Supporting Information

Structural and electronic factors relating to the stability of imidazolidine nitroxide radicals

CONTENTS

1,Experimental section

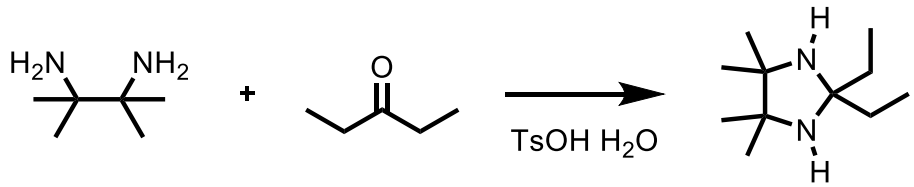
General Remarks

FT-IR spectra were recorded on a Nicolet iS10 FT-IR Spectrometer (KBr pellet method). ^{1}H and ^{13}C NMR spectra were recorded on BRUKER DRX-300, JEOL ECX-400 and BRUKER DRX-500 instruments. Date for ^{1}H NMR are reported as chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constant (Hz), integration, and assignment.Date for ^{13}C NMR are reported as chemical shift. Electron spin resonance (ESR) were recorded on JEOL ME-3X. Liquid chromatography–mass spectrometry (LC/MS) were recorded on Shimadzu LC-2010C HT and Shimadzu LCMS-2020, column：Wakopack Navi C18-5 φ 2.0 mm × 150 mm (D), tRet = retention time.

Procedure, NMR, IR, ESR spectra for all new compounds (3, 7, 11, 14, and 15)

The known nitroxides (1-2, 3-6, 8-10, 12-13) were synthesized in 4 to 5 steps using common synthetic routes[24,25,26].

Procedure of 2,2-diethyl-4,4,5,5-tetramethylimidazolidine(16)

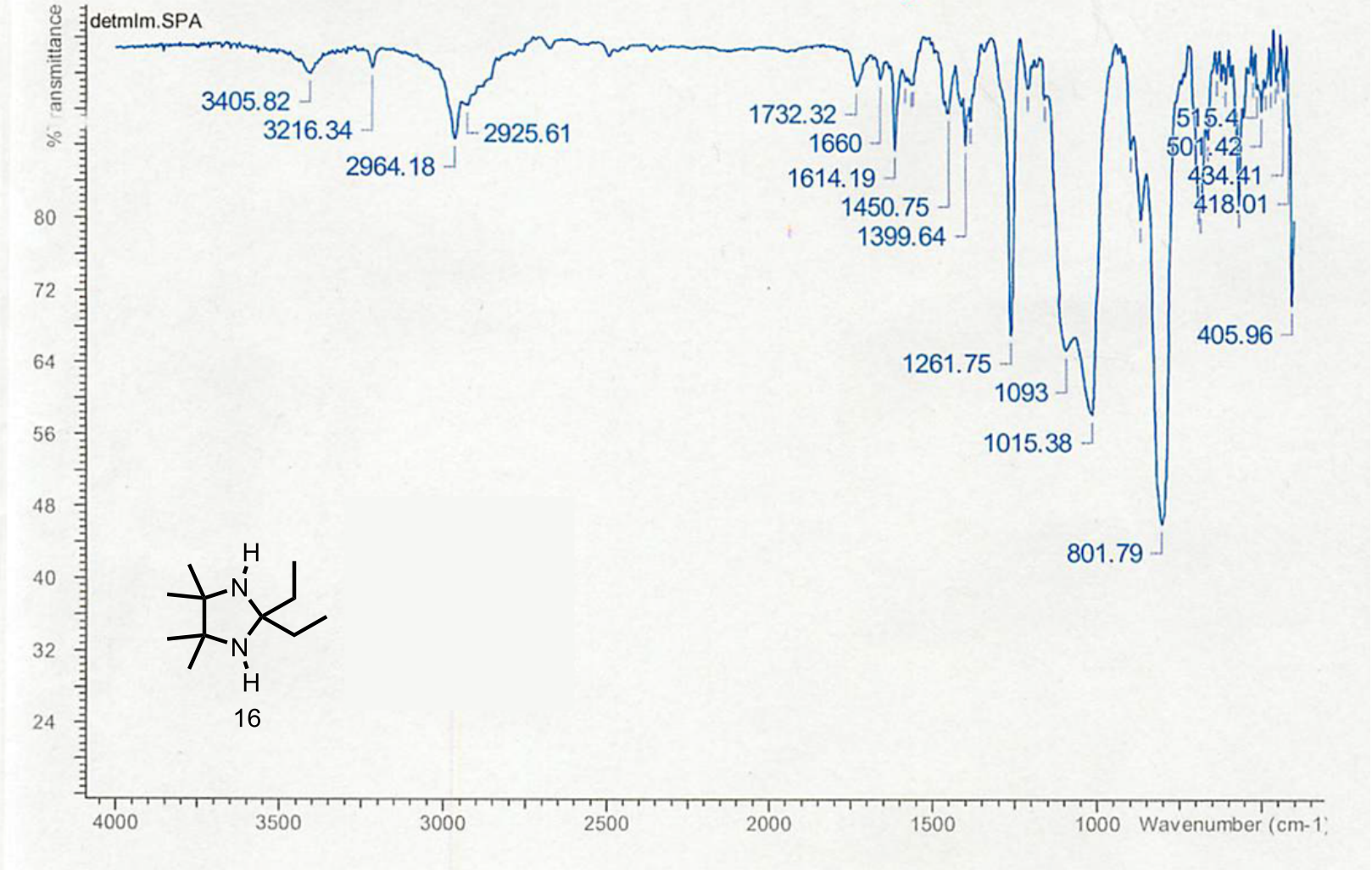


16

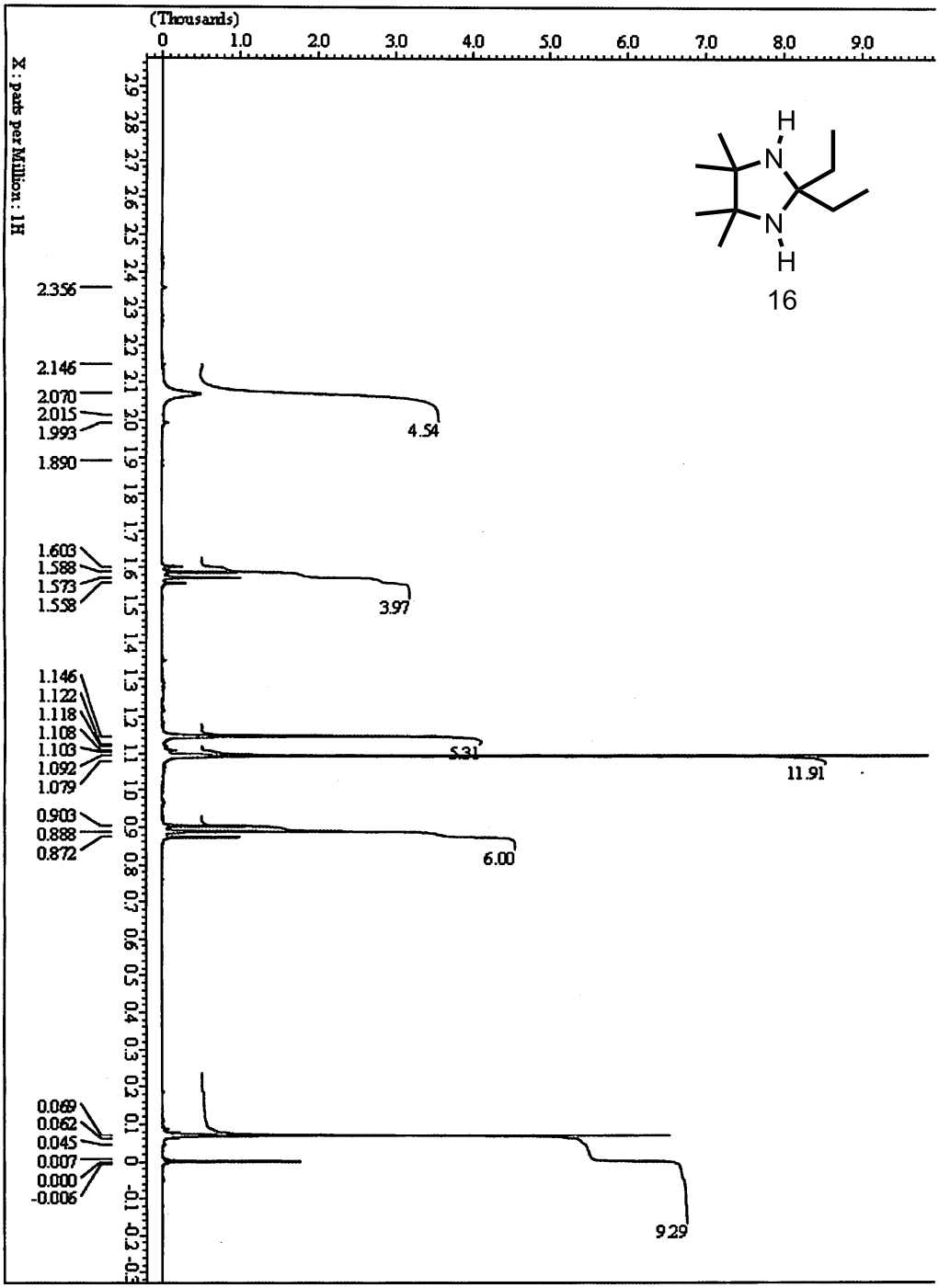
A 100 mL flask was charged with 10 mL of benzene, 348 mg (3 mmol) of 2,3-diamino-2,3-dimethylbutane and 6.46 g (75 mmol) of 3-pentanone, and 3 mg (0.02 mmol) of toluenesulfonic acid monohydrate. After a 48-h reflux and evaporation in vacuo quantitativelyafforded imidazolidine as a slight yellow solid. It was used in the next reaction without purification.

^{1}H -NMR ($CDCl_3$) δ =0.89 (6H, t, J= 4.5 Hz), 1.10(12H, s), 1.58(4H, q, J= 4.5 Hz), 2.07(2H, br, NH); ^{13}C-NMR δ = 78.4, 62.5, 32.7, 25.3, 9.2;IR(KBr film) : 2964, 1262, 1015, 802

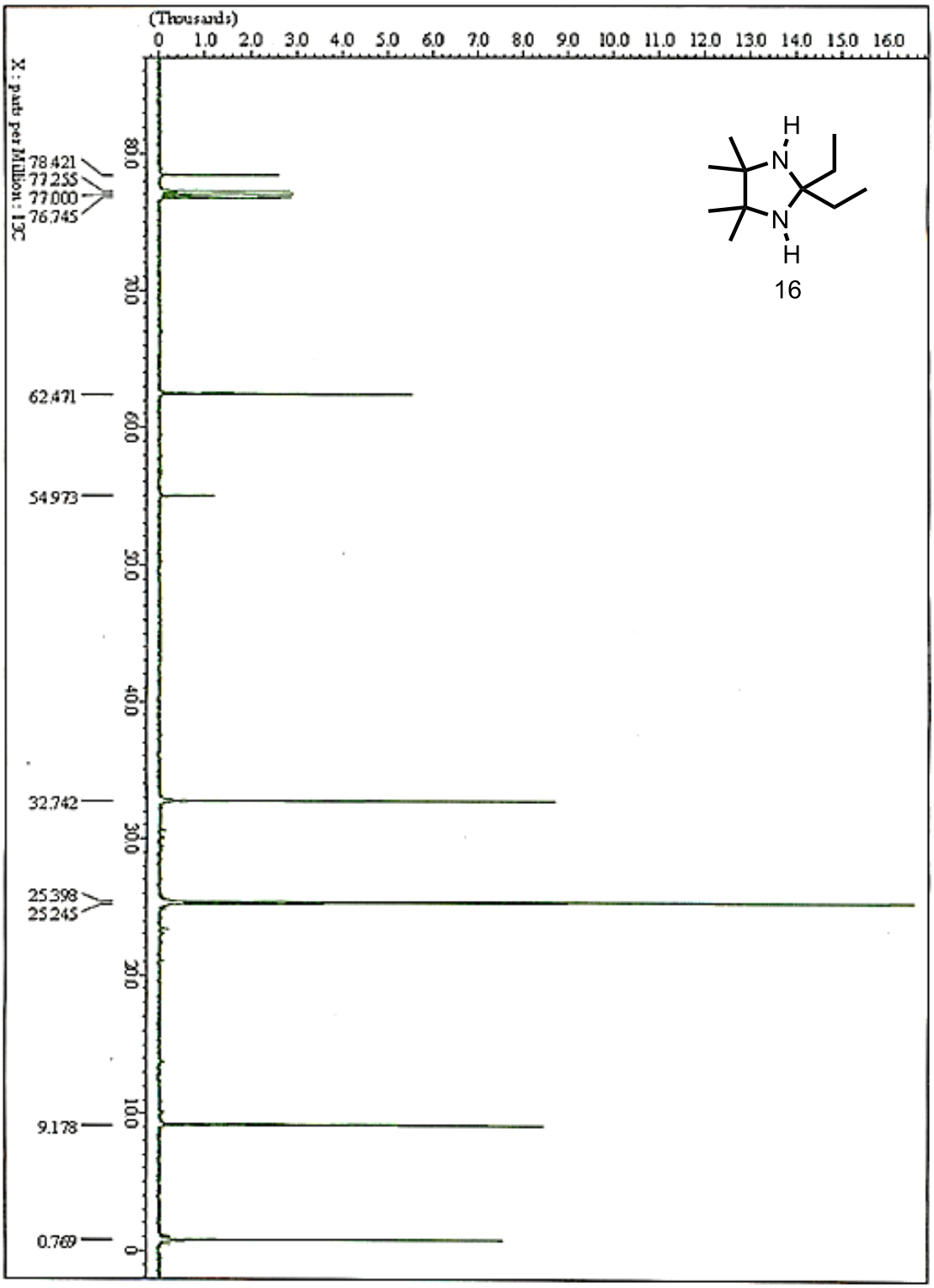
IR spectra of 2,2-diethyl-4,4,5,5-tetramethylimidazolidine(16)



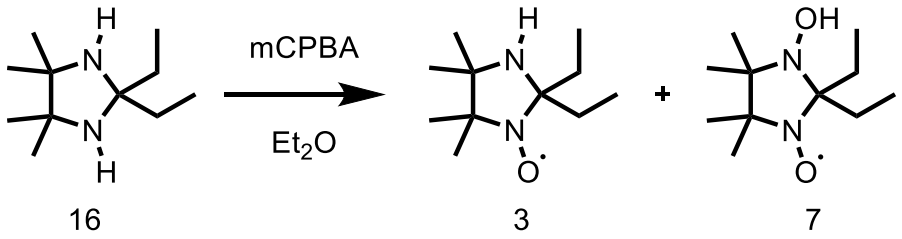
^{1}H NMR spectra of 2,2-diethyl-4,4,5,5-tetramethylimidazolidine(16)



^{13}C NMR spectra of 2,2-diethyl-4,4,5,5-tetramethylimidazolidine(16)

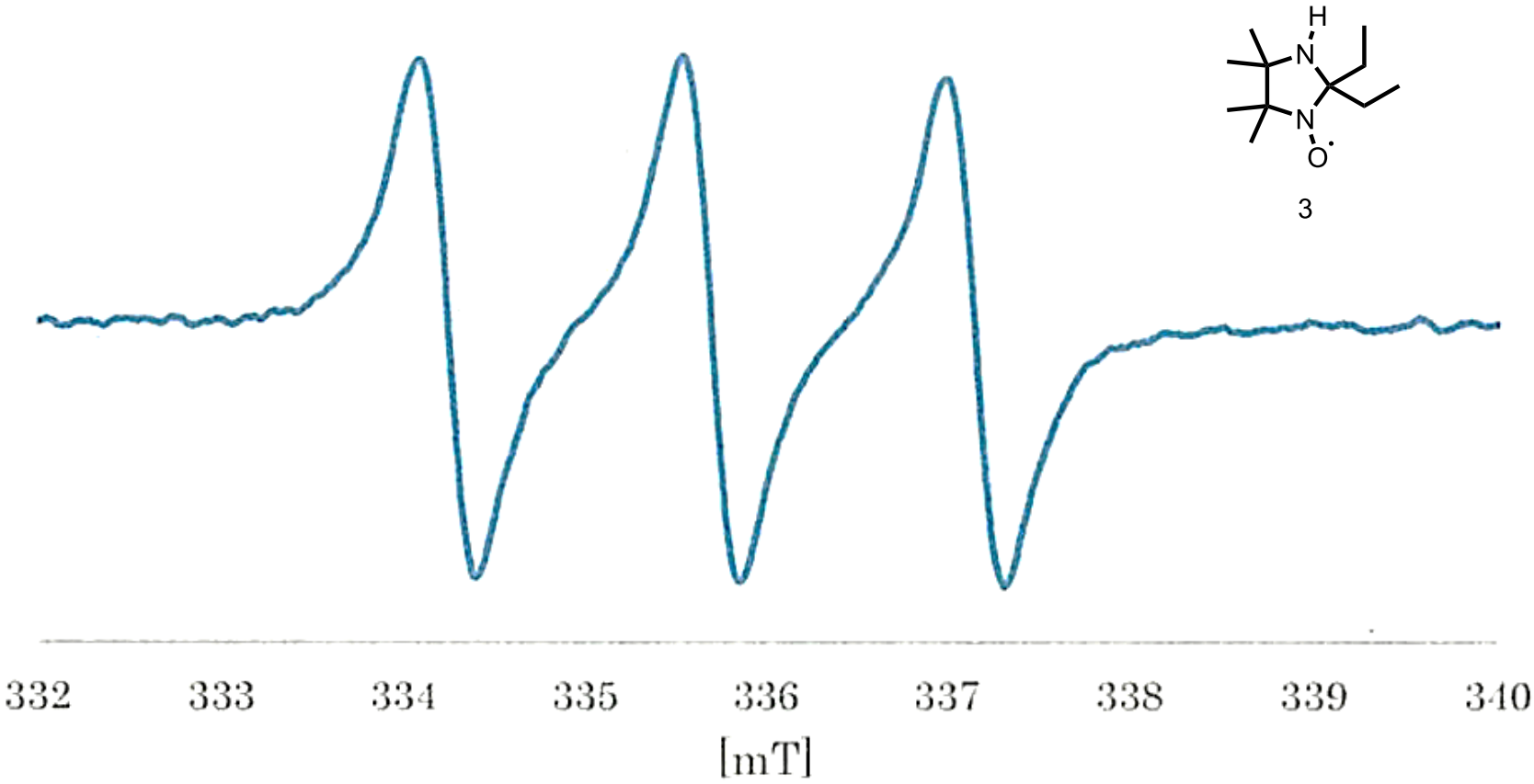


Procedure of 2,2-diethyl-4,4,5,5-tetramethylimidazolidine-1-oxyl (3) and 1-hydroxy-2,2-diethyl-4,4,5,5-tetramethylimidazolidine-3-oxyl (7)



