

## Supporting information

# Landscape of Structure- O-H Bond Dissociation Energy Relationship of Oximes and Hydroxylamines

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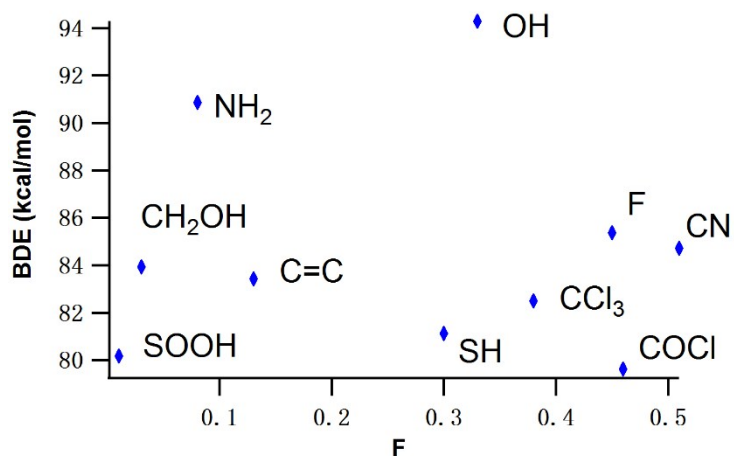
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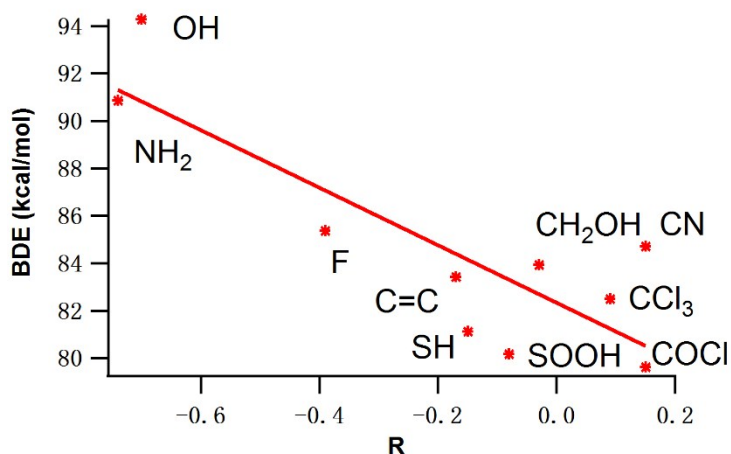
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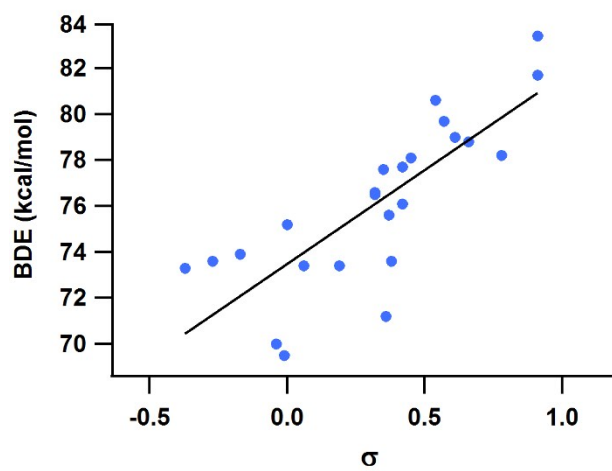
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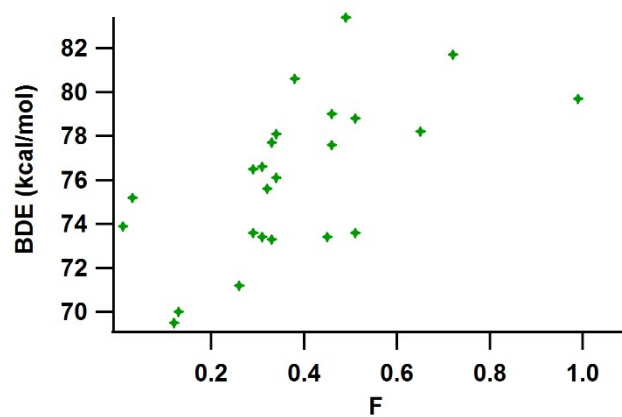
**Figure S1.** Relationship between O-H BDE of *Z*-oximes and the inductive parameter (F) of the substituents.



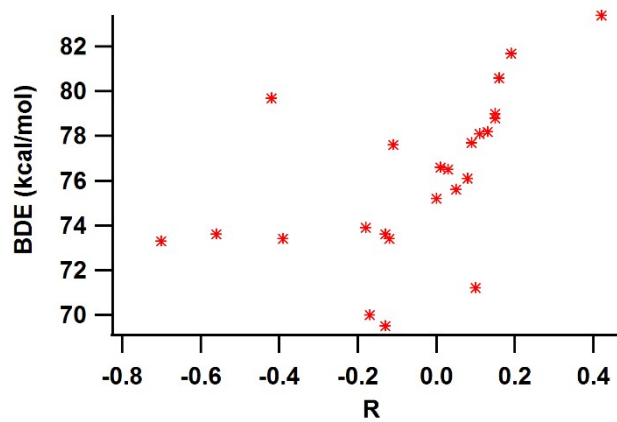
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**Figure S3.** Relationship between O-H BDE of hydroxylamines and the para-Hammett constants ( $\sigma$ ) of the substituents.

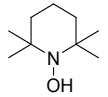
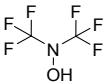
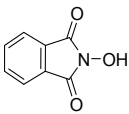
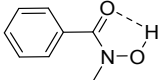
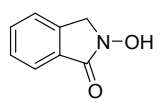
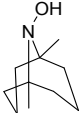
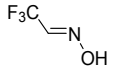
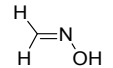
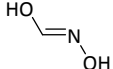
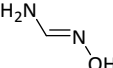
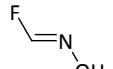
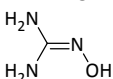



**Figure S4.** Relationship between O-H BDE of hydroxylamines and the inductive parameter (F) of the substituents.



**Figure S5.** Relationship between O-H BDE of hydroxylamines and the resonance parameter (R) of the substituents.

**Table S1.** Gas phase BDEs of selected compounds calculated by B3LYP/6-311+G (d,p) with or without the D3BJ correction (units: kcal/mol).

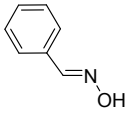
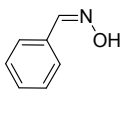
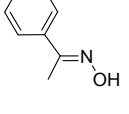
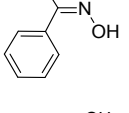
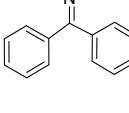
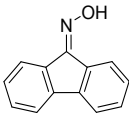
Entry	Structure	B3LYP <sup>a</sup>	B3LYP-D3BJ
1		69.6	70.3
2		85.2	84.7
3		83.0	82.9
20		77.2	77.8
42		77.6	77.6
81		70.4	70.7
94		85.0	84.8
95		84.0	83.8
112		90.2	89.9
113		89.1	88.8
124		88.7	88.4
155		84.2	84.0
223		80.6	80.6

104		80.5	79.8
120		85.6	85.5

**Table S2. Gas phase O-H BDEs calculated by different computational methods in kcal/mol.**

Entry	Structure	Literature BDE		Calculated BDE <sup>b</sup>
		Computational Method	Reaction <sup>a</sup> BDE	
4		CBS-APNO	N 77.4 <sup>1</sup>	77.6
5		G2M	N 81.2 <sup>2</sup>	77.8
		B3LYP/6-311++G(2df,2pd)	N 78.4 <sup>2</sup>	
1		CCSD	N 69.2 <sup>3</sup>	69.6
		B3LYP/ EPR-III// B3LYP/ 6-311+G(d,p)	I (entry 7) 69.5 <sup>3</sup>	
7		CCSD	N 71.8 <sup>3</sup>	70.5
		B3LYP/ EPR-III// B3LYP / 6-311+G(d,p)	N 64.8 <sup>3</sup>	
6		G3B3	N 83.2 <sup>4</sup>	83.5
		CBS-APNO	N 82.7 <sup>4</sup>	
		G3B3	I(avg.) 83.3±1.0 <sup>4</sup>	
3		G3B3	N 83.0 <sup>4</sup>	83.0
		G3B3	I(avg.) 83.5±1.0 <sup>4</sup>	
		B3LYP/6-311++G(2df,2pd)	N 78.6 <sup>2</sup>	
		B3LYP/6-311+G(d)	N 80.9 <sup>5</sup>	
		B3LYP/6-311++G(d,p)	N 85.7 <sup>5</sup>	
		B3LYP/6-311++G(3df,3pd)	I(phenol) 82.52 <sup>6</sup>	
		B3LYP/6-311+G(d)	I(phenol) 83.44 <sup>7</sup>	
95		Corrected DFT <sup>c</sup>	N 83.4	84.0
96		ONIOM-G3B3 <sup>d</sup>	N 85.9	85.5

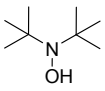
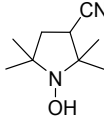
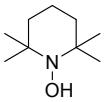
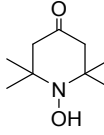
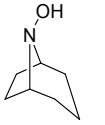
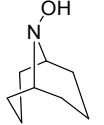
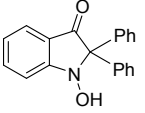
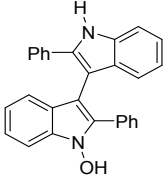
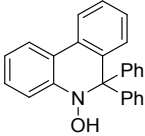
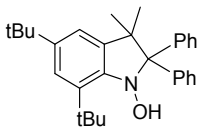
Entry	Structure	Literature BDE			Calculated BDE <sup>b</sup>
		Computational Method	Reaction <sup>a</sup>	BDE	
97		Corrected DFT <sup>c</sup>	N	84.7	85.0
		ONIOM-G3B3 <sup>d</sup>	N	84.9	
		Corrected DFT <sup>c</sup>	N	82.6	
94		Corrected DFT <sup>c</sup>	N	84.4	85.0
98		Corrected DFT <sup>c</sup>	N	82.2	83.3
		G3MP2	N	86.5 <sup>8</sup>	
		G3	N	85.9 <sup>8</sup>	
		CBS-QB3	N	85.1 <sup>8</sup>	
99		CBS-APNO	N	84.6 <sup>8</sup>	85.8
		(RO)B3LYP/6-311+G(2d,2p)/(U)B3LYP/6-31G(d)	N	82.6 <sup>8</sup>	
		Corrected DFT <sup>c</sup>	N	83.8	
		ONIOM-G3B3 <sup>d</sup>	N	83.0	
100		Corrected DFT <sup>c</sup>	N	83.8	84.6
101		ONIOM-G3B3 <sup>d</sup>	N	83.0	82.1
		Corrected DFT <sup>c</sup>	N	82.7	
102		ONIOM-G3B3 <sup>d</sup>	N	83.0	81.5
		Corrected DFT <sup>c</sup>	N	81.5	
103		ONIOM-G3B3 <sup>d</sup>	N	79.0	78.5
		Corrected DFT <sup>c</sup>	N	77.6	
104		ONIOM-G3B3 <sup>d</sup>	N	78.7	80.5
		Corrected DFT <sup>c</sup>	N	77.2	
105		ONIOM-G3B3 <sup>d</sup>	N	78.3	79.5

Entry	Structure	Literature BDE		Calculated BDE <sup>b</sup>
		Computational Method	Reaction <sup>a</sup> BDE	
		Corrected DFT <sup>c</sup>	N 76.9	
106		Corrected DFT <sup>c</sup>	N 83.9	84.5
107		Corrected DFT <sup>c</sup>	N 79.4	81.4
108		Corrected DFT <sup>c</sup>	N 82.8	83.6
109		Corrected DFT <sup>c</sup>	N 80.1	81.6
110		ONIOM-G3B3 <sup>d</sup>	N 81.8	82.2
		Corrected DFT <sup>c</sup>	N 81.6	
111		ONIOM-G3B3 <sup>d</sup>	N 80.4	82.5
		Corrected DFT <sup>c</sup>	N 81.8	

<sup>a</sup> The label “I” indicates an isodesmic reaction was used to calculate the BDEs referencing the compound in parentheses, and “N” means a non-isodesmic reaction. <sup>b</sup> UB3LYP/6-311+G(d,p) level of computation using an isodesmic reaction referencing the experiment BDE of phenol. <sup>c</sup> “Corrected DFT” indicate the data obtained by combination of the results of (RO)B3LYP/6-311+G(2d,2p)//(U)B3LYP/6-31G(d) with the difference between (RO)B3LYP/6-311+G(2d,2p)//(U)B3LYP/6-31G(d) and CBS-APNO in acetone oxime (entry 99) BDE. <sup>d</sup> “ONIOM-G3B3” is a multilayer composite ab initio method proposed by Fu et al. <sup>9</sup>



**Table S3. Gas phase BDEs of alkyl hydroxylamines calculated at the UB3LYP/6-311+G(d,p) level and their discrepancies from experiment values.**

Entry	Structure	Calculated BDE	Discrepancy <sup>a</sup>	Entry	Structure	Calculated BDE	Discrepancy <sup>a</sup>
8		68.7	-0.3 <sup>3</sup>	9		67.9	-1.1 <sup>3</sup>
1		69.6	0.0 <sup>10</sup> , -0.5, <sup>3</sup> - 0.1 <sup>11</sup>	7		70.5	-1.3 <sup>10</sup> , -0.1 <sup>3</sup> , -1.4 <sup>11</sup>
10		75.0	-2.0 <sup>10</sup>	11		71.7	-4.5 <sup>10</sup>
12		69.4	-1.2 <sup>7</sup>	13 <sup>b</sup>		-	-
14		69.0	-1.4 <sup>7</sup>	15		67.9	-1.8 <sup>7</sup>

<sup>a</sup> When multiple experiment values are present, discrepancies from each data are listed besides their reference labels. <sup>b</sup> BDE of entry 13 is not calculated because of the large size of the molecule.

**Table S4. Gas phase and solution BDEs of acyl hydroxylamines calculated at the UB3LYP/6-311+G(d,p) level and their discrepancies from experiment values in kcal/mol.**

Entry	Structure	Gas phase BDE	Discrepancies of gas phase BDE <sup>a</sup>	Solution BDE	Discrepancies of solution BDE <sup>a,b</sup>
16		72.2	-4.6 <sup>12</sup>	73.4	-3.4 <sup>12</sup>
17		73.3	-2.9 <sup>12</sup>	74.4	-1.8 <sup>12</sup>
18		73.0	-2.8 <sup>12</sup>	74.0	-1.8 <sup>12</sup>
19		74.2	-6.0 <sup>13</sup>	76.8	-3.4 <sup>13</sup>
20		77.2	-2.0 <sup>13</sup>	79.1	-0.1 <sup>13</sup>
21		73.4	-3.8 <sup>12</sup> -6.5 <sup>14</sup>	75.1	-2.1 <sup>12</sup> -4.8 <sup>14</sup>
22		71.3	-3.1 <sup>12</sup>	72.1	-2.3 <sup>12</sup>
3		83.0	-6.6 <sup>14</sup> -5.1 <sup>13</sup>	83.9	-5.7 <sup>14</sup> -4.2 <sup>13</sup>
23		76.5	-2.0 <sup>13</sup>	76.1	-2.4 <sup>13</sup>

<sup>a</sup> When multiple experiment values are present, discrepancies from each BDE are listed besides the reference label. <sup>b</sup> The solvents are: entries 16, 17, 18, 21, 22 CCl<sub>4</sub>, 3, 19, 20 BuOH, and 23 benzene, which are the solvents used in ref. <sup>12,13</sup>

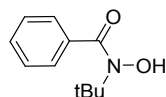
**Table S5. Gas phase BDEs of oximes calculated at the UB3LYP/6-311+G(d,p) level and their discrepancies from experiment values in kcal/mol.**

Entry	Structure	BDE	Discrepancy <sup>a</sup>	Entry	Structure	BDE	Discrepancy <sup>a</sup>
99		85.8	+1.5 <sup>b</sup> , -8.3 <sup>d</sup>	101		82.1	-0.7 <sup>b</sup> , -3.9 <sup>d</sup>
102		81.5	+2.2 <sup>b</sup> , -1.1 <sup>c</sup> , -2.8 <sup>d</sup>	103		78.5	-0.3 <sup>b</sup> , +0.9 <sup>c</sup> , +2.4 <sup>d</sup>
104		79.8	+2.8 <sup>b</sup> , +0.6 <sup>c</sup> , -0.2 <sup>d</sup>	105		79.5	+3.0 <sup>b</sup>
110		82.2	-0.2 <sup>b</sup>	111		82.5	+0.5 <sup>b</sup>

<sup>a</sup> When multiple experiment values are present, discrepancies from each BDE are listed besides the reference label. <sup>b</sup> values obtained based on a relationship between the rate of thermolysis of O-Benzyl oxime ethers and NO-H BDE. <sup>8</sup> <sup>c</sup> Ingold *et al.* corrected the calorimetric values <sup>10</sup> downward by 1.7 kcal/mol considering the revised heat of formation of the reference compound and H-bonding energy between oximes and the solvent. <sup>10</sup> <sup>d</sup> values obtained from ref. <sup>15</sup>

**Table S6. Gas phase and solution BDEs of entries 3, 20 and 21 calculated using different solvation model for single point energy (units: kcal/mol).**

Entry	Structure	Gas phase	Defult PCM	IEFPCM radii=pauling	SMD	Experiment
3		83.0	83.9	84.6	85.2	88.1 <sup>13</sup>
20		77.2	79.1	80.3	79.1	79.2 <sup>13</sup>



73.4

75.1

75.4

74.8

77.2<sup>16</sup>

**Table S7.** BDEs mono-substituted *E*- and *Z*-aldoximes in kcal/mol, and resonance (R), and inductive (F) parameters of the substituents.

Entry	Substituent	R	F	BDE- <i>E</i>	Entry	BDE- <i>Z</i>
95	H	0	0.03	84.0		
123	Cl	-0.19	0.42	87.2		
124	F	-0.39	0.45	88.7	145	85.4
125	Br	-0.22	0.45	86.8		
112	OH	-0.7	0.33	90.2	146	94.3
113	NH <sub>2</sub>	-0.74	0.08	89.1	147	90.9
126	OMe	-0.56	0.29	89.2		
127	CCl <sub>3</sub>	0.09	0.38	85.0	148	77.3
96	Me	-0.18	0.01	85.5	97	
128	NH-NO <sub>2</sub>	-0.42	0.99	89.0		
114	NH-Me	-0.73	0.03	88.1		
129	N(Me) <sub>2</sub>	-0.98	0.15	86.5		
130	CH=O	0.09	0.33	83.2		
131	CH=CH <sub>2</sub>	-0.17	0.13	84.6	149	83.4
132	CH <sub>2</sub> OH	-0.03	0.03		150	83.9
133	CN	0.15	0.51	84.9	151	84.7
134	COCl	0.15	0.46	82.7	152	79.6
135	COOH	0.11	0.34	82.7		
136	N=N-CN	0.47	0.56	83.1		
137	NO <sub>2</sub>	0.13	0.65	84.6		
106	Ph	-0.13	0.12	84.5		
138	SH	-0.15	0.30		153	87.6
139	SO <sub>2</sub> F	0.19	0.72	85.3		
140	SO <sub>2</sub> Cl	-0.05	1.16	85.3		
141	SO <sub>2</sub> CF <sub>3</sub>	0.22	0.74	84.6		
142	SO <sub>2</sub> CN	0.29	0.97	84.6		
143	SOOH	-0.08	0.01	84.9	154	80.2
144	POF <sub>2</sub>	0.15	0.74	84.3		

**Table S8.** BDEs of selected mono-substituted *E*-aldoximes in kcal/mol calculated by B2PLYP/6-311+G (d,p) method and CCSD/6-311+G (d,p) method. (units: kcal/mol)

Entry	Substituent	B3LYP	B2PLYP	CCSD
95	H	84	82.3	82.0
124	F	88.7	87.3	86.1
112	OH	90.2	88.9	87.3

113	NH <sub>2</sub>	89.1	87.7	86.2
94	CF <sub>3</sub>	85.0	83.2	82.8
96	Me	85.5	83.9	83.2

**Table S9.** BDEs of mono-substituted hydroxylamines XCH<sub>3</sub>NOH in kcal/mol, and resonance (R), and inductive (F) parameters of the substituents.

Entry	substituent	R	F	$\sigma_p$	BDE
219	H	0	0.03	0	75.2
220	F	-0.39	0.45	0.06	73.4
221	OH	-0.7	0.33	-0.37	73.3
222	OMe	-0.56	0.29	-0.27	73.6
223	CF <sub>3</sub>	0.16	0.38	0.54	80.6
66	Me	-0.18	0.01	-0.17	73.9
224	NH-NO <sub>2</sub>	-0.42	0.99	0.57	79.7
24	CH=O	0.09	0.33	0.42	77.7
225	COCH <sub>3</sub>	0.17	0.33	0.50	75.4
226	CH=CH <sub>2</sub>	-0.17	0.13	-0.04	70.0
227	CN	0.15	0.51	0.66	78.8
26	COCl	0.15	0.46	0.61	79.0
29	COOH	0.11	0.34	0.45	78.1
228	CONH <sub>2</sub>	0.10	0.26	0.36	71.2
229	NCO	-0.12	0.31	0.19	73.4
230	NO	0.42	0.49	0.91	83.4
231	NO <sub>2</sub>	0.13	0.65	0.78	78.2
232	Ph	-0.13	0.12	-0.01	69.5
233	SO <sub>2</sub> F	0.19	0.72	0.91	81.7
234	PO(OH) <sub>2</sub>	0.08	0.34	0.42	76.1
235	OCCL <sub>3</sub>	-0.11	0.46	0.35	77.6
236	CHCl <sub>2</sub>	0.01	0.31	0.32	76.6
237	CHF <sub>2</sub>	0.03	0.29	0.32	76.5
238	CF <sub>2</sub> CH <sub>3</sub>				74.8
239	SCHF <sub>2</sub>	0.05	0.32	0.37	75.6
33	CONH <sub>2</sub>	0.1	0.26	0.36	71.2
240	N=C=S	-0.13	0.51	0.38	73.6

**Table S10.** Predicted and calculated  $\Delta$ BDEs of symmetrically di-substituted oximes WWC=NOH in kcal/mol. ( $\Delta$ BDE (W) = BDE (*E*-WCH=NOH)-BDE (H<sub>2</sub>C=NOH)). The  $\Delta$ BDEs in Tables S2, S4, and S5 are defined in text.

Entry	R <sub>a</sub>	$\Delta$ BDE (W)	2 $\times$ $\Delta$ BDE(W)	BDE	$\Delta$ BDE
155	NH <sub>2</sub>	4.6	9.2	84.2	0.2
156	OMe	4.9	9.8	89.6	5.6

157	OH	6.2	12.4	87.8	3.8
158	F	4.7	9.4	100.3	16.3
159	Cl	3.2	6.4	98.8	14.8
100	Et	-0.2	-0.4	84.5	0.5
160	C=C	-0.5	-1	76.1	-7.9
161	CHO	-3.4	-6.8	77.2	-6.8
162	COCl	-1.4	-2.8	78.8	-5.2
163	COOH	1	2	79.6	-4.4
164	SOOH	0.9	1.8	81.2	-2.8

**Table S11.** Predicted and calculated  $\Delta$ BDEs of unsymmetrically di-substituted oximes WZC=NOH in kcal/mol. ( $\Delta$ BDE (W) =BDE (*E*- WCH=NOH)-BDE (H<sub>2</sub>C=NOH))

Entry	W	$\Delta$ BDE(W)	Z	$\Delta$ BDE(Z)	$\frac{\Delta$ BDE(W)+ $\Delta$ BDE(Z)}	BDE	$\Delta$ BDE
165	NH <sub>2</sub>	4.6	C=C	-0.2	4.4	87.3	3.3
166	NH <sub>2</sub>	4.6	COCl	-3.4	1.2	88.6	4.6
167	OH	6.2	NH <sub>2</sub>	4.6	10.8	82.2	-1.8
168	OH	6.2	OME	4.9	11.1	85.7	1.7
169	OH	6.2	CHO	-0.5	5.7	85.5	1.5
170	OH	6.2	N=NCN	-0.9	5.3	89.3	5.3
171	Cl	3.2	NH <sub>2</sub>	4.6	7.8	85.8	1.8
172	Cl	3.2	OH	6.2	9.4	89.8	5.8
173	Cl	3.2	C=C	-0.2	3	84.0	0.0
174	Cl	3.2	NO <sub>2</sub>	0.6	3.8	82.4	-1.6
175	Cl	3.2	CHO	-0.5	2.7	83.4	-0.6
176	Cl	3.2	N=NCN	-0.9	2.3	84.5	0.5
177	Me	1.5	OH	6.2	7.7	92.6	8.6
178	Me	1.5	C=C	-0.2	1.3	83.8	-0.2
179	Me	1.5	CHO	-0.5	1	83.5	-0.5
180	Me	1.5	N=NCN	-0.9	0.6	82.3	-1.7
181	C=C	-0.2	NH <sub>2</sub>	4.6	4.4	86.8	2.8
182	C=C	-0.2	Me	1.5	1.3	83.8	-0.2
183	C=C	-0.2	NO <sub>2</sub>	0.6	0.4	82.2	-1.8
184	C=C	-0.2	COCl	-3.4	-3.6	79.5	-4.5
185	C=C	-0.2	CHO	-0.5	-0.7	78.8	-5.2
186	C=C	-0.2	N=NCN	-0.9	-1.1	74.6	-9.4
187	NO <sub>2</sub>	0.6	NH <sub>2</sub>	4.6	5.2	85.6	1.6
188	NO <sub>2</sub>	0.6	OH	6.2	6.8	83.7	-0.3
189	NO <sub>2</sub>	0.6	F	4.7	5.3	86.5	2.5
190	NO <sub>2</sub>	0.6	Me	1.5	2.1	83.1	-0.9
191	NO <sub>2</sub>	0.6	C=C	-0.2	0.4	82.2	-1.8
192	NO <sub>2</sub>	0.6	COCl	-3.4	-2.8	82.7	-1.3
193	NO <sub>2</sub>	0.6	CHO	-0.5	0.1	83.2	-0.8
194	NO <sub>2</sub>	0.6	N=NCN	-0.9	-0.3	81.1	-2.9
195	COCl	-3.4	NH <sub>2</sub>	4.6	1.2	82.9	-1.1

196	COCl	-3.4	OH	6.2	2.8	85.4	1.4
197	COCl	-3.4	F	4.7	1.3	83.6	-0.4
198	COCl	-3.4	Me	1.5	-1.9	80.0	-4.0
199	COCl	-3.4	C=C	-0.2	-3.6	79.2	-4.8
200	COCl	-3.4	NO <sub>2</sub>	0.6	-2.8	82.0	-2.0
201	COCl	-3.4	CHO	-0.5	-3.9	80.2	-3.8
202	COCl	-3.4	N=NCN	-0.9	-4.3	78.6	-5.4
203	CHO	-0.5	NH <sub>2</sub>	4.6	4.1	82.8	-1.2
204	CHO	-0.5	OH	6.2	5.7	85.1	1.1
205	CHO	-0.5	F	4.7	4.2	83.5	-0.5
206	CHO	-0.5	Cl	3.2	2.7	81.8	-2.2
207	CHO	-0.5	Me	1.5	1	80.1	-3.9
208	CHO	-0.5	NO <sub>2</sub>	0.6	0.1	80.8	-3.2
209	CHO	-0.5	COCl	-3.4	-3.9	78.0	-6.0
210	CHO	-0.5	N=NCN	-0.9	-1.4	78.4	-5.6
211	N=NCN	-0.9	NH <sub>2</sub>	4.6	3.7	82.9	-1.1
212	N=NCN	-0.9	OH	6.2	5.3	85.5	1.5
213	N=NCN	-0.9	F	4.7	3.8	85.0	1.0
214	N=NCN	-0.9	Me	1.5	0.6	83.1	-0.9
215	N=NCN	-0.9	C=C	-0.2	-1.1	80.9	-3.1
216	N=NCN	-0.9	NO <sub>2</sub>	0.6	-0.3	84.3	0.3
217	N=NCN	-0.9	COCl	-3.4	-4.3	82.4	-1.6
218	N=NCN	-0.9	CHO	-0.5	-1.4	82.3	-1.7

**Table S12.** Predicted and calculated  $\Delta$ BDEs of di-substituted hydroxylamines XYNOH in kcal/mol. ( $\Delta$ BDE(X)=BDE(XCH<sub>3</sub>NOH)-BDE(CH<sub>3</sub>)<sub>2</sub>NOH))

Entry	X	$\Delta$ BDE(X)	Y	$\Delta$ BDE(Y)	$\Delta$ BDE(X) + $\Delta$ BDE(Y)	BDE	$\Delta$ BDE
30	CHO	3.8	OH	-0.6	3.2	71.8	-2.1
31	CHO	3.8	F	-0.5	3.3	73.0	-0.9
32	CHO	3.8	OCH <sub>3</sub>	-0.3	3.5	71.9	-2.0
25	COCl	5.1	NH-NO <sub>2</sub>	5.8	10.9	84.7	10.8
241	CN	4.9	OH	-0.6	4.3	77.8	3.9
242	CN	4.9	F	-0.5	4.4	79.0	5.1
243	CN	4.9	OCH <sub>3</sub>	-0.3	4.6	77.5	3.6
27	COCl	5.1	F	-0.5	4.6	75.2	1.3
28	COCl	5.1	OCH <sub>3</sub>	-0.3	4.8	75.1	1.2
244	Ph	-4.4	OH	-0.6	-5.0	68.8	-5.1
245	Ph	-4.4	F	-0.5	-4.9	70.3	-3.6
246	COCH <sub>3</sub>	1.5	CF <sub>3</sub>	6.7	8.2	80.3	6.4
247	COCH <sub>3</sub>	1.5	CF <sub>2</sub> CH <sub>3</sub>	0.9	2.4	82.1	8.2
2	CF <sub>3</sub>	6.7	CF <sub>3</sub>	6.7	13.4	85.2	11.3
58	CF <sub>2</sub> CH <sub>3</sub>	0.9	CF <sub>2</sub> CH <sub>3</sub>	0.9	1.8	80.3	6.4

Total energy and Sum of electronic and thermal enthalpies of precursor and corresponding radicals in Hartree.

Entry	Precursor total energy	Radical total energy r	Sum of electronic and thermal enthalpies of precursor	Sum of electronic and thermal enthalpies of radical
1	-484.4692999	-483.8558292	-284.388538	-283.7658
2	-806.0462542	-805.4074068	-805.987062	-805.360817
3	-588.4153467	-587.7798177	-588.286179	-587.663416
4	-131.7667883	-131.1386729	-131.10813	-131.722352
5	-284.4724789	-283.8452794	-284.388109	-283.773598
6	-434.7168312	-434.0804844	-434.637607	-434.014051
7	-558.5051886	-557.8897609	-558.238035	-557.635203
8	-446.3409067	-445.7289228	-446.063466	-445.463561
9	-537.4096376	-536.7986558	-537.15352	-536.554811
10	-404.611185	-403.9868838	-404.404878	-403.792566
11	-523.0488393	-443.3130254	-443.693193	-443.088429
12	-976.5553625	-975.9419812	-976.238704	-975.637624
13				
14	-1094.299864	-1093.687156	-1093.909332	-1093.308893
15	-1295.730816	-1295.119785	-1295.102923	-1294.504174
16	710.7946251	-710.1791187	-710.674766	-710.069209
17	-712.1930277	-711.5733662	-711.876532	-711.269208
18	-795.4942009	-795.0608273	-795.211548	-794.604759
19	-1042.65802	-1042.368699	-1042.39122	-1041.782526
20	-515.5725256	-514.9464717	-515.402637	-514.789116
21	-633.5398946	-632.9195953	-633.282505	-632.67459
22	-653.2168339	-652.6005225	-652.899976	-652.295801
23	-907.6019754	-906.9769459	-907.16178	-906.549346
24	-284.4606838	-283.8336851	-284.376205	-283.761829
25	-964.6450338	-964.0070642	-964.572459	-963.95064
26	-744.0876082	-743.3448105	-744.011197	-743.394889
27	-803.9563052	-803.3325624	-803.917789	-803.307504
28	-819.2658595	-818.6433927	-819.185016	-818.574903
29	-359.7273864	-359.0991462	-359.636787	-359.021835
30	-320.3272228	-319.7100889	-320.26769	-319.662754
31	-344.3303709	-343.7108908	-344.283717	-343.676872
32	-359.6370236	-359.0196956	-359.548192	-358.943113
33	-339.8524674	-339.2362646	-339.749601	-339.145708



Entry	Precursor total energy	Radical total energy r	Sum of electronic and thermal enthalpies of precursor	Sum of electronic and thermal enthalpies of radical
34	-441.7627291	-441.1433451	-441.56152	-440.954541
35	-477.6996825	-477.0741458	-477.52146	-476.908306
36	-517.008683	-516.3843727	-516.801121	-516.189149
37	-418.4514901	-417.8177269	-418.291265	-417.67001
38	-476.4790316	-475.851894	-476.323154	-475.708459
39	-438.0093707	-439.932946	-440.382903	-439.765749
40	-416.016022	-415.3960864	-415.90124	-415.295024
41	-417.2293878	-416.6136247	-417.091013	-416.487343
42	-514.3680389	-513.7413393	-514.220815	-513.606634
43	-514.3683824	-513.7417136	-514.220815	-513.606634
44	-439.3288503	-438.7042275	-439.173296	-438.56101
45	-593.0230786	-592.3979521	-592.817628	-592.204877
46	-479.8886505	-479.2521713	-479.678765	-479.054955
47	-456.5558732	-455.9331474	-456.387279	-455.776935
48	-587.6446074	-587.0133945	-587.509389	-586.888619
49	-820.708652	-820.0862943	-820.473169	-819.862193
50	-437.1714933	-436.526934	-437.046952	-436.416328
51	-475.285817	-474.6389882	-475.152466	-474.518681
52	-435.9582339	-435.3173275	-435.857493	-435.227009
53	-604.7941837	-604.1454567	-604.663547	-604.027854
54	-506.3001179	-505.6876628	-506.059175	-505.459084
55	-566.2568235	-565.6404932	-566.055038	-565.4481
56	-626.2065735	-625.5792339	-626.038171	-625.423237
57	-686.1629442	-685.5320512	-686.031203	-685.412676
58	-684.9518623	-684.3188389	-684.840945	-684.220912
59	-396.1580717	-395.5239228	-396.031599	-395.412294

Entry	Precursor total energy	Radical total energy r	Sum of electronic and thermal enthalpies of precursor	Sum of electronic and thermal enthalpies of radical
60	-471.1544319	-470.5266018	-471.037419	-470.422516
61	-490.8737019	-490.2497677	-490.69936	-490.087726
62	-1023.533796	-1023.032888	-1023.664416	-1022.915069
63	-872.4286531	-871.7931335	-872.302738	-871.679959
64	-1379.518768	-1378.883842	-1379.438753	-1378.816492
65	-584.5254186	-583.8825923	-584.397004	-583.767255
66	-806.0462542	-805.4074068	-210.306024	-209.697796
67	-641.7129649	-641.1043591	-641.311261	-640.714285
68	-484.4539642	-483.8427743	-484.170136	-483.571081
69	-677.448577	-676.8383061	-677.085258	-676.486849
70	-754.8485189	-754.2368061	-754.449858	-753.850001
71	-563.1204663	-562.50234	-562.774605	-562.16853
72	-641.7413581	-641.1349789	-641.336387	-640.742009
73	-715.7819992	-715.1734257	-715.395284	-714.798947
74	-602.4287553	-601.823047	-602.053781	-601.460242
75	-1132.085528	-1131.473835	-1131.688731	-1131.088984
76	-1247.641067	-1247.027621	-1247.196257	-1246.595107
77	-445.1457055	-444.5372479	-444.890177	-444.293806
78	-523.7759441	-523.1667354	-523.460356	-522.863186
79	-483.263712	-482.6427472	-482.999656	-482.390915
80	-597.6075433	-596.9984523	-597.326568	-596.729531
81	-522.5717484	-521.9568045	-522.277332	-521.674616
82	-560.7115013	-560.0936581	-560.410289	-559.804586
83	-596.3931034	-595.7772708	-596.134526	-595.531035
84	-287.8443072	-287.2278098	-287.704702	-287.10054
85	-285.4125	-284.7868085	-285.320932	-284.707787

Entry	Precursor total energy	Radical total energy r	Sum of electronic and thermal enthalpies of precursor	Sum of electronic and thermal enthalpies of radical
86	-443.9144326	-443.3055217	-443.683323	-443.086454
87	-481.0569481	-480.447344	-480.825791	-480.228441
88	-440.3067701	-439.6966703	-440.142134	-439.543964
89	-592.7834702	-592.1685109	-592.59277	-591.990117
90	-822.851128	-822.2445608	-822.583957	-821.989835
91	-710.7467433	-710.1344695	-710.467723	-709.867811
92	-706.1557367	-705.5393967	-705.953028	-705.348917
93	-483.245691	-482.633183	-482.983984	-482.383727
94	-507.0173983	-506.3785853	-506.960169	-506.334193
95	-169.871703	-169.2343976	-169.822849	-169.198444
96	-209.2051286	-208.5657243	-209.126879	-208.500179
97	-209.2043778	-208.5667047	-209.126794	-209.126794
98	-507.01307140	-506.37711646	-506.955703	-506.332449
99	-248.5363989	-247.8976295	-248.429728	-247.802571
100	-327.183023	-326.5452757	-327.015626	-326.390484
101	-405.8269881	-405.1929026	-405.600836	-404.979474
102	-445.1484151	-444.5152835	-444.893287	-444.272871
103	-484.4550902	-483.8267718	-484.170903	-483.555264
104	-716.7814095	-716.1500448	-716.384217	-715.765508
105	-716.7770217	-716.1471807	-716.379698	-715.762513
106	-400.9902313	-400.3522135	-400.855764	-400.230627
107	-400.9872771	-400.3541254	-400.852298	-400.232033
108	-440.3178498	-439.6815444	-440.153964	-439.530328
109	-440.3071436	-439.6744802	-440.144828	-439.524375
110	-632.0959389	-631.4619432	-631.876109	-631.254668
111	-630.9005913	-630.2658095	-630.70337	-630.081354
112	-245.1266051	-244.4793676	-245.071549	-244.437357
113	-225.2557387	-224.6104133	-225.188164	-224.555748
114	-264.5724019	-263.9285425	-264.475286	-263.844384
115	-247.2621185	-246.6225377	-247.178243	-246.551079
116	-286.6119916	-285.972495	-286.497618	-285.870592
117	-325.9700466	-325.3305876	-325.824785	-325.197853
118	-365.2996604	-364.661531	-403.213013	-402.586517
119	-403.3950859	-402.7560459	-403.213013	-402.586517
120	-327.1779639	-326.5393038	-327.01179	-326.38592
121	-327.1736503	-326.5397801	-327.006991	-326.385929

Entry	Precursor total energy	Radical total energy r	Sum of electronic and thermal enthalpies of precursor	Sum of electronic and thermal enthalpies of radical
122	-949.0981189	-948.4702562	-948.587898	-947.972521
123	-629.4926864	-628.8504123	-629.451909	-628.822411
124	-269.1384363	-268.493786	-269.096364	-268.464596
125	-2743.412956	-2742.771416	-2743.372679	-2742.743878
126	-284.4368761	-283.79123	-284.352345	-283.719702
127	-1588.044689	-1587.405944	-1587.991389	-1587.365455
128	-429.7920443	-429.1468373	-429.719788	-429.087506
129	-303.8886014	-303.2473182	-303.762415	-303.134008
130	-283.2287146	-282.5926656	-283.168304	-282.545152
131	-247.2990203	-246.6609505	-247.214667	-246.589427
132				
133	-262.132366	-261.4938393	-262.082885	-261.457168
134	-742.8632181	-742.2281811	-742.810616	-742.188397
135	-358.5038189	-357.8686939	-358.436903	-357.814619
136	-371.6006414	-370.9648917	-371.540085	-370.91723
137	-374.4250921	-373.7869734	-374.371005	-373.745775
138				
139	-817.7761195	-817.1369095	-817.72067	-817.094249
140	-1178.125773	-1177.486517	-1178.07128	-1177.44484
141	-1055.627173	-1054.98905	-1055.556948	-1054.931622
142	-810.7298756	-810.0912422	-1055.556948	-1054.931622
143	-793.7528021	-793.1141941	-793.685261	-793.059449
144	-785.7272322	-785.0896399	-785.672568	-785.04775
145	-269.1357157	-268.496746	-269.093683	-268.467151
146	-245.1325254	-244.4780869	-245.077089	-244.436339
147	-225.2617667	-224.6128407	-225.193852	-224.558557
148	-1588.039391	-1587.404692	-1587.985934	-1587.363993
149	-247.2974475	-246.6612068	-247.212799	-246.589372
150	-284.4410891	-283.8022244	-284.35451	-283.730276
151	-262.1319028	-261.4936857	-262.082181	-261.456682
152	-742.8589411	-742.2291066	-742.806397	-742.189021
153	-568.0954649	-567.4525524	-568.045167	-567.415026
154	-718.5198202	-717.8888636	-718.458435	-717.840176
155	-280.645077	-280.0071088	-280.558672	-279.934006
156	-398.9976734	-398.351177	-398.877814	-398.244563
157	-320.3846233	-319.7413387	-320.323945	-319.693617
158	-368.4057104	-367.7423742	-368.370352	-367.720011
159	-1089.110624	-1088.449162	-1089.077856	-1088.429859
160	-324.7062008	-324.0822669	-324.586943	-323.975185
161	-396.5685529	-395.9423133	-396.496968	-395.883379
162	-1315.835578	-1315.20712	-1315.780069	-1315.163957

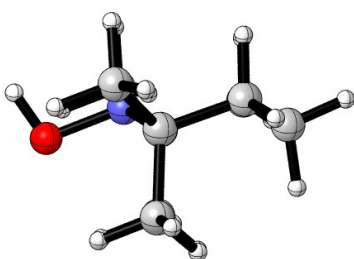
Entry	Precursor total energy	Radical total energy r	Sum of electronic and thermal enthalpies of precursor	Sum of electronic and thermal enthalpies of radical
163	-547.1240994	-546.4938664	-547.039536	-546.422255
164	-1267.17589	-1266.543616	-1267.10164	-1266.481805
165	-302.685255	-302.0418203	-302.582212	-301.952677
166	-798.2489285	-797.6044297	-798.17803	-797.546374
167	-300.5181508	-299.883437	-300.444555	-299.823078
168	-359.6919776	-359.0528984	-359.602663	-358.975682
169	-358.4838675	-357.8445562	-358.417546	-357.790865
170	-446.8489021	-446.2018693	-446.782676	-446.1499
171	-684.8727579	-684.2324332	-684.813814	-684.186528
172	-704.7407685	-704.0942105	-704.69451	-704.060875
173	-706.9176626	-706.2810683	-706.841749	-706.217452
174	-834.0326171	-833.3985501	-833.987197	-833.365391
175	-742.8460497	-742.2102359	-742.794048	-742.170629
176	-831.2187361	-830.5808258	-831.16632	-830.541171
177	-284.4530639	-283.8012439	-284.369986	-283.731928
178	-286.6286563	-285.9919448	-286.514812	-285.89079
179	-322.5635621	-321.9272394	-322.473653	-321.850104
180	-410.9272538	-410.2926547	-410.837589	-410.215911
181	-302.6775895	-302.0349831	-302.574532	-301.945654
182	-286.6286561	-285.9919449	-286.514812	-285.890788
183	-451.8434375	-451.209615	-451.754486	-451.133018
184	-820.2725371	-819.6429536	-820.185034	-819.567803
185	-360.6436416	-360.0148541	-360.547893	-359.931816
186	-449.0117134	-448.3895678	-448.916242	-448.306802
187	-429.8049997	-429.1655579	-429.733072	-429.10624
188	-449.6699496	-449.0332564	-449.61056	-448.986652
189	-473.6789999	-473.038203	-473.632432	-473.004132
190	-413.7582624	-413.1229712	-413.675288	-413.05233
191	-451.8434375	-451.209615	-451.754486	-451.133018
192	-947.3970288	-946.7623586	-947.340197	-946.717859
193	-487.7685576	-487.1330607	-487.703747	-487.080678
194	-576.1314772	-575.4987644	-576.066417	-575.446734
195	-798.2359364	-797.6007947	-798.165377	-797.542769
196	-818.1059141	-817.4666308	-818.047961	-817.42138
197	-842.1173592	-841.481117	-842.072221	-841.448438
198	-782.1890254	-781.5586772	-782.107381	-781.489337
199	-820.2754127	-819.6463097	-820.187949	-819.57123
200	-947.396304	-946.7626343	-947.339203	-946.718017
201	-856.2049393	-855.5741105	-856.141463	-855.523097
202	-944.5706589	-943.9423061	-944.507377	-943.891588
203	-338.5997296	-337.9646055	-338.521185	-337.898824

Entry	Precursor total energy	Radical total energy r	Sum of electronic and thermal enthalpies of precursor	Sum of electronic and thermal enthalpies of radical
204	-358.4730075	-357.8339994	-358.407108	-357.781014
205	-382.484784	-381.8486374	-382.43175	-381.808258
206	-742.8390703	-742.205681	-742.787198	-742.166373
207	-322.5525924	-321.9218654	-322.46314	-321.844963
208	-487.7703157	-487.1394194	-487.706221	-487.08696
209	-856.2056173	-855.5784082	-856.142163	-855.52741
210	-484.9431538	-484.3152133	-484.871727	-484.256378
211	-426.9786286	-426.3430174	-426.89993	-426.277381
212	-446.8435681	-446.2039488	-446.777604	-446.150937
213	-470.8566362	-470.21791	-470.803318	-470.1774
214	-831.2104374	-830.5748635	-831.1584	-830.535508
215	-449.0147512	-448.382788	-448.919053	-448.299708
216	-576.133653	-575.4950554	-576.068538	-575.443645
217	-944.5710621	-943.9365393	-944.50747	-943.885686
218	-484.9410012	-484.3063718	-484.869512	-484.247797
219	-171.0871611	-170.4636917	-171.013668	-170.403362
220	-270.3076734	-269.6878354	-270.242719	-269.635255
221	-246.293281	-245.6737434	-246.215497	-245.608262
222	-285.6059843	-284.9860586	-285.499073	-284.891225
223	-508.2354603	-507.604173	-508.154633	-507.535773
224	-430.9801798	-430.3520724	-430.884938	-430.269163
225	-323.7926414	-323.1693873	-323.678918	-323.068257
226	-248.5014727	-247.8870981	-248.393749	-247.791766
227	-263.3346912	-262.706166	-263.261799	-262.645696
228	-339.8524674	-339.2362646	-339.749601	-339.145708
229	-338.5771017	-337.9574685	-338.498956	-337.891563
230	-300.4330226	-299.7964103	-300.361479	-299.738027
231	-375.6341609	-375.0061577	-375.556739	-374.941597
232	-402.1906195	-401.5772712	-402.032964	-401.431794
233	-818.9959634	-818.3624635	-818.916856	-818.296092
234	-738.89917	-738.2749278	-738.796781	-738.184989
235	-744.0876082	-743.4586263	-1664.379312	-1663.765154
236	-1129.650609	-1129.025751	-1129.564719	-1128.952118
237	-408.9564333	-408.3316544	-408.867845	-408.255435
238	-448.2886718	-447.6667316	-448.171727	-447.562069
239	-807.1458165	-806.5225928	-807.055289	-806.444258
240	-661.5367753	-660.9166437	-661.460743	-660.852921
241	-299.2030715	-298.5760146	-299.154931	-298.540421
242	-323.2082273	-322.5793531	-323.172951	-322.556605
243	-338.5172353	-337.8909709	-338.439911	-337.825863
244	-438.0726715	-437.4602161	-437.939557	-437.339477

Entry	Precursor total energy	Radical total energy r	Sum of electronic and thermal enthalpies of precursor	Sum of electronic and thermal enthalpies of radical
245	-462.0850055	-461.4700664	-461.96471	-461.362138
246	-621.6040673	-620.9729126	-621.51228	-620.893751
247	-561.6674709	-561.0335403	-561.539283	-560.917955

Cartesian coordinates for compounds

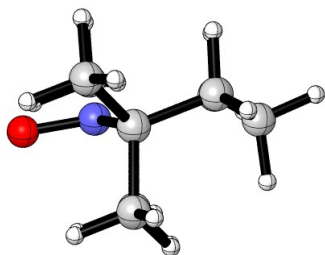
**Entry 1**



C	1.2950380	-0.1514722	-0.0782644
C	-1.2950370	-0.1515072	-0.0782104
C	-1.2503890	1.3368848	-0.4859134
C	-0.0000270	2.0650838	0.0067696
C	1.2503330	1.3369178	-0.4859654
C	1.6301610	-0.3128842	1.4209056
C	2.4000950	-0.8467882	-0.8935984
C	-1.6300940	-0.3129272	1.4209736
C	-2.4001090	-0.8468512	-0.893499441
N	-0.0000000	-0.7609202	-0.5031064
O	0.0000270	-2.1440992	-0.0776734
H	-1.2866870	1.3979818	-1.5799474
H	-2.1583480	1.8235398	-0.1141304
H	-0.0000490	3.0961708	-0.3628764
H	-0.0000060	2.1384158	1.0992976
H	1.2865840	1.3980158	-1.5800014
H	2.1582950	1.8235968	-0.1142204
H	1.4700540	-1.3442582	1.7377006
H	2.6829390	-0.0687712	1.5910096
H	1.0398700	0.3370718	2.0662016
H	3.3558400	-0.3344822	-0.7505874
H	2.5304860	-1.8849952	-0.5820824
H	2.1594600	-0.8302262	-1.9597354
H	-1.4699460	-1.3442972	1.7377616
H	-1.0397930	0.3370438	2.0662446

H	-2.6828710	-0.0688422	1.5911206
H	-2.5304600	-1.8850622	-0.5819774
H	-3.3558620	-0.3345712	-0.7504484
H	-2.1595190	-0.8302832	-1.9596454
H	0.0000160	-2.6374852	-0.9061014

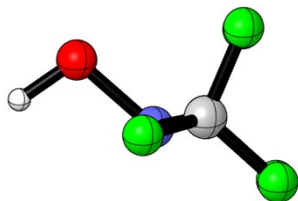
### 1-radical



C	1.3326434	-0.2399568	-0.0553921
C	-1.3326466	-0.2399308	-0.0554071
C	-1.2454186	1.1968712	-0.6049171
C	0.0000194	1.9557032	-0.1516051
C	1.2454484	1.1968462	-0.6049031
O	-0.0000216	-2.1909898	0.0196119
N	-0.0000076	-0.9283188	-0.1903501
C	1.7614884	-0.2530068	1.4257749
C	2.3477064	-1.0423258	-0.8819961
C	-1.7615096	-0.2529728	1.4257549
C	-2.3477166	-1.0422808	-0.8820221
H	-1.2494096	1.1555632	-1.7006791
H	-2.1573366	1.7281612	-0.3134391
H	0.0000314	2.9606462	-0.5861501
H	0.0000154	2.0970422	0.9343579
H	1.2494514	1.1555392	-1.7006651
H	2.1573734	1.7281192	-0.3134151
H	1.7113194	-1.2694418	1.8199679
H	2.7925144	0.0998052	1.5191009
H	1.1341284	0.3865362	2.0493139
H	3.3203774	-0.5433018	-0.8514451
H	2.4609004	-2.0534978	-0.4934331
H	2.0316294	-1.1125858	-1.9257081
H	-2.7925296	0.0998592	1.5190699
H	-1.7113646	-1.2694088	1.8199489
H	-1.1341436	0.3865582	2.0493009
H	-2.4609346	-2.0534498	-0.4934611
H	-3.3203776	-0.5432368	-0.8514821
H	-2.0316296	-1.1125468	-1.9257301

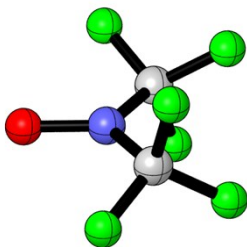


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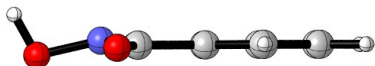
N	0.0000000	0.2670634	-0.3622782
C	1.2461640	-0.3541526	0.0345088
C	-1.2461640	-0.3541536	0.0345088
F	-1.4371900	-0.3933506	1.3632708
F	-1.2976700	-1.6035176	-0.4296282
F	-2.2488610	0.3498414	-0.5005212
F	1.2976850	-1.6035066	-0.4296552
F	2.2488610	0.3498614	-0.5004962
F	1.4371770	-0.3933776	1.3632728
O	-0.0000030	1.5974444	0.1147068
H	0.0000010	2.1378484	-0.6876892

### 2-radical



N	0.0000408	0.5826883	0.0000433
C	-1.2807342	-0.1369937	0.0673953
C	1.2807888	-0.1372067	-0.0676787
O	-0.0000722	1.8512563	0.0014233
F	-1.1946442	-1.2806287	-0.6176367
F	-1.6014862	-0.4229787	1.3343563
F	1.5984788	-0.4280157	-1.3343217
F	2.2293958	0.6260353	0.4468323
F	-2.2283132	0.6241783	-0.4522537
F	1.1965458	-1.2783347	0.6218403

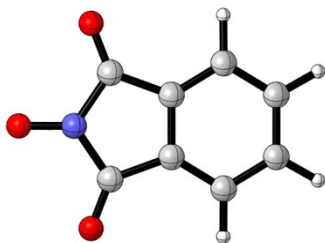
### Entry 3



C	1.1870760	-1.4206944	-0.0297020
C	0.0049170	-0.6983944	-0.0263250
C	0.0050050	0.6984216	-0.0261400
C	1.1872570	1.4205706	-0.0294880

C	2.3857430	0.6989406	-0.0391690
C	2.3856540	-0.6992164	-0.0392620
C	-1.4060670	1.1835316	-0.0176910
C	-1.4062200	-1.1833214	-0.0185890
O	-1.8429100	2.3032046	-0.0680920
O	-1.8431620	-2.3029744	-0.0685910
N	-2.1737260	0.0001146	0.0841030
O	-3.5170750	0.0002916	-0.2071860
H	1.1773710	-2.5048714	-0.0298000
H	1.1776920	2.5047486	-0.0292640
H	3.3309860	1.2312366	-0.0483340
H	3.3308280	-1.2316314	-0.0485500
H	-3.9833690	0.0000436	0.6420800

### 3-radical



C	0.9350869	-1.4206116	-0.0000382
C	-0.2510701	-0.7001586	-0.0000543
C	-0.2510691	0.7001594	-0.0001353
C	0.9350899	1.4206094	0.0000038
C	2.1316669	0.7000554	0.0000727
C	2.1316659	-0.7000596	0.0000308
C	-1.6439461	1.2042064	-0.0005182
C	-1.6439491	-1.2042036	0.0001478
O	-2.0790481	2.3191484	0.0000907
O	-2.0790531	-2.3191446	-0.0000833
N	-2.4663281	0.0000024	0.0000348
O	-3.7240171	0.0000044	0.0002648
H	0.9253269	-2.5046976	0.0000158
H	0.9253309	2.5046954	-0.0000493
H	3.0771579	1.2318154	0.0001228
H	3.0771559	-1.2318206	0.0000947

### Entry 4

N	-0.5015858	0.0000484	0.1393380
O	0.9126192	0.0001294	-0.1527430
H	-0.8611128	0.8145364	-0.3552470
H	-0.8604768	-0.8146276	-0.3554010
H	1.3105562	-0.0000866	0.7240530

#### 4-radical

N	-0.54089100	0.00000000	-0.01690800
O	0.73527800	0.00000000	0.00420700
H	-1.04799400	-0.87892700	0.04234900
H	-1.04799400	0.87892800	0.04234900

#### Entry 5

N	-0.60702700	-0.72063500	-0.10826900
C	0.43252300	0.15794300	-0.00990200
O	-1.89118900	-0.18432800	0.03372700
O	0.20950100	1.36314900	-0.00114700
C	1.81155200	-0.45163500	0.02021600
H	-0.55914000	-1.65370900	0.27449600
H	-1.69914700	0.77466200	0.07982800
H	1.79702800	-1.54174000	-0.03831500
H	2.31320300	-0.14395200	0.94011500
H	2.38629800	-0.05923000	-0.82076400

#### 5-radical

N	0.81331100	-0.58381700	0.00005300
C	-0.53683000	-0.15337300	0.00002500
O	1.81938000	0.19161500	-0.00005900
O	-1.39969900	-1.00350200	-0.00005300
C	-0.74065800	1.33334100	0.00002600
H	0.95965900	-1.59810400	0.00019400
H	-0.26876100	1.78112500	-0.87765900
H	-0.26752300	1.78126400	0.87697200
H	-1.80907200	1.53772000	0.00071700

#### Entry 6

C	-1.16505400	0.17429500	0.02299400
C	1.16503700	0.17419200	0.02238300
N	-0.00000300	-0.60691900	0.16549600
O	-0.00012000	-1.94675100	-0.15656400
O	-2.29274900	-0.23587900	-0.04424400
O	2.29277000	-0.23599800	-0.04411000
C	-0.66726500	1.58926900	-0.00968600
C	0.66737900	1.58922400	-0.00943000
H	0.00005500	-2.41969200	0.68674000
H	-1.34876500	2.42768500	-0.02194800
H	1.34894800	2.42758700	-0.02149400

#### 6-radical

C	1.18664400	0.13699300	-0.00010400
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C	-1.18664400	0.13699300	-0.00003100
N	0.00000000	-0.69556800	-0.00005700
O	0.00000000	-1.95607000	-0.00010300
O	2.31095500	-0.26925400	-0.00009600
O	-2.31095500	-0.26925400	0.00002700
C	0.66908400	1.53459200	0.00014800
C	-0.66908400	1.53459200	0.00018200
H	1.33858200	2.38329600	0.00027100
H	-1.33858200	2.38329600	0.00034100

**Entry 7**

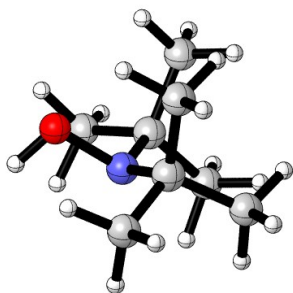
C	1.2964110	-0.0965941	-0.0670472
C	-1.2964110	-0.0965941	-0.0670472
C	-1.2643800	1.3353839	-0.6570892
C	0.0000000	2.0834829	-0.2958762
C	1.2643800	1.3353839	-0.6570892
N	0.0000000	-0.7469291	-0.4251952
C	1.6156520	-0.0478401	1.4436468
C	2.4073760	-0.8900151	-0.7777692
C	-1.6156520	-0.0478411	1.4436468
C	-2.4073760	-0.8900151	-0.7777692
O	0.0000000	3.1783459	0.2251138
H	-1.3025400	1.2643199	-1.7506052
H	-2.1332590	1.9009719	-0.3173012
H	1.3025400	1.2643199	-1.7506052
H	2.1332590	1.9009719	-0.3173012
H	1.4420380	-1.0238241	1.8986418
H	2.6692800	0.2093219	1.5828788
H	1.0286890	0.6987509	1.9781778
H	3.3590170	-0.3586511	-0.6934372
H	2.5319890	-1.8761291	-0.3270492
H	2.1711840	-1.0134691	-1.8377392
H	-2.6692800	0.2093219	1.5828788
H	-1.4420380	-1.0238241	1.8986418
H	-1.0286890	0.6987509	1.9781778
H	-2.5319890	-1.8761291	-0.3270492
H	-3.3590170	-0.3586511	-0.6934372
H	-2.1711840	-1.0134701	-1.8377392
O	0.0000000	-2.0692641	0.1567928
H	0.0000000	-2.6500851	-0.6114492

