

Supporting Information

Computational Study on N-N Homolytic Bond Dissociation Enthalpies of Hydrazine Derivatives

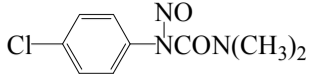
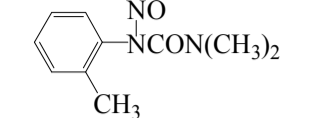
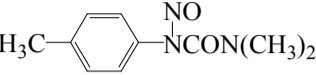
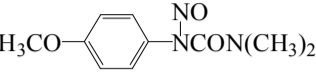
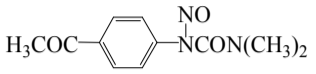
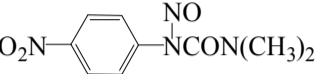

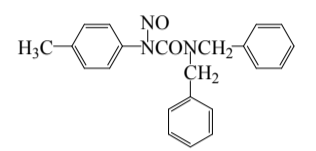
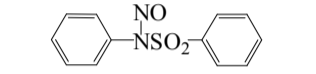
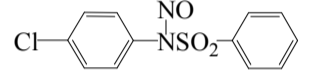
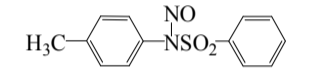
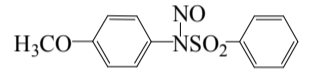
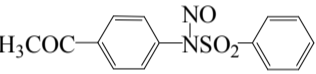
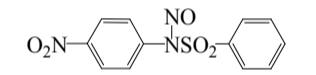
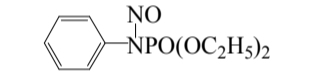
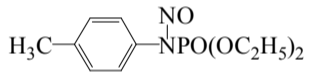
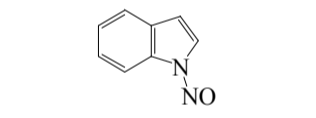
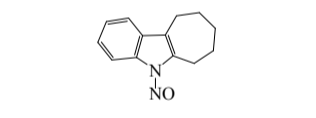
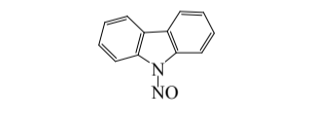
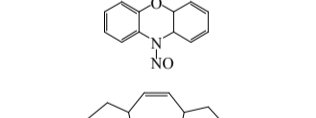
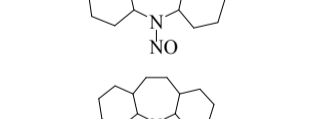
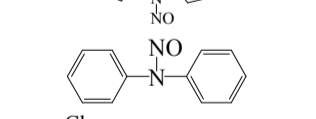
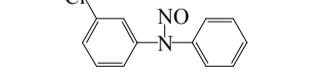
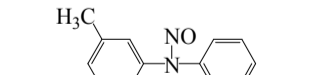
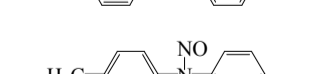
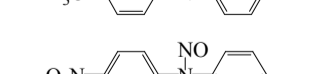
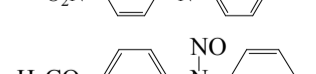
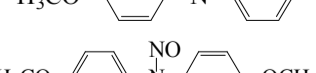

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









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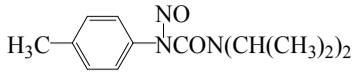
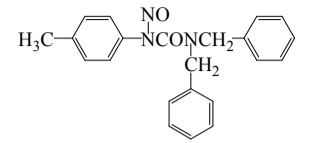
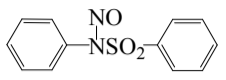
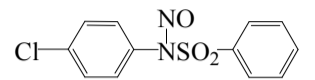
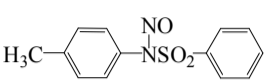
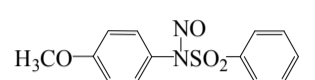
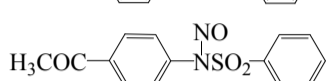
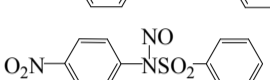
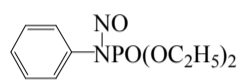
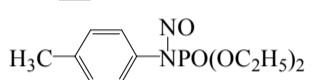
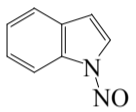
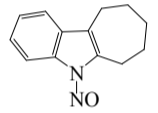
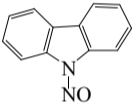
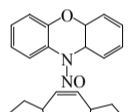
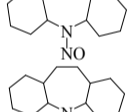
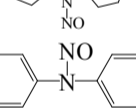
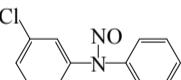
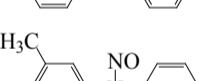
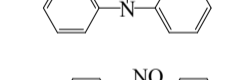
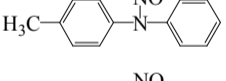
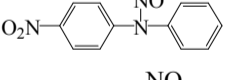
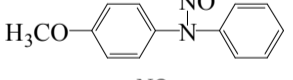
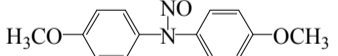
Table S1 The calculated 58 N-N BDEs by using 25 kinds of DFTs (kJ/mol)