To a −15℃ stirred solution of 184 mg (1.0 mmol) of 2,2-diethyl-4,4,5,5-tetramethylimidazolidine (16)in 10 mL of diethyl ether was added 585 mg (3.39 mmol) of *m*CPBA dissolved in 10 mL of ether dropwise during 1-h. After 3-h stirring, the mixture was then washed thrice with Na_2CO_3 and evaporated. Chromatography of the resulting oil over silica gel afforded 40.3 mg(0.20mmol,20.2%) of2,2-diethyl-4,4,5,5-tetramethylimidazolidine-1-oxyl (3) and 31.4 mg (0.15 mmol, 14.6%) of 1-hydroxy-2,2-diethyl-4,4,5,5-tetramethylimidazolidine-3-oxyl (7). Purity was confirmed by HPLC.
ESR(acetonitrile) three lines, a_N=1.45 mT (3) and a_N=1.52 mT (7) respectively
IR(KBr film) : 3300, 2967, 1262, 1094, 1019, 798 (3) and 3420, 2979, 1458, 1371, 1147, 1020 (7) respectively

ESR spectra of2,2-diethyl-4,4,5,5-tetramethylimidazolidine-1-oxyl (3)



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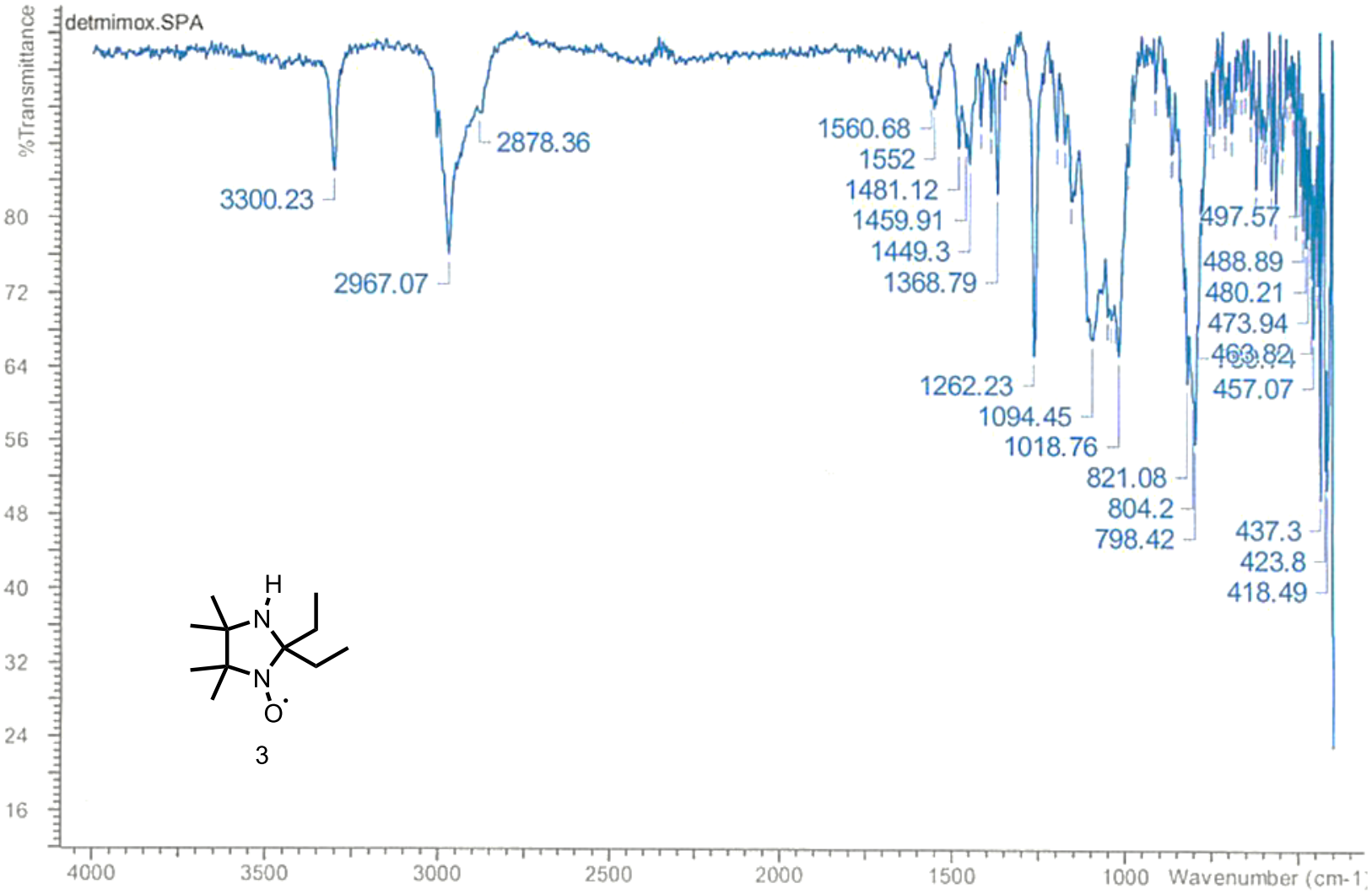
IR spectra of 2,2-diethyl-4,4,5,5-tetramethylimidazolidine-1-oxyl (3)



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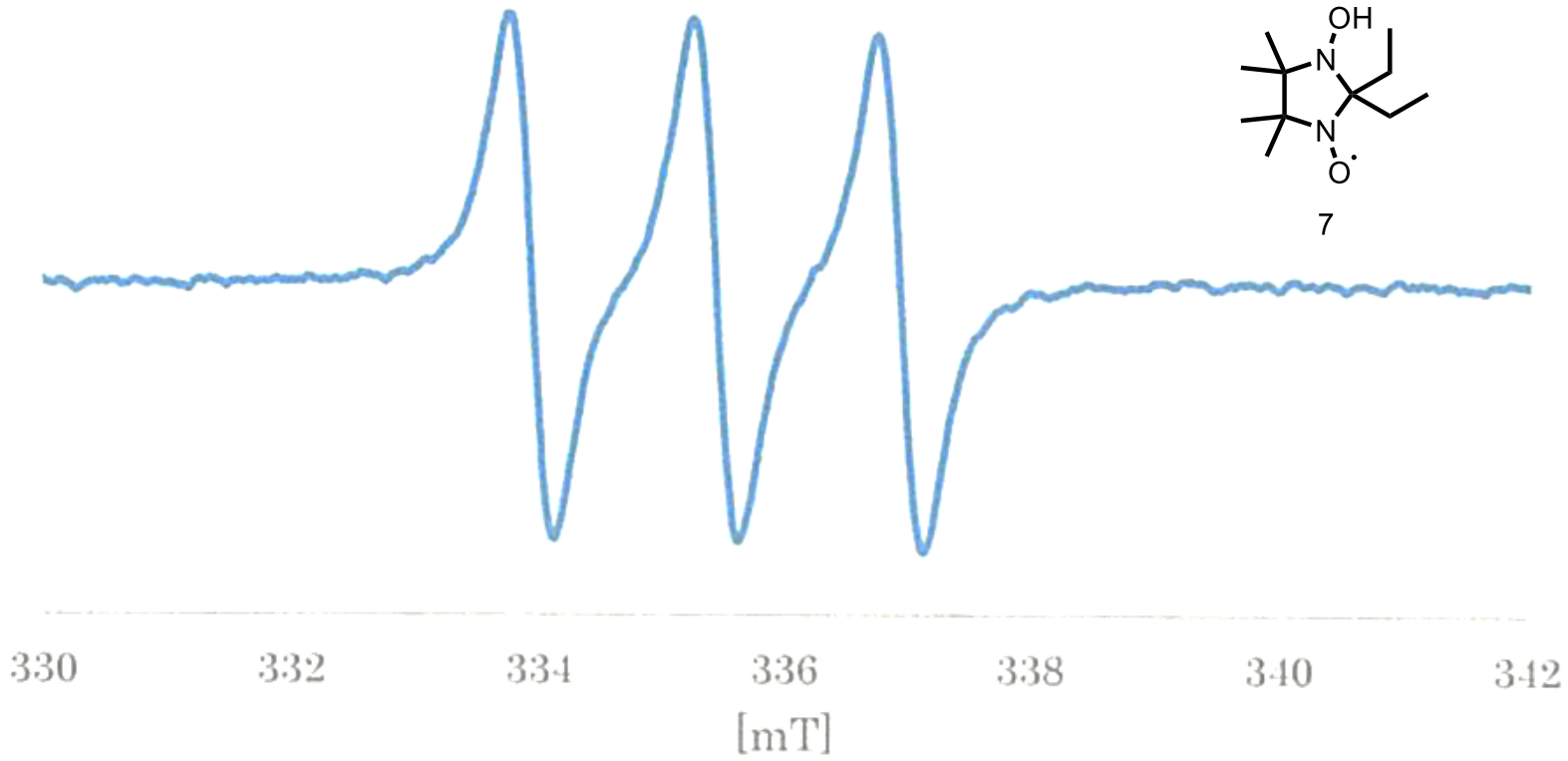
ESR spectra of 1-hydroxy-2,2-diethyl-4,4,5,5-tetramethylimidazolidine-3-oxyl (7)



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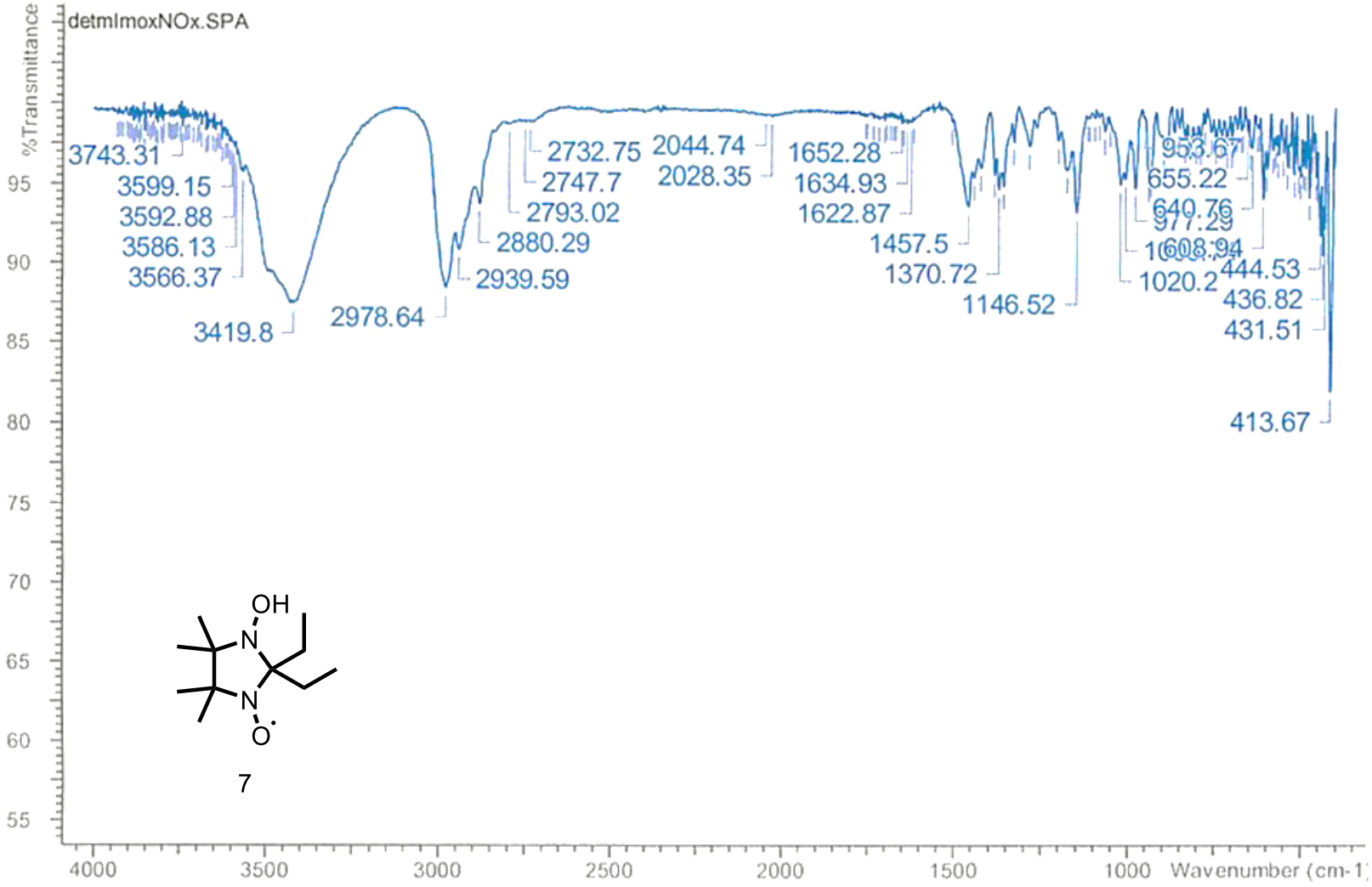
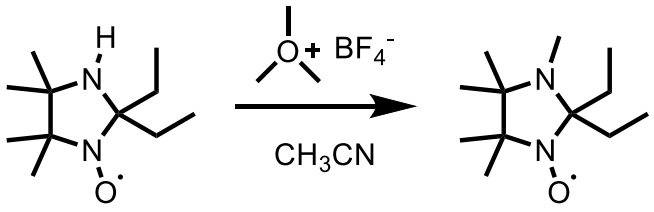
IR spectra of 1-hydroxy-2,2-diethyl-4,4,5,5-tetramethylimidazolidine-3-oxyl (7)



Procedure of 1-*N*-methyl-2,2-dietyl-4,4,5,5-tetramethylimidazolidine-1-oxyl (11)

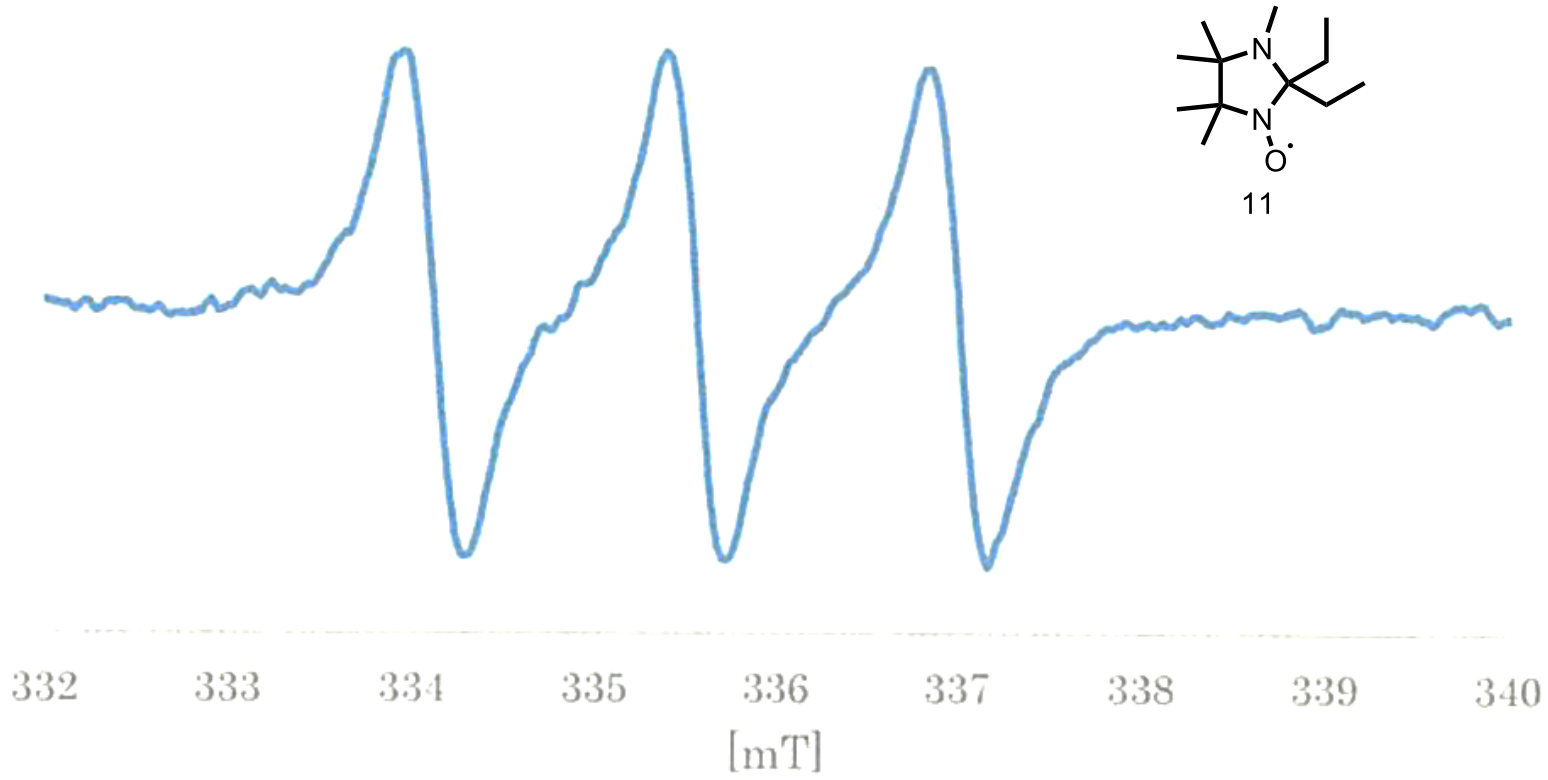


3 11

To a stirred solution of 29.9 mg (0.15 mmol) of 2,2-diethyl-4,4,5,5-tetramethylimidazolidine-1-oxyl (3) dissolved in 5 mL of acetonitrile at 0℃ was added 39.9 mg (0.27 mmol) of trimethyloxonium tetrafluoroboronate in 5 mL of acetonitrile over a 15-min period. After a 1-h stir at 0℃ the solution was diluted with 20 mL of CH_2Cl_2, washed thrice with cold 10% Na_2CO_3solution, and then evaporated. Chromatography of the resulting oil over silica gel afforded 4.1 mg (0.02 mmol,12.8%) of 1-*N*-methyl-2,2-dietyl-4,4,5,5-tetramethylimidazolidine-1-oxyl (11) as an oil. Purity was confirmed by HPLC.