**7-radical**

C	-1.1554255	1.2295994	0.5548707
C	-1.3243335	-0.1882736	-0.0232813
C	1.3229355	-0.1973586	0.0237487
C	1.1642375	1.2195224	-0.5597593

C	0.0069455	2.0284014	-0.0044293
N	-0.0031305	-0.8961316	0.0012197
O	-0.0075695	-2.1737516	0.0035307
C	-2.3146625	-0.9744886	0.8477757
C	-1.8354175	-0.1450036	-1.4780823
C	2.3082155	-0.9936776	-0.8438473
C	1.8335805	-0.1522316	1.4786427
O	0.0117045	3.2393954	-0.0054553
H	-0.9927165	1.1634374	1.6378257
H	-2.0714245	1.8079704	0.4159037
H	1.0018875	1.1504764	-1.6425813
H	2.0841155	1.7920524	-0.4222163
H	-1.9405885	-1.0743666	1.8692597
H	-3.2707215	-0.4452486	0.8771747
H	-2.4748565	-1.9740336	0.4464547
H	-1.1941575	0.4599944	-2.1233103
H	-1.8721715	-1.1577536	-1.8837303
H	-2.8426325	0.2792304	-1.5114603
H	2.4612265	-1.9928256	-0.4387533
H	1.9339935	-1.0947286	-1.8651623
H	3.2679545	-0.4712246	-0.8746683
H	2.8436835	0.2651594	1.5109797
H	1.1961875	0.4595614	2.1212937
H	1.8631395	-1.1637016	1.8880577

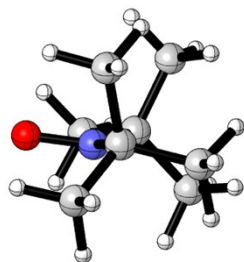
### Entry 8



N	0.0111575	-0.5772953	-0.4585436
O	-0.0623465	-1.9496333	0.0142014
C	-1.3222825	0.0606467	-0.1618206
C	-2.3966075	-0.8953893	-0.7248606
C	-1.6142725	0.2986987	1.3318514
C	-1.4604735	1.3765147	-0.9530406
C	1.3346205	-0.0708333	0.0580684
C	1.5279115	1.4233257	-0.2357536
C	1.5735675	-0.3276923	1.5623774
C	2.4032425	-0.8416483	-0.7462886
H	-0.0974865	-2.4681283	-0.7978196
H	-2.1863605	-1.1414113	-1.7700496

H	-2.4599675	-1.8203893	-0.1535406
H	-3.3743895	-0.4089983	-0.6874836
H	-0.9997235	1.0978587	1.7511294
H	-2.6598175	0.5923287	1.4672694
H	-1.4454015	-0.6104003	1.9122864
H	-2.5084285	1.6877967	-0.9431276
H	-0.8833795	2.1999547	-0.5392316
H	-1.1629185	1.2347617	-1.9946716
H	1.3190785	1.6649717	-1.2795356
H	0.9185725	2.0629127	0.4035824
H	2.5714105	1.6814577	-0.0376196
H	1.3743295	-1.3685933	1.8159594
H	2.6185385	-0.1151933	1.8071054
H	0.9564205	0.3068827	2.1988224
H	3.4045385	-0.4894443	-0.4837996
H	2.3631835	-1.9111633	-0.5362986
H	2.2572835	-0.6918973	-1.8191686

### 8-radical



N	-0.0034616	-0.7714753	0.0115207
O	0.0353914	-1.9716753	0.4615617
C	-1.3655966	-0.0981883	0.0146417
C	-2.4176706	-1.2086203	0.1649557
C	-1.4919826	0.8657817	1.2098427
C	-1.6336696	0.6293497	-1.3165533
C	1.3620214	-0.1095743	-0.0382493
C	1.3810194	1.2567127	-0.7344663
C	1.8824624	0.0299177	1.4058117
C	2.2761204	-1.0637753	-0.8282643
H	-2.3495946	-1.9337393	-0.6473903
H	-2.3052876	-1.7502213	1.1022077
H	-3.4108326	-0.7524203	0.1398377
H	-0.8020106	1.7085887	1.1493097
H	-2.5050776	1.2770587	1.2446977
H	-1.3115526	0.3401987	2.1502337
H	-2.6914126	0.9010237	-1.3672423
H	-1.0622716	1.5473757	-1.4346683
H	-1.4191436	-0.0244543	-2.1654533
H	1.0850574	1.1892937	-1.7822813

H	0.7618534	2.0055687	-0.2402493
H	2.4080444	1.6301617	-0.7115353
H	1.8354324	-0.9323453	1.9170957
H	2.9230644	0.3666707	1.3992107
H	1.3008774	0.7558057	1.9786177
H	3.2860854	-0.6483513	-0.8804173
H	2.3229144	-2.0418613	-0.3532093
H	1.9092204	-1.1968063	-1.8495643

### Entry 9

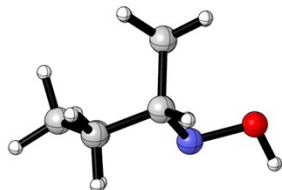
C	0.61338700	0.81559900	-0.09364700
C	-1.35054500	-0.67986600	-0.02442700
C	-0.05347600	-1.53507200	0.01151900
C	1.06100500	-0.60772800	-0.53368900
C	-2.30987500	-1.14752600	-1.12941500
C	-2.07958400	-0.70625200	1.32879100
C	0.92109900	1.10456500	1.38702000
C	1.22058300	1.90972600	-0.97503500
C	2.40165700	-0.98228600	-0.10324700
N	3.46221800	-1.28767700	0.23357600
N	-0.83020700	0.67254400	-0.41685100
O	-1.59479800	1.72806700	0.17109600
H	0.17984200	-1.83631500	1.03385300
H	-0.14019000	-2.44383300	-0.58546700
H	1.05054600	-0.63339800	-1.62778300
H	-2.70954400	-2.14113600	-0.90506600
H	-3.15367600	-0.45749500	-1.21757800
H	-1.80073100	-1.18514800	-2.09548300
H	-2.99136300	-0.10899900	1.29285400
H	-2.35384500	-1.73774300	1.56850700
H	-1.45942500	-0.32172000	2.13897500
H	0.37003900	1.98978200	1.70706000
H	0.65046200	0.27749300	2.04458800
H	1.98863100	1.29464700	1.51834000
H	0.82691500	2.88766100	-0.68692700
H	2.30743800	1.94062700	-0.86194300
H	0.97904500	1.73567400	-2.02634600
H	-1.95534800	2.19434500	-0.59063600

### 9-radical

C	0.64480100	0.83806800	-0.03267400
C	-1.40073500	-0.64788100	0.00555000
C	-0.12044800	-1.49952100	0.10829600
C	0.99575500	-0.60842100	-0.49327300
C	-2.16133200	-0.87624800	-1.31198500
C	-2.33778900	-0.83145800	1.20346500

C	1.16997300	1.18064500	1.37129200
C	1.07342200	1.90048600	-1.04549500
N	-0.84187700	0.73729600	0.00589600
O	-1.57753300	1.76405600	0.13264800
C	2.34060500	-1.04660200	-0.14210700
N	3.40322700	-1.40285000	0.13116900
H	0.10805600	-1.72359000	1.15227400
H	-0.20717000	-2.44720600	-0.42462800
H	0.92486500	-0.63836300	-1.58541700
H	-2.62289400	-1.86729500	-1.31621300
H	-2.94707300	-0.12585600	-1.41920500
H	-1.49954900	-0.80159200	-2.17897900
H	-3.17194400	-0.13122300	1.13676600
H	-2.73480900	-1.84998200	1.21694600
H	-1.81327600	-0.65124400	2.14472700
H	2.25483800	1.30414900	1.35748100
H	0.71297600	2.11564100	1.70031000
H	0.92318300	0.40466400	2.09933700
H	0.69100700	2.87627300	-0.74294300
H	2.16381700	1.95146500	-1.09827600
H	0.68328600	1.67617600	-2.04123500

### Entry 10

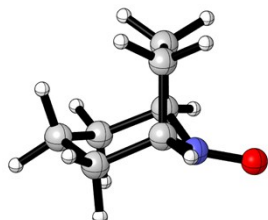


C	-1.0250559	1.2697278	-0.5823044
C	0.4657801	1.1509448	-0.2182334
C	0.4656381	-1.1510242	-0.2181184
C	-1.0252129	-1.2696592	-0.5821784
C	-1.7990479	0.0001018	-0.1859924
C	0.7000201	0.7774118	1.2703906
C	0.6999251	-0.7773722	1.2704676
N	0.9915131	-0.0001102	-0.9924224
H	-1.4518519	2.1485138	-0.0883884
H	-1.0996639	1.4348548	-1.6617724
H	1.0044971	2.0494308	-0.5208964
H	1.0042441	-2.0496062	-0.5206934
H	-1.4521169	-2.1483432	-0.0881754
H	-1.0998409	-1.4348832	-1.6616304
H	-1.9678109	0.0001658	0.8961756
H	-2.7909469	0.0001398	-0.6471154
H	-0.0718659	1.1995488	1.9186666
H	1.6624281	1.1634188	1.6076546



H	1.6622851	-1.1634642	1.6077696
H	-0.0720129	-1.1993502	1.9187866
O	2.4392641	-0.0001902	-0.8072764
H	2.7598321	-0.0002562	-1.7147144

### 10-radical



C	-0.8208173	1.2783869	-0.7225463
C	0.6265007	1.1764499	-0.2111083
C	0.6264497	-1.1764461	-0.2112803
C	-0.8208733	-1.2782461	-0.7227343
C	-1.6202623	0.0000649	-0.4031013
C	0.7173027	0.7812169	1.2853797
C	0.7172687	-0.7814361	1.2852647
N	1.2444307	0.0000379	-0.8750063
O	2.4864207	0.0000329	-1.1779773
H	-1.3078593	2.1514839	-0.2764603
H	-0.7892983	1.4443089	-1.8042733
H	1.2114497	2.0578659	-0.4690793
H	1.2113607	-2.0578491	-0.4693813
H	-1.3079523	-2.1513871	-0.2767763
H	-0.7893603	-1.4440101	-1.8044853
H	-1.8932023	-0.0000071	0.6576077
H	-2.5635983	0.0001259	-0.9561033
H	-0.1098743	1.1985819	1.8638257
H	1.6459457	1.1629079	1.7123787
H	1.6458957	-1.1632311	1.7122077
H	-0.1099263	-1.1988511	1.8636487

### Entry 11

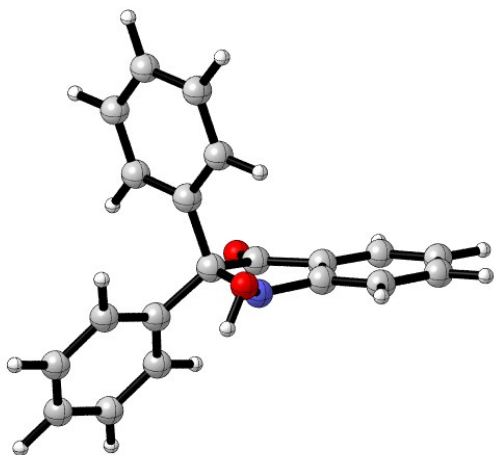
C	-1.08971200	0.00003100	-1.64660300
C	-1.11171800	-1.26441900	-0.77458800
C	1.42230800	1.26885900	-0.23473300
C	-0.03230600	-1.21814400	0.32615400
C	2.22366400	0.00001000	0.09573100
C	1.42232400	-1.26884100	-0.23477800
C	-1.11173300	1.26444200	-0.77453100
C	-0.03232100	1.21812800	0.32620800

N	-0.13757400	-0.00002500	1.16270600
O	-1.45166200	-0.00003900	1.77781800
H	-1.94381300	0.00004300	-2.33077200
H	-0.19601800	0.00005000	-2.28098700
H	-0.96417500	-2.16150800	-1.38597500
H	-2.08986500	-1.36078100	-0.29450500
H	1.93955500	2.14538200	0.16422300
H	1.38572300	1.40249100	-1.32074100
H	-0.18806700	-2.05829700	1.00644600
H	2.48009200	-0.00001100	1.15765900
H	3.16641000	0.00002100	-0.46066800
H	1.93958200	-2.14536700	0.16415600
H	1.38575100	-1.40244000	-1.32079000
H	-2.08988400	1.36077300	-0.29445000
H	-0.96419300	2.16156100	-1.38587500
H	-0.18808200	2.05825000	1.00653800
H	-1.23973700	-0.00008500	2.71708000

### 11-radical

C	-1.40085600	-0.00000100	-1.41650800
C	-1.27317700	-1.27492500	-0.56382600
C	1.32384200	1.26905900	-0.45579100
C	-0.01654000	-1.23904600	0.33375900
C	2.15707200	0.00000000	-0.22003400
C	1.32384300	-1.26905900	-0.45579000
C	-1.27317700	1.27492400	-0.56382600
C	-0.01654000	1.23904600	0.33375900
N	-0.07975100	0.00000000	1.13818400
O	-0.76217400	0.00000100	2.22172900
H	-2.36277100	-0.00000100	-1.93745400
H	-0.63532400	-0.00000100	-2.19986100
H	-1.24258000	-2.16463600	-1.20155200
H	-2.14711600	-1.37261000	0.08833900
H	1.89973800	2.15030800	-0.16232200
H	1.11954200	1.37725700	-1.52570300
H	-0.05836400	-2.05277200	1.05767600
H	2.53154500	0.00000100	0.80830400
H	3.03295800	0.00000000	-0.87545000
H	1.89973900	-2.15030700	-0.16232000
H	1.11954200	-1.37725800	-1.52570200
H	-2.14711600	1.37260900	0.08833800
H	-1.24258100	2.16463500	-1.20155300
H	-0.05836400	2.05277300	1.05767500

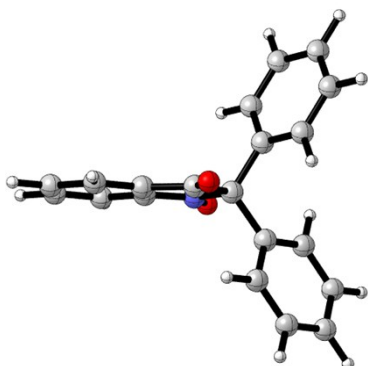
### Entry 12



C	2.0185028	-0.6847658	0.5640479
C	2.0720048	-0.6397358	-0.8397561
C	3.2849678	-0.7686298	-1.5158171
C	4.4496278	-0.9109398	-0.7708931
C	4.3880088	-0.9227208	0.6327079
C	3.1842238	-0.8136138	1.3230969
C	0.7121938	-0.4577118	-1.3516611
O	0.3184208	-0.4730038	-2.4955371
C	-0.1992642	-0.1897638	-0.0914511
N	0.7028238	-0.6561618	0.9956239
C	-1.4862872	-1.0124858	-0.0363281
C	-2.4884432	-0.6530068	0.8744019
C	-1.6589912	-2.1697198	-0.8015621
C	-3.6321742	-1.4347708	1.0206309
C	-2.8074262	-2.9478938	-0.6598241
C	-3.7960462	-2.5859748	0.2519869
C	-0.4374922	1.3292392	-0.1069881
C	-1.4308122	1.8400112	-0.9528441
C	0.3583768	2.2244832	0.6136769
C	-1.6361102	3.2123472	-1.0580641
C	0.1482978	3.5991442	0.5088309
C	-0.8492652	4.0986612	-0.3238441
H	3.3029178	-0.7405198	-2.5991321
H	5.4081408	-1.0033968	-1.2668311
H	5.3078428	-1.0215768	1.1990879
H	3.1472948	-0.8229388	2.4042859
H	-2.3787332	0.2512132	1.4618189
H	-0.9085382	-2.4617728	-1.5242031
H	-4.3978152	-1.1393998	1.7295799
H	-2.9280402	-3.8372018	-1.2683381
H	-4.6889272	-3.1916958	0.3591109
H	-2.0397322	1.1609802	-1.5365511
H	1.1374948	1.8611612	1.2689449
H	-2.4100352	3.5883722	-1.7178441

H	0.7693478	4.2781192	1.0824939
H	-1.0104642	5.1678712	-0.4035441
O	0.4737918	-0.1751698	2.2984839
H	0.0003178	-0.8970308	2.7322019

### 12-radical



C	-2.1722393	-0.1005741	-0.6164751
C	-2.2037593	0.0897429	0.7721769
C	-3.4194003	0.2071599	1.4426799
C	-4.5930493	0.1292409	0.6990599
C	-4.5450303	-0.0660491	-0.6938331
C	-3.3409423	-0.1850971	-1.3775721
C	-0.8281753	0.1100209	1.2863869
O	-0.4645573	0.2250939	2.4334979
C	0.1310287	-0.0378801	0.0536069
N	-0.8633543	-0.1813981	-1.0727391
O	-0.5355163	-0.3644321	-2.2811391
C	1.0030937	-1.2929731	0.1029479
C	2.0232567	-1.4456121	-0.8436661
C	0.7735477	-2.3203111	1.0229729
C	2.7949607	-2.6030321	-0.8697991
C	1.5526827	-3.4768701	0.9987989
C	2.5632247	-3.6226471	0.0527989
C	0.9310947	1.2612329	-0.0806431
C	1.9579927	1.5054529	0.8400089
C	0.6369017	2.2299389	-1.0434141
C	2.6785177	2.6943639	0.7927019
C	1.3657667	3.4188929	-1.0904511
C	2.3862237	3.6558549	-0.1744911
H	-3.4346583	0.3541739	2.5160639
H	-5.5539503	0.2174179	1.1914759
H	-5.4743723	-0.1254801	-1.2492481
H	-3.2933083	-0.3363341	-2.4476321
H	2.2078957	-0.6581191	-1.5628981

H	0.0026417	-2.2234501	1.7764229
H	3.5793867	-2.7071551	-1.6109231
H	1.3677947	-4.2606671	1.7246599
H	3.1686697	-4.5219311	0.0354539
H	2.1868787	0.7658929	1.5969869
H	-0.1430183	2.0591399	-1.7735271
H	3.4698977	2.8692359	1.5128419
H	1.1324807	4.1569279	-1.8496441
H	2.9513927	4.5802309	-0.2134491

#### Entry 14

C	-3.88941800	0.75643000	-2.04109400
C	-2.50477800	0.87129800	-2.12276000
C	-1.68620100	0.11758900	-1.27232800
C	-2.26236700	-0.78291700	-0.35094600
C	-3.65755900	-0.86020800	-0.27966300
C	-4.47346100	-0.10123400	-1.11239400
C	-1.36244100	-1.59566800	0.48217300
C	-0.01054900	-1.22064800	0.61831400
C	0.82592800	-1.97433100	1.44579800
C	0.35424300	-3.09379600	2.12338000
C	-0.97264200	-3.48788500	1.96501800
C	-1.81489200	-2.74739400	1.14806100
N	-0.28438700	0.16998700	-1.35899500
O	0.18053800	1.20438000	-2.18692200
C	0.52731300	0.03422000	-0.10485200
C	0.35998000	1.31609200	0.74844600
C	1.00338600	2.50844700	0.37269300
C	-0.50423900	1.35926200	1.84894800
C	0.77730200	3.69766100	1.06429600
C	-0.72467600	2.54685800	2.54523000
C	-0.09029600	3.72265400	2.15374400
C	1.98991600	-0.21612000	-0.52805000
C	2.26693400	-0.93166000	-1.69768900
C	3.06080200	0.17270300	0.28227800
C	3.57729700	-1.23871400	-2.05182000
C	4.37509800	-0.13870900	-0.06881800
C	4.63938700	-0.84390600	-1.23904300
H	-4.51020800	1.34705000	-2.70546600
H	-2.05568700	1.52201900	-2.85875700
H	-4.11642000	-1.51756500	0.44873900
H	-5.55138300	-0.17900400	-1.03523800
H	1.86439000	-1.69331400	1.55583100
H	1.02551900	-3.66279300	2.75629800
H	-1.34631900	-4.37353500	2.46651700

H	-2.83772600	-3.07516400	1.01090900
H	-0.03682800	2.04334700	-1.74035300
H	1.71728700	2.50120100	-0.44182000
H	-1.00538300	0.45806600	2.17627300
H	1.29056900	4.60165400	0.75531800
H	-1.39547400	2.54842200	3.39721200
H	-0.26306900	4.64573900	2.69543400
H	1.44779900	-1.23842300	-2.33494100
H	2.87718600	0.72289000	1.19704300
H	3.76856000	-1.78740400	-2.96745700
H	5.18915800	0.17434600	0.57569300
H	5.66003300	-1.08263000	-1.51642200

#### 14-radical

C	3.91319600	0.75888800	-2.09284800
C	2.53224800	0.82311900	-2.19531400
C	1.73612900	0.13521100	-1.26960600
C	2.31280800	-0.66015600	-0.25780100
C	3.71116200	-0.68600200	-0.17041400
C	4.50667900	0.01312600	-1.07037700
C	1.43143100	-1.45948400	0.60781900
C	0.05416500	-1.17012700	0.65490200
C	-0.78389100	-1.94742800	1.45849600
C	-0.28071600	-3.00265200	2.21289800
C	1.07856600	-3.30425700	2.15648800
C	1.91928400	-2.54447100	1.35507200
N	0.33566000	0.22468600	-1.36364800
O	-0.19410000	0.77914700	-2.38130400
C	-0.51033300	0.02938400	-0.12082200
C	-1.94963000	-0.26670500	-0.57584800
C	-3.05074100	0.36212100	0.00430600
C	-2.17380600	-1.25515800	-1.54296100
C	-4.35043200	0.01557300	-0.37421000
C	-3.46517800	-1.59535000	-1.92603400
C	-4.56239200	-0.96047900	-1.34104900
C	-0.39809200	1.34348200	0.69277300
C	-0.06997800	1.35194700	2.05032600
C	-0.63723200	2.56794700	0.05245500
C	0.01330400	2.55421800	2.75560800
C	-0.54966800	3.76517400	0.75514300
C	-0.22519500	3.76400700	2.11220800
H	4.52944800	1.30257900	-2.79960000
H	2.04373200	1.40187900	-2.96663100
H	4.18624100	-1.25917800	0.61577800
H	5.58568400	-0.02203500	-0.97596900
H	-1.84264400	-1.72624200	1.49410600

H	-0.94939100	-3.59148300	2.83014100
H	1.47982800	-4.13636200	2.72383500
H	2.96705500	-2.80978200	1.29267100
H	-2.90471700	1.12607200	0.75675500
H	-1.33150600	-1.75536900	-2.00533200
H	-5.19291100	0.51651000	0.08953100
H	-3.61706000	-2.35557000	-2.68412900
H	-5.57027900	-1.22579600	-1.64001200
H	0.12274300	0.42213400	2.56923000
H	-0.89025900	2.57767400	-1.00070400
H	0.27007000	2.53800500	3.80903000
H	-0.73574500	4.70159900	0.24098100
H	-0.15722300	4.69781500	2.65902400

### Entry 15

C	-0.63944700	0.59711800	-0.08155500
C	-0.70936500	-0.63903800	-0.73327800
C	-1.91653400	-1.27230100	-0.97710500
C	-3.10680700	-0.67279700	-0.55323800
C	-3.01104100	0.59690200	0.02787400
C	-1.81698400	1.30613600	0.25181700
C	0.67557600	-1.06717800	-1.19962500
C	1.60032600	-0.23839900	-0.19553300
N	0.73312500	0.97640200	0.01661500
O	1.10628200	1.71238000	1.16256300
C	0.91307900	-2.58430800	-1.21944400
C	0.83812900	-0.54763200	-2.65358100
C	1.83182100	-0.93090600	1.17974400
C	3.04406800	-0.77289900	1.86908600
C	0.80472400	-1.62471300	1.84581600
C	3.23893200	-1.31378700	3.13969100
C	0.99687600	-2.16475400	3.11624700
C	2.21847000	-2.01958200	3.76891200
C	2.92586600	0.16964600	-0.84829700
C	3.18043400	1.49022400	-1.22615300
C	3.90504000	-0.79608100	-1.12347800
C	4.37063300	1.83516500	-1.86747300
C	5.09030900	-0.45557000	-1.76976600
C	5.32920300	0.86542600	-2.14669300
C	-4.48608200	-1.33703000	-0.72267700
C	-5.39805100	-0.44445900	-1.59665400
C	-4.38603200	-2.71826400	-1.39660700
C	-5.14099700	-1.52879100	0.66554300
C	-1.89561900	2.76869000	0.76458700
C	-1.58860400	2.86001100	2.27906100

C	-0.93988400	3.68040300	-0.04011800
C	-3.31380000	3.35793800	0.56808200
H	-1.92278500	-2.23094500	-1.47896000
H	-3.93471500	1.07900300	0.31034100
H	1.06744500	1.09818600	1.91732300
H	0.21534800	-3.05113100	-1.92001500
H	1.91859300	-2.81327600	-1.57873200
H	0.78098100	-3.05787000	-0.24792100
H	1.81385800	-0.81274400	-3.06541700
H	0.06565600	-1.00316700	-3.27841100
H	0.72411300	0.53562900	-2.71025300
H	3.85072600	-0.21414700	1.41530400
H	-0.16186700	-1.74596600	1.37845200
H	4.19224700	-1.17286000	3.63697200
H	0.18372600	-2.70017000	3.59383700
H	2.36859600	-2.44232700	4.75594400
H	2.43937600	2.24915100	-1.01749600
H	3.75166400	-1.82438000	-0.81919900
H	4.54456400	2.86815800	-2.14842800
H	5.82914800	-1.22274300	-1.97425300
H	6.25292400	1.13376700	-2.64705300
H	-5.55576100	0.53886300	-1.14794500
H	-4.96119100	-0.29324100	-2.58764200
H	-6.37923700	-0.91276900	-1.72485200
H	-3.77524700	-3.41268700	-0.81288200
H	-5.38393500	-3.15555700	-1.48910500
H	-3.96260600	-2.65136000	-2.40275700
H	-6.12338700	-2.00088100	0.56305800
H	-4.52239400	-2.16652100	1.30335300
H	-5.28141100	-0.57657700	1.18260600
H	-0.55808600	2.59336700	2.50026200
H	-1.75274800	3.88442800	2.62949600
H	-2.25239700	2.20141900	2.84705700
H	0.10228600	3.39640700	0.07368100
H	-1.19426200	3.65666800	-1.10411400
H	-1.04557700	4.71367200	0.30497600
H	-3.29055900	4.41868500	0.83056000
H	-3.65055600	3.27768200	-0.46876500
H	-4.06009500	2.88736100	1.21305100

### 15-radical

C	0.64590200	0.45700100	-0.39782700
C	0.70239300	-0.93915900	-0.25695200
C	1.90648300	-1.60869200	-0.13285600
C	3.10309100	-0.88564300	-0.15196700
C	3.01699500	0.50595100	-0.31739100



C	1.83186900	1.24109400	-0.44951600
C	-0.68296200	-1.55852400	-0.37731000
C	-1.61316000	-0.32164600	-0.01404200
N	-0.71560300	0.83006100	-0.44708800
O	-1.18302300	2.00735600	-0.51755900
C	-0.84498700	-1.96077900	-1.86902800
C	-0.91780000	-2.82447900	0.46052600
C	-1.85205100	-0.05577700	1.49335300
C	-2.99719700	0.63868700	1.90474200
C	-0.88149300	-0.33980000	2.46605200
C	-3.18910100	0.99261900	3.23907900
C	-1.07279900	0.01015100	3.80060400
C	-2.23232800	0.67218500	4.19715700
C	-2.92250900	-0.36243600	-0.80313600
C	-3.92488500	-1.25276400	-0.39158100
C	-3.14234300	0.38679200	-1.96289200
C	-5.10218600	-1.39933600	-1.12012100
C	-4.32460200	0.24501500	-2.68976300
C	-5.30830700	-0.64865000	-2.27614800
C	4.48308400	-1.55138100	-0.00730600
C	5.33281200	-1.26449400	-1.26788800
C	5.20576900	-0.98258600	1.23660300
C	4.37856800	-3.07866200	0.15941900
C	1.89868600	2.77615500	-0.62781300
C	1.22895000	3.48574800	0.57408600
C	3.35448100	3.29019700	-0.68852700
C	1.23261700	3.18786800	-1.96329400
H	1.90768800	-2.68485100	-0.02421800
H	3.94554900	1.05483100	-0.33875300
H	-0.07140600	-2.69078200	-2.11968400
H	-0.72688100	-1.10584800	-2.53660100
H	-1.82033200	-2.41230400	-2.05792500
H	-1.92766000	-3.20492500	0.29195400
H	-0.78691300	-2.67371400	1.52973200
H	-0.22706900	-3.60887800	0.14023800
H	-3.74738300	0.91691000	1.17764800
H	0.04701800	-0.81993200	2.19106600
H	-4.08798900	1.52835800	3.52350400
H	-0.30647000	-0.23093600	4.52909700
H	-2.38086800	0.94497700	5.23595500
H	-3.79327100	-1.82896200	0.51628200
H	-2.40102100	1.09872000	-2.29540500
H	-5.86014900	-2.09580400	-0.77889900
H	-4.47382900	0.84272900	-3.58218400
H	-6.22654800	-0.75542600	-2.84263600
H	5.49284500	-0.19420300	-1.41590100

H	4.84499600	-1.65662700	-2.16456600
H	6.31506000	-1.73937000	-1.17952000
H	5.35322000	0.09714400	1.16313900
H	4.63134700	-1.18043800	2.14588400
H	6.19063400	-1.44685200	1.34861800
H	3.80952400	-3.35348700	1.05191200
H	5.37990100	-3.50489100	0.26466900
H	3.90961900	-3.55289200	-0.70727800
H	0.17931800	3.21931400	0.67412100
H	1.29161700	4.57063900	0.44059600
H	1.74917900	3.23157300	1.50261000
H	3.90664200	3.09503000	0.23488500
H	3.91298900	2.86463000	-1.52696600
H	3.33303500	4.37376400	-0.82855300
H	1.73595400	2.70207500	-2.80511700
H	1.32137900	4.27046100	-2.10002000
H	0.17573800	2.93277400	-1.98518000

### Entry 16

N	2.17772600	0.40611300	-0.25639600
C	1.09805400	-0.46547400	-0.10693500
O	1.27328100	-1.67512100	-0.03672700
C	-0.25591500	0.14707800	-0.10961900
C	-1.33456100	-0.64747000	-0.01849600
C	-2.74133000	-0.24273600	-0.00656600
C	-3.72770200	-1.24193500	0.03871200
C	-3.16060500	1.09956200	-0.03509000
C	-5.08163700	-0.91826600	0.04962200
C	-4.51091600	1.42337700	-0.02298400
C	-5.47852700	0.41644400	0.01848100
C	3.60065000	-0.00333700	0.01969100
C	4.50902800	1.19639800	-0.29856300
C	3.75500200	-0.40559300	1.49603400
C	3.98719000	-1.15737600	-0.92322100
O	1.89223600	1.73691100	0.15177600
H	-0.33630100	1.22154300	-0.17625300
H	-1.14631400	-1.71587700	0.05220300
H	-3.42169000	-2.28246500	0.06433900
H	-2.42548200	1.89521900	-0.06132200
H	-5.82470500	-1.70696600	0.08369600
H	-4.81422200	2.46422700	-0.04356100
H	-6.53163300	0.67362500	0.02844500
H	4.36796600	1.53801300	-1.32907100
H	4.34025000	2.03244200	0.38019700
H	5.55012700	0.88296900	-0.19684800
H	3.13473000	-1.27248400	1.72633100

H	4.79703000	-0.66099900	1.70830100
H	3.46711200	0.42172800	2.14990800
H	5.05458300	-1.36405500	-0.80441100
H	3.42424000	-2.06126100	-0.70828200
H	3.80986700	-0.87623000	-1.96483600
H	2.03384600	2.26942200	-0.64085100

### 16-radical

N	2.18205000	0.48603100	-0.00003800
C	1.09361300	-0.45136900	-0.00002300
O	1.32297400	-1.64910900	0.00006700
C	-0.24881600	0.15278400	-0.00003600
C	-1.33107900	-0.64634000	0.00002500
C	-2.73440400	-0.23856200	0.00001900
C	-3.72424700	-1.23591300	-0.00004100
C	-3.14619200	1.10681700	0.00007200
C	-5.07650000	-0.90682900	-0.00006100
C	-4.49507200	1.43499000	0.00005500
C	-5.46641200	0.43047400	-0.00001400
C	3.63870300	0.03471100	0.00000500
C	4.50959200	1.29459700	-0.00008100
C	3.90945700	-0.78621000	1.27357400
C	3.90947200	-0.78639300	-1.27344200
O	1.92185500	1.73274000	-0.00009300
H	-0.30956300	1.23054100	-0.00010000
H	-1.14986200	-1.71860600	0.00007600
H	-3.42249300	-2.27803000	-0.00007600
H	-2.40728100	1.89921100	0.00013300
H	-5.82354900	-1.69234900	-0.00011000
H	-4.79456100	2.47698100	0.00009900
H	-6.51851900	0.69185700	-0.00002600
H	4.32929200	1.90939300	-0.88253900
H	4.32927800	1.90952300	0.88228300
H	5.55662600	0.98253900	-0.00005000
H	3.32485600	-1.70392600	1.29290000
H	4.97067800	-1.04720500	1.30821100
H	3.67891800	-0.19795500	2.16578600
H	4.97069600	-1.04737800	-1.30803900
H	3.32488400	-1.70412000	-1.29263800
H	3.67892700	-0.19827300	-2.16574200

### Entry 17

N	-2.14850600	-0.40781300	-0.27304100
C	-1.12496200	0.50849400	-0.05427200

O	-1.35184000	1.69953100	0.07495200
C	2.75878900	0.47648800	-0.01883400
C	3.39187100	0.18033600	1.19401000
C	3.44779000	0.20695300	-1.20685500
C	4.67063900	-0.37308600	1.22062900
C	4.72703000	-0.34646500	-1.18643100
C	5.34301300	-0.63992500	0.02891600
C	-3.59811200	-0.11056700	0.00709000
C	-4.42133200	-1.34097400	-0.40848000
C	-3.79591800	0.17923900	1.50416400
C	-4.04353600	1.08063100	-0.86007300
C	1.35723900	1.04569800	-0.04501400
C	0.28936900	-0.05900900	-0.04115200
O	-1.77241300	-1.73467300	0.06575500
H	2.88016000	0.39288600	2.12780800
H	2.98011600	0.44110000	-2.15849600
H	5.14433000	-0.59018700	2.17184200
H	5.24476500	-0.54249100	-2.11912900
H	6.33975700	-1.06611200	0.04753100
H	-4.24836700	-1.59584300	-1.45877700
H	-4.20037400	-2.21139600	0.20927900
H	-5.48210100	-1.10666300	-0.29663000
H	-4.85472200	0.35032600	1.71756100
H	-3.46049300	-0.66924600	2.10624200
H	-3.23924500	1.06872500	1.80291600
H	-3.83908300	0.88306800	-1.91580900
H	-5.12238000	1.21556000	-0.74269400
H	-3.53856300	1.99955200	-0.57524500
H	1.19845400	1.69938100	0.81549300
H	1.22419600	1.67192100	-0.93092100
H	0.39683700	-0.69692700	0.84178300
H	0.42467300	-0.72725700	-0.89676700
H	-1.82568400	-2.22744300	-0.76254100

### 17-radical

N	-2.15655800	0.50308900	-0.00003200
O	-1.81132000	1.72994500	0.00017000
C	-1.12061100	-0.48062500	0.00002900
O	-1.39216000	-1.66333200	0.00027200
C	2.75449500	-0.46448900	-0.00014200
C	3.41561800	-0.18426400	-1.20123700
C	3.41543700	-0.18438600	1.20108700
C	4.69660800	0.36481200	-1.20402800
C	4.69642200	0.36469400	1.20412600
C	5.34144200	0.64238000	0.00011100

C	-3.63777300	0.14103500	-0.00006800
C	-4.42974100	1.45172600	0.00024900
C	-3.95536100	-0.66328600	-1.27282200
C	-3.95522700	-0.66385300	1.27236200
C	1.35066700	-1.02943600	-0.00029000
C	0.28623000	0.07810400	0.00017900
H	2.92485600	-0.40460100	-2.14443500
H	2.92454500	-0.40483100	2.14419400
H	5.19277600	0.57076600	-2.14612800
H	5.19244700	0.57055200	2.14632100
H	6.33943100	1.06591600	0.00020900
H	-4.21215400	2.05453700	0.88264100
H	-4.21216000	2.05494400	-0.88186800
H	-5.49424000	1.20555700	0.00019400
H	-5.02960600	-0.86297700	-1.30823100
H	-3.69064300	-0.09080200	-2.16577100
H	-3.42574100	-1.61414300	-1.29061800
H	-3.69039500	-0.09177500	2.16553700
H	-5.02946900	-0.86355700	1.30781000
H	-3.42560600	-1.61472200	1.28966500
H	1.20484200	-1.66907300	-0.87445000
H	1.20491000	-1.66978900	0.87335700
H	0.40033800	0.73787200	-0.86555900
H	0.40038100	0.73712700	0.86649200

### Entry 18

N	4.31242700	0.49269100	0.22316400
C	5.69224600	-0.07253800	0.01155100
C	5.82382800	-0.62068300	-1.41921900
C	6.70734600	1.05976400	0.23982800
C	5.95209900	-1.16898200	1.06023100
C	3.15238300	-0.27157000	0.12496200
O	3.18942000	-1.48883400	0.18047900
C	1.84634600	0.50318100	0.00014100
C	0.61443400	-0.39558500	0.11216600
C	-0.69611700	0.38467100	-0.03964900
C	-1.94273800	-0.50306800	0.04879200
C	-3.25900500	0.26606500	-0.11103200
C	-4.50295800	-0.62678000	-0.03769500
C	-5.82140800	0.13585100	-0.21337800
C	-7.05753500	-0.77081100	-0.15106100
C	-8.39457600	-0.05868000	-0.40861100
C	-8.78862000	0.96390400	0.66339700
H	5.12828300	-1.44495000	-1.58291600
H	5.62152900	0.16618000	-2.15064200

H	6.83917300	-0.98968400	-1.58930900
H	6.58707900	1.50460600	1.23268400
H	7.71532200	0.64290500	0.18572500
H	6.62418100	1.84353700	-0.51306700
H	6.99307800	-1.49387300	0.97754500
H	5.79778300	-0.77762600	2.06944900
H	5.30039200	-2.02668000	0.91812100
H	1.85603900	1.03156800	-0.95946700
H	1.82304400	1.29087000	0.76093100
H	0.67106800	-1.18020300	-0.64812000
H	0.62842600	-0.91471900	1.07607100
H	-0.75233700	1.16365800	0.73235600
H	-0.69759000	0.91228700	-1.00263300
H	-1.88375200	-1.28269300	-0.72140000
H	-1.94445600	-1.02908200	1.01209300
H	-3.25254100	0.79766200	-1.07159000
H	-3.32312300	1.04104600	0.66394800
H	-4.43222400	-1.40681000	-0.80683700
H	-4.51461700	-1.15250300	0.92593600
H	-5.88842800	0.91460200	0.55532900
H	-5.80946900	0.65990300	-1.17846000
H	-6.93985700	-1.57355900	-0.88930400
H	-7.09567600	-1.26447400	0.82915700
H	-9.18413400	-0.81509800	-0.48314100
H	-8.35599000	0.43536200	-1.38753600
H	-8.83522700	0.49704400	1.65294800
H	-8.07636100	1.79137300	0.72118500
H	-9.77226900	1.39375900	0.45396700
O	4.15315200	1.79838100	-0.31333700
H	4.29073300	2.39194200	0.43516400

### 18-radical

N	4.34467900	0.54609500	-0.06801000
O	4.20294900	1.79290000	-0.29174900
C	5.74778400	-0.03800100	0.05166800
C	5.93902900	-1.11300800	-1.03271100
C	6.74121000	1.10645800	-0.16949000
C	5.92629600	-0.62136900	1.46436300
C	3.16290700	-0.24771900	0.06982000
O	3.24547200	-1.43709300	0.29492900
C	1.86354100	0.51282600	-0.08225400
C	0.63438400	-0.39071300	0.02094400
C	-0.67745100	0.39079900	-0.11273900
C	-1.92223300	-0.50105100	-0.04292700
C	-3.23994100	0.27380500	-0.15731100
C	-4.48329900	-0.62155900	-0.10940700

C	-5.80342800	0.15116900	-0.21464300
C	-7.04028200	-0.75582900	-0.18176600
C	-8.38131300	-0.02416000	-0.34888000
C	-8.74359300	0.91433700	0.80786400
H	5.26659800	-1.95640400	-0.88685900
H	5.77081900	-0.69106000	-2.02719500
H	6.96880000	-1.47793800	-0.99270200
H	6.62060700	1.89506700	0.57400400
H	7.75204000	0.70008100	-0.08603000
H	6.62666900	1.55439900	-1.15734600
H	6.95212600	-0.98349900	1.57317600
H	5.75950000	0.14867700	2.22229200
H	5.24534500	-1.45130600	1.64509000
H	1.88716200	1.04848400	-1.03700300
H	1.84202000	1.30320000	0.67649500
H	0.68598600	-1.16317300	-0.75344400
H	0.65261500	-0.92447700	0.97640800
H	-0.73168200	1.15070200	0.67771200
H	-0.68088900	0.94110500	-1.06265700
H	-1.87274300	-1.25154500	-0.84229800
H	-1.91284600	-1.06216000	0.90034200
H	-3.24319200	0.84664300	-1.09382600
H	-3.29545200	1.01429000	0.65122000
H	-4.42942400	-1.35757100	-0.92211500
H	-4.47680100	-1.20001800	0.82361000
H	-5.85340600	0.88242900	0.60050600
H	-5.80931200	0.73214200	-1.14660600
H	-6.94696700	-1.50421100	-0.97840100
H	-7.05214200	-1.31804700	0.76156700
H	-9.17513500	-0.77168100	-0.45950700
H	-8.36700200	0.54267300	-1.28823800
H	-8.76638600	0.37357000	1.75988800
H	-8.02776600	1.73444400	0.91007500
H	-9.73091800	1.36016800	0.65729000

### Entry 19

N	2.35769800	-0.03553800	0.37597600
C	1.38525300	-0.63387600	-0.38990500
O	1.64184800	-1.50037700	-1.21042800
C	3.83528400	-0.10487100	0.05881600
C	4.28134200	-1.57805100	0.06209600
C	4.09543600	0.56046500	-1.30233600
C	4.59749700	0.63683700	1.16725400
C	-0.06637100	-0.26437800	-0.15467300
C	-0.96138500	-1.33311200	-0.05653200
C	-0.55736700	1.04263900	-0.17901200

C	-2.32143600	-1.07469500	0.05629400
C	-1.93038900	1.24989000	-0.09658300
C	-2.84093200	0.21173200	0.03304600
N	-2.44504800	2.64219500	-0.13606900
O	-1.62700700	3.54106300	-0.27153100
O	-3.65227000	2.79893000	-0.02929600
N	-3.26058800	-2.21627200	0.19462200
O	-4.45489900	-1.95952200	0.23362800
O	-2.77687300	-3.33660700	0.26420900
O	1.94750000	1.12702400	1.06180800
H	3.81452000	-2.14609400	-0.73823000
H	4.03631300	-2.05169800	1.01643100
H	5.36651600	-1.61503100	-0.06517800
H	3.57070400	0.03383200	-2.10057700
H	3.77106600	1.60432100	-1.28969100
H	5.16500500	0.54104000	-1.52699400
H	4.35888200	1.69969000	1.19328300
H	5.66710300	0.53274700	0.97529700
H	4.39861800	0.20205000	2.15158300
H	-0.60553300	-2.35393500	-0.07631000
H	0.09916700	1.89441500	-0.26655800
H	-3.90257800	0.39517600	0.10867800
H	1.96780600	0.89123100	1.99866200

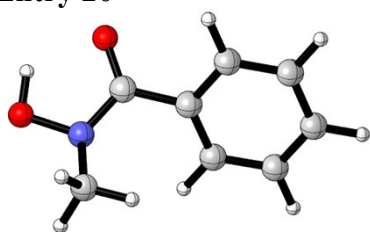
### 19-radical

N	-2.36810000	-0.14834800	0.27324400
O	-2.00540800	-1.08074700	1.06050300
C	-1.37258200	0.70051200	-0.27814900
O	-1.67211500	1.72831900	-0.85093000
C	-3.86071000	0.08816000	0.03285700
C	-4.61027200	-1.08372100	0.67328400
C	-4.26595300	1.40862300	0.71104900
C	-4.12679200	0.11595500	-1.48146800
C	0.06606400	0.29352800	-0.11260300
C	0.99141000	1.33874100	-0.04116300
C	0.51858400	-1.02919700	-0.13558700
C	2.34529100	1.04356500	0.04187700
C	1.88525700	-1.27205700	-0.07775100
C	2.82636100	-0.25746500	0.02407700
N	2.36219700	-2.67850700	-0.12160200
O	1.52255600	-3.55147200	-0.28411700
O	3.56255000	-2.86723700	0.00523900
N	3.31946200	2.16008500	0.14463700
O	4.50503200	1.86736100	0.18496600
O	2.86924200	3.29535700	0.18352400
H	-4.44596200	-1.13085300	1.74962100



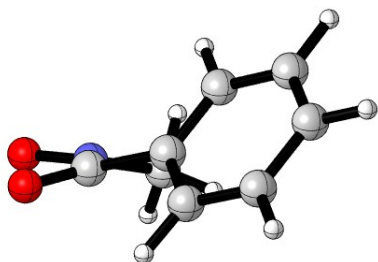
H	-4.30985900	-2.03996200	0.24196900
H	-5.67744700	-0.94172900	0.48962700
H	-4.02329600	1.38397800	1.77640200
H	-3.77437100	2.26520300	0.25309900
H	-5.34716700	1.53711200	0.61595600
H	-3.63549000	0.95567300	-1.96928700
H	-5.20327600	0.20658300	-1.64514400
H	-3.79542200	-0.81411100	-1.95088900
H	0.65993400	2.36787100	-0.05157000
H	-0.16111000	-1.86460800	-0.19912300
H	3.88375100	-0.47029200	0.08335700

### Entry 20



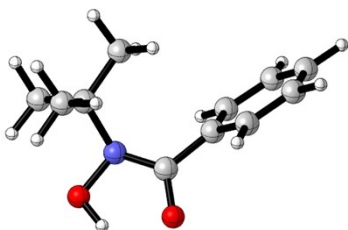
N	-2.1472141	-0.1897924	-0.1408259
O	-3.4774132	0.2461636	-0.2479829
C	-1.2305471	0.8087676	-0.3218759
O	-1.6271531	1.9414476	-0.6087829
C	0.2211309	0.4715826	-0.2275329
C	0.7620088	-0.6891154	-0.7921819
C	1.0707659	1.4040096	0.3784171
C	2.1339438	-0.9227604	-0.7309599
C	2.4384418	1.1598246	0.4512421
C	2.9725418	-0.0040704	-0.1018549
C	-2.0641372	-1.3382154	0.7442601
H	-3.3545542	1.1944266	-0.4710169
H	0.1165498	-1.3932144	-1.3043559
H	0.6482849	2.3166856	0.7806281
H	2.5481588	-1.8167994	-1.1829109
H	3.0893589	1.8814416	0.9314591
H	4.0396909	-0.1887654	-0.0529079
H	-2.5905712	-2.1820464	0.2945211
H	-1.0207692	-1.6005964	0.8965701
H	-2.5285172	-1.0989734	1.7060911

### 20-radical



N	-2.3948801	0.0295267	0.2315143
O	-3.5876181	-0.3632743	0.4141433
C	-1.4559901	-0.8852473	-0.3730197
O	-1.8630841	-1.8722173	-0.9347797
C	-0.0017541	-0.5619453	-0.2460377
C	0.8271659	-0.8369253	-1.3404307
C	0.5646969	-0.1080983	0.9509623
C	2.1986479	-0.6248133	-1.2495077
C	1.9409459	0.0815377	1.0457383
C	2.7577389	-0.1661323	-0.0564977
C	-2.1229161	1.4567577	0.4800773
H	0.3848569	-1.2205813	-2.2518507
H	-0.0613381	0.0701627	1.8176163
H	2.8331019	-0.8263203	-2.1048847
H	2.3752539	0.4164817	1.9806263
H	3.8281429	-0.0109053	0.0167503
H	-1.1698371	1.7481967	0.0464793
H	-2.1203471	1.6516947	1.5548123
H	-2.9327871	2.0221027	0.0182893

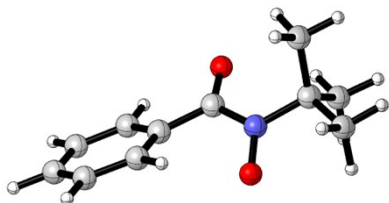
### Entry 21



N	0.4422991	-1.3499012	-0.6291461
O	0.8971931	-2.6637432	-0.8885491
C	1.4489371	-0.5911562	-0.0764731
O	2.5534091	-1.1117942	0.1132719
C	1.2638531	0.8714498	0.1671349
C	1.5607601	1.3884538	1.4322389
C	0.9459791	1.7425238	-0.8787611
C	1.4914091	2.7597188	1.6597549
C	0.8984451	3.1162608	-0.6528741
C	1.1593201	3.6260248	0.6179389

C	-1.0277289	-1.4080332	-0.3067681
C	-1.6451649	-0.0150072	-0.1425881
C	-1.2151109	-2.2147962	0.9920239
C	-1.7156189	-2.1142262	-1.4887371
H	1.8193451	-2.6180182	-0.5509111
H	1.8486601	0.7133418	2.2295099
H	0.7540551	1.3448938	-1.8683271
H	1.7083801	3.1537358	2.6460949
H	0.6626641	3.7882318	-1.4703041
H	1.1166801	4.6950108	0.7933669
H	-1.2433509	0.5304728	0.7103559
H	-1.5197039	0.5951638	-1.0373231
H	-2.7165559	-0.1513932	0.0233549
H	-0.7535969	-1.7005222	1.8395579
H	-2.2809159	-2.3298072	1.2053569
H	-0.7718889	-3.2064902	0.9012599
H	-2.7895609	-2.1761512	-1.2963981
H	-1.5628469	-1.5519592	-2.4131211
H	-1.3293459	-3.1222842	-1.6309391

### 21-radical



N	0.8134438	0.0558003	-0.1892661
O	1.3208997	-1.0243847	0.2561089
C	-0.6071433	0.1520333	-0.3291491
O	-1.0803843	1.0340353	-1.0213241
C	-1.4629533	-0.8471757	0.3803409
C	-1.1262173	-1.4667727	1.5917769
C	-2.7271602	-1.0801007	-0.1795981
C	-2.0410132	-2.3046367	2.2228699
C	-3.6277132	-1.9370188	0.4421669
C	-3.2869792	-2.5497607	1.6477039
C	1.7484547	1.1565843	-0.6854771
C	1.7114027	1.1845213	-2.2238671
C	1.3206277	2.5043982	-0.0807041
C	3.1593238	0.8025952	-0.2031931
H	-0.1579623	-1.2973038	2.0397299
H	-2.9890533	-0.5786287	-1.1028871
H	-1.7761153	-2.7721058	3.1643229
H	-4.5961583	-2.1212387	-0.0085461
H	-3.9903672	-3.2133608	2.1382519

H	0.7251188	1.4591323	-2.5940651
H	1.9863648	0.2079823	-2.6306511
H	2.4379427	1.9172933	-2.5856761
H	0.3433047	2.8225523	-0.4374951
H	1.2995978	2.4491273	1.0111629
H	2.0548908	3.2636302	-0.3620061
H	3.2063608	0.7340163	0.8852659
H	3.8382488	1.5938373	-0.5293601
H	3.5032388	-0.1450507	-0.6164361

## Entry 22

N	-1.32302100	-0.23135600	-0.68616700
C	-2.04492100	0.63601100	0.33208500
C	-3.10064000	1.42731000	-0.45457900
C	-2.71803200	-0.20381300	1.43363400
C	-1.05300100	1.61898300	0.96800500
C	-0.24473700	-1.05355400	-0.18663700
O	-0.46197500	-2.19461800	0.20806100
C	2.11834800	-1.27717200	0.31183500
C	1.38497500	0.57069500	-1.16094900
C	3.15478000	-0.36271300	0.97096100
C	2.40768100	1.51899100	-0.53178200
C	3.61412600	0.74691400	0.01759700
N	0.99472900	-0.49150300	-0.21838500
O	-2.27040700	-1.12278900	-1.27932200
H	-2.62670900	2.02962000	-1.23343300
H	-3.81618300	0.75636800	-0.92891300
H	-3.64129300	2.09547100	0.22129600
H	-3.25037800	0.45823600	2.12207300
H	-3.44692000	-0.89832500	1.01283500
H	-1.98751800	-0.77691500	2.00896600
H	-1.60274500	2.27984300	1.64249500
H	-0.28236600	1.11402100	1.55250000
H	-0.56978400	2.24311600	0.21409100
H	2.58179200	-1.83803400	-0.51302800
H	1.71861200	-2.00678000	1.01281500
H	1.83237400	0.09137800	-2.04492300
H	0.48971900	1.08862100	-1.49094600
H	4.00512500	-0.97029700	1.29557500
H	2.71678500	0.08184000	1.87202200
H	2.72563800	2.24482800	-1.28675900
H	1.93148600	2.08270500	0.27727000
H	4.30370000	1.42689500	0.52640000
H	4.17076600	0.30129900	-0.81693400
H	-2.20646800	-1.93453300	-0.74247000

## 22-radical

N	-1.19833300	0.26293100	-0.43035000
O	-1.16460400	1.07873400	-1.41719300
C	-2.50645800	0.07487000	0.30694500
C	-3.17763200	1.45439500	0.37313300
C	-3.38388700	-0.91129800	-0.48367700
C	-2.23381100	-0.43160500	1.73110800
C	-0.11661600	-0.70354100	-0.31466300
O	-0.38446400	-1.87584400	-0.10555400
C	2.24695400	-1.16401000	-0.62201200
C	1.53733200	1.20225900	-0.48219500
C	3.30120200	-0.95106900	0.46769600
C	2.58976600	1.46402300	0.60358800
C	3.78139900	0.50541900	0.48876200
N	1.13684300	-0.21120300	-0.48228000
H	-2.55333900	2.17069500	0.91382200
H	-3.37093500	1.85174400	-0.62215700
H	-4.12693900	1.35761300	0.90504900
H	-2.91520700	-1.89416700	-0.53034200
H	-4.35945900	-1.00629600	0.00150900
H	-3.54176900	-0.54427100	-1.50054800
H	-3.17528200	-0.44152100	2.28571300
H	-1.82076400	-1.43843400	1.73430400
H	-1.54562500	0.23568800	2.25850700
H	2.69892100	-1.01026700	-1.61148000
H	1.83204100	-2.16849800	-0.58713600
H	1.94548900	1.44431000	-1.47166200
H	0.66561000	1.83080800	-0.33777000
H	4.13880500	-1.63338600	0.29209800
H	2.86746100	-1.21637100	1.43847300
H	2.92107100	2.50447500	0.52553100
H	2.11958000	1.34990900	1.58745300
H	4.48177600	0.66698200	1.31357300
H	4.33204400	0.71910200	-0.43666200

## Entry 23

C	-0.05634600	1.25558500	-0.00000700
C	0.86228400	0.18810400	-0.00000700
C	0.43873900	-1.15314500	0.00001200
C	-0.90460100	-1.47958600	0.00001600
C	-1.86582700	-0.46352400	-0.00000600
C	-1.40537000	0.85818500	-0.00001900
C	1.62566000	-2.10530500	0.00003800
C	2.79812900	-1.12997200	-0.00000700

N	2.27918300	0.12759500	0.00004800
O	4.00627300	-1.33787800	-0.00010500
C	1.68853700	-2.97889000	1.26901600
C	1.68853400	-2.97899500	-1.26886500
C	-3.38014200	-0.74504200	-0.00002400
C	-4.02445300	-0.12387600	-1.26162900
C	-3.69123400	-2.25342500	-0.00007000
C	-4.02447900	-0.12395100	1.26160600
C	0.31280800	2.75707500	0.00002200
C	1.11354100	3.11033700	1.27728200
C	1.11336200	3.11043300	-1.27732300
C	-0.93942500	3.66039000	0.00015600
O	3.17429500	1.18596900	-0.00013100
H	-1.19452600	-2.52244700	0.00003200
H	-2.15008800	1.63963600	-0.00003600
H	2.62119700	-3.54728700	1.28505400
H	1.63878000	-2.36877400	2.17370900
H	0.85116800	-3.68075800	1.28397800
H	0.85117300	-3.68087400	-1.28376200
H	1.63876300	-2.36895500	-2.17360800
H	2.62120100	-3.54738000	-1.28486500
H	-3.87870100	0.95796200	-1.30167300
H	-3.59394200	-0.55263500	-2.17083100
H	-5.10197900	-0.31549700	-1.27218400
H	-3.29066200	-2.75288400	0.88655700
H	-4.77405500	-2.40431700	-0.00006300
H	-3.29068200	-2.75282700	-0.88673700
H	-5.10200100	-0.31559400	1.27213700
H	-3.59397100	-0.55274800	2.17079100
H	-3.87875100	0.95788800	1.30170700
H	0.51522300	2.90253100	2.16941200
H	2.04699800	2.55720700	1.35053400
H	1.35639900	4.17773500	1.27819300
H	0.51493400	2.90265600	-2.16938700
H	1.35619300	4.17783700	-1.27820900
H	2.04681400	2.55731900	-1.35071400
H	-0.61742100	4.70477900	0.00004300
H	-1.55889400	3.51015100	-0.88786000
H	-1.55861400	3.51026000	0.88838300
H	4.02832500	0.70272600	-0.00018900

### 23-radical

C	-0.06050600	1.26868300	-0.00005100
C	0.89684300	0.22099100	-0.00002300
C	0.51207900	-1.12933000	-0.00004700
C	-0.82190000	-1.49825700	-0.00005900