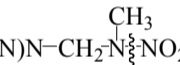








Entry	compounds	Exp.	B3LYP	B3LYP-D3	CAM-B3LYP	BP86	B3P86	B3PW91	B97D	M11	B97D3
1	ON-NO ₂	36.6 ^a	31.3	35.9	19.9	68.8	44.6	34.5	55.8	28.1	62.6
2	O ₂ N-NO ₂	54.4 ^a	46.3	53.0	42.5	75.4	63.4	52.6	63.9	59.4	71.3
3	H ₂ N-NH ₂	262.7 ^a	241.0	243.0	251.0	266.1	262.5	249.4	246.9	276.2	252.4
4	F ₂ N-NF ₂	87.3 ^a	48.7	53.3	57.4	67.1	66.9	53.6	43.9	78.3	49.2
5	H ₃ CHN-NH ₂	257.5 ^a	226.6	231.6	238.9	248.1	248.1	234.8	231.6	263.7	236.3
6	H ₂ N-N(CH ₃) ₂	253.7 ^a	213.7	221.6	228.1	233.9	235.9	221.7	221.1	252.7	224.5
7	H ₃ CHN-NHCH ₃	260.2 ^a	222.4	231.0	237.9	238.2	244.8	231.2	226.2	262.3	229.8
8	(H ₃ C) ₂ N-NHCH ₃	255.2 ^a	206.2	219.6	223.8	222.4	229.9	215.2	215.5	250.3	217.4
9	(H ₃ C) ₂ N-N(CH ₃) ₂	237.2 ^a	177.1	197.4	197.3	193.0	203.1	187.2	194.0	231.2	194.3
10	H ₂ N-NO ₂	214.3 ^a	199.1	203.3	214.1	212.6	223.3	209.7	193.4	237.6	201.0
11	H ₃ CHN-NO ₂	212.8 ^a	188.8	196.8	206.0	199.2	213.5	199.3	181.6	232.6	189.6
12	(H ₃ C) ₂ N-NO ₂	199.8 ^a	168.3	179.8	186.9	178.2	194.2	179.2	162.2	217.6	170.6
13	H ₂ N(H ₃ C)N ⁺ (NO)	137.6 ^a	119.2	133.3	123.1	135.1	132.0	132.7	130.3	140.7	125.7
14		227.6±8.4	201.5	209.9	217.9	220.9	227.8	215.2	206.1	251.9	210.7
15		162.3±8.4	140.0	154.6	161.1	154.0	169.3	157.5	142.3	202.5	148.3
16		118.4	95.9	107.9	112.4	108.4	121.1	106.5	91.7	146.5	101.2
17		121.5	92.8	109.1	110.7	104.9	119.2	103.8	93.0	149.8	101.3
18		129.7	92.7	109.7	110.7	104.9	119.2	103.8	93.8	150.0	101.9
19		123.8	92.9	110.1	110.8	105.0	119.3	104.0	94.2	150.2	102.3
20		167.4	165.5	183.3	186.3	175.2	192.9	176.7	165.5	225.3	171.5
21	((NO ₂) ₃ CCH ₂) ₂ N-NO ₂	167.4	104.5	133.9	127.4	120.1	134.0	114.7	117.9	179.8	124.1
22	(H(NO ₂) ₂ CCH ₂) ₂ N-NO ₂	190.4	133.4	159.8	155.2	144.9	161.3	143.6	143.9	199.8	150.4
23		167.4	148.0	175.0	171.7	157.8	176.7	159.4	158.2	214.9	165.6
24		167.4	123.4	144.8	150.9	122.9	151.1	135.6	119.0	190.9	128.9
25		167.4	140.3	163.5	162.5	149.4	168.6	152.0	144.9	201.2	151.7
26	O ₂ N-N+(CH ₂ C(NO ₂) ₃) ₂	163.2	110.9	136.2	131.4	128.7	141.0	123.0	122.5	175.7	129.1
27		167.4	119.9	139.1	134.8	142.4	147.7	132.0	134.3	170.8	143.2
28		121.8	85.5	99.2	95.0	111.6	110.4	98.4	101.7	123.9	109.2
29		96.7	87.2	104.4	98.2	111.1	111.8	99.4	105.6	128.8	113.0

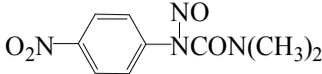
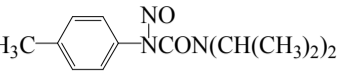
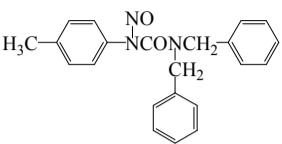
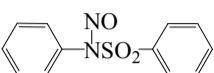
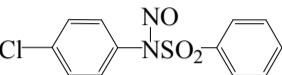
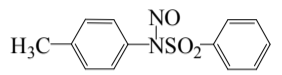
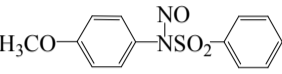
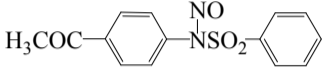
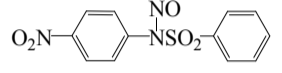
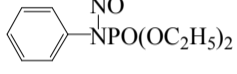
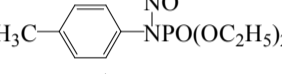
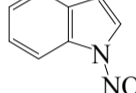
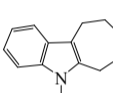
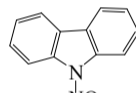
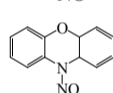
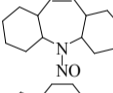
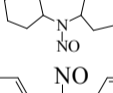
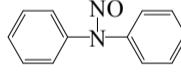
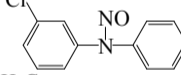
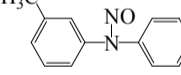
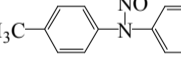
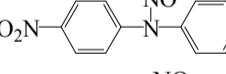
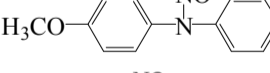
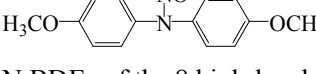
* Corresponding author. Tel.: +86 21 67791216; fax: +86 21 67791220.
E-mail address: wrzheng@sues.edu.cn (W.R. Zheng).

