40)	120.0	(18-22-26)	119.0	(18-22-46)	120.5	(26-22-46)	120.4
(20-24-28)	119.4	(20-24-48)	120.3	(28-24-48)	120.3	(14-26-22)	120.9
(14-26-42)	119.0	(22-26-42)	120.1	(16-28-24)	120.6	(16-28-44)	119.3
(24-28-44)	120.1						

(3-1-2-4)	-67.7	(1-2-4-6)	105.1	(1-2-4-8)	-78.9
(2-4-6-10)	-19.2	(2-4-6-14)	158.1	(8-4-6-10)	165.3
(8-4-6-14)	-17.4	(2-4-8-12)	-30.5	(2-4-8-16)	146.1
(6-4-8-12)	145.0	(6-4-8-16)	-38.3	(4-6-10-18)	179.3
(4-6-10-30)	0.1	(14-6-10-18)	2.0	(14-6-10-30)	-177.2
(4-6-14-26)	-179.1	(4-6-14-34)	-1.0	(10-6-14-26)	-1.9
(10-6-14-34)	176.2	(4-8-12-20)	178.3	(4-8-12-32)	-1.5
(16-8-12-20)	1.5	(16-8-12-32)	-178.3	(4-8-16-28)	-178.4
(4-8-16-36)	-0.1	(12-8-16-28)	-1.7	(12-8-16-36)	176.5
(6-10-18-22)	-0.6	(6-10-18-38)	179.5	(30-10-18-22)	178.6
(30-10-18-38)	-1.3	(8-12-20-24)	-0.3	(8-12-20-40)	179.5
(32-12-20-24)	179.5	(32-12-20-40)	-0.7	(6-14-26-22)	0.5
(6-14-26-42)	179.6	(34-14-26-22)	-177.6	(34-14-26-42)	1.4
(8-16-28-24)	0.7	(8-16-28-44)	179.5	(36-16-28-24)	-177.6
(36-16-28-44)	1.3	(10-18-22-26)	-0.9	(10-18-22-46)	180.0
(38-18-22-26)	179.0	(38-18-22-46)	-0.1	(12-20-24-28)	-0.7
(12-20-24-48)	180.0	(40-20-24-28)	179.5	(40-20-24-48)	0.2
(18-22-26-14)	0.9	(18-22-26-42)	-178.1	(46-22-26-14)	180.0
(46-22-26-42)	1.0	(20-24-28-16)	0.5	(20-24-28-44)	-178.3
(48-24-28-16)	179.8	(48-24-28-44)	1.0		

(bond)-(plane) angle (2-4)-(6-4-8) 4.0

Frequencies(cm^{-1}): -2774.3	5.4	18.9	19.6	34.6	41.5	51.7	53.9		
71.4	75.8	108.2	115.4	147.5	170.7	238.2	240.3	251.3	267.9
322.8	324.5	372.7	374.9	422.5	424.6	428.6	434.6	437.5	438.2
487.7	490.3	532.9	540.0	584.5	588.8	637.8	638.8	639.8	640.6
647.1	651.7	684.6	716.9	720.0	726.2	728.2	760.7	771.7	787.9
789.9	801.4	804.3	865.7	872.3	884.1	885.9	942.1	946.3	961.4
963.3	971.2	971.3	1019.2	1021.3	1028.0	1029.2	1031.6	1032.8	1035.1
1036.2	1038.5	1038.6	1040.0	1040.1	1083.3	1083.4	1085.3	1085.8	1137.7
1137.9	1143.4	1144.3	1201.4	1202.8	1207.3	1207.4	1208.5	1208.6	1222.6
1225.1	1238.4	1239.1	1244.4	1357.3	1358.6	1361.4	1363.6	1398.7	1398.8
1403.6	1404.3	1407.8	1408.4	1429.0	1440.6	1531.6	1531.7	1547.3	1548.7
1569.8	1570.1	1573.0	1573.3	1688.9	1689.0	1694.5	1701.6	1702.1	1704.0
1705.0	1714.5	1715.9	3274.4	3274.6	3274.8	3275.0	3282.9	3283.1	3283.6
3283.7	3297.4	3297.5	3299.5	3299.7	3304.8	3304.9	3312.4	3312.5	3318.6
3318.6	3334.1	3335.4							