C	-1.80923800	-0.51058100	-0.00002600
C	-1.39009600	0.83079800	-0.00001700
C	1.70953000	-2.05859200	-0.00004300
C	2.87345500	-1.07686600	0.00002400
N	2.32274600	0.25920500	0.00005300
O	4.05232800	-1.29812300	0.00007200
O	3.07752800	1.27177400	0.00017400
C	1.78311000	-2.93439000	1.26830700
C	1.78317900	-2.93430900	-1.26844400
C	-3.31345200	-0.83429900	0.00002500
C	-3.97174800	-0.22915000	1.26266200
C	-3.97187800	-0.22902500	-1.26248200
C	-3.58314600	-2.35035100	-0.00004000
C	0.25447700	2.78251600	-0.00003500
C	1.04154300	3.16389400	-1.27746300
C	-1.03138800	3.63860500	-0.00013600
C	1.04135700	3.16388900	1.27750600
H	-1.08204000	-2.54854700	-0.00006900
H	-2.16150800	1.58503900	0.00002200
H	0.95282600	-3.64458600	1.28325100
H	1.73018300	-2.32768100	2.17518700
H	2.72086000	-3.49401700	1.28041500
H	0.95289500	-3.64450300	-1.28348000
H	2.72092900	-3.49393700	-1.28053700
H	1.73030300	-2.32754300	-2.17529000
H	-3.85712200	0.85628800	1.30225600
H	-3.52963000	-0.64582000	2.17184700
H	-5.04305800	-0.45138900	1.27302100
H	-3.85726300	0.85641800	-1.30198400
H	-3.52985700	-0.64560400	-2.17175700
H	-5.04318900	-0.45126400	-1.27275000
H	-3.17003000	-2.83870700	-0.88700100
H	-4.66133600	-2.53008300	0.00002200
H	-3.16991200	-2.83880600	0.88681100
H	0.45683900	2.92509800	-2.17101900
H	2.00145600	2.65588900	-1.33697200
H	1.23308400	4.24140000	-1.28084900
H	-1.64504000	3.46912800	-0.88905800
H	-1.64554300	3.46855600	0.88833100
H	-0.74592800	4.69330200	0.00027800
H	0.45656400	2.92500100	2.17097800
H	1.23281500	4.24141100	1.28097000
H	2.00130600	2.65595800	1.33710600

**Entry 24**

N	-0.36513000	-0.02376400	-0.04339400
C	0.78870000	-0.71380600	-0.00949000
C	-1.72143500	-0.50311900	0.01896400
O	-0.25772500	1.36710000	0.00032900
H	0.64415900	-1.80382000	-0.02110700
H	-2.29542000	-0.12721500	-0.83147200
H	-1.69582800	-1.59288200	-0.01828300
H	-2.20022200	-0.18227200	0.94836300
H	0.71381900	1.49029400	0.01930700
O	1.88095100	-0.15662600	0.01843400

#### 24-radical

N	0.42969000	-0.14294600	-0.00000300
C	-0.92007300	-0.54798400	-0.00002100
C	0.81198200	1.27302300	-0.00000900
O	1.33521400	-1.03925900	0.00014700
O	-1.84717400	0.22327000	-0.00011800
H	-0.98817200	-1.64550300	-0.00002600
H	-0.09297000	1.87678000	-0.00077600
H	1.40812000	1.47372700	0.89116000
H	1.40942000	1.47329400	-0.89039500

#### Entry 25

N	-0.17992600	0.67436800	-0.62429400
C	-1.34259000	0.33193800	0.07580000
N	1.79127500	-0.34360200	0.22961600
O	2.85464500	-0.80280100	-0.11237500
O	1.41472800	-0.01991700	1.33332000
N	0.80453600	-0.22002000	-0.84926200
O	-1.99992600	1.11686600	0.67646200
Cl	-1.78141900	-1.37391100	-0.10020600
O	0.21590300	2.01315700	-0.49575800
H	1.31546500	-0.07039300	-1.71568400
H	0.23021400	2.20158500	0.45877500

#### 25-radical

N	-0.13676800	0.57397900	0.34992300
C	-1.10950200	-0.49050300	0.30764900
O	-0.35805200	1.75830700	-0.01749200
N	2.06671700	-0.14557700	-0.23184000
O	3.22483000	-0.01084300	0.08272600
O	1.58958400	-0.58507600	-1.24612300
N	1.11959800	0.21523100	0.84112200
O	-0.87512600	-1.58808000	0.67986700
Cl	-2.63945000	0.04908400	-0.34608200



H	1.53094700	1.00869600	1.33125000
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### Entry 26

N	-0.85017200	-0.18952400	-0.07788200
C	0.25982700	0.56154500	-0.00067800
C	-1.08184700	-1.61411700	0.04121200
O	-2.05346400	0.53217900	-0.01082700
H	-1.78372100	-1.91850900	-0.73681700
H	-0.14081300	-2.13832900	-0.09167400
H	-1.50325300	-1.84443900	1.02335400
H	-1.75602100	1.46079700	0.00505900
O	0.25767100	1.76810900	0.04000400
Cl	1.79020400	-0.37174800	-0.00772800

### 26-radical

N	0.86275900	-0.34998200	0.00028900
C	-0.23050500	0.54354700	0.00112700
C	2.21676100	0.24022000	-0.00042700
O	0.71822100	-1.60809400	0.00013300
O	-0.08743900	1.72879200	-0.00010800
Cl	-1.80099100	-0.25526500	-0.00027400
H	2.35248400	0.85784100	0.88804500
H	2.91030400	-0.59583900	-0.00165000
H	2.35096200	0.85920700	-0.88816900

### Entry 27

N	0.90595900	-0.20929900	0.38017700
C	-0.23289800	0.59894800	0.02534600
O	-0.16666700	1.77332400	-0.08827200
Cl	-1.73674800	-0.31412500	0.00423100
F	0.76327900	-1.52358900	-0.15053200
O	2.04116800	0.31740800	-0.16764500
H	2.71486700	0.19798700	0.51688700

### 27-radical

N	-0.86250600	-0.35740000	0.00087000
C	0.23774300	0.55788700	-0.00001800
O	-0.90831400	-1.56382000	-0.00043600
O	0.10944500	1.73377800	-0.00020400
Cl	1.75739800	-0.31223600	0.00000700
F	-2.09708000	0.34475800	-0.00011000

### Entry 28

N	-0.42652900	-0.40901600	0.50921200
C	0.50286300	0.56646200	0.13736100
O	0.30620700	1.73804800	0.14984400

Cl	2.11586000	-0.12964900	-0.18874800
O	-1.73137100	0.02375100	0.61506100
C	-2.35412900	0.31165800	-0.66129100
H	-1.86259900	1.15832800	-1.14284000
H	-2.33768600	-0.57404200	-1.29812600
H	-3.37948000	0.57180200	-0.40500600
O	-0.32488500	-1.64578400	-0.13441600
H	-0.29617900	-2.28577400	0.58986000

### 28-radical

N	0.46818500	-0.20243300	-0.00004000
C	-0.72297500	0.57084900	-0.00001500
O	0.56247900	-1.43561900	-0.00004700
O	-0.74359700	1.75825500	0.00001500
Cl	-2.15541200	-0.45699200	0.00002600
O	1.60452400	0.61878500	-0.00009000
C	2.82189200	-0.14424300	0.00008600
H	2.89593800	-0.76479400	0.89430200
H	2.89610600	-0.76494400	-0.89401000
H	3.59191200	0.62463100	0.00009400

### Entry 29

N	0.41990100	-0.02703100	0.38437400
C	-0.84756100	-0.61461400	0.05548500
O	-1.85109600	0.00607100	-0.10768900
F	0.44628300	1.31351000	-0.06473800
H	-0.75303900	-1.71171400	0.08197000
O	1.43832700	-0.70379200	-0.25270700
H	2.18469600	-0.65120300	0.36031700

### 29-radical

N	0.47907200	-0.13423700	-0.00000700
C	-0.87340000	-0.60570200	-0.00006800
O	1.50746600	-0.77219000	0.00001600
O	-1.82555600	0.11225600	0.00003000
F	0.58678400	1.28405400	-0.00000100
H	-0.84944400	-1.70314000	0.00009800

### Entry 30

N	0.41632200	0.00140300	0.35229700
C	-0.79816100	-0.65530800	0.10262900
O	-1.82324100	-0.06422300	-0.12378400
O	0.41816300	1.35051900	0.03344200
O	1.47878700	-0.68397300	-0.27681700
H	-0.68683900	-1.74467300	0.18148400
H	-0.23270400	1.46615800	-0.68343600

H	2.20458000	-0.61803700	0.35737600
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### 30-radical

N	0.49066000	-0.08972200	-0.00003000
C	-0.78644700	-0.67566800	-0.00007700
O	1.56016800	-0.70102800	0.00003200
O	-1.78204800	0.01601800	0.00004000
O	0.52595900	1.29814100	-0.00000100
H	-0.72754300	-1.76823400	0.00009500
H	-0.42103100	1.54524400	0.00000900

### Entry 31

N	0.41990100	-0.02703100	0.38437400
C	-0.84756100	-0.61461400	0.05548500
O	-1.85109600	0.00607100	-0.10768900
F	0.44628300	1.31351000	-0.06473800
H	-0.75303900	-1.71171400	0.08197000
O	1.43832700	-0.70379200	-0.25270700
H	2.18469600	-0.65120300	0.36031700

### 31-radical

N	0.47907200	-0.13423700	-0.00000700
C	-0.87340000	-0.60570200	-0.00006800
O	1.50746600	-0.77219000	0.00001600
O	-1.82555600	0.11225600	0.00003000
F	0.58678400	1.28405400	-0.00000100
H	-0.84944400	-1.70314000	0.00009800

### Entry 32

N	-0.11543500	0.28705700	-0.47948500
C	-1.07391100	-0.68485600	-0.17079400
O	1.18105000	-0.17595000	-0.68148700
C	1.85527200	-0.51425500	0.55000200
O	-2.14120100	-0.46118100	0.33461500
H	-0.74308300	-1.66457300	-0.55363500
H	1.92551200	0.35819700	1.20068800
H	1.33754700	-1.33100700	1.06307700
H	2.84899700	-0.83628900	0.24254400
O	-0.16345200	1.44950100	0.28348100
H	-0.26026700	2.15998400	-0.36440400

### 32-radical

N	-0.10185700	0.41257000	-0.00005200
O	0.45839700	1.52238100	-0.00003200
C	-1.51009400	0.23526900	0.00007200
O	0.63091500	-0.77444600	-0.00026300

C	2.04850700	-0.54551600	0.00015500
O	-2.05306800	-0.83510800	0.00006000
H	-1.98683400	1.22452300	0.00012000
H	2.35792400	-0.00122400	0.89379100
H	2.46306400	-1.55151100	0.00009200
H	2.35841400	-0.00091000	-0.89311700

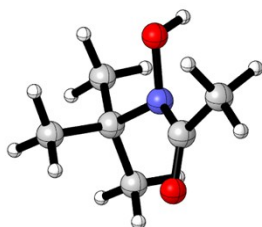
### Entry 33

N	-0.58865800	0.09083400	-0.24370100
C	-1.66975700	-0.83048700	0.05080700
C	0.74104700	-0.27605200	-0.03111200
O	1.07307100	-1.44715800	0.03919500
N	1.61661100	0.77801300	0.07770500
O	-0.91368800	1.44619700	-0.03345800
H	-1.33389700	-1.83200200	-0.20862900
H	-1.94418100	-0.81444200	1.11554100
H	-2.53661800	-0.56050500	-0.55239100
H	1.33556300	1.68162900	-0.27005700
H	2.58746600	0.52337500	-0.01323300
H	-1.00681200	1.56694700	0.92667400

### 33-radical

N	0.61287700	-0.23252400	0.00010400
O	0.80238600	-1.49391700	0.00015600
C	1.76640400	0.66843200	-0.00015700
C	-0.72880500	0.29600200	0.00005200
O	-0.92543700	1.49446000	0.00016000
N	-1.66472000	-0.67765600	-0.00039400
H	1.40875200	1.69440000	0.00068900
H	2.36602300	0.46944000	0.88983600
H	2.36485700	0.47058300	-0.89120600
H	-1.38488400	-1.64597800	0.00031700
H	-2.63304200	-0.40813100	0.00049000

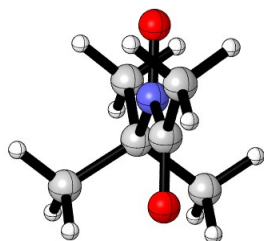
### Entry 34



N	0.5344384	0.3464742	-0.2678605
C	1.6648244	-0.4410658	-0.0727615
O	1.5908664	-1.6539238	0.0242635
C	2.9923654	0.2896982	-0.0385965

C	-1.0200396	-0.4859048	1.4940235
C	-0.8655226	-0.1356998	0.0047895
C	-1.8372486	0.9922882	-0.3792215
C	-1.1614046	-1.3508288	-0.8925515
O	0.7457864	1.7010072	0.1052405
H	3.1028914	0.9759072	-0.8804675
H	3.0780664	0.8813792	0.8755385
H	3.7799394	-0.4613998	-0.0649735
H	-0.3525276	-1.3036648	1.7694065
H	-0.7943146	0.3829192	2.1178965
H	-2.0475626	-0.7965728	1.7030225
H	-1.7012356	1.2930342	-1.4229285
H	-2.8603536	0.6252332	-0.2731155
H	-1.7238476	1.8676442	0.2604715
H	-0.5466336	-2.2072558	-0.6295575
H	-2.2155646	-1.6199758	-0.7811715
H	-0.9833736	-1.1034278	-1.9425455
H	0.6204514	2.2041352	-0.7089015

### 34-radical



N	0.5643089	0.5244160	0.0000361
O	0.7419569	1.7867910	0.0000331
C	1.7231719	-0.3100560	0.0000791
O	1.6164319	-1.5184840	0.0000121
C	3.0357389	0.4296630	-0.0000179
C	-1.0596301	-0.8740240	-1.2729399
C	-0.8535591	-0.0342290	0.0000071
C	-1.0596581	-0.8740690	1.2729201
C	-1.8160731	1.1567030	0.0000161
H	3.8356169	-0.3083840	-0.0000829
H	3.1154829	1.0764570	-0.8760519
H	3.1156089	1.0764370	0.8760211
H	-0.8779261	-0.2697170	-2.1656959
H	-0.4050281	-1.7436230	-1.2939219
H	-2.0963441	-1.2194700	-1.3068989
H	-0.8779831	-0.2697890	2.1657011
H	-2.0963701	-1.2195240	1.3068401
H	-0.4050491	-1.7436630	1.2938901

H	-1.6818171	1.7833800	-0.8823109
H	-2.8370331	0.7678410	-0.0000089
H	-1.6818461	1.7833440	0.8823721

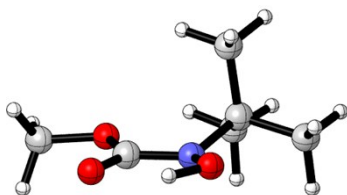
### Entry 35

N	-0.27294900	0.42105500	-0.29271400
C	-1.49708400	-0.13336500	-0.07550600
O	-2.51020400	0.54202100	0.05381900
C	1.26820900	-1.49507600	-0.67299300
C	1.08289700	-0.13725800	0.02367800
C	2.12252600	0.84292100	-0.54798400
C	1.24127900	-0.26280200	1.54811900
O	-1.51602600	-1.48591800	-0.05764600
O	-0.31232200	1.82527900	-0.09959000
H	0.63593900	-2.27228300	-0.25115100
H	1.05521600	-1.41355100	-1.74134400
H	2.31130900	-1.79844500	-0.55589700
H	2.07157700	1.81651900	-0.06376800
H	3.11901500	0.42504400	-0.38804500
H	1.97437300	0.98300800	-1.62099100
H	0.53245500	-0.98710700	1.95719400
H	2.25098700	-0.60121000	1.79528300
H	1.07631800	0.70312400	2.03029200
H	-2.44651700	-1.72903900	0.04467100
H	-1.26857400	1.98897500	0.01820500

### 35-radical

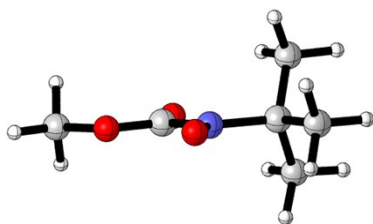
N	-0.28520800	0.53781000	0.00003200
C	-1.45990300	-0.25155500	-0.00016000
O	-1.45921900	-1.46078200	-0.00023900
C	1.25660100	-0.95515000	1.27348900
C	1.09757600	-0.10713700	0.00009300
C	1.25653400	-0.95547900	-1.27309000
C	2.12237200	1.03077300	-0.00007700
O	-0.39776000	1.80543600	0.00006800
O	-2.56421200	0.50950900	-0.00014300
H	1.10748200	-0.34079800	2.16527200
H	0.55613300	-1.78852500	1.29557400
H	2.27250400	-1.35714100	1.30799500
H	1.10739300	-0.34135300	-2.16502600
H	2.27242500	-1.35750500	-1.30753200
H	0.55604400	-1.78884400	-1.29493400
H	2.02234200	1.66370900	0.88223000
H	3.12050400	0.58683400	-0.00003800
H	2.02230700	1.66347900	-0.88254500
H	-3.31023700	-0.10654300	-0.00024200

### Entry 36



N	0.0160743	0.9153355	-0.3734451
C	1.3629273	0.7982365	-0.1490651
O	2.0825703	1.7792085	-0.0135321
C	-0.8317637	-1.3838975	-0.7907031
C	-1.0641847	-0.0668465	-0.0315421
C	-1.0991987	-0.2932745	1.4893249
C	-2.3968607	0.5331655	-0.5147691
O	1.8124233	-0.4688255	-0.1401791
C	3.2424653	-0.6112715	-0.0320211
O	-0.4116667	2.2503175	-0.1408741
H	-1.7058417	-2.0234725	-0.6452761
H	-0.7215687	-1.1954365	-1.8611731
H	0.0477683	-1.9173735	-0.4393871
H	-1.2315107	0.6561305	2.0128739
H	-1.9326637	-0.9491615	1.7545749
H	-0.1756867	-0.7627585	1.8367859
H	-2.3551377	0.7608625	-1.5821511
H	-3.1890917	-0.2004445	-0.3483711
H	-2.6495457	1.4463135	0.0212409
H	3.6033623	-0.1634675	0.8939979
H	3.4209573	-1.6844055	-0.0352371
H	3.7374173	-0.1377925	-0.8804391
H	0.4387543	2.7188585	-0.0306331

### 36-radical



N	-0.1802109	0.7416611	0.0005888
C	-1.3975289	0.0051011	0.0007128
O	-1.4416189	-1.2042739	-0.0001022
C	1.2879361	-0.8260849	1.2728248
C	1.1681421	0.0298321	0.0001628

C	1.2879541	-0.8246509	-1.2734642
C	2.2488081	1.1153481	0.0007708
O	-0.2266359	2.0132431	0.0008998
O	-2.4514129	0.8194971	0.0002588
C	-3.7322929	0.1613211	-0.0005462
H	1.1691271	-0.2056319	2.1650358
H	0.5474691	-1.6239849	1.2944188
H	2.2834411	-1.2764989	1.3065818
H	1.1690991	-0.2032009	-2.1649762
H	2.2834841	-1.2749699	-1.3077472
H	0.5475331	-1.6225649	-1.2959442
H	2.1802221	1.7521801	0.8833158
H	3.2239061	0.6225661	0.0004658
H	2.1801871	1.7531981	-0.8810362
H	-3.8426999	-0.4593319	0.8894878
H	-4.4631599	0.9662921	-0.0008112
H	-3.8417499	-0.4590479	-0.8908962

### Entry 37

N	-0.06685200	0.34304200	-0.27324200
C	-1.35313400	-0.10450900	-0.08019500
O	-2.24584300	0.71770600	0.10172200
C	2.08770600	-0.22039900	-1.03067400
C	-1.58358500	-1.59261600	-0.15709100
O	0.11030700	1.74097100	-0.01943900
N	1.03755900	-0.43346400	-0.02911000
C	1.52444700	-0.34968300	1.35642100
H	2.85319500	-0.98711000	-0.89600500
H	1.65361500	-0.32490600	-2.02482700
H	2.55444100	0.76922500	-0.94517200
H	-0.93179600	-2.07225600	-0.88541700
H	-1.38537600	-2.04641700	0.81831700
H	-2.63066800	-1.75655400	-0.40845900
H	-0.81474200	2.01983100	0.13968100
H	1.95039500	0.63268500	1.59122900
H	0.69975400	-0.55084400	2.04194400
H	2.28790800	-1.11687600	1.49614300

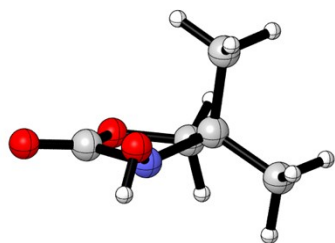
### 37-radical

N	0.08053400	-0.48110600	-0.00001200
C	1.42806900	0.04663400	-0.00001600
O	2.35534600	-0.71877700	0.00003000
C	-1.81166200	0.25924100	-1.22183400
C	1.54486600	1.55023400	-0.00004900
O	-0.13167100	-1.72380200	0.00000900
N	-1.01377200	0.43691200	-0.00001000



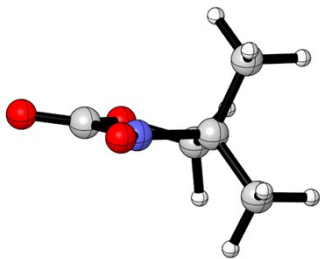
C	-1.81159500	0.25931500	1.22187000
H	-2.59091500	1.02292400	-1.22802500
H	-1.17399700	0.40721500	-2.09490300
H	-2.27511100	-0.73354700	-1.27980400
H	1.05990600	1.98331400	0.87663300
H	2.60536100	1.79735400	-0.00014900
H	1.05971800	1.98331300	-0.87662300
H	-1.17388100	0.40733800	2.09489500
H	-2.59084500	1.02300000	1.22806100
H	-2.27504300	-0.73347000	1.27992400

### Entry 38



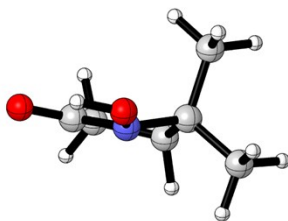
O	1.6633912	-1.3236671	0.5062461
C	0.2937032	-1.5307841	0.0945981
C	-0.3077438	-0.1174231	-0.0423249
C	-0.8480738	0.4070159	1.2972541
C	-1.3561218	-0.0241181	-1.1475909
N	0.9439062	0.5662399	-0.4296609
C	2.0367392	-0.0512081	0.1970391
O	3.1223812	0.4085779	0.3958191
O	0.9155822	1.9660699	-0.3239079
H	0.2979372	-2.0600731	-0.8618649
H	-0.1992718	-2.1373641	0.8532101
H	-1.0942848	1.4668569	1.2209261
H	-1.7535148	-0.1395961	1.5736391
H	-0.1135978	0.2838359	2.0972661
H	-2.2266108	-0.6392011	-0.9029199
H	-1.6974958	1.0074999	-1.2601089
H	-0.9469428	-0.3611261	-2.1024499
H	1.2700182	2.2784639	-1.1651689

### 38-radical



O	-1.7718674	-1.2149422	-0.2844696
C	-0.3858094	-1.3784882	0.1041004
C	0.2496666	0.0249468	0.0480294
C	0.9357926	0.3079648	-1.2956746
C	1.1680686	0.3197378	1.2311484
N	-0.9923544	0.8401768	0.1375544
C	-2.1617344	0.0745138	-0.1544606
O	-3.2718184	0.4860728	-0.2793336
O	-1.0020014	2.0942438	0.2799864
H	-0.3687694	-1.7941672	1.1141444
H	0.0681816	-2.0831182	-0.5909496
H	1.1988406	1.3653108	-1.3640946
H	1.8496386	-0.2853462	-1.3822276
H	0.2809326	0.0594638	-2.1346056
H	2.0448426	-0.3320172	1.1956624
H	1.5062736	1.3565838	1.1949044
H	0.6521176	0.1590638	2.1802854

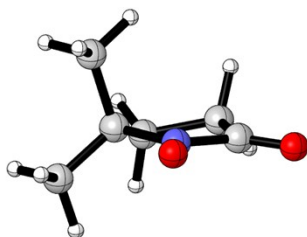
### Entry 39



C	-1.8209677	-0.2083145	-0.2880720
N	-0.6231157	-0.8334685	-0.4307040
O	-2.8886037	-0.8070155	-0.2677799
C	0.5571164	-0.0616325	-0.0136099
C	0.0068793	1.3697525	-0.2830600
C	-1.5259417	1.2706865	-0.1233539
C	0.8650034	-0.2988335	1.4743791
C	1.7650424	-0.4086675	-0.8855479
O	-0.5972387	-2.2227396	-0.2964590
H	0.4586393	2.0942285	0.3958351
H	0.2586843	1.6650355	-1.3036860
H	-1.8696897	1.5693565	0.8712791
H	-2.0835317	1.8635455	-0.8497900

H	1.0712144	-1.3547345	1.6592270
H	1.7420274	0.2810065	1.7734710
H	0.0247003	-0.0004385	2.1072771
H	2.6049933	0.2473835	-0.6411860
H	2.0799033	-1.4414425	-0.7198520
H	1.5244803	-0.2876485	-1.9440579
H	-1.5495957	-2.4360585	-0.2343099

### 39-radical



C	1.9797449	-0.3085751	-0.0043882
N	0.7649909	-1.0309751	-0.2140882
O	3.0720699	-0.8111221	-0.0210072
O	0.7175399	-2.2804821	-0.3762672
C	-0.4691471	-0.1864711	-0.0902562
C	0.1234089	1.2379959	-0.2174492
C	1.5840879	1.1308379	0.2546408
C	-1.4441221	-0.5406601	-1.2114042
C	-1.0930871	-0.4436821	1.2901468
H	0.0962139	1.5498449	-1.2644932
H	-0.4560331	1.9612319	0.3580608
H	2.2673209	1.8068659	-0.2599712
H	1.6896789	1.3200489	1.3280718
H	-1.7723231	-1.5776211	-1.1229152
H	-2.3212101	0.1093109	-1.1553072
H	-0.9784711	-0.4096361	-2.1909982
H	-2.0139781	0.1351949	1.3971228
H	-1.3333201	-1.5029561	1.4027048
H	-0.4133651	-0.1591511	2.0977978

### Entry 40

C	-1.25878300	0.21790500	-0.12945700
C	-0.75452400	1.56451400	0.05520600
C	0.58681800	1.47199600	0.24002900
N	-0.05931200	-0.59709300	-0.22989700
N	1.02845700	0.17280300	0.21861300
O	-2.37097100	-0.25439900	-0.20463500
O	-0.11238500	-1.83140200	0.44341600

C	2.33738900	-0.20339500	-0.30377100
H	-1.36791400	2.44724300	0.12236800
H	1.31235900	2.26127600	0.37892500
H	-0.34192300	-2.46124600	-0.25132700
H	3.08401500	0.44709700	0.15353600
H	2.54801600	-1.23147200	-0.01184600
H	2.38286800	-0.11256900	-1.39496200

#### 40-radical

C	-1.33008900	0.08249600	-0.00006700
C	-0.92629000	1.46503900	-0.00007900
C	0.43479400	1.52683400	0.00018600
N	-0.03587400	-0.64952400	0.00007900
N	0.99606100	0.28094100	0.00011000
O	-2.38610400	-0.50556300	-0.00033500
O	0.16475600	-1.87552000	0.00005800
C	2.38658600	-0.12750800	0.00007500
H	-1.61203700	2.29448600	-0.00025900
H	1.07981000	2.39290700	0.00024600
H	2.89477500	0.23842700	0.89501100
H	2.40214300	-1.21668400	0.00006700
H	2.89477900	0.23843400	-0.89485900

#### Entry 41

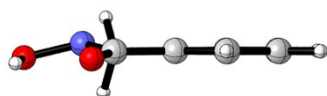
C	-1.25137400	0.10654100	0.09464300
N	1.03024900	0.14458400	-0.36077700
O	-2.35140000	-0.37723000	0.16463100
C	2.30990700	-0.28389600	0.19116100
H	3.09112600	0.33858500	-0.24961100
H	2.34539600	-0.19227800	1.28822600
H	2.49746000	-1.31878900	-0.09485000
C	-0.85176600	1.55086500	-0.13884000
H	-1.36491200	2.22842500	0.54262900
H	-1.15250800	1.79940200	-1.16109100
C	0.66859400	1.52130300	0.02051500
H	1.19773200	2.22440800	-0.62285400
H	0.94401800	1.72235400	1.06797400
N	-0.05022400	-0.62326800	0.22576300
O	-0.09058300	-1.91344500	-0.32402000
H	-0.13479300	-2.49479100	0.44491400

#### 41-radical

C	-1.28603100	-0.02164600	0.01668100
N	-0.02743100	-0.69073700	-0.05884800
N	1.01934100	0.22918500	-0.33938200
O	-2.33644300	-0.59349100	0.14789100

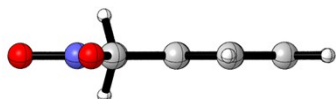
O	0.16181800	-1.92242600	-0.04952200
C	2.32288800	-0.21196400	0.13320600
H	3.06694000	0.49207700	-0.24107600
H	2.37417200	-0.25021000	1.23126900
H	2.53135700	-1.20152200	-0.26837900
C	-0.97991500	1.45489800	-0.11181100
H	-1.57102300	2.03509700	0.59565600
H	-1.24389800	1.77607700	-1.12427500
C	0.53091100	1.53154600	0.13276500
H	1.02503400	2.32919700	-0.42216500
H	0.74393300	1.66048600	1.20459500

### Entry 42



C	-1.0304143	1.5972776	-0.0128013
C	0.0337747	0.7046026	0.0378917
C	-0.1674633	-0.6793104	0.0318627
C	-1.4522353	-1.2030564	-0.0030903
C	-2.5276593	-0.3117594	-0.0528033
C	-2.3209543	1.0718996	-0.0592003
C	1.4925197	0.9701126	0.0724807
O	2.1417747	1.9966986	-0.0687903
N	2.0616937	-0.2611384	0.2835997
C	1.1699167	-1.3866474	0.0692207
O	3.4184417	-0.4250684	0.0116527
H	-0.8510123	2.6658646	-0.0145273
H	-1.6252733	-2.2737084	-0.0003963
H	-3.5395163	-0.6993024	-0.0891863
H	-3.1741823	1.7391506	-0.0988583
H	1.2494017	-2.1185474	0.8782537
H	1.4048087	-1.8847394	-0.8793183
H	3.7163787	0.4976726	-0.1059903

### 42-radical



C	-0.8313224	1.6114577	-0.0000681
C	0.2503066	0.7333827	-0.0000051
C	0.0686226	-0.6523433	-0.0000041
C	-1.2114064	-1.1918643	-0.0000801
C	-2.2995644	-0.3168443	-0.0001491
C	-2.1136334	1.0711237	-0.0001411
C	1.6887416	1.0643967	0.0000429

O	2.2594666	2.1240047	0.0001399
N	2.3516276	-0.2169573	0.0001649
O	3.5999626	-0.3739673	0.0002859
C	1.4022296	-1.3499193	0.0001039
H	-0.6638854	2.6819997	-0.0000691
H	-1.3693694	-2.2646863	-0.0000801
H	-3.3063054	-0.7189703	-0.0002081
H	-2.9769144	1.7262157	-0.0001961
H	1.5757956	-1.9635323	-0.8883931
H	1.5756486	-1.9634963	0.8886569

### Entry 43

C	0.26249100	0.46032900	0.00000500
C	0.53103500	-0.91888700	0.00000800
C	1.84498800	-1.34967500	-0.00000100
C	2.87500500	-0.39699200	0.00000500
C	2.58063200	0.96498400	0.00000100
C	1.25777200	1.42320600	-0.00000700
C	-1.83075700	-0.55628800	0.00008000
N	-1.12358300	0.61319200	-0.00001500
O	-1.75174000	1.84236000	-0.00001100
O	-3.05027500	-0.59987600	-0.00002300
C	-0.78291200	-1.66927800	-0.00001900
H	2.07946200	-2.40863700	-0.00000900
H	3.90775400	-0.72423800	0.00000500
H	3.38852800	1.68753200	0.00000000
H	1.01801100	2.47830800	-0.00001400
H	-2.69532400	1.59172200	0.00007900
H	-0.92339000	-2.30059800	-0.88177500
H	-0.92337400	-2.30069500	0.88166800

### 43-radical

C	-0.24300800	0.47784900	-0.00005600
C	-0.44619900	-0.90579700	-0.00008800
C	-1.74203200	-1.39841200	-0.00005100
C	-2.80850900	-0.49194900	-0.00003100
C	-2.57926400	0.88821600	0.00000300
C	-1.28284400	1.39926000	0.00001500
C	1.90507100	-0.47479600	-0.00045400
N	1.14120500	0.75860200	-0.00000400
O	1.65283200	1.91078800	0.00024300
O	3.10131100	-0.51641400	0.00023600
C	0.88651600	-1.60958200	-0.00002100
H	-1.92999800	-2.46633300	-0.00003600
H	-3.82620000	-0.86419100	-0.00001400
H	-3.42146000	1.57022800	0.00004500

H	-1.07673000	2.46183100	0.00006600
H	1.04726500	-2.23754100	0.88115100
H	1.04714700	-2.23794500	-0.88092200

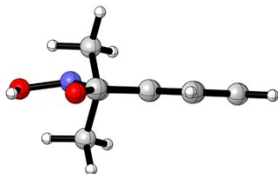
#### Entry 44

C	-1.40238100	0.28273700	-0.08980900
N	-0.31519800	-0.52430200	-0.31231400
O	-2.54721500	-0.13721100	0.01103700
C	0.96529700	0.12165600	0.00707300
C	1.51301700	-0.36919100	1.36027200
C	1.98376800	-0.09438300	-1.12240700
C	-0.83804100	1.65095400	0.02736100
C	0.49396500	1.56192800	0.09106900
O	-0.46141100	-1.89550100	-0.08770400
H	1.73841300	-1.43569300	1.30537900
H	2.42933000	0.17022700	1.61084300
H	0.78470200	-0.20861000	2.15736600
H	2.90921200	0.44721100	-0.90997400
H	2.22123900	-1.15656400	-1.21379700
H	1.58155000	0.25425800	-2.07530000
H	-1.45482100	2.53655400	0.07299800
H	1.19864700	2.37985300	0.17176200
H	-1.42662300	-1.97762200	0.03891000

#### 44-radical

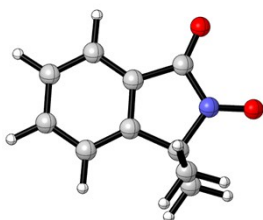
C	1.48799400	0.12850100	0.00051600
N	0.28905400	-0.66726400	-0.00003600
O	2.60651800	-0.31782200	-0.00012800
O	0.26231900	-1.92547400	-0.00035700
C	-0.94645000	0.17316600	0.00006500
C	-1.76150700	-0.11185700	-1.27002000
C	-1.76126800	-0.11176900	1.27031700
C	1.00011300	1.52285100	-0.00017700
C	-0.33620700	1.55320500	-0.00005500
H	-2.06832000	-1.15953400	-1.28078000
H	-2.65629500	0.51488700	-1.29116300
H	-1.17303900	0.08922200	-2.16743400
H	-2.65606300	0.51495900	1.29156500
H	-2.06805200	-1.15945200	1.28121400
H	-1.17264100	0.08939400	2.16760700
H	1.68080000	2.36187700	-0.00050000
H	-0.95651000	2.44128100	-0.00024900

#### Entry 45



C	1.9243490	1.7917832	-0.0497230
C	0.6660880	1.2027462	-0.0835500
C	0.4991220	-0.1844888	-0.0324910
C	1.6070980	-1.0179818	0.0381060
C	2.8772730	-0.4345978	0.0710310
C	3.0362780	0.9540462	0.0291070
C	-0.6711250	1.8383972	-0.1530670
O	-1.0285190	3.0085182	-0.0824300
N	-1.5348480	0.7923402	-0.3050370
C	-0.9821420	-0.5481158	-0.0527940
C	-1.4576040	-1.0864398	1.3093030
C	-1.3531140	-1.5051248	-1.1949220
H	2.0259320	2.8700442	-0.0850450
H	1.5025540	-2.0967818	0.0740940
H	3.7536770	-1.0699998	0.1324190
H	4.0327830	1.3794622	0.0571310
H	-2.5422550	-1.2092078	1.3069830
H	-0.9965460	-2.0563158	1.5085790
H	-1.1858990	-0.4014408	2.1148750
H	-0.8932370	-2.4834758	-1.0365690
H	-2.4363650	-1.6390858	-1.2356730
H	-1.0139690	-1.1094958	-2.1538130
O	-2.8975080	1.0162902	-0.1322600
H	-2.9320220	1.9889252	-0.0442530

#### 45-radical

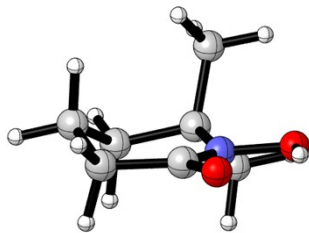


C	-1.4170211	2.1322777	-0.4461753
C	-0.2841881	1.3459007	-0.2456973
C	-0.3739121	-0.0291043	-0.0168803
C	-1.6178111	-0.6486223	0.0155737
C	-2.7578761	0.1325017	-0.1843813
C	-2.6612311	1.5105027	-0.4133663
C	1.1250389	1.7781307	-0.2363343
O	1.6223889	2.8645207	-0.3927003



N	1.8667759	0.5710957	0.0120907
O	3.1203689	0.5172357	0.0942977
C	0.9985709	-0.6456633	0.1685417
C	1.3574659	-1.6581823	-0.9280993
C	1.2111209	-1.2324483	1.5710817
H	-1.3161141	3.1968937	-0.6214903
H	-1.7122891	-1.7143763	0.1914587
H	-3.7353211	-0.3361813	-0.1619853
H	-3.5625651	2.0926887	-0.5654243
H	2.4030539	-1.9556773	-0.8278583
H	0.7303389	-2.5478573	-0.8362733
H	1.2080799	-1.2297443	-1.9211963
H	0.5813989	-2.1145423	1.7074637
H	2.2553899	-1.5260733	1.6939237
H	0.9583369	-0.5032743	2.3434307

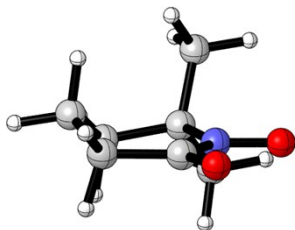
#### Entry 46



C	-2.0916092	0.6916095	-0.3491544
C	-1.7005792	-0.7674365	-0.2454274
C	0.7848958	-0.1723015	0.0140366
C	0.3532528	1.2618615	-0.3587664
C	-1.0218992	1.6438015	0.1927106
N	-0.3746512	-1.0533535	-0.2307944
O	-2.5207942	-1.6905285	-0.2201354
C	1.9414498	-0.6173415	-0.8959454
C	1.2065938	-0.2776365	1.4924116
O	-0.0815552	-2.4167475	-0.0678524
H	-2.2873522	0.8965905	-1.4083154
H	-3.0451502	0.7995295	0.1708996
H	1.1234218	1.9477455	0.0044336
H	0.3377038	1.3503575	-1.4508214
H	-1.0161302	1.6108225	1.2866816
H	-1.2632002	2.6737955	-0.0838424
H	2.7843388	0.0685185	-0.7772324
H	2.2755268	-1.6239165	-0.6432014
H	1.6320718	-0.6101445	-1.9436204
H	1.4255038	-1.3148815	1.7489956
H	2.1052908	0.3192325	1.6683446
H	0.4197418	0.0779705	2.1610856

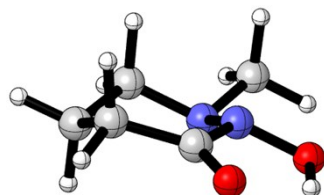
H -0.9868702 -2.7975475 -0.0644904

#### 46-radical



C	-2.1217260	0.6043200	-0.3395563
C	-1.8320190	-0.8711240	-0.1416833
C	0.7381800	-0.3158460	0.0255507
C	0.3186070	1.0884550	-0.4450483
C	-1.0163150	1.5443390	0.1379687
N	-0.4478500	-1.2588090	-0.0217593
O	-0.1955400	-2.4896980	0.1539827
O	-2.6938390	-1.7124030	-0.1059793
C	1.8184590	-0.8807100	-0.9069883
C	1.2448360	-0.3029320	1.4785497
H	-2.2891200	0.7423190	-1.4153973
H	-3.0793680	0.7985760	0.1474587
H	1.1218840	1.7819580	-0.1807613
H	0.2485600	1.0938370	-1.5391003
H	-0.9768770	1.5578630	1.2316597
H	-1.2389640	2.5675150	-0.1764673
H	2.6812260	-0.2095480	-0.9084803
H	2.1415320	-1.8676160	-0.5774323
H	1.4448990	-0.9628590	-1.9307243
H	1.4656410	-1.3204880	1.8042467
H	2.1599880	0.2907090	1.5464207
H	0.5078050	0.1221430	2.1635407

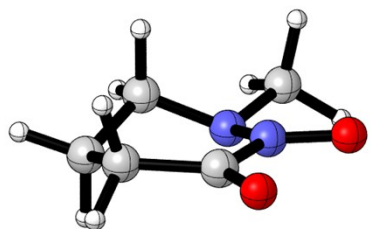
#### Entry 47



C	-0.6806333	1.6029602	-0.4192104
C	0.6846117	1.0997882	0.0278986
C	-1.4944093	-0.7210628	0.0695516
C	-1.7771563	0.7538472	0.2316766
N	-0.1731563	-1.1119358	0.1423646
O	-2.3603303	-1.5802448	-0.0728464
N	0.8980657	-0.2934108	-0.3872334

H	-0.7972843	2.6541852	-0.1444014
H	-0.7509363	1.5374962	-1.5088854
H	1.4864007	1.6765532	-0.4369724
H	0.7850767	1.2042392	1.1223536
H	-2.7619323	0.9372162	-0.1994384
H	-1.8471603	0.9710102	1.3031506
C	2.1706407	-0.7975488	0.1457076
H	2.3158997	-1.8269968	-0.1719484
H	2.9655037	-0.1832318	-0.2799074
H	2.2133217	-0.7441518	1.2437746
O	0.0232897	-2.4427248	-0.2542124
H	-0.8998113	-2.7359878	-0.4114224

#### 47-radical



C	-0.8328680	1.4311304	-0.3123000
C	0.5066760	0.9870204	0.2551390
C	-1.4947390	-1.0437406	-0.0522560
C	-1.9109690	0.4111774	0.0514260
N	-0.0800470	-1.3331736	-0.0551780
O	-2.2770560	-1.9603606	-0.0463400
O	0.3197520	-2.5214556	-0.0343920
N	0.8738140	-0.3054836	-0.3304260
H	-1.1000510	2.4168694	0.0769790
H	-0.7402160	1.5192184	-1.3982380
H	1.2968060	1.6879764	-0.0185940
H	0.4725390	0.9323944	1.3559920
H	-2.8110990	0.5249344	-0.5557730
H	-2.2261550	0.5479124	1.0933070
C	2.2383920	-0.7472306	-0.0516240
H	2.4653290	-1.6366916	-0.6331290
H	2.9016900	0.0623424	-0.3564710
H	2.3982020	-0.9728396	1.0118780

#### Entry 48

N	0.00237700	-0.31539100	-0.00002200
C	1.26249100	0.30759500	0.00003500
O	1.42633000	1.49766100	0.00011700
C	-1.21330400	0.36410700	-0.00012200

O	-1.36887500	1.55175100	-0.00025800
O	2.22555700	-0.62097600	0.00002600
O	-2.21132600	-0.56691500	0.00012200
C	3.56769200	-0.09747200	0.00009100
C	-3.57115600	-0.08147400	0.00016400
O	0.00914700	-1.72616000	-0.00037500
H	3.74010400	0.50832900	-0.89001800
H	3.74005800	0.50823000	0.89027700
H	4.21143900	-0.97370100	0.00005800
H	-4.05893900	-0.46723300	0.89475900
H	-3.57420200	1.00648900	-0.00048700
H	-4.05932800	-0.46833000	-0.89374000
H	-0.93676200	-1.94547700	0.00123400

#### 48-radical

N	-0.00005500	0.50728400	0.00044100
O	-0.00001200	1.77929000	0.00093100
C	-1.24127400	-0.23186300	-0.14764700
O	-1.28926000	-1.33385500	-0.61437200
C	1.24137100	-0.23183200	0.14802300
O	1.28974600	-1.33342300	0.61566200
O	-2.25249900	0.51644100	0.26693700
O	2.25211800	0.51620900	-0.26799300
C	-3.56226200	-0.06490500	0.08736800
C	3.56214600	-0.06472700	-0.08895400
H	-3.74328800	-0.26193700	-0.96954000
H	-3.64179900	-0.99339600	0.65305500
H	-4.25621900	0.68076100	0.46596500
H	4.25567900	0.68093600	-0.46832000
H	3.74382400	-0.26122300	0.96794000
H	3.64156300	-0.99346500	-0.65425200

#### Entry 49

N	-0.00004100	0.49295700	0.09327500
C	-1.27026700	1.06962300	-0.19945700
O	-1.36905500	2.21663900	-0.55857700
C	1.26994400	1.06872700	-0.20186600
O	1.36848500	2.21459700	-0.56472300
C	2.47858600	0.18892800	-0.03871000
C	2.53460400	-1.14910500	-0.44706700
C	3.64027100	0.81304300	0.43190700
C	3.73594700	-1.84879600	-0.37891400
C	4.83200200	0.10159700	0.52671500
C	4.88273000	-1.23039500	0.11809300
C	-2.47869500	0.18931300	-0.03790900

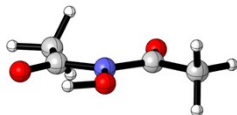
C	-3.64052200	0.81215000	0.43403200
C	-2.53431800	-1.14793800	-0.44886600
C	-4.83203300	0.10016100	0.52748900
C	-3.73542700	-1.84814000	-0.38201000
C	-4.88237200	-1.23104700	0.11626200
O	0.00001800	-0.74706200	0.75055200
H	1.64877400	-1.64043900	-0.82563800
H	3.59754400	1.85867200	0.71151300
H	3.77588700	-2.87937000	-0.71279200
H	5.72228800	0.58948800	0.90655200
H	5.81354200	-1.78293900	0.17993800
H	-3.59806700	1.85723200	0.71571400
H	-1.64834500	-1.63823700	-0.82845800
H	-5.72245300	0.58702600	0.90832800
H	-3.77507200	-2.87807600	-0.71788000
H	-5.81301300	-1.78399200	0.17708000
H	0.00091700	-0.54217900	1.69650600

#### 49-radical

N	0.00000000	-0.00572800	-0.00007900
O	-0.00000200	-1.28173500	-0.00022700
C	-1.17855500	0.73512400	0.46743500
O	-0.99513200	1.75106100	1.08713900
C	1.17858700	0.73520500	-0.46741400
O	0.99520200	1.75123500	-1.08697100
C	2.50648000	0.14612600	-0.17061900
C	3.58703000	0.59444900	-0.94393300
C	2.73199500	-0.75272300	0.88076400
C	4.87190600	0.13696500	-0.68129600
C	4.02349200	-1.19417800	1.14956600
C	5.09189100	-0.75698000	0.36764300
C	-2.50647200	0.14610300	0.17062600
C	-3.58695600	0.59427100	0.94412100
C	-2.73207900	-0.75252800	-0.88092400
C	-4.87185700	0.13684600	0.68149800
C	-4.02360000	-1.19392100	-1.14971000
C	-5.09193200	-0.75688100	-0.36760700
H	3.40040300	1.30129500	-1.74291400
H	1.90800700	-1.10332900	1.48655100
H	5.70202900	0.47941800	-1.28808400
H	4.19540200	-1.88275200	1.96855600
H	6.09537000	-1.11062300	0.57639000
H	-3.40026100	1.30095400	1.74323100
H	-1.90814400	-1.10301000	-1.48685300
H	-5.70192700	0.47917700	1.28842600

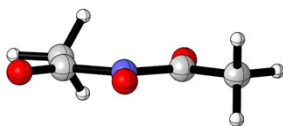
H	-4.19558100	-1.88232300	-1.96882900
H	-6.09543100	-1.11047800	-0.57634400

### Entry 50



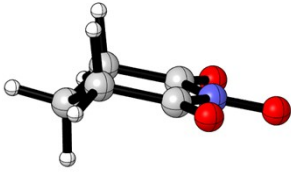
N	-0.1096728	-0.4966855	-0.0002949
C	1.0267092	0.3308435	0.0002791
O	0.9136462	1.5375425	0.0008891
C	-1.4702718	-0.1673175	-0.0003869
O	-2.2604838	-1.1004405	-0.0007259
C	2.3427442	-0.4015005	0.0002111
C	-1.8813378	1.2754615	0.0002851
H	3.1406242	0.3382435	0.0007251
H	2.4283412	-1.0481395	0.8760821
H	2.4287052	-1.0473205	-0.8762269
H	-1.4892988	1.7986415	0.8733841
H	-1.4892248	1.7994605	-0.8722879
H	-2.9698948	1.3031865	0.0002531
O	0.1480012	-1.8733945	-0.0008939
H	-0.7585868	-2.2485815	-0.0012919

### 50-radical



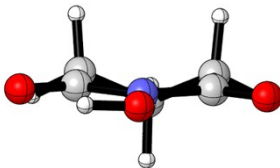
N	-0.1451026	-0.7502043	0.0000989
O	0.1111354	-1.9960663	0.0000469
C	0.9831524	0.1650707	0.0001909
O	0.8117854	1.3579387	0.0002089
C	-1.5921416	-0.3697473	0.0000669
O	-2.3796346	-1.2680803	0.0001509
C	2.3240424	-0.5159493	-0.0000511
C	-1.9510426	1.0883987	-0.0000781
H	3.0927704	0.2542007	-0.0001871
H	2.4353664	-1.1591883	0.8750169
H	2.4350704	-1.1592213	-0.8751301
H	-1.5436896	1.5995287	0.8730299
H	-1.5434856	1.5994177	-0.8731571
H	-3.0382256	1.1539017	-0.0002071

### Entry 51



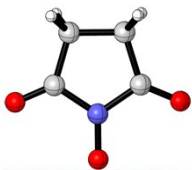
C	-0.0095606	1.4196446	-0.4685283
C	1.2793504	0.8456526	0.1204457
C	1.3648654	-0.6687754	0.0395067
C	-1.1558836	-0.7597954	0.1055357
C	-1.2290646	0.7470356	0.1617917
N	0.1148554	-1.3174634	0.0363767
O	2.3950714	-1.2904424	0.0014037
O	-2.1218466	-1.5049584	0.1293927
O	0.1638354	-2.7032704	-0.0102953
H	-0.0502746	2.4994016	-0.3055823
H	-0.0221986	1.2649256	-1.5524883
H	2.1703204	1.2341346	-0.3750483
H	1.3692104	1.1159176	1.1804487
H	-2.1644826	1.0386966	-0.3188903
H	-1.3215536	1.0270856	1.2189007
H	-0.7826436	-2.9477884	0.0370307

### 51-radical



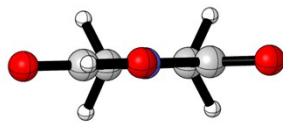
C	0.0001671	1.2245587	-0.4264070
C	1.2527831	0.5929607	0.1779190
C	1.3019671	-0.9117013	0.0319120
C	-1.3018359	-0.9119453	0.0302520
C	-1.2531259	0.5927317	0.1762760
N	0.0001671	-1.5917653	-0.0272640
O	2.3033981	-1.5635113	-0.0224310
O	-2.3030729	-1.5639343	-0.0254760
O	0.0003551	-2.8530063	-0.1370970
H	-0.0000529	2.3013777	-0.2413190
H	0.0008931	1.0944897	-1.5137200
H	2.1726481	0.9823187	-0.2616560
H	1.3057701	0.8128667	1.2526280
H	-2.1724829	0.9819047	-0.2645250
H	-1.3075789	0.8126547	1.2509080

### Entry 52



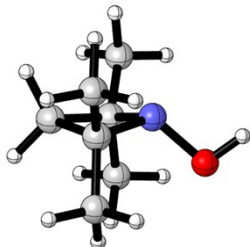
C	1.2703768	-0.3543173	-0.0013187
C	-1.0918632	-0.3541833	-0.0159487
N	0.0801518	-1.0820773	-0.0274307
O	0.0503288	-2.4554943	-0.0631597
O	2.3793098	-0.8155723	-0.0067157
O	-2.1835672	-0.8830653	-0.0363067
C	0.8404098	1.1105927	0.0344263
C	-0.7026292	1.1090917	0.0239393
H	-0.9078112	-2.6447653	-0.0741917
H	1.2743788	1.6182037	-0.8287427
H	1.2622428	1.5714757	0.9292743
H	-1.1417322	1.5678527	0.9120003
H	-1.1295962	1.6122587	-0.8458257

### 52-radical



C	1.2049706	-0.5731752	0.0000970
C	-1.2050164	-0.5730782	-0.0002460
N	-0.0000554	-1.3763562	-0.0000940
O	-0.0001054	-2.6367462	-0.0001420
O	2.3058476	-1.0378592	0.0004980
O	-2.3059304	-1.0376742	-0.0006220
C	0.7704266	0.8784088	0.0001230
C	-0.7703564	0.8784708	-0.0000120
H	1.1990256	1.3694498	-0.8762920
H	1.1989096	1.3694588	0.8765860
H	-1.1989134	1.3693918	0.8764910
H	-1.1988024	1.3697088	-0.8763870

### Entry 53

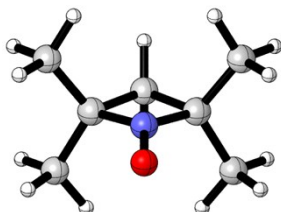


C	-1.0889021	0.1296622	-0.0664104
C	-0.0000061	0.5914112	-1.0789874



C	1.0889009	0.1296642	-0.0664204
N	0.0000049	0.0320872	0.9680846
C	2.1322089	1.1731052	0.3273506
C	1.7646589	-1.1922648	-0.4351794
C	-2.1322081	1.1731002	0.3273716
C	-1.7646601	-1.1922688	-0.4351614
H	-0.0000081	1.6681022	-1.2581204
H	-0.0000101	0.0672592	-2.0360084
H	2.7171419	0.8259362	1.1849486
H	2.8247369	1.3627372	-0.4992024
H	1.6529669	2.1149172	0.6028226
H	2.4375849	-1.0271918	-1.2821934
H	2.3540319	-1.5715298	0.4024566
H	1.0502809	-1.9663918	-0.7143394
H	-2.7171321	0.8259302	1.1849756
H	-1.6529651	2.1149142	0.6028396
H	-2.8247441	1.3627312	-0.4991744
H	-2.4375961	-1.0271978	-1.2821684
H	-1.0502841	-1.9663938	-0.7143294
H	-2.3540251	-1.5715358	0.4024806
O	0.0000099	-1.1837228	1.7266796
H	0.0000139	-0.8730598	2.6376856

### 53-radical



C	-1.1101300	0.0425438	0.0059278
C	0.0000000	0.4789528	-1.0031792
C	1.1101300	0.0425438	0.0059278
N	0.0000000	-0.2523192	0.9676548
O	0.0000000	-1.0180742	1.9728978
C	2.0382950	1.1468908	0.5085838
C	1.8921080	-1.2127872	-0.3804452
C	-2.0382950	1.1468908	0.5085838
C	-1.8921080	-1.2127872	-0.3804452
H	0.0000000	1.5472358	-1.2241202
H	0.0000000	-0.0841822	-1.9369442
H	2.5955240	0.8035358	1.3842568
H	2.7576130	1.4222518	-0.2685092
H	1.4753400	2.0395808	0.7903718
H	2.6139340	-0.9759002	-1.1674652
H	2.4370500	-1.5998012	0.4836868

H	1.2313880	-2.0021212	-0.7445612
H	-2.5955240	0.8035358	1.3842568
H	-1.4753400	2.0395808	0.7903718
H	-2.7576140	1.4222518	-0.2685092
H	-2.6139330	-0.9759002	-1.1674662
H	-1.2313880	-2.0021212	-0.7445612
H	-2.4370500	-1.5998012	0.4836868

#### Entry 54

N	-0.01699600	0.49050200	0.38285700
C	1.31250400	-0.12227400	0.03534600
C	-1.31289200	-0.13887500	0.04259100
F	-1.37577900	-1.29993100	0.84729200
C	-1.52358600	-0.58834000	-1.40107100
C	2.34795600	0.68224900	0.84812600
C	1.68459500	-0.03447500	-1.46075300
C	-2.45003900	0.75882300	0.52147900
C	1.36425600	-1.58266700	0.51241500
H	-2.55572700	-0.91974500	-1.53443900
H	-1.33391000	0.24475900	-2.08033600
H	-0.86632500	-1.41727200	-1.65805600
H	2.09808100	0.65786500	1.91151000
H	3.34344200	0.25078000	0.71620000
H	2.38894300	1.72229700	0.51909700
H	1.09707600	-0.71273600	-2.07950400
H	1.55297600	0.98186400	-1.83379700
H	2.73611100	-0.30786200	-1.58539400
H	-3.37236900	0.17500900	0.51425700
H	-2.25668900	1.09346800	1.54218500
H	-2.57438800	1.62348500	-0.12934600
H	0.70610700	-2.23777900	-0.05796700
H	2.38805200	-1.94596600	0.38977600
H	1.09088900	-1.66474000	1.56529400
O	-0.05128200	1.81003800	-0.20653100
H	-0.06779500	2.39548600	0.55834200

#### 54-radical

N	-0.01321700	-0.57162100	-0.00020700
C	1.34105400	0.10262300	-0.00004200
C	-1.34052900	0.11033600	-0.00003100
F	-1.11053800	1.49826100	-0.00086800
C	-2.09895800	-0.22555100	1.27561000
C	2.39705400	-1.00936800	-0.00016900

C	1.50233500	0.95686600	1.27228500
C	-2.09985400	-0.22689700	-1.27477500
O	-0.09866900	-1.84889000	0.00022100
C	1.50238900	0.95718500	-1.27214700
H	-3.07422000	0.26484300	1.26249000
H	-2.23517400	-1.30459000	1.34509100
H	-1.53875800	0.11831200	2.14657600
H	2.30946300	-1.64499600	-0.88150500
H	3.38498400	-0.54178900	-0.00014100
H	2.30949100	-1.64518300	0.88103200
H	0.78840200	1.77846000	1.30872600
H	1.37682100	0.33904600	2.16524600
H	2.51041300	1.38029200	1.29617400
H	-3.07509800	0.26353000	-1.26148500
H	-1.54023600	0.11606200	-2.14647300
H	-2.23612800	-1.30600400	-1.34304800
H	0.78845200	1.77878000	-1.30841600
H	2.51047200	1.38060300	-1.29590100
H	1.37688300	0.33958400	-2.16526100