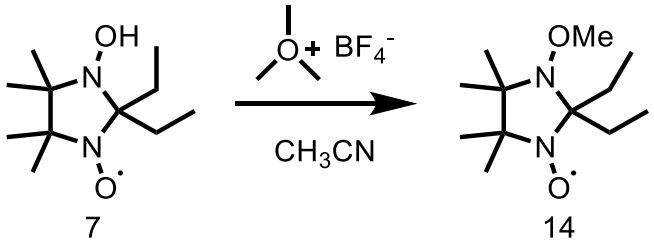
ESR(acetonitrile) three lines, a_N=1.42 mT

ESR spectra of 1-*N*- methyl-2,2-dietyl-4,4,5,5-tetramethylimidazolidine-1-oxyl (11)



11

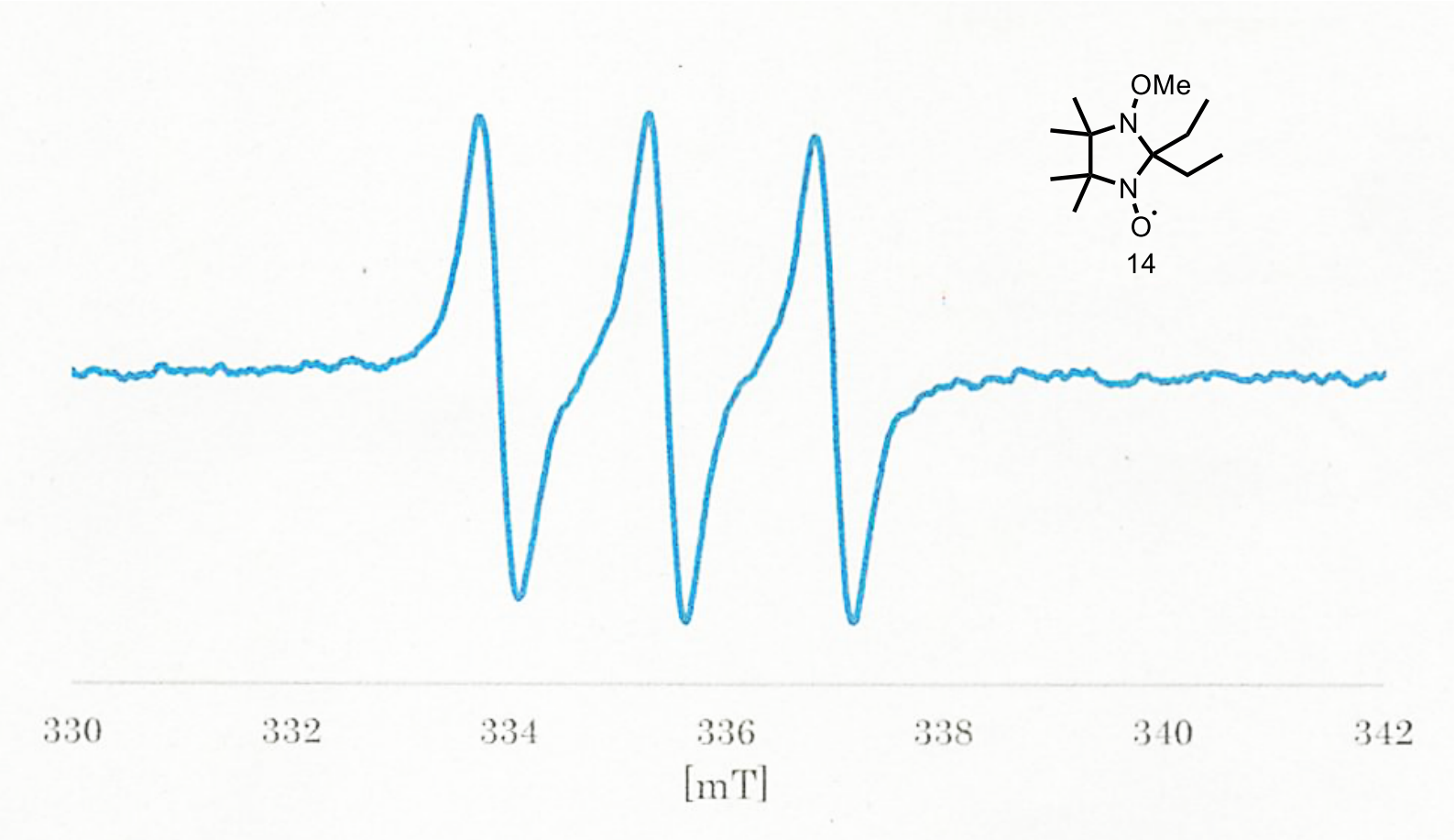
Procedure of 1-*N*- methoxy-2,2-dietyl-4,4,5,5-tetramethylimidazolidine-1-oxyl (14)



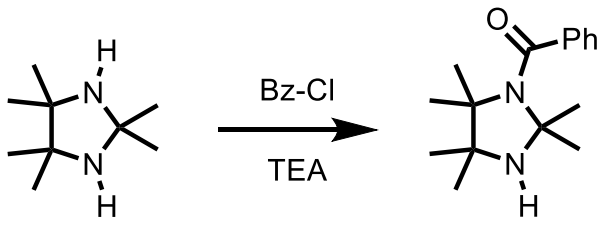
To a stirred solution of 43.1 mg (0.2 mmol) of 1-hydroxy-2,2-diethyl-4,4,5,5-tetramethylimidazolidine-3-oxyl (7) dissolved in 5 mL of acetonitrile portionwise over a 15-min period. After a 1-h stir at 0°Cthe solution was diluted with 20 mL of CH_2Cl_2, washed thrice with cold 10% Na_2CO_3solution, and then evaporated. Chromatography of the resulting oil over silica gel afforded 0.6 mg (3.0×10^{-3} mmol,1.4%) of 1-*N*-methoxy-2,2-dietyl-4,4,5,5-tetramethylimidazolidine-1-oxyl (14) as an oil. Purity was confirmed by HPLC.

ESR(acetonitrile) three lines, a_N=1.57 mT

ESR spectra of 1-N-methoxy-2,2-dietyl-4,4,5,5-tetramethylimidazolidine-1-oxyl (14)



Procedure of1-Benzoyl-2,2,4,4,5,5-hexamethylimidazolidine (18)

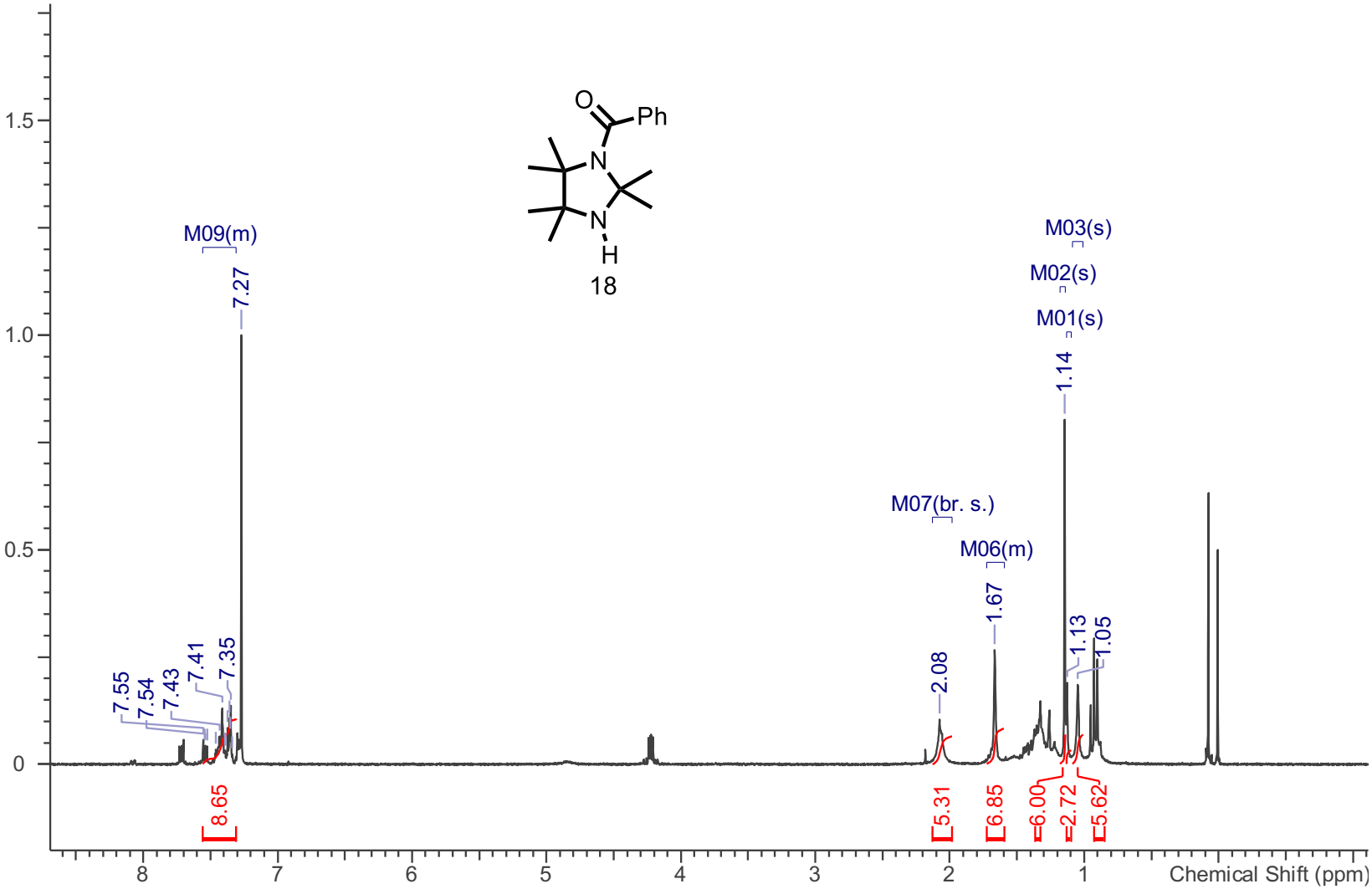


17 18

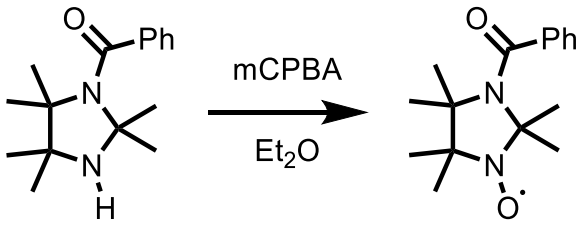
To a 50 mL round bottom flask in a constant temperature oven at 0℃, 2,2,4,4,5,5-hexamethylimidazolidine (17) (15 mg,0.1 mmol) in 2 mL of THF, 0.2 equivalents of benzoyl chloride (2.2 μL,0.02 mmol) and 2 equivalents of triethylamine (25 μL,0.2 mmol) were added, and the mixture was stirred at room temperature for 3 hours.After extracting with ethyl acetate, it was washed with sodium bicarbonate, dehydrated with sodium sulfate and concentrated on a rotary evaporator. 1-benzoyl-2,2,4,4,5,5-hexamethylimidazolidine (18) as white crystals was obtained in a yield of 11%(2.9 mg, 0.011 mmol). Purity was confirmed by HPLC.

^{1}H -NMR ($CDCl_3$) δ = 1.05 (6H, s), 1.14 (6H, s), 1.67 (6H, s), 2.08 (1H, br, NH), 7.35-7.55 (m, 5H)

^{1}H NMR spectra of 1-benzoyl-2,2,4,4,5,5-hexamethylimidazolidine (18)



Procedure of1-benzoyl-2,2,4,4,5,5-hexamethylimidazolidine-3-oxyl (15)

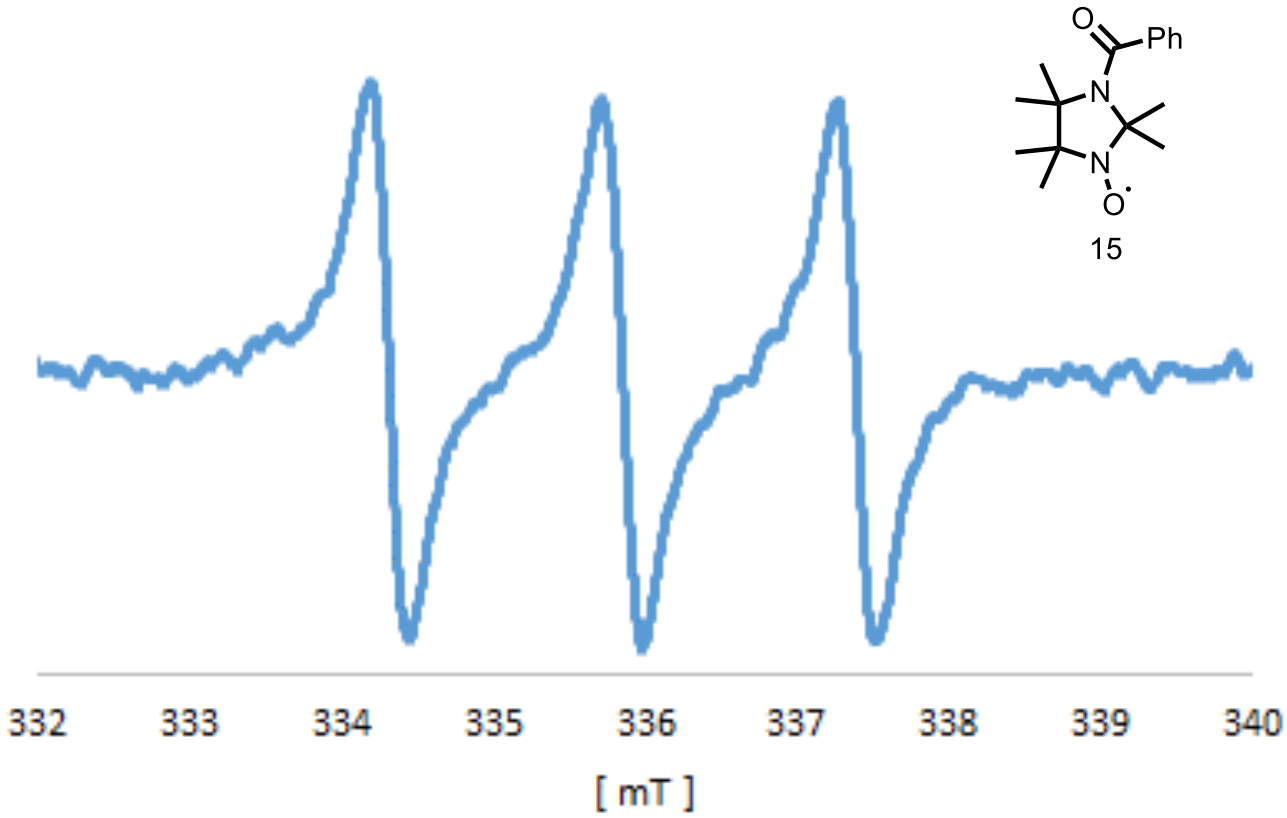


18 15

To a 50 mL round bottom flaskin a constant temperature oven at -8℃, 2 mg (0.01 mmol) of 1-benzoyl-2,2,4,4,5,5-hexamethylimidazolidine(18) and 5 mL of diethyl ether were added, and 5 mg (0.03 mmol) of *m*CPBA in 5 mL of diethyl ether was dropwised. After dropwising, the mixture was stirred for 3 hours in a constant temperature bath.Washing with sodium thiosulfate and sodium bicarbonate, dehydration with magnesium sulfate and concentration with a rotary evaporator afforded 1-benzoyl-2,2,4,4,5,5-hexamethylimidazolidine-3-oxyl (15) of yellow crystal was obtained in a yield of 85%(2.1 mg, 8.5×10^{-3} mmol). Purity was confirmed by HPLC.

ESR(acetonitrile) three lines, a_N=1.42 mT

ESR spectra of 1-benzoyl-2,2,4,4,5,5-hexamethylimidazolidine-3-oxyl (15)



15

Kinetics study

To measure the half-lives of the various compounds, they were exposed to a 20-fold molar excess of ascorbate in an organic solvent and the stabilities of the radicals were determined from the degree of reduction in theelectron spin resonance signal.

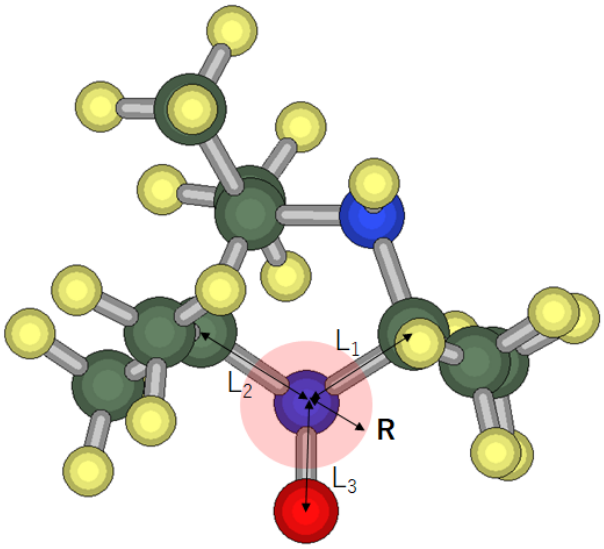
ESR condition:

FREQUENCY=9441MHz, MODURATION:Fq=100.0 kHz, Width=0.6 mT, POWER=4.000mW, SWEEP TIME=1.0min, TIME CONSTANT=0.1 sec, AMPLITUDE=6.000

2. Calculation section

Making close-packed model

As it is mentioned in the text, we used a close-packed model in which atoms and atoms are in close contact with each otherin calculating the volume ratio. the close-packed model was constructed byconsidering thatthe bond length of the target atom is L_n (n is number), and by calculating the volumes of the balls with a radius of half of L_n.Subsequently, setting the average volume as the volume of the target atom, the radius of the target atom was determined from the calculated volume.