30		122.2	81.6	95.8	91.8	106.6	106.3	94.5	97.8	120.6	104.8
31		115.1	79.1	97.8	89.1	105.5	103.7	90.9	101.9	119.5	107.1
32		120.1	81.9	95.7	91.6	107.7	106.7	94.9	98.3	119.7	105.6
33		118.4	73.2	87.3	83.7	97.9	97.8	86.3	89.9	111.3	96.9
34		127.6	88.1	103.6	96.6	115.9	114.2	101.7	108.4	128.7	115.3
35		138.5	85.6	99.8	96.2	109.9	110.9	98.6	100.3	126.7	107.4
36		111.3	72.8	92.9	82.1	102.3	99.2	85.9	99.0	117.1	105.5
37		106.3	85.7	94.1	93.9	114.1	111.3	100.0	97.1	118.2	104.9
38		55.2	75.1	91.8	80.6	105.9	100.1	87.6	96.5	111.1	104.9
39		54.8	74.4	90.5	83.3	100.3	99.7	87.9	91.7	112.0	100.8
40		47.7	73.6	89.7	81.9	100.5	99.0	87.2	91.7	110.3	100.9
41		51.9	66.4	82.4	75.2	92.4	91.7	80.1	84.1	103.1	93.2
42		60.7	73.9	90.7	79.6	104.0	99.1	86.5	94.9	110.8	103.1
43		75.3	79.4	96.3	85.6	108.9	104.7	92.0	99.7	116.8	107.9
44		146.4	90.2	106.7	99.7	118.1	115.3	102.9	108.9	131.0	119.1
45		144.3	89.5	107.6	98.7	116.8	115.1	102.6	176.6	129.7	119.3
46		120.1	117.3	126.3	123.9	144.9	142.5	130.4	127.3	146.1	135.8
47		124.3	83.6	95.9	89.0	113.0	109.4	96.4	98.2	112.8	105.9
48		114.6	109.4	121.4	120.3	134.6	135.9	123.1	120.1	148.9	128.5
49		56.9	42.8	55.3	65.1	71.9	68.9	56.1	57.5	79.1	65.7
50		80.3	63.3	77.7	77.4	90.5	89.1	77.1	78.2	105.9	88.0
51		95.8	63.3	77.7	77.4	90.5	89.1	77.1	78.2	105.9	88.0
52		94.6	94.5	106.8	106.2	120.2	120.1	108.1	105.4	133.8	115.4
53		100.8	93.0	105.2	105.0	118.5	118.8	106.8	103.6	132.7	113.7
54		93.3	94.9	107.0	106.7	120.3	120.4	108.4	105.4	133.9	115.5
55		89.5	92.5	104.8	104.3	117.9	117.9	106.0	103.4	131.6	113.4
56		101.7	92.3	104.3	105.1	117.0	118.3	106.4	101.6	132.7	112.1
57		89.5	88.7	101.2	100.7	113.4	114.0	102.0	99.5	127.2	109.2
58		87.9	88.0	100.6	100.7	112.0	113.3	101.5	98.1	127.5	108.0

Entry	compounds	Exp.	M05-2X	M06-2X	M06-HF	MPW1B95	MPW1KCIS	TPSS1KCIS	TPSSLYP1W
1	ON-NO ₂	36.6 ^a	35.7	29.1	21.5	29.7	47.1	41.3	47.7
2	O ₂ N-NO ₂	54.4 ^a	53.1	55.8	35.6	51.2	61.2	53.5	49.6
3	H ₂ N-NH ₂	262.7 ^a	265.3	270.1	296.3	266.2	261.5	242.2	221.8
4	F ₂ N-NF ₂	87.3 ^a	74.8	89.4	100.5	65.7	61.9	51.1	37.4
5	H ₃ CHN-NH ₂	257.5 ^a	256.0	262.6	294.7	252.6	245.1	228.1	207.3
6	H ₂ N-N(CH ₃) ₂	253.7 ^a	249.5	256.5	293.8	241.1	230.6	215.6	194.9
7	H ₃ CHN-NHCH ₃	260.2 ^a	283.4	264.1	292.0	250.0	239.5	223.7	200.1
8	(H ₃ C) ₂ N-NHCH ₃	255.2 ^a	247.9	257.0	301.4	236.1	222.0	208.3	184.5
9	(H ₃ C) ₂ N-N(CH ₃) ₂	237.2 ^a	236.9	236.9	284.6	211.2	191.7	180.4	155.6
10	H ₂ N-NO ₂	214.3 ^a	225.1	233.8	266.8	223.9	214.8	197.8	169.7
11	H ₃ CHN-NO ₂	212.8 ^a	218.3	230.4	270.1	214.9	201.9	188.4	160.9
12	(H ₃ C) ₂ N-NO ₂	199.8 ^a	182.1	216.5	262.7	196.6	179.2	169.8	143.6
13	H ₂ N(H ₃ C)N ^{δ+} NO	137.6 ^a	132.7	137.6	134.2	136.0	140.0	129.1	111.7
14	H ₂ N-NH- 	227.6±8.4	228.6	248.8	286.0	234.4	223.4	204.8	172.9
15	 -HN-NH- 	162.3±8.4	171.9	203.5	252.0	178.0	161.4	146.3	107.8
16	H ₃ CN ^{δ+} NO ₂	118.4	122.6	145.2	173.3	123.4	108.2	99.4	75.2
17	C ₂ H ₅ N ^{δ+} NO ₂	121.5	121.9	146.9	175.5	123.0	105.2	96.6	70.9
18	C ₃ H ₇ N ^{δ+} NO ₂	129.7	121.9	146.9	176.2	123.2	105.2	96.7	71.1
19	C ₄ H ₉ N ^{δ+} NO ₂	123.8	122.0	147.1	175.8	123.4	105.3	96.9	71.2
20	H ₃ C(O ₂ N)N-CH ₂ -N ^{δ+} (CH ₃)NO ₂	167.4	180.9	219.7	265.3	199.1	176.4	168.0	140.8
21	((NO ₂) ₃ CCH ₂) ₂ N-NO ₂	167.4	161.6	171.2	205.8	148.6	117.6	110.5	85.0
22	(H(NO ₂) ₂ CCH ₂) ₂ N-NO ₂	190.4	190.1	195.5	237.6	169.3	144.6	136.9	111.1
23	(O ₂ N) ₃ CH ₂ C-N ^{δ+} (NO ₂)-(CH ₂) ₂ C(NO ₂) ₃	167.4	180.9	209.5	255.0	184.7	160.5	150.8	121.2
24	O ₂ N ^{δ+} N(CH ₂) ₂ N(NO ₂)CH ₂ C(NO ₂) ₃	167.4	159.6	188.7	232.6	160.0	133.7	125.4	90.8
25	O ₂ N ^{δ+} N(CH ₂) ₂ N(NO ₂)CH ₂ CH(NO ₂) ₂	167.4	175.5	196.9	236.2	174.7	152.5	143.6	114.3
26	O ₂ N ^{δ+} N(CH ₂ C(NO ₂) ₃) ₂	163.2	161.0	168.9	207.3	148.9	125.3	116.7	89.9
27	C(NO ₂) ₃ ON ^{δ+} N(CH ₂) ₂ N(NO)CH ₂ C(NO ₂) ₃	167.4	157.4	166.5	179.3	149.9	137.4	129.3	106.9
28	 -N ^{δ+} (NO)CON(CH ₃) ₂	121.8	113.2	123.4	135.6	107.9	105.3	94.6	74.4
29	 -N ^{δ+} (NO)CON(CH ₃) ₂	96.7	108.9	128.1	140.9	108.9	105.9	95.8	75.6
30	 -N ^{δ+} (NO)CON(CH ₃) ₂	122.2	110.1	119.9	132.1	104.1	100.9	90.6	70.3
31	 -N ^{δ+} (NO)CON(CH ₃) ₂	115.1	108.5	119.0	130.5	102.4	98.8	87.8	68.7
32	 -N ^{δ+} (NO)CON(CH ₃) ₂	120.1	109.3	119.3	132.0	104.0	101.5	91.1	71.1
33	 -N ^{δ+} (NO)CON(CH ₃) ₂	118.4	114.4	109.6	120.1	94.9	92.5	81.9	61.2
34	 -N ^{δ+} (NO)CON(CH ₃) ₂	127.6	116.8	127.0	137.1	111.9	109.1	98.1	77.2
35	 -N ^{δ+} (NO)CON(CH ₃) ₂	138.5	126.4	126.1	139.0	109.8	104.8	94.7	73.3