### Entry 55

N	0.04547100	0.43244300	-0.45731600
C	1.28341700	-0.16724700	-0.04820000
C	-1.30299600	-0.10798900	-0.04488000
F	1.21000700	-1.52017000	-0.22227600
F	1.48950300	0.00061500	1.34278100
O	0.15762000	1.82109800	-0.15666700
C	2.49856600	0.36839700	-0.76810100
C	-1.50775300	-1.50819300	-0.65205400
C	-2.34029800	0.83628100	-0.68117900
C	-1.50140200	-0.15532200	1.48280500
H	0.23012000	1.89070000	0.80976300
H	3.38374500	-0.13123000	-0.37302700
H	2.40087900	0.15669700	-1.83289200
H	2.58482100	1.44261300	-0.62301300
H	-0.93119600	-2.27795100	-0.14359400
H	-2.56594300	-1.76840000	-0.56911800
H	-1.23816100	-1.51237100	-1.71023200
H	-2.18694900	0.89860400	-1.76072800
H	-3.34213700	0.44270100	-0.49376300
H	-2.28299200	1.84397400	-0.27162300
H	-2.52180700	-0.47851900	1.70503400
H	-0.81102500	-0.85139000	1.96043300
H	-1.37139600	0.82912000	1.94242700

### 55-radical

N	0.04008500	0.57348600	-0.13697700
C	1.31532100	-0.12320300	-0.02148800
C	-1.31918300	-0.08818400	-0.00272500
F	1.43083400	-1.01498500	-1.06594100
F	1.29475100	-0.91372800	1.11531400
O	0.08083900	1.85032300	-0.07456200
C	2.51409100	0.78498700	0.00982200
C	-1.27096200	-1.58379800	-0.34377200
C	-2.25211900	0.63477800	-0.98590200
C	-1.79028500	0.12417500	1.44735100
H	3.39955800	0.15172600	0.07644200
H	2.55325900	1.38495200	-0.89751600
H	2.46253400	1.44829000	0.87075000
H	-0.62196000	-2.14488300	0.32763900
H	-2.28361600	-1.98075500	-0.23963700
H	-0.94449600	-1.75485800	-1.37004400
H	-1.90947500	0.50187700	-2.01497600
H	-3.25688900	0.21416400	-0.90067700
H	-2.29777000	1.70158600	-0.77016000
H	-2.80618000	-0.26198500	1.56450800
H	-1.14011900	-0.39882900	2.15143000
H	-1.79360200	1.18761400	1.69348800

### Entry 56

N	0.04379400	0.45643800	-0.44547100
C	1.28096800	-0.13590300	-0.05459800
C	-1.27589700	-0.13958300	-0.01442700
C	-1.34568200	-1.61879400	-0.42256600
C	-1.52060000	0.01293400	1.49743600
C	-2.34403100	0.63798700	-0.80109400
F	1.40287500	-1.36425300	-0.58834300
F	1.48056300	-0.27083900	1.28373900
F	2.30189300	0.60991300	-0.51704200
O	0.09551800	1.81587200	0.00154000
H	-1.10151800	-1.75762500	-1.47739400
H	-0.68860900	-2.25413200	0.17096600
H	-2.36859900	-1.96741700	-0.26304200
H	-1.41128800	1.05222000	1.80918600
H	-2.53905500	-0.30648600	1.73368300
H	-0.83420100	-0.59641600	2.08656900
H	-3.33219800	0.22464600	-0.58668400
H	-2.35541100	1.69255600	-0.52442100

H	-2.16748500	0.55899200	-1.87675300
H	0.29113600	2.31838200	-0.79982800

### 56-radical

N	-0.03575500	0.58989800	-0.16563900
O	-0.04255800	1.86189800	-0.07307600
C	-1.32351700	-0.07439500	-0.02430900
C	1.29353800	-0.13013000	-0.00472400
C	1.75874200	0.08148900	1.44574800
C	1.17773000	-1.62458700	-0.32718100
C	2.26001700	0.54155900	-0.98946900
F	-1.51454900	-0.97624400	-1.00750200
F	-2.30887800	0.80630400	-0.06892800
F	-1.40998200	-0.74884400	1.14818300
H	1.08488900	-0.40269100	2.15560200
H	2.75623000	-0.34452500	1.58001300
H	1.80613000	1.14578900	1.68189900
H	2.16774300	-2.07114000	-0.21030000
H	0.50322300	-2.15374800	0.34676700
H	0.85451400	-1.79942000	-1.35405100
H	3.25037300	0.09163600	-0.88844000
H	1.92611200	0.40533300	-2.02087700
H	2.34315300	1.60973800	-0.79270600

### Entry 57

N	0.02474800	0.48612300	-0.40466000
C	1.24998800	-0.17729500	-0.03081800
C	-1.25432400	-0.08350700	-0.02886800
F	-2.19072000	0.63688100	-0.74254000
F	-1.54624700	0.17146500	1.28849400
F	1.33737700	-1.31481200	-0.80448700
F	1.20817400	-0.64919600	1.27067200
O	0.06474800	1.84825900	-0.00192500
C	2.49044000	0.65862300	-0.21590300
C	-1.43403000	-1.55451900	-0.31460100
H	-0.17724000	2.32743100	-0.80450500
H	3.34837000	0.01174400	-0.03056100
H	2.53674800	1.03830700	-1.23652000
H	2.49566400	1.48940100	0.48574700
H	-0.78412700	-2.15462400	0.31882500
H	-2.47437600	-1.79337000	-0.09142100
H	-1.22595300	-1.76667300	-1.36164800

### 57-radical

N	-0.03180400	0.58289600	-0.12611900
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C	1.30347700	-0.04537800	-0.00366100
C	-1.29051800	-0.15664700	-0.00587400
O	-0.07223200	1.85647500	-0.11140200
F	1.78054400	0.26278800	1.24298700
F	-1.24353700	-0.92048800	1.13819600
F	2.10646700	0.60717300	-0.88652100
F	-1.35872900	-1.06304500	-1.03755900
C	-2.50432800	0.72836100	-0.00033500
C	1.38488300	-1.53303800	-0.23588700
H	-3.37732600	0.07949900	0.07650900
H	-2.46912100	1.40885800	0.84820000
H	-2.55111300	1.30733400	-0.92096700
H	1.05993100	-1.77874400	-1.24506300
H	2.43215100	-1.81126400	-0.11316100
H	0.78217100	-2.07540600	0.48914500

### Entry 59

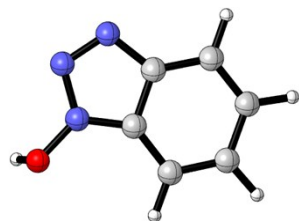
C	-1.10573800	-0.29859400	0.00622600
N	0.00000000	0.51836700	0.04102200
C	1.10573800	-0.29859400	0.00622700
C	2.51008200	0.18802900	-0.01003700
C	-2.51008200	0.18803000	-0.01003900
N	0.69510000	-1.53917400	0.00167900
N	-0.69510100	-1.53917500	0.00169000
O	0.00000100	1.89416900	-0.11921700
H	2.68244500	0.87196700	-0.84521800
H	2.76714100	0.71503400	0.91405300
H	3.16961000	-0.67289100	-0.11190400
H	-2.76713900	0.71504000	0.91404800
H	-2.68244500	0.87196400	-0.84522300
H	-3.16961000	-0.67289000	-0.11190000
H	0.00000100	2.26506700	0.77489500

### 59-radical

C	1.12392300	-0.26958000	-0.00003200
N	0.00000000	0.59243600	-0.00003100
O	0.00000000	1.85766300	-0.00002300
C	-1.12392300	-0.26958000	0.00003500
C	-2.51983200	0.24168500	0.00007100
C	2.51983200	0.24168500	0.00004400
N	-0.71308800	-1.49123500	-0.00003700
N	0.71308800	-1.49123500	-0.00007200
H	-2.52041600	1.33199500	0.00070600
H	-3.05338600	-0.11454000	-0.88343700
H	-3.05370900	-0.11561300	0.88294300

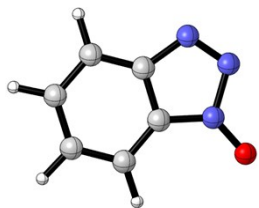
H	2.52041600	1.33199500	-0.00114000
H	3.05316000	-0.11407300	0.88388000
H	3.05393500	-0.11607900	-0.88249900

### Entry 60



C	-0.5770113	-0.2194461	0.0304903
C	-0.1164313	1.1104259	0.0380273
C	1.2602477	1.3819429	0.0411813
C	2.1200407	0.2992539	0.0423013
C	1.6362927	-1.0325271	0.0392653
C	0.2831677	-1.3234821	0.0319653
N	-1.2031413	1.9608449	0.0423933
N	-2.2835923	1.2505669	0.0527063
N	-1.9291143	-0.0530161	0.0119413
H	1.6202087	2.4033899	0.0446463
H	3.1908497	0.4649939	0.0474253
H	2.3506877	-1.8477511	0.0441363
H	-0.0896903	-2.3394251	0.0342843
O	-2.8658353	-1.0410931	0.1546233
H	-3.3966793	-1.0146781	-0.6553867

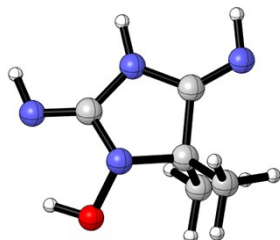
### 60-radical



C	0.7972162	-0.3297959	-0.0000113
C	0.3949522	1.0047781	0.0000047
C	-0.9533868	1.3470641	0.0000137
C	-1.8682998	0.2963651	0.0000117
C	-1.4476848	-1.0470999	0.0000127
C	-0.0985428	-1.3925219	0.0000047
N	1.5363002	1.8223631	-0.0000533
N	2.5843462	1.1095651	0.0002567
N	2.1899722	-0.2630879	-0.0001003
H	-1.2672188	2.3833991	0.0000017
H	-2.9296528	0.5139221	0.0000007

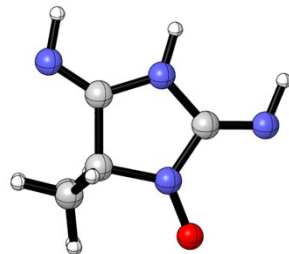
H	-2.1944918	-1.8322219	-0.0000013
H	0.2375372	-2.4214329	-0.0000203
O	3.0189532	-1.1912969	-0.0001203

### Entry 61



C	-1.6128110	0.6484599	0.0144094
N	-0.9313911	-0.4456741	0.5123355
C	0.5076840	-0.3654171	0.1675544
C	1.3723930	-0.9237821	1.2954865
C	0.8187730	-1.0427261	-1.1798655
N	-2.8660450	0.6049819	-0.2225756
O	-1.5576690	-1.6844621	0.2733174
N	-0.6496420	1.6436049	-0.1616746
C	0.6451069	1.1571579	0.0171074
N	1.7546000	1.7692329	0.0291724
H	1.1303690	-0.4380431	2.2420004
H	2.4267130	-0.7524631	1.0742794
H	1.1971460	-1.9970261	1.3980134
H	0.1920180	-0.6447121	-1.9817646
H	0.6406000	-2.1160311	-1.1068715
H	1.8649440	-0.8657611	-1.4342616
H	-3.2466210	1.4679479	-0.5954246
H	-2.4589660	-1.4124921	0.0076234
H	-0.8800271	2.6222779	-0.2399766
H	1.6528260	2.7749269	-0.10888566

### 61-radical



C	1.8380722	0.4482522	-0.0298800
N	1.0446642	-0.7244638	-0.0296120
C	-0.4206588	-0.4343858	0.0025500
C	-1.0883178	-0.9846188	-1.2628020
C	-1.0390398	-1.0174098	1.2782180
N	3.1034472	0.4434082	-0.0544730



O	1.5083022	-1.8968398	-0.0537250
N	0.9084292	1.4953582	0.0016560
C	-0.4217918	1.0917052	0.0222600
N	-1.4833858	1.7848362	0.0518300
H	-0.6341838	-0.5648958	-2.1631160
H	-2.1473098	-0.7243218	-1.2532360
H	-0.9781678	-2.0700628	-1.2893130
H	-0.5501358	-0.6208248	2.1707770
H	-0.9284888	-2.1031218	1.2724320
H	-2.0974758	-0.7574818	1.3164300
H	3.4920972	1.3838322	-0.0498760
H	1.1954352	2.4623592	0.0086140
H	-1.3014908	2.7886752	0.0612660

### Entry 62

C	2.13517600	1.33505800	-0.02085400
C	0.85490100	0.79087700	-0.02267200
C	0.69323300	-0.59178400	0.00339900
C	1.76292200	-1.47216300	0.01408300
C	3.04387100	-0.91720200	0.02101400
C	3.22706000	0.46900300	0.00504300
S	-1.04161700	-1.02538700	0.01762000
O	-1.50717700	-1.40039700	1.34259900
O	-1.40629900	-1.83272800	-1.13576000
N	-1.46775500	0.66362200	-0.31163300
C	-0.41678500	1.56715200	-0.05781400
O	-0.55038400	2.75765100	0.06319100
O	-2.73903800	1.02685900	0.09663700
H	2.26019600	2.41074700	-0.04114200
H	1.61350400	-2.54452200	0.02449400
H	3.90642100	-1.57278100	0.03995100
H	4.23213100	0.87368600	0.01075900
H	-3.25117300	1.09697400	-0.72109000

### 62-radical

C	2.14064200	1.27246400	-0.00013800
C	0.83776400	0.77786900	0.00000100
C	0.62773000	-0.60320700	0.00027900
C	1.67029200	-1.51619500	0.00034600
C	2.97013700	-1.00809200	0.00022000
C	3.20178300	0.37077700	-0.00005000
S	-1.11055100	-1.01624100	-0.00009000
O	-1.53203700	-1.59177300	1.26484000
O	-1.53115600	-1.59159600	-1.26546600
N	-1.53256300	0.77696000	0.00001700
C	-0.37333100	1.63095600	-0.00003000

O	-0.44183900	2.82961900	-0.00002800
O	-2.71622200	1.16210400	0.00030100
H	2.30333300	2.34324900	-0.00032200
H	1.48486300	-2.58302100	0.00058300
H	3.80854700	-1.69441100	0.00032300
H	4.21993300	0.74104800	-0.00020500

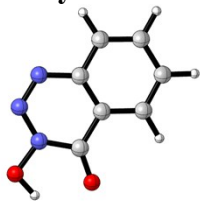
#### Entry 64

S	-1.42624700	-0.25368500	0.09339600
O	-1.89817700	0.14184700	1.39720100
O	-1.09972700	-1.62227700	-0.25010800
O	-2.47691600	0.28641500	-1.01181500
S	1.56134200	-0.05222600	0.08350800
O	2.51772900	0.90396700	-0.40257200
O	1.50692900	-0.48932100	1.45868300
O	1.60108900	-1.30709600	-0.91240300
N	-0.02572000	0.63276700	-0.43571200
O	-0.12954400	1.96182100	0.00689200
H	-3.08550200	0.91021200	-0.58411500
H	0.87459500	-1.92410100	-0.69154600
H	0.05836200	2.47623900	-0.79183200

#### 64-radical

S	1.58560700	-0.26692300	0.02739100
O	1.69935100	-1.29794800	-0.96198900
O	1.70391800	-0.48234900	1.45142700
S	-1.58710200	-0.22510500	0.11070100
O	-2.15451900	0.36619200	1.29795900
N	-0.01891500	0.65789600	-0.25081100
O	-0.00535200	1.88498200	-0.04438600
O	2.54205400	0.93782600	-0.44705900
H	2.48667700	1.68839900	0.16860900
O	-2.42142500	0.26732000	-1.18117200
H	-2.83290000	1.12895000	-1.00066600
O	-1.30120700	-1.61979500	-0.06749800

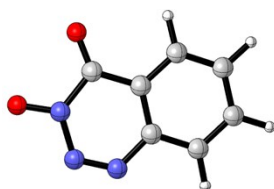
#### Entry 65



C	-0.4978943	-1.5959979	0.3331807
C	0.1832337	-0.3655129	-0.0040033
C	-0.5661133	0.8297021	0.0497367

C	1.5380327	-0.3414319	-0.3730873
C	0.0581067	2.0510031	-0.2709063
C	1.3901797	2.0624151	-0.6322613
C	2.1329997	0.8660611	-0.6841093
N	-1.9052593	0.8655221	0.4071067
N	-2.5151963	-0.2116129	0.7059067
O	-0.0753043	-2.7458979	0.3619667
N	-1.8366253	-1.3586909	0.6653107
O	-2.5859793	-2.4582299	1.0045857
H	2.0886477	-1.2731939	-0.4059173
H	-0.5322713	2.9575591	-0.2241953
H	1.8722787	3.0011261	-0.8793393
H	3.1776737	0.8960601	-0.9701213
H	-1.9265093	-3.1788799	0.9161467

### 65-radical



C	-1.7610645	0.8581419	-0.0003260
C	-0.3611335	0.4475909	-0.0001540
C	-0.0568795	-0.9253271	0.0002390
C	0.6705765	1.3937489	-0.0003780
C	1.2796515	-1.3480021	0.0003960
C	2.2944275	-0.4035781	0.0001680
C	1.9906075	0.9657669	-0.0002170
N	-1.0381205	-1.9184601	0.0004960
N	-2.2645615	-1.6530581	0.0004050
O	-2.2015545	1.9768799	-0.0005680
N	-2.6714395	-0.2928411	0.0000050
O	-3.9042775	-0.1055321	0.0000140
H	0.4167405	2.4463729	-0.0006770
H	1.4852365	-2.4111581	0.0006990
H	3.3292575	-0.7249901	0.0002900
H	2.7925335	1.6944449	-0.0003920

### Entry 66

N	0.00000000	0.01644800	-0.40827600
C	1.20901300	-0.64881100	0.06727800
C	-1.20901300	-0.64881100	0.06727800
H	1.23229500	-1.65729100	-0.35271700
H	2.08365400	-0.10295900	-0.28737700
H	1.24709600	-0.71245700	1.16527700
H	-2.08365400	-0.10295900	-0.28737700

H	-1.23229500	-1.65729100	-0.35271700
H	-1.24709600	-0.71245700	1.16527700
O	0.00000000	1.33634800	0.19586100
H	0.00000000	1.92523100	-0.56666400

### 66-radical

N	0.00000000	0.11837200	-0.15233300
O	0.00000000	1.38313500	0.04296200
C	1.25748000	-0.60258400	0.02552900
C	-1.25748000	-0.60258400	0.02552900
H	1.22684600	-1.54682700	-0.52196600
H	2.06023200	0.02471900	-0.35834500
H	1.43997800	-0.80923100	1.08845600
H	-2.06023200	0.02471800	-0.35834500
H	-1.22684500	-1.54682700	-0.52196700
H	-1.43997700	-0.80923100	1.08845600

### Entry 67

C	-0.49810900	0.51658600	-0.11983700
C	0.78528400	0.09696600	-0.10280900
C	1.17590500	-1.41441100	-0.03910000
C	1.16696500	-1.89173800	1.43817000
C	0.20464000	-2.30171100	-0.86059500
C	2.56696200	-1.76451700	-0.62871300
C	1.87152300	1.22627200	-0.06576900
C	2.81049300	1.06792800	1.15768700
C	2.70147000	1.27335300	-1.37643300
C	1.26865300	2.64652000	0.07993600
N	-1.70217600	-0.24484600	-0.09233400
C	-2.90245400	0.52390300	-0.49052700
C	-3.34487600	1.58779100	0.52614300
C	-4.04312000	-0.43850600	-0.82802500
O	-1.93159900	-0.78224000	1.24091900
H	-0.68481100	1.57946300	-0.17902500
H	1.96479200	-1.42294600	2.01740000
H	0.22067200	-1.65543900	1.92362600
H	1.32412200	-2.97523800	1.47749200
H	0.14868600	-1.95875700	-1.89708200
H	0.58283700	-3.32834800	-0.86400200
H	-0.81106400	-2.31767000	-0.47792400
H	2.73575300	-2.83535300	-0.48271300
H	3.39714100	-1.24614300	-0.15399000
H	2.60894100	-1.57554600	-1.70332900
H	2.24146800	1.12676200	2.08952300
H	3.36744300	0.13328800	1.16533000

H	3.54216900	1.88181900	1.16193700
H	2.04015800	1.35751800	-2.24350700
H	3.34991500	2.15515600	-1.36572000
H	3.33977600	0.40642100	-1.52168400
H	2.08900700	3.36505000	0.15576700
H	0.66801800	2.93901300	-0.78511600
H	0.65838100	2.74706000	0.98039200
H	-2.59453300	1.02056500	-1.41760600
H	-2.54457500	2.29510000	0.75633800
H	-4.18840800	2.15732000	0.12663900
H	-3.65761700	1.11636200	1.45938700
H	-3.72332000	-1.17315400	-1.57073800
H	-4.37985700	-0.96957300	0.06630300
H	-4.89869700	0.11070000	-1.23020100
H	-2.00838200	-1.73220200	1.09072000

### 67-radical

C	-0.50185500	-0.53987700	0.07613100
C	0.80155000	-0.10841800	0.06143500
C	1.19473900	1.39796100	-0.00509800
C	0.37364700	2.20423800	1.03682000
C	2.66698300	1.74621200	0.33328300
C	0.93238100	1.93491400	-1.43839100
C	1.86514900	-1.25647100	0.05028100
C	1.24716400	-2.67714000	0.09418000
C	2.66928800	-1.20600700	-1.27593500
C	2.82621700	-1.20059500	1.26757600
N	-1.73395900	0.07415900	-0.10475000
C	-2.97516300	-0.70339400	0.20591300
C	-3.79747000	-0.88863800	-1.07063700
C	-3.75689400	0.01063900	1.31047200
O	-1.92517900	1.24960900	-0.56844300
H	-0.67277200	-1.58977000	0.24000300
H	-0.69266000	2.19381500	0.83327000
H	0.55255700	1.81365000	2.04313300
H	0.70227400	3.24826900	1.02309400
H	3.40696500	1.24184200	-0.28594700
H	2.79316500	2.81901300	0.16473400
H	2.90333400	1.56105300	1.38208600
H	1.59781600	1.45369100	-2.16076800
H	1.13204900	3.01154300	-1.46863600
H	-0.09921900	1.77363600	-1.74303300
H	0.70776300	-2.86916000	1.02622700
H	0.57829300	-2.87260300	-0.74739100
H	2.05740100	-3.40796500	0.03786400

H	3.18437600	-0.26087200	-1.43366600
H	3.42460900	-1.99840400	-1.27910000
H	2.00626300	-1.37000800	-2.12974100
H	3.41541200	-2.12175200	1.30631600
H	3.52827900	-0.37382500	1.22905500
H	2.26359800	-1.12810700	2.20268900
H	-2.64493800	-1.67758600	0.57297000
H	-3.22674600	-1.42440400	-1.83334700
H	-4.70174400	-1.46202600	-0.85163300
H	-4.08650200	0.08287900	-1.47472200
H	-3.15751000	0.10658100	2.21911100
H	-4.04726800	1.00926600	0.97949300
H	-4.66006300	-0.55527600	1.55255600

### Entry 68

C	0.11001200	-0.05757500	0.47258600
C	-0.97418800	-0.41577300	-0.21996200
C	-2.39598600	0.05627400	0.02361100
C	-2.50387800	1.07125100	1.17335000
C	-2.92431300	0.70734900	-1.27557400
C	-3.27274000	-1.17405000	0.35423500
N	1.41963000	-0.56061600	0.32983900
C	2.50659300	0.44686900	0.38442900
C	2.52872000	1.37995100	-0.83304800
C	3.84988300	-0.24776700	0.60655200
H	0.05474900	0.64660000	1.29605000
H	-0.84932400	-1.12034800	-1.03673100
H	-2.16396700	0.64332300	2.12108900
H	-1.91444000	1.97076000	0.97236800
H	-3.54471400	1.38089400	1.30528900
H	-2.86146300	0.01059000	-2.11683600
H	-3.97189000	1.00608700	-1.16368100
H	-2.34026500	1.59517500	-1.53321900
H	-4.32180300	-0.88424700	0.47628000
H	-3.22147500	-1.91830000	-0.44617100
H	-2.93954300	-1.65241300	1.27937700
H	2.27188000	1.03423700	1.27900200
H	1.56516200	1.87745800	-0.96658300
H	3.29638400	2.14841300	-0.70699700
H	2.75130000	0.81802700	-1.74247400
H	3.80878000	-0.90038900	1.48210100
H	4.12475100	-0.84793500	-0.26422600
H	4.63785000	0.49306000	0.76513300
O	1.55351500	-1.34278900	-0.86222900
H	1.70787800	-2.23353800	-0.52788900

**68-radical**

C	0.09970000	0.00418100	0.25778600
C	-1.03656200	-0.01041300	-0.46825400
C	-2.45010700	0.00165700	0.06803600
C	-2.50988100	0.03883700	1.60404600
C	-3.17360900	1.24580100	-0.50036800
C	-3.17281700	-1.26925300	-0.43884900
N	1.36934800	-0.00889700	-0.31207000
C	2.58881900	0.01199600	0.54107600
C	3.39536800	1.28103700	0.25459000
C	3.40059100	-1.26476900	0.30930100
O	1.53646500	-0.03707600	-1.57588500
H	0.10894900	0.02705700	1.33925100
H	-0.92848000	-0.03318900	-1.54909300
H	-2.02675400	-0.83707400	2.04695400
H	-2.02857500	0.93607900	2.00413400
H	-3.55093900	0.04566100	1.93865000
H	-3.15016800	1.24881900	-1.59377800
H	-4.22191300	1.25737300	-0.18516700
H	-2.70088200	2.16791000	-0.15175300
H	-4.22090700	-1.26601100	-0.12259100
H	-3.15027600	-1.32572000	-1.53080300
H	-2.69933800	-2.17293400	-0.04578000
H	2.23099200	0.03345800	1.57379500
H	2.80226200	2.17762000	0.45043800
H	4.28438700	1.30996100	0.88957300
H	3.70958600	1.29659200	-0.79046200
H	2.81190600	-2.15449000	0.54562500
H	3.71300400	-1.32485600	-0.73465100
H	4.29096600	-1.26181700	0.94304200

**Entry 69**

N	-1.31791700	0.13258800	-0.45265500
C	-2.12211400	-0.98353700	0.16648600
C	-1.20214400	-2.15604600	0.54149200
C	-2.90850100	-0.52160800	1.41093800
C	-3.10561200	-1.47314600	-0.91176000
C	-0.19300100	0.67186900	0.37742300
C	0.05327300	2.19712100	0.14051700
C	0.53405500	2.55590200	-1.27239200
C	1.01757700	2.76985900	1.18971900
C	1.07055300	-0.14716300	0.12499100
C	1.93351400	-0.44478200	1.18560800
C	1.42559800	-0.58154100	-1.15680300
C	3.11946700	-1.14666800	0.97609400
C	2.60933900	-1.28468500	-1.37105100

C	3.46319100	-1.56939700	-0.30626200
O	-2.27618100	1.19111700	-0.71054500
H	-0.61567900	-2.49633500	-0.31353500
H	-0.51372500	-1.90907400	1.34975900
H	-1.82520500	-2.98737000	0.88209700
H	-3.55783800	0.32042800	1.16909900
H	-3.53098100	-1.34193600	1.77862800
H	-2.24635800	-0.22605300	2.22897800
H	-2.56339800	-1.76624400	-1.81492700
H	-3.65766900	-2.34311600	-0.54643700
H	-3.82890900	-0.69939100	-1.17109300
H	-0.43605500	0.58376200	1.44498400
H	-0.91594800	2.67256000	0.29579200
H	-0.11557000	2.14751100	-2.04972900
H	0.55024100	3.64317100	-1.39269400
H	1.54591600	2.18673400	-1.45771200
H	0.67071800	2.57080500	2.20846300
H	2.02601800	2.36024800	1.08934600
H	1.08830800	3.85514100	1.07260900
H	1.67079200	-0.13329900	2.19172900
H	0.75542700	-0.38397100	-1.98347900
H	3.76939700	-1.36872500	1.81548300
H	2.86353600	-1.61508200	-2.37252600
H	4.38193500	-2.12052700	-0.47304500
H	-2.25125100	1.27664500	-1.66884400

### 69-radical

N	1.26676500	-0.03346100	0.45952400
O	1.40262400	0.24267100	1.70215700
C	2.34496300	-0.81504500	-0.24277100
C	1.70785500	-1.83986300	-1.19728300
C	3.24467500	0.16829600	-1.01807900
C	3.16861100	-1.55043800	0.82025300
C	0.16710800	0.61366600	-0.29523500
C	0.06978300	2.14383900	0.02123100
C	-0.65444200	2.49761600	1.32630500
C	-0.57009900	2.88790500	-1.16120800
C	-1.14168800	-0.15582700	-0.14230700
C	-1.98089300	-0.31760700	-1.24991100
C	-1.53742300	-0.70565600	1.08289900
C	-3.19299200	-0.99801400	-1.13914800
C	-2.74615900	-1.38964700	1.19368900
C	-3.58036000	-1.53586100	0.08578900
H	1.03595900	-2.51047900	-0.65781100
H	1.14338900	-1.37034400	-2.00527100
H	2.49682000	-2.44081800	-1.65688500



H	3.68756100	0.89866000	-0.33710600
H	4.05503400	-0.37432600	-1.51285600
H	2.68833400	0.70729100	-1.78970100
H	2.54121100	-2.22885700	1.40130400
H	3.94686500	-2.13435000	0.32236500
H	3.63800600	-0.85308300	1.51263000
H	0.45657400	0.54465900	-1.34528800
H	1.10763500	2.48400500	0.10962800
H	-0.60240600	3.57834400	1.49051300
H	-1.71148600	2.22127600	1.27996800
H	-0.19981900	1.99802200	2.18037400
H	-0.56382200	3.96539200	-0.97476400
H	-0.03175000	2.71046300	-2.09787300
H	-1.61195300	2.58730100	-1.30602600
H	-1.68278000	0.08462900	-2.21298800
H	-0.89160700	-0.60066500	1.94597600
H	-3.82754100	-1.11382400	-2.01093800
H	-3.03648300	-1.81082800	2.14999900
H	-4.51973600	-2.06979700	0.17546700

### Entry 70

N	0.97566100	-0.64347800	-0.40245400
O	0.93326600	-1.48137900	-1.56493200
C	2.27438400	-0.16200800	-0.13653600
C	3.40902900	-0.66902500	-0.78574200
C	2.43882500	0.81604200	0.85925200
C	4.67483100	-0.20264100	-0.43998800
C	3.71056800	1.27364800	1.18918000
C	4.83936000	0.76899300	0.54528400
C	-0.08773300	0.30908800	-0.41667400
C	-1.36872100	0.12123000	-0.04480700
C	-2.33278000	1.33012600	-0.29760900
C	-2.77384000	1.99306300	1.03417200
C	-1.67391800	2.46387400	-1.12329500
C	-3.57607500	0.90924200	-1.12250900
C	-1.88406000	-1.23466500	0.53497800
C	-2.32775500	-2.15963400	-0.63012600
C	-0.80575500	-1.98155300	1.36493200
C	-3.07593900	-1.10302900	1.51772500
H	0.77257500	-2.36540600	-1.20884000
H	3.29132500	-1.41061200	-1.56237600
H	1.57220400	1.19962300	1.38327600
H	5.54115100	-0.60317000	-0.95538200
H	3.81662200	2.02718900	1.96203500
H	5.82820700	1.12623000	0.80733800

H	0.22881500	1.27003700	-0.80027700
H	-3.41361500	1.36235100	1.64569200
H	-1.90063400	2.27060400	1.63109700
H	-3.33176000	2.90897000	0.81587400
H	-1.30383600	2.11010200	-2.08808400
H	-2.42651100	3.23246800	-1.31774800
H	-0.85214900	2.95005000	-0.59247100
H	-4.20743800	1.78612400	-1.29396800
H	-3.27793900	0.51976200	-2.09968400
H	-4.19405600	0.15770700	-0.63572500
H	-3.21282400	-1.77925100	-1.14165300
H	-1.53725400	-2.26536000	-1.37458100
H	-2.57268000	-3.15231900	-0.23833000
H	-0.35268200	-1.32493500	2.11116900
H	-1.28562600	-2.81093300	1.89261800
H	0.00254200	-2.39808200	0.76874200
H	-3.38592000	-2.10846600	1.81552400
H	-2.78645700	-0.57070800	2.42652800
H	-3.95034500	-0.61309900	1.09644600

### 70-radical

N	0.99719100	-0.50276600	-0.62968900
C	2.29092800	-0.07976400	-0.23038100
C	3.41461600	-0.73962100	-0.74792300
C	2.45318400	0.97158100	0.68336600
C	4.68526700	-0.33524800	-0.36022100
C	3.73417600	1.36697500	1.05751300
C	4.85477500	0.71996200	0.53912400
C	-0.11564500	0.37377200	-0.46705400
C	-1.37970800	0.11007200	-0.07350400
O	0.87476200	-1.60216700	-1.27741500
C	-2.38729200	1.29566200	-0.25004100
C	-1.78215600	2.49450600	-1.02269300
C	-3.61311400	0.85514300	-1.09175800
C	-2.85017900	1.87540400	1.11256000
C	-1.81957900	-1.28000900	0.48366300
C	-0.68641200	-1.94997900	1.30715000
C	-3.01870400	-1.23162400	1.46510200
C	-2.20143500	-2.21776400	-0.69247100
H	3.26516000	-1.55386200	-1.44322200
H	1.58748400	1.45651000	1.11556000
H	5.55172900	-0.84544500	-0.76566200
H	3.85399100	2.17762700	1.76730000
H	5.84975900	1.02986700	0.83640200
H	0.16543800	1.37442800	-0.75785300

H	-1.40117500	2.20530200	-2.00480400
H	-0.98186400	2.99324600	-0.46940900
H	-2.56797000	3.23772500	-1.17902900
H	-3.30155200	0.54160900	-2.09165100
H	-4.17850800	0.03958200	-0.64707000
H	-4.29521700	1.70301500	-1.20551000
H	-3.47667000	1.19758400	1.68525500
H	-3.43054600	2.78666900	0.93860700
H	-1.98768900	2.14428100	1.72907700
H	-1.10145600	-2.81197000	1.83666700
H	-0.28692100	-1.26335800	2.05906300
H	0.13061700	-2.31610400	0.69254000
H	-3.92483000	-0.79702800	1.04854800
H	-3.26028100	-2.26017400	1.74589600
H	-2.76813900	-0.69708900	2.38407500
H	-2.44445500	-3.20998100	-0.29828400
H	-1.37105500	-2.31606900	-1.38976200
H	-3.07660100	-1.85407800	-1.23419700

### Entry 71

N	1.27971900	0.11342300	0.40247800
C	2.63839700	0.12688000	-0.23125000
C	3.56512500	0.93219100	0.69538300
C	3.21642700	-1.28445400	-0.44938200
C	2.52638100	0.87908100	-1.56960400
C	0.24800400	-0.66220100	-0.29768900
C	-1.16933100	-0.33061300	0.18992000
C	-1.56534600	1.12385700	-0.11305100
C	-2.19203300	-1.30490500	-0.42142900
C	-2.99581300	1.43941600	0.34667400
C	-3.62652400	-0.99539200	0.03208700
C	-4.01151100	0.46134900	-0.25983300
O	1.40332600	-0.52149100	1.70501100
H	3.71347300	0.42215100	1.64773800
H	4.54294700	1.06195800	0.22450900
H	3.14353200	1.92272000	0.88890300
H	2.62534800	-1.85851400	-1.16748900
H	4.23562700	-1.21755300	-0.84045400
H	3.24786800	-1.83620200	0.49217800
H	3.52857000	1.07093800	-1.96117600
H	1.98648500	0.31043600	-2.32926300
H	2.02299600	1.83931000	-1.43196400
H	0.43311500	-1.73945800	-0.18196000
H	0.31671900	-0.42545500	-1.36197900
H	-1.18582600	-0.47360100	1.27833000
H	-1.49153400	1.29141000	-1.19742500

H	-0.85034900	1.80623900	0.35422700
H	-2.13918100	-1.24092800	-1.51770500
H	-1.92916200	-2.33549100	-0.15780100
H	-3.25722000	2.46964300	0.08252400
H	-3.04608000	1.37812700	1.44193200
H	-4.32991300	-1.67889200	-0.45512400
H	-3.70975400	-1.18124000	1.11088700
H	-5.01694200	0.67070900	0.12053000
H	-4.05173200	0.61235200	-1.34675600
H	1.22371300	0.19805200	2.31896100

### 71-radical

N	-1.36676000	0.39838100	-0.42221100
O	-1.48012400	1.54648900	-0.98097600
C	-2.57253800	-0.17336700	0.27027800
C	-3.33550400	0.98560700	0.92362900
C	-3.45673700	-0.86523500	-0.78598600
C	-2.13316100	-1.17162500	1.35260800
C	-0.25197300	-0.45007300	-0.87749100
C	1.04319600	-0.27722800	-0.06346300
C	2.09629300	-1.29813900	-0.53300500
C	1.60532500	1.15220900	-0.14058000
C	3.41539800	-1.16217800	0.24177400
C	2.91914100	1.28965200	0.64237500
C	3.96599500	0.26893500	0.17663500
H	-2.70647800	1.50307300	1.65177200
H	-3.65706500	1.71226200	0.17942900
H	-4.21358500	0.59116200	1.44132800
H	-2.93726500	-1.70346700	-1.25868600
H	-4.36746500	-1.25465300	-0.32244000
H	-3.74145600	-0.15214600	-1.56252500
H	-3.01715100	-1.54211100	1.87769900
H	-1.61310500	-2.03936600	0.94159500
H	-1.48175300	-0.69295800	2.08773800
H	-0.07330900	-0.18309200	-1.92293400
H	-0.56556100	-1.49647300	-0.84886100
H	0.81086200	-0.49551600	0.98792900
H	2.28819600	-1.14478000	-1.60392000
H	1.70489900	-2.31710000	-0.43004600
H	1.78110400	1.40548900	-1.19462900
H	0.86442700	1.86828700	0.22224700
H	4.15219700	-1.87204300	-0.14845900
H	3.24555600	-1.43624000	1.29127100
H	3.30887200	2.30738500	0.53806800
H	2.72197400	1.14225100	1.71269000
H	4.87561300	0.35110600	0.78068900

H 4.25618800 0.49701700 -0.85730700

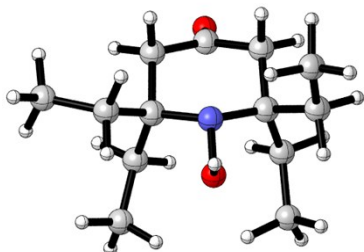
**Entry 72**

C -1.48929200 -1.00918900 -1.23433800  
C -1.38443500 -0.00389600 -0.04031300  
C 1.23497200 -0.06663600 -0.23048200  
C 0.96064700 -0.77187500 -1.58758300  
C -0.19136000 -1.76997500 -1.51325500  
C 2.26967800 -0.89088300 0.58961800  
C 3.70307500 -0.95416800 0.04743900  
C -2.41353200 -0.39346600 1.05620800  
C -2.18238800 -1.74381000 1.74154100  
N -0.02818500 -0.15433300 0.56592800  
C 1.77812200 1.36023600 -0.54684300  
C 2.32201100 2.23611000 0.59000100  
C -1.66607300 1.45070700 -0.51669100  
C -3.10648200 1.75722200 -0.95073800  
O 0.06822700 0.72276400 1.70510200  
H -2.30808000 -1.71202200 -1.06075700  
H -1.75579000 -0.45180800 -2.13796700  
H 0.71601600 -0.01884400 -2.34603300  
H 1.87881300 -1.25485000 -1.92877700  
H -0.28129200 -2.31309000 -2.45980100  
H -0.00298600 -2.51587000 -0.73570100  
H 1.87217900 -1.90687600 0.68145800  
H 2.29815100 -0.48323800 1.60361200  
H 3.75117800 -1.37241200 -0.96179400  
H 4.18257900 0.02700300 0.02165200  
H 4.31320900 -1.59694700 0.68858500  
H -3.40143200 -0.40558200 0.58691600  
H -2.44297700 0.39880500 1.80985300  
H -2.18335100 -2.57145200 1.02670300  
H -1.22651300 -1.78026600 2.26923600  
H -2.97631400 -1.93900200 2.46835200  
H 2.58024100 1.21291400 -1.28053700  
H 1.00234300 1.91488000 -1.07915900  
H 2.80214900 3.12465700 0.16728200  
H 1.53158300 2.55974800 1.26432900  
H 3.07362700 1.71668400 1.18984900  
H -1.00382000 1.66494900 -1.35995400  
H -1.38165900 2.13143800 0.29039700  
H -3.46491700 1.06006400 -1.71455200  
H -3.80685500 1.72242900 -0.11340600  
H -3.16271000 2.76271600 -1.37765200  
H 0.03844100 0.12192600 2.45816500

**72-radical**

C	-1.41691300	-1.27490200	-1.26830300
C	-1.49385100	-0.09123100	-0.25742000
C	1.20154300	-0.09824900	-0.22817100
C	1.04729200	-1.06877100	-1.42066000
C	-0.10316000	-2.05188800	-1.22683300
C	2.04716600	-0.75235000	0.89902900
C	3.52734800	-0.99058700	0.58180100
C	-2.49186300	-0.42489200	0.87884100
C	-2.16166700	-1.66820200	1.70883800
O	-0.16283400	0.83284300	1.47739600
N	-0.15232700	0.17200400	0.37765600
C	1.83012000	1.22492500	-0.74730700
C	2.20592900	2.29914800	0.27760200
C	-1.96352600	1.17652900	-1.03137600
C	-2.15967500	2.46976900	-0.23652800
H	-2.26707200	-1.94048300	-1.09836000
H	-1.53782900	-0.88145100	-2.28295800
H	0.86807600	-0.49924100	-2.34017600
H	1.99542400	-1.59014300	-1.56865500
H	-0.09697700	-2.80425900	-2.02159900
H	0.00637900	-2.59187500	-0.28125700
H	1.57700900	-1.70675100	1.15956200
H	1.95845400	-0.12254400	1.78464200
H	4.00994800	-1.47767600	1.43362200
H	3.67673600	-1.64094300	-0.28464600
H	4.06641200	-0.05902500	0.39442400
H	-3.47139900	-0.54696500	0.40170700
H	-2.56334100	0.43107600	1.54847800
H	-2.93268700	-1.82666400	2.46790000
H	-2.11281900	-2.57666600	1.10187300
H	-1.20834600	-1.54838100	2.22697400
H	2.72312300	0.94423100	-1.31842700
H	1.13660500	1.65236900	-1.47943700
H	2.95331300	1.94298200	0.99054900
H	2.63146400	3.16526100	-0.23849800
H	1.34034000	2.62899500	0.85125300
H	-2.90595000	0.90896300	-1.52544700
H	-1.24543100	1.35448400	-1.83978200
H	-2.43345300	3.28096400	-0.91788400
H	-2.95899900	2.38032300	0.50221500
H	-1.25248100	2.76086400	0.29408600

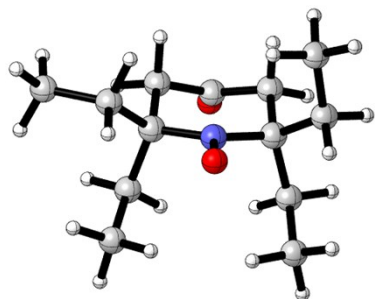
**Entry 73**



C	1.4041955	1.8450107	-0.2414719
C	1.4764555	0.2994617	-0.1144439
C	-1.1370825	0.2612117	0.1392431
C	-1.1108755	1.8050427	-0.0503389
C	0.0888465	2.3007497	-0.8254959
C	-2.0843575	-0.0653333	1.3259951
C	-3.5412205	0.3878287	1.1753261
C	2.6874075	-0.0791963	0.7821031
C	2.6541545	0.4016797	2.2361241
N	0.2346455	-0.1243303	0.5956331
C	-1.6546735	-0.3893093	-1.1812789
C	-2.0315955	-1.8770753	-1.1579959
C	1.7339965	-0.2593573	-1.5505899
C	1.8147855	-1.7762023	-1.7585099
O	0.0001585	3.0110257	-1.8047709
O	0.2847115	-1.5476963	0.8152551
H	1.4863135	2.2937317	0.7529461
H	2.2263595	2.2121147	-0.8568509
H	-2.0189035	2.1477377	-0.5444169
H	-1.0606585	2.2730167	0.9402831
H	-1.6503825	0.3992547	2.2178901
H	-2.0656195	-1.1434983	1.4960251
H	-4.1086995	0.1085227	2.0672381
H	-3.6310985	1.4712907	1.0625671
H	-4.0342685	-0.0786973	0.3189711
H	3.5842505	0.3153627	0.2920381
H	2.7894895	-1.1657143	0.7728631
H	3.5166845	0.0054547	2.7791801
H	2.6966775	1.4907637	2.3189261
H	1.7493845	0.0724937	2.7523791
H	-2.5429655	0.1769807	-1.4804229
H	-0.9283525	-0.2123703	-1.9757909
H	-2.8541605	-2.0768793	-0.4665149
H	-2.3660895	-2.1833063	-2.1536409
H	-1.1971315	-2.5121353	-0.8667489
H	2.6874725	0.1788377	-1.8686719
H	0.9941005	0.1572867	-2.2384429
H	2.5924155	-2.2360983	-1.1448019
H	0.8767255	-2.2770483	-1.5269049

H	2.0606965	-1.9835583	-2.8044079
H	0.3782075	-1.6270533	1.7715231

### 73-radical



C	1.4116187	1.7912078	-0.2793941
C	1.5142417	0.2528888	-0.1140921
C	-1.1628393	0.2354498	0.1258630
C	-1.0945973	1.7740428	-0.0588210
C	0.0945377	2.2249808	-0.8748970
C	-2.0405263	-0.0948732	1.3580370
C	-3.4944733	0.3811678	1.2732660
C	2.6445107	-0.0967472	0.8837120
C	2.4661517	0.3916168	2.3239670
O	0.2826417	-1.4605622	0.9609049
N	0.2198267	-0.2962032	0.4283590
C	-1.7217783	-0.4009602	-1.1793680
C	-2.0083373	-1.9050332	-1.1457610
C	1.8398577	-0.3499642	-1.5147530
C	1.9695807	-1.8718942	-1.6197891
O	-0.0010793	2.8802728	-1.8902280
H	1.4923837	2.2715488	0.7004890
H	2.2319227	2.1494998	-0.9023720
H	-2.0089073	2.1373028	-0.5267680
H	-1.0055273	2.2425218	0.9286530
H	-1.5596363	0.3553158	2.2329709
H	-2.0112563	-1.1714172	1.5213679
H	-3.5774493	1.4654968	1.1599330
H	-4.0340353	-0.0838272	0.4442760
H	-4.0211623	0.1118808	2.1924309
H	3.5677687	0.3179418	0.4629930
H	2.7604387	-1.1797842	0.9003920
H	1.5596957	-0.0212992	2.7697079
H	3.3130037	0.0607308	2.9311060
H	2.4261937	1.4817338	2.4026260
H	-2.6466393	0.1315898	-1.4235981
H	-1.0354653	-0.1736432	-1.9994811
H	-2.8217813	-2.1458442	-0.4571970



H	-2.3096483	-2.2452872	-2.1404091
H	-1.1371143	-2.4818492	-0.8358760
H	2.7827017	0.1098728	-1.8322330
H	1.0905817	0.0013058	-2.2299811
H	1.0704847	-2.3852422	-1.2799980
H	2.1465227	-2.1500512	-2.6626831
H	2.8075887	-2.2538862	-1.0333541

#### Entry 74

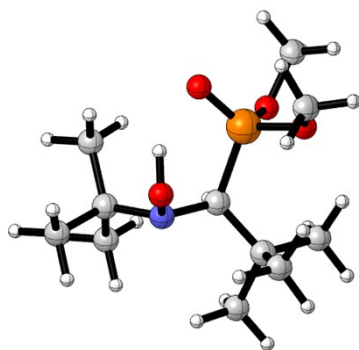
C	-1.15358900	0.14445500	0.19689200
C	1.32036900	0.04548300	0.02827600
C	0.90664600	0.36856000	1.49186600
C	-0.55359500	0.85904600	1.42764700
C	2.35739800	1.04264200	-0.54721600
C	1.86473100	-1.40021300	-0.11556500
C	-1.60825600	-1.28848500	0.60373900
C	-2.30128200	0.94696600	-0.45133500
N	0.02812500	0.25134100	-0.69873800
C	-2.20187400	-2.19740700	-0.48081300
C	1.96543900	2.52172100	-0.50569400
C	-3.57095200	1.10117500	0.39397000
C	3.14197100	-1.70939800	0.67708200
O	-0.07282300	-0.55790300	-1.87705800
H	0.97148500	-0.53539900	2.10134900
H	1.56467400	1.10656700	1.95433300
H	-1.10448300	0.63607900	2.34325700
H	-0.58869200	1.94053200	1.27234100
H	2.55267000	0.75184400	-1.58687900
H	3.30335900	0.90940400	-0.01321900
H	1.08254700	-2.09943400	0.19058800
H	2.04073400	-1.59625600	-1.17579800
H	-2.35442600	-1.16265000	1.39661000
H	-0.77075500	-1.80426500	1.08061800
H	-2.55808100	0.47997900	-1.40749300
H	-1.90085900	1.93720900	-0.69148600
H	-1.47612000	-2.42528000	-1.26001400
H	-2.53531200	-3.13821900	-0.03171400
H	-3.07204900	-1.74281700	-0.96220400
H	1.02653400	2.69442600	-1.03494900
H	1.84462200	2.88521000	0.51929100
H	2.74060800	3.13408200	-0.97541300
H	-4.29328200	1.74077600	-0.12088800
H	-4.06223600	0.14310900	0.58211900
H	-3.35927100	1.56284100	1.36297400
H	3.39244400	-2.76984400	0.58200000
H	4.00254500	-1.14243300	0.31476200

H	3.02998700	-1.49764900	1.74476900
H	-0.09298100	0.08875100	-2.59041700

**74-radical**

C	-1.13694600	-0.17358300	0.30291500
C	1.37373800	0.03069800	0.07227300
C	0.94238000	0.38764400	1.50680200
C	-0.44655500	-0.25323200	1.68411400
C	2.23579900	1.10165000	-0.62748200
C	2.06064400	-1.36026600	-0.01075600
C	-1.95766400	-1.45702100	0.02517900
C	-1.96494900	1.12314300	0.12651900
N	0.04811800	-0.08859100	-0.60569300
O	-0.05076600	-0.12654600	-1.87471700
C	-2.75270400	-1.52290300	-1.28360100
C	1.58535400	2.47200800	-0.83694700
C	-3.25972800	1.19780900	0.94279400
C	3.48377900	-1.44495600	0.55245600
H	1.65640500	0.02801100	2.24995300
H	0.87617800	1.47160600	1.62266500
H	-0.34492100	-1.30012900	1.98352400
H	-1.03113800	0.24426300	2.45960400
H	2.53237700	0.70184000	-1.60172800
H	3.15355100	1.21948600	-0.04286900
H	1.42713300	-2.08774100	0.50773000
H	2.06380600	-1.65184700	-1.06556400
H	-2.63999000	-1.58979000	0.87303400
H	-1.26216800	-2.30210500	0.06492400
H	-2.18876800	1.23118400	-0.93814100
H	-1.32477500	1.97205700	0.38859600
H	-3.26455600	-2.48722500	-1.35478300
H	-3.51753100	-0.74407100	-1.33958000
H	-2.09841000	-1.41239300	-2.14773500
H	0.69592900	2.39338600	-1.46414300
H	1.30315200	2.95063000	0.10508600
H	2.28824700	3.14246600	-1.33901600
H	-3.74214900	2.16743800	0.79189500
H	-3.97712000	0.42778300	0.65004700
H	-3.07763400	1.09072200	2.01613400
H	4.18886700	-0.83838900	-0.02003400
H	3.53504400	-1.12209300	1.59676900
H	3.83887600	-2.47853100	0.51561500

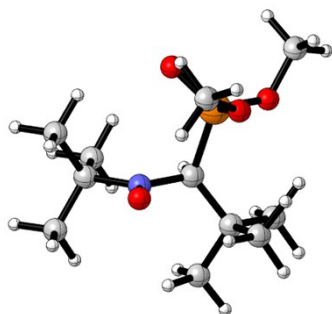
**Entry 75**



N	0.9388165	-0.4063829	0.8254985
C	0.7845925	-0.2750059	2.3135405
C	2.1581785	-0.6138029	2.9218475
C	0.3312905	1.1163081	2.8005925
C	-0.2235985	-1.3313469	2.7994915
C	-0.2214085	-0.3150009	-0.0697685
C	-0.2350505	-1.4662449	-1.1484725
P	-0.4938685	1.4297891	-0.7093635
O	0.2565355	2.4864171	0.0350575
O	-2.1029435	1.5235311	-0.6336035
O	-0.2328405	1.5398081	-2.3080525
C	-2.7965315	2.7115391	-1.0683325
C	0.9137415	2.2423781	-2.8354865
C	-1.5074075	-1.3787859	-2.0162775
C	-0.2687115	-2.8120199	-0.3963145
C	1.0182075	-1.4472469	-2.0412565
O	2.0340885	0.3691471	0.3375315
H	2.0823365	-0.6293219	4.0122575
H	2.4945765	-1.5954519	2.5802095
H	2.9125975	0.1190141	2.6380255
H	0.3079905	1.1253981	3.8943185
H	1.0049135	1.9082941	2.4721775
H	-0.6705305	1.3668061	2.4441895
H	-0.2475645	-1.3167779	3.8917395
H	-1.2425245	-1.1350589	2.4567335
H	0.0660225	-2.3326639	2.4783675
H	-1.1187545	-0.4636559	0.5354215
H	-3.8483345	2.5477731	-0.8418625
H	-2.4313855	3.5861691	-0.5263725
H	-2.6658565	2.8514621	-2.1432325
H	0.7146765	2.3838301	-3.8967005
H	1.0349235	3.2049531	-2.3388305
H	1.8183495	1.6450511	-2.7045245
H	-2.4125875	-1.3745409	-1.4016025
H	-1.5564435	-2.2524539	-2.6726985
H	-1.5198665	-0.4906459	-2.6487075
H	-1.1569005	-2.8979129	0.2372455

H	0.6168305	-2.9342089	0.2278525
H	-0.2963045	-3.6332149	-1.1182225
H	1.0123475	-2.3262249	-2.6933005
H	1.9288015	-1.4713029	-1.4412905
H	1.0474995	-0.5649279	-2.6813295
H	1.7720955	1.3065321	0.4335055

### 75-radical



N	0.9966227	-0.3861889	0.3809191
O	0.8546537	-0.7387139	1.6035761
C	2.1722937	-0.9858709	-0.3648439
C	3.4498277	-0.4852909	0.3308851
C	2.0647437	-2.5172229	-0.2502889
C	2.1733137	-0.5751329	-1.8409599
C	-0.0770583	0.4356981	-0.2104479
C	-0.2921243	1.8158951	0.5221331
P	-1.5084823	-0.7298109	-0.5036239
O	-1.0820733	-1.9501069	-1.2394769
O	-2.5589533	0.2191041	-1.2739939
O	-2.3105463	-1.0355269	0.8615451
C	-3.7725133	-0.3387239	-1.8218709
C	-2.0412403	-2.1993129	1.6784651
C	-1.0500603	2.7693661	-0.4257119
C	1.0968287	2.4301651	0.7983751
C	-1.0590123	1.7050821	1.8526911
H	4.3223857	-0.9753599	-0.1085079
H	3.5692857	0.5946451	0.2143751
H	3.4184987	-0.7205699	1.3954691
H	2.9237957	-2.9789109	-0.7446239
H	2.0638687	-2.8190319	0.7977431
H	1.1477727	-2.8709279	-0.7236469
H	3.0418007	-1.0316079	-2.3215789
H	1.2820727	-0.9347349	-2.3589809
H	2.2642857	0.5066951	-1.9715819
H	0.2290517	0.6714981	-1.2292569
H	-4.2496563	0.4647741	-2.3799229
H	-3.5402603	-1.1710539	-2.4885649
H	-4.4296313	-0.6729289	-1.0165249

H	-1.1554093	-2.0198679	2.2874431
H	-2.9197143	-2.3298169	2.3085911
H	-1.8961993	-3.0774029	1.0478111
H	-2.0524373	2.4100581	-0.6534809
H	-0.5144653	2.9024941	-1.3716619
H	-1.1365553	3.7519911	0.0464901
H	1.6884167	2.5216561	-0.1182679
H	1.6631127	1.8408461	1.5202591
H	0.9707097	3.4357611	1.2090911
H	-0.5526403	1.0308651	2.5432161
H	-2.0768773	1.3412431	1.7055671
H	-1.1174323	2.6962781	2.3131741

**Entry 76**

N	-0.76590900	-0.45750900	-0.48542600
C	-2.14638500	0.02433500	-0.23874200
C	-3.04163400	-0.42362300	-1.40823300
C	-2.78306000	-0.39036100	1.10499700
C	-4.47343500	0.11389700	-1.27734200
C	-4.20524700	0.17761900	1.23761100
C	-5.10123600	-0.26003000	0.07180300
C	0.39005800	0.39933800	-0.09531400
C	0.43700400	1.56674800	-1.12469900
C	0.34694500	0.94616100	1.35387100
C	1.37606900	2.73787300	-0.78261000
C	1.39451100	2.03042600	1.64586200
C	1.23956900	3.20468900	0.67201800
P	1.86413800	-0.76160500	-0.35223500
O	1.70996200	-1.80643500	-1.40450800
O	2.29970700	-1.35753500	1.09460800
O	3.07915200	0.27201500	-0.60523700
C	2.00934200	-2.70862800	1.49980100
C	4.40039700	-0.23078900	-0.88693300
O	-0.63043600	-1.76463800	0.11702000
H	-2.09554200	1.11770000	-0.26100700
H	-3.05634000	-1.51984500	-1.43109700
H	-2.58913100	-0.09525800	-2.34783000
H	-2.81942800	-1.48162700	1.15195500
H	-2.16816000	-0.06359800	1.94618100
H	-5.08850900	-0.26065600	-2.10200500
H	-4.45949900	1.20787700	-1.37597400
H	-4.63966200	-0.14213200	2.19052600
H	-4.16404100	1.27484300	1.27020100
H	-6.09576700	0.18847000	0.16629000
H	-5.24247000	-1.34761300	0.11621800
H	-0.58138000	1.96164900	-1.19033400

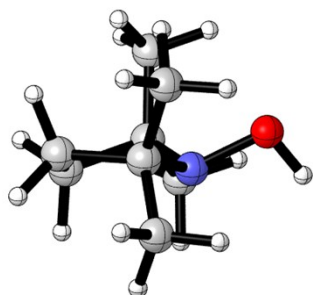
H	0.66424100	1.16398700	-2.11494700
H	-0.64018000	1.39873000	1.49258800
H	0.42630200	0.12261300	2.06523300
H	1.15145000	3.56428300	-1.46529500
H	2.40940300	2.44519500	-0.96877300
H	1.27047500	2.37311700	2.67833600
H	2.40422900	1.61588200	1.57145800
H	1.98334200	3.97935200	0.88458300
H	0.25508300	3.66780600	0.82397000
H	0.97562000	-2.78341200	1.83987000
H	2.17838200	-3.39968900	0.67235000
H	2.69353000	-2.93165800	2.31785600
H	5.00222100	0.63388900	-1.16197700
H	4.81961600	-0.70541100	0.00295500
H	4.36927200	-0.94203300	-1.71427300
H	-0.28823800	-2.28901100	-0.62313900