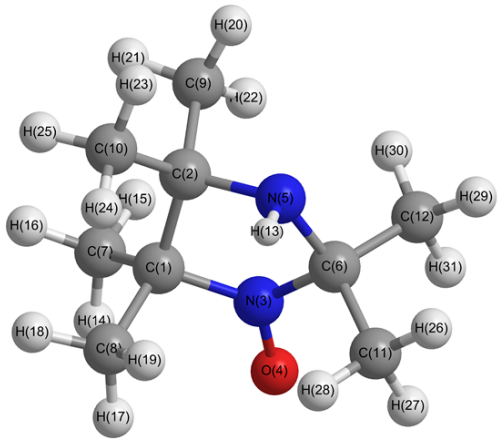
Let the radius of target atm **R**

$$\frac{4}{3}\pi R^3 = \frac{\frac{4}{3}\pi(\frac{L_1}{2})^3+\frac{4}{3}\pi(\frac{L_2}{2})^3+\frac{4}{3}\pi(\frac{L_3}{2})^3}{3}$$

$$\Leftrightarrow R^3 = \frac{(\frac{L_1}{2})^3+(\frac{L_2}{2})^3+(\frac{L_3}{2})^3}{3}$$

$$\Leftrightarrow R = \sqrt[3]{\frac{(\frac{L_1}{2})^3+(\frac{L_2}{2})^3+(\frac{L_3}{2})^3}{3}}$$

Labeled models of nitroxide radicals



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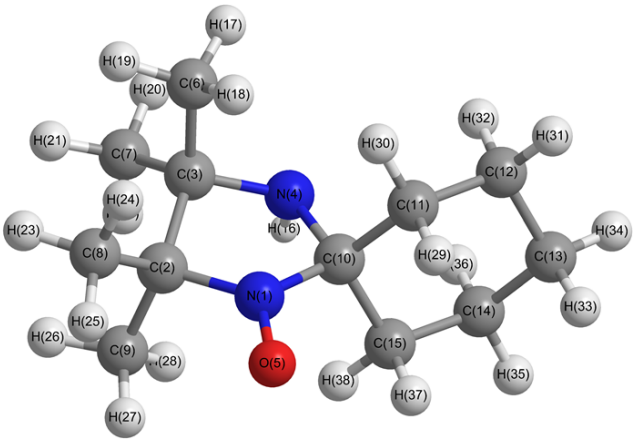

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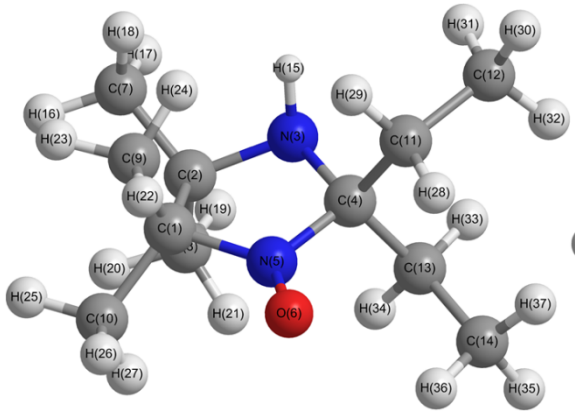

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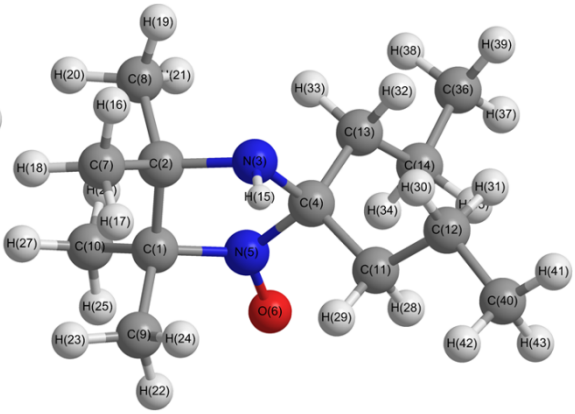

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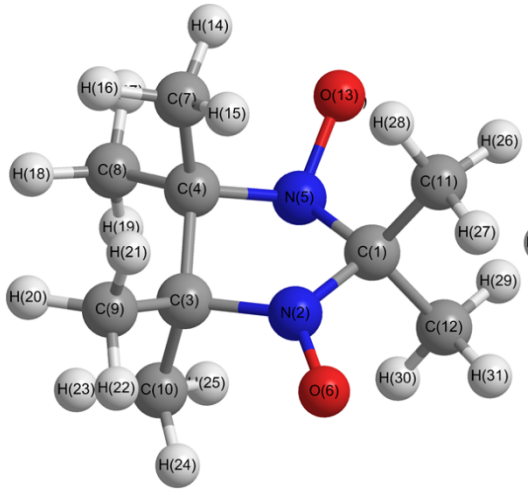

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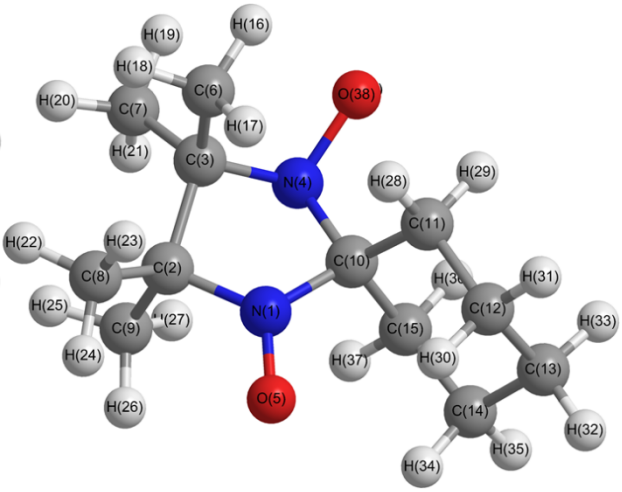

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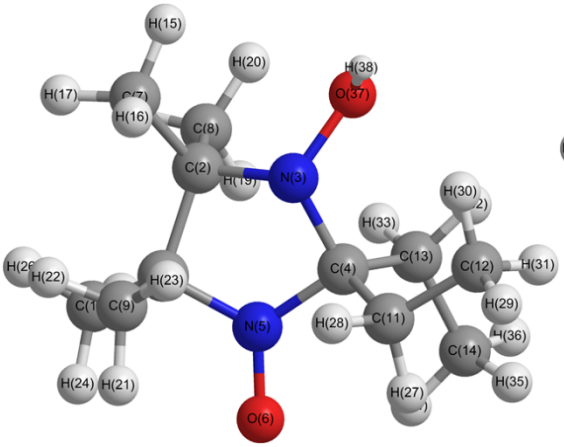
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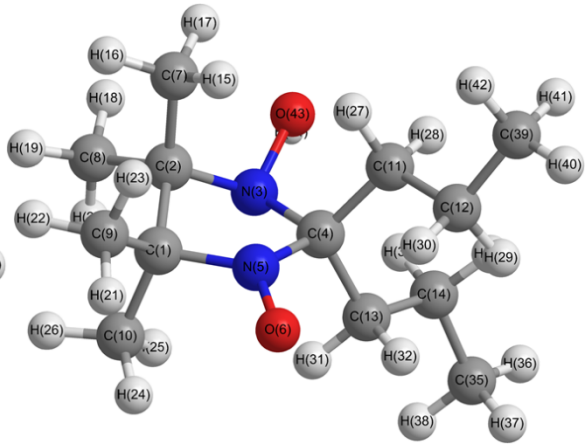
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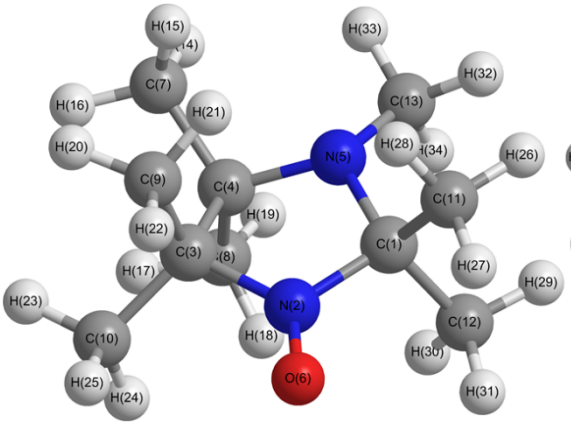
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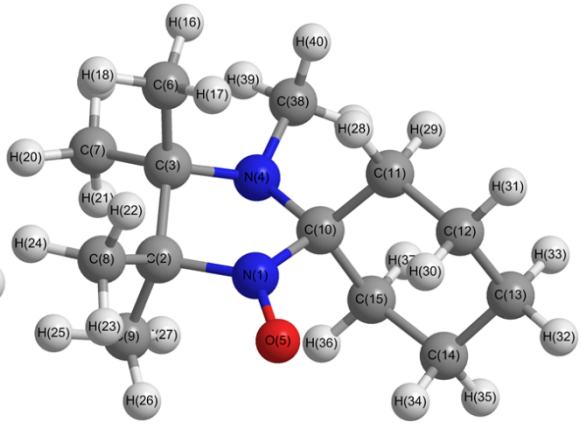
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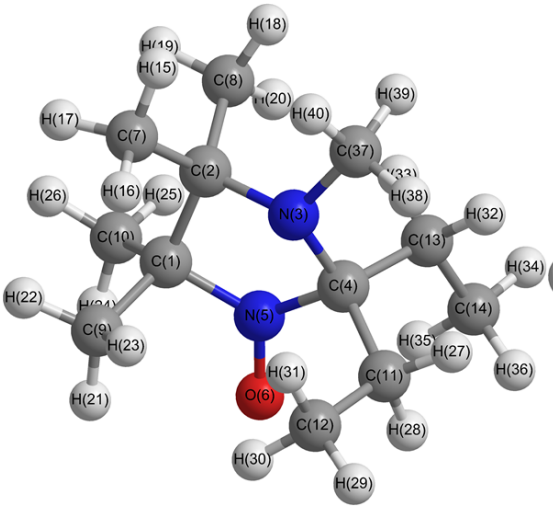
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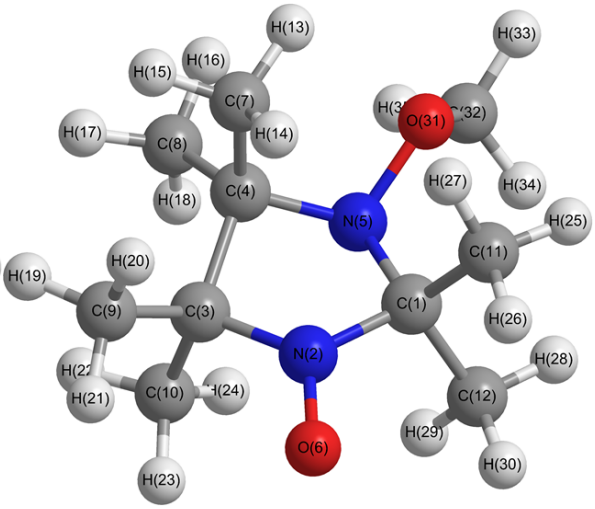
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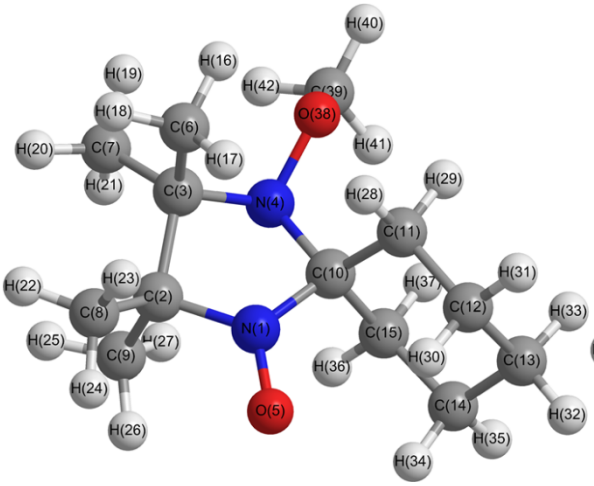
12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C(13)
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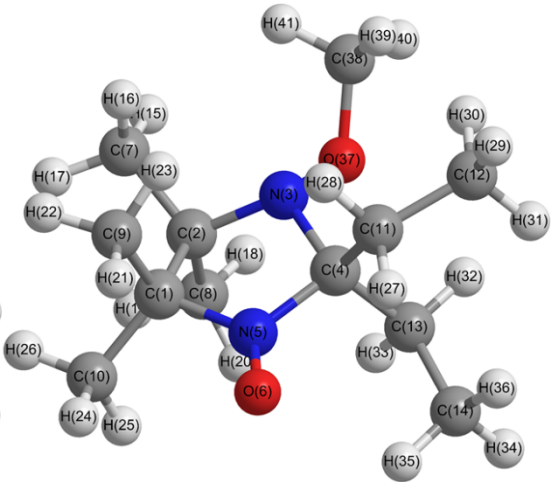
H(24)
O(5)
C(14)
H(32)
H(26)
H(35)
H(34)

13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C(12)
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N(3)
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H(31)
C(9)
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H(18)
H(21)
C(4)
C(1)
C(8)
H(27)
H(32)
H(1)
N(5)
C(13)
H(26)
H(33)
C(10)
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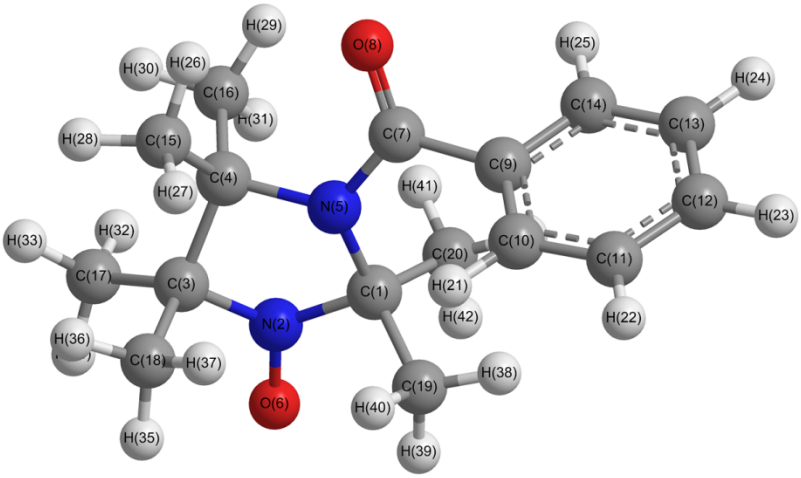
O(6)
H(36)
H(24)
H(25)
C(14)
H(35)
H(34)

14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C(10)
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C(11)
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C(3)
C(1)
H(21)
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N(2)
H(36)
C(18)
H(37)
C(19)
H(38)
O(6)
H(40)
H(35)
H(39)

15

Electron density of each atoms

The atomic charge of each atom was calculated by the Breneman model. [1]

1,2,3

1		2		3	
1	C 0.305494	1	N −0.088277	1	C 0.303017
2	C 0.561852	2	C 0.374359	2	C 0.561964
3	N −0.017893	3	C 0.540346	3	N −0.922409
4	O −0.388697	4	N −0.883399	4	C 0.440945
5	N −0.929567	5	O −0.376943	5	N −0.022429
6	C 0.734202	6	C −0.308690	6	O −0.377596
7	C −0.368229	7	C −0.329974	7	C −0.348059
8	C −0.284148	8	C −0.298099	8	C −0.363017
9	C −0.281582	9	C −0.311331	9	C −0.281699
10	C −0.323438	10	C 0.563516	10	C −0.304138
11	C −0.293493	11	C −0.067298	11	C 0.176778
12	C −0.389781	12	C 0.059823	12	C −0.251395
13	H 0.328722	13	C −0.007668	13	C 0.098634
14	H 0.109712	14	C 0.002209	14	C −0.254614
15	H 0.088710	15	C −0.012715	15	H 0.346616
16	H 0.079902	16	H 0.319116	16	H 0.072669
17	H 0.095238	17	H 0.080475	17	H 0.103253
18	H 0.059260	18	H 0.081703	18	H 0.065255
19	H 0.048093	19	H 0.044459	19	H 0.095031
20	H 0.074664	20	H 0.094742	20	H 0.061238
21	H 0.040599	21	H 0.064415	21	H 0.099387
22	H 0.062614	22	H 0.061884	22	H 0.089486
23	H 0.091942	23	H 0.055918	23	H 0.060083
24	H 0.063638	24	H 0.067186	24	H 0.056947
25	H 0.062077	25	H 0.090805	25	H 0.063964
26	H 0.068329	26	H 0.058040	26	H 0.094610
27	H 0.075682	27	H 0.096849	27	H 0.069265
28	H 0.056199	28	H 0.063038	28	H −0.021831
29	H 0.090179	29	H 0.003868	29	H −0.043688
30	H 0.098721	30	H 0.007803	30	H 0.055921
31	H 0.081002	31	H −0.012710	31	H 0.052756
		32	H −0.016720	32	H 0.066696

	33 H −0.002116	33 H −0.011383
	34 H −0.003249	34 H −0.009800
	35 H −0.000594	35 H 0.056876
	36 H −0.002881	36 H 0.070310
	37 H 0.014551	37 H 0.050356
	38 H −0.022440	

4,5,6

4	5	6
1 C 0.300828	1 C 0.734918	1 N −0.082838
2 C 0.559340	2 N −0.056046	2 C 0.169470
3 N −0.842408	3 C 0.330037	3 C 0.708594
4 C 0.209062	4 C 0.504272	4 N −0.700818
5 N 0.052911	5 N −0.594559	5 O −0.338353
6 O −0.379495	6 O −0.369649	6 C −0.288484
7 C −0.351472	7 C −0.233668	7 C −0.278975
8 C −0.313984	8 C −0.280867	8 C −0.329177
9 C −0.275102	9 C −0.359608	9 C −0.217641
10 C −0.321265	10 C −0.228239	10 C 0.698228
11 C 0.102271	11 C −0.380242	11 C −0.037141
12 C 0.119512	12 C −0.305411	12 C −0.053155
13 C −0.017726	13 O −0.452487	13 C 0.005986
14 C 0.147890	14 H 0.078071	14 C −0.008016
15 H 0.332512	15 H 0.039076	15 C −0.071624
16 H 0.098420	16 H 0.030849	16 H 0.079739
17 H 0.067749	17 H 0.073279	17 H 0.070153
18 H 0.073839	18 H 0.049564	18 H 0.027206
19 H 0.084228	19 H 0.064924	19 H 0.063055
20 H 0.046691	20 H 0.079378	20 H 0.039345
21 H 0.086110	21 H 0.088505	21 H 0.063715
22 H 0.088022	22 H 0.104088	22 H 0.081055
23 H 0.056191	23 H 0.041529	23 H 0.078069
24 H 0.057995	24 H 0.082932	24 H 0.107378
25 H 0.095437	25 H 0.041731	25 H 0.045719
26 H 0.072685	26 H 0.090850	26 H 0.087380
27 H 0.069843	27 H 0.077737	27 H 0.047071
28 H −0.013840	28 H 0.109975	28 H −0.003001
29 H −0.018677	29 H 0.068022	29 H 0.016339
30 H −0.013923	30 H 0.071006	30 H 0.010924
31 H −0.004199	31 H 0.072024	31 H 0.013018
32 H 0.008304	32 H 0.428008	32 H 0.003482
33 H 0.019192		33 H −0.011441