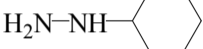
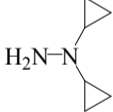
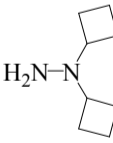
36		111.3	103.3	115.0	124.8	97.1	94.1	82.9	63.0
37		106.3	108.7	116.8	131.3	105.6	106.3	95.5	74.6
38		55.2	68.5	109.1	110.7	96.2	95.9	91.5	68.5
39		54.8	55.7	110.8	119.3	95.6	94.5	84.0	62.9
40		47.7	62.6	109.5	117.8	94.6	94.1	83.4	62.6
41		51.9	54.7	100.8	107.2	86.5	86.5	75.8	54.7
42		60.7	66.8	108.9	111.1	95.4	94.5	84.6	66.8
43		75.3	71.9	115.5	118.2	101.2	99.8	89.9	71.9
44		146.4	139.2	128.7	137.5	114.3	110.6	100.9	81.6
45		144.3	137.9	128.8	139.1	112.9	109.4	99.8	79.9
46		120.1	134.5	143.2	151.5	137.1	137.3	125.9	105.6
47		124.3	133.2	109.4	119.4	103.2	102.7	93.5	75.7
48		114.6	106.7	143.2	156.5	130.5	128.7	118.3	96.0
49		56.9	65.1	72.7	81.9	63.5	62.0	52.9	34.3
50		80.3	92.7	99.4	112.6	85.9	82.9	72.6	52.0
51		95.8	92.8	99.4	112.6	85.9	82.9	72.6	52.0
52		94.6	91.9	129.1	143.3	115.4	114.1	103.3	81.9
53		100.8	105.5	127.9	143.0	114.3	112.8	101.9	80.1
54		93.3	105.8	129.4	143.7	115.6	114.5	103.6	82.1
55		89.5	103.1	126.9	141.2	113.0	111.9	101.2	80.1
56		101.7	104.7	128.3	144.4	114.0	112.0	101.4	78.6
57		89.5	99.1	122.2	135.4	108.7	107.7	97.1	75.9
58		87.9	99.3	121.4	135.1	108.7	106.9	96.3	74.6

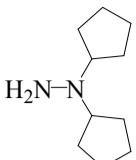
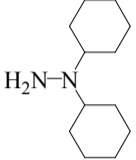