#### 76-radical

N	-0.77531100	-0.44255800	-0.01549700
O	-0.63379200	-1.70726600	0.13808500
C	-2.15806200	0.08936200	-0.01290000
C	-2.86337400	-0.28061800	-1.33001100
C	-2.94291300	-0.42829800	1.20477000
C	-4.31880200	0.20758300	-1.34488200
C	-4.39561600	0.06972200	1.18111700
C	-5.10187200	-0.30391900	-0.12874200
C	0.44688400	0.41039100	0.02742600
C	0.37623600	1.48841600	-1.09158600
C	0.55250100	1.05113000	1.44027500
C	1.35616500	2.66210900	-0.92916700
C	1.53318300	2.22792100	1.55557900
C	1.27869000	3.28106400	0.47125700
P	1.84715000	-0.79778100	-0.36517500
O	1.77719000	-1.46888800	-1.68620400
O	2.13238300	-1.75723600	0.90305200
O	3.09718200	0.22562600	-0.20148400
C	1.76835300	-3.15440000	0.92198500
C	4.43192600	-0.23788300	-0.47864200
H	-2.08350400	1.17762900	0.06006600
H	-2.82747700	-1.36992100	-1.43388600
H	-2.30867600	0.13618100	-2.17553800
H	-2.91862300	-1.52122600	1.18659900
H	-2.44410500	-0.11388700	2.12674600
H	-4.80241400	-0.11206200	-2.27316300
H	-4.33674300	1.30574500	-1.34985000
H	-4.93663800	-0.34450300	2.03769800

H	-4.41409300	1.16108700	1.30326100
H	-6.12004900	0.09811500	-0.13756100
H	-5.19460800	-1.39545800	-0.19086700
H	-0.63616000	1.90280700	-1.08241500
H	0.50424300	1.00342900	-2.06270300
H	-0.44955100	1.42150700	1.68747400
H	0.78546800	0.27174000	2.17001600
H	1.11705600	3.41279200	-1.68946600
H	2.37626000	2.32644900	-1.12275700
H	1.42245600	2.67240700	2.55019800
H	2.55939000	1.86435000	1.47865500
H	2.00388700	4.09593700	0.56139800
H	0.28687200	3.72967400	0.62117300
H	0.77445100	-3.26512900	1.35185300
H	1.78031900	-3.56475400	-0.08817900
H	2.51485300	-3.65100900	1.54189500
H	4.48210800	-0.68870600	-1.47187200
H	5.07641700	0.63911800	-0.43690500
H	4.74531200	-0.96106200	0.27777200

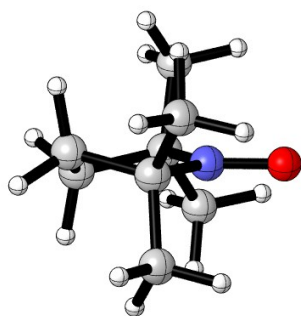
### Entry 77



C	1.2374328	0.0804471	-0.0951200
C	-1.2251412	0.0049901	-0.0378630
C	-0.7345802	1.4220071	0.3775330
C	0.7187638	1.5285061	-0.1219270
C	-1.8198212	-0.7632539	1.1542580
C	-2.2628332	0.0673281	-1.1692050
C	2.3897088	-0.1564779	-1.0760670
C	1.6709318	-0.3459889	1.3221410
N	0.0227998	-0.6112469	-0.6015240
O	0.0804908	-2.0231329	-0.3527260
H	-1.3698702	2.2064351	-0.0390510
H	-0.7731622	1.5240551	1.4647970
H	0.7465268	1.9050051	-1.1481800
H	1.3298578	2.1924711	0.4936120
H	-2.1615932	-1.7546349	0.8537470
H	-1.0986312	-0.8901169	1.9629020

H	-2.6772852	-0.2077369	1.5458420
H	-2.4926712	-0.9382689	-1.5336440
H	-3.1960672	0.5206641	-0.8202530
H	-1.8816172	0.6533451	-2.0089240
H	3.2621658	0.4433771	-0.8008890
H	2.6925538	-1.2074409	-1.0692790
H	2.0880198	0.1102181	-2.0917000
H	2.6215568	0.1314301	1.5764790
H	0.9430388	-0.0616619	2.0839400
H	1.8074768	-1.4276909	1.3684450
H	0.0819498	-2.4026289	-1.2373430

### 77-radical



C	-1.2607992	-0.0489240	0.0290559
C	1.2603598	-0.0644160	-0.0129241
C	0.7191938	1.3031780	-0.4759661
C	-0.7090272	1.3893770	0.0952439
C	2.1799118	-0.7349780	-1.0367831
C	1.9498258	0.0076210	1.3613489
C	-2.1845082	-0.4023240	1.1975489
C	-1.9508302	-0.3558250	-1.3121611
N	-0.0032222	-0.8479200	0.1201909
O	-0.0079942	-2.1064690	0.2980959
H	1.3520998	2.1260410	-0.1375711
H	0.6932048	1.3379570	-1.5688151
H	-0.6816222	1.7256420	1.1356199
H	-1.3361662	2.0908050	-0.4587231
H	2.4486058	-1.7392460	-0.7043621
H	1.6880968	-0.8174380	-2.0090331
H	3.0950758	-0.1491190	-1.1594331
H	2.1379868	-1.0011220	1.7350409
H	2.9054288	0.5330680	1.2791299
H	1.3307678	0.5328190	2.0931259
H	-3.0952082	0.2012630	1.1516529
H	-2.4609042	-1.4573940	1.1564369
H	-1.6925572	-0.2154240	2.1551519
H	-2.1468562	-1.4272150	-1.3916011



H	-2.9023962	0.1788970	-1.3801511
H	-1.3284652	-0.0588540	-2.1601181

**Entry 78**

C	-1.27949900	-0.41271200	0.05654300
C	-1.75714300	0.96006200	-0.49290900
C	-1.06651500	2.25085700	-0.05025800
C	0.43151400	2.31186800	-0.35261500
C	1.36083600	-0.13745600	0.06611700
C	1.24035800	1.34026100	0.51405500
C	-1.40409600	-0.51178200	1.59068800
C	-2.25250400	-1.44642500	-0.55385200
C	1.90537500	-0.94232800	1.26990900
C	2.39063300	-0.22262800	-1.08110300
N	0.08564600	-0.69478500	-0.50889400
H	-1.70268400	0.89337000	-1.58500300
H	-2.81968000	1.04613400	-0.23917700
H	-1.21819800	2.41520400	1.02388800
H	-1.57350000	3.08231100	-0.55347100
H	0.60944700	2.12723600	-1.41777200
H	0.78780800	3.32837800	-0.15310300
H	2.27151500	1.69942100	0.58804500
H	0.84646100	1.38321700	1.53472600
H	-2.44954600	-0.37651800	1.88535500
H	-1.08796700	-1.49933600	1.93373300
H	-0.81749900	0.24062100	2.11700400
H	-2.06398000	-2.45058900	-0.17780300
H	-3.27689900	-1.16813600	-0.29499200
H	-2.17501400	-1.45981000	-1.64475400
H	2.85117000	-0.50035500	1.59730400
H	1.22086900	-0.92430700	2.11881200
H	2.08934700	-1.98102700	0.99880400
H	3.37155000	0.12124000	-0.74091800
H	2.49874300	-1.25244300	-1.42533200
H	2.08120400	0.39228000	-1.92915000
O	0.29257900	-2.13157300	-0.54863500
H	0.20294500	-2.33911800	-1.48430800

**78-radical**

C	-1.33050000	-0.38962600	0.06727700
C	-1.64910200	0.96601000	-0.61542100
C	-0.96325300	2.23850000	-0.11309500
C	0.55679100	2.26506200	-0.28126200
C	1.38196200	-0.22538700	0.08515900
C	1.29429500	1.23444700	0.58291500
C	-1.51100400	-0.34870700	1.59845800

C	-2.32077200	-1.42246800	-0.49787000
C	2.00589000	-1.08826600	1.20128700
C	2.27711200	-0.29486200	-1.16845800
N	0.06087600	-0.85766300	-0.29717500
O	0.17493400	-2.04572300	-0.76659100
H	-1.44709900	0.84572900	-1.68612100
H	-2.73122000	1.10962000	-0.52457800
H	-1.21296100	2.40922100	0.94110100
H	-1.39493000	3.08368400	-0.66089100
H	0.81557600	2.13532100	-1.33790100
H	0.91888800	3.26087300	-0.00372900
H	2.33689200	1.55130900	0.68858900
H	0.88383500	1.26227300	1.59672200
H	-2.53650900	-0.05181800	1.83745100
H	-1.34097200	-1.34209100	2.01989300
H	-0.84241500	0.35180700	2.09543900
H	-2.14777900	-2.41235500	-0.07908300
H	-3.33479400	-1.10192100	-0.24524100
H	-2.23759400	-1.50099100	-1.58254700
H	3.00723000	-0.72159500	1.44334000
H	1.40234700	-1.05424500	2.11174000
H	2.08239300	-2.12512900	0.87273200
H	3.27341900	0.08666300	-0.93028500
H	2.36440800	-1.32498400	-1.51009200
H	1.86717300	0.29983500	-1.98752000

### Entry 79

C	1.25842100	1.39952700	-0.49804700
C	1.17334500	-0.06281100	-0.00212800
C	-1.17334500	-0.06281100	-0.00212800
C	-1.25842100	1.39952700	-0.49804700
C	0.00000000	2.20542600	-0.15991700
C	0.77470100	-0.13088500	1.50218100
C	-0.77470100	-0.13088500	1.50218100
N	0.00000000	-0.65744800	-0.72038800
C	2.47234300	-0.79385900	-0.32734900
C	-2.47234300	-0.79385900	-0.32734900
H	2.14501600	1.86925300	-0.05943000
H	1.40774900	1.37559800	-1.58257400
H	-2.14501600	1.86925300	-0.05943000
H	-1.40774900	1.37559800	-1.58257400
H	0.00000000	2.46073500	0.90513600
H	0.00000000	3.15738400	-0.69964700
H	1.20070100	0.70293400	2.06629000
H	1.15852500	-1.05245300	1.94350000
H	-1.15852500	-1.05245300	1.94350000

H	-1.20070100	0.70293400	2.06629000
H	3.30485700	-0.31169300	0.19309400
H	2.42824300	-1.83619700	-0.01282000
H	2.68023400	-0.76003300	-1.40083100
H	-3.30485700	-0.31169300	0.19309400
H	-2.68023400	-0.76003300	-1.40083100
H	-2.42824300	-1.83619700	-0.01282000
O	0.00000000	-2.08552900	-0.41305600
H	0.00000000	-2.48279700	-1.28917500

### 79-radical

C	1.27411400	1.30631300	-0.59003900
C	1.20104100	-0.09559700	0.05620000
C	-1.20104100	-0.09559700	0.05620000
C	-1.27411400	1.30631300	-0.59003900
C	0.00000000	2.13012100	-0.34289000
C	0.77804300	-0.01022100	1.55050400
C	-0.77804300	-0.01022100	1.55050400
N	0.00000000	-0.76030000	-0.55040500
O	0.00000000	-2.00161400	-0.84370700
C	2.46793800	-0.89885800	-0.18828200
C	-2.46793800	-0.89885800	-0.18828200
H	2.14906200	1.83713500	-0.19983800
H	1.43258600	1.17091400	-1.66526800
H	-2.14906200	1.83713500	-0.19983800
H	-1.43258600	1.17091500	-1.66526800
H	0.00000000	2.49835900	0.68841100
H	0.00000000	3.01980000	-0.97959000
H	1.19841200	0.87537600	2.03313100
H	1.15861600	-0.88395700	2.08360900
H	-1.15861600	-0.88395600	2.08360900
H	-1.19841100	0.87537600	2.03313100
H	3.30791900	-0.41776900	0.32058600
H	2.36419500	-1.91699000	0.18786700
H	2.69715200	-0.95647700	-1.25487800
H	-3.30791900	-0.41776800	0.32058400
H	-2.69715100	-0.95647900	-1.25487800
H	-2.36419600	-1.91699000	0.18786900

### Entry 80

C	-0.72210200	0.69753000	0.03436800
C	-0.72210200	-0.69753000	0.03436800
C	-1.92048700	-1.40429900	0.00176000
C	-3.12399100	-0.69804400	-0.03518300
C	-3.12399100	0.69804400	-0.03518300

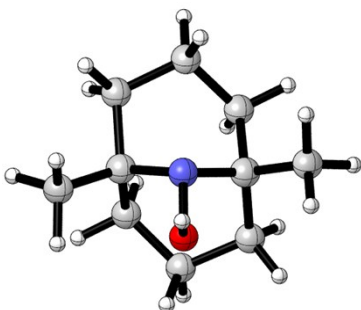
C	-1.92048700	1.40429900	0.00176000
C	0.69474200	-1.23756600	0.04891600
C	0.69474200	1.23756600	0.04891600
N	1.43025100	0.00000000	0.46241600
C	1.09730500	1.79061500	-1.33531300
C	0.92230400	2.31571700	1.11889300
C	0.92230400	-2.31571700	1.11889300
C	1.09730500	-1.79061500	-1.33531300
O	2.77774100	0.00000000	-0.01905100
H	-1.92761800	-2.48917800	0.00614000
H	-4.06464400	-1.23685900	-0.06075100
H	-4.06464400	1.23685900	-0.06075100
H	-1.92761800	2.48917800	0.00614000
H	0.50895200	2.68588400	-1.55366400
H	2.15491900	2.05877100	-1.34563700
H	0.91763500	1.06983200	-2.13320400
H	1.98111400	2.58734600	1.15745000
H	0.35532500	3.22283000	0.89102100
H	0.62023300	1.94877300	2.10122500
H	0.35532500	-3.22283000	0.89102100
H	1.98111400	-2.58734600	1.15745000
H	0.62023300	-1.94877300	2.10122500
H	2.15491900	-2.05877100	-1.34563700
H	0.50895200	-2.68588400	-1.55366400
H	0.91763500	-1.06983200	-2.13320400
H	3.30123300	0.00000000	0.78903700

### 80-radical

C	-0.00003800	0.68889900	-0.69831900
C	-0.00003800	0.68889900	0.69831900
C	-0.00002600	1.88944200	1.40307400
C	-0.00000200	3.09307100	0.69802000
C	-0.00000200	3.09307100	-0.69802000
C	-0.00002600	1.88944200	-1.40307400
C	-0.00004400	-0.71519500	1.26320300
C	-0.00004400	-0.71519500	-1.26320300
N	-0.00073800	-1.51131900	0.00000000
O	-0.00055100	-2.78090100	0.00000000
C	-1.26418500	-1.04177500	-2.07680300
C	1.26474300	-1.04208700	-2.07571500
C	1.26474300	-1.04208700	2.07571500
C	-1.26418500	-1.04177500	2.07680300
H	-0.00004800	1.89568700	2.48784000
H	0.00000100	4.03354000	1.23722800
H	0.00000100	4.03354000	-1.23722800
H	-0.00004800	1.89568700	-2.48784000

H	-1.27225300	-0.47175500	-3.00920800
H	-1.28043800	-2.10686900	-2.31663200
H	-2.16660900	-0.79588600	-1.51351200
H	1.28089900	-2.10716000	-2.31563900
H	1.27379900	-0.47194800	-3.00803700
H	2.16674600	-0.79651500	-1.51161000
H	1.27379900	-0.47194800	3.00803700
H	1.28089900	-2.10716000	2.31563900
H	2.16674600	-0.79651500	1.51161000
H	-1.28043800	-2.10686900	2.31663200
H	-1.27225300	-0.47175500	3.00920800
H	-2.16660900	-0.79588600	1.51351200

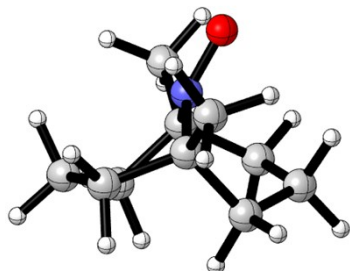
### Entry 81



C	-0.0446823	-1.9235745	-1.0265873
C	1.3391257	-1.3274045	-0.6844303
C	-1.3278963	1.5616865	-0.2275303
C	1.2317527	-0.0150295	0.1423447
C	0.0579047	2.2304415	-0.3327533
C	1.1199857	1.2320135	-0.7994213
C	-1.1371223	-0.8497495	-1.1318363
C	-1.2300203	0.0546555	0.1459337
N	0.0038617	-0.0243075	0.9893577
C	2.4481597	0.1476585	1.0605437
C	-2.4496323	-0.3406665	0.9828747
H	-0.3231473	-2.6351185	-0.2468833
H	0.0079397	-2.4856225	-1.9638143
H	1.9061327	-1.1131435	-1.5969263
H	1.9174207	-2.0666795	-0.1252893
H	-1.9211793	2.0828245	0.5293027
H	-1.8754343	1.6493465	-1.1716623
H	0.3429087	2.6267645	0.6451597
H	0.0182267	3.0829915	-1.0178393
H	2.0991877	1.7166505	-0.8487973
H	0.8926497	0.9110155	-1.8190943
H	-2.1059483	-1.3296775	-1.3008093
H	-0.9540323	-0.2313015	-2.0149423

H	3.3685617	0.1269335	0.4692887
H	2.4050657	1.0999995	1.5971857
H	2.4959537	-0.6629875	1.7897077
H	-2.4636303	0.2051895	1.9305497
H	-3.3605483	-0.0879385	0.4323287
H	-2.4615503	-1.4100655	1.1971207
O	0.0154327	-1.2665785	1.7429017
H	-0.0154463	-0.9583265	2.6540177

### 81-radical



C	-0.0406800	-1.9759236	-0.8839269
C	1.3532020	-1.3623916	-0.6265889
C	-1.3406950	1.5198694	-0.1755859
C	1.2549220	-0.0437916	0.1983951
C	0.0499990	2.1829414	-0.2257389
C	1.1186490	1.2077654	-0.7280839
C	-1.1258180	-0.9051476	-1.0611509
C	-1.2547720	0.0167674	0.2065811
N	0.0012540	-0.1440776	1.0084461
O	0.0048550	-0.8834916	2.0524151
C	2.4468410	0.1181954	1.1414381
C	-2.4536110	-0.4036906	1.0528291
H	-0.3086520	-2.6088156	-0.0327759
H	-0.0102830	-2.6281076	-1.7613369
H	1.8654000	-1.1452866	-1.5699089
H	1.9716590	-2.0856926	-0.0890069
H	-1.9659040	2.0449074	0.5522041
H	-1.8461320	1.6062104	-1.1430229
H	0.3232030	2.5242734	0.7777171
H	0.0220330	3.0735314	-0.8603159
H	2.0909090	1.7052504	-0.7811819
H	0.8819630	0.9008824	-1.7497469
H	-2.0937900	-1.3803386	-1.2442569
H	-0.9103290	-0.3019336	-1.9468119
H	3.3729080	0.0903064	0.5604341
H	2.4014820	1.0736404	1.6714551
H	2.4651400	-0.6825696	1.8799931
H	-2.4747490	0.1389884	1.9993081

H	-3.3702360	-0.1817956	0.4987651
H	-2.4287670	-1.4704766	1.2794591

### Entry 83

C	-2.85772700	0.01169400	0.00971100
C	-1.52509700	0.42014900	0.04547700
C	-0.42805800	-0.48418600	0.02177300
C	-0.72036900	-1.85995900	0.01037500
C	-2.04340200	-2.27952400	-0.01346600
C	-3.10297600	-1.35412200	-0.02343500
N	-0.98462100	1.68482200	0.12773600
C	0.79276300	0.30595700	0.00810600
C	0.39480300	1.61766900	0.03130700
O	-1.69656400	2.83530300	-0.19644600
C	2.22884400	-0.19616900	-0.00751000
C	2.50906900	-1.04220600	1.25647600
C	3.21793600	0.98412300	-0.02775200
C	2.47406300	-1.05291100	-1.27166500
H	-3.66403600	0.73475400	-0.00288600
H	0.07310100	-2.59676100	0.01179800
H	-2.26589800	-3.34037100	-0.03036000
H	-4.12542800	-1.71249800	-0.05776600
H	0.96455400	2.53161800	0.01388900
H	-1.96752300	3.21238200	0.65170500
H	2.36959300	-0.44402300	2.16115900
H	3.53992500	-1.41073500	1.24740800
H	1.84518400	-1.90621300	1.32494100
H	4.24526700	0.61009900	-0.04536200
H	3.10961300	1.61387500	0.85998900
H	3.07718600	1.60932400	-0.91408300
H	1.80821700	-1.91670900	-1.31684100
H	3.50444000	-1.42246400	-1.28576600
H	2.31157400	-0.46156000	-2.17679100

### 83-radical

C	2.86849700	0.14676700	0.00000300
C	1.52694500	0.49125500	0.00004400
C	0.46926800	-0.44226300	0.00009200
C	0.79890500	-1.80021900	0.00003200
C	2.14508200	-2.17177000	-0.00003200
C	3.16796500	-1.21503600	-0.00005300
N	0.95296600	1.77676000	-0.00002200
C	-0.78846900	0.32087200	-0.00002900
C	-0.43778400	1.64271000	-0.00012000
O	1.59512200	2.87146000	0.00003800

C	-2.20123900	-0.23327400	0.00000300
C	-2.42526000	-1.09448700	-1.26600700
C	-3.23511800	0.90819100	-0.00004900
C	-2.42515100	-1.09434400	1.26611900
H	3.63553900	0.91068800	0.00000100
H	0.03414800	-2.56612300	-0.00002100
H	2.40323600	-3.22457200	-0.00012800
H	4.20281800	-1.53644700	-0.00008400
H	-1.03163100	2.54072000	-0.00016700
H	-2.29203800	-0.49614000	-2.17115900
H	-3.44355200	-1.49485800	-1.27003800
H	-1.73397500	-1.93745500	-1.31934200
H	-4.24613900	0.49250200	-0.00029200
H	-3.13624600	1.54021000	-0.88683100
H	-3.13660200	1.53999900	0.88692300
H	-1.73384000	-1.93729000	1.31948500
H	-3.44343500	-1.49473800	1.27028100
H	-2.29186800	-0.49590600	2.17120300

#### Entry 84

C	-0.44080200	-0.29953400	1.15599700
C	-0.44080200	1.20173200	0.77681500
C	-0.44080200	-0.29953400	-1.15599700
C	-0.44080200	1.20173200	-0.77681500
N	0.09952800	-1.03938600	0.00000000
O	1.54073500	-0.78578800	0.00000000
H	0.14152700	-0.53818900	2.04464900
H	-1.46085800	-0.66764300	1.30561200
H	-1.30767800	1.71820900	1.19462300
H	0.45315800	1.69388600	1.16231900
H	-1.46085800	-0.66764300	-1.30561200
H	0.14152700	-0.53818900	-2.04464900
H	0.45315800	1.69388600	-1.16231900
H	-1.30767800	1.71820900	-1.19462300
H	1.90436000	-1.67689900	0.00000000

#### 84-radical

C	0.00000000	-0.77277200	-1.38689900
C	0.00000000	0.77277200	-1.38689900
C	0.46230500	1.13881100	0.02743400
C	-0.46230500	-1.13881100	0.02743400
H	-0.64379400	-1.19282800	-2.16104000
H	1.01375200	-1.14710300	-1.55614600
H	-1.01375200	1.14710300	-1.55614600
H	0.64379400	1.19282800	-2.16104000
H	1.55406600	1.21877800	0.10469400



H	0.02565000	2.05957100	0.41998500
H	-0.02565000	-2.05957100	0.41998500
H	-1.55406600	-1.21877800	0.10469400
N	0.00000000	0.00000000	0.83614000
O	0.00000000	0.00000000	2.10570200

### Entry 85

C	0.13384700	-1.13246100	-0.00317600
C	1.44750600	-0.71177300	0.00495200
C	1.44751200	0.71176400	0.00556300
C	0.13386500	1.13246000	-0.00357700
N	-0.63768900	0.00000800	0.01356700
O	-2.01741800	-0.00000800	-0.11050100
H	-0.31834900	-2.10961000	-0.02471400
H	2.31093800	-1.35829300	0.01029100
H	2.31094700	1.35827500	0.01137000
H	-0.31831200	2.10961100	-0.02539600
H	-2.35843900	0.00009000	0.79491800

### 85-radical

C	-0.07888400	-1.14592300	-0.00048700
C	-1.37166400	-0.72666000	-0.00005800
C	-1.37166400	0.72666000	-0.00003200
C	-0.07888400	1.14592300	-0.00032100
N	0.73218300	0.00000000	0.00041000
O	2.00078000	0.00000000	0.00051700
H	0.38258800	-2.11850300	-0.00085400
H	-2.24506100	-1.35984900	-0.00013800
H	-2.24506100	1.35984900	-0.00007600
H	0.38258800	2.11850300	-0.00055000

### Entry 86

C	1.23032800	-0.19232000	0.00829800
C	0.66451400	-1.55503400	-0.32315500
C	-0.66451400	-1.55503400	-0.32315500
C	-1.23032800	-0.19232000	0.00829800
C	2.29257900	-0.24671100	1.11746800
C	1.82379600	0.48281700	-1.24591400
C	-2.29257900	-0.24671100	1.11746800
C	-1.82379600	0.48281700	-1.24591400
N	0.00000000	0.47008200	0.54910800
O	0.00000000	1.88010900	0.29569000
H	1.30306100	-2.40259400	-0.54365800
H	-1.30306100	-2.40259400	-0.54365800

H	3.18552400	-0.78079500	0.77797000
H	2.59604500	0.76538700	1.40075500
H	1.89614500	-0.74920300	2.00172400
H	2.16639500	1.49265200	-1.01396400
H	2.67841700	-0.09948000	-1.60213400
H	1.09581600	0.54500100	-2.05528400
H	-2.59604500	0.76538700	1.40075500
H	-3.18552400	-0.78079500	0.77797000
H	-1.89614500	-0.74920300	2.00172400
H	-2.67841700	-0.09948000	-1.60213400
H	-2.16639500	1.49265200	-1.01396400
H	-1.09581600	0.54500100	-2.05528400
H	0.00000000	2.26161300	1.17953400

### 86-radical

C	-1.25352900	0.16940800	0.00003900
C	-0.66536300	1.55993900	0.00050500
C	0.66536300	1.55993900	0.00050500
C	1.25352900	0.16940800	0.00003900
C	-2.07491200	-0.13762800	1.26401600
C	-2.07514300	-0.13665500	-1.26402600
C	2.07491200	-0.13762700	1.26401600
C	2.07514300	-0.13665500	-1.26402600
N	0.00000000	-0.63942600	-0.00039800
O	0.00000000	-1.90963700	-0.00061500
H	-1.29549800	2.44119400	0.00077300
H	1.29549800	2.44119400	0.00077300
H	-2.99361800	0.45492800	1.27300000
H	-2.34174300	-1.19650300	1.28032900
H	-1.50456900	0.09224300	2.16625200
H	-2.34200100	-1.19551300	-1.28111700
H	-2.99384900	0.45591200	-1.27239500
H	-1.50495400	0.09389700	-2.16618600
H	2.34174300	-1.19650300	1.28032900
H	2.99361800	0.45492900	1.27300000
H	1.50456900	0.09224400	2.16625200
H	2.99384900	0.45591200	-1.27239500
H	2.34200100	-1.19551300	-1.28111700
H	1.50495400	0.09389700	-2.16618600

### Entry 87

C	-0.61128700	-0.58577000	1.36039700
C	-1.21911300	-0.14952400	0.02014400
C	1.19834700	-0.13804200	-0.01410700
N	-0.02313100	0.45092600	-0.67980900

O	0.69355100	-1.02342700	1.00715000
C	-1.66143500	-1.37498000	-0.79653600
C	-2.38064900	0.82883400	0.17003000
C	1.96526100	-0.99685400	-1.01666100
C	2.11010600	0.90597800	0.63310500
O	-0.01825500	1.88483300	-0.51684400
H	-0.57317700	0.25523700	2.06715200
H	-1.12867300	-1.42325000	1.83198900
H	-2.53544400	-1.84141800	-0.33178300
H	-1.92594700	-1.07539200	-1.81294500
H	-0.87052600	-2.12415800	-0.85237300
H	-2.10537600	1.70412600	0.75660200
H	-2.73651300	1.16856000	-0.80593000
H	-3.21043900	0.31867300	0.66775700
H	1.30242000	-1.72326400	-1.48731400
H	2.39859200	-0.36639900	-1.79647300
H	2.77028800	-1.53337600	-0.50875200
H	2.92951800	0.37134500	1.11812000
H	2.52417900	1.59404200	-0.10464700
H	1.57970700	1.49311100	1.38247600
H	-0.06644400	2.19658500	-1.42589500

### 87-radical

C	0.609925	-1.521394	-0.207210
C	1.244398	-0.136985	-0.001030
C	-1.232273	-0.121045	0.012690
N	0.012910	0.689446	-0.113070
O	0.012415	1.957488	-0.161477
O	-0.718971	-1.416294	0.317160
C	1.852737	0.030017	1.400786
C	2.241956	0.252427	-1.091350
C	-2.086251	0.361562	1.176771
C	-1.996120	-0.108471	-1.314239
H	0.585113	-1.785236	-1.272122
H	1.115557	-2.314353	0.343882
H	1.165334	-0.326659	2.170875
H	2.785511	-0.535475	1.479159
H	2.069032	1.083995	1.588053
H	2.547402	1.292493	-0.963216
H	3.131854	-0.380284	-1.033692
H	1.802155	0.145933	-2.085731
H	-2.969957	-0.272633	1.271529
H	-1.518402	0.317367	2.107015
H	-2.400633	1.391583	1.001297
H	-2.910854	-0.697598	-1.220842

H	-2.257076	0.918043	-1.580275
H	-1.389193	-0.529518	-2.118411

### Entry 88

C	0.32428500	0.94379900	-0.03529100
C	-0.08910000	-0.38694800	-0.17140600
C	0.81569900	-1.44290500	-0.15496400
C	2.17006500	-1.13347100	0.00019900
C	2.59852200	0.18849200	0.12738200
C	1.67132400	1.23794300	0.10758300
N	-1.48753100	-0.44220200	-0.36203500
C	-0.89742800	1.83440600	-0.11371400
O	-2.12091700	-1.58679000	0.16674900
C	-2.03621200	0.82736800	0.15338300
H	0.47659700	-2.46566100	-0.26207000
H	2.89814300	-1.93664800	0.02177100
H	3.65376900	0.40387000	0.24801200
H	2.00488000	2.26486600	0.21541000
H	-0.99767600	2.26236500	-1.11750500
H	-0.89060200	2.65853600	0.60201900
H	-1.91334200	-1.61198700	1.11926000
H	-2.21829700	0.73570600	1.23669000
H	-2.97635400	1.06657900	-0.34237300

### 88-radical

C	0.265646	0.923708	-0.000041
C	-0.086019	-0.431291	0.000027
C	0.861069	-1.455454	0.000020
C	2.202634	-1.080884	-0.000060
C	2.575779	0.267645	-0.000130
C	1.604635	1.278040	-0.000120
N	-1.472490	-0.567163	0.000098
C	-0.984419	1.782753	0.000012
O	-2.113747	-1.660685	0.000163
C	-2.142640	0.756132	0.000014
H	0.545422	-2.490621	0.000074
H	2.969486	-1.847034	-0.000069
H	3.626268	0.533555	-0.000193
H	1.902214	2.321296	-0.000174
H	-1.023413	2.430195	-0.879740
H	-1.023362	2.430131	0.879814
H	-2.779697	0.817143	0.885022
H	-2.779615	0.817065	-0.885060

**Entry 89**

N	0.00000000	1.38503900	0.17648300
C	-1.13962100	0.59286500	0.06134900
O	-0.00000300	2.71968300	-0.22325800
C	1.13962100	0.59286600	0.06134800
C	-0.72648900	-0.76162200	0.03724900
C	-1.69828700	-1.76507200	0.00102500
C	-3.04184300	-1.40500300	-0.03960500
C	-3.42449100	-0.05473000	-0.04463800
C	-2.47912500	0.96619800	0.00956100
C	0.72648900	-0.76162200	0.03725000
C	1.69828800	-1.76507200	0.00102600
C	3.04184400	-1.40500200	-0.03960400
C	3.42449100	-0.05472900	-0.04463900
C	2.47912500	0.96619800	0.00956000
H	0.00000700	3.22785900	0.59919100
H	-1.41073000	-2.81055600	-0.00693100
H	-3.80369600	-2.17488800	-0.07525600
H	-4.47704800	0.20046400	-0.09189100
H	-2.77119100	2.00885600	0.00018000
H	1.41073100	-2.81055600	-0.00692800
H	3.80369700	-2.17488700	-0.07525500
H	4.47704800	0.20046600	-0.09189300
H	2.77119200	2.00885600	0.00017700

**89-radical**

N	0.00000000	1.44258800	-0.00024500
C	-1.14537700	0.61835100	-0.00020600
O	0.00000000	2.71032600	0.00020300
C	1.14537700	0.61835100	-0.00020600
C	-0.73126300	-0.72995800	-0.00026500
C	-1.69914400	-1.73072300	-0.00010900
C	-3.04615600	-1.36176200	0.00021300
C	-3.42979600	-0.01359400	0.00028800
C	-2.47802500	1.00508800	-0.00004300
C	0.73126300	-0.72995800	-0.00026500
C	1.69914400	-1.73072300	-0.00010900
C	3.04615600	-1.36176200	0.00021300
C	3.42979600	-0.01359400	0.00028800
C	2.47802500	1.00508800	-0.00004300
H	-1.41824700	-2.77766700	-0.00015400
H	-3.80948400	-2.13111400	0.00045100
H	-4.48310800	0.24124700	0.00051000
H	-2.75019800	2.05276000	-0.00003000

H	1.41824700	-2.77766700	-0.00015400
H	3.80948400	-2.13111400	0.00045100
H	4.48310800	0.24124700	0.00051000
H	2.75019800	2.05276000	-0.00003000

### Entry 90

C	-1.17855300	0.63259400	-0.10897800
C	-1.18249300	1.95843800	-0.31503500
C	1.17518300	1.97225300	-0.25251600
C	1.17758000	0.63942900	-0.09574700
N	-0.00382300	2.74396100	-0.37065000
O	-0.00088300	-0.07365500	0.00924700
C	-2.37041200	-0.23370500	-0.07931800
C	-2.27782000	-1.58010200	-0.45962700
C	-3.61316700	0.26677300	0.33670700
C	-3.40532900	-2.39673600	-0.44490100
C	-4.73781300	-0.55092700	0.34471300
C	-4.63937000	-1.88612500	-0.04730800
C	2.37265400	-0.21583500	-0.02390500
C	2.31161000	-1.45402200	0.63375900
C	3.59348300	0.18633800	-0.58793100
C	3.44634400	-2.25284200	0.74367500
C	4.72523200	-0.61292400	-0.47076700
C	4.65820600	-1.83588600	0.19689500
O	-0.03933900	3.67599900	0.79757100
H	-2.10435500	2.49265500	-0.48890000
H	2.09854000	2.52913500	-0.30788000
H	-1.32138900	-1.97884400	-0.77230900
H	-3.69405200	1.29215100	0.67751100
H	-3.31880700	-3.43453100	-0.74674000
H	-5.68999800	-0.14963100	0.67295100
H	-5.51581900	-2.52398300	-0.03423300
H	1.37466000	-1.77953400	1.06653100
H	3.65373100	1.11611900	-1.14058400
H	3.38261700	-3.20347800	1.26127900
H	5.65874000	-0.28718600	-0.91568900
H	5.54021200	-2.46030500	0.28198500
H	-0.04755400	4.54063000	0.36779000

### 90-radical

C	-1.190895	0.650818	-0.000898
C	-1.185983	2.003587	-0.018836
C	1.185983	2.003587	0.018835

C	1.190895	0.650818	0.000898
N	0.000000	2.726109	0.000000
O	0.000000	-0.058305	0.000000
C	-2.378032	-0.203979	-0.017567
C	-2.270249	-1.554830	-0.388508
C	-3.644699	0.298377	0.330989
C	-3.398395	-2.368954	-0.427995
C	-4.766240	-0.518836	0.286005
C	-4.650377	-1.857194	-0.094871
C	2.378032	-0.203979	0.017567
C	3.644699	0.298377	-0.330989
C	2.270249	-1.554830	0.388508
C	4.766241	-0.518836	-0.286005
C	3.398395	-2.368954	0.427995
C	4.650377	-1.857195	0.094872
O	0.000000	4.010180	0.000000
H	-2.079874	2.604123	-0.060000
H	2.079874	2.604123	0.060000
H	-1.302679	-1.957127	-0.656853
H	-3.752255	1.325323	0.658730
H	-3.297191	-3.407273	-0.723067
H	-5.733393	-0.114203	0.561638
H	-5.527161	-2.493661	-0.124324
H	3.752255	1.325323	-0.658729
H	1.302679	-1.957127	0.656853
H	5.733393	-0.114203	-0.561638
H	3.297191	-3.407273	0.723066
H	5.527161	-2.493661	0.124324

### Entry 91

N	0.00001800	1.35939700	0.57565900
C	-1.20921600	0.78140300	0.11639400
C	-2.33399500	1.55983100	-0.16537100
C	-1.23750000	-0.61923600	-0.02838700
C	-3.50274300	0.94692800	-0.60796900
C	-2.41928600	-1.19958500	-0.49056900
C	-3.54835100	-0.43273800	-0.77797000
C	1.20924100	0.78137700	0.11639700
C	2.33403200	1.55978900	-0.16536100
C	1.23749800	-0.61926400	-0.02838700
C	3.50277100	0.94687300	-0.60796100
C	2.41928000	-1.19962400	-0.49057500
C	3.54835600	-0.43279200	-0.77797100
C	-0.00001600	-1.41930100	0.39497400
C	-0.00002600	-1.54057600	1.94786200

C	-0.00007300	-2.83944500	-0.19232700
O	0.00003800	2.77013700	0.54072400
H	-2.27911900	2.63348000	-0.05822700
H	-4.37184800	1.55587700	-0.83011100
H	-2.47161600	-2.27214900	-0.62478200
H	-4.45344700	-0.91421700	-1.12938600
H	2.27917000	2.63343800	-0.05821200
H	4.37188400	1.55581100	-0.83009900
H	2.47160200	-2.27218500	-0.62480300
H	4.45344500	-0.91428200	-1.12939000
H	-0.88850400	-2.08353200	2.28219800
H	0.88839100	-2.08362800	2.28220200
H	0.00002600	-0.55919700	2.42516700
H	-0.87466800	-3.39686700	0.14821400
H	0.00005300	-2.82964100	-1.28513100
H	0.87433400	-3.39703200	0.14841800
H	0.00004400	3.02541200	1.47186300

### 91-radical

N	-0.00000100	1.54601800	-0.00022600
C	1.23200500	0.85128600	-0.00012400
C	2.41132800	1.61245200	-0.00022100
C	1.26592400	-0.55269900	0.00007200
C	3.64170700	0.97813300	-0.00012200
C	2.52791900	-1.15861700	0.00017000
C	3.70367000	-0.41644500	0.00007500
C	-1.23200600	0.85128500	-0.00012600
C	-2.41132900	1.61245100	-0.00022300
C	-1.26592400	-0.55270000	0.00007100
C	-3.64170800	0.97813200	-0.00012500
C	-2.52791900	-1.15861800	0.00016800
C	-3.70367100	-0.41644700	0.00007300
C	0.00000000	-1.41213200	0.00018800
C	0.00000000	-2.30822800	1.26845400
C	0.00000300	-2.30857500	-1.26783400
O	-0.00000100	2.82437000	-0.00040600
H	2.32411800	2.68945900	-0.00037000
H	4.55095500	1.56790100	-0.00019600
H	2.59669500	-2.23990800	0.00032300
H	4.66162700	-0.92327900	0.00015500
H	-2.32411900	2.68945800	-0.00037300
H	-4.55095600	1.56789900	-0.00020000
H	-2.59669500	-2.23990900	0.00032200
H	-4.66162700	-0.92328100	0.00015300
H	0.88210700	-2.95139700	1.29154400



H	-0.88210400	-2.95139900	1.29154200
H	-0.00000200	-1.69710100	2.17370300
H	0.00000100	-1.69769600	-2.17325000
H	-0.88210100	-2.95175500	-1.29074800
H	0.88210900	-2.95175000	-1.29074800

### Entry 92

C	-0.70796100	-0.06058400	3.67391900
C	-1.41882100	-0.01552000	2.48861800
C	-0.76185600	0.02196200	1.24913800
C	0.65077600	0.01949600	1.22452800
C	1.37526700	-0.03298300	2.42893100
C	0.69336600	-0.07405200	3.63359700
C	-1.54958500	0.04932900	0.00000000
C	0.65077600	0.01949600	-1.22452800
C	-0.76185600	0.02196200	-1.24913800
C	-1.41882100	-0.01552000	-2.48861800
C	-0.70796100	-0.06058400	-3.67391900
C	0.69336600	-0.07405200	-3.63359700
C	1.37526700	-0.03298300	-2.42893100
N	1.29609700	0.09781600	0.00000000
O	2.68361000	-0.02701700	0.00000000
O	-2.77649800	0.07859400	0.00000000
H	-1.22632900	-0.09126800	4.62464800
H	-2.50204100	-0.01100400	2.47434300
H	2.45510300	-0.06260200	2.40475000
H	1.26004000	-0.12170500	4.55688000
H	-2.50204100	-0.01100400	-2.47434300
H	-1.22632900	-0.09126800	-4.62464800
H	1.26004000	-0.12170500	-4.55688000
H	2.45510300	-0.06260200	-2.40475000
H	3.02512500	0.88002100	0.00000000

### 92-radical

C	-3.672062	-0.669594	0.000079
C	-2.489856	-1.391220	0.000059
C	-1.250923	-0.736124	-0.000013
C	-1.228733	0.672269	-0.000055
C	-2.423311	1.406802	-0.000038
C	-3.632513	0.732076	0.000029
C	0.000000	-1.524301	-0.000065
C	1.228733	0.672269	-0.000058
C	1.250923	-0.736124	-0.000016
C	2.489856	-1.391220	0.000054

C	3.672062	-0.669594	0.000072
C	3.632513	0.732076	0.000022
C	2.423311	1.406802	-0.000043
N	0.000000	1.367786	-0.000100
O	0.000000	2.642827	-0.000118
O	0.000000	-2.749076	0.000142
H	-4.624887	-1.185522	0.000131
H	-2.485421	-2.474246	0.000089
H	-2.372551	2.486234	-0.000071
H	-4.556444	1.298931	0.000045
H	2.485421	-2.474246	0.000084
H	4.624887	-1.185522	0.000122
H	4.556444	1.298931	0.000036
H	2.372551	2.486234	-0.000076

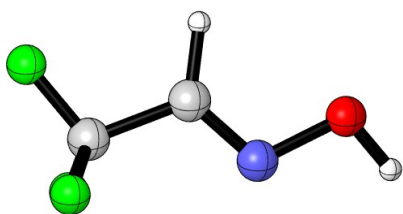
### Entry 93

C	-0.43403400	0.02991400	-0.01586300
C	0.36504300	1.07597000	-0.25803500
N	1.73591200	0.72221500	-0.35471000
O	2.55930000	1.68900200	0.33817000
C	-1.94949300	-0.00689000	0.00376700
C	-2.43382400	-0.52842700	1.37722500
C	-2.54138200	1.39433100	-0.23006100
C	-2.46200500	-0.95818000	-1.10314600
C	0.44631500	-1.20380300	0.11325600
C	1.85191000	-0.59965100	0.31666200
C	3.01383300	-1.42541400	-0.21337400
H	0.10276600	2.10415000	-0.45827600
H	3.19369600	1.96003800	-0.33437700
H	-2.06003200	-1.53531700	1.58072600
H	-2.09751000	0.12762100	2.18456700
H	-3.52711900	-0.56998000	1.40365500
H	-2.25487000	1.79055400	-1.20820600
H	-3.63380600	1.35306100	-0.19401100
H	-2.20889400	2.10058700	0.53587500
H	-3.55594600	-0.99317900	-1.09926400
H	-2.13601500	-0.62033100	-2.09090500
H	-2.09710900	-1.97837500	-0.95661300
H	0.42158600	-1.79531000	-0.81202700
H	0.16352100	-1.87203800	0.93088000
H	1.99600400	-0.39594600	1.38640900
H	3.96329500	-0.90693100	-0.05648300
H	3.06955100	-2.38640500	0.30652600
H	2.89692600	-1.61681600	-1.28345000

### 93-radical

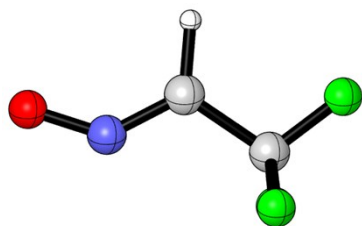
C	-0.39857300	0.04942600	0.06588200
C	0.40455500	1.12864500	-0.07985800
N	1.74311100	0.81715900	0.08244800
O	2.71494900	1.63541300	0.03716600
C	-1.90835200	-0.00334100	-0.04187500
C	-2.50747700	-0.48946100	1.29986000
C	-2.48766500	1.38487300	-0.36914900
C	-2.31679300	-0.99121100	-1.16102600
C	0.47146100	-1.17192000	0.33362300
C	1.91433000	-0.62174600	0.43341400
C	2.94307300	-1.28788500	-0.47163400
H	0.15703700	2.15632200	-0.29707500
H	-2.15778000	-1.49219900	1.55853600
H	-2.23822100	0.18617800	2.11618800
H	-3.59904200	-0.52685800	1.23510300
H	-2.10808300	1.76311000	-1.32245600
H	-3.57702400	1.32846400	-0.44415100
H	-2.24571600	2.11373500	0.40935400
H	-3.40645600	-1.03063500	-1.25070500
H	-1.90796000	-0.68111000	-2.12667000
H	-1.96565000	-2.00524500	-0.95293200
H	0.38962100	-1.89803200	-0.48360800
H	0.17781100	-1.69462300	1.24827000
H	2.27220400	-0.64174900	1.46880700
H	3.89300600	-0.75353000	-0.41878600
H	3.10486900	-2.32279600	-0.15878600
H	2.60267800	-1.28872600	-1.51098300

### Entry 94



C	0.1214119	0.3914074	-0.0000284
N	1.0398839	-0.4807726	-0.0000224
H	0.2966319	1.4651104	-0.0000104
C	-1.3080921	-0.0930926	-0.0000024
F	-1.6012171	-0.8363916	-1.0844644
F	-2.1388221	0.9731244	-0.0005744
F	-1.6014821	-0.8354116	1.0850686
O	2.2990629	0.0883184	0.0000186
H	2.8926229	-0.6722926	0.0000156

### 94-radical



C	-0.3616659	0.4836482	-0.0000691
N	-1.4984819	-0.1023527	0.0002199
H	-0.2722909	1.5656723	-0.0004061
O	-2.6522039	0.2682652	0.0002359
C	0.8828231	-0.3568908	-0.0000041
F	0.9707371	-1.1567328	1.0830499
F	1.9599941	0.4547542	0.0002859
F	0.9710881	-1.1563638	-1.0833121

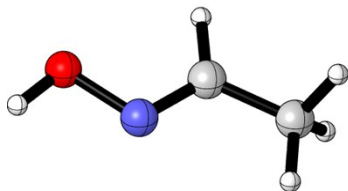
### Entry 95

C	-1.12586700	0.17839400	-0.00000500
N	-0.07381000	-0.53007800	-0.00000400
H	-1.10576200	1.26740200	0.00000800
H	-2.06825900	-0.35618100	0.00003100
O	1.08146100	0.26414400	0.00000000
H	1.79420400	-0.38418700	0.00002400

### 95-radical

C	-1.12305200	0.11646600	-0.00001700
O	1.18666800	0.14189600	0.00001700
N	0.06871800	-0.34695700	-0.00000600
H	-1.30014400	1.18907200	0.00000800
H	-1.93591100	-0.59433400	-0.00000100

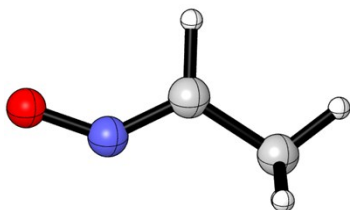
### Entry 96



C	-0.0246444	0.3062361	-0.1719368
N	-1.0604004	-0.2771679	0.2766002
H	-0.1173704	1.2559711	-0.7036938
C	1.3257676	-0.3028859	0.0249582
H	1.9770126	0.3790061	0.5815162

H	1.2471086	-1.2434009	0.5710512
H	1.8067106	-0.4905939	-0.9406138
O	-2.2291124	0.4572691	-0.0123308
H	-2.9250714	-0.0844339	0.3744492

### 96-radical



C	-0.3271155	0.4378724	-0.0000280
O	-2.6380295	0.2852164	0.0001370
N	-1.4790995	-0.1183346	0.0001500
H	-0.2916185	1.5272464	-0.0002580
C	0.9347345	-0.3780846	-0.0000040
H	1.8016705	0.2834814	0.0002130
H	0.9996115	-1.0188476	0.8836170
H	0.9998465	-1.0185496	-0.8838270

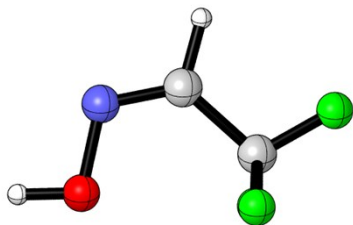
### Entry 97

C	0.52163200	0.68377200	-0.00000700
N	-0.75214400	0.68866000	0.00000600
C	1.45143300	-0.48984100	-0.00001000
O	-1.29860100	-0.61246500	0.00000900
H	0.94604500	1.68556100	0.00000400
H	0.91090400	-1.43356400	-0.00067200
H	2.10154300	-0.44903200	0.87993700
H	2.10248400	-0.44827900	-0.87921700
H	-2.24555000	-0.43916600	-0.00007000

### 97-radical

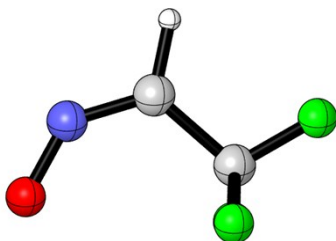
C	0.46644100	0.66554000	-0.00000900
N	-0.79916300	0.47339000	0.00000700
C	1.48191100	-0.44128000	-0.00000200
O	-1.51448200	-0.52591300	-0.00000200
H	0.77378600	1.70451900	0.00000900
H	0.99412700	-1.41634100	-0.00057300
H	2.12562000	-0.37042700	0.88244300
H	2.12635600	-0.36973400	-0.88184700

### Entry 98



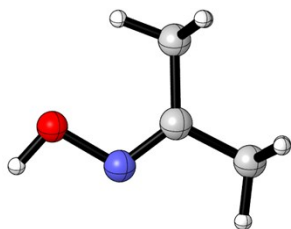
C	-0.0726468	0.8198947	-0.0001296
N	-1.3195618	0.5721307	-0.0000116
C	1.0568472	-0.1892473	-0.0000296
O	-1.6143588	-0.7776963	0.0002194
F	1.0404772	-0.9815873	1.0877734
F	2.2367112	0.4724687	-0.0003416
F	1.0402062	-0.9821363	-1.0874236
H	0.2106342	1.8655407	-0.0003196
H	-2.5783088	-0.7993673	0.0002624

### 98-radical



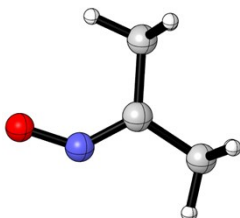
C	-0.3577995	0.7040099	-0.0000630
N	-1.5849815	0.3372659	0.0000010
C	0.7800945	-0.2850261	0.0000090
O	-2.1702415	-0.7250211	0.0000990
F	0.7602285	-1.0866251	1.0842730
F	1.9505785	0.3816259	-0.0004430
F	0.7597675	-1.0873181	-1.0837280
H	-0.1376465	1.7610889	-0.0001480

### Entry 99



C	-0.0221014	-0.1929573	-0.0000362
C	1.2836036	-0.9392483	0.0000068
C	0.0176116	1.3100037	0.0000308
N	-1.0772154	-0.9135833	-0.0000772
H	1.1103906	-2.0151552	0.0000568
H	1.8775336	-0.6740383	0.8811838
H	1.8775496	-0.6741183	-0.8811822
H	-0.9794904	1.7426887	-0.0007982
H	0.5641216	1.6668728	-0.8790312
H	0.5625706	1.6668227	0.8800828
O	-2.2676394	-0.1478183	-0.0000432
H	-2.9469344	-0.8294693	-0.0001922

### 99-radical



C	-0.2755861	-0.2200019	-0.0000437
C	0.9762069	-1.0487749	0.0000253
C	-0.1830341	1.2840351	0.0000283
O	-2.5825761	-0.4343519	-0.0001967
N	-1.4095621	-0.8181379	-0.0001237
H	0.7397039	-2.1128549	0.0000013
H	1.5874559	-0.8261539	0.8812933
H	1.5875669	-0.8261359	-0.8811617
H	-1.1724881	1.7406061	-0.0005537
H	0.3666909	1.6308901	-0.8813367
H	0.3656219	1.6308801	0.8820683

### Entry 100

C	0.10958000	-0.03759400	0.24606100
N	0.18387900	1.19997000	-0.05995300
C	1.38677100	-0.84329800	0.20055500
C	-1.16511600	-0.75088300	0.63207300
O	-1.07706600	1.84467300	0.01290100
C	2.63435000	-0.10848700	-0.28741800
C	-1.99048500	-1.18697300	-0.59291400
H	1.19791700	-1.72392100	-0.42824500
H	1.55665400	-1.24500300	1.20862500
H	-1.76755700	-0.08766000	1.25672100
H	-0.90611400	-1.62870900	1.23188600
H	-0.85514500	2.75398800	-0.21139600

H	3.49405400	-0.78378500	-0.28200600
H	2.86439300	0.74696000	0.35041000
H	2.49920600	0.26901700	-1.30300200
H	-2.89073500	-1.71951100	-0.27512900
H	-1.41812200	-1.85593800	-1.24182500
H	-2.29577600	-0.31920000	-1.17971600

### 100-radical

C	0.06706200	-0.06529800	0.26071700
N	0.17074800	1.18374200	-0.01108200
C	1.28530100	-0.94810700	0.18049400
C	-1.28070300	-0.64993200	0.63058700
O	-0.64226800	2.11538200	-0.02503100
C	2.56323900	-0.25929800	-0.29754300
C	-2.16044500	-0.94359400	-0.59670700
H	1.04728300	-1.79449100	-0.47753400
H	1.44699200	-1.39144500	1.17218400
H	-1.79744700	0.05310600	1.29137500
H	-1.11353000	-1.56963700	1.19920800
H	3.39165100	-0.97120400	-0.32168900
H	2.84135500	0.56303800	0.36573600
H	2.43919500	0.15284400	-1.30171100
H	-3.11955700	-1.36726100	-0.28716900
H	-1.67841500	-1.65809800	-1.26934400
H	-2.36133700	-0.02872700	-1.15852000

### Entry 101

C	-0.11958000	0.17698500	0.06496200
C	-1.52677900	-0.31402600	0.38446500
C	1.02917400	-0.79566800	0.31442100
N	-0.03115200	1.37291500	-0.37307200
C	1.81905000	-1.14938000	-0.96012400
C	1.95384200	-0.30535800	1.44652700
C	-1.96204400	-1.39287900	-0.62927500
C	-2.57570000	0.79822300	0.47763400
O	1.29809000	1.77374300	-0.65824900
H	-1.45576000	-0.79930900	1.36844800
H	0.56101100	-1.72101100	0.66733700
H	1.15692800	-1.51796700	-1.74822100
H	2.35651200	-0.28382700	-1.34593100
H	2.54397800	-1.93765000	-0.73522500
H	1.38860000	-0.10403300	2.36099100
H	2.69709600	-1.07504600	1.67508400
H	2.47620800	0.60727100	1.15985800
H	-1.24639700	-2.21635000	-0.69399200
H	-2.92837800	-1.81519700	-0.34011300



H	-2.06784300	-0.95658000	-1.62678300
H	-3.53992700	0.37398200	0.77244700
H	-2.29114500	1.55435100	1.21192200
H	-2.70149900	1.30331600	-0.48227600
H	1.17617400	2.68031800	-0.95771500

### 101-radical

C	-0.09993600	0.14273600	0.07670800
C	-1.50057200	-0.33301200	0.40950700
C	1.10351400	-0.76893900	0.31119300
O	1.04393800	1.98394900	-0.74974000
N	0.05947400	1.32432000	-0.39464800
C	1.87381800	-1.05310700	-0.98859700
C	2.02408200	-0.19368400	1.40228800
C	-1.94324800	-1.45396400	-0.55362500
C	-2.53205700	0.79931900	0.44522300
H	-1.44050000	-0.77189900	1.41559900
H	0.69562900	-1.71634300	0.68002100
H	1.23055300	-1.51738600	-1.74036100
H	2.28081100	-0.13170800	-1.41213700
H	2.70946700	-1.73075100	-0.79098100
H	1.48361300	-0.04145000	2.34026100
H	2.85324200	-0.88010900	1.59624000
H	2.44579600	0.76563800	1.09231700
H	-1.22693200	-2.27906200	-0.58207900
H	-2.90820700	-1.86328100	-0.24198400
H	-2.05152000	-1.06465400	-1.57012400
H	-3.51060600	0.40721300	0.73447900
H	-2.24916600	1.57582900	1.15936500
H	-2.63360600	1.27002700	-0.53634800

### Entry 102

C	0.07315300	0.26969100	0.00000200
C	-1.42455200	-0.08717300	-0.00000100
C	1.10211500	-0.86034700	-0.00000500
N	0.33459800	1.52018100	0.00001000
C	1.96700000	-0.87121400	-1.27650700
C	1.96699300	-0.87123800	1.27650100
C	-1.75002900	-0.91764700	1.26376500
C	-2.31432500	1.16840100	0.00003700
C	-1.75004300	-0.91757800	-1.26380900
O	1.72096900	1.81382500	0.00000700
H	0.53378800	-1.79401500	-0.00001500
H	1.34743900	-0.90544500	-2.17650600
H	2.60125500	0.01269300	-1.33272900
H	2.60708000	-1.75881500	-1.27704700

H	2.60707100	-1.75884200	1.27703000
H	2.60125100	0.01266600	1.33274300
H	1.34742700	-0.90548300	2.17649600
H	-2.80991900	-1.18861200	1.26434300
H	-1.17402100	-1.84448000	1.31536300
H	-1.55035300	-0.34110900	2.17108400
H	-2.13239400	1.78701300	-0.88028700
H	-3.36585600	0.86581900	0.00003200
H	-2.13238800	1.78696300	0.88039500
H	-2.80993500	-1.18853800	-1.26439200
H	-1.55037200	-0.34099300	-2.17109900
H	-1.17404100	-1.84441200	-1.31546100
H	1.72214900	2.77634800	0.00001100