34 H -0.009861		34 H 0.014104
35 H -0.023870		35 H -0.003944
36 C -0.220911		36 H 0.007121
37 H 0.049379		37 H 0.012671
38 H 0.047147		38 O -0.462866
39 H 0.041784		39 H 0.437651
40 C -0.254554		
41 H 0.061231		
42 H 0.052072		
43 H 0.060644		

7,8,9

7		8		9	
1	C 0.317391	1	C 0.300583	1	C 0.758722
2	C 0.561612	2	C 0.587918	2	N −0.074801
3	N −0.607908	3	N −0.578248	3	C 0.365790
4	C 0.525259	4	C 0.314342	4	C 0.545781
5	N −0.087502	5	N −0.006851	5	N −0.674940
6	O −0.355870	6	O −0.356515	6	O −0.374100
7	C −0.296246	7	C −0.287282	7	C −0.352105
8	C −0.296028	8	C −0.301170	8	C −0.269895
9	C −0.269513	9	C −0.361212	9	C −0.249964
10	C −0.317632	10	C −0.264228	10	C −0.362790
11	C 0.103648	11	C −0.008732	11	C −0.315133
12	C −0.198456	12	C 0.101831	12	C −0.393897
13	C 0.113792	13	C 0.028176	13	C −0.080038
14	C −0.300862	14	C 0.183053	14	H 0.085019
15	H 0.077059	15	H 0.064465	15	H 0.087912
16	H 0.065561	16	H 0.036323	16	H 0.061773
17	H 0.052729	17	H 0.091523	17	H 0.035286
18	H 0.039769	18	H 0.074032	18	H 0.044096
19	H 0.068490	19	H 0.052849	19	H 0.069602
20	H 0.091516	20	H 0.067709	20	H 0.043091
21	H 0.089360	21	H 0.107743	21	H 0.040888
22	H 0.052808	22	H 0.082627	22	H 0.084052
23	H 0.063032	23	H 0.086627	23	H 0.077526
24	H 0.099077	24	H 0.090913	24	H 0.086394
25	H 0.075780	25	H 0.064554	25	H 0.100178
26	H 0.068095	26	H 0.051073	26	H 0.069270
27	H −0.019556	27	H 0.030067	27	H 0.068979
28	H −0.012159	28	H 0.017507	28	H 0.072698
29	H 0.052020	29	H −0.009561	29	H 0.083735
30	H 0.029037	30	H −0.003584	30	H 0.094732
31	H 0.045694	31	H 0.008367	31	H 0.083873
32	H −0.004330	32	H −0.013885	32	H 0.073813
33	H −0.003096	33	H −0.026220	33	H 0.083125

34 H 0.077286	34 H −0.043775	34 H 0.031328
35 H 0.067703	35 C −0.249319	
36 H 0.065115	36 H 0.054479	
37 O −0.476244	37 H 0.056867	
38 H 0.443570	38 H 0.053654	
	39 C −0.205039	
	40 H 0.049911	
	41 H 0.038752	
	42 H 0.042863	
	43 O −0.465647	
	44 H 0.442460	

10,11,12

10		11		12	
1	N −0.116461	1	C 0.329519	1	C 0.822201
2	C 0.276848	2	C 0.493182	2	N −0.094519
3	C 0.644426	3	N −0.504269	3	C 0.426432
4	N −0.741658	4	C 0.439473	4	C 0.462796
5	O −0.343467	5	N −0.025135	5	N −0.623398
6	C −0.309934	6	O −0.369426	6	O −0.370918
7	C −0.353182	7	C −0.407983	7	C −0.248359
8	C −0.330564	8	C −0.348350	8	C −0.428684
9	C −0.236918	9	C −0.287909	9	C −0.378838
10	C 0.728916	10	C −0.307738	10	C −0.265177
11	C −0.079090	11	C 0.125547	11	C −0.435989
12	C −0.017657	12	C −0.222038	12	C −0.330878
13	C −0.020104	13	C −0.035638	13	H 0.065051
14	C 0.002604	14	C −0.216344	14	H 0.046511
15	C −0.121353	15	H 0.104326	15	H 0.045894
16	H 0.071867	16	H 0.097449	16	H 0.132434
17	H 0.067470	17	H 0.087476	17	H 0.081973
18	H 0.037322	18	H 0.089199	18	H 0.113645
19	H 0.080071	19	H 0.062806	19	H 0.080160
20	H 0.060034	20	H 0.073205	20	H 0.089556
21	H 0.087048	21	H 0.092926	21	H 0.104972
22	H 0.077959	22	H 0.059185	22	H 0.048396
23	H 0.096364	23	H 0.053163	23	H 0.084531
24	H 0.075065	24	H 0.088653	24	H 0.051359
25	H 0.043921	25	H 0.070762	25	H 0.095163
26	H 0.084930	26	H 0.067657	26	H 0.094818
27	H 0.043488	27	H −0.023226	27	H 0.103394
28	H −0.005706	28	H −0.011114	28	H 0.083404
29	H 0.014597	29	H 0.043236	29	H 0.078526
30	H 0.011021	30	H 0.063286	30	H 0.065892
31	H 0.004187	31	H 0.040732	31	O −0.190757
32	H 0.008203	32	H 0.014465	32	C 0.055493
33	H −0.009326	33	H 0.022126	33	H 0.054100

34 H 0.017254	34 H 0.055082	34 H 0.036369
35 H −0.003395	35 H 0.068018	35 H 0.044450
36 H 0.016831	36 H 0.041588	
37 H 0.028605	37 C −0.104125	
38 C −0.044100	38 H 0.074292	
39 H 0.078125	39 H 0.027687	
40 H 0.018902	40 H 0.078255	
41 H 0.056856		

13,14,15

13		14		15	
1	N −0.131904	1	C 0.426850	1	C 0.664294
2	C 0.316884	2	C 0.518629	2	N −0.146942
3	C 0.612589	3	N −0.607170	3	C 0.451445
4	N −0.688056	4	C 0.540189	4	C 0.581596
5	O −0.339109	5	N −0.123190	5	N −0.650210
6	C −0.331034	6	O −0.353651	6	O −0.348137
7	C −0.389764	7	C −0.386673	7	C 0.596515
8	C −0.337374	8	C −0.378228	8	O −0.552671
9	C −0.252395	9	C −0.333768	9	C −0.005664
10	C 0.764367	10	C −0.327259	10	C −0.046358
11	C −0.114480	11	C 0.246867	11	C −0.112029
12	C 0.024474	12	C −0.247234	12	C −0.079122
13	C −0.033673	13	C 0.084869	13	C −0.088919
14	C 0.001767	14	C −0.243726	14	C −0.088502
15	C −0.108002	15	H 0.120973	15	C −0.365762
16	H 0.078768	16	H 0.096221	16	C −0.404404
17	H 0.079976	17	H 0.071168	17	C −0.352785
18	H 0.053028	18	H 0.101078	18	C −0.317104
19	H 0.112806	19	H 0.068144	19	C −0.259665
20	H 0.066366	20	H 0.095538	20	C −0.185834
21	H 0.102289	21	H 0.094922	21	H 0.059350
22	H 0.075524	22	H 0.064689	22	H 0.098925
23	H 0.078077	23	H 0.083415	23	H 0.091966
24	H 0.099789	24	H 0.095834	24	H 0.092929
25	H 0.047733	25	H 0.073367	25	H 0.096070
26	H 0.085503	26	H 0.067552	26	H 0.127759
27	H 0.055200	27	H −0.055630	27	H 0.074124
28	H 0.001112	28	H −0.057761	28	H 0.053017
29	H 0.019532	29	H 0.047868	29	H 0.137010
30	H −0.003362	30	H 0.060590	30	H 0.061037
31	H −0.000033	31	H 0.049100	31	H 0.074450
32	H 0.007946	32	H −0.015171	32	H 0.088707
33	H −0.005133	33	H −0.018197	33	H 0.072987

34 H 0.016924	34 H 0.056308	34 H 0.095725
35 H −0.005694	35 H 0.064403	35 H 0.094962
36 H 0.013212	36 H 0.048170	36 H 0.063362
37 H 0.040664	37 O −0.234810	37 H 0.055639
38 O −0.215316	38 C 0.113240	38 H 0.030256
39 C 0.088883	39 H 0.021249	39 H 0.068780
40 H 0.050805	40 H 0.044454	40 H 0.071141
41 H 0.023523	41 H 0.026777	41 H 0.040364
42 H 0.037591		42 H 0.051614
		43 H 0.010085

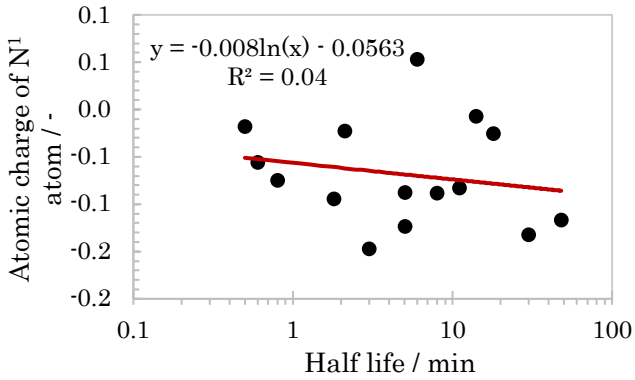


Fig. S1Plot of Atomic charge of N1 atom against half life of nitroxides in ascorbatesolution

Mulliken spin densitiesof each atoms

1,2,3

1		2		3	
1	C −0.022274	1	N 0.449988	1	C −0.020470
2	C 0.002307	2	C −0.022837	2	C 0.001408
3	N 0.448770	3	C 0.002498	3	N 0.002868
4	O 0.512072	4	N 0.001065	4	C −0.020478
5	N 0.001445	5	O 0.509910	5	N 0.451724
6	C −0.020174	6	C 0.001249	6	O 0.508556
7	C 0.010081	7	C −0.000124	7	C −0.000386
8	C 0.031487	8	C 0.010248	8	C 0.001185
9	C 0.001340	9	C 0.031351	9	C 0.031479
10	C −0.000135	10	C −0.022173	10	C 0.010116
11	C 0.022678	11	C 0.018335	11	C 0.020375
12	C 0.016702	12	C 0.000557	12	C −0.000230
13	H −0.000301	13	C −0.000061	13	C 0.015131
14	H −0.001141	14	C 0.000053	14	C −0.000369
15	H 0.000242	15	C 0.022684	15	H −0.000314
16	H −0.000690	16	H −0.000331	16	H 0.000014
17	H −0.002219	17	H −0.000139	17	H −0.000177
18	H 0.003301	18	H 0.000417	18	H 0.000041
19	H −0.001115	19	H 0.000370	19	H −0.000126
20	H −0.000139	20	H −0.000163	20	H 0.000300
21	H 0.000359	21	H 0.000013	21	H 0.000302
22	H 0.000411	22	H 0.000023	22	H −0.002098
23	H −0.000169	23	H −0.000696	23	H 0.002429
24	H 0.000025	24	H 0.000219	24	H −0.001073
25	H 0.000013	25	H −0.001127	25	H −0.000615
26	H 0.000363	26	H 0.003448	26	H −0.001180
27	H −0.001561	27	H −0.002252	27	H 0.000353
28	H −0.000662	28	H −0.001071	28	H −0.001296
29	H 0.000946	29	H −0.001615	29	H −0.000765
30	H −0.000477	30	H −0.000486	30	H 0.001538
31	H −0.001487	31	H 0.001043	31	H 0.000279
		32	H 0.000052	32	H −0.000048

	33 H -0.000021	33 H 0.002355
	34 H -0.000063	34 H -0.000332
	35 H 0.001638	35 H 0.000796
	36 H 0.000149	36 H -0.001254
	37 H -0.001582	37 H -0.000034
	38 H -0.000571	

4,5,6

4		5		6	
1	C	-0.020793	1 C -0.019255	1 N 0.446023	
2	C	0.001363	2 N 0.437748	2 C -0.020555	
3	N	0.002988	3 C -0.019492	3 C 0.001746	
4	C	-0.020684	4 C 0.001755	4 N 0.000387	
5	N	0.452959	5 N 0.000089	5 O 0.508787	
6	O	0.507501	6 O 0.517996	6 C 0.001317	
7	C	-0.000391	7 C 0.001514	7 C -0.000268	
8	C	0.001104	8 C -0.000249	8 C 0.010969	
9	C	0.031555	9 C 0.010450	9 C 0.030669	
10	C	0.010427	10 C 0.030660	10 C -0.021636	
11	C	0.020119	11 C 0.019104	11 C 0.018701	
12	C	-0.000148	12 C 0.023039	12 C -0.000588	
13	C	0.015290	13 O 0.001268	13 C 0.000065	
14	C	-0.000275	14 H -0.000086	14 C -0.000280	
15	H	-0.000304	15 H 0.000550	15 C 0.021969	
16	H	-0.000176	16 H 0.000609	16 H -0.000086	
17	H	0.000041	17 H -0.000182	17 H 0.000426	
18	H	0.000014	18 H 0.000018	18 H 0.000520	
19	H	-0.000123	19 H 0.000028	19 H -0.000179	
20	H	0.000277	20 H -0.000825	20 H 0.000019	
21	H	0.000273	21 H 0.000191	21 H 0.000025	
22	H	-0.002108	22 H -0.001036	22 H -0.000882	
23	H	0.002359	23 H 0.002926	23 H 0.000189	
24	H	-0.001069	24 H -0.001998	24 H -0.001080	
25	H	-0.001190	25 H -0.000974	25 H 0.002734	
26	H	0.000349	26 H 0.001322	26 H -0.002003	
27	H	-0.000581	27 H -0.001688	27 H -0.000952	
28	H	-0.001264	28 H -0.000605	28 H -0.000419	
29	H	-0.000776	29 H -0.000443	29 H 0.002045	
30	H	0.000271	30 H -0.000754	30 H -0.000916	
31	H	-0.000023	31 H -0.001565	31 H 0.001332	
32	H	0.002533	32 H -0.000117	32 H -0.000041	
33	H	-0.000357		33 H -0.000029	

34 H -0.001335		34 H -0.000657
35 H -0.000037		35 H 0.001475
36 C 0.000546		36 H 0.001149
37 H 0.000140		37 H -0.001038
38 H -0.000036		38 O 0.001165
39 H 0.000081		39 H -0.000101
40 C 0.001105		
41 H 0.000473		
42 H -0.000057		
43 H -0.000043		

7,8,9

7			8			9		
1	C	−0.018078	1	C	−0.018167	1	C	−0.019788
2	C	0.001202	2	C	0.001193	2	N	0.444418
3	N	0.000150	3	N	0.000183	3	C	−0.021942
4	C	−0.019195	4	C	−0.019154	4	C	0.002871
5	N	0.440335	5	N	0.440922	5	N	0.001090
6	O	0.514311	6	O	0.513668	6	O	0.513988
7	C	−0.000344	7	C	0.001319	7	C	−0.000197
8	C	0.001351	8	C	−0.000348	8	C	0.001452
9	C	0.030435	9	C	0.010646	9	C	0.031943
10	C	0.010577	10	C	0.030579	10	C	0.009993
11	C	0.021437	11	C	0.017663	11	C	0.022815
12	C	−0.000671	12	C	−0.000391	12	C	0.017268
13	C	0.017635	13	C	0.021206	13	C	0.000178
14	C	−0.000521	14	C	−0.000542	14	H	−0.000192
15	H	−0.000161	15	H	0.000455	15	H	0.000024
16	H	0.000038	16	H	0.000609	16	H	0.000015
17	H	0.000014	17	H	−0.000075	17	H	0.000367
18	H	0.000623	18	H	−0.000158	18	H	0.000494
19	H	0.000470	19	H	0.000014	19	H	−0.000114
20	H	−0.000078	20	H	0.000038	20	H	0.003238
21	H	−0.001919	21	H	−0.001040	21	H	−0.001118
22	H	0.002367	22	H	−0.000830	22	H	−0.002144
23	H	−0.000911	23	H	0.000252	23	H	−0.000805
24	H	−0.001035	24	H	−0.001905	24	H	0.000206
25	H	0.000244	25	H	−0.000920	25	H	−0.001025
26	H	−0.000830	26	H	0.002342	26	H	0.000075
27	H	−0.001510	27	H	−0.000471	27	H	−0.001560
28	H	−0.000844	28	H	0.002635	28	H	−0.000715
29	H	0.001756	29	H	−0.000028	29	H	0.001218
30	H	0.000301	30	H	−0.001370	30	H	−0.000440
31	H	−0.000057	31	H	−0.000860	31	H	−0.001673
32	H	0.002560	32	H	−0.001475	32	H	−0.000008
33	H	−0.000444	33	H	−0.000031	33	H	−0.000199

34 H -0.001290	34 H 0.000290	34 H 0.000268
35 H -0.000028	35 C 0.001298	
36 H 0.000999	36 H 0.000493	
37 O 0.001190	37 H -0.000039	
38 H -0.000080	38 H -0.000068	
	39 C 0.000687	
	40 H 0.000192	
	41 H 0.000060	
	42 H -0.000041	
	43 O 0.001244	
	44 H -0.000077	

10,11,12

10		11		12	
1	N 0.451573	1	C −0.022566	1	C −0.018974
2	C −0.022452	2	C 0.001081	2	N 0.438078
3	C 0.003012	3	N 0.003042	3	C −0.019608
4	N 0.001105	4	C −0.023551	4	C 0.002022
5	O 0.505254	5	N 0.454118	5	N −0.000110
6	C 0.001418	6	O 0.505796	6	O 0.517389
7	C −0.000219	7	C −0.000429	7	C 0.001586
8	C 0.010023	8	C 0.000573	8	C −0.000216
9	C 0.032087	9	C 0.030427	9	C 0.010201
10	C −0.021799	10	C 0.013822	10	C 0.030772
11	C 0.016301	11	C 0.020466	11	C 0.018879
12	C −0.000442	12	C −0.000407	12	C 0.023382
13	C 0.000058	13	C 0.018339	13	H −0.000089
14	C 0.000036	14	C −0.000663	14	H 0.000564
15	C 0.021639	15	H −0.000127	15	H 0.000652
16	H −0.000123	16	H 0.000035	16	H −0.000187
17	H 0.000404	17	H 0.000002	17	H 0.000020
18	H 0.000333	18	H −0.000098	18	H 0.000027
19	H −0.000192	19	H 0.000171	19	H −0.000845
20	H 0.000017	20	H 0.000167	20	H 0.000185
21	H 0.000024	21	H −0.002076	21	H −0.001008
22	H 0.000208	22	H 0.001939	22	H 0.003027
23	H −0.001032	23	H −0.000708	23	H −0.002018
24	H −0.000902	24	H −0.001299	24	H −0.000990
25	H 0.003040	25	H 0.000197	25	H 0.001233
26	H −0.002143	26	H −0.000331	26	H −0.001699
27	H −0.001103	27	H −0.000385	27	H −0.000597
28	H −0.000266	28	H −0.001423	28	H −0.000372
29	H 0.001943	29	H 0.000194	29	H −0.000713
30	H −0.000917	30	H −0.000611	30	H −0.001632
31	H 0.001171	31	H −0.000028	31	O 0.001186
32	H −0.000036	32	H 0.004251	32	C −0.000145
33	H −0.000030	33	H −0.000393	33	H −0.000009