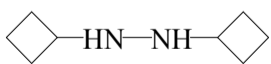
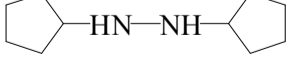
Entry	compounds	Exp.	N12	MN12-L	MN12-SX	PBE1W	PBE1PBE	SOGGA11	SPGGA11-X	WB97	WB97-X
1	ON-NO ₂	36.6 ^a	63.0	60.0	51.0	67.4	35.3	55.3	22.9	17.8	21.9
2	O ₂ N-NO ₂	54.4 ^a	77.1	72.1	64.7	72.9	57.0	66.8	45.0	43.1	45.7
3	H ₂ N-NH ₂	262.7 ^a	271.0	256.2	269.4	263.5	255.4	275.3	259.1	265.8	263.6
4	F ₂ N-NF ₂	87.3 ^a	63.1	90.1	95.6	65.3	62.9	50.1	67.8	77.8	65.1
5	H ₃ CHN-NH ₂	257.5 ^a	254.4	244.7	257.2	245.9	242.6	255.5	246.3	254.7	251.6
6	H ₂ N-N(CH ₃) ₂	253.7 ^a	238.8	234.6	246.6	231.3	231.1	238.7	235.1	245.5	241.5
7	H ₃ CHN-NHCH ₃	260.2 ^a	249.7	242.4	255.4	237.2	241.1	248.5	244.2	254.0	250.1
8	(H ₃ C) ₂ N-NHCH ₃	255.2 ^a	230.9	230.5	242.0	220.0	226.8	230.7	229.9	242.9	237.8
9	(H ₃ C) ₂ N-N(CH ₃) ₂	237.2 ^a	199.8	210.8	218.5	189.6	200.4	191.4	203.6	221.3	214.6
10	H ₂ N-NO ₂	214.3 ^a	228.9	232.5	239.6	208.6	220.0	214.8	223.9	224.4	223.6
11	H ₃ CHN-NO ₂	212.8 ^a	217.8	225.7	230.9	195.0	210.9	193.9	214.5	216.6	215.2
12	(H ₃ C) ₂ N-NO ₂	199.8 ^a	196.4	207.6	211.4	173.0	191.4	162.7	194.7	198.2	196.2
13	H ₂ N(H ₃ C)N $\frac{5}{3}$ NO	137.6 ^a	135.2	129.8	136.1	130.8	140.0	139.4	130.4	130.1	131.3
14	H ₂ N-NH- 	227.6±8.4	235.0	225.5	236.1	217.9	225.4	234.4	222.8	233.4	231.4
15	 -HN-NH- 	162.3±8.4	172.9	172.2	180.8	150.6	170.8	169.0	164.1	176.8	175.2
16	H ₃ CN $\frac{5}{3}$ NO ₂ NO ₂	118.4	120.8	140.0	141.0	103.6	118.7	94.8	120.4	126.1	103.6
17	C ₂ H ₅ N $\frac{5}{3}$ NO ₂ NO ₂	121.5	118.7	141.8	141.2	100.2	117.3	90.3	118.8	126.4	123.3
18	C ₃ H ₇ N $\frac{5}{3}$ NO ₂ NO ₂	129.7	119.2	142.1	141.4	100.2	117.3	90.4	118.8	126.5	123.3
19	C ₄ H ₉ N $\frac{5}{3}$ NO ₂ NO ₂	123.8	119.3	142.1	141.5	100.3	117.4	90.8	118.9	126.5	123.4
20	H ₃ C(O ₂ N)N-  NO ₂	167.4	196.1	210.6	213.6	170.2	190.6	154.7	193.1	165.5	197.1
21	((NO ₂) ₃ CCH ₂) ₂ N-NO ₂	167.4	136.2	170.7	162.8	116.9	133.9	102.0	134.8	148.5	143.7
22	(H(NO ₂) ₂ CCH ₂) ₂ N-NO ₂	190.4	162.0	190.2	188.1	141.1	160.3	128.9	163.4	174.4	170.2
23	(O ₂ N) ₃ CH ₂ C- 	167.4	176.1	203.0	202.7	154.2	176.6	145.4	178.6	189.7	186.0
24	O ₂ N $\frac{5}{3}$ N(CH ₂) ₂ N(NO ₂)CH ₂ C(NO ₂) ₃ C(NO ₂) ₃	167.4	142.7	173.5	178.5	119.7	154.1	122.3	156.8	170.9	166.2
25	O ₂ N $\frac{5}{3}$ N(CH ₂) ₂ N(NO ₂)CH ₂ CH(NO ₂) ₂ CH(NO ₂) ₂	167.4	168.4	187.8	189.0	145.2	168.2	133.8	169.0	178.8	175.6
26	O ₂ N $\frac{5}{3}$ N(CH ₂ C(NO ₂) ₃) ₂	163.2	146.7	164.6	161.3	123.5	139.2	109.3	138.4	147.4	144.1
27	C(NO ₂) ₃ ON $\frac{5}{3}$ N(CH ₂) ₂ N(NO)CH ₂ C(NO ₂) ₃	167.4	153.9	172.9	169.6	139.7	146.1	135.4	141.0	154.6	151.0
28	 -N(NO)CON(CH ₃) ₂	121.8	119.7	125.0	125.7	109.0	107.8	108.1	100.3	107.4	107.6
29	 -N(NO)CON(CH ₃) ₂	96.7	119.1	130.4	130.3	109.3	110.0	110.1	103.3	112.9	112.3
30	 -N(NO)CON(CH ₃) ₂	122.2	115.0	120.9	121.3	104.2	104.1	103.9	96.5	104.9	104.9
31	 -N(NO)CON(CH ₃) ₂	115.1	113.6	120.5	120.2	103.8	101.6	103.5	93.8	103.1	102.8
32	 -N(NO)CON(CH ₃) ₂	120.1	115.8	120.6	121.5	105.3	104.3	104.8	96.5	103.9	104.1
33	 -N(NO)CON(CH ₃) ₂	118.4	106.2	112.3	112.9	95.6	96.2	96.6	88.2	96.8	96.8
34	 -N(NO)CON(CH ₃) ₂	127.6	124.5	131.4	129.9	113.4	111.8	113.8	102.1	109.1	109.1

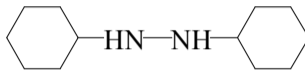
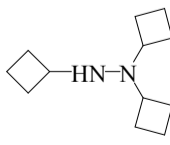
35		138.5	118.2	126.0	127.2	107.1	108.6	103.9	102.0	126.4	109.3
36		111.3	108.5	119.1	116.7	100.4	97.0	98.7	87.9	98.1	97.2
37		106.3	123.1	116.3	117.9	110.1	108.1	107.0	98.2	102.5	103.5
38		55.2	113.1	118.0	114.2	103.3	96.8	101.3	85.9	83.1	91.4
39		54.8	108.4	115.2	114.2	97.8	55.7	101.1	89.0	85.3	96.2
40		47.7	108.2	114.2	113.3	98.0	96.9	101.1	88.0	83.9	94.5
41		51.9	100.3	107.4	106.4	89.8	90.0	91.9	81.1	76.4	87.9
42		60.7	111.4	116.5	113.2	101.4	95.9	97.5	85.5	82.3	90.5
43		75.3	116.2	121.8	118.8	106.2	101.5	102.1	91.4	88.4	96.5
44		146.4	125.7	135.5	132.7	116.2	113.2	119.7	103.2	139.2	112.2
45		144.3	124.0	135.0	132.2	114.6	113.2	116.4	104.4	137.9	111.9
46		120.1	157.6	156.3	152.4	141.8	139.4	140.7	129.1	129.8	131.3
47		124.3	125.2	123.2	118.5	109.4	105.6	99.9	95.0	126.7	96.0
48		114.6	146.7	148.0	146.1	131.4	133.3	125.5	123.9	131.4	131.3
49		56.9	82.9	81.5	78.1	68.0	65.6	55.9	55.7	64.2	63.7
50		80.3	98.1	97.6	98.3	87.1	87.2	83.2	78.3	92.9	91.8
51		95.8	98.1	97.6	98.3	87.1	87.2	83.2	78.3	92.9	91.8
52		94.6	129.8	130.3	131.1	117.1	117.4	114.4	108.7	76.2	118.6
53		100.8	128.3	129.0	130.1	115.4	116.2	113.1	107.6	105.5	117.8
54		93.3	130.0	130.1	131.1	117.2	117.7	114.6	109.1	105.8	119.1
55		89.5	127.2	127.8	128.6	114.9	115.3	112.6	106.5	103.1	116.4
56		101.7	126.0	127.4	129.2	113.7	116.2	112.1	108.0	104.7	118.1
57		89.5	123.1	123.8	124.5	110.3	111.4	107.5	102.7	99.1	101.7
58		87.9	122.1	123.6	124.1	108.9	111.0	105.4	102.4	99.3	113.1