### 102-radical

C	0.08747600	0.23283800	0.00015800
C	-1.40178100	-0.11602500	-0.00005900
C	1.17459700	-0.84390000	-0.00028000
O	1.50371900	2.07235800	0.00055400
N	0.42321700	1.47067300	0.00045600
C	2.03818700	-0.77040300	-1.27183000
C	2.03781700	-0.77184600	1.27160200
C	-1.73367200	-0.94567000	1.26207400
C	-2.26625900	1.15654800	-0.00012000
C	-1.73330200	-0.94556000	-1.26236100
H	0.65836300	-1.80811500	-0.00089700
H	1.43186400	-0.88300600	-2.17395500
H	2.56571300	0.18451000	-1.33321500
H	2.78629900	-1.56837800	-1.26412600
H	1.43122700	-0.88546200	2.17342100
H	2.78591800	-1.56982400	1.26321400
H	2.56534000	0.18298700	1.33422500
H	-2.79289300	-1.21910300	1.26050400
H	-1.15541300	-1.87171000	1.31055300
H	-1.53431900	-0.37178100	2.17097800
H	-2.07315400	1.76999600	-0.88314200
H	-3.32496900	0.88268500	-0.00028600
H	-2.07340600	1.76991000	0.88301600
H	-2.79251300	-1.21903400	-1.26111000
H	-1.53371400	-0.37157900	-2.17115400
H	-1.15498800	-1.87157300	-1.31076000

### Entry 103

C	-0.02565600	0.38083600	-0.04946200
C	-1.51791800	-0.06891000	-0.00993500
C	1.21016200	-0.56837500	-0.00150300

N	0.06539600	1.65951700	-0.05901800
C	-1.84017600	-0.67388000	1.37811100
H	-2.89445000	-0.96508200	1.41355700
H	-1.24873300	-1.55875200	1.61230300
H	-1.66994400	0.06471400	2.16597400
C	-2.46262600	1.14108300	-0.19842900
H	-2.30811600	1.62509300	-1.16462600
H	-3.49629000	0.78525500	-0.15190300
H	-2.32117800	1.89568500	0.57463500
C	1.94748700	-0.33526700	1.34308000
H	1.31968300	-0.63831700	2.18592900
H	2.85624100	-0.94475400	1.36892200
H	2.22915100	0.70674000	1.47846900
C	2.15215300	-0.26461200	-1.19705100
H	1.62725800	-0.41166100	-2.14564400
H	2.54355800	0.74797100	-1.17487400
H	2.99360000	-0.96407100	-1.17283500
C	0.91278300	-2.08223300	-0.09265600
H	0.54351800	-2.37225900	-1.07638100
H	1.85548700	-2.61455000	0.06315000
H	0.21576200	-2.44149400	0.66366500
C	-1.86680300	-1.07564900	-1.13308600
H	-1.51418500	-0.72004900	-2.10560600
H	-1.46330500	-2.07095400	-0.96352100
H	-2.95417000	-1.17495800	-1.19534300
O	1.37232500	2.19678600	-0.02044400
H	1.19331100	3.14258100	-0.03360600

### 103-radical

C	-0.02823300	0.35294600	-0.05465600
C	-1.50056800	-0.11657600	-0.01057000
C	1.27227900	-0.50890900	-0.00312100
O	1.07164400	2.41627400	-0.02092100
N	0.12176700	1.62941000	-0.04909200
C	-1.80663800	-0.78591800	1.35078100
H	-2.85800600	-1.08734800	1.38453700
H	-1.20483500	-1.67741100	1.52901100
H	-1.63066800	-0.08793400	2.17354000
C	-2.43930500	1.10271500	-0.14741100
H	-2.29425800	1.61623800	-1.10067500
H	-3.47749000	0.76296500	-0.09850700
H	-2.28233600	1.82886500	0.65262700
C	1.94942300	-0.25607800	1.36516100
H	1.32613800	-0.62210200	2.18536200
H	2.90712900	-0.78365500	1.40787900
H	2.14399000	0.80571800	1.52752200

C	2.21963300	-0.06875800	-1.14372200
H	1.76256100	-0.24865700	-2.12079400
H	2.48490100	0.98648300	-1.07894800
H	3.14429400	-0.65132100	-1.09264500
C	1.05800800	-2.02674000	-0.16459000
H	0.69834300	-2.28600800	-1.16093100
H	2.02524200	-2.51992600	-0.03228900
H	0.37803000	-2.44938700	0.57499600
C	-1.84214700	-1.08474200	-1.16751500
H	-1.55413100	-0.65959300	-2.13305500
H	-1.36624600	-2.05803100	-1.06439700
H	-2.92289500	-1.25258900	-1.18835900

#### Entry 104

C	1.31233100	0.29484200	-0.19542000
C	2.55990300	-0.60982400	-0.00496400
N	1.31378300	1.57425300	-0.16756100
C	3.62367400	-0.26404700	-1.07722500
C	3.14055300	-0.40045600	1.41514300
C	2.24444000	-2.11339100	-0.16438500
C	-0.06102100	-0.33284000	-0.43022500
C	-1.09035900	0.47211600	-1.27586200
C	-0.76609700	-0.77394300	0.89267400
C	-1.71087800	1.66352500	-0.51580500
C	-2.23094800	-0.50278900	-1.65211400
C	-1.33987800	0.44455800	1.64405700
C	-1.91196400	-1.73901800	0.52290000
C	-2.39040000	1.16093000	0.77109800
C	-2.93351800	-1.01337100	-0.37521100
C	-3.52147200	0.18047700	0.40404300
O	2.57465100	2.17395000	0.07594100
H	3.21836200	-0.40402600	-2.08390100
H	3.97653200	0.76040700	-0.98901900
H	4.47823700	-0.93893900	-0.96633900
H	2.41618600	-0.69466100	2.18022900
H	4.02975800	-1.02624900	1.54092100
H	3.42128700	0.63680800	1.58749000
H	1.48919800	-2.46820400	0.53949200
H	1.91672800	-2.36211000	-1.17689400
H	3.15977000	-2.68074800	0.02602600
H	0.12972400	-1.24724400	-0.99762800
H	-0.59668700	0.83420800	-2.18316700
H	-0.05215900	-1.29114800	1.54077100
H	-2.45174800	2.14983900	-1.16248200
H	-0.94463000	2.40055600	-0.27971500
H	-1.83719400	-1.34809900	-2.22923800

H	-2.95552200	0.00943400	-2.29576100
H	-0.53823600	1.14049400	1.90933500
H	-1.79505300	0.10609100	2.58250300
H	-1.51020900	-2.62020800	0.00882300
H	-2.40455000	-2.09806900	1.43424100
H	-2.80525800	2.01057300	1.32460600
H	-3.73579400	-1.70658200	-0.65146500
H	-4.02675200	-0.17697000	1.30948300
H	-4.27822500	0.69180500	-0.20264400
H	2.35635300	3.11105600	0.04749800

#### 104-radical

C	1.33766500	0.27154300	0.00005200
C	2.65540400	-0.54449800	0.00011200
O	2.11354200	2.49250100	-0.00016700
N	1.31340300	1.55201600	-0.00008100
C	2.69242800	-1.43445400	-1.26422700
C	3.90641400	0.35114900	-0.00038100
C	2.69283200	-1.43362300	1.26502400
C	0.00261400	-0.46566900	0.00003700
C	-0.88140700	-0.23481600	-1.26266400
C	-0.88149800	-0.23475000	1.26266200
C	-1.52149500	1.16789200	-1.25721300
C	-2.00245100	-1.29699700	-1.25935900
C	-1.52159500	1.16795300	1.25709800
C	-2.00254200	-1.29693300	1.25932600
C	-2.39761300	1.33944300	-0.00009600
C	-2.87781200	-1.13274600	-0.00005200
C	-3.51132600	0.27310100	-0.00011400
H	1.84875100	-2.12651600	-1.31237500
H	2.68613700	-0.82525500	-2.17177900
H	3.60894500	-2.03224300	-1.26623100
H	3.95077800	0.99225200	0.88173600
H	4.79712200	-0.28406000	-0.00029900
H	3.95051100	0.99165100	-0.88294800
H	2.68681500	-0.82382600	2.17217600
H	1.84918200	-2.12566600	1.31389100
H	3.60936000	-2.03139700	1.26713800
H	0.26106100	-1.52767700	0.00007400
H	-0.26495300	-0.35489200	-2.15979200
H	-0.26510900	-0.35478200	2.15984100
H	-2.13190900	1.28808800	-2.16019900
H	-0.75243400	1.94381500	-1.29035300
H	-1.56966400	-2.30420300	-1.29039400
H	-2.61772700	-1.18788200	-2.15993500
H	-0.75254500	1.94388500	1.29026900

H	-2.13208500	1.28818200	2.16003000
H	-1.56975800	-2.30413700	1.29044500
H	-2.61788400	-1.18777000	2.15985200
H	-2.84465100	2.33924200	-0.00013800
H	-3.66572500	-1.89388500	-0.00006100
H	-4.15207900	0.39671600	0.88089600
H	-4.15200700	0.39667000	-0.88118300

### Entry 105

C	1.46453600	0.44308400	0.00003500
C	2.72642900	-0.45952900	0.00000300
N	1.74684200	1.68812000	0.00000900
C	4.02768900	0.36404600	0.00000700
C	2.72639300	-1.34892500	1.26584800
C	2.72638500	-1.34888900	-1.26586800
C	0.11282200	-0.28496000	0.00005100
C	-0.79502300	-0.16229900	-1.26594700
C	-0.79509600	-0.16228000	1.26599900
C	-1.69360100	1.09138400	-1.26209300
C	-1.71040700	-1.41117600	-1.26684600
C	-1.69370600	1.09138200	1.26210200
C	-1.71047700	-1.41116200	1.26684900
C	-2.58089600	1.09870100	-0.00003100
C	-2.59391200	-1.41567600	-0.00002400
C	-3.47949700	-0.15371900	-0.00006400
O	0.64366700	2.56823100	-0.00000400
H	4.09743000	1.00522300	-0.88007900
H	4.09745300	1.00518100	0.88012000
H	4.88310100	-0.31839300	-0.00002100
H	1.85567700	-2.00583700	1.32357800
H	3.61610500	-1.98546800	1.26783000
H	2.75074900	-0.73601600	2.17099700
H	1.85568500	-2.00582000	-1.32360300
H	2.75071400	-0.73595600	-2.17100100
H	3.61611200	-1.98541200	-1.26788400
H	0.41620300	-1.33263300	0.00007700
H	-0.16947400	-0.16624900	-2.16428100
H	-0.16959800	-0.16622400	2.16436800
H	-2.32804100	1.06893800	-2.15685200
H	-1.09254800	1.99729700	-1.30956600
H	-1.10782500	-2.32608600	-1.31385500
H	-2.34513400	-1.40333300	-2.16035500
H	-1.09268600	1.99730800	1.30965200
H	-2.32822000	1.06888900	2.15680700
H	-1.10789700	-2.32607200	1.31389800
H	-2.34525400	-1.40331600	2.16032200

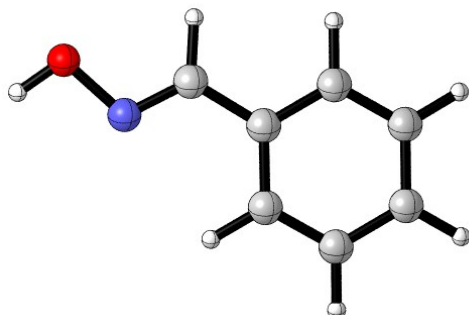
H	-3.20539000	1.99890500	-0.00005600
H	-3.22531800	-2.31132900	-0.00003600
H	-4.13264700	-0.15239800	0.88086000
H	-4.13257800	-0.15240600	-0.88103900
H	1.07632100	3.42862700	-0.00003300

### 105-radical

C	-1.40684100	0.44117400	-0.15671400
C	-2.61926900	-0.51144500	-0.00460400
O	-1.11553800	2.77605000	-0.04069300
N	-1.68238600	1.68235700	0.01002300
C	-2.58945300	-1.61630600	-1.08321400
C	-2.64204000	-1.14777100	1.40630000
C	-3.93512400	0.27654900	-0.18118700
C	-0.02426200	-0.04704600	-0.62226600
C	0.59318500	-1.20596200	0.22061800
C	1.06444400	1.04894000	-0.78856700
C	1.09786400	-0.69161000	1.58314900
C	1.77592800	-1.80586500	-0.57040200
C	1.58703200	1.54573700	0.57804000
C	2.24633100	0.44178300	-1.57766100
C	2.19129300	0.37219600	1.36865900
C	2.85861500	-0.73477000	-0.79279200
C	3.36455300	-0.23674700	0.57599700
H	-2.60221900	-1.18621300	-2.08885000
H	-1.71769000	-2.26788200	-1.00403500
H	-3.47811600	-2.24545200	-0.98169400
H	-2.68993200	-0.37242100	2.17527900
H	-3.52810800	-1.78148000	1.51213200
H	-1.76707600	-1.76710400	1.60567300
H	-4.04254500	1.05742000	0.57412000
H	-3.98605400	0.75109300	-1.16425800
H	-4.78463900	-0.40569900	-0.08601800
H	-0.21416900	-0.45838100	-1.62342300
H	-0.14682600	-1.99127300	0.37894300
H	0.65487000	1.89052000	-1.35125500
H	1.49358600	-1.53204600	2.16557600
H	0.27128100	-0.26548300	2.16200300
H	1.42417000	-2.19630200	-1.53283000
H	2.19253600	-2.65485100	-0.01606300
H	0.78697000	2.01848300	1.15171400
H	2.34497200	2.31940700	0.40921100
H	1.90980500	0.10258700	-2.56454600
H	3.00338400	1.21513900	-1.74988000
H	2.54948100	0.72983500	2.34001800
H	3.69063900	-1.16401700	-1.36163900

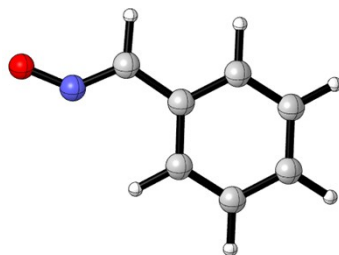
H	4.15195100	0.51315500	0.43707000
H	3.81120100	-1.06707100	1.13598900

**Entry 106**



C	-1.4506638	1.0289574	-0.0001690
N	-2.5890448	0.4522614	0.0000450
H	-1.3927718	2.1192474	-0.0005120
C	-0.1968828	0.2687814	-0.0000460
C	1.0160182	0.9707194	-0.0002920
C	-0.1687608	-1.1355856	0.0003160
C	2.2313852	0.2897534	-0.0001730
H	1.0050332	2.0558354	-0.0005730
C	1.0442552	-1.8111086	0.0004310
H	-1.1039568	-1.6815626	0.0005060
C	2.2490552	-1.1026226	0.0001880
H	3.1615452	0.8465604	-0.0003630
H	1.0549032	-2.8953376	0.0007130
H	3.1933072	-1.6352156	0.0002790
O	-3.6316198	1.3901834	-0.0002450
H	-4.4218018	0.8391334	-0.0001050

**106-radical**



C	-1.6698250	1.2080048	-0.0000569
O	-3.9827100	1.1757138	0.0004461
N	-2.8526180	0.7027928	0.0002981
H	-1.5814060	2.2940798	-0.0002649
C	-0.4628920	0.3849058	-0.0000359
C	0.7864030	1.0215378	-0.0004019
C	-0.5074480	-1.0190552	0.0003401



C	1.9627670	0.2764208	-0.0004129
H	0.8348260	2.1055288	-0.0006889
C	0.6680840	-1.7580312	0.0003301
H	-1.4672490	-1.5228022	0.0006321
C	1.9085910	-1.1152872	-0.0000459
H	2.9204890	0.7842018	-0.0007049
H	0.6198060	-2.8411182	0.0006161
H	2.8231820	-1.6968922	-0.0000499

**Entry 107**

C	-0.09327300	-0.39923700	0.00004900
C	0.98586200	-1.30259000	-0.00003300
C	2.30091400	-0.85427100	-0.00008400
C	2.56728900	0.51445100	-0.00003700
C	1.50957300	1.42259100	0.00005900
C	0.18998300	0.97961800	0.00009800
C	-1.43670100	-0.99217900	0.00010300
N	-2.62090100	-0.50287800	0.00002100
O	-2.66303300	0.89986000	-0.00013900
H	0.78370100	-2.36864900	-0.00005900
H	3.11575700	-1.56928900	-0.00015500
H	3.59146400	0.87027100	-0.00007300
H	1.71199600	2.48783000	0.00010200
H	-0.62004400	1.69131400	0.00016700
H	-1.46494500	-2.07997500	0.00024000
H	-3.60924500	1.07946200	-0.00018800

**107-radical**

C	0.12658300	-0.42300200	0.00000500
C	-0.96147400	-1.31273200	-0.00005400
C	-2.26649200	-0.83523700	-0.00012200
C	-2.50841400	0.53864100	-0.00013200
C	-1.43544500	1.42921400	-0.00007400
C	-0.12594700	0.95827500	-0.00000600
C	1.47622000	-0.98963900	0.00007600
N	2.57822400	-0.32303400	0.00013700
O	2.85485400	0.87258500	0.00015600
H	-0.77706100	-2.38185400	-0.00004700
H	-3.09523700	-1.53408000	-0.00016800
H	-3.52594800	0.91219200	-0.00018500
H	-1.61779200	2.49778700	-0.00008100
H	0.69937200	1.65909900	0.00003900
H	1.60008300	-2.06569000	0.00007600

**Entry 108**

C	1.26389100	0.19776000	0.04618600
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N	1.93110800	-0.87002400	-0.20249700
C	-0.21621400	0.05852600	0.02653900
C	-1.03545300	1.17959800	-0.16492100
C	-0.82683200	-1.19560700	0.19089000
C	-2.42300700	1.05181100	-0.20198500
H	-0.59362300	2.15931900	-0.30055900
C	-2.21016300	-1.31991300	0.15825000
H	-0.20198300	-2.06527200	0.34772100
C	-3.01603000	-0.19696500	-0.03928200
H	-3.03826400	1.93083700	-0.35814400
H	-2.66394000	-2.29548200	0.29346900
H	-4.09540100	-0.29622300	-0.06156200
C	1.90211400	1.53331000	0.32870000
H	2.02782700	2.10361400	-0.59800500
H	1.28782200	2.12313700	1.00947000
H	2.89090300	1.39422600	0.76243100
O	3.32138900	-0.65948400	-0.17351700
H	3.66795300	-1.53924100	-0.35546300

#### 108-radical

C	-1.31027600	0.25092500	-0.00003700
O	-3.26318100	-1.00049800	0.00012000
N	-2.04960600	-0.80650200	0.00012900
C	0.15499200	0.07847200	-0.00000700
C	1.00168400	1.19635800	0.00027700
C	0.74027100	-1.20045300	-0.00027600
C	2.38730500	1.04213800	0.00031500
H	0.58573600	2.19614000	0.00048900
C	2.11980200	-1.35017100	-0.00023400
H	0.10129000	-2.07576900	-0.00052700
C	2.95316800	-0.22884400	0.00006100
H	3.02249400	1.92077000	0.00054500
H	2.54974800	-2.34551500	-0.00044700
H	4.03043300	-0.34854900	0.00008500
C	-1.95892000	1.61428000	-0.00027000
H	-1.66115800	2.18552300	0.88376500
H	-1.66048400	2.18552700	-0.88406900
H	-3.04352600	1.51514800	-0.00067000

#### Entry 109

C	1.49566000	0.35931200	0.00148700
N	2.32933200	-0.61280700	-0.00274500
C	2.06384500	1.75229100	0.00755900
C	0.00536700	0.19366000	0.00081200
O	1.81482200	-1.90260600	-0.00827700

C	-0.70191200	0.12202900	1.20814800
C	-2.08947100	-0.00822600	1.20623400
C	-2.78535500	-0.06513700	-0.00018000
C	-2.08981600	0.00483600	-1.20610900
C	-0.70226700	0.13514800	-1.20702200
H	3.15323200	1.71065400	0.00747900
H	1.72347100	2.30336200	0.89029700
H	1.72365500	2.31096000	-0.87046700
H	0.84118100	-1.86205700	-0.00810000
H	-0.16216100	0.16556900	2.14792400
H	-2.62570500	-0.06415400	2.14677000
H	-3.86474100	-0.16532500	-0.00057300
H	-2.62632600	-0.04089500	-2.14703900
H	-0.16281100	0.18890000	-2.14643900

### 109-radical

C	-1.46798900	-0.35681900	-0.00319600
N	-2.25328700	0.65965600	0.00619300
C	-2.06773400	-1.73535800	-0.01588500
C	0.01833600	-0.17851100	-0.00165200
O	-2.09126900	1.87916700	0.01737100
C	0.72085700	-0.11506400	1.20614500
C	2.10618800	0.03554400	1.20629800
C	2.80061400	0.12321300	0.00101400
C	2.10568200	0.06154500	-1.20559100
C	0.72034400	-0.08901200	-1.20809500
H	-3.15722000	-1.68321900	-0.01462700
H	-1.73939300	-2.30635900	0.85861000
H	-1.74066000	-2.28957600	-0.90158500
H	0.18171300	-0.17692500	2.14509700
H	2.64141000	0.08732400	2.14772800
H	3.87823200	0.24157400	0.00207300
H	2.64050800	0.13362900	-2.14590800
H	0.18078400	-0.13061600	-2.14792500

### Entry 110

C	-1.36351700	0.21114100	0.04245800
C	-1.46649300	-1.06984300	0.60211600
C	-2.69806400	-1.71776700	0.67028400
C	-3.84327800	-1.10132500	0.17178700
C	-3.74969200	0.17099800	-0.39456400
C	-2.52313500	0.82185500	-0.46038100
C	-0.05233700	0.91524100	0.00283500
N	-0.11029600	2.19965800	0.00261100
C	1.21114700	0.12118900	-0.03920900
C	2.21552400	0.30680500	0.91820700

C	1.39861000	-0.83607400	-1.04367700
C	3.37966900	-0.45524700	0.87384400
C	2.57208400	-1.58449700	-1.09747400
C	3.56345600	-1.39953200	-0.13554500
H	-0.58198000	-1.55672900	0.99432000
H	-2.76053100	-2.70522700	1.11372200
H	-4.80052900	-1.60824500	0.21907800
H	-4.63532200	0.65398200	-0.79241100
H	-2.44755400	1.80701700	-0.90245200
H	2.08253400	1.04900600	1.69508000
H	0.62438000	-0.99149700	-1.78650000
H	4.14662600	-0.30795900	1.62599900
H	2.70880100	-2.31452200	-1.88737900
H	4.47378000	-1.98740200	-0.17191700
O	1.14736200	2.81449800	-0.08780800
H	0.91911500	3.75032600	-0.08743000

### 110-radical

C	-1.34536000	0.20159000	0.04171400
C	-1.56600500	-0.95890800	0.79642300
C	-2.82781700	-1.54611700	0.83811300
C	-3.88793900	-0.98605300	0.12694700
C	-3.67794200	0.16814500	-0.62662200
C	-2.41747500	0.75612800	-0.67164700
C	-0.01287800	0.85872400	0.02844600
N	-0.02174000	2.15341800	0.05334100
O	0.84182100	3.02660100	0.04055900
C	1.26032300	0.09562400	-0.02507500
C	2.44674400	0.61503000	0.51499400
C	1.29863000	-1.16144700	-0.64998800
C	3.63213500	-0.11060300	0.44450300
C	2.48913500	-1.87766600	-0.72762300
C	3.65950200	-1.35802300	-0.17708000
H	-0.75197100	-1.39368800	1.36413700
H	-2.98376800	-2.43875000	1.43342200
H	-4.86916800	-1.44577600	0.15856600
H	-4.49529200	0.60775500	-1.18715000
H	-2.25416500	1.64761700	-1.26583800
H	2.44335600	1.58688800	0.99204200
H	0.39689900	-1.57249800	-1.08622200
H	4.53749700	0.30286300	0.87414700
H	2.50200900	-2.84176700	-1.22344400
H	4.58589400	-1.91792300	-0.23614600

### Entry 111

C	-1.19932000	0.56240500	0.00000600
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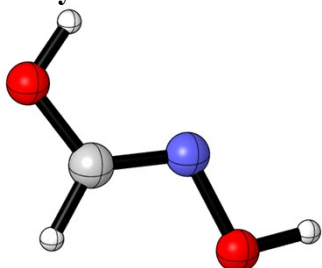
C	-0.94911700	-0.82417400	-0.00001400
C	-2.00797800	-1.72675600	-0.00002800
C	-3.31348900	-1.22957300	-0.00002200
C	-3.55636500	0.14685200	-0.00000200
C	-2.49697400	1.05728000	0.00001200
C	0.10120800	1.27144900	0.00001800
N	0.14589000	2.55381800	0.00003700
C	1.15234900	0.22990400	0.00000500
C	2.54260200	0.31495900	0.00000800
C	0.50884800	-1.03189900	-0.00001500
C	3.28638400	-0.86895200	-0.00000800
C	1.25711700	-2.20257600	-0.00003100
C	2.65184500	-2.11165400	-0.00002800
O	1.45137200	3.05109600	0.00004800
H	-1.83166500	-2.79667500	-0.00004300
H	-4.14936300	-1.92016600	-0.00003300
H	-4.57752700	0.51068900	0.00000200
H	-2.67786600	2.12548300	0.00002800
H	3.03422000	1.27667300	0.00002300
H	4.36923400	-0.81926400	-0.00000600
H	0.77369500	-3.17315800	-0.00004600
H	3.24740100	-3.01783600	-0.00004000
H	1.31699800	4.00516500	0.00006300

### 111-radical

C	-1.19588900	0.55263000	0.00003000
C	-0.90443500	-0.83061000	-0.00011600
C	-1.94046200	-1.75995500	-0.00024500
C	-3.25866900	-1.29973800	-0.00022800
C	-3.54035300	0.06986000	-0.00008500
C	-2.50860200	1.00998100	0.00004600
C	0.08271600	1.27605200	0.00015500
N	0.20422800	2.56113600	0.00030900
O	1.17388400	3.30987900	0.00041900
C	1.16246200	0.27773500	0.00006000
C	2.54381900	0.42732600	0.00010800
C	0.55722000	-1.00151900	-0.00010100
C	3.33378800	-0.72525700	-0.00000600
C	1.35497100	-2.14071700	-0.00021600
C	2.74465300	-1.99218200	-0.00016700
H	-1.73468400	-2.82451200	-0.00035900
H	-4.07497100	-2.01306600	-0.00032800
H	-4.57110700	0.40506500	-0.00007300
H	-2.72660000	2.07185200	0.00016200
H	2.99671700	1.41192300	0.00023500
H	4.41378400	-0.63528300	0.00003000

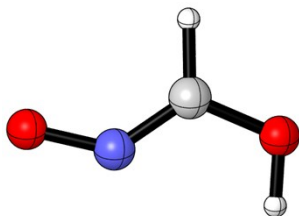
H	0.91313000	-3.13088000	-0.00034200
H	3.37575500	-2.87372200	-0.00025500

**Entry 112**



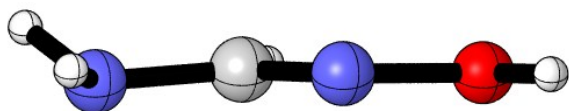
C	-0.6243573	-0.0217079	0.0632519
N	0.6288737	0.1229791	-0.0681091
O	-1.4472283	1.0442571	0.1080789
H	-1.1364813	-0.9754509	0.1496679
H	-0.9110083	1.8462821	0.0250689
O	1.2826457	-1.1312329	-0.0881491
H	2.2075557	-0.8851269	-0.1898091

**112-radical**



C	0.1512182	0.3507337	-0.0000005
N	-0.8988398	-0.3663753	0.0000695
O	-2.1140738	-0.0882723	-0.0000135
O	1.3954052	-0.1831183	0.0000185
H	0.1323142	1.4346177	0.0000305
H	1.3339762	-1.1475853	-0.0001045

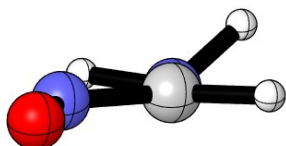
**Entry 113**



C	-0.1762404	0.3020661	-0.0491614
N	0.7858386	-0.5342659	-0.0229714
N	-1.4902764	-0.1134859	-0.1320474
H	-2.1706624	0.4836061	0.3132376
H	-1.6403914	-1.0995249	0.0345936
H	-0.0053044	1.3781411	-0.0643334

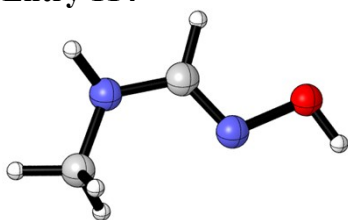
O	2.0305346	0.1521171	-0.0595474
H	2.6665016	-0.5686539	-0.0197704

### 113-radical



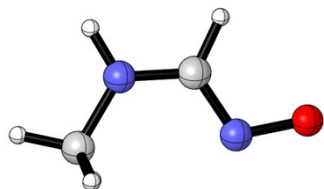
C	0.1613584	0.3234174	-0.0625577
O	2.4344144	-0.0883766	-0.0859667
N	1.2250644	-0.3841806	-0.0232817
N	-1.1070516	-0.2433206	-0.1408417
H	-1.8113166	0.2292594	0.4094533
H	-1.1259416	-1.2454846	-0.0024617
H	0.2234724	1.4086854	-0.0943437

### Entry 114



C	0.3392255	0.8448722	-0.0918943
N	1.3291805	0.0347252	-0.0611023
N	-0.9586315	0.4033082	-0.1201323
H	0.4820485	1.9243742	-0.1352563
O	2.5486195	0.7707012	-0.1343373
H	3.2116225	0.0754392	-0.0873983
C	-1.2665585	-1.0050028	0.0777357
H	-0.7601845	-1.5982058	-0.6856753
H	-0.9385315	-1.3712248	1.0582407
H	-2.3430945	-1.1472268	-0.0213593
H	-1.6436965	1.0682402	0.2011787

### 114-radical



C	0.8848298	0.6543250	0.0028137
N	1.6266848	-0.4504430	-0.0005253
N	-0.4526272	0.5797260	0.0018027

H	1.3466328	1.6414680	0.0064827
O	2.8941048	-0.1941510	0.0011417
C	-1.1913072	-0.6799540	-0.0030673
H	-0.9408622	-1.2657110	-0.8893483
H	-0.9401892	-1.2728360	0.8782527
H	-2.2573592	-0.4558850	-0.0017723
H	-0.9699072	1.4434610	0.0042197

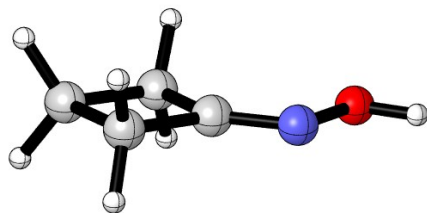
### Entry 115

C	-1.14825300	0.92141700	0.00005200
C	-1.63679600	-0.55310200	0.00009700
C	-0.22024300	-0.20654700	-0.00005800
N	0.94467400	-0.68027300	-0.00003300
O	1.91941000	0.35271300	-0.00007800
H	-1.26337600	1.49561800	-0.91379500
H	-1.26312400	1.49563100	0.91392200
H	-2.07746700	-0.93870800	-0.91394100
H	-2.07724500	-0.93876900	0.91421700
H	2.74496400	-0.14417900	-0.00008800

### 115-radical

C	-1.23255200	0.87886800	0.00020900
C	-1.53271400	-0.64462200	0.00019000
C	-0.16997500	-0.13407400	-0.00018400
N	1.05465200	-0.42161700	-0.00014600
H	-1.41960000	1.43248400	-0.91491600
H	-1.41899600	1.43238600	0.91551700
H	-1.92975100	-1.07550100	-0.91426800
H	-1.92917600	-1.07568400	0.91481100
O	2.11580100	0.20457600	-0.00017700

### Entry 116

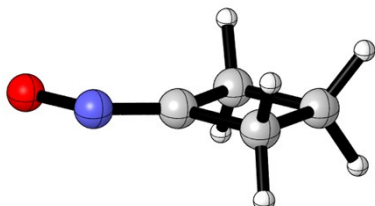


C	-0.7558658	-1.1154695	0.0001518
C	-1.5196428	0.2517395	-0.0002892
C	-0.1577998	1.0187555	0.0001668
C	0.5385812	-0.3269295	0.0001458
N	1.7358902	-0.7346435	-0.0000322
O	2.6399252	0.3585835	-0.0000832
H	-0.9064058	-1.7355525	0.8869368
H	-0.9061908	-1.7361635	-0.8862352



H	-2.1317378	0.4227095	0.8853888
H	-2.1308798	0.4224835	-0.8866062
H	0.0480252	1.6265875	0.8847318
H	0.0485312	1.6269905	-0.8839982
H	3.4975702	-0.0790905	-0.0002772

### 116-radical



C	0.3551794	-1.1390448	0.0000234
C	1.2626994	0.1381852	-0.0005936
C	-0.0008546	1.0590872	0.0003374
C	-0.8379846	-0.2101088	0.0002184
N	-2.0877586	-0.4358608	0.0001594
O	-3.0949186	0.2792712	0.0002634
H	0.4443494	-1.7709338	-0.8870676
H	0.4449574	-1.7703668	0.8874684
H	1.8871884	0.2404482	-0.8876506
H	1.8886094	0.2404242	0.8854564
H	-0.1311496	1.6848602	-0.8865416
H	-0.1303176	1.6840392	0.8879264

### Entry 117

C	-0.11271500	1.12554100	-0.01806100
C	-1.63810200	0.99703000	0.17841000
C	-1.96780700	-0.42739300	-0.31150600
C	-0.76709200	-1.26606700	0.16834400
C	0.39411400	-0.29892500	0.06471900
N	1.59716300	-0.70768800	0.02412200
O	2.50207600	0.38129200	-0.07873600
H	0.13820600	1.53122300	-1.00493900
H	0.38058200	1.77062900	0.71243600
H	-1.88461400	1.08666600	1.24171600
H	-2.19920300	1.77007700	-0.35055200
H	-2.92300300	-0.79931300	0.06495100
H	-2.01643100	-0.44265300	-1.40571100
H	-0.90354800	-1.55320400	1.21835100
H	-0.59617500	-2.18055700	-0.40107200
H	3.35705300	-0.06050300	-0.10558300

### 117-radical

C	-0.16378500	1.17407800	0.05437400
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C	-1.66726500	0.92876200	-0.18930600
C	-1.90333700	-0.51863200	0.28874100
C	-0.63621200	-1.27371700	-0.16239900
C	0.43948900	-0.21585200	-0.05128500
N	1.68855100	-0.47230600	-0.02169000
O	2.69859200	0.23598200	0.06832900
H	0.29206100	1.86875000	-0.65620000
H	0.02192400	1.57616700	1.05776100
H	-2.30030000	1.65443600	0.32508800
H	-1.88561500	1.00423300	-1.25947100
H	-1.97719400	-0.54071100	1.38109500
H	-2.82038900	-0.95484200	-0.11185800
H	-0.41431200	-2.16070500	0.43379700
H	-0.73810800	-1.59687600	-1.20576800

### Entry 118

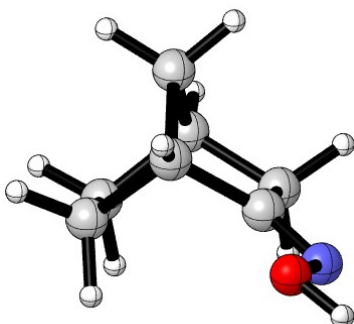
C	1.08272500	1.42418600	-0.25622800
C	-0.21142400	1.09295600	0.51685100
C	0.39405600	-1.39589100	0.38633800
C	1.67234600	-1.03711500	-0.39574400
C	2.17365500	0.36789400	-0.03529100
C	-0.65388900	-0.32108100	0.23538000
N	-1.81459600	-0.69871000	-0.13951200
O	-2.73250800	0.37652500	-0.25150000
H	0.85022100	1.48668500	-1.32583000
H	1.44087600	2.41342600	0.04477800
H	-0.01588400	1.17528400	1.59466100
H	-1.00602400	1.79714000	0.27632900
H	0.64447900	-1.48605100	1.45242200
H	-0.01899500	-2.35381300	0.06506800
H	2.44664500	-1.78416500	-0.19550300
H	1.45927500	-1.08353700	-1.47048300
H	2.48811700	0.38301400	1.01669200
H	3.06003200	0.61531400	-0.62816700
H	-3.53131700	-0.07022600	-0.54922000

### 118-radical

C	1.13456300	1.39527400	-0.27215600
C	-0.18352300	1.15609700	0.49083700
C	0.26954700	-1.38584000	0.38791400
C	1.57405400	-1.10336000	-0.38280300
C	2.15199500	0.27286000	-0.02226000
C	-0.69861700	-0.24286800	0.23699500
N	-1.90674800	-0.47394300	-0.11894700
O	-2.89543500	0.23804700	-0.32144800
H	0.91926200	1.45766800	-1.34512700

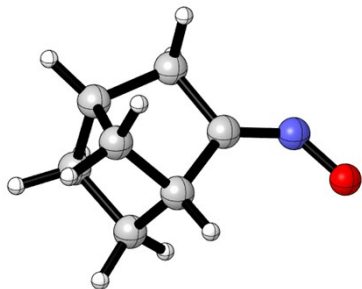
H	1.55279600	2.36266200	0.02252000
H	-0.00190300	1.26701500	1.56881400
H	-0.94331200	1.88884400	0.21270500
H	0.50881800	-1.50620100	1.45376700
H	-0.19663600	-2.31517300	0.05479300
H	2.30306500	-1.89108800	-0.17007300
H	1.37046800	-1.14175800	-1.45949900
H	2.44785200	0.27754900	1.03515600
H	3.06219200	0.46073600	-0.59999600

### Entry 119



C	-0.4067130	-1.4002852	-0.5001538
C	0.3983790	-0.6890772	0.6270453
C	-1.2286000	0.8161968	0.1108133
C	-1.5128190	-0.3555202	-0.8616358
C	-0.7315240	0.0667958	1.3675183
C	0.0672940	1.5312898	-0.3420457
C	1.1152130	0.4669938	-0.0389987
N	2.3376370	0.6122948	-0.3503917
O	3.1125920	-0.5194212	0.0265133
H	0.2249740	-1.6670352	-1.3488188
H	-0.8438840	-2.3234892	-0.1107957
H	1.0430860	-1.3429492	1.2082062
H	-2.0728770	1.4911308	0.2541773
H	-1.4637360	-0.0388642	-1.9064548
H	-2.5120570	-0.7648962	-0.6933377
H	-0.3646900	0.7334328	2.1524453
H	-1.4775840	-0.6083022	1.7954192
H	0.2519670	2.4299058	0.2555583
H	0.0654130	1.8242628	-1.3943998
H	3.9979290	-0.2624632	-0.2506637

### 119-radical



C	-0.3177803	-1.4363907	-0.4447607
C	0.5158287	-0.7406267	0.6671893
C	-0.9580353	0.8735843	0.0413013
C	-1.3128013	-0.3140257	-0.8891107
C	-0.5604213	0.1413233	1.3439423
C	0.4021317	1.4674273	-0.4047667
C	1.3412717	0.3347893	-0.0217657
N	2.5895837	0.3047623	-0.2688067
O	3.4961307	-0.5086527	-0.0489267
H	0.3079057	-1.8017317	-1.2607127
H	-0.8480923	-2.2958767	-0.0255657
H	1.0973927	-1.4119877	1.2969733
H	-1.7481573	1.6191673	0.1308823
H	-1.2025063	-0.0520247	-1.9441037
H	-2.3493543	-0.6252987	-0.7391207
H	-0.1560513	0.8064583	2.1109123
H	-1.3745303	-0.4475947	1.7745733
H	0.6370587	2.3805593	0.1525563
H	0.4404257	1.7061393	-1.4706897

### Entry 120

C	0.62157800	0.44451400	0.00002700
C	-0.82574300	0.00484600	-0.00001000
N	1.58183000	-0.38493600	0.00001200
C	-1.49763900	0.59621800	-1.26013900
C	-1.49759400	0.59596600	1.26028000
C	-0.96245100	-1.52462300	-0.00015000
O	2.83050600	0.27490100	-0.00000300
H	0.82744100	1.51902100	0.00001800
H	-2.56448900	0.35452600	-1.26735500
H	-1.40078600	1.68579500	-1.29060800
H	-1.04975100	0.19049100	-2.17110000
H	-1.40073000	1.68553400	1.29096600
H	-2.56444200	0.35427100	1.26747000
H	-1.04966600	0.19003700	2.17112900
H	-0.49067700	-1.96441000	-0.88126900
H	-0.49063400	-1.96457400	0.88086100
H	-2.02071300	-1.80178900	-0.00015400

H	3.45868500	-0.45509100	-0.00006100
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**120-radical**

C	-0.62591800	-0.58768200	-0.00000600
C	0.76854300	-0.00037700	0.00000000
O	-2.88955400	-0.10088600	0.00000000
N	-1.68234300	0.13121200	-0.00000100
C	1.50576600	-0.50766800	-1.25997200
C	1.50575200	-0.50765700	1.25998400
C	0.72814100	1.53548400	-0.00000700
H	-0.74771500	-1.67306300	-0.00000800
H	2.53817700	-0.14595500	-1.26605400
H	1.53485900	-1.60098700	-1.29149000
H	1.01500600	-0.15534200	-2.17095400
H	1.53484400	-1.60097600	1.29151300
H	2.53816400	-0.14594500	1.26607400
H	1.01498300	-0.15532300	2.17095700
H	0.21232200	1.91980900	-0.88337000
H	0.21231200	1.91981700	0.88334700
H	1.74618400	1.93396300	-0.00000300

**Entry 121**

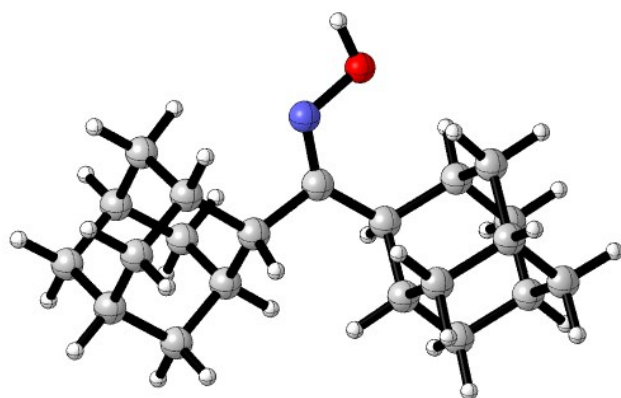
C	0.42471700	1.01773000	-0.00000800
N	1.69210100	0.88356600	-0.00000800
C	-0.69557500	-0.01622000	0.00000000
C	-0.61459700	-0.89658000	-1.26756700
C	-2.03516800	0.74625800	-0.00000800
C	-0.61459400	-0.89655300	1.26758600
O	2.11470900	-0.46372000	0.00000100
H	0.13811500	2.06858100	-0.00001200
H	-1.45153800	-1.60179600	-1.27696300
H	-0.67914600	-0.28668000	-2.17317800
H	0.31637800	-1.46134500	-1.30028800
H	-2.13101800	1.38206400	0.88559700
H	-2.13101700	1.38204500	-0.88562700
H	-2.87246100	0.04342500	-0.00000100
H	-1.45153000	-1.60177400	1.27699700
H	0.31638600	-1.46131100	1.30031900
H	-0.67914600	-0.28663300	2.17318400
H	3.07389500	-0.37959300	-0.00000200

**121-radical**

C	-0.45949300	1.00556600	-0.00004900
O	-2.32824200	-0.35832600	0.00000800
N	-1.70295100	0.70092500	-0.00003000
C	0.67820300	-0.01568000	-0.00000100

C	2.00657700	0.76133500	0.00004700
C	0.58394300	-0.89608000	-1.26345600
C	0.58384200	-0.89606500	1.26345800
H	-0.25066000	2.06938100	-0.00003700
H	2.85082400	0.06694400	0.00008600
H	2.09457000	1.39695000	-0.88607500
H	2.09449900	1.39696400	0.88616600
H	-0.36512600	-1.43533000	-1.30331600
H	0.67302700	-0.29290000	-2.17086500
H	1.39175400	-1.63408100	-1.26464000
H	1.39165000	-1.63406800	1.26471400
H	0.67285600	-0.29287400	2.17086600
H	-0.36523200	-1.43531100	1.30324700

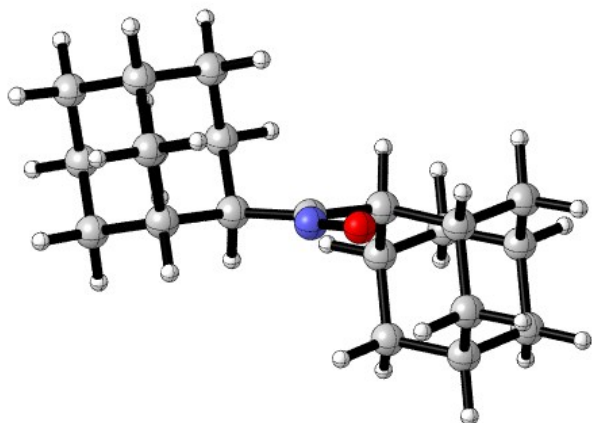
### Entry 122



C	-0.0003522	1.0359034	0.0213254
N	-0.2424062	2.2779424	0.2056934
C	-1.1727222	0.1302264	0.4266414
C	-1.7105172	-0.7798346	-0.7222346
C	-2.3895742	0.8334184	1.0889634
C	-2.5378332	0.0384264	-1.7339216
C	-2.6036452	-1.8704776	-0.0925976
C	-3.2410942	1.6225544	0.0713404
C	-3.2769792	-0.2612986	1.7224674
C	-3.7516892	0.6758204	-1.0295656
C	-3.7977432	-1.2180576	0.6300914
C	-4.6287322	-0.4239616	-0.3972656
C	1.2416798	0.3483574	-0.5783246
C	1.5767788	-1.0124136	0.1166384
C	2.5717448	1.1567804	-0.6691846
C	2.1648718	-0.7674686	1.5216324
C	2.6003658	-1.7898736	-0.7358386
C	3.1652308	1.3894394	0.7353164
C	3.5887498	0.3629634	-1.5178406

C	3.4731668	0.0373704	1.4069574
C	3.9069308	-0.9879746	-0.8555656
C	4.4890678	-0.7474566	0.5520924
O	0.7782168	3.1866404	-0.1519986
H	-0.7615462	-0.5414466	1.1901074
H	-0.8790432	-1.2600066	-1.2448006
H	-2.0294782	1.5127374	1.8651124
H	-2.8713452	-0.6194856	-2.5452786
H	-1.9196822	0.8193754	-2.1904506
H	-2.0184772	-2.4759486	0.6100684
H	-2.9634792	-2.5508216	-0.8735366
H	-2.6537282	2.4323634	-0.3633406
H	-4.0893772	2.0811014	0.5941164
H	-2.7110112	-0.8223976	2.4758384
H	-4.1217192	0.2044844	2.2432804
H	-4.3412692	1.2421694	-1.7590446
H	-4.4197342	-1.9959826	1.0867134
H	-5.5000902	0.0283274	0.0908134
H	-5.0120922	-1.0983146	-1.1725826
H	0.9412818	0.1133944	-1.6105086
H	0.6796818	-1.6257316	0.2038084
H	2.3876678	2.1122724	-1.1511626
H	2.3518998	-1.7301726	2.0119584
H	1.4485768	-0.2254216	2.1497664
H	2.1858858	-1.9883746	-1.7316566
H	2.7929168	-2.7645326	-0.2720516
H	2.4687878	1.9708134	1.3454394
H	4.0822478	1.9841014	0.6475964
H	3.1954438	0.2048204	-2.5294066
H	4.5042958	0.9566054	-1.6248766
H	3.8877578	0.2073714	2.4067504
H	4.6288788	-1.5430616	-1.4648136
H	5.4295028	-0.1885606	0.4799644
H	4.7248698	-1.7059596	1.0302414
H	0.3788638	4.0292544	0.0871154

**122-radical**



C	-0.0036864	0.9447027	0.0496276
O	0.5654066	3.2185847	-0.0956094
N	-0.1148704	2.2173487	0.1495826
C	-1.1976694	0.1064517	0.4888816
C	-1.7462244	-0.8264433	-0.6339794
C	-2.3904304	0.9064257	1.0792176
C	-2.4701144	-0.0020923	-1.7177254
C	-2.7346984	-1.8263593	0.0001066
C	-3.1394274	1.7071937	-0.0085844
C	-3.3750764	-0.0999873	1.7137746
C	-3.6639514	0.7492097	-1.0942244
C	-3.9130694	-1.0647163	0.6366386
C	-4.6410444	-0.2606383	-0.4592544
C	1.2313876	0.2551877	-0.5475404
C	1.6784866	-1.0066853	0.2513056
C	2.4753376	1.1583817	-0.7558714
C	2.3049006	-0.6005653	1.5999856
C	2.7198986	-1.7776063	-0.5877394
C	3.1114586	1.5476797	0.5957846
C	3.5130006	0.3789797	-1.5927674
C	3.5460996	0.2805157	1.3547166
C	3.9535646	-0.8913193	-0.8399324
C	4.5784596	-0.4975063	0.5136786
H	-0.8271954	-0.5477603	1.2895246
H	-0.9221214	-1.3832533	-1.0894594
H	-2.0181244	1.5907427	1.8477216
H	-2.8165774	-0.6706263	-2.5145784
H	-1.7798514	0.7119007	-2.1809964
H	-2.2220934	-2.4338453	0.7554536
H	-3.1034854	-2.5175893	-0.7667354
H	-2.4886374	2.4636877	-0.4523354
H	-3.9756794	2.2439997	0.4547546
H	-2.8786344	-0.6652363	2.5114386
H	-4.2060834	0.4423637	2.1789306



H	-4.1807924	1.3231097	-1.8709684
H	-4.6070874	-1.7775443	1.0952236
H	-5.4997314	0.2694667	-0.0309624
H	-5.0361324	-0.9395373	-1.2244544
H	0.9102046	-0.0913363	-1.5410284
H	0.8201016	-1.6598433	0.4271826
H	2.1869046	2.0620107	-1.2968184
H	2.5808146	-1.5014533	2.1603376
H	1.5763056	-0.0564753	2.2119656
H	2.2772396	-2.0927493	-1.5401044
H	3.0125836	-2.6905253	-0.0559074
H	2.4111546	2.1320057	1.1978986
H	3.9777166	2.1935197	0.4118556
H	3.0891436	0.1127597	-2.5683854
H	4.3790106	1.0214937	-1.7875234
H	3.9908806	0.5609407	2.3156026
H	4.6863256	-1.4414763	-1.4402944
H	5.4697306	0.1197717	0.3514306
H	4.9063746	-1.3952633	1.0511586

#### Entry 123

C	0.03890000	0.42034700	-0.00016600
N	0.94471800	-0.46019700	-0.00013500
H	0.20824100	1.49283100	0.00006000
O	2.21453200	0.13426800	0.00009600
H	2.80638600	-0.62642000	0.00022900
Cl	-1.62219500	-0.07301500	0.00005200

#### 123-radical

C	-0.06511400	0.51801600	-0.00008600
N	-1.06582700	-0.26375500	-0.00004700
H	-0.15687200	1.59820700	0.00002200
O	-2.28119200	-0.09484400	0.00004100
Cl	1.54458100	-0.12360400	0.00002900

#### Entry 124

C	-0.49217000	0.34946000	-0.00064900
N	0.45582700	-0.47762000	-0.00049800
H	-0.42505500	1.43293000	0.00014600
F	-1.74156400	-0.12371700	0.00042400
O	1.69232400	0.18391300	0.00031300
H	2.32277200	-0.54420100	0.00092200

#### 124-radical

C	0.47523400	0.41317300	0.00047900
O	-1.78060800	-0.00641500	-0.00033300

N	-0.57835700	-0.28433700	0.00041300
H	0.52358900	1.49529600	-0.00061300
F	1.65759700	-0.21474000	-0.00027600

#### Entry 125

C	-0.64639800	0.45516100	-0.00001700
N	-1.52771600	-0.44841600	0.00002600
H	-0.84240900	1.52340100	-0.00002100
Br	1.18083700	-0.03766200	-0.00001700
O	-2.81619300	0.10901100	0.00005600
H	-3.38493000	-0.66936800	0.00010200

#### 125-radical

C	-0.66590800	0.57075200	-0.00002900
N	-1.63549700	-0.24702700	-0.00001600
H	-0.79807200	1.64726000	0.00001500
O	-2.85676500	-0.14157500	0.00002000
Br	1.11703200	-0.06314200	0.00000300

#### Entry 126

C	-0.12335900	0.66630100	-0.00002800
N	-0.80617000	-0.40654300	0.00002300
O	1.21616900	0.67045100	-0.00004700
C	1.86867500	-0.60802800	-0.00002200
H	-0.55233600	1.66499100	-0.00003800
H	2.93443600	-0.39006800	-0.00004500
H	1.59177500	-1.17812800	0.88946000
H	1.59174600	-1.17817800	-0.88946200
O	-2.19090700	-0.10150100	0.00006100
H	-2.59642800	-0.97405400	0.00010900

#### 126-radical

C	0.15250300	0.75905900	-0.00000500
N	0.93645000	-0.24736500	-0.00002800
O	2.18108600	-0.33615100	0.00001700
O	-1.18794300	0.64813600	0.00000600
C	-1.72137700	-0.68130600	0.00000400
H	0.51004700	1.78325000	0.00000800
H	-2.80272500	-0.56522900	0.00010400
H	-1.39725900	-1.22439800	-0.89189100
H	-1.39710700	-1.22447200	0.89179700

#### Entry 127

C	1.02635100	-0.55837300	0.00086000
N	2.02698000	0.21886300	-0.00033600
H	1.11698900	-1.64298600	0.00252900

C	-0.37294800	-0.01789400	0.00005700
Cl	-0.45026000	1.75991700	-0.00277700
Cl	-1.21257000	-0.66326200	1.47107800
Cl	-1.21254800	-0.66796100	-1.46898800
O	3.22048900	-0.49024500	0.00078800
H	3.89124500	0.20272200	-0.00029300

### 127-radical

C	0.97307200	-0.00010200	0.75873900
N	2.08016600	0.00002000	0.12027200
H	0.95170600	-0.00046200	1.84495900
C	-0.33350500	0.00003000	0.03646800
Cl	-0.12727500	0.00066100	-1.73639600
Cl	-1.27026300	1.46757600	0.54265900
Cl	-1.27004500	-1.46812000	0.54160100
O	3.24982900	-0.00015600	0.45352400

### Entry 128

C	-0.83785700	0.14106400	0.11233200
N	-1.90227100	-0.53256100	-0.06049400
N	0.36043200	-0.56075700	0.21365100
H	0.39287800	-1.55998100	0.05264200
H	-0.78024600	1.21854200	0.22142700
O	-3.02347300	0.30427200	-0.06463500
H	-3.75304400	-0.30693800	-0.21483800
N	1.58281500	0.05771300	-0.00956600
O	2.53340900	-0.69965700	-0.12553500
O	1.60015500	1.27678800	-0.02712400

### 128-radical

C	-0.87676600	0.24797500	0.28661300
N	-1.94824600	-0.31058500	-0.13177200
N	0.28895300	-0.52195500	0.37936000
H	0.25226500	-1.51356900	0.17390700
H	-0.83012800	1.28046300	0.60992200
O	-3.11766500	0.06380200	-0.19816400
N	1.51030700	0.03259900	-0.02792700
O	2.41137900	-0.76788700	-0.20630500
O	1.56645600	1.24718900	-0.10067200

### Entry 129

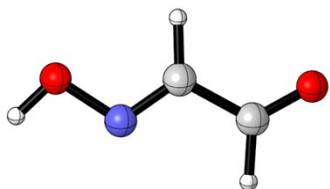
C	-0.38693100	-0.43309800	-0.12040000
N	-1.34345100	0.39432800	0.08535400
N	0.92264000	-0.03633400	-0.23030800
H	-0.57739700	-1.49777500	-0.25577100
O	-2.58962700	-0.29678600	0.01609200

H	-3.22180000	0.39906300	0.21964200
C	1.95230000	-1.00231200	0.12384800
H	1.64510200	-2.00120100	-0.19140200
H	2.88098000	-0.75173500	-0.39412500
H	2.15402800	-1.02716000	1.20516400
C	1.23850500	1.36327100	0.01249800
H	0.52192500	1.99181800	-0.51556900
H	1.19185600	1.61984500	1.08046700
H	2.24476000	1.56831500	-0.35814700

### 129-radical

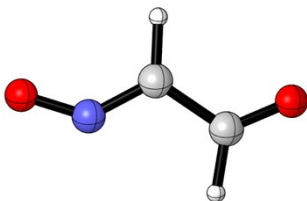
C	-0.45078300	-0.46754500	-0.00010600
N	-1.48214600	0.37570100	0.00007600
N	0.82124300	-0.04158400	-0.00028800
H	-0.62573400	-1.54296400	-0.00021000
O	-2.62076200	-0.23609600	0.00005400
C	1.92971800	-0.98300600	0.00012800
H	1.55061900	-2.00410000	-0.00059200
H	2.55369000	-0.83682100	-0.88752300
H	2.55245900	-0.83760900	0.88879000
C	1.15837200	1.37927400	0.00002100
H	0.23996300	1.96009600	-0.00109800
H	1.74772100	1.61962800	0.89019000
H	1.74985900	1.61938900	-0.88877600

### Entry 130



C	0.1637633	0.3633664	0.0001581
N	-0.8849368	-0.3663696	-0.0003139
H	0.1350413	1.4523714	0.0005221
C	1.4619573	-0.3410496	0.0002011
H	1.3916663	-1.4449026	-0.0001899
O	-2.0440728	0.3793504	-0.0003129
H	-2.7463967	-0.2826936	-0.0006889
O	2.5229783	0.2399274	0.0006241

### 130-radical



C	-0.1690043	0.4072546	-0.0000351
N	-1.3119893	-0.1980274	0.0000459
H	-0.1209313	1.4941596	-0.0001291
C	1.0440657	-0.4144844	0.0000079
H	0.8659367	-1.5076964	0.0001179
O	-2.4662593	0.1608416	0.0000439
O	2.1581817	0.0579526	-0.0000511

### Entry 131

C	0.04210200	0.22496800	-0.00001000
N	1.10376300	-0.48860000	0.00016800
H	0.10528600	1.31484300	-0.00005100
C	-1.25822400	-0.42134100	-0.00015100
C	-2.41151900	0.25643700	-0.00035600
H	-1.25042400	-1.50698300	-0.00008800
H	-3.36678700	-0.25370200	-0.00046700
H	-2.43410600	1.34146900	-0.00042400
O	2.25206000	0.31197300	0.00031200
H	2.96905800	-0.33159000	0.00046400

### 131-radical

C	0.07747000	0.32956900	0.00002800
O	2.37774700	0.09065800	-0.00005600
N	1.21304300	-0.28221300	0.00000500
H	0.08019800	1.41930900	-0.00002300
C	-1.16491800	-0.41257300	0.00002400
C	-2.37151400	0.16697000	0.00000900
H	-1.07417000	-1.49472500	0.00005400
H	-3.27835800	-0.42399600	0.00003700
H	-2.48717100	1.24583600	-0.00001000