34 H -0.000668	34 H 0.001030	34 H -0.000020
35 H 0.001560	35 H -0.001373	35 H 0.000028
36 H -0.000989	36 H -0.000004	
37 H 0.002036	37 C 0.000440	
38 C 0.000012	38 H 0.000007	
39 H -0.000139	39 H 0.000477	
40 H 0.000221	40 H -0.000101	
41 H -0.000026		

13,14,15

13		14		15	
1	N 0.446109	1	C −0.018253	1	C −0.017890
2	C −0.020844	2	C 0.001500	2	N 0.440129
3	C 0.002033	3	N 0.000043	3	C −0.021286
4	N 0.000241	4	C −0.019195	4	C 0.003675
5	O 0.508572	5	N 0.440647	5	N −0.000358
6	C 0.001430	6	O 0.512329	6	O 0.514350
7	C −0.000211	7	C −0.000297	7	C −0.000609
8	C 0.010686	8	C 0.001449	8	O −0.000069
9	C 0.030790	9	C 0.030904	9	C 0.000126
10	C −0.021520	10	C 0.010282	10	C −0.000012
11	C 0.018555	11	C 0.022135	11	C −0.000022
12	C −0.000607	12	C −0.000578	12	C −0.000009
13	C 0.000058	13	C 0.017836	13	C −0.000024
14	C −0.000174	14	C −0.000660	14	C 0.000009
15	C 0.022114	15	H −0.000177	15	C 0.000021
16	H −0.000089	16	H 0.000042	16	C 0.001794
17	H 0.000467	17	H 0.000012	17	C 0.008765
18	H 0.000572	18	H −0.000086	18	C 0.033068
19	H −0.000186	19	H 0.000689	19	C 0.025430
20	H 0.000019	20	H 0.000533	20	C 0.016473
21	H 0.000024	21	H −0.001943	21	H −0.000004
22	H −0.000922	22	H 0.002626	22	H 0.000005
23	H 0.000156	23	H −0.000947	23	H 0.000001
24	H −0.001032	24	H −0.001015	24	H 0.000000
25	H 0.002872	25	H 0.000239	25	H 0.000000
26	H −0.002038	26	H −0.000882	26	H −0.000188
27	H −0.000966	27	H −0.001509	27	H 0.000034
28	H −0.000447	28	H −0.000685	28	H −0.000009
29	H 0.001954	29	H 0.001771	29	H −0.000129
30	H −0.000904	30	H 0.000259	30	H 0.000570
31	H 0.001332	31	H −0.000042	31	H 0.000458
32	H −0.000042	32	H 0.002658	32	H 0.000171
33	H −0.000019	33	H −0.000506	33	H −0.000957

34 H −0.000704	34 H 0.001061	34 H −0.000850
35 H 0.001488	35 H −0.001298	35 H −0.002163
36 H −0.001026	36 H 0.000004	36 H 0.003669
37 H 0.001236	37 O 0.001131	37 H −0.001195
38 O 0.001157	38 C −0.000104	38 H 0.000503
39 C −0.000105	39 H 0.000006	39 H −0.001291
40 H −0.000005	40 H 0.000023	40 H −0.000705
41 H −0.000023	41 H −0.000005	41 H −0.000304
42 H −0.000003		42 H −0.001640
		43 H 0.000461

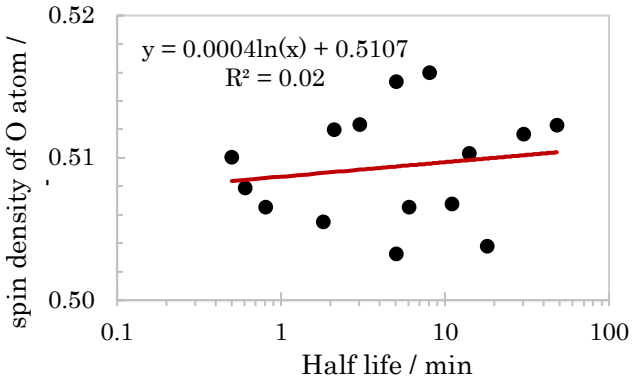


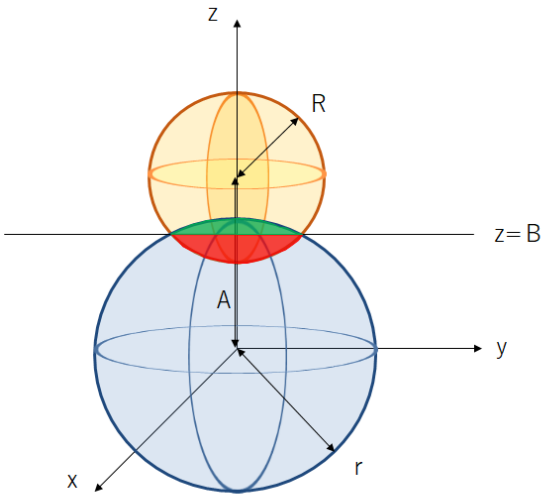
Fig. S2Plot of Spin density of O atom against half life of nitroxides in ascorbatesolution

SOMO-LUMO energy gap of all compounds

Compound	SOMO (α-HOMO) [au]	LUMO (β-LUMO) [au]	E.G. [au]
1	-0.18135	-0.03871	0.14264
2	-0.17941	-0.03779	0.14162
3	-0.18221	-0.04029	0.14192
4	-0.18191	-0.04011	0.14180
5	-0.18614	-0.04405	0.14209
6	-0.18514	-0.04445	0.14069
7	-0.18684	-0.04595	0.14089
8	-0.18685	-0.04606	0.14079
9	-0.18182	-0.03923	0.14259
10	-0.18148	-0.04037	0.14111
11	-0.18104	-0.03958	0.14146
12	-0.18618	-0.04417	0.14201
13	-0.18487	-0.04423	0.14064
14	-0.18668	-0.04639	0.14029
15	-0.19559	-0.05388	0.14171

Volume ratio calcuration

In calculating the volume ratio, it is necessary to calculate the overlapping volume of the 3.42 Å sphere and the atomic sphere.Calculation formulas are shown below with the figures.



$$V_1 = \int_{A-R}^{B} \pi\{r^2 - (t^2 - 2At + A^2)\}dt$$

$$V_2 = \int_{B}^{r} \pi(r^2 - t^2)dt$$

$\Leftrightarrow$

$$V_1 = \frac{\pi}{3} \times \{2R^3 + (3B - 3A)R^2 + A^3 - 3BA^2 + 3B^2A - B^3)\}$$

$$V_2 = \frac{\pi}{3} \times \ (2r^3 - 3r^2B + B^3)$$

$V_1 + V_2$ = overlapping volume

$\frac{sum\ of\ (V_1+V_2)}{\frac{4}{3}\pi r^3}$ = volume ratio

Multiple regression analysis

Summary of Multiple regression analysis for Variables Predicting Radical's stability (N = 15).

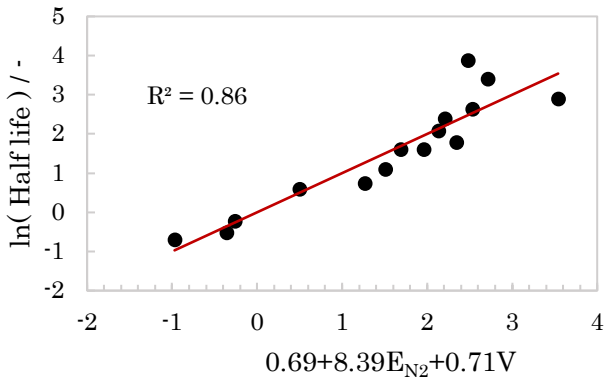


Fig. S3 Correlation of ln(Half life) vs $f(C_{N^2}, V)$

Regressuion Statics	
Multiple R	0.93
R Square	0.86
Adjusted R square	0.83
Standard Error	0.57
Observations	15.00

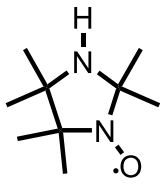
analysis of variance	N	SS	MS	F	Significance F
Regression	2.00	23.20	11.60	35.98	0.00
Residual	12.00	3.87	0.32		
Total	14.00	27.07			

	Coefficient	Standardized Partial Regression Coefficient	Standard Deviation	Standard Error	t Stat	P-Value	Lower 95%	Upper 95%
Segment	0.68			2.55	0.27	0.79	-4.86	6.23
C_{N2}	8.39	0.80	0.13	1.16	7.23	0.00	5.86	10.92
V	0.71	0.33	0.63	0.24	3.00	0.01	0.20	1.23

3. DFT Calculation section

Geometry optimization

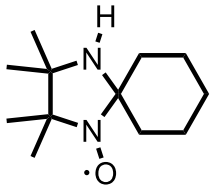
Each molecules were calculated five stable conformations bymolecular mechanics method using medit program, andthey are optimized by Gaussian 09 programat the UB3LYP/6-31G* level. We defined the most stable conformation from the comparison of enthalpy.



1

C	0.803917	0.755785	-0.009790
C	1.020292	-0.800076	0.052899
N	-0.650308	0.787193	-0.328560
O	-1.267327	1.863579	-0.625148
N	-0.286318	-1.330965	0.548045
C	-1.374800	-0.443315	0.117039
C	1.572552	1.509235	-1.100017
C	1.019526	1.473531	1.339213
C	1.311520	-1.407113	-1.333047
C	2.132126	-1.241959	1.010574
C	-2.329198	-0.100664	1.269190
C	-2.174667	-1.011348	-1.065218
H	-0.262067	-1.340892	1.565889
H	1.246516	2.553242	-1.113721
H	1.391706	1.092381	-2.093199
H	2.649287	1.482992	-0.898895
H	0.569211	2.469144	1.278849
H	2.085293	1.587618	1.564275
H	0.549456	0.941729	2.172765
H	1.245034	-2.496801	-1.262636
H	2.315598	-1.140329	-1.680429
H	0.597361	-1.074034	-2.090611
H	2.192965	-2.335583	1.023489
H	1.959489	-0.901228	2.036727
H	3.103852	-0.854056	0.686458
H	-2.867030	-0.997287	1.595427
H	-3.054000	0.645156	0.932987
H	-1.786747	0.315761	2.124952
H	-2.776485	-1.863180	-0.732893
H	-1.514418	-1.353720	-1.864640
H	-2.837628	-0.237602	-1.465059

Zero-point correction=	0.278592 (Hartree/Particle)
Thermal correction to Energy=	0.292300
Thermal correction to Enthalpy=	0.293244
Thermal correction to Gibbs Free Energy=	0.240318
Sum of electronic and zero-point Energies=	-538.784707
Sum of electronic and thermal Energies=	-538.770999
Sum of electronic and thermal Enthalpies=	-538.770055
Sum of electronic and thermal Free Energies=	-538.822981



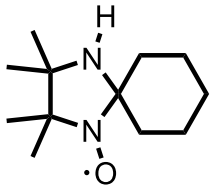
2

The N^2 atom takes the axial position.

N	0.473560	-1.021789	-0.471209
C	1.777269	-0.490082	0.011782
C	1.396068	1.025828	0.173712
N	-0.055081	1.000963	0.532495
O	0.334960	-2.216254	-0.898402
C	1.572872	1.818617	-1.135744
C	2.168454	1.754386	1.279143
C	2.864836	-0.813617	-1.017739
C	2.124548	-1.194244	1.340582
C	-0.691299	-0.182207	-0.063674
C	-1.535090	0.155578	-1.313407
C	-2.813859	0.924560	-0.955350
C	-3.671514	0.156246	0.059293
C	-2.855582	-0.191652	1.312021
C	-1.568236	-0.948355	0.949320
H	-0.130984	0.932757	1.545845
H	1.103197	2.800011	-1.021138
H	1.107110	1.319819	-1.989590
H	2.632795	1.964347	-1.371101
H	1.821664	2.791198	1.347401
H	3.241482	1.771931	1.059842
H	2.033523	1.288009	2.260520
H	3.830593	-0.407301	-0.697176
H	2.627337	-0.413311	-2.005626
H	2.958511	-1.899099	-1.113618
H	3.128461	-0.923103	1.684415
H	2.092871	-2.276144	1.179057
H	1.412824	-0.952687	2.136511
H	-1.780429	-0.793826	-1.806444
H	-0.930972	0.736307	-2.016565

H	-3.389742	1.125175	-1.867575
H	-2.532642	1.899038	-0.534554
H	-4.038637	-0.772347	-0.402142
H	-4.557322	0.742560	0.334587
H	-3.451901	-0.800144	2.003744
H	-2.605586	0.734189	1.850013
H	-1.812539	-1.914341	0.492198
H	-0.979450	-1.167575	1.849975

Zero-point correction=	0.345389 (Hartree/Particle)
Thermal correction to Energy=	0.360720
Thermal correction to Enthalpy=	0.361664
Thermal correction to Gibbs Free Energy=	0.304643
Sum of electronic and zero-point Energies=	-655.455116
Sum of electronic and thermal Energies=	-655.439785
Sum of electronic and thermal Enthalpies=	-655.438841
Sum of electronic and thermal Free Energies=	-655.495861



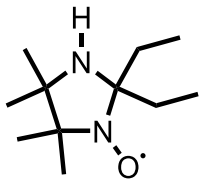
2

The N^2 atom takes the equatorial position.

N	0.059496	0.697875	-0.430002
C	1.530523	0.739267	-0.188247
C	1.776957	-0.762603	0.194842
N	0.504791	-1.177392	0.854556
O	-0.558729	1.692049	-0.944562
C	2.938900	-0.983621	1.169915
C	2.013600	-1.655103	-1.038902
C	1.800069	1.731116	0.962794
C	2.233824	1.244369	-1.452076
C	-0.624677	-0.419461	0.293281
C	-1.537164	0.098783	1.430206
C	-2.839626	0.758929	0.952030
C	-3.622219	-0.157918	0.001878
C	-2.744161	-0.601065	-1.175609
C	-1.458672	-1.283807	-0.683360
H	0.573789	-0.957767	1.847160
H	3.015785	-2.048814	1.413489
H	2.809713	-0.432220	2.106998
H	3.888963	-0.670804	0.723493
H	1.971569	-2.703413	-0.728893
H	2.995050	-1.462841	-1.485958
H	1.257846	-1.503842	-1.813873
H	1.369433	1.392670	1.910653
H	1.341080	2.691407	0.708162
H	2.873844	1.887731	1.110476
H	3.319802	1.255996	-1.306717
H	2.004620	0.627191	-2.323623
H	1.900794	2.263122	-1.668888
H	-0.967657	0.794248	2.059928
H	-1.779499	-0.775504	2.052768

H	-2.595790	1.693439	0.437214
H	-3.450398	1.016495	1.827069
H	-4.519091	0.357870	-0.363362
H	-3.971504	-1.045494	0.551820
H	-2.482610	0.271451	-1.784214
H	-3.295187	-1.295960	-1.822439
H	-1.709684	-2.202484	-0.136663
H	-0.835175	-1.585573	-1.530496

Zero-point correction=	0.345497 (Hartree/Particle)
Thermal correction to Energy=	0.360772
Thermal correction to Enthalpy=	0.361717
Thermal correction to Gibbs Free Energy=	0.304984
Sum of electronic and zero-point Energies=	-655.453122
Sum of electronic and thermal Energies=	-655.437847
Sum of electronic and thermal Enthalpies=	-655.436903
Sum of electronic and thermal Free Energies=	-655.493635

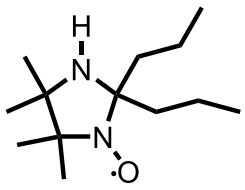


3

C	-1.397742	0.507981	-0.424504
C	-1.373403	-0.732538	0.537603
N	0.008435	-1.281066	0.389094
C	0.948416	-0.195681	0.063315
N	0.033719	0.923025	-0.343056
O	0.454560	1.967557	-0.947225
C	-2.381024	-1.830198	0.174459
C	-1.612089	-0.344574	2.010134
C	-1.710947	0.155018	-1.893507
C	-2.283111	1.684754	-0.000722
C	1.853000	-0.563437	-1.133250
C	2.855228	-1.692756	-0.865839
C	1.765801	0.207809	1.316445
C	2.760142	1.360483	1.133324
H	0.001627	-1.939942	-0.387615
H	-3.408705	-1.458454	0.248169
H	-2.275461	-2.669264	0.870613
H	-2.234610	-2.213695	-0.840450
H	-1.373079	-1.202703	2.645192
H	-2.658065	-0.066284	2.179678
H	-0.989962	0.494688	2.330390
H	-1.425262	1.003397	-2.522564
H	-2.779008	-0.040878	-2.035567
H	-1.153416	-0.721964	-2.237987
H	-3.341610	1.404402	-0.040383
H	-2.119352	2.521663	-0.685758
H	-2.050819	2.031199	1.008708
H	2.374230	0.345657	-1.447360
H	1.202466	-0.841336	-1.973133
H	3.391955	-1.946217	-1.786827
H	2.361020	-2.603321	-0.507310

H	3.601483	-1.406266	-0.118077
H	2.284843	-0.693872	1.661335
H	1.058513	0.463630	2.110623
H	3.222574	1.610984	2.095068
H	2.264968	2.253378	0.743285
H	3.568494	1.099863	0.440762

Zero-point correction=	0.336264 (Hartree/Particle)
Thermal correction to Energy=	0.352565
Thermal correction to Enthalpy=	0.353509
Thermal correction to Gibbs Free Energy=	0.294601
Sum of electronic and zero-point Energies=	-617.350120
Sum of electronic and thermal Energies=	-617.333819
Sum of electronic and thermal Enthalpies=	-617.332875
Sum of electronic and thermal Free Energies=	-617.391783