^a Average N-N BDEs of the 8 high-level *ab initio* methods which are regarded as the standard reference values

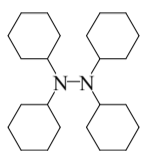
Table S2 The Cartesian coordinates and absolute energy values (hartrees) of selected molecules and radicals

Molecules:							
							
SCF energy= -228.6080124				SCF energy= -267.9310785			
N	-0.90736400	-0.66418600	-0.09621100	N	-1.30634700	0.61976800	0.20878800
H	-0.74996300	-0.95884200	-1.05639100	H	-1.21063800	0.75815000	1.21297400
N	-1.99932000	0.25983100	-0.11009200	N	-2.40588600	-0.27367000	0.01697000
H	-2.51184500	0.15072600	0.76210300	H	-2.84211700	-0.04908500	-0.87433200
H	-1.65540200	1.22395500	-0.15255800	H	-2.09254000	-1.24802400	-0.02034300
C	0.30687200	-0.16901200	0.50287700	C	-0.04783500	0.18651300	-0.36716000
C	1.62955500	-0.51327700	-0.11445000	C	1.20225900	1.02080100	0.00086800
C	1.14288200	0.92339600	-0.14957300	C	0.70521800	-1.09298200	0.13996900
H	0.26136200	-0.15685300	1.59143900	H	-0.17725000	0.13951700	-1.45658200
H	1.62231700	-1.06903300	-1.05034200	C	2.03033000	-0.29372100	0.00084500
H	2.45501200	-0.77391000	0.54267500	H	1.10938100	1.43686200	1.01249200
H	1.63762000	1.65539100	0.48477200	H	1.49376100	1.82619900	-0.68068100
H	0.81183100	1.31241200	-1.11069600	H	0.46681900	-1.30015900	1.19154700
							
SCF energy= -307.2814800				SCF energy= -346.5980409			
N	-1.53541800	-0.54537100	-0.38700400	N	1.78165200	-0.57453100	-0.28587700
H	-1.32304000	-0.40492200	-1.37321000	H	2.14024600	-1.41650600	0.16725100
N	-2.69183900	0.23927800	-0.09709500	N	2.89309200	0.38814600	-0.13561600
H	-3.20883000	-0.22876900	0.64384100	H	3.66418000	-0.02932500	-0.66117700
H	-2.44469100	1.17578800	0.23474000	H	2.62158500	1.18951600	-0.70862700
C	-0.35030600	-0.27730500	0.43754800	C	0.63904500	-0.12355900	0.53267800
C	0.78984300	-1.25632000	0.04460900	C	0.03517600	1.16817500	-0.06654000
C	0.27798300	1.15498600	0.31435600	C	-0.40977800	-1.26343400	0.58425100
H	-0.66433900	-0.45412500	1.47389300	C	-1.44999400	1.30915200	0.29877900
C	2.08604600	-0.42802200	0.07118000	H	0.13922200	1.12970200	-1.16100800
H	0.60403700	-1.62215600	-0.97522600	C	-1.47377900	-1.12463700	-0.51263200
H	0.81723400	-2.13789000	0.69328200	H	-0.89759500	-1.25552400	1.56855300
C	1.62424100	0.95756500	-0.41140800	C	-2.29493900	0.17477500	-0.33114800
H	0.45640900	1.57420500	1.31344700	H	-1.54782000	1.28725500	1.39352600
H	-0.38444600	1.85638900	-0.20947900	H	-0.97082400	-1.12025400	-1.48772100
H	2.47307500	-0.35426500	1.09748800	H	-3.17163400	-0.02018900	0.30084400
H	2.88127000	-0.86088300	-0.54685300	H	0.09788400	-2.23453100	0.50347400
H	2.34419700	1.75677900	-0.20074200	H	0.98344100	0.10064500	1.55762500
H	1.47308200	0.93707700	-1.50019800	H	0.59727900	2.04320500	0.28216100
							