### Entry 133

C	-0.02379500	0.44897400	-0.00005900
N	0.87459200	-0.46119400	-0.00005200
H	0.21882800	1.51055100	0.00004600
C	-1.39589200	0.05938600	-0.00000200
N	-2.52251200	-0.19312600	0.00003700
O	2.13901200	0.08757600	0.00004200
H	2.72263900	-0.68107500	0.00008200

### 133-radical

C	-0.01242900	0.54187000	0.00001100
O	-2.20224000	-0.15072700	0.00001500
N	-1.00093000	-0.29002200	0.00000800
H	-0.20254800	1.61194400	0.00001700
C	1.32046700	0.05638000	-0.00001100
N	2.42553600	-0.28078200	-0.00002800

#### Entry 134

C	-0.72985600	0.67540900	0.00010900
N	-1.43055400	-0.38901400	-0.00005600
H	-1.16539200	1.67306400	0.00026300
C	0.74766800	0.61615600	0.00005600
O	1.43654400	1.58600000	-0.00009700
O	-2.77679900	-0.11512700	-0.00001400
H	-3.18980700	-0.98783400	-0.00016300
Cl	1.46966200	-1.02814700	0.00001100

#### 134-radical

C	-0.71385600	0.82603700	-0.00000300
N	-1.52819700	-0.17410100	0.00000000
H	-1.08725800	1.84652900	-0.00000300
C	0.73463300	0.61696900	-0.00000600
O	1.53593700	1.49507000	0.00000400
O	-2.72748800	-0.28557200	0.00000200
Cl	1.24661100	-1.11540200	0.00000000

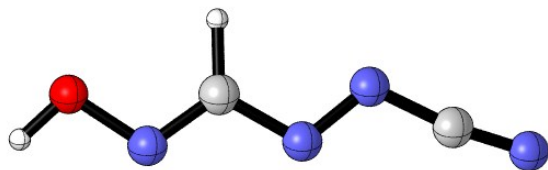
#### Entry 135

C	-0.35344800	-0.50404500	0.00001900
N	-1.26210300	0.38859300	0.00002100
H	-0.56945400	-1.57007000	-0.00003800
C	1.07987700	-0.12232600	0.00013300
O	1.96121900	-0.94912800	-0.00005200
O	1.30187000	1.20523200	-0.00002600
H	2.26274500	1.32894200	-0.00011600
O	-2.52607700	-0.17057500	-0.00003500
H	-3.11324000	0.59497700	0.00000400

#### 135-radical

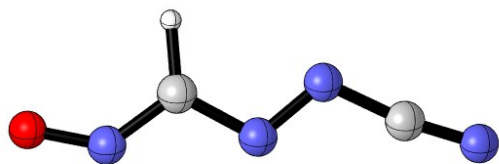
C	-0.35684400	-0.62839200	0.00000200
N	-1.36696400	0.17013500	0.00000100
H	-0.50226300	-1.70445500	-0.00000100
C	1.01957600	-0.10850500	0.00000700
O	-2.56680700	0.02353700	-0.00000200
O	1.98712700	-0.83132800	-0.00000400
O	1.08811300	1.23992500	-0.00000100
H	2.02715800	1.47781700	-0.00000600

### Entry 136



C	-0.5745949	0.2418698	0.0061673
N	-1.6160629	-0.5029942	0.0966603
H	-0.6012959	1.3296528	-0.0654307
O	-2.7607849	0.2440818	0.0915693
H	-3.4680369	-0.4099072	0.1630473
N	0.6351961	-0.4394162	0.0046533
N	1.6162681	0.3539638	-0.0864727
C	2.8317571	-0.2357512	-0.0951697
N	3.9375541	-0.5814992	-0.1150247

### 136-radical



C	-0.9927746	0.2326974	0.0000323
N	-2.0419136	-0.5365666	-0.0001928
H	-1.0839326	1.3181764	0.0005753
O	-3.2237286	-0.3089326	0.0000713
N	0.2164884	-0.4146426	-0.0005957
N	1.1920474	0.3972414	-0.0003777
C	2.4120714	-0.1763686	0.0000533
N	3.5217424	-0.5116046	0.0004343

### Entry 137

C	-0.29689900	-0.47670500	-0.00005200
N	-1.22632200	0.37944500	-0.00005100
H	-0.38548100	-1.55672400	-0.00000500
N	1.09091100	0.01890600	0.00000300
O	1.93688300	-0.87015900	0.00002100
O	1.30307000	1.21574400	0.00001300
O	-2.46618400	-0.20949600	0.00003500
H	-3.07540400	0.53979200	0.00010100

### 137-radical

C	0.29584900	-0.60044000	0.00001900
O	2.51275700	-0.02415700	0.00000900

N	1.31998900	0.16351200	0.00001400
H	0.31355700	-1.68243200	0.00002000
N	-1.01504200	0.03660800	0.00002700
O	-1.95980600	-0.74456800	-0.00003000
O	-1.08086200	1.25425500	-0.00003200

### Entry 139

C	-0.82721700	0.51864800	-0.07757100
N	-1.73755500	-0.35568500	-0.00126300
S	0.85725200	-0.07654100	-0.13552700
O	0.93795200	-1.50991500	-0.08730500
O	1.57963700	0.73585100	-1.08306300
F	1.30675200	0.46704400	1.34517000
O	-2.99477800	0.19556700	-0.00191600
H	-0.95145600	1.59690900	-0.14149100
H	-3.58165500	-0.56977200	0.05593700

### 139-radical

C	0.82057900	0.66437200	-0.04490100
N	1.82150500	-0.12939800	-0.01764200
O	3.01976100	0.00167700	0.02160600
S	-0.79702900	-0.05633600	-0.14684800
O	-1.64012900	0.85196900	-0.88078100
O	-0.72101600	-1.47036400	-0.39487600
F	-1.23131100	0.11191100	1.42221800
H	0.89132500	1.74747300	-0.02507500

### Entry 140

C	1.03133600	0.02211700	-0.53085300
N	1.94857500	0.04245800	0.33639700
O	3.15272100	0.46139700	-0.17651600
H	3.75109400	0.42129200	0.58089700
S	-0.58459600	-0.54750300	0.01271500
O	-1.15401000	-1.29992600	-1.08747500
O	-0.54463400	-1.04175200	1.36845900
Cl	-1.58562400	1.33258700	0.04652500
H	1.09739500	0.29711700	-1.58067500

### 140-radical

C	1.03925500	-0.06867700	-0.67466600
N	2.00674200	0.17234400	0.12040900
O	3.16631000	0.48642700	0.00308300
S	-0.52069600	-0.54553800	0.04678400
O	-1.18327600	-1.40099700	-0.91542700
O	-0.33928200	-0.89729100	1.43680100
Cl	-1.54051800	1.31945600	0.00107100



H	1.08721200	-0.00160200	-1.75728500
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### Entry 141

C	1.41644900	0.15025100	-0.54527300
N	2.23147400	-0.23656400	0.34253500
S	-0.13118100	0.87310000	0.03746400
O	-0.03006200	1.28387700	1.42535000
O	-0.59086400	1.75460300	-1.02697200
C	-1.28453400	-0.64418700	0.00174100
F	-0.92756000	-1.52100200	0.93727200
F	-2.52951800	-0.23838500	0.21872100
F	-1.20701600	-1.23144900	-1.19808500
O	3.39460900	-0.73545900	-0.18855900
H	1.55750300	0.12076800	-1.62335900
H	3.91695700	-0.97743800	0.58765800

### 141-radical

C	1.41488300	0.12441900	0.67275800
N	2.30651500	-0.33616500	-0.12025300
O	3.39528000	-0.83849100	0.00014400
S	-0.04791200	0.85023200	-0.05962800
O	-0.54286800	1.83288000	0.89151600
O	0.18743000	1.13259100	-1.46403200
C	-1.27302200	-0.60644500	0.00179100
F	-1.33039000	-1.08577700	1.24841500
F	-2.47154700	-0.17376700	-0.36606900
F	-0.87114400	-1.57536000	-0.81870800
H	1.50880800	0.13988800	1.75474900

### Entry 142

C	0.98154900	-0.71858600	0.00004900
N	1.71704100	0.30655800	-0.00005800
S	-0.79647600	-0.46075300	-0.00000700
O	-1.33211500	-0.92218900	-1.26669400
O	-1.33217900	-0.92222900	1.26664000
C	-0.89704500	1.31862900	0.00001400
N	-1.10270900	2.45396400	0.00003100
O	3.05939200	0.01105400	0.00002500
H	1.28917200	-1.76288500	0.00018600
H	3.48631200	0.87794500	-0.00003800

### 142-radical

C	-0.97689900	-0.02763800	-0.67881000
N	-1.94074700	0.23826500	0.11887700
O	-3.09559800	0.55843100	0.00126300
S	0.57463500	-0.52028700	0.04777200

O	0.38556800	-0.85733200	1.44147400
O	1.23218200	-1.38539600	-0.91030900
C	1.46293000	1.02600600	0.01380800
N	2.04927800	2.02033100	-0.01476500
H	-1.04728300	-0.00140700	-1.76254900

### Entry 143

C	-0.83578700	-0.49210600	-0.14159200
N	-1.76338800	0.33734400	0.07922900
O	-3.01282100	-0.23757700	-0.02046800
H	-3.61424100	0.49488700	0.16475000
S	0.84787400	0.11971700	-0.09958400
O	1.53236800	-0.42049500	-1.26606200
O	0.87840700	1.52082300	0.23505300
H	-0.95225800	-1.54456300	-0.38997300
O	1.38036900	-0.73713000	1.20103300
H	2.13236800	-1.27955200	0.91705600

### 143-radical

C	0.83021000	-0.61463800	0.22496800
N	1.84609200	0.10968900	-0.04363600
O	3.04418100	-0.05169600	-0.03298000
S	-0.78249600	0.12725500	0.09607300
O	-1.56943900	-0.31513700	1.23636800
O	-0.64698100	1.51826200	-0.26058500
H	0.89031600	-1.64726200	0.55502000
O	-1.33702900	-0.69992300	-1.21155400
H	-2.20013600	-1.08085200	-0.98654100

### Entry 144

C	0.87059600	-0.48069500	-0.00000800
N	1.80679500	0.38210800	-0.00003900
P	-0.81166200	0.14657800	0.00001100
O	-1.06747800	1.58167200	0.00007400
F	-1.45913200	-0.66743800	-1.19781900
F	-1.45915800	-0.66755600	1.19774800
O	3.05034900	-0.20229800	0.00002300
H	1.04639400	-1.55709700	0.00001200
H	3.65903800	0.54780100	0.00002300

### 144-radical

C	-0.85085200	0.72284700	0.00404800
O	-3.03880800	-0.00677400	0.00024800
N	-1.83750800	-0.10315400	-0.00074300
P	0.82891000	0.12040900	-0.00099700
O	1.85145500	1.16221000	-0.01053100

F	0.89815400	-0.90883700	1.19757900
F	0.88541900	-0.92031000	-1.19011800
H	-1.01931600	1.79769200	0.01099500

### Entry 145

C	0.61960900	0.60453700	0.00005700
N	-0.63404700	0.71903300	-0.00002700
F	1.25138100	-0.59811100	-0.00001500
O	-1.38048900	-0.44078200	-0.00003600
H	1.28380700	1.45563000	0.00012800
H	-0.78165700	-1.20682800	0.00015000

### 145-radical

C	0.57782600	0.56582600	0.00004700
N	-0.68506300	0.49476000	0.00001600
F	1.34725600	-0.53672400	-0.00000500
O	-1.48732200	-0.44190200	-0.00005900
H	1.10174700	1.50746000	0.00011600

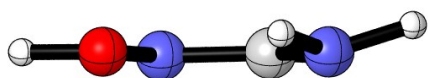
### Entry 146

C	-0.65319600	0.59522300	-0.00000100
N	0.61193700	0.75685600	0.00000000
O	-1.31508000	-0.57050500	0.00000000
O	1.24004400	-0.52346900	-0.00000200
H	-1.28346200	1.47461200	0.00000300
H	-0.65799400	-1.28413200	0.00000300
H	2.17736100	-0.30802200	0.00001100

### 146-radical

C	-0.58844800	0.60455300	0.00000100
N	0.75650600	0.64949300	-0.00000100
O	-1.25288100	-0.51859000	0.00000100
O	1.24587300	-0.54156000	-0.00000100
H	-1.16231100	1.52162400	0.00000100
H	-0.54648200	-1.21419100	0.00000100

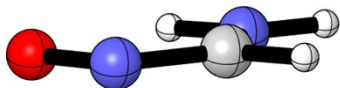
### Entry 147



C	0.3337402	0.6883702	-0.0299969
N	-0.9444738	0.7777783	-0.0540669
N	1.0780123	-0.4594648	-0.0744979
O	-1.5081597	-0.5346158	-0.0743899

H	0.8705262	1.6304843	-0.0140159
H	2.0357022	-0.4192298	0.2310241
H	0.5877822	-1.3264947	0.0861311
H	-2.4531298	-0.3568278	-0.0701879

### 147-radical



C	0.0150597	0.6329459	-0.0208284
N	-1.3336493	0.6625279	-0.0743294
N	0.7197607	-0.4961671	0.0445776
O	-1.8482943	-0.5145011	-0.0545354
H	0.5344067	1.5831639	-0.0327594
H	1.7242187	-0.5074541	0.0845186
H	0.1884977	-1.3605151	0.0533566

### Entry 148

C	0.62011200	-0.00089000	1.25733200
N	1.89325300	-0.00079200	1.24909900
C	-0.33475400	-0.00000600	0.08138700
Cl	-2.01770500	-0.00050600	0.74014500
O	2.45524100	0.00026300	-0.01208200
Cl	-0.11424000	1.47331100	-0.93065500
Cl	-0.11389800	-1.47222700	-0.93228500
H	0.16938200	-0.00166100	2.24244100
H	3.40309400	0.00064700	0.16571500

### 148-radical

C	0.64708700	-0.00001000	1.24213600
N	1.91922400	-0.00000900	1.09141400
C	-0.32270200	-0.00000100	0.08689300
Cl	-1.98798400	-0.00004200	0.76503100
O	2.67077900	0.00000000	0.13668400
Cl	-0.09459400	1.46685800	-0.94010200
Cl	-0.09454700	-1.46680700	-0.94016500
H	0.26400400	-0.00002600	2.25146600

### Entry 149

C	-0.01231700	0.72238300	0.00006300
N	-1.29185600	0.65210600	0.00001600
C	0.94836700	-0.37234400	-0.00001100
O	-1.75566100	-0.67350300	-0.00012400
C	2.26882700	-0.15776700	0.00007700
H	0.36196100	1.74349400	0.00017100
H	0.55030500	-1.37978200	-0.00014200

H	-2.71204700	-0.56272100	-0.00014700
H	2.97691300	-0.97769000	0.00002200
H	2.68189000	0.84634700	0.00020700

#### 149-radical

C	-0.05843000	0.68181500	0.00006900
N	-1.32803100	0.45249800	-0.00000500
C	0.94501200	-0.36989300	0.00000000
O	-2.00261900	-0.56964000	-0.00013700
C	2.26093300	-0.12772300	0.00007400
H	0.22489600	1.72724100	0.00018700
H	0.57034900	-1.38912800	-0.00011800
H	2.98085100	-0.93662900	0.00001900
H	2.65598300	0.88295700	0.00019200

#### Entry 150

C	-0.11642100	0.04037400	0.41016300
N	-1.08581100	0.28153400	-0.37619000
C	1.24784400	0.55998200	0.06379000
O	-2.28263800	-0.28565300	0.08357300
O	2.18880500	-0.50221300	-0.10063200
H	-0.24872000	-0.55864400	1.31281400
H	1.63743600	1.16460700	0.88636600
H	1.18149700	1.19041300	-0.82895700
H	-2.92152500	-0.02930700	-0.59075200
H	1.91410900	-1.03700700	-0.85339200

#### 150-radical

C	-0.15300400	0.20019800	0.46432500
N	-1.19861400	0.04831600	-0.26161200
C	1.16231600	0.54185100	-0.16818900
O	-2.36865600	-0.23276500	-0.04393100
O	2.13603800	-0.48450200	0.02482900
H	-0.22811200	0.04256100	1.53992100
H	1.58831500	1.42806200	0.30724000
H	1.00881500	0.76369900	-1.23017400
H	1.82635100	-1.28670200	-0.40969600

#### Entry 151

C	0.02355100	0.92211200	0.00004900
N	1.23566900	0.50932100	0.00008700
C	-1.14188800	0.09300000	-0.00005100
O	1.33411200	-0.86275400	0.00002100
N	-2.11254200	-0.53231600	-0.00013100
H	-0.11008300	1.99730700	0.00009800
H	2.28532100	-1.02498200	0.00005900

**151-radical**

C	0.03386500	0.86600100	0.00004700
N	1.21562100	0.34120400	0.00007700
C	-1.15309600	0.08256700	-0.00005200
O	1.64471100	-0.78912400	0.00003900
N	-2.13287700	-0.53025200	-0.00013200
H	-0.02150900	1.94491700	0.00010000

**Entry 152**

C	0.54123400	-0.91954800	-0.00022100
N	1.83292200	-0.85774100	-0.00012900
C	-0.34799900	0.24655100	-0.00038400
O	2.44496000	0.33691900	0.00033300
O	0.00770700	1.39455900	-0.00031500
Cl	-2.08865900	-0.17383000	0.00020000
H	0.11852100	-1.91495700	-0.00024400
H	1.77748100	1.06041400	0.00124000

**152-radical**

C	-0.56916800	-0.86808200	-0.00010000
N	-1.85217800	-0.69356500	-0.00016700
C	0.32593400	0.29860400	0.00006300
O	-2.56877200	0.27446100	-0.00012500
O	0.00973800	1.44173600	0.00013000
Cl	2.06439800	-0.21042600	0.00009000
H	-0.19784200	-1.88050000	-0.00017300

**Entry 153**

C	0.01748900	0.88673200	0.00000200
N	-1.23279000	0.63899900	-0.00000600
S	1.38360500	-0.23068300	0.00000100
O	-1.50858200	-0.73972700	0.00000500
H	0.29068500	1.93594000	0.00000000
H	0.63646700	-1.35242900	-0.00003300
H	-2.47158400	-0.76814300	-0.00000100

**153-radical**

C	0.03393900	0.84107000	-0.00004700
N	1.24610100	0.44466300	-0.00004400
S	-1.39664700	-0.21208200	0.00007900
O	1.78455000	-0.66273600	0.00009100
H	-0.15282400	1.90563000	-0.00024500
H	-0.70356800	-1.36949300	-0.00116000

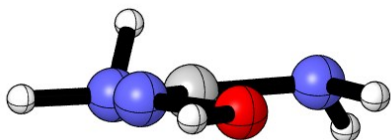
**Entry 154**

C	-0.52270600	-1.00772800	-0.37883900
N	-1.71984500	-0.74461000	-0.01790200
S	0.91441800	0.11240800	-0.48334900
O	-2.07392100	0.48920700	0.42113900
O	0.35767900	1.44509600	-0.05994200
O	1.82152000	-0.56493700	0.75213900
H	-0.31980100	-2.01871100	-0.71949800
H	-1.30282000	1.10178400	0.35773600
H	1.32484900	-0.57789500	1.58701300

### 154-radical

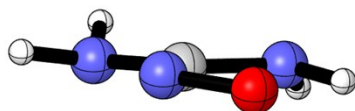
C	-0.58256800	-0.96576100	-0.44509700
N	-1.71282300	-0.55922100	-0.01615400
S	0.90916300	0.12530500	-0.47341700
O	-2.15874900	0.46393800	0.46243100
O	0.41555100	1.44911700	-0.02619700
O	1.75965600	-0.63537400	0.76289600
H	-0.47949000	-1.96715200	-0.84178900
H	1.28637600	-0.55005800	1.60708300

### Entry 155



C	-0.2061835	-0.1172180	0.0092639
N	0.8137165	-0.9019200	0.0427959
O	2.0161645	-0.1216650	-0.0242841
N	-1.4812655	-0.6755200	-0.0975531
N	-0.1668865	1.2593450	0.0741609
H	2.6993915	-0.7976860	-0.0127141
H	-1.4436905	-1.6869210	-0.1077141
H	-2.1260025	-0.3359790	0.6068069
H	-0.8685375	1.7333760	-0.4758581
H	0.7632935	1.6441880	-0.0149041

### 155-radical



C	0.0875023	-0.1705898	-0.0013822
N	1.2703173	-0.8357628	-0.0017742

O	2.2827853	-0.0340958	-0.0445892
N	-1.0405647	-0.9211558	-0.0694602
N	0.0239773	1.1722272	0.0706018
H	-0.8825697	-1.9165488	0.0075798
H	-1.9000827	-0.5700958	0.3230128
H	-0.7823767	1.6729462	-0.2651012
H	0.9410113	1.6030752	-0.0188872

**Entry 156**

**156-radical**

**Entry 157**

**157-radical**

**Entry 158**

**158-radical**

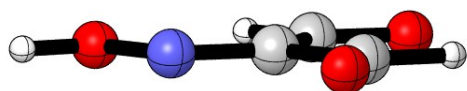
**Entry 159**

**159-radical**

**Entry 160**

**160-radical**

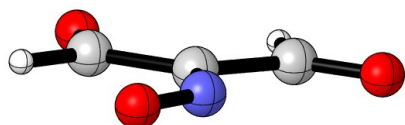
**Entry 161**



C	0.1381019	-0.1221692	0.0279427
N	-0.7822341	-1.0209632	-0.0222453
C	1.5455429	-0.6149532	0.2524617
C	-0.0898901	1.3491608	-0.1185453
O	-2.0420661	-0.5186352	-0.2280133
O	1.8442379	-1.7747332	0.3831647
O	0.8207889	2.1444038	-0.0610023
H	2.2953939	0.1927738	0.2871157
H	-1.1297351	1.6715848	-0.2816393
H	-2.6001401	-1.3064692	-0.2392393

**161-radical**





C	-0.0438273	-0.2328280	0.0000277
N	-0.7854793	-1.3057270	0.0001657
C	1.4370457	-0.3841790	0.0001637
C	-0.7088313	1.0974580	-0.0002733
O	-1.9711883	-1.5000950	0.0001147
O	2.0068307	-1.4479720	0.0003767
O	-0.0947203	2.1347380	-0.0003393
H	1.9761817	0.5776650	0.0000557
H	-1.8160113	1.0609400	-0.0002913

### Entry 161

C	0.00419800	-0.04389800	0.00001500
N	-0.62267600	-1.16835200	0.00009900
C	1.51051800	-0.11557300	0.00014600
C	-0.64793000	1.30257100	-0.00020100
O	-1.98896500	-1.04546200	0.00002100
O	2.13961300	-1.14301200	-0.00012300
O	0.00003500	2.32492200	0.00015800
H	1.99910600	0.87295100	-0.00019700
H	-1.74868600	1.31558800	-0.00079700
H	-2.29787300	-1.96024700	0.00009600

### 161-radical

C	-0.00356300	-0.01763900	0.00000500
N	-0.27677900	-1.29298900	-0.00013300
C	-1.12853700	0.95720600	-0.00013200
C	1.42099900	0.40957500	0.00030600
O	0.39414400	-2.28975600	-0.00008300
O	-2.29375900	0.64325000	-0.00034500
O	1.75566700	1.56762500	0.00037200
H	-0.79743600	2.00895900	-0.00002300
H	2.15307800	-0.42183500	0.00032400

### Entry 162

C	-0.02522800	0.45212300	0.12395800
N	-0.44356000	1.68132900	0.07184800
C	-1.08649100	-0.58536600	0.34182500
C	1.41559200	0.09460800	0.03653200
O	0.41032300	2.69472000	0.02140400
O	-0.91868700	-1.58232100	0.96296400
Cl	-2.67130000	-0.20211900	-0.38695800
O	2.28298700	0.92707800	0.12594600

Cl	1.83281300	-1.57495700	-0.34682300
H	1.33896900	2.35698300	0.07495100

### 162-radical

C	-0.05349700	0.37251500	0.05209600
N	-0.61714000	1.54971700	-0.00332800
C	-0.95972400	-0.79794300	0.13963100
C	1.44534900	0.35372200	0.06304100
O	-0.20278100	2.66807300	-0.03565200
O	-0.64685900	-1.91364100	0.37939500
Cl	-2.69777800	-0.37493800	-0.14093400
O	2.09314700	1.34294300	0.18730800
Cl	2.21419900	-1.22487200	-0.19751900

### Entry 163

C	0.03281700	-0.23399700	0.00002500
N	0.35440800	-1.47813700	0.00004500
C	-1.46785800	-0.03274200	0.00018400
C	0.99419800	0.95409700	-0.00004600
O	1.66709200	-1.79569300	0.00001100
O	-1.96790600	1.07197000	0.00022800
O	-2.21566000	-1.13091200	-0.00020400
O	2.18374600	0.80091800	0.00007600
O	0.41781800	2.15662900	-0.00018700
H	1.66929200	-2.76285900	0.00004400
H	-1.62229000	-1.90363500	-0.00038300
H	-0.56351900	2.06600900	-0.00034700

### 163-radical

C	0.00869500	0.24691100	0.00003100
N	0.35854200	1.49647300	-0.00005500
C	-1.44390100	-0.06733300	-0.00016000
C	1.09630800	-0.81548000	0.00028200
O	1.43484500	2.04049500	0.00005000
O	-1.83497600	-1.21563800	-0.00027000
O	-2.31156200	0.94859700	-0.00032000
O	2.25399000	-0.49616000	0.00029300
O	0.66911600	-2.07322300	0.00018500
H	-1.85078100	1.80061800	-0.00024600
H	-0.31693200	-2.09309100	0.00020900

### Entry 164

C	0.13882700	0.61602700	-0.13054300
N	0.68894500	1.74222300	0.07981300
S	-1.69802600	0.60539500	-0.29478700
S	0.94828200	-1.01443700	-0.42394300

O	2.02359100	1.89561800	0.22536100
O	-1.91917800	-0.56700800	-1.18783900
O	-2.03933000	0.18208900	1.27805100
O	2.38947100	-0.72524700	-0.14109900
O	0.20510300	-1.67627600	0.97359500
H	2.46536900	1.01596500	0.17598400
H	-1.51890200	-0.60430300	1.52693600
H	0.11660400	-2.63212100	0.83679200

#### 164-radical

C	0.14119200	0.61775200	-0.12047700
N	0.74618800	1.70537100	0.11502200
S	-1.69629800	0.58434100	-0.24621500
S	1.06663100	-0.97421300	-0.44369000
O	1.87368900	2.13001000	0.23691200
O	-1.92884400	-0.49992600	-1.23508400
O	-1.99524500	0.02314200	1.28705600
O	2.46217400	-0.68053100	-0.07268900
O	0.24026600	-1.71900500	0.88072100
H	-1.43744700	-0.76066400	1.45970900
H	0.22534700	-2.67500700	0.72115800

#### Entry 165

C	-0.02756500	-0.02152200	0.01888800
N	-1.04380200	-0.82324600	-0.00495200
C	1.28447500	-0.67528800	0.04898000
C	2.46545400	-0.06086100	-0.05305000
N	-0.12529900	1.34879400	-0.03490900
O	-2.24815400	-0.07558400	-0.02920900
H	1.22980700	-1.75225600	0.16097900
H	3.38900900	-0.62503100	-0.01531900
H	2.56245800	1.00995000	-0.19615800
H	0.62736800	1.87880200	0.37400800
H	-1.05006800	1.72068600	0.12458500
H	-2.92382000	-0.76028100	-0.02430100

#### 165-radical

C	-0.06105700	0.00729800	-0.00025600
N	-1.16102800	-0.82501300	-0.00032200
C	1.22090600	-0.65494800	-0.00032100
C	2.42442200	-0.05903600	0.00048400
N	-0.23452300	1.33317200	-0.00057200
O	-2.26100200	-0.19938700	0.00064800
H	1.13887400	-1.73631500	-0.00083800
H	3.33441800	-0.64559600	0.00061600
H	2.55285000	1.01857300	0.00114500

H	0.52368900	1.99197200	0.00012900
H	-1.19858600	1.64946700	0.00058100

### Entry 166

C	0.62055900	-0.10433700	0.03153700
N	1.64920800	0.67133200	-0.05318800
C	-0.68097600	0.63918800	0.03452300
N	0.65445500	-1.46079400	0.15237300
O	2.81602800	-0.10451200	-0.05886200
O	-0.83876800	1.80586400	0.07975400
Cl	-2.14433200	-0.46758800	-0.06372000
H	-0.18595400	-1.98870100	-0.01474900
H	1.54186500	-1.90788100	-0.01883200
H	3.51651900	0.55190400	-0.14096900

### 166-radical

C	0.63786800	-0.18417500	0.01340500
N	1.73521800	0.50614800	-0.02859700
C	-0.59776300	0.62920300	0.01707900
N	0.63938400	-1.56240100	0.11571400
O	2.89659200	0.10106700	-0.03180400
O	-0.67139200	1.81012500	0.03292700
Cl	-2.11454000	-0.38327800	-0.02713700
H	-0.20936900	-2.02909600	-0.16786700
H	1.49210400	-2.02111700	-0.17251300

### Entry 167

C	0.42151600	-0.02915800	-0.00062100
N	-0.57751500	-0.83900600	0.02932600
N	1.71411900	-0.49155400	-0.08600000
O	0.33177100	1.31201400	-0.00235900
O	-1.78282000	-0.05379400	-0.02871400
H	2.39777000	0.08355900	0.38558900
H	1.80952700	-1.48122300	0.08929300
H	-0.61330800	1.52806000	0.05002500
H	-2.47092200	-0.70728300	0.12412000

### 167-radical

C	0.38823300	0.00838300	-0.00009600
N	-0.66017600	-0.85185100	0.00008400
N	1.63852100	-0.45683900	0.00029700
O	0.19734800	1.30582800	-0.00009900
O	-1.76972000	-0.17530100	0.00001600
H	2.42613400	0.16934100	0.00024300
H	1.77715100	-1.45518900	-0.00168500
H	-0.80212100	1.35216100	0.00001800

**Entry 168**

C	0.06929600	-0.12134300	0.00005100
N	1.14025000	-0.82708600	-0.00020200
O	-1.10748200	-0.74652200	0.00068000
O	0.02177500	1.22066200	0.00023800
O	2.24910200	0.09062200	0.00023200
C	-2.30413000	0.04870400	-0.00047900
H	0.94400700	1.52841900	-0.00049100
H	3.01065300	-0.49608100	-0.00250100
H	-2.35827500	0.67392400	-0.89328100
H	-2.35926100	0.67494800	0.89155400
H	-3.11703100	-0.67386900	-0.00050300

**168-radical**

C	-0.10425900	-0.09648200	0.00007600
N	-1.24628300	-0.81580500	0.00020600
O	1.03716600	-0.72753700	0.00001500
O	-0.12532500	1.21253300	0.00005000
O	-2.25386000	0.00612800	-0.00026200
C	2.25614400	0.05216500	-0.00009900
H	-1.11460300	1.38194600	0.00065200
H	2.30356000	0.67429700	0.89368300
H	2.30364000	0.67388100	-0.89417000
H	3.05622800	-0.68258100	0.00010400

**Entry 169**

C	-0.02273100	-0.05130400	-0.00001500
N	-1.06388100	-0.79972900	0.00006500
C	1.30914200	-0.67968700	-0.00014900
O	-0.08044000	1.29709400	-0.00006300
O	-2.26555200	-0.14686800	0.00004800
O	2.30520300	0.01488000	0.00017200
H	1.32915300	-1.77927700	-0.00046900
H	0.83473000	1.62736500	-0.00021000
H	-2.10886800	0.81511000	-0.00005300

**169-radical**

C	0.05542700	0.04655900	0.00009200
N	1.17984100	-0.58891800	-0.00002400
C	-1.18803400	-0.72649700	0.00036700
O	-0.00560300	1.38918000	0.00008100
O	2.33648800	-0.18551900	-0.00013300
O	-2.25930500	-0.15287600	-0.00030800
H	-1.08437700	-1.82288700	0.00013700
H	-0.95150700	1.61865900	0.00015600

**Entry 170**

C	-0.85590900	0.32687700	0.02353800
N	-1.32464600	-0.86845900	0.06710900
N	0.52195000	0.57068600	0.18747600
O	-1.55607800	1.45909700	-0.06001200
O	-2.72281100	-0.80795000	-0.01284900
N	1.26015200	-0.34829500	-0.24423800
C	2.58347300	-0.16519400	-0.02837800
N	3.73770500	-0.16648200	0.06958900
H	-2.49834700	1.22871100	-0.07530400
H	-3.00205600	-1.72012900	0.12768700

**170-radical**

C	0.88809900	0.37410900	0.00434300
N	1.35175700	-0.94387900	0.02297100
N	-0.41513300	0.62463400	-0.07396300
O	1.73129500	1.38347300	0.01442600
O	2.57052700	-1.03999400	-0.11266700
N	-1.21723000	-0.26490300	0.38643400
C	-2.49487600	-0.13367600	0.01343200
N	-3.63331800	-0.15950000	-0.21767300
H	2.62355400	1.01511600	-0.14511900

**Entry 171**

C	-0.18170600	0.50411800	0.01721300
N	1.04182500	0.83087600	0.05422700
N	-1.20550000	1.42064700	-0.09971000
Cl	-0.74038700	-1.19050100	-0.00279600
O	2.01603200	-0.14389000	-0.01377100
H	-2.01253900	1.24275200	0.48352300
H	-0.87482600	2.37643100	-0.04764800
H	1.58166400	-1.01491000	-0.06307900

**171-radical**

C	-0.03838700	0.46936200	0.00000600
N	1.29354500	0.48277000	0.00012700
N	-0.70230800	1.63551700	-0.00010500
Cl	-1.00632700	-0.97891300	0.00000600
O	1.88340600	-0.64503300	-0.00007200
H	-1.70744300	1.66991400	0.00028400
H	-0.16058600	2.48770400	0.00000500

**Entry 172**

C	-0.12319000	0.50596300	-0.00002000
N	1.12961100	0.67681400	-0.00002200

O	-0.99374000	1.52669900	0.00000800
Cl	-0.93601400	-1.04449900	0.00000000
O	1.96816800	-0.41866600	0.00001200
H	-0.47665400	2.34675000	0.00007300
H	1.42532600	-1.22801000	0.00004400

### 172-radical

C	0.00185400	0.45919500	-0.00001800
N	1.32478100	0.30920400	-0.00000900
O	-0.49885200	1.67849200	0.00000900
Cl	-1.15853000	-0.79868700	0.00000100
O	1.76819000	-0.88302200	0.00001000
H	0.25571900	2.29432900	0.00001500

### Entry 173

C	0.00808800	-0.37346300	0.00064700
N	-1.00509600	-1.14735700	-0.00014400
C	1.35520700	-0.92701500	0.00044600
C	2.49635300	-0.23571800	-0.00054500
Cl	-0.18512900	1.40323600	0.00011000
O	-2.26219200	-0.62933200	-0.00046700
H	1.35888300	-2.01207600	0.00119400
H	3.44756200	-0.75259300	-0.00059700
H	2.51823400	0.84673200	-0.00136000
H	-2.20216500	0.34625200	0.00034600

### 173-radical

C	0.04965300	-0.29854500	-0.00051400
N	1.15019600	-0.95663100	-0.00014300
C	-1.22558200	-0.99532900	-0.00000200
C	-2.43143700	-0.42198900	0.00016300
Cl	0.11157400	1.45954700	0.00003200
O	2.33845900	-0.67083700	0.00026000
H	-1.12674400	-2.07635900	0.00020800
H	-3.32628400	-1.03085300	0.00038200
H	-2.55857200	0.65320600	-0.00009500

### Entry 174

C	-0.14044900	-0.14085600	-0.00004500
N	-0.75993100	-1.24206800	0.00007200
N	1.36467500	-0.19179000	-0.00005900
Cl	-0.85709700	1.43505800	0.00015800
O	-2.10718200	-1.24083200	-0.00016900
O	1.93593300	0.88329400	-0.00033900
O	1.87351000	-1.29173400	0.00027300
H	-2.43795400	-0.31965600	-0.00062600

**174-radical**

C	0.19264200	-0.06094200	0.00043600
N	0.86497900	-1.14427700	0.00016100
N	-1.28617100	-0.21799400	0.00001100
Cl	0.86301800	1.51499000	-0.00011300
O	2.04130700	-1.42543400	-0.00009300
O	-1.94305300	0.80517600	0.00010000
O	-1.70810600	-1.36140300	-0.00024500

**Entry 175**

C	0.02825900	-0.32132800	-0.00009700
N	-0.95382900	-1.13705200	-0.00008600
C	1.40211200	-0.89625200	0.00006000
Cl	-0.15541900	1.42407600	0.00000100
O	-2.21660100	-0.66784500	0.00004900
O	2.40901600	-0.23905200	0.00000200
H	1.39360900	-2.00028100	0.00018800
H	-2.19622800	0.31101600	0.00022300

**175-radical**

C	-0.02955500	-0.24460300	0.00005100
N	-1.11822900	-0.93479200	0.00001100
C	1.24660400	-0.99329200	0.00023500
Cl	-0.04870800	1.48967700	0.00000500
O	-2.30189600	-0.67994000	-0.00006500
O	2.33390700	-0.47806000	-0.00013900
H	1.09726000	-2.08959600	-0.00025000

**Entry 176**

C	0.67425900	-0.24936200	0.00020800
N	1.51059800	-1.22733400	0.00007800
N	-0.65510100	-0.66496400	0.00011800
N	-1.50249200	0.26551000	0.00009600
Cl	1.11817200	1.42865200	-0.00002400
O	2.80923600	-0.83875500	-0.00016600
C	-2.79082000	-0.13795100	-0.00003100
N	-3.93609000	-0.31324100	-0.00016000
H	3.29815100	-1.67294900	-0.00026000

**176-radical**

C	0.70693300	-0.21192900	0.00034700
N	1.58284400	-1.17367600	0.00010000
N	-0.59794300	-0.63541000	-0.00016800
N	-1.46194100	0.28660000	-0.00045900
Cl	1.20340100	1.45265700	0.00004200



O	2.78495100	-1.20337000	-0.00010000
C	-2.74202900	-0.13481500	-0.00000500
N	-3.88394000	-0.33290600	0.00024600

**Entry 177**

C	0.39107300	-0.11847800	-0.00001000
N	-0.69734700	-0.77884900	-0.00001000
O	1.52311400	-0.88263700	0.00000600
C	0.56255400	1.37053100	0.00000000
O	-1.82572700	0.07740700	0.00000400
H	2.29340400	-0.30659000	0.00001200
H	1.12253000	1.68569600	-0.88661500
H	1.12264500	1.68567100	0.88655100
H	-0.40400000	1.86831300	0.00006800
H	-2.55400900	-0.55162100	0.00002600

**177-radical**

C	-0.34241700	-0.10540200	0.00003900
N	0.82197300	-0.75691000	-0.00006900
O	-1.40677300	-0.91311200	0.00002000
C	-0.53734400	1.37315500	-0.00001500
O	1.84545400	0.02046000	0.00003600
H	-2.22116400	-0.39622200	-0.00004400
H	-1.09956000	1.68403500	0.88688000
H	-1.09927400	1.68407000	-0.88707900
H	0.43530900	1.86118900	0.00014500

**Entry 178**

C	0.02918700	-0.02440900	0.00003300
N	1.04654200	-0.81355700	0.00001100
C	-1.26104200	-0.72181500	0.00003400
C	0.09558900	1.47795100	0.00003100
O	2.27248900	-0.13263500	-0.00004900
C	-2.46001900	-0.13058200	-0.00004200
H	-1.18691600	-1.80493000	0.00007400
H	-0.41466700	1.87684400	0.88129600
H	-0.41354800	1.87681400	-0.88190200
H	1.12489800	1.82625000	0.00064200
H	2.91113100	-0.85339300	0.00002200
H	-3.36931600	-0.71928400	-0.00005900
H	-2.57957100	0.94681000	-0.00009800

**178-radical**

C	-0.06845400	0.01942300	-0.00002100
N	-1.16910100	-0.66253300	0.00000400
C	1.17303500	-0.74217900	-0.00001900

C	-0.09927600	1.52637600	-0.00000900
O	-2.35682900	-0.35704900	0.00001600
C	2.40074400	-0.20893900	0.00002000
H	1.05186800	-1.82128700	-0.00004400
H	0.41317700	1.91840200	-0.88332400
H	0.41257100	1.91838400	0.88366900
H	-1.12599200	1.89005200	-0.00035200
H	3.27976800	-0.84103800	0.00002200
H	2.57065500	0.86151600	0.00005500

### Entry 179

C	-0.00407700	0.00803700	0.00003700
N	0.98324400	-0.81425100	-0.00008900
C	-1.32038100	-0.68715900	-0.00011700
C	0.08561400	1.50041000	-0.00008600
O	2.20680500	-0.16562600	0.00015000
O	-2.38136400	-0.10623500	0.00018000
H	-1.25109200	-1.79026600	-0.00051200
H	0.63495500	1.84873600	0.87851700
H	-0.91595800	1.92833200	0.00063300
H	0.63350100	1.84874600	-0.87961500
H	2.84542700	-0.88863900	-0.00004200

### 179-radical

C	-0.03113500	0.05718500	0.00006600
N	-1.11227000	-0.66168700	0.00008200
C	1.22042200	-0.71811800	-0.00010300
C	-0.06722300	1.55748900	-0.00005200
O	-2.29450600	-0.38230900	-0.00001000
O	2.31918400	-0.20889800	0.00009200
H	1.08082600	-1.81602400	-0.00047200
H	-0.59031300	1.93241900	-0.88416100
H	0.95550000	1.93320800	-0.00029900
H	-0.58992600	1.93252900	0.88424000

### Entry 180

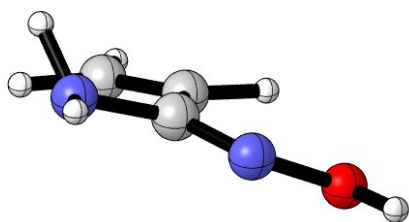
C	-0.86799600	0.31369100	-0.04251300
N	-1.26649700	-0.90660900	-0.08626800
N	0.51636500	0.54187800	-0.22849100
C	-1.72708300	1.53397600	0.06177400
O	-2.64222000	-0.99256100	0.02633700
N	1.26936400	-0.32714800	0.28074000
C	2.58953100	-0.14898000	0.03809400
N	3.74290800	-0.14069800	-0.07084600
H	-2.12671700	1.62559400	1.07599500
H	-2.57840800	1.46083000	-0.61793400

H	-1.13993800	2.42162900	-0.16954200
H	-2.81886600	-1.93165600	-0.10929300

### 180-radical

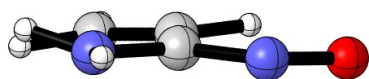
C	-0.91846500	0.35518900	-0.00016300
N	-1.34499300	-0.88550400	-0.00018500
N	0.43938200	0.61560700	-0.00077700
C	-1.87746400	1.50938700	0.00023700
O	-2.46688600	-1.33396000	-0.00021900
N	1.19860000	-0.39964500	0.00139300
C	2.51598700	-0.13071200	0.00013700
N	3.67392700	-0.06289100	-0.00052300
H	-2.51844900	1.47936200	0.88564700
H	-2.52284100	1.47627300	-0.88184400
H	-1.31238900	2.43989300	-0.00266900

### Entry 181



C	-0.4085066	0.0877002	0.3859588
N	-0.4362806	0.2115482	1.6688568
C	0.8117784	0.0031872	-0.4271112
O	0.8552034	0.1197492	2.2404367
C	0.8422904	-0.4345378	-1.6885683
N	-1.6412426	-0.0109708	-0.2627063
H	1.7187314	0.3237202	0.0694768
H	0.6767844	0.2845342	3.1713527
H	1.7708724	-0.4575468	-2.2467733
H	-0.0432436	-0.8070428	-2.1911132
H	-1.7242056	0.5667682	-1.0891632
H	-2.4221816	0.1128902	0.3693538

### 181-radical



C	-0.3156573	0.0511880	0.6679348
N	-0.2778783	0.0856670	2.0333358
C	0.8691937	-0.0155580	-0.1657062
O	0.8789207	0.0251510	2.5453368

C	0.8818387	-0.1904170	-1.4939882
N	-1.5657163	0.0684480	0.1544288
H	1.7922897	0.0790370	0.3935048
H	1.8168067	-0.2200620	-2.0404072
H	-0.0174553	-0.3290870	-2.0861062
H	-1.7354173	0.2634920	-0.8173582
H	-2.3269253	0.1821410	0.8090248

### Entry 182

C	-0.02918100	-0.02440000	0.00102000
N	-1.04657300	-0.81352500	0.00011600
C	1.26100800	-0.72180200	0.00090000
O	-2.27239800	-0.13268600	-0.00114400
C	2.46001900	-0.13061200	-0.00098900
C	-0.09562200	1.47800500	0.00070900
H	1.18686000	-1.80492600	0.00163300
H	-2.91102600	-0.85346500	0.00070100
H	3.36925000	-0.71939200	-0.00164600
H	2.57950900	0.94678200	-0.00230200
H	-1.12477900	1.82625200	0.01878000
H	0.39764700	1.87592700	-0.89075400
H	0.43039600	1.87783700	0.87210100

### 182-radical

C	0.06867900	0.01927300	-0.00004700
N	1.16922700	-0.66242300	0.00000500
C	-1.17296800	-0.74232800	-0.00003900
O	2.35687000	-0.35681200	0.00003600
C	-2.40058100	-0.20899900	0.00004200
C	0.09883100	1.52642400	-0.00001900
H	-1.05183000	-1.82144700	-0.00008900
H	-3.27959200	-0.84110500	0.00004800
H	-2.57042000	0.86146400	0.00011300
H	1.12544200	1.89039900	-0.00071900
H	-0.41283500	1.91794400	0.88392800
H	-0.41407400	1.91798300	-0.88321900

### Entry 183

C	0.05613400	-0.48287600	0.00005100
N	-0.91574000	-1.34141300	0.00027500
C	1.40912800	-1.04313400	-0.00008900
O	-2.20387900	-0.99370700	0.00026400
C	2.60598600	-0.44860000	-0.00041700
N	-0.16994900	0.98307400	0.00000100
O	-1.35084200	1.37953100	-0.00096200
O	0.78446700	1.73159200	0.00096800

H	1.35728700	-2.12691200	-0.00000300
H	-2.26164900	-0.00566300	-0.00027600
H	3.49273000	-1.07133500	-0.00059900
H	2.74599900	0.62062000	-0.00048400

#### 183-radical

C	-0.03548500	-0.46227600	-0.00002700
N	1.00133400	-1.23655900	-0.00005500
C	-1.36431900	-1.06079000	0.00007600
O	2.20002600	-1.07261200	-0.00010900
C	-2.56790900	-0.47923800	0.00007200
N	0.22627400	1.00599600	-0.00009900
O	1.38961000	1.37278800	0.00032900
O	-0.75546300	1.73619100	-0.00021900
H	-1.30210000	-2.14470700	0.00019200
H	-3.44958200	-1.10860200	0.00020500
H	-2.70867200	0.59013800	-0.00006000

#### Entry 184

C	-0.46825300	0.62307500	-0.03656000
N	-1.73682400	0.86830900	-0.23753900
C	0.37624300	1.82551100	-0.09360900
O	-2.66644000	-0.09429400	-0.14687600
C	1.61296700	2.00262100	0.37559800
C	-0.00755300	-0.77405700	0.18381100
O	-0.72583200	-1.66080700	0.56154000
Cl	1.66811300	-1.17898000	-0.29645200
H	-0.15642400	2.66904800	-0.52106400
H	-2.26120200	-0.92568100	0.18863300
H	2.07889800	2.97749800	0.29896300
H	2.19631400	1.22154300	0.84317800

#### 184-radical

C	-0.52050400	0.55527300	-0.02310400
N	-1.82477000	0.63267300	-0.12249600
C	0.18726500	1.83826500	-0.07031800
O	-2.72153600	-0.17405600	-0.10727200
C	1.44946000	2.13255900	0.25141200
C	-0.00689100	-0.83882800	0.12323000
O	-0.68214400	-1.78318500	0.36969800
Cl	1.75639000	-1.06496200	-0.19511200
H	-0.46927400	2.64710900	-0.37707100
H	1.78528300	3.15978500	0.17974500
H	2.17221800	1.40304500	0.58496200

#### Entry 185

C	0.16049300	-0.26290900	-0.00002500
N	1.29357100	-0.89098500	0.00001600
C	-1.01340500	-1.14318400	-0.00002300
O	2.40782600	-0.06346300	0.00007000
C	-2.30052200	-0.78088200	-0.00000400
C	0.08238500	1.23801100	-0.00017800
O	-0.95629100	1.85760200	0.00016000
H	-0.75025200	-2.19714900	-0.00003000
H	3.14073800	-0.68909200	0.00010200
H	-3.06997300	-1.54440300	-0.00000600
H	-2.61454800	0.25276600	0.00001100
H	1.05304800	1.75545600	-0.00065400

### 185-radical

C	-0.18636600	-0.23952500	0.00000500
N	-1.39380600	-0.74087000	0.00000200
C	0.94137200	-1.16625400	0.00001100
O	-2.50450700	-0.24864400	-0.00000800
C	2.23735900	-0.83621100	-0.00001200
C	-0.10749000	1.24939900	-0.00000800
O	0.92097000	1.87836000	0.00000800
H	0.65115300	-2.21277300	0.00003200
H	2.98869000	-1.61661600	-0.00001200
H	2.57548400	0.19031800	-0.00002700
H	-1.09963400	1.74297900	0.00001200

### Entry 186

C	1.01269600	0.19604000	-0.01300200
N	1.27630300	1.46015700	0.02896800
C	2.14407200	-0.72594700	0.07743800
O	0.18014800	2.29031600	-0.07425800
C	2.05476500	-2.05446700	-0.02760000
N	-0.25117600	-0.38002400	-0.30968900
N	-1.20553400	0.04346500	0.38328900
C	-2.42157100	-0.46397000	0.05510900
N	-3.52078100	-0.79913400	-0.08709600
H	3.09654200	-0.23763400	0.25230600
H	0.57873600	3.16411700	-0.16513400
H	2.93968800	-2.67308700	0.05473700
H	1.11239800	-2.55711000	-0.20781700

### 186-radical

C	0.98384000	0.22654600	0.00009900
N	0.96059400	1.55470300	-0.00008500
C	2.27148400	-0.45797700	0.00038200
O	-0.00517300	2.28516000	-0.00024100

C	2.43006100	-1.78346000	-0.00041700
N	-0.18981300	-0.49791800	0.00036200
N	-1.26419300	0.16391400	-0.00015600
C	-2.40889300	-0.54011700	0.00003000
N	-3.47180000	-1.00321000	0.00007600
H	3.12978700	0.20514900	0.00144400
H	3.42235600	-2.21597900	0.00000100
H	1.58677800	-2.46282100	-0.00144600

### Entry 187

C	0.02838700	0.65880500	-0.01073900
N	1.30132700	0.79050700	0.07133300
N	-0.81025700	1.74049000	-0.14403900
N	-0.69883700	-0.63698100	-0.01387300
O	2.15022100	-0.27064000	0.04765700
O	-1.90911700	-0.60846900	0.11755800
O	-0.02478000	-1.67022000	-0.11097100
H	-1.71929700	1.64766100	0.28747800
H	-0.35035600	2.62813900	0.00110500
H	1.62310200	-1.09211600	-0.05204500

### 187-radical

C	0.09508500	0.62413400	-0.00929000
N	1.37146800	0.54929200	0.02414700
N	-0.61891400	1.79612100	-0.11554000
N	-0.71747600	-0.61774400	-0.00771400
O	2.17291200	-0.38564200	0.03801600
O	-1.93247700	-0.45518500	0.07343000
O	-0.13031300	-1.68270400	-0.06712100
H	-1.57160900	1.72345600	0.21567600
H	-0.12542500	2.62630900	0.17921300

### Entry 188

C	0.09649800	0.65430300	-0.00009400
N	1.36383500	0.72046200	0.00009800
O	-0.63680100	1.76292800	-0.00024700
N	-0.75723700	-0.59696900	0.00007700
O	2.06116200	-0.46558500	0.00011600
O	-1.97169000	-0.37586300	0.00029700
O	-0.23157700	-1.68521300	-0.00033500
H	-1.57159500	1.48224400	0.00035800
H	2.97766500	-0.16265300	0.00032600

### 188-radical

C	0.11976500	0.62857400	0.00007500
N	1.39104200	0.54228200	-0.00009400

O	-0.52669700	1.79232200	0.00022700
N	-0.72959100	-0.58470400	0.00008600
O	2.17767900	-0.39686100	-0.00023100
O	-1.94155200	-0.35407900	-0.00046600
O	-0.19323100	-1.67345100	0.00039200
H	-1.47835300	1.58205900	0.00023100

### Entry 189

C	0.08676600	0.64436200	0.00006400
N	1.35126300	0.69045700	0.00001700
F	-0.60865200	1.76235500	0.00001400
N	-0.78609900	-0.54453300	0.00002300
O	2.11159400	-0.41904300	-0.00007400
O	-1.98392100	-0.38974800	-0.00010000
O	-0.19244500	-1.63411300	0.00009000
H	1.51931000	-1.20560700	-0.00012100

### 189-radical

C	0.15509900	0.59187300	-0.00001600
N	1.41064800	0.42000300	-0.00001300
F	-0.36567400	1.79772000	0.00000600
N	-0.82672700	-0.51339700	0.00002600
O	2.14334900	-0.55464800	0.00001000
O	-1.99995500	-0.19032100	-0.00000700
O	-0.35926600	-1.63965200	-0.00001000

### Entry 190

C	-0.05055200	0.64331500	0.00004000
N	1.20229500	0.92292600	0.00009400
C	-1.07332700	1.73201800	0.00017700
N	-0.58814000	-0.73902200	-0.00002600
O	2.16068000	-0.01956600	-0.00030000
O	-1.79551500	-0.87934100	-0.00048800
O	0.22196900	-1.68276700	0.00062400
H	-1.71539000	1.66724200	0.88138400
H	-1.71555700	1.66731800	-0.88091300
H	-0.54997200	2.68653900	0.00017400
H	1.72804300	-0.90703400	-0.00111000

### 190-radical

C	0.04431500	0.61235200	-0.00004100
N	1.32566100	0.61473400	0.00003200
C	-0.78005500	1.85434700	0.00001400
N	-0.65518500	-0.69981600	-0.00023200
O	2.19634900	-0.23136800	0.00001400
O	-1.87982800	-0.64075600	0.00009800



O	0.01916200	-1.71633000	0.00006800
H	-1.42397300	1.89218000	0.88109200
H	-1.42389600	1.89234400	-0.88111100
H	-0.11648800	2.71849500	0.00013300

### Entry 191

C	0.05613400	-0.48287600	0.00005100
N	-0.91574000	-1.34141300	0.00027600
C	1.40912900	-1.04313400	-0.00008900
N	-0.16995000	0.98307400	0.00000100
O	-2.20387900	-0.99370800	0.00026400
O	0.78446700	1.73159200	0.00097000
O	-1.35084200	1.37953200	-0.00096400
C	2.60598700	-0.44860000	-0.00041800
H	1.35728700	-2.12691100	-0.00000200
H	-2.26164900	-0.00566400	-0.00027600
H	3.49273000	-1.07133600	-0.00060000
H	2.74600000	0.62061900	-0.00048400

### 191-radical

C	-0.03548500	-0.46227600	-0.00002700
N	1.00133400	-1.23655800	-0.00005500
C	-1.36431900	-1.06079100	0.00007600
N	0.22627300	1.00599700	-0.00009800
O	2.20002600	-1.07261300	-0.00010900
O	-0.75546300	1.73619100	-0.00022000
O	1.38961000	1.37278800	0.00033000
C	-2.56790900	-0.47923900	0.00007200
H	-1.30209900	-2.14470800	0.00019200
H	-3.44958100	-1.10860300	0.00020500
H	-2.70867300	0.59013700	-0.00005900

### Entry 192

C	-0.37032700	-0.35981400	0.10938100
N	-1.06036500	-1.40184100	-0.16556000
C	1.09849000	-0.55527200	0.38690500
N	-0.88905500	1.01382000	0.22676900
O	-2.35892100	-1.34002100	-0.45886400
O	-0.18123800	1.84309300	0.75594200
O	-2.04036900	1.21239400	-0.18748000
O	1.54187300	-1.23459100	1.24445800
Cl	2.13103000	0.27958200	-0.80990200
H	-2.64130900	-0.39322800	-0.47028000

### 192-radical

C	-0.40642700	-0.34067500	0.06094800
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N	-1.27372300	-1.27322400	-0.11761500
C	1.02654800	-0.73324400	0.19303600
N	-0.87852300	1.07011500	0.17468700
O	-2.46060700	-1.32174700	-0.28901500
O	-0.20372400	1.79513100	0.88336400
O	-1.90914300	1.35568700	-0.40546000
O	1.38054700	-1.77541100	0.63410600
Cl	2.16990700	0.43741200	-0.50043400

### Entry 193

C	-0.08383400	-0.46947400	0.05222500
N	0.87213000	-1.32949900	0.12514400
C	-1.46664300	-1.03775600	-0.00534900
N	0.13065400	0.99342400	0.01213000
O	2.15344900	-0.98044600	0.08581500
O	1.23164700	1.37143000	-0.42894600
O	-0.73207100	1.71950300	0.44151100
O	-2.46279300	-0.41784800	-0.25820000
H	-1.45304600	-2.12833800	0.17171400
H	2.21456200	-0.01686000	-0.13532800

### 193-radical

C	0.03901600	-0.45046900	-0.04406000
N	-1.00465800	-1.20329000	-0.11010200
C	1.37486400	-1.09407400	0.04083900
N	-0.14608000	1.03191100	-0.00436300
O	-2.19425700	-1.03295600	-0.13985900
O	-1.14653200	1.44625700	0.55594900
O	0.71735800	1.68588700	-0.55411900
O	2.40627000	-0.51681900	0.25054500
H	1.30917300	-2.19203700	-0.07954500

### Entry 194

C	0.43321600	0.20439300	-0.01863800
N	0.72088900	1.44321200	0.04583100
N	-0.85316700	-0.31674000	-0.16744400
N	1.45977200	-0.88468800	-0.02252700
O	2.05738600	1.68979200	0.12546400
O	1.53735500	-1.53122200	1.00576600
O	2.11142300	-1.02385300	-1.03756300
N	-1.77713000	0.46299600	0.17810000
C	-3.02579200	-0.01112700	-0.02122500
N	-4.15228200	-0.26077100	-0.12650300
H	2.11955900	2.65460600	0.13764400

### 194-radical

C	-0.45982000	0.13235700	-0.00005600
N	-0.75346300	1.39793700	-0.00007400
N	0.81833000	-0.37168100	-0.00007700
N	-1.56491000	-0.88413900	0.00002000
O	-1.77158900	2.02607900	-0.00002800
O	-1.23277700	-2.05017100	-0.00011200
O	-2.69832500	-0.43425800	0.00019400
N	1.73162900	0.49997200	0.00002900
C	2.98783600	0.01117600	0.00001400
N	4.11890500	-0.24128900	0.00007600