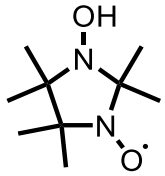


4

C	1.874884	0.020357	0.636323
C	1.800334	-0.173142	-0.920390
N	0.400877	-0.636261	-1.163414
C	-0.499144	-0.084082	-0.136878
N	0.456696	0.389697	0.919506
O	0.076929	0.698764	2.099830
C	2.769958	-1.226710	-1.469996
C	2.043958	1.136917	-1.694705
C	2.195741	-1.272254	1.416074
C	2.792236	1.139006	1.142672
C	-1.412114	-1.175150	0.463375
C	-2.456191	-1.764311	-0.496110
C	-1.302828	1.112954	-0.705206
C	-2.263278	1.820769	0.261788
C	-2.920694	3.046649	-0.382791
C	-3.235396	-2.921491	0.139955
H	0.389909	-1.651398	-1.082007
H	2.624714	-1.328888	-2.550883
H	2.621090	-2.211128	-1.014890
H	3.810027	-0.930104	-1.296766
H	1.774762	0.981833	-2.743686
H	3.097064	1.434699	-1.645193
H	1.445675	1.967902	-1.313820
H	1.944745	-1.111379	2.468750
H	3.258869	-1.525083	1.345540
H	1.615302	-2.129449	1.059864
H	2.666245	1.243787	2.224164
H	2.556774	2.102600	0.685782
H	3.841518	0.900409	0.936111

H	-1.903278	-0.752982	1.345916
H	-0.768120	-1.983645	0.837718
H	-1.968081	-2.112771	-1.416443
H	-3.161209	-0.983080	-0.805083
H	-1.852168	0.744754	-1.580531
H	-0.588156	1.845863	-1.093806
H	-1.720292	2.116133	1.165380
H	-3.047414	1.126047	0.590874
H	-3.611101	3.538137	0.312081
H	-2.169445	3.787277	-0.684226
H	-3.490055	2.771709	-1.279845
H	-3.984730	-3.323379	-0.551266
H	-2.567571	-3.744426	0.423381
H	-3.758308	-2.594677	1.046940

Zero-point correction=	0.392934 (Hartree/Particle)
Thermal correction to Energy=	0.412184
Thermal correction to Enthalpy=	0.413128
Thermal correction to Gibbs Free Energy=	0.346575
Sum of electronic and zero-point Energies=	-695.920446
Sum of electronic and thermal Energies=	-695.901196
Sum of electronic and thermal Enthalpies=	-695.900251
Sum of electronic and thermal Free Energies=	-695.966804

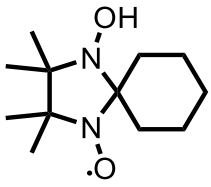


5

C	1.357101	-0.139006	-0.039121
N	0.318485	-1.146396	0.296617
C	-1.062883	-0.710874	-0.054713
C	-0.882023	0.840819	0.034675
N	0.494885	0.961383	-0.538453
O	0.618199	-2.375909	0.458228
C	-0.997047	1.369938	1.479787
C	-1.843484	1.639958	-0.854446
C	-2.056522	-1.321021	0.938438
C	-1.391323	-1.219713	-1.474451
C	2.210271	0.168376	1.201781
C	2.255572	-0.652491	-1.172776
O	1.071594	2.235752	-0.221951
H	-0.585939	2.381132	1.528607
H	-0.463922	0.746409	2.201072
H	-2.047061	1.413054	1.787487
H	-1.635266	2.709896	-0.747505
H	-2.884626	1.472562	-0.555929
H	-1.733482	1.375586	-1.908760
H	-3.073788	-0.978818	0.719282
H	-1.816262	-1.067578	1.972995
H	-2.029991	-2.410073	0.845942
H	-2.439235	-1.027725	-1.728317
H	-1.221499	-2.300370	-1.503579
H	-0.758889	-0.746605	-2.229973
H	3.021428	0.854531	0.947189
H	2.637500	-0.773246	1.560311
H	1.625718	0.614900	2.007308
H	2.990540	0.116141	-1.434863
H	1.662848	-0.885933	-2.060964
H	2.783776	-1.554808	-0.852926

H 1.218242 2.621374 -1.099782

Zero-point correction=	0.281551 (Hartree/Particle)
Thermal correction to Energy=	0.296579
Thermal correction to Enthalpy=	0.297523
Thermal correction to Gibbs Free Energy=	0.241982
Sum of electronic and zero-point Energies=	-613.944877
Sum of electronic and thermal Energies=	-613.929850
Sum of electronic and thermal Enthalpies=	-613.928906
Sum of electronic and thermal Free Energies=	-613.984447



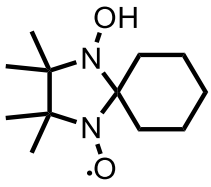
6

The N^2 atom takes the equatorial position.

N	-0.015340	-0.960864	0.252099
C	-1.488601	-0.967950	0.015080
C	-1.781106	0.566616	0.060274
N	-0.546462	1.063799	-0.614618
O	0.624144	-2.056363	0.412480
C	-1.961707	1.103975	1.496013
C	-2.994532	1.000958	-0.773224
C	-2.173544	-1.803075	1.101396
C	-1.754486	-1.615774	-1.360323
C	0.650015	0.302031	-0.158208
C	1.442604	0.926467	1.015814
C	2.739443	0.162407	1.330284
C	3.649932	0.074078	0.098949
C	2.915620	-0.591730	-1.072079
C	1.584485	0.110737	-1.377659
O	-0.378772	2.471281	-0.406041
H	-1.872687	2.193055	1.485322
H	-1.222452	0.706857	2.195220
H	-2.955131	0.845904	1.877732
H	-3.114284	2.087393	-0.705218
H	-3.914458	0.541310	-0.394386
H	-2.878279	0.736537	-1.826857
H	-3.260316	-1.786083	0.964851
H	-1.941011	-1.445411	2.106538
H	-1.830662	-2.838335	1.026498
H	-2.827352	-1.757546	-1.527428
H	-1.269609	-2.596472	-1.379028
H	-1.351264	-1.011014	-2.176442
H	0.810839	0.983824	1.906153
H	1.680197	1.957311	0.730663

H	2.493957	-0.848192	1.675932
H	3.258325	0.669596	2.154014
H	4.563269	-0.484556	0.339442
H	3.967995	1.087222	-0.191796
H	2.717763	-1.639967	-0.827646
H	3.541585	-0.580045	-1.974107
H	1.783181	1.123445	-1.758273
H	1.034118	-0.418095	-2.162828
H	-0.412820	2.820926	-1.310130

Zero-point correction=	0.348255 (Hartree/Particle)
Thermal correction to Energy=	0.364915
Thermal correction to Enthalpy=	0.365859
Thermal correction to Gibbs Free Energy=	0.306352
Sum of electronic and zero-point Energies=	-730.612993
Sum of electronic and thermal Energies=	-730.596333
Sum of electronic and thermal Enthalpies=	-730.595389
Sum of electronic and thermal Free Energies=	-730.654896



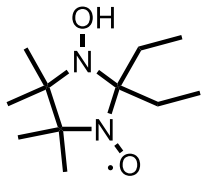
6

The N^2 atom takes the axial position.

N	0.507699	-1.154714	-0.403293
C	1.821112	-0.619757	0.047029
C	1.493687	0.907684	0.045881
N	0.084381	0.865381	0.552629
O	0.347906	-2.386695	-0.692947
C	1.620629	1.537932	-1.357305
C	2.331743	1.734472	1.029255
C	2.913867	-1.062344	-0.931149
C	2.135574	-1.192266	1.445527
C	-0.647194	-0.285637	-0.043639
C	-1.491025	-0.026692	-1.317929
C	-2.885296	0.578400	-1.076778
C	-3.669877	-0.173620	0.005768
C	-2.844125	-0.287684	1.292492
C	-1.507778	-0.993437	1.027115
O	-0.574733	2.109786	0.272200
H	1.131771	2.514883	-1.360275
H	1.165972	0.923579	-2.138156
H	2.674562	1.683175	-1.616508
H	2.019570	2.783160	0.982789
H	3.395552	1.692852	0.769047
H	2.208026	1.387557	2.057739
H	3.877903	-0.627339	-0.645863
H	2.689505	-0.774151	-1.960171
H	3.002410	-2.151525	-0.900913
H	3.149010	-0.922530	1.761417
H	2.068493	-2.283436	1.396686
H	1.430066	-0.832931	2.198784
H	-1.597213	-1.014078	-1.786314
H	-0.930719	0.599587	-2.016692

H	-3.440804	0.566620	-2.023578
H	-2.777770	1.627992	-0.784741
H	-3.918795	-1.184347	-0.349954
H	-4.622883	0.333714	0.203061
H	-3.399825	-0.840808	2.060372
H	-2.662612	0.715805	1.703924
H	-0.921213	-1.074623	1.948148
H	-1.693775	-2.011865	0.664831
H	-0.805083	2.426993	1.159386

Zero-point correction=	0.348637 (Hartree/Particle)
Thermal correction to Energy=	0.365137
Thermal correction to Enthalpy=	0.366081
Thermal correction to Gibbs Free Energy=	0.307009
Sum of electronic and zero-point Energies=	-730.612509
Sum of electronic and thermal Energies=	-730.596010
Sum of electronic and thermal Enthalpies=	-730.595066
Sum of electronic and thermal Free Energies=	-730.654137

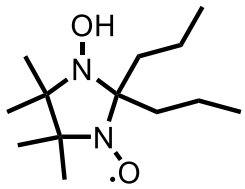


7

C	1.447021	-0.732824	-0.270980
C	1.389984	0.742262	0.239531
N	0.021221	1.118621	-0.234647
C	-0.932375	-0.011950	-0.042039
N	0.033293	-1.147816	-0.028982
O	-0.340202	-2.347256	-0.263533
C	2.401704	1.681389	-0.432287
C	1.571978	0.851764	1.768205
C	1.744396	-0.858684	-1.779714
C	2.385639	-1.666146	0.501011
C	-1.842415	-0.144935	-1.285205
C	-2.880401	0.968925	-1.453076
C	-1.737462	0.042595	1.280222
C	-2.678082	-1.146426	1.516737
O	-0.428395	2.305917	0.435381
H	2.280285	2.693631	-0.032114
H	2.258739	1.723597	-1.514498
H	3.430094	1.364165	-0.224936
H	2.627494	0.730590	2.033507
H	1.002751	0.100010	2.319205
H	1.248407	1.840695	2.101493
H	1.494584	-1.874808	-2.099165
H	2.805609	-0.681865	-1.983671
H	1.155380	-0.152098	-2.369694
H	2.281698	-2.681229	0.108467
H	2.155029	-1.694318	1.567980
H	3.426860	-1.350072	0.374964
H	-2.334889	-1.120937	-1.237760
H	-1.189903	-0.166926	-2.164246
H	-3.435856	0.826843	-2.386862
H	-2.409731	1.957235	-1.497291

H	-3.608932	0.983418	-0.635708
H	-2.301493	0.979361	1.288185
H	-1.033033	0.113219	2.112803
H	-2.143702	-2.097796	1.453601
H	-3.496451	-1.176193	0.789133
H	-3.129283	-1.066470	2.512453
H	-0.536405	2.929209	-0.299660

Zero-point correction=	0.339350 (Hartree/Particle)
Thermal correction to Energy=	0.356938
Thermal correction to Enthalpy=	0.357882
Thermal correction to Gibbs Free Energy=	0.296426
Sum of electronic and zero-point Energies=	-692.509724
Sum of electronic and thermal Energies=	-692.492137
Sum of electronic and thermal Enthalpies=	-692.491192
Sum of electronic and thermal Free Energies=	-692.552648

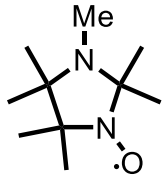


8

C	1.863198	0.077778	-0.792674
C	1.828081	-0.168330	0.748801
N	0.456607	-0.753212	0.877288
C	-0.506297	-0.041665	-0.013813
N	0.448870	0.496698	-1.024080
O	0.060992	0.855619	-2.187577
C	2.032575	1.125377	1.565994
C	2.839487	-1.211639	1.243860
C	2.803603	1.191381	-1.265369
C	2.137864	-1.194253	-1.622617
C	-1.288362	1.108037	0.668649
C	-2.257004	1.881531	-0.240386
C	-1.435192	-1.069533	-0.700740
C	-2.464649	-1.746847	0.213045
C	-3.280586	-2.810692	-0.530081
C	-2.878913	3.079999	0.485598
O	0.028149	-0.721481	2.246702
H	1.462920	1.970847	1.174348
H	3.090355	1.408918	1.568677
H	1.723328	0.952901	2.599569
H	2.733853	-1.335461	2.326884
H	3.867217	-0.886637	1.045668
H	2.681617	-2.184585	0.773047
H	2.684147	1.325045	-2.343849
H	3.845873	0.922453	-1.062131
H	2.588404	2.147348	-0.783808
H	1.867953	-0.992990	-2.663554
H	1.551102	-2.045575	-1.268544
H	3.198638	-1.463743	-1.585682
H	-0.569075	1.812419	1.096804

H	-1.832175	0.685772	1.519500
H	-3.059816	1.217835	-0.586160
H	-1.730310	2.218033	-1.139246
H	-0.794479	-1.838149	-1.148008
H	-1.942155	-0.565384	-1.530555
H	-3.147236	-0.998881	0.635775
H	-1.954041	-2.210685	1.066951
H	-4.015077	-3.283945	0.131530
H	-3.825386	-2.371535	-1.374595
H	-2.632825	-3.600103	-0.930524
H	-3.581784	3.614535	-0.163533
H	-3.426475	2.764831	1.382824
H	-2.110080	3.795225	0.803176
H	-0.088791	-1.662850	2.448360

Zero-point correction=	0.396524 (Hartree/Particle)
Thermal correction to Energy=	0.416862
Thermal correction to Enthalpy=	0.417806
Thermal correction to Gibbs Free Energy=	0.349522
Sum of electronic and zero-point Energies=	-771.079679
Sum of electronic and thermal Energies=	-771.059341
Sum of electronic and thermal Enthalpies=	-771.058397
Sum of electronic and thermal Free Energies=	-771.126681

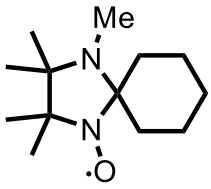


9

C	-1.346322	-0.181277	-0.023079
N	-0.275293	-1.169136	0.258364
C	1.082542	-0.678441	-0.088411
C	0.855970	0.863755	0.071302
N	-0.542586	0.985183	-0.421222
O	-0.536429	-2.408361	0.413460
C	1.801585	1.694864	-0.811984
C	1.037730	1.326730	1.537014
C	1.402609	-1.111891	-1.534768
C	2.105412	-1.308762	0.861701
C	-2.222982	-0.674437	-1.187313
C	-2.217000	-0.028769	1.242140
C	-1.193398	2.279230	-0.339826
H	1.682104	2.765281	-0.612960
H	1.613785	1.523814	-1.874413
H	2.846215	1.444226	-0.594620
H	2.092979	1.301236	1.828779
H	0.480357	0.704849	2.242462
H	0.694791	2.360401	1.651983
H	2.444377	-0.894218	-1.793376
H	0.751911	-0.611901	-2.256391
H	1.247305	-2.192352	-1.614208
H	3.109060	-0.920753	0.655773
H	1.865481	-1.122748	1.910803
H	2.115016	-2.391384	0.709897
H	-3.028260	0.039676	-1.390604
H	-2.669046	-1.638995	-0.928805
H	-1.624960	-0.790530	-2.094386
H	-3.081305	0.615112	1.049313
H	-1.653479	0.388609	2.080370
H	-2.581899	-1.018475	1.532848

H	-2.145628	2.240597	-0.879828
H	-0.575084	3.033736	-0.835478
H	-1.404009	2.632367	0.684507

Zero-point correction=	0.306506 (Hartree/Particle)
Thermal correction to Energy=	0.321598
Thermal correction to Enthalpy=	0.322542
Thermal correction to Gibbs Free Energy=	0.266965
Sum of electronic and zero-point Energies=	-578.060548
Sum of electronic and thermal Energies=	-578.045456
Sum of electronic and thermal Enthalpies=	-578.044512
Sum of electronic and thermal Free Energies=	-578.100089



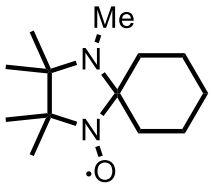
10

The N^2 atom takes the equatorial position.

N	0.000087	-0.955079	0.233341
C	-1.462262	-0.983642	-0.032265
C	-1.790294	0.539291	0.094206
N	-0.553001	1.129484	-0.476758
O	0.660399	-2.038897	0.391765
C	-2.051659	0.960382	1.561421
C	-3.014088	0.951123	-0.742287
C	-2.142675	-1.902458	0.987182
C	-1.685832	-1.552275	-1.450137
C	0.641664	0.336850	-0.121363
C	1.470838	0.871488	1.079026
C	2.768798	0.084628	1.330288
C	3.649484	0.049242	0.074702
C	2.881845	-0.543225	-1.114867
C	1.560210	0.200153	-1.364643
C	-0.426686	2.574540	-0.483341
H	-2.091350	2.052162	1.637517
H	-1.274622	0.603958	2.243120
H	-3.013683	0.576452	1.917489
H	-3.285223	1.995025	-0.552123
H	-3.883458	0.341429	-0.471131
H	-2.827059	0.837346	-1.812521
H	-1.922837	-1.612860	2.017065
H	-1.783066	-2.924829	0.845231
H	-3.228739	-1.893709	0.843110
H	-2.749348	-1.727375	-1.643853
H	-1.160764	-2.509543	-1.524513
H	-1.296673	-0.879178	-2.217958
H	0.850370	0.882597	1.981132
H	1.732519	1.915812	0.860803

H	2.519658	-0.938250	1.631131
H	3.311027	0.547993	2.164985
H	4.559680	-0.533112	0.265815
H	3.977055	1.071924	-0.169701
H	2.667724	-1.598186	-0.918600
H	3.494325	-0.498610	-2.025132
H	0.989477	-0.276679	-2.167642
H	1.784103	1.221327	-1.704604
H	-1.291229	3.012998	-0.991129
H	-0.345889	3.044150	0.512039
H	0.459139	2.862922	-1.058259

Zero-point correction=	0.373051 (Hartree/Particle)
Thermal correction to Energy=	0.389832
Thermal correction to Enthalpy=	0.390776
Thermal correction to Gibbs Free Energy=	0.331149
Sum of electronic and zero-point Energies=	-694.727928
Sum of electronic and thermal Energies=	-694.711147
Sum of electronic and thermal Enthalpies=	-694.710203
Sum of electronic and thermal Free Energies=	-694.769830



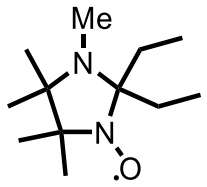
10

The N^2 atom takes the axial position.