SCF energy= -345.3245460				SCF energy= -423.9728186			
N	0.08936200	1.99991000	-0.00284500	N	0.04188700	0.54982300	-0.33264600
H	-0.65487200	2.18521300	0.67908600	N	-0.28147800	1.86637100	0.12463200
H	-0.11592200	2.55182700	-0.83392200	H	-0.09499500	1.96023300	1.13010500
N	0.06985200	0.61686900	-0.38418500	H	0.32743500	2.52067100	-0.36091700
C	-1.28310100	0.11293500	-0.52796900	C	1.23130600	0.01575500	0.32084100
C	-1.68648700	-1.29593900	-0.20465200	C	1.84173400	-1.29777100	-0.23663900
C	-2.20198600	-0.15829200	0.65655500	C	2.58116500	0.72302800	0.02734100
H	-1.76953600	0.55353700	-1.39778200	H	1.07881100	-0.06860200	1.41616800
H	-0.94721800	-1.95569800	0.23761500	C	3.25041500	-0.67826600	-0.02605700
H	-2.37507300	-1.79211500	-0.88435100	H	1.60620300	-1.40753300	-1.30108600
H	-3.24763800	0.13027400	0.58089600	H	1.60634900	-2.23241500	0.28314000
H	-1.78819200	-0.07778200	1.65943600	H	2.55680700	1.19357000	-0.96255400
C	0.97553300	-0.14447800	0.43758300	H	2.95582900	1.44402000	0.76191500
C	1.72241100	-1.28514600	-0.21307700	H	3.99685200	-0.84945400	-0.80793400
C	2.44207900	-0.00561600	0.14192600	H	3.68455700	-0.96343500	0.93838300
H	0.70462400	-0.26522500	1.49280400				
H	1.51133200	-1.47078200	-1.26233400				
H	1.91558200	-2.17705400	0.37858300				
H	3.13214900	-0.01048400	0.98151100				
H	2.70957300	0.67005000	-0.66452300				

							
SCF energy= -502.6698855				SCF energy= -581.3127917			
N	0.04583500	0.72659800	-0.21937700	N	-0.01606400	0.37148300	0.37620700
N	-0.19730900	1.93232600	0.50917100	N	-0.59659300	1.67683200	0.28379400
H	-0.67138100	2.59219400	-0.10083000	H	-0.02782200	2.31520900	0.83434300
H	-0.79226100	1.77163500	1.32799700	H	-0.57823000	2.01730100	-0.68565700
C	1.25202100	0.08704800	0.33468100	C	-1.05714000	-0.68300800	0.30896000
C	1.68132500	-1.19276100	-0.41391800	C	-2.12202300	-0.51479500	1.41924900
C	2.49236700	1.02302500	0.25363300	C	-1.72609900	-0.92558400	-1.07158300
H	1.08078500	-0.18185600	1.39551600	C	-3.32964300	0.37369100	1.07240900
C	3.17737300	-1.31373100	-0.08556400	H	-2.49735600	-1.52353500	1.65118700
H	1.54611400	-1.04300500	-1.49470600	C	-2.90544500	0.00779500	-1.39797100
H	1.11094200	-2.08234600	-0.12225900	H	-2.10362200	-1.96021700	-1.07030800
C	3.68588900	0.13716400	-0.19845800	C	-3.95509500	-0.01262200	-0.27643200
H	2.67935300	1.50226000	1.21919400	H	-3.01076000	1.41979500	1.03660000
H	2.29142500	1.82647900	-0.46102900	H	-2.55195700	1.03726100	-1.54107400
H	3.30323000	-1.68389900	0.94183000	H	-4.38738000	-1.02412600	-0.20907600
H	3.70464600	-2.01053500	-0.74783600	C	1.15450500	0.24042300	-0.52652200
H	4.59140600	0.31245900	0.39373800	C	1.80658900	-1.16576500	-0.52757800
H	3.94341300	0.35456600	-1.24308700	C	2.21687200	1.30603700	-0.12001900
C	-1.12136900	-0.17236500	-0.33725800	C	2.82346800	-1.33115700	0.61052000
C	-1.75397400	-0.72927000	0.96984100	H	2.32410200	-1.28960300	-1.48866800
C	-2.30833000	0.46071800	-1.12745200	C	3.65196000	0.85672900	-0.42939200
H	-0.76256800	-1.03049600	-0.91340800	H	2.12894600	1.47854500	0.96223600
C	-3.18139300	-1.10551700	0.54444400	C	4.03691500	-0.38919400	0.40037300
H	-1.80103400	0.04368200	1.75080800	H	2.32749600	-1.10468000	1.56293600
H	-1.18737300	-1.57071700	1.38415000	H	3.74250200	0.64021300	-1.50309200
C	-3.60025100	0.06404200	-0.36911700	H	4.43332100	-0.07626300	1.37528800
H	-2.31413700	0.08171100	-2.15553600	H	1.05427900	-1.95746600	-0.50089400
H	-2.20546400	1.54801900	-1.20196300	H	0.83473200	0.45986700	-1.56642200
H	-3.16479100	-2.04506600	-0.02609400	H	2.00915000	2.26254700	-0.61409400
H	-3.86161100	-1.25277200	1.39164900	H	3.15764500	-2.37402300	0.67487600
H	-4.42455400	-0.19654900	-1.04244600	H	4.85009500	-0.92668000	-0.10508800
H	-3.94777600	0.90165400	0.25075700	H	4.35190900	1.67713600	-0.22745600
							
SCF energy= -345.321128				SCF energy= -423.9694523			
N	0.51778400	-0.49331200	-0.36012900	N	0.50455800	0.50514800	-0.17889400
H	1.08215600	-0.43527600	0.49416200	H	0.50339300	1.02713000	0.70324800
N	-0.51778400	0.49331200	-0.36012900	N	-0.50454200	-0.50504700	-0.17887400
H	-1.08215600	0.43527600	0.49416200	H	-0.50333300	-1.02703800	0.70325600
C	0.03147300	1.81477800	-0.51787200	C	-1.82139100	0.04750900	-0.42432500
C	-0.68080900	2.98155100	0.09690500	C	-3.00432300	-0.94960400	-0.39493100
C	0.68080900	2.57036900	0.63086600	C	-2.57814200	0.91289300	0.63891800
H	0.46975900	1.95385800	-1.50299200	H	-1.77309800	0.58078100	-1.37927000
H	-1.54940900	2.78054600	0.72126100				
H	-0.76241300	3.89751800	-0.48226300				
H	1.53842300	3.20602500	0.42302600				
H	0.70592100	2.09132600	1.60831100				
C	-0.03147300	-1.81477800	-0.51787200				
C	0.68080900	-2.98155100	0.09690500				
C	-0.68080900	-2.57036900	0.63086600				
H	-0.46975900	-1.95385800	-1.50299200				
H	1.54940900	-2.78054600	0.72126100				
H	0.76241300	-3.89751800	-0.48226300				
H	-1.53842300	-3.20602500	0.42302600				
H	-0.70592100	-2.09132600	1.60831100				
							