### Entry 195

C	-0.56313300	0.64810800	-0.00897200
N	-1.85155600	0.52983300	0.08106600
N	-0.03382200	1.92682600	-0.14117000
C	0.35075600	-0.52119500	-0.04258600
O	-2.45133200	-0.68979800	0.04342700
O	-0.00823200	-1.66367800	-0.08173100
Cl	2.10860900	-0.14694600	0.04266900
H	0.81254300	2.11369400	0.37833200
H	-0.73612800	2.64715100	-0.03210400
H	-1.77433700	-1.39303400	-0.03508900

### 195-radical

C	-0.58723400	0.60082200	-0.00042700
N	-1.85776300	0.35008100	0.05766200
N	-0.12731800	1.90819500	-0.11166800
C	0.33404200	-0.56207200	-0.02334600
O	-2.50790800	-0.68776200	0.01022200
O	0.00941700	-1.70139200	-0.03408000
Cl	2.09110800	-0.09702700	0.01702700
H	0.70509500	2.11729300	0.42232200
H	-0.85128600	2.60496800	-0.00024100

### Entry 196

C	-0.55829400	0.63383600	0.00007000
N	-1.84028800	0.52607800	0.00005000
O	-0.00789700	1.86768200	-0.00004800
C	0.38742700	-0.50854900	0.00003400
O	-2.44335800	-0.69131300	-0.00003500
O	0.01984700	-1.65306500	-0.00001500
Cl	2.10870600	-0.10230500	-0.00000200
H	-0.73032300	2.51231300	-0.00006400
H	-1.75919600	-1.39380900	-0.00009500

### 196-radical

C	0.58407400	0.58465000	-0.00001100
N	1.84960000	0.34787400	-0.00001800
O	0.10220000	1.84683700	0.00001300
C	-0.37475700	-0.54898400	0.00005400
O	2.50669400	-0.68852800	0.00000800
O	-0.04741900	-1.69117100	-0.00001700
Cl	-2.09014700	-0.05057000	-0.00000700
H	0.83759500	2.47346100	-0.00005000

#### Entry 197

C	0.55881800	0.63074600	0.00027900
N	1.83457300	0.56757600	0.00009200
F	0.02728700	1.85537400	-0.00014600
C	-0.37851000	-0.50979500	0.00005000
O	2.45500000	-0.62876900	-0.00011400
O	0.00522500	-1.64943400	-0.00005300
Cl	-2.09645700	-0.10709700	-0.00000300
H	1.78852800	-1.35082900	0.00008600

#### 197 radical

C	0.58244500	0.56861400	-0.00029600
N	1.85031400	0.38075700	-0.00011700
F	0.14580200	1.82540300	0.00010900
C	-0.37797300	-0.55501100	0.00000800
O	2.54151200	-0.61946800	0.00016700
O	-0.05022900	-1.69706200	-0.00003000
Cl	-2.08361900	-0.03784100	0.00002800

#### Entry 198

C	-0.55839500	0.63947600	0.00001500
N	-1.85171600	0.51299300	-0.00000200
C	-0.02354200	2.04470500	0.00000400
C	0.33369500	-0.54140100	0.00004300
O	-2.43562100	-0.69922000	-0.00002200
O	-0.03127200	-1.68704900	0.00001700
Cl	2.09509200	-0.18583800	-0.00001600
H	-0.86676600	2.73404700	-0.00002600
H	0.59293000	2.23587700	-0.88142800
H	0.59288800	2.23590400	0.88145900
H	-1.74900100	-1.40404900	-0.00005000

#### 198-radical

C	-0.58216700	0.58869600	0.00000400
N	-1.85267300	0.31894700	-0.00000900
C	-0.13729000	2.02206900	0.00000000
C	0.32440400	-0.58441900	0.00002900

O	-2.50105700	-0.70234700	0.00000000
O	0.00048200	-1.72549300	-0.00000700
Cl	2.08371000	-0.12543200	-0.00000400
H	-1.01361000	2.67007100	-0.00002100
H	0.46709900	2.24713900	-0.88130200
H	0.46707000	2.24715600	0.88131800

### Entry 199

C	0.58789600	0.04605500	0.10156900
N	1.62171100	-0.74976600	0.12264200
C	0.85536600	1.49483100	0.19204800
C	-0.78989900	-0.49062700	-0.01336400
O	1.48345800	-2.07849000	0.00620600
O	-1.06176800	-1.65840100	-0.10899600
Cl	-2.12597700	0.70769400	-0.01733300
C	1.99361000	2.06644300	-0.20336500
H	0.06180900	2.10244600	0.60848100
H	0.53009700	-2.31201200	-0.08120100
H	2.14526100	3.13219500	-0.08424000
H	2.79710800	1.48986700	-0.64589600

### 199-radical

C	0.56414400	-0.02154700	-0.06189100
N	1.51517300	0.87322300	-0.06357500
C	0.90866600	-1.44589800	-0.12502300
C	-0.81661800	0.52828100	0.00940600
O	1.53578200	2.07864300	-0.00615100
O	-1.09911800	1.67907200	0.06112800
Cl	-2.12451600	-0.72974500	0.01656100
C	2.12079800	-1.94842900	0.12211400
H	0.09475200	-2.10640100	-0.39238100
H	2.30317300	-3.01152600	0.03079200
H	2.95738700	-1.32514500	0.41762200

### Entry 200

C	0.55331100	0.23623000	0.01854200
N	1.82812400	0.37530000	-0.02420000
N	-0.18443100	1.53195500	0.06634400
C	-0.18492000	-1.04283200	0.03654300
O	2.62432600	-0.69362100	0.00500700
O	0.39964900	-2.08981900	0.13998300
Cl	-1.92519800	-0.98361800	-0.20511400
O	-0.86380000	1.70024400	1.06609300
O	-0.04405100	2.29880700	-0.86368700
H	2.08316700	-1.51455400	0.08225900

**200-radical**

C	0.53680700	-0.16791800	0.03415700
N	1.55832200	-0.94950400	-0.06161900
N	0.87538500	1.27107700	0.09129300
C	-0.84154500	-0.73015900	0.11293000
O	1.69831300	-2.14033400	-0.07472000
O	-1.03648700	-1.87692700	0.35506900
Cl	-2.15090700	0.38217100	-0.31849100
O	0.18202300	1.94916100	0.82987700
O	1.82588900	1.64817000	-0.56971500

**Entry 201**

C	-0.51558100	0.55126000	-0.00003300
N	-1.81136200	0.72750100	-0.00004700
C	0.19901400	1.86971000	-0.00004200
C	0.09323500	-0.80109100	0.00001500
O	-2.64901400	-0.29830700	0.00000200
O	-0.58012800	-1.80540200	0.00008300
Cl	1.84625200	-0.93191200	-0.00004700
O	1.39033800	2.03732200	0.00011400
H	-0.52187400	2.70802300	-0.00016700
H	-2.13445400	-1.14620200	0.00005400

**201-radical**

C	0.55528000	0.48500600	0.00001600
N	1.86550800	0.46638800	0.00002800
C	-0.01429500	1.86031600	0.00000400
C	-0.11924200	-0.84881500	-0.00000700
O	2.68246400	-0.40896100	0.00002600
O	0.47705400	-1.87885100	-0.00008700
Cl	-1.89358900	-0.80924200	0.00003900
O	-1.18207300	2.14826100	-0.00006000
H	0.78243000	2.62977000	0.00004100

**Entry 202**

C	0.28671300	-0.51016300	-0.04773500
N	0.32744300	-1.81207200	-0.08336000
N	-0.96035000	0.12890900	-0.19502800
C	1.49035300	0.35057500	0.01930100
O	1.49166300	-2.44678300	-0.03853800
O	2.60050700	-0.10838700	0.11468900
Cl	1.23168000	2.09283000	-0.01618800
N	-1.93571200	-0.52364500	0.25065100
C	-3.14497600	0.04741700	0.04632400
N	-4.24546900	0.39709000	-0.04465400
H	2.23016800	-1.79572100	0.06536900

**202-radical**

C	-0.26927800	0.48236200	0.00012600
N	-0.29257600	1.80269600	0.00039400
N	0.92402800	-0.21162300	-0.00014300
C	-1.57890700	-0.23375900	-0.00019700
O	-1.19623100	2.58187300	0.00003100
O	-2.62685800	0.32658000	-0.00057900
Cl	-1.45265600	-2.00533200	0.00021800
N	1.96461400	0.50269600	0.00039500
C	3.12800300	-0.17784100	-0.00038900
N	4.20407000	-0.60827700	-0.00015500

**Entry 203**

C	0.60791500	-0.04659100	0.01262500
N	0.08031000	-1.22936800	0.03924700
N	2.00346900	0.05815600	-0.08876300
C	-0.13910700	1.22725600	-0.02500200
O	-1.27879100	-1.34585900	-0.01284900
O	-1.35617200	1.29453600	0.01516500
H	2.43316800	0.68065700	0.58491300
H	2.45308000	-0.84956100	-0.08130800
H	0.47487700	2.14377400	-0.09509100
H	-1.68072800	-0.44979100	-0.00617000

**203-radical**

C	-0.58089700	-0.00407900	0.01221600
N	-0.02219100	1.16676100	0.05337600
N	-1.97274200	-0.14567900	-0.07765800
C	0.26567400	-1.21929400	-0.04290300
O	1.15634000	1.49573700	-0.02439700
O	1.47009900	-1.20915800	0.02962700
H	-2.38890900	-0.67683300	0.67841000
H	-2.45610500	0.73458600	-0.20090600
H	-0.31063400	-2.15772300	-0.16525300

**Entry 204**

C	0.61369200	-0.01664800	-0.00012400
N	0.14961200	-1.21583900	-0.00003700
O	1.95970900	0.17265800	0.00003100
C	-0.15824000	1.24125800	-0.00000100
O	-1.20273100	-1.40096100	0.00004700
O	-1.37680200	1.25481500	0.00001400
H	2.38809800	-0.69502100	0.00022500
H	0.43563900	2.17004200	0.00007900
H	-1.64514700	-0.52390400	-0.00002800

**204-radical**

C	-0.57933400	-0.04104500	-0.00003000
N	-0.12237700	1.16265800	-0.00001400
O	-1.91263400	-0.30299000	0.00000200
C	0.31214500	-1.22288000	-0.00001100
O	1.03491500	1.58294800	0.00001500
O	1.51508100	-1.14135300	0.00000400
H	-2.41111600	0.52385800	0.00008900
H	-0.22800700	-2.18775200	0.00008100

**Entry 205**

C	-0.60551300	-0.07455900	0.00001700
N	-0.071115100	-1.23546300	0.00002500
F	-1.95031700	-0.03381300	-0.00001400
C	0.04866500	1.24012000	-0.00000100
O	1.27987900	-1.31455900	-0.00001400
O	1.26361000	1.34555100	0.00000900
H	-0.61764200	2.11799100	-0.00002100
H	1.66172100	-0.40673900	-0.00008400

**205-radical**

C	0.57110000	0.01454600	0.00000700
N	0.09717200	-1.17712000	0.00001400
F	1.90330300	0.15833300	0.00000200
C	-0.24956000	1.24011900	-0.00003100
O	-1.05501100	-1.57757000	-0.00001500
O	-1.45497000	1.21654500	0.00002100
H	0.34068200	2.17505200	-0.00002300

**Entry 206**

C	-0.20366600	-0.06591700	0.00070100
N	0.33869800	-1.23239400	0.00021100
Cl	-1.95261600	-0.00489100	-0.00018500
C	0.49210800	1.23519500	0.00018600
O	1.68653800	-1.31429100	-0.00024700
O	1.70919100	1.31002800	-0.00019300
H	-0.14403300	2.13423000	0.00002800
H	2.07112600	-0.40588700	-0.00016900

**206-radical**

C	-0.17634000	-0.03086000	0.00021100
N	0.42301900	-1.17241300	0.00011400
Cl	-1.91418400	0.01341200	-0.00004200
C	0.58705900	1.24279600	-0.00002400
O	1.60413100	-1.45707800	-0.00013500



O	1.79076400	1.27670000	0.00002300
H	-0.04348700	2.15029300	-0.00030100

### Entry 207

C	0.59071700	-0.04106300	0.00009700
N	0.05313500	-1.22406600	0.00000900
C	2.09478800	0.03185900	0.00002600
C	-0.17918900	1.21303500	-0.00019700
O	-1.29397000	-1.33175300	-0.00008800
O	-1.40234300	1.26711300	0.00017700
H	2.46647100	0.56018000	0.88356900
H	2.46653200	0.56145800	-0.88271500
H	2.50766200	-0.97597800	-0.00064600
H	0.41398300	2.14583600	-0.00054400
H	-1.69399100	-0.42890400	0.00000800

### 207-radical

C	-0.56465100	0.00773700	0.00001600
N	0.03706600	1.15934300	0.00004600
C	-2.06459400	-0.06281700	0.00001100
C	0.27159300	-1.21272900	-0.00009000
O	1.21485000	1.45615500	-0.00005600
O	1.47984100	-1.21983200	0.00008000
H	-2.43516900	-0.59083300	0.88377100
H	-2.43509400	-0.59275400	-0.88262400
H	-2.48912400	0.94074500	-0.00109300
H	-0.31168800	-2.15628800	-0.00019300

### Entry 208

C	0.04018100	-0.04248800	-0.00013800
N	0.55366400	-1.22653600	0.00043200
N	-1.44952000	-0.00717100	-0.00009800
C	0.76919200	1.23673500	-0.00078900
O	1.87653300	-1.34052800	0.00085800
O	1.99230000	1.23816500	-0.00066200
O	-2.06322200	-1.05060600	-0.00147600
O	-1.93731400	1.12075700	0.00174200
H	0.18224700	2.16193400	-0.00113700
H	2.28614400	-0.43376000	0.00067100

### 208-radical

C	-0.06675000	-0.00589300	-0.00007300
N	-0.61852400	-1.17845400	-0.00009900
N	1.39916600	0.01894800	-0.00030000
C	-0.86962900	1.24404300	0.00010600
O	-1.77485600	-1.49713400	-0.00007100

O	-2.07406600	1.21358600	0.00013900
O	1.99999600	-1.03922700	0.00034500
O	1.90295600	1.13719500	-0.00007900
H	-0.27846200	2.17228000	-0.00008400

### Entry 209

C	-0.40695600	-0.17525400	0.04372300
N	-1.25610300	-1.15500700	-0.14504200
C	1.00866200	-0.64481500	0.10997000
C	-0.79938100	1.23554300	0.20382700
O	-2.54451200	-0.87050000	-0.23214100
O	-1.97392500	1.58002300	0.14513100
O	1.38704700	-1.74490900	0.30439400
Cl	2.21855300	0.69357500	-0.18511100
H	-0.00910800	1.97141700	0.39655100
H	-2.67640200	0.11310200	-0.11857400

### 209-radical

C	0.42038800	0.13367300	-0.00002900
N	1.35450200	1.05785500	0.00017900
C	-0.96323400	0.64689600	-0.00014800
C	0.86015700	-1.28960100	-0.00024800
O	2.54593800	0.95171900	0.00029200
O	2.02479300	-1.60181000	-0.00016800
O	-1.29710100	1.78332500	-0.00037800
Cl	-2.21310900	-0.66962500	0.00022200
H	0.04843200	-2.03304100	-0.00044200

### Entry 210

C	0.58378100	-0.21823200	0.00002900
N	1.38011900	-1.26228900	0.00001300
N	-0.76243600	-0.60376100	0.00006300
C	1.03717700	1.19061400	0.00004200
O	2.68474700	-1.05354100	-0.00004100
O	2.22780800	1.47124000	-0.00005600
N	-1.57145800	0.36532600	0.00007600
C	-2.87886900	0.02339800	-0.00004100
N	-4.03039100	-0.10095500	-0.00007100
H	0.26477900	1.96947300	0.00009000
H	2.87140900	-0.07400200	-0.00005900

### 210-radical

C	0.60417300	-0.19137900	-0.00020500
N	1.46754000	-1.19004300	0.00004800
N	-0.71885900	-0.58204200	-0.00056000
C	1.12905000	1.20885600	-0.00012800

O	2.66375900	-1.15463700	0.00026900
O	2.30875500	1.45003200	0.00036000
N	-1.54121500	0.38163300	-0.00069400
C	-2.84126900	0.02201400	0.00015100
N	-3.99092700	-0.12226700	0.00067700
H	0.35239500	1.98892300	-0.00023900

### Entry 211

C	0.99170000	0.43617900	-0.00850700
N	2.13578900	-0.17583600	0.03444200
N	-0.20386600	-0.29774300	-0.03299500
N	-1.22667100	0.44581400	0.01178600
N	0.96638100	1.80865300	-0.07411000
O	2.05060700	-1.54827800	-0.00561700
C	-2.41231500	-0.19992800	0.00504900
N	-3.49964700	-0.60036400	0.00722000
H	0.11306300	2.24734600	0.23935500
H	1.82617700	2.27595600	0.16937400
H	2.97569600	-1.81825300	0.03255100

### 211-radical

C	0.99291100	0.37760500	-0.00806300
N	2.10426100	-0.32750300	0.00399200
N	-0.18733100	-0.33241100	-0.01861300
N	-1.20919100	0.43817500	0.00903400
N	1.04694200	1.74782200	-0.06816300
O	2.31404700	-1.52580000	0.01029300
C	-2.39850100	-0.18449000	0.00395600
N	-3.49047700	-0.57652100	0.00451800
H	0.17989100	2.20938200	0.16944400
H	1.89185100	2.19139000	0.25748200

### Entry 212

C	-1.01970200	0.42919800	-0.00002100
N	-2.11711400	-0.25989200	-0.00001000
O	-1.06288500	1.76890800	-0.00000500
N	0.19901700	-0.22094600	0.00000300
O	-2.02445100	-1.61170700	0.00000900
N	1.21676500	0.52997600	0.00003600
C	2.39935700	-0.11684800	0.00000200
N	3.48553500	-0.52251100	-0.00002000
H	-1.99111900	2.04302100	0.00001600
H	-1.07755300	-1.86111900	0.00000800

### 212-radical

C	-0.98704100	0.37857200	0.00001600
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N	-2.08429800	-0.32023000	0.00003300
O	-1.02571100	1.72172400	0.00003000
N	0.21441700	-0.29825500	-0.00007200
O	-2.30512000	-1.52021000	0.00000200
N	1.22548600	0.46883400	-0.00010800
C	2.41372900	-0.16365900	0.00000700
N	3.50566800	-0.55437000	0.00008000
H	-1.94238200	2.02655500	0.00008100

#### Entry 214

C	-0.86892400	0.00520800	0.00003800
N	-1.89731000	0.77781800	0.00001100
N	0.42997200	0.50316900	-0.00000300
O	-1.60388900	2.10989500	-0.00000900
N	1.33563200	-0.37113200	-0.00002900
Cl	-1.19018600	-1.70555200	-0.00000300
C	2.59617900	0.11266300	-0.00000300
N	3.72847200	0.35918100	0.00001500
H	-2.47661700	2.52474000	-0.00004000

#### 214-radical

C	-0.85117200	0.05053900	-0.00014100
N	-1.81894700	0.91809400	-0.00011500
N	0.44340100	0.52565000	0.00019400
O	-1.85379400	2.12424200	0.00002400
N	1.33768900	-0.36721600	0.00042300
Cl	-1.26978900	-1.62951200	-0.00005000
C	2.60328300	0.09427600	-0.00000600
N	3.73844100	0.32902500	-0.00028100

#### Entry 215

C	-1.01658400	-0.01036700	-0.00002100
N	-1.93896700	-0.95129700	0.00000800
C	-1.52479100	1.36329600	-0.00006300
C	-0.84002100	2.51128700	0.00003600
N	0.29283600	-0.47004600	-0.00002100
N	1.21533300	0.39496400	0.00004900
O	-1.54357600	-2.22706700	0.00002300
C	2.46795700	-0.10822700	0.00000200
N	3.59424200	-0.38250600	-0.00003300
H	-2.61023200	1.38522600	-0.00012900
H	-1.38260200	3.44943200	0.00003600
H	0.23792700	2.55772700	0.00011900
H	-0.55996300	-2.24958600	0.00004400

#### 215-radical

C	-0.97994300	-0.00557000	0.00000100
N	-1.93526600	-0.91801000	-0.00001100
C	-1.42490000	1.38794100	-0.00001900
C	-0.68299500	2.50054000	0.00000000
N	0.29668000	-0.56154300	0.00002800
N	1.24194000	0.28201800	0.00004800
O	-1.93592900	-2.11996800	-0.00000200
C	2.48001400	-0.25392700	-0.00000500
N	3.60041500	-0.55139000	-0.00003600
H	-2.50740600	1.47439300	-0.00005300
H	-1.17998800	3.46346000	-0.00002200
H	0.39538800	2.49045900	0.00003000

### Entry 216

C	0.73997900	0.27957400	0.00000400
N	1.76082300	1.04655000	0.00000400
N	-0.58519000	0.68539500	0.00001000
O	1.47335200	2.37100000	0.00001200
N	-1.40514800	-0.27316200	-0.00000500
N	1.07074400	-1.18694800	0.00000200
C	-2.70574200	0.08323900	-0.00001300
N	-3.85547000	0.22613900	-0.00002500
O	1.17281400	-1.71396000	-1.09075200
O	1.17267500	-1.71398600	1.09075800
H	2.34353700	2.79285300	0.00001400

### 216-radical

C	0.71017300	0.32459800	0.00004500
N	1.66567300	1.18897600	0.00004500
N	-0.61400500	0.69813300	0.00008200
O	1.70105200	2.39339100	0.00008900
N	-1.41713900	-0.27866400	0.00004100
N	1.13069500	-1.11472700	0.00000200
C	-2.72208100	0.05313400	-0.00009400
N	-3.87399900	0.17943800	-0.00019300
O	1.26446700	-1.63270200	-1.09132600
O	1.26359100	-1.63300000	1.09129400

### Entry 217

C	0.45743000	0.69459300	0.12267100
N	1.21810500	1.71973100	-0.02172000
N	-0.92589300	0.73484200	-0.07020900
O	0.57769200	2.86218900	-0.37854000
N	-1.47707700	-0.37068200	0.19085900
C	1.16342000	-0.57944900	0.54994000
C	-2.81664000	-0.40124300	0.02679200

N	-3.95637800	-0.58767600	-0.06480800
O	1.48717000	-0.84442900	1.65368800
Cl	1.49133300	-1.67113700	-0.83481100
H	1.29187100	3.51034100	-0.44466600

### 217-radical

C	0.53602200	0.67731600	0.01837700
N	1.22986800	1.77117400	-0.15912200
N	-0.84690200	0.79591300	-0.10119000
O	0.93670400	2.89704500	-0.44417600
N	-1.48392000	-0.22730500	0.27293500
C	1.35694800	-0.53832100	0.35419300
C	-2.82575400	-0.13447800	0.17481200
N	-3.98188300	-0.20955700	0.15334300
O	2.27380000	-0.53043000	1.10481400
Cl	0.91132500	-1.99244700	-0.57242100

### Entry 218

C	-0.98709100	0.09202600	0.03798300
N	-2.04113100	-0.64096300	-0.05144600
N	0.28732200	-0.42796000	0.32773500
O	-1.78293700	-1.97973100	-0.01188500
N	1.20264500	0.08814700	-0.36011300
C	-1.25324500	1.56922300	-0.02143300
C	2.45644100	-0.32600200	-0.04956600
N	3.57941900	-0.57692300	0.07921000
O	-0.40553000	2.41536000	0.06587700
H	-2.65740700	-2.38709800	-0.06634600
H	-2.32926300	1.79447200	-0.13520500

### 218-radical

C	0.95604600	0.01057700	0.00567700
N	1.94050800	-0.86014800	0.00792200
N	-0.32679800	-0.54632900	-0.03942100
O	1.98813400	-2.05656300	-0.00642800
N	-1.26245100	0.29239800	0.06256800
C	1.39994900	1.43613500	0.01249900
C	-2.50364300	-0.23560000	0.00794000
N	-3.62539100	-0.52562500	-0.01873000
O	0.67444700	2.39242700	-0.03031100
H	2.50415600	1.52435100	0.05084400

### Entry 219

N	-0.04316600	0.56698700	-0.15040400
C	1.16930700	-0.23209400	0.00369000
H	-0.07994800	1.24755400	0.60514200

H	1.23795000	-0.94705800	-0.81788500
H	2.02231000	0.44998900	-0.05794400
H	1.20915800	-0.77855400	0.95476600
O	-1.17389400	-0.29257100	0.12675700
H	-1.71199300	-0.20771500	-0.66744300

### 219-radical

N	-0.17798700	0.42577900	-0.05500100
O	-1.22483000	-0.30073900	0.01473500
C	1.14739200	-0.17094800	0.00920500
H	-0.28237800	1.41823300	0.15533400
H	1.19828200	-0.98793200	-0.71206100
H	1.89146600	0.58781700	-0.24173900
H	1.35282900	-0.56697400	1.01036200

### Entry 220

N	-0.04765100	-0.04280200	-0.45964800
C	1.28566300	-0.31031600	0.07779900
F	-0.36670000	1.28100000	0.10688200
H	1.95150900	0.46328300	-0.29907600
H	1.27727300	-0.31933200	1.17092600
H	1.59093100	-1.28339000	-0.30918000
O	-0.90127800	-0.91164900	0.19834800
H	-1.68961300	-0.93485400	-0.36065100

### 220-radical

N	0.04748300	0.20295200	-0.27886100
O	0.46403000	1.26722200	0.09734700
C	-1.30812800	-0.28184100	0.05368900
F	0.96165100	-0.96836000	0.05250900
H	-1.46907800	-1.22061300	-0.46761900
H	-1.38025700	-0.41690400	1.13465900
H	-2.00137400	0.48535800	-0.28850300

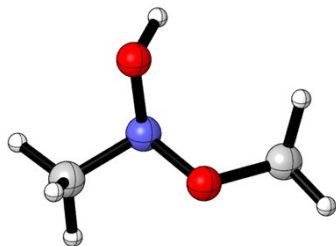
### Entry 221

N	0.04582000	0.00000100	-0.42396500
C	-1.33938500	0.00016400	0.04752000
O	0.63653900	-1.14913100	0.19654200
H	-1.82451900	0.89259500	-0.34534600
H	-1.82478800	-0.89204600	-0.34552100
H	-1.38094500	0.00006100	1.14183700
H	1.27918300	-1.45017200	-0.45653500
O	0.63685400	1.14896500	0.19655500
H	1.27949500	1.44990500	-0.45657300

### 221-radical

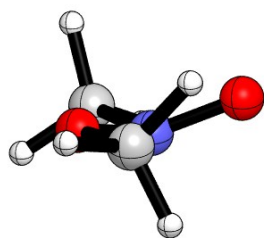
N	0.04486700	0.13144800	-0.23406500
O	0.49057200	1.25501500	0.07324000
C	-1.34626600	-0.23784900	0.04675900
O	0.88654700	-0.99738200	0.04617900
H	-1.97092800	0.56579900	-0.33668800
H	-1.56702900	-1.17569400	-0.45877200
H	-1.48490400	-0.34704500	1.12650600
H	1.76943800	-0.59716800	0.07150000

### Entry 222



N	-0.4423206	0.2381129	-0.2469962
C	-1.6884276	-0.5060931	-0.0612882
O	0.5395054	-0.5681981	0.3957068
H	-2.4969346	0.0908859	-0.4807772
H	-1.5986766	-1.4457241	-0.6053252
H	-1.8757606	-0.7011121	0.9996908
C	1.8388384	-0.2167251	-0.0656172
H	2.1146934	0.7929089	0.2574748
H	2.5168434	-0.9344241	0.3969098
H	1.8990694	-0.2907681	-1.1556952
O	-0.5952146	1.4251499	0.5591438
H	-0.2116156	2.1159869	0.0067728

### 222-radical

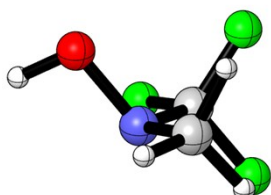


N	-0.4080893	0.4180214	-0.3086141
O	-0.0024673	1.5822654	-0.1282531
C	-1.8101343	0.0685514	-0.0546541
O	0.4041987	-0.6772796	0.1773729
H	-2.4196613	0.7931714	-0.5905341
H	-1.9908923	-0.9389636	-0.4227021



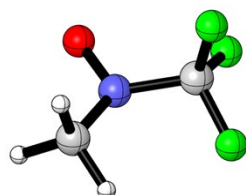
H	-2.0138453	0.1229484	1.0188529
C	1.7981397	-0.3793076	0.0886029
H	2.0583237	0.4882134	0.6968059
H	2.2892967	-1.2724946	0.4729219
H	2.0951307	-0.2051256	-0.9497991

### Entry 223



N	-0.1549105	0.2553985	-0.4020044
C	-1.0015835	-0.8592275	0.0359686
C	1.2062085	0.1565755	0.0154736
F	1.3883685	0.0899725	1.3573456
F	1.9050245	1.2124425	-0.4238674
F	1.7413295	-0.9617145	-0.5098024
H	-1.1012655	-0.8929435	1.1255666
H	-1.9822005	-0.7253625	-0.4173464
H	-0.5650575	-1.7882415	-0.3291564
O	-0.6870005	1.4607245	0.1538526
H	-0.7489125	2.0523765	-0.6060304

### 223-radical



N	-0.2063609	0.5323510	-0.1827653
O	-0.5846879	1.7363020	0.0008537
C	-1.1722059	-0.5615470	-0.0034723
C	1.2094621	0.2626350	-0.0220893
F	1.5424341	0.1099800	1.2780277
F	1.9330961	1.2509460	-0.5249413
F	1.5243471	-0.8838840	-0.6512653
H	-1.3300989	-0.7557030	1.0614137
H	-2.1037909	-0.2299220	-0.4572853
H	-0.8121949	-1.4611580	-0.4984763

### Entry 224

N	1.00904900	0.10958800	0.23846000
C	2.19769600	-0.73437600	0.38672700

O	1.31059600	1.08924600	-0.78334300
N	-1.34475800	-0.06930200	0.09373100
O	-2.24098500	-0.52424900	-0.59343900
O	-1.42769200	0.75175500	0.97601800
N	-0.05741200	-0.65701200	-0.17238000
H	2.48816100	-1.20934400	-0.55909400
H	1.97370000	-1.49510200	1.13332400
H	3.01261200	-0.10333500	0.73631300
H	1.02451700	1.92088800	-0.38328700
H	-0.06867600	-0.92378400	-1.16017700

#### 224-radical

N	1.11177700	-0.32248900	-0.13478400
C	1.88686600	0.89256200	-0.39617000
O	1.39731900	-1.09596000	0.82726200
N	-1.24920700	0.13607900	0.01982700
O	-0.98866500	1.08637400	0.71815900
O	-2.32425600	-0.37087600	-0.20612700
N	-0.12877200	-0.44398300	-0.75793100
H	1.60282200	1.67605200	0.30978600
H	1.69005000	1.21827100	-1.41587200
H	2.93791400	0.63857500	-0.26875700
H	-0.36374200	-1.43183300	-0.85228100

#### Entry 225

N	0.60362300	0.05383700	-0.15814000
C	1.33674600	1.27590300	0.08220400
O	1.42964500	-1.07282900	-0.02335500
C	-0.72592400	-0.19707000	-0.01684900
O	-1.10646700	-1.36510600	0.08206200
C	-1.67486900	0.98051800	-0.02572100
H	2.18639700	1.32183300	-0.60132900
H	1.70569100	1.31645300	1.11292700
H	0.68660800	2.12747600	-0.10709600
H	0.76331300	-1.78847500	0.05587000
H	-1.45754800	1.68336100	-0.83213600
H	-1.62868000	1.52102600	0.92423200
H	-2.68228000	0.58883900	-0.15294700

#### 225-radical

N	-0.61099000	0.26415700	-0.00004100
C	-1.84626900	-0.52985000	-0.00000200
O	-0.70037700	1.53446600	0.00002500
C	0.67030400	-0.36367500	-0.00001100
O	0.74622700	-1.57352500	0.00001600
C	1.83898000	0.58287700	-0.00000400

H	-2.42318800	-0.27332900	-0.88977900
H	-2.42260700	-0.27427400	0.89043200
H	-1.58843400	-1.58534200	-0.00061100
H	1.80661900	1.23359100	0.87630500
H	1.80654000	1.23373700	-0.87619900
H	2.75310800	-0.00711000	-0.00008400

### Entry 226

N	0.43217400	-0.04411700	-0.34089300
C	0.60690900	1.35141400	0.03482000
O	1.46990000	-0.83678500	0.26447500
H	1.62401800	1.65454500	-0.21102400
H	-0.08514900	1.95660100	-0.55305800
H	0.42269300	1.52060600	1.10387700
H	2.03792200	-1.07006000	-0.47944100
C	-0.80942100	-0.63924600	-0.09517800
C	-1.97616200	-0.01284600	0.09609000
H	-0.75474200	-1.72122600	-0.12859300
H	-2.88242000	-0.59691600	0.18149400
H	-2.07469000	1.06361200	0.14280100

### 226-radical

N	0.48061900	-0.14262300	-0.00000400
C	0.75163300	1.29697400	0.00000000
O	1.47347700	-0.95226200	0.00000400
H	1.83172700	1.41204700	-0.00004300
H	0.32349400	1.76399700	-0.89120600
H	0.32356500	1.76398000	0.89124800
C	-0.81300900	-0.63759700	-0.00000300
C	-1.93467700	0.10629600	0.00000200
H	-0.82885900	-1.72027300	-0.00000500
H	-2.89746200	-0.38539800	0.00000200
H	-1.92829500	1.18807000	0.00000800

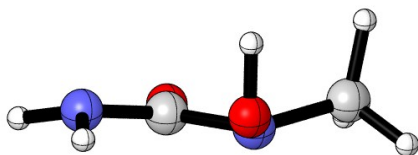
### Entry 227

N	-0.31712000	0.03349300	-0.32850000
C	-1.12445600	-1.12398300	0.07605100
O	-0.88076200	1.23927300	0.20638600
H	-2.11101700	-1.02485800	-0.37458400
H	-0.63879000	-2.02041700	-0.31111600
H	-1.21488200	-1.18904900	1.16438300
H	-1.06385100	1.76996800	-0.57999100
C	1.00161600	-0.03299600	-0.06052800
N	2.14736000	-0.10605900	0.09379700

### 227-radical

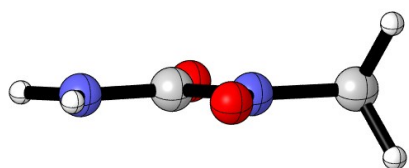
N	-0.34317000	0.14359000	-0.00008700
C	-1.25600600	-1.01133500	0.00002100
O	-0.82025900	1.33144500	0.00003400
H	-1.88077300	-0.95848700	-0.89240300
H	-0.67062500	-1.92973600	-0.00085600
H	-1.87953900	-0.95942100	0.89337200
C	0.99303600	-0.04137600	-0.00001300
N	2.13900300	-0.21325400	0.00002600

### Entry 228



N	-0.3744081	0.0745685	-0.3058488
C	-1.4635301	-0.8342365	-0.0021597
C	0.9535379	-0.3166755	-0.1286367
O	1.2680719	-1.4938675	-0.0843467
N	1.8481769	0.7215235	-0.0224827
O	-0.6728321	1.4312955	-0.0669157
H	-1.1496451	-1.8365765	-0.2848777
H	-1.7142791	-0.8311795	1.0685132
H	-2.3389211	-0.5408245	-0.5816328
H	1.5742059	1.6350015	-0.3495098
H	2.8125709	0.4531015	-0.1389477
H	-0.7429481	1.5378695	0.8968453

### 228-radical



N	0.4240521	-0.3020832	0.0145795
O	0.5778161	-1.5677922	0.0515115
C	1.6024601	0.5660498	0.0078395
C	-0.9020129	0.2634088	-0.0203785
O	-1.0646759	1.4664328	-0.0555665
N	-1.8649629	-0.6834512	-0.0090345
H	1.2739721	1.6012208	-0.0244485
H	2.1831141	0.3748438	0.9120015
H	2.2080721	0.3273178	-0.8682315
H	-1.6126449	-1.6588102	0.0220585
H	-2.8251899	-0.3871372	-0.0303305

**Entry 229**

N	-0.83884600	0.02190400	-0.42891700
C	-1.98661300	-0.68790300	0.14793700
N	0.32956500	-0.67300400	-0.03378600
C	1.46834500	-0.24875900	-0.00470500
O	2.59979500	0.02793600	0.07704100
H	-1.94014000	-0.70672200	1.24148900
H	-1.97427400	-1.70442000	-0.24441600
H	-2.88849300	-0.17482100	-0.18158600
O	-0.82429900	1.32737200	0.18918700
H	-0.72649500	1.92116900	-0.56577900

**229-radical**

N	-0.83227500	0.13259500	-0.17480000
C	-2.08352800	-0.58898100	0.07166200
O	-0.74831800	1.37100300	0.03808600
N	0.30531700	-0.68659900	-0.03528000
C	1.45061800	-0.24893800	0.00068800
O	2.57806400	0.02513500	0.04332200
H	-2.21753200	-0.74832300	1.14623000
H	-2.04562100	-1.54630000	-0.44499100
H	-2.88864100	0.03107400	-0.31604300

**Entry 230**

N	-0.34111800	-0.01197700	0.00017300
C	-1.72132200	-0.43420400	-0.00002400
O	-0.10981900	1.34386600	-0.00001800
H	-2.22340500	-0.05720200	-0.89325000
H	-1.71602600	-1.52267600	0.00014400
H	-2.22374200	-0.05693200	0.89289300
H	0.88178000	1.34490300	-0.00032900
O	1.77104200	-0.24576000	0.00005000
N	0.67248200	-0.82912700	-0.00011100

**230-radical**

N	0.36092200	0.12771300	-0.00008800
C	1.64765600	-0.57472400	0.00008800
O	0.27909700	1.35868100	-0.00000400
H	2.20613200	-0.28552900	0.89167800
H	1.44811700	-1.64434800	-0.00002400
H	2.20643000	-0.28539800	-0.89127200
O	-1.83950800	-0.11371500	0.00026200
N	-0.82711100	-0.74144300	-0.00033700

**Entry 231**

N	-0.59642000	0.07612400	-0.38281100
C	-1.44036200	-1.01712100	0.10999500
O	-1.07598400	1.27595600	0.14853200
H	-2.43672800	-0.83867300	-0.28991300
H	-1.05004200	-1.95423400	-0.27462600
H	-1.47417800	-1.03658000	1.20367300
H	-0.77741500	1.95772500	-0.46855900
N	0.81564900	-0.08143400	-0.02136900
O	1.44571000	0.94683500	0.09927400
O	1.23601500	-1.22133300	0.00203400

### 231-radical

N	-0.64831800	0.25341500	-0.14140700
C	-1.60169700	-0.85179600	0.05231000
O	-0.93190900	1.44271900	0.02218700
H	-2.57236600	-0.45593200	-0.23809400
H	-1.32034900	-1.69329400	-0.57470200
H	-1.61442400	-1.15874300	1.10126400
N	0.83995100	-0.12136400	-0.00722400
O	1.59348100	0.80810600	0.04669800
O	1.06041400	-1.31402700	-0.01412400

### Entry 232

N	1.59029300	-0.13314900	0.34031600
C	2.29427600	-1.02767700	-0.58284800
O	2.20869900	1.15464400	0.21514400
H	3.33512200	-1.10677300	-0.26870900
H	1.83899400	-2.01611400	-0.53807000
H	2.25193500	-0.65656900	-1.61505600
H	2.53424000	1.33051200	1.10549900
C	0.17811400	-0.04003900	0.15172100
C	-0.59151700	-1.20464400	0.29895500
C	-0.46631400	1.17135700	-0.11837000
C	-1.97351000	-1.15497100	0.15913300
H	-0.11063400	-2.14325600	0.54721100
C	-1.85482000	1.20922100	-0.24625600
H	0.12093100	2.07148800	-0.22704600
C	-2.61726900	0.05252300	-0.11464100
H	-2.55156500	-2.06468100	0.27897700
H	-2.33885400	2.15684200	-0.45643000
H	-3.69557200	0.08880100	-0.21591200

### 232-radical

N	-1.60614700	0.14677000	0.00002300
C	-2.46217100	-1.04288100	0.00000600
O	-2.17643900	1.29123600	-0.00003000

H	-3.48636500	-0.68114100	0.00016600
H	-2.28289200	-1.64973600	-0.89177000
H	-2.28268000	-1.64991900	0.89161000
C	-0.20214100	0.04847700	0.00001000
C	0.43935800	-1.20138800	-0.00000200
C	0.56418900	1.22599800	0.00001100
C	1.82976500	-1.26257100	-0.00000900
H	-0.13247200	-2.11955700	-0.00001500
C	1.94899300	1.14399400	0.00000500
H	0.05088400	2.17726700	0.00001700
C	2.59242900	-0.09637800	-0.00000400
H	2.31710300	-2.23087600	-0.00002000
H	2.53393900	2.05677800	0.00000600
H	3.67449600	-0.15160100	-0.00001000

### Entry 233

N	-0.98439900	0.07351600	-0.44489500
C	-1.78392700	-1.07782700	-0.00049500
S	0.68678500	-0.01826200	-0.13778000
O	1.16264400	-1.26889900	-0.66707100
O	1.26802300	1.26090500	-0.43914600
F	0.75115400	-0.17082800	1.49585400
H	-1.30922500	-1.98515100	-0.36983100
H	-1.87379500	-1.10672600	1.08857500
H	-2.76860300	-0.97163300	-0.45329400
O	-1.52306100	1.25045900	0.12803700
H	-1.46381400	1.90579700	-0.58096600

### 233-radical

N	-1.06157400	-0.23916900	0.20596700
O	-1.46626800	-1.40511700	-0.02199200
C	-1.94825100	0.92453500	-0.00072100
S	0.69020000	0.03241500	0.14559000
O	0.96288900	1.30716200	0.75722800
O	1.35834900	-1.19374500	0.46082100
F	0.85936500	0.26405400	-1.46741100
H	-1.49209100	1.80762100	0.44027800
H	-2.11934100	1.06999700	-1.06987700
H	-2.88528700	0.68782900	0.50096000

### Entry 234

N	0.98998200	-0.01761600	-0.44270100
C	1.96048900	0.98946700	-0.00941900
P	-0.64672600	0.19104000	0.00918600
O	-1.10137600	1.58116000	-0.15149700
O	-0.80758900	-0.42411700	1.48261100

O	-1.40490600	-0.92791100	-0.88016900
O	1.41897000	-1.32160300	0.01515800
H	1.55979300	1.96800300	-0.27461800
H	2.14666700	0.95099800	1.06948200
H	2.89628400	0.82578000	-0.54559900
H	-0.31734400	-1.25130900	1.59561600
H	-1.63778900	-0.60124600	-1.75794400
H	1.51967400	-1.83154200	-0.79813300

### 234-radical

N	-0.83227500	0.13259500	-0.17480000
C	-2.08352800	-0.58898100	0.07166200
O	-0.74831800	1.37100300	0.03808600
N	0.30531700	-0.68659900	-0.03528000
C	1.45061800	-0.24893800	0.00068800
O	2.57806400	0.02513500	0.04332200
H	-2.21753200	-0.74832300	1.14623000
H	-2.04562100	-1.54630000	-0.44499100
H	-2.88864100	0.03107400	-0.31604300

### Entry 235

N	-1.76196100	-0.03349100	0.11306200
C	-2.62884300	-1.12019600	-0.34694000
O	-0.54955600	-0.17769200	-0.77077800
C	0.59973900	-0.03833200	-0.07570400
Cl	1.90958500	-0.15885400	-1.28454900
Cl	0.70980600	1.58743600	0.76724400
Cl	0.81615800	-1.32504800	1.18820200
O	-2.37378800	1.14570900	-0.30585300
H	-2.12717800	-2.06048000	-0.12747100
H	-3.55147700	-1.04694900	0.22854500
H	-2.84288200	-1.03514500	-1.41585500
H	-1.98770500	1.82398200	0.26701500

### 235-radical

N	-1.90444300	-0.17840800	0.07190700
O	-2.37921800	-1.25925100	0.28857900
C	-2.66504500	1.06710500	0.33483600
O	-0.48188700	0.07874300	0.87904000
C	0.58934700	0.01262600	0.09451900
Cl	2.00853900	0.34656600	1.15261200
Cl	0.80633000	-1.60961400	-0.70239900
Cl	0.54997200	1.27454400	-1.24949200
H	-2.85458500	1.14208200	1.40693900
H	-2.07475400	1.90521800	-0.02091600
H	-3.59881300	0.97181000	-0.21871000



**Entry 236**

N	1.14034700	-0.18662600	-0.15395900
O	2.01774400	0.00490300	-1.06201200
C	1.56143300	-0.27040100	1.24559100
C	-0.22729000	0.01138800	-0.52655100
Cl	-1.27184700	-1.36265500	0.00097600
Cl	-0.89750700	1.57625600	0.12369500
H	0.76123600	-0.70109800	1.84548500
H	2.44397700	-0.90664100	1.28345300
H	1.80864700	0.72704500	1.61822900
H	-0.26409100	0.07071600	-1.60699800

**236-radical**

N	0.90190900	-0.72545400	-0.26342700
C	1.20143300	-1.09996100	1.11457600
C	-0.24470800	0.02826300	-0.54757000
Cl	-1.73990100	-0.84234800	-0.12379400
Cl	-0.25450700	1.72670100	0.31052200
O	2.01751300	-0.11672900	-0.88209800
H	1.41374800	-0.22319400	1.73975700
H	0.35013500	-1.63986800	1.52704200
H	2.06813900	-1.75837100	1.09399900
H	-0.26717400	0.28725000	-1.59838000
H	2.14626500	0.74236500	-0.43805400

**Entry 237**

N	0.62513300	0.27044400	-0.40104200
C	1.75273000	-0.65544400	-0.29799000
C	-0.64568100	-0.36306000	-0.34546300
F	-0.91315000	-0.98743300	0.85519100
F	-1.62646300	0.56596400	-0.51407900
O	0.72901700	1.21394000	0.67086300
H	1.80475600	-1.13626800	0.68470900
H	1.64555100	-1.41738700	-1.07325400
H	2.67038800	-0.09808100	-0.48003100
H	-0.71556800	-1.11336200	-1.13491700
H	0.60103700	2.06472100	0.23459300

**237-radical**

N	-0.70933800	-0.11383400	-0.15823400
O	-1.50810100	-1.10655900	-0.27241400
C	-1.20708900	1.18005300	0.31349600
C	0.69700800	-0.40216700	-0.16441000
F	1.36203400	0.52483700	-0.91206800
F	1.21994000	-0.31351600	1.09928000

H	-0.45994600	1.94777600	0.11496000
H	-2.12322900	1.40084300	-0.23231100
H	-1.41855100	1.13449400	1.38514400
H	0.85462200	-1.40301000	-0.56025800

### Entry 238

N	0.74924800	0.16327200	-0.49124500
C	1.77562900	-0.81067100	-0.11891300
O	1.13017100	1.46243000	-0.06051900
C	-0.57692500	-0.11326200	-0.02079300
F	-0.88736500	-1.38545200	-0.42079500
F	-0.59706900	-0.16479800	1.38747500
C	-1.63076600	0.85672700	-0.48650100
H	1.92748300	-0.86827400	0.96792800
H	2.70343200	-0.50706100	-0.60159500
H	1.48203800	-1.79081500	-0.49156100
H	1.20961800	1.42419500	0.90894000
H	-1.67406000	0.83895300	-1.57540100
H	-1.38973300	1.86453300	-0.15468200
H	-2.59260800	0.55161100	-0.07364600

### 238-radical

N	0.80877300	0.30876200	-0.11895400
C	1.88096600	-0.68744700	-0.03011000
O	1.09147100	1.54515100	0.02487100
C	-0.57621000	-0.11340600	-0.00522900
F	-0.79655000	-1.06956100	-0.97127200
F	-0.72917500	-0.78973600	1.19206000
C	-1.57777300	0.99991900	-0.11366500
H	2.21483300	-0.78546300	1.00629000
H	2.70600200	-0.33762500	-0.64913200
H	1.51947900	-1.64722100	-0.39501800
H	-1.46191400	1.51170400	-1.06814200
H	-1.42894500	1.71545000	0.69253800
H	-2.57300900	0.55988800	-0.04588600

### Entry 239

N	1.05871600	0.07512900	-0.31928300
C	2.20289200	-0.82146200	-0.51958400
S	0.02756700	-0.45804800	0.99851000
C	-1.55884100	-0.11236900	0.19111700
F	-1.64703200	1.19472100	-0.20908600
F	-1.76567300	-0.86884700	-0.92248200
O	1.61316900	1.36839400	-0.03205700
H	1.81698600	-1.81818600	-0.73076400
H	2.75749000	-0.45430500	-1.38347900

H	2.87375600	-0.85585200	0.34726000
H	-2.35503500	-0.31530400	0.91108300
H	0.99940800	1.96948500	-0.47390400

### 239-radical

N	1.35071500	0.21680300	0.09453400
O	1.46846100	1.02678600	1.05168100
C	2.55214200	-0.20420500	-0.64113400
S	-0.00651500	-0.96823200	0.09618200
C	-1.31249000	0.31611300	0.09542400
F	-1.54429300	0.80638200	-1.15260400
F	-2.45995500	-0.26920300	0.52519800
H	2.25161100	-0.64399100	-1.59079200
H	3.15469800	0.68890800	-0.80332400
H	3.12614600	-0.92796600	-0.05365600
H	-1.03059000	1.13679300	0.75458600

### Entry 240

N	1.05871600	0.07512900	-0.31928300
C	2.20289200	-0.82146200	-0.51958400
S	0.02756700	-0.45804800	0.99851000
C	-1.55884100	-0.11236900	0.19111700
F	-1.64703200	1.19472100	-0.20908600
F	-1.76567300	-0.86884700	-0.92248200
O	1.61316900	1.36839400	-0.03205700
H	1.81698600	-1.81818600	-0.73076400
H	2.75749000	-0.45430500	-1.38347900
H	2.87375600	-0.85585200	0.34726000
H	-2.35503500	-0.31530400	0.91108300
H	0.99940800	1.96948500	-0.47390400

### 240-radical

N	1.34283700	0.12992500	-0.13154900
O	1.27574900	1.37719800	0.02759500
C	2.60298000	-0.59102600	0.06208300
N	0.21431600	-0.66416600	-0.03550400
C	-0.95302400	-0.29932100	-0.01176800
S	-2.48280300	0.02093600	0.02039400
H	2.80130000	-0.71522400	1.13110600
H	2.52904500	-1.56465400	-0.41881100
H	3.38870700	0.00908500	-0.39187800

### Entry 241

N	-0.35807300	0.00480200	-0.39506500
O	-0.99791400	1.10460200	0.22919600
C	0.96747800	0.04039500	-0.07916600

N	2.10822800	0.04683200	0.10463200
H	-1.61819000	1.41268800	-0.44638200
O	-0.95042900	-1.20011600	0.01701700
H	-0.85102000	-1.25237700	0.98470000

#### 241-radical

N	-0.36133900	0.11534800	-0.00013100
O	-0.99433800	1.19074000	-0.00009700
O	-1.03662000	-1.11573200	-0.00048600
C	0.97301500	-0.00645800	0.00017800
N	2.12996100	-0.07485700	0.00009500
H	-1.97077400	-0.84475500	0.00384800

#### Entry 242

N	0.36631400	-0.03414000	0.42175700
F	0.88226500	1.20435900	-0.12837100
C	-0.95563000	-0.05565800	0.06661000
N	-2.09635100	-0.07374400	-0.10499400
O	1.02007500	-1.05780100	-0.22939800
H	1.74305300	-1.28768900	0.37352500

#### 242-radical

N	0.39216000	-0.15935200	0.16606700
O	1.07541900	-1.13417400	-0.06905800
F	1.00069200	1.14263800	-0.04220800
C	-0.94434400	-0.04257900	0.00512500
N	-2.09837700	0.02294100	-0.03726900

#### Entry 243

N	-0.10023100	0.22209000	-0.31214600
O	0.83831200	-0.43788700	0.51494100
C	2.09420700	-0.54562800	-0.17904300
C	-1.32557900	-0.33145100	-0.09164600
N	-2.37790500	-0.79865900	0.00836300
H	2.48254800	0.44544900	-0.42149000
H	2.75541100	-1.04608800	0.52735700
H	1.97785100	-1.14553700	-1.08334100
O	-0.10581400	1.60548100	-0.03683600
H	-0.34061300	1.70388600	0.90324700

#### 243-radical

N	-0.16451200	0.27123000	0.00013300
O	0.20375800	1.46339900	0.00005400
O	0.74884800	-0.80934300	0.00039900
C	2.11324000	-0.35576700	-0.00027600
C	-1.43887700	-0.14472400	-0.00007500

N	-2.55104600	-0.47130500	-0.00016700
H	2.33180900	0.22881600	0.89426600
H	2.67882700	-1.28557300	0.00008500
H	2.33124700	0.22778700	-0.89563400

#### Entry 244

N	1.61071400	0.04873600	0.39866200
C	0.19333800	0.00663800	0.16183900
C	-0.52394300	1.20832900	0.15184800
C	-0.47961500	-1.21305700	0.04674800
C	-1.90876200	1.18212000	0.01419500
C	-1.86596100	-1.22117800	-0.08897800
C	-2.58733700	-0.02938200	-0.10749900
O	2.20572800	1.16394000	-0.22516100
H	0.00217900	2.14664800	0.26334800
H	0.08019200	-2.13679700	0.05685300
H	-2.45800500	2.11683900	0.00666800
H	-2.38195600	-2.16999500	-0.18432900
H	-3.66577700	-0.04403900	-0.21337900
H	1.99613500	1.09892500	-1.17534700
O	2.19811900	-1.12328200	-0.15453900
H	2.95513300	-1.27882100	0.42423300

#### 244-radical

N	-1.59797300	-0.12241500	-0.00006900
O	-2.28785500	-1.16209700	0.00009500
C	-0.20671200	-0.03686300	-0.00001500
C	0.44570200	1.20738900	0.00001700
C	0.52713100	-1.23572000	-0.00003900
C	1.83463600	1.23660200	0.00003700
C	1.91298900	-1.17683900	-0.00001800
C	2.57552100	0.05350700	0.00001700
O	-2.27427300	1.11373300	-0.00008200
H	-0.13130900	2.12067300	0.00003800
H	-0.00252400	-2.17843100	-0.00006400
H	2.34238900	2.19420700	0.00007000
H	2.48201600	-2.09935600	-0.00003100
H	3.65836900	0.08903000	0.00003000
H	-3.20170700	0.82924300	0.00035000

#### Entry 245

N	-1.61127300	0.11323700	-0.42555700
C	-0.19473400	0.01644600	-0.17507200
C	0.54305000	1.19969400	-0.26140800
C	0.43572000	-1.20599100	0.04668100

C	1.92285400	1.15462700	-0.10912900
C	1.82329600	-1.23702200	0.18594600
C	2.56824600	-0.06367200	0.11266700
F	-2.09693400	1.09328500	0.58746300
H	0.03009500	2.13672000	-0.43449300
H	-0.14679700	-2.11409700	0.10174700
H	2.49708800	2.07189400	-0.16847500
H	2.31834600	-2.18620500	0.35601600
H	3.64590000	-0.09528000	0.22389400
O	-2.21797200	-1.07069200	-0.07523200
H	-3.04012500	-1.06420400	-0.58320100

#### 245-radical

N	-1.59797300	-0.12241500	-0.00006900
O	-2.28785500	-1.16209700	0.00009500
C	-0.20671200	-0.03686300	-0.00001500
C	0.44570200	1.20738900	0.00001700
C	0.52713100	-1.23572000	-0.00003900
C	1.83463600	1.23660200	0.00003700
C	1.91298900	-1.17683900	-0.00001800
C	2.57552100	0.05350700	0.00001700
O	-2.27427300	1.11373300	-0.00008200
H	-0.13130900	2.12067300	0.00003800
H	-0.00252400	-2.17843100	-0.00006400
H	2.34238900	2.19420700	0.00007000
H	2.48201600	-2.09935600	-0.00003100
H	3.65836900	0.08903000	0.00003000
H	-3.20170700	0.82924300	0.00035000

#### Entry 246

N	-0.23008500	0.40153700	-0.29251900
C	-1.37403500	-0.41813100	-0.06329200
O	-0.37452100	1.73828700	0.12920300
C	1.09336400	-0.09675500	-0.01212400
O	-1.26049400	-1.61375100	0.02409400
C	-2.68145800	0.32919000	0.00336100
F	1.33526400	-1.20342200	-0.70835800
F	1.30208500	-0.35781900	1.29125300
F	1.98802600	0.83975200	-0.37988300
H	-0.15946000	2.26747100	-0.65078000
H	-2.72293600	0.93629300	0.91039400
H	-3.48246900	-0.40719400	0.01346300
H	-2.80002800	1.00395800	-0.84659100

#### 246-radical

N	-0.25063200	0.50857400	0.00022200
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C	-1.39788000	-0.38212500	0.00008400
O	-0.38953600	1.77037700	0.00028900
C	1.12179500	-0.05649300	-0.00005500
O	-1.21746400	-1.56957600	0.00022700
C	-2.71690800	0.33239300	-0.00019900
F	1.31804200	-0.80631600	-1.08694300
F	1.31833100	-0.80711300	1.08629200
F	1.99497000	0.93959000	0.00022400
H	-2.80427500	0.97627000	0.87755700
H	-3.50554300	-0.41699300	-0.00032800
H	-2.80389400	0.97619300	-0.87805400

### Entry 247

N	0.20022200	0.48849800	-0.26476700
C	1.48050300	-0.01404100	-0.05387600
O	0.10788100	1.88116800	-0.07943000
C	-1.04008700	-0.17989300	0.00995500
O	2.37974900	0.79874300	0.11282300
C	1.69905900	-1.50204100	-0.09721600
F	-1.06133300	-1.32885900	-0.74322400
F	-1.06829500	-0.62482900	1.32538900
C	-2.26752200	0.64754300	-0.26528000
H	1.04724100	2.10276900	0.10382700
H	1.08325900	-2.01578200	0.64253300
H	2.75216300	-1.68109300	0.11052800
H	1.44266600	-1.90137800	-1.07972700
H	-3.13623700	0.00957400	-0.10121100
H	-2.25496900	0.99821100	-1.29678400
H	-2.30179200	1.50271400	0.40608000

### 247-radical

N	0.27950100	0.50071400	0.06364400
C	1.40184400	-0.39704200	0.00147600
O	0.46271800	1.74892900	0.20267000
C	-1.12852100	-0.02436900	-0.04204900
O	1.21528100	-1.58894700	-0.04134600
C	2.73950900	0.28673400	0.00626400
F	-1.92762600	1.06198200	-0.09708700
F	-1.22756200	-0.65184700	-1.24886600
C	-1.54728700	-0.93422300	1.08404000
H	2.81153500	0.99651100	-0.82031500
H	3.50888900	-0.47775000	-0.07964800
H	2.87466900	0.85807700	0.92718300
H	-2.58888400	-1.21645400	0.92262400
H	-1.46240700	-0.39999700	2.03150900

H            -0.92088700   -1.82306900   1.09773100

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