N	0.456259	-1.149504	-0.359239
C	1.793247	-0.672175	0.063380
C	1.549410	0.869997	0.001053
N	0.133321	0.949316	0.460635
O	0.231788	-2.373385	-0.638618
C	1.764746	1.430416	-1.426188
C	2.465407	1.647631	0.961792
C	2.855006	-1.222490	-0.894101
C	2.077147	-1.200265	1.486314
C	-0.650460	-0.206958	-0.023060
C	-1.503623	-0.027788	-1.313130
C	-2.918585	0.543232	-1.110030
C	-3.696848	-0.224092	-0.034016
C	-2.914755	-0.251422	1.284792
C	-1.514105	-0.853225	1.094481
C	-0.491790	2.259476	0.424483
H	1.421215	2.468661	-1.480961
H	1.226435	0.855522	-2.184789
H	2.826853	1.427701	-1.693050
H	3.515666	1.400641	0.768462
H	2.238560	1.419768	2.005740
H	2.361835	2.728262	0.817572
H	2.638580	-0.979174	-1.936496
H	2.887220	-2.311635	-0.807337
H	3.843035	-0.824831	-0.637149
H	1.396088	-0.763739	2.220886
H	3.106331	-0.982152	1.790816
H	1.941278	-2.286244	1.485979
H	-1.589672	-1.034669	-1.740696
H	-0.951343	0.576731	-2.040332

H	-3.452866	0.501575	-2.067992
H	-2.871248	1.603974	-0.833820
H	-3.868106	-1.255953	-0.373664
H	-4.686055	0.227223	0.114762
H	-3.454177	-0.845392	2.034051
H	-2.848938	0.764948	1.696407
H	-1.622150	-1.908965	0.815858
H	-0.947866	-0.815362	2.030454
H	0.157307	2.982420	0.927460
H	-0.705013	2.647229	-0.586635
H	-1.433107	2.237844	0.979023

Zero-point correction=	0.373467 (Hartree/Particle)
Thermal correction to Energy=	0.390085
Thermal correction to Enthalpy=	0.391029
Thermal correction to Gibbs Free Energy=	0.331794
Sum of electronic and zero-point Energies=	-694.724604
Sum of electronic and thermal Energies=	-694.707987
Sum of electronic and thermal Enthalpies=	-694.707043
Sum of electronic and thermal Free Energies=	-694.766278

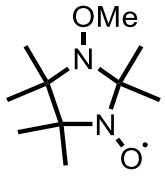


11

C	-1.181444	-0.936067	-0.026229
C	-1.400057	0.607228	-0.218587
N	-0.124949	1.143966	0.325467
C	1.012418	0.264413	0.012259
N	0.299991	-1.027762	-0.145932
O	0.902237	-2.151880	-0.064943
C	-2.586295	1.142371	0.606134
C	-1.668677	0.991999	-1.696166
C	-1.592173	-1.457720	1.365306
C	-1.820858	-1.840358	-1.089317
C	2.037885	0.189935	1.170388
C	1.475628	-0.045723	2.571736
C	1.760595	0.629047	-1.308940
C	2.853197	-0.347788	-1.765609
C	0.105760	2.575047	0.256774
H	-2.783979	2.192523	0.365776
H	-2.398208	1.068524	1.679241
H	-3.499141	0.584178	0.370062
H	-1.633758	2.080541	-1.811679
H	-2.667360	0.665908	-2.006221
H	-0.948676	0.557690	-2.392617
H	-1.158098	-2.452743	1.501417
H	-2.680840	-1.541600	1.446651
H	-1.229988	-0.810482	2.165697
H	-1.527934	-2.875489	-0.893453
H	-1.495855	-1.588393	-2.101158
H	-2.913636	-1.775417	-1.045473
H	2.620483	1.120769	1.156172
H	2.734679	-0.616255	0.924395
H	2.283302	0.002246	3.311225
H	1.017417	-1.036043	2.649581

H	0.723983	0.704312	2.835570
H	2.201803	1.625295	-1.174399
H	1.021660	0.728876	-2.108892
H	3.231147	-0.046059	-2.749509
H	2.468418	-1.368067	-1.840406
H	3.706084	-0.363063	-1.079489
H	0.998983	2.825887	0.838454
H	0.244826	2.979343	-0.760532
H	-0.734374	3.104816	0.715902

Zero-point correction=	0.364268 (Hartree/Particle)
Thermal correction to Energy=	0.381998
Thermal correction to Enthalpy=	0.382942
Thermal correction to Gibbs Free Energy=	0.321150
Sum of electronic and zero-point Energies=	-656.623798
Sum of electronic and thermal Energies=	-656.606068
Sum of electronic and thermal Enthalpies=	-656.605124
Sum of electronic and thermal Free Energies=	-656.666917

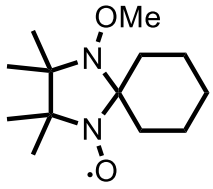


12

C	-0.476544	1.210838	0.080697
N	0.996874	1.024673	0.153578
C	1.434908	-0.352432	-0.206819
C	0.152098	-1.149862	0.197532
N	-0.897513	-0.177438	-0.248599
O	1.791834	2.021202	0.104696
C	0.101506	-1.460489	1.708891
C	-0.037985	-2.463273	-0.572828
C	2.705772	-0.702019	0.573508
C	1.743240	-0.393191	-1.718279
C	-0.997586	1.784269	1.407632
C	-0.828217	2.164106	-1.071033
O	-2.155451	-0.482526	0.359933
C	-3.134665	-0.701145	-0.650799
H	-0.914919	-1.752489	1.982893
H	0.393259	-0.607350	2.325817
H	0.772991	-2.291338	1.949298
H	-0.956344	-2.956133	-0.237032
H	0.794325	-3.150538	-0.381778
H	-0.115001	-2.294915	-1.649267
H	3.015501	-1.730118	0.356741
H	2.571810	-0.595426	1.651976
H	3.509527	-0.026691	0.268090
H	2.185801	-1.353967	-2.001817
H	2.462134	0.399273	-1.947821
H	0.843881	-0.234760	-2.318597
H	-2.065821	2.003238	1.337566
H	-0.456048	2.713612	1.610141
H	-0.844068	1.100804	2.243725
H	-1.912523	2.308172	-1.119729
H	-0.487092	1.759013	-2.027030

H	-0.349375	3.133489	-0.906572
H	-4.055124	-0.944475	-0.111063
H	-3.295268	0.195139	-1.262017
H	-2.859384	-1.535403	-1.306415

Zero-point correction=	0.309932 (Hartree/Particle)
Thermal correction to Energy=	0.326402
Thermal correction to Enthalpy=	0.327346
Thermal correction to Gibbs Free Energy=	0.268296
Sum of electronic and zero-point Energies=	-653.224667
Sum of electronic and thermal Energies=	-653.208196
Sum of electronic and thermal Enthalpies=	-653.207252
Sum of electronic and thermal Free Energies=	-653.266303



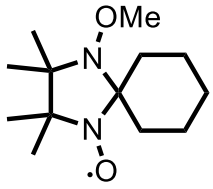
13

The N^2 atom takes the equatorial position.

N	0.083071	-1.201897	0.036762
C	-1.389769	-1.234253	-0.190185
C	-1.766347	0.207293	0.276069
N	-0.583015	0.949578	-0.259553
O	0.785713	-2.262274	-0.093180
C	-1.926371	0.317001	1.807821
C	-3.039513	0.760339	-0.379163
C	-2.005062	-2.374729	0.626773
C	-1.649729	-1.491502	-1.689801
C	0.667974	0.162802	-0.033572
C	1.451706	0.508067	1.254993
C	2.788843	-0.244650	1.361691
C	3.679916	0.019455	0.140924
C	2.953644	-0.360308	-1.156197
C	1.589773	0.339460	-1.265827
O	-0.492955	2.248344	0.330976
C	-0.596996	3.249019	-0.678151
H	-1.892312	1.369822	2.097824
H	-1.145673	-0.215103	2.355727
H	-2.892300	-0.093602	2.120247
H	-3.247146	1.764186	0.005745
H	-3.903256	0.130086	-0.137762
H	-2.943942	0.822736	-1.465384
H	-3.094636	-2.377316	0.513888
H	-1.762612	-2.301307	1.688985
H	-1.616473	-3.328283	0.259949
H	-2.716887	-1.645963	-1.881462
H	-1.111521	-2.397571	-1.984414
H	-1.301962	-0.660198	-2.308058
H	0.834639	0.310764	2.135323

H	1.636478	1.587808	1.237384
H	2.598551	-1.320354	1.448848
H	3.298737	0.069429	2.281663
H	4.619142	-0.541476	0.226049
H	3.952049	1.085956	0.113291
H	2.803174	-1.443502	-1.185480
H	3.562830	-0.091274	-2.029205
H	1.050407	0.010594	-2.160082
H	1.747057	1.421872	-1.370861
H	-0.526329	4.201229	-0.143270
H	0.217236	3.177363	-1.408451
H	-1.556122	3.193826	-1.205571

Zero-point correction=	0.376895 (Hartree/Particle)
Thermal correction to Energy=	0.394897
Thermal correction to Enthalpy=	0.395842
Thermal correction to Gibbs Free Energy=	0.333248
Sum of electronic and zero-point Energies=	-769.892071
Sum of electronic and thermal Energies=	-769.874068
Sum of electronic and thermal Enthalpies=	-769.873124
Sum of electronic and thermal Free Energies=	-769.935718



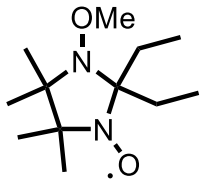
13

The N^2 atom takes the axial position.

N	-0.585547	-1.355267	-0.204865
C	-1.857224	-0.598887	-0.302622
C	-1.479680	0.638919	0.574855
N	0.008820	0.847761	0.331575
O	-0.476164	-2.570810	-0.576711
C	-1.645199	0.356097	2.082781
C	-2.290638	1.895004	0.245219
C	-3.002018	-1.472300	0.222911
C	-2.124835	-0.257961	-1.785115
C	0.610214	-0.487559	0.022206
C	1.395196	-1.027941	1.240978
C	2.757330	-0.347061	1.422109
C	3.630628	-0.492030	0.170051
C	2.905178	0.062046	-1.063137
C	1.508968	-0.553219	-1.233232
O	0.189202	1.726607	-0.801453
C	0.770135	2.945931	-0.357773
H	-1.140176	1.142011	2.651743
H	-1.225226	-0.606602	2.382170
H	-2.705120	0.355527	2.358203
H	-2.015205	2.714865	0.916980
H	-3.353921	1.684729	0.405427
H	-2.152746	2.228494	-0.782406
H	-3.946035	-0.916687	0.205643
H	-3.104968	-2.351140	-0.419395
H	-2.820254	-1.825708	1.240263
H	-3.114527	0.194711	-1.910015
H	-2.096718	-1.186603	-2.364176
H	-1.377545	0.430049	-2.186662
H	1.528163	-2.104431	1.074097

H	0.796916	-0.913954	2.148288
H	3.263272	-0.776764	2.295924
H	2.598689	0.717667	1.642945
H	3.861030	-1.555729	0.011668
H	4.591064	0.020405	0.309651
H	3.490229	-0.137314	-1.970274
H	2.825519	1.152315	-0.981454
H	1.605309	-1.625618	-1.441163
H	0.993202	-0.104785	-2.084099
H	0.095457	3.504810	0.301919
H	0.950625	3.526689	-1.267922
H	1.717433	2.772991	0.165613

Zero-point correction=	0.377320 (Hartree/Particle)
Thermal correction to Energy=	0.395071
Thermal correction to Enthalpy=	0.396015
Thermal correction to Gibbs Free Energy=	0.334107
Sum of electronic and zero-point Energies=	-769.890148
Sum of electronic and thermal Energies=	-769.872397
Sum of electronic and thermal Enthalpies=	-769.871453
Sum of electronic and thermal Free Energies=	-769.933361

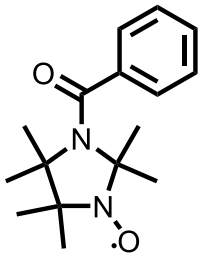


14

C	1.567057	-0.759393	-0.326105
C	1.371729	0.656343	0.298739
N	-0.035302	0.938345	-0.148274
C	-0.868936	-0.300644	-0.029859
N	0.210337	-1.331024	-0.098720
O	-0.039264	-2.546251	-0.403956
C	2.310539	1.718647	-0.291575
C	1.550714	0.658203	1.831982
C	1.841672	-0.739148	-1.845271
C	2.612865	-1.647058	0.356659
C	-1.780900	-0.473172	-1.270069
C	-3.068101	0.356837	-1.294255
C	-1.655120	-0.419706	1.300013
C	-2.396796	-1.748486	1.497909
O	-0.601795	2.006168	0.621004
C	-0.792003	3.155690	-0.197427
H	2.171819	2.672743	0.227270
H	2.127191	1.876628	-1.356580
H	3.357303	1.422628	-0.155452
H	1.121082	1.574009	2.244372
H	2.614832	0.633363	2.089381
H	1.071836	-0.194996	2.317046
H	1.679557	-1.747046	-2.238760
H	2.877160	-0.449322	-2.052325
H	1.175956	-0.048089	-2.368183
H	2.604204	-2.634057	-0.113350
H	2.410597	-1.781546	1.421248
H	3.613478	-1.216368	0.240514
H	-2.026861	-1.537877	-1.337463
H	-1.176030	-0.234667	-2.151235
H	-3.595534	0.191447	-2.240715

H	-2.872509	1.430297	-1.211404
H	-3.753371	0.080107	-0.486582
H	-2.358780	0.416200	1.343903
H	-0.963820	-0.268418	2.132301
H	-2.880190	-1.755996	2.481711
H	-1.715581	-2.600985	1.440343
H	-3.178824	-1.901186	0.746564
H	-1.420059	2.935929	-1.067375
H	-1.296162	3.882918	0.446600
H	0.159613	3.575026	-0.543692

Zero-point correction=	0.367958 (Hartree/Particle)
Thermal correction to Energy=	0.386819
Thermal correction to Enthalpy=	0.387763
Thermal correction to Gibbs Free Energy=	0.323598
Sum of electronic and zero-point Energies=	-731.787090
Sum of electronic and thermal Energies=	-731.768229
Sum of electronic and thermal Enthalpies=	-731.767285
Sum of electronic and thermal Free Energies=	-731.831450



15

C	-0.458754	-1.038169	-0.432759
N	-1.942183	-1.179288	-0.409562
C	-2.629350	-0.110249	0.348326
C	-1.657539	1.082962	0.074573
N	-0.322553	0.371045	0.041302
O	-2.484870	-2.309075	-0.640602
C	0.834598	1.120667	-0.073266
O	0.818310	2.341878	-0.216933
C	2.180614	0.450792	0.051273
C	2.571486	-0.203117	1.226158
C	3.877880	-0.674196	1.369361
C	4.800414	-0.505639	0.335964
C	4.420386	0.158975	-0.832996
C	3.123970	0.652577	-0.966010
C	-1.708528	2.135752	1.192578
C	-1.945142	1.762520	-1.280791
C	-4.050708	0.059850	-0.197672
C	-2.711807	-0.524830	1.834278
C	0.139342	-2.116835	0.486606
C	0.021560	-1.251673	-1.877604
H	1.857940	-0.328067	2.034767
H	4.174019	-1.170168	2.289806
H	5.814669	-0.880148	0.444707
H	5.138663	0.304955	-1.635179
H	2.834183	1.204541	-1.855316
H	-1.117549	3.009982	0.922230
H	-1.326703	1.742766	2.138500
H	-2.747671	2.449549	1.346310
H	-1.136662	2.457704	-1.509961

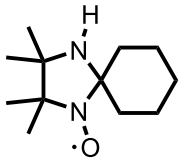
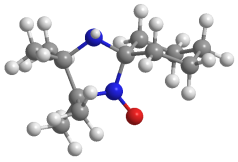
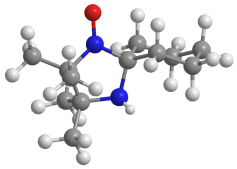
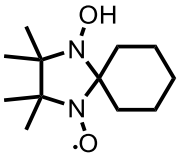
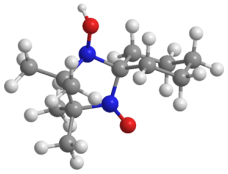
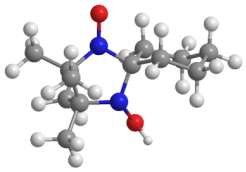
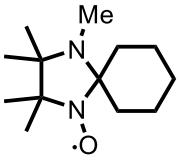
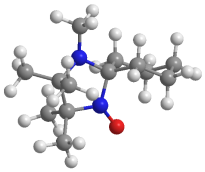
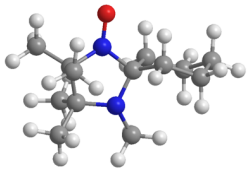
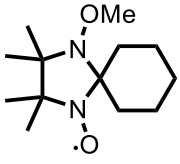
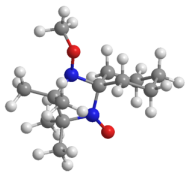
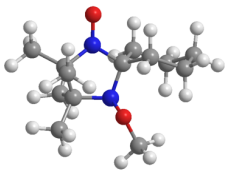
H	-2.881796	2.327578	-1.234816
H	-2.029695	1.033763	-2.092508
H	-4.060652	0.229986	-1.275843
H	-4.550371	0.899674	0.296716
H	-4.622267	-0.850069	0.002400
H	-3.162196	-1.520386	1.893132
H	-3.338589	0.171619	2.399884
H	-1.727729	-0.559703	2.308652
H	1.216583	-2.211333	0.346843
H	-0.337276	-3.065925	0.225308
H	-0.063909	-1.902653	1.538747
H	-0.380783	-0.484198	-2.544048
H	-0.330157	-2.229567	-2.219745
H	1.113042	-1.230943	-1.930598

Zero-point correction=	0.369632 (Hartree/Particle)
Thermal correction to Energy=	0.389609
Thermal correction to Enthalpy=	0.390553
Thermal correction to Gibbs Free Energy=	0.322691
Sum of electronic and zero-point Energies=	-883.081168
Sum of electronic and thermal Energies=	-883.061191
Sum of electronic and thermal Enthalpies=	-883.060247
Sum of electronic and thermal Free Energies=	-883.128109

Difference of enthalpies between the equatorial and axial compounds

Table S1 shows the structures and the enthalpy differences for both the equatorial and axial structures of Entry 2, 6, 10, and 13.

Table S1 Difference of enthalpies between the equatorial and axial compounds

Entry	Structures		Enthalpy differences
	Equatorial N^2 atom	Axial N^2 atom	H_{axial} - $H_{equatorial}$ / kJ mol^{-1}
 2			-5.09
 6			0.848
 10			8.30
 13			4.39

4. References

1. Breneman CM, Wiberg KB (1990) Determining atom-centered monopoles from molecular electrostatic potentials. The need for high sampling density in formamide conformational analysis. J Comp Chem 11:361-373.