SCF energy= -502.6709141							
N	0.01919200	0.71329700	-0.06290300				
H	-0.30983600	1.09350100	0.83029200				
N	-0.01919200	-0.71329700	-0.06290300				

H	0.30983600	-1.09350100	0.83029200	C	-3.88070900	0.17409600	0.22559300
C	-1.35512300	-1.22699500	-0.35199200	H	-2.82235500	-1.75769200	0.32586500
C	-1.35512300	-2.76793800	-0.44249100	H	-3.31477700	-1.39619400	-1.34525600
C	-2.48307200	-0.93180900	0.66273900	H	-2.27141400	0.64311500	1.65911000
H	-1.63967400	-0.79557500	-1.32010600	H	-2.54625600	2.00309500	0.53610800
C	-2.82146100	-3.21033200	-0.17692100	H	-4.57676300	-0.10967200	1.02146500
H	-0.68667300	-3.17228500	0.33095400	H	-4.43559300	0.72660700	-0.54064300
H	-0.96534900	-3.11490300	-1.40485400	C	1.82140300	-0.04745700	-0.42434800
C	-3.58469500	-1.92429800	0.25423300	C	3.00437800	0.94958300	-0.39489300
H	-2.81512200	0.11248000	0.64595600	C	2.57807500	-0.91293600	0.63887800
H	-2.12355800	-1.15525000	1.68058500	H	1.77309400	-0.58069300	-1.37931200
H	-3.27680400	-3.66229700	-1.06520700	C	3.88069300	-0.17417500	0.22562100
H	-2.85988700	-3.96928000	0.61320000	H	2.82244100	1.75765600	0.32592900
H	-4.14530600	-1.51523500	-0.59659000	H	3.31488000	1.39619400	-1.34519300
H	-4.31148000	-2.11184500	1.05269100	H	2.27133300	-0.64316900	1.65906900
C	1.35512300	1.22699500	-0.35199200	H	2.54614100	-2.00312900	0.53601900
C	1.35512300	2.76793800	-0.44249100	H	4.57673200	0.10953700	1.02152300
C	2.48307200	0.93180900	0.66273900	H	4.43556300	-0.72668500	-0.54062500
H	1.63967400	0.79557500	-1.32010600				
C	2.82146100	3.21033200	-0.17692100		SCF energy= -581.3336789		
H	0.68667300	3.17228500	0.33095400	N	0.01852500	-0.71372200	0.08164600
H	0.96534900	3.11490300	-1.40485400	H	0.32831500	-1.07678000	0.98760800
C	3.58469500	1.92429800	0.25423300	N	-0.01852500	0.71372200	0.08164600
H	2.81512200	-0.11248000	0.64595600	H	-0.32831500	1.07678000	0.98760800
H	2.12355800	1.15525000	1.68058500	C	1.28045100	1.30880100	-0.26273100
H	3.27680400	3.66229700	-1.06520700	C	1.10421700	2.82885600	-0.40134900
H	2.85988700	3.96928000	0.61320000	C	2.41872200	0.98160600	0.72591400
H	4.14530600	1.51523500	-0.59659000	H	1.54454300	0.89127400	-1.24386900
H	4.31148000	2.11184500	1.05269100	C	2.41872200	3.52846100	-0.78490100
				H	0.74500500	3.23831200	0.55736300
				H	0.32264400	3.03430600	-1.14296200
				C	3.73590700	1.67512900	0.33786100
				H	2.11635100	1.31347700	1.73383900
				H	2.56528100	-0.10476400	0.77439100
				C	3.55197100	3.19387700	0.19785000
				H	2.26358300	4.61444200	-0.83282300
				H	2.71363700	3.21178300	-1.79691500
				H	4.51328500	1.45032000	1.08029000
				H	4.09215500	1.26357900	-0.61888500
				H	4.48952600	3.66284700	-0.12955500
				H	3.31508700	3.62237500	1.18413000
				C	-1.28045100	-1.30880100	-0.26273100
				C	-1.10421700	-2.82885600	-0.40134900
				C	-2.41872200	-0.98160600	0.72591400
				H	-1.54454300	-0.89127400	-1.24386900
				C	-2.41872200	-3.52846100	-0.78490100
				H	-0.74500500	-3.23831200	0.55736300
				H	-0.32264400	-3.03430600	-1.14296200
				C	-3.73590700	-1.67512900	0.33786100
				H	-2.11635100	-1.31347700	1.73383900
				H	-2.56528100	0.10476400	0.77439100
				C	-3.55197100	-3.19387700	0.19785000
				H	-2.26358300	-4.61444200	-0.83282300
				H	-2.71363700	-3.21178300	-1.79691500
				H	-4.51328500	-1.45032000	1.08029000
				H	-4.09215500	-1.26357900	-0.61888500
				H	-4.48952600	-3.66284700	-0.12955500
				H	-3.31508700	-3.62237500	1.18413000
					SCF energy= -580.0065995		
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				N	0.55792100	0.42232700	-0.58644300

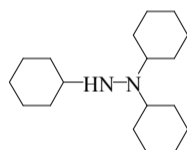
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H	-4.13641700	0.52468400	2.28594300
H	-2.79752500	0.17509200	3.40382700
C	-0.85531800	-0.05450500	-1.29004300
C	-1.45088500	-1.42170400	-1.79370200
C	-2.11960700	0.65156400	-1.85843400
H	-0.02201000	0.18532900	-1.95680400
C	-2.35498000	-0.59848200	-2.75098200
H	-2.03172900	-1.94036100	-1.02692500
H	-0.74899600	-2.13314000	-2.24314700
H	-2.91123300	0.75386000	-1.11184600
H	-1.97286800	1.62399200	-2.34321100
H	-3.38964900	-0.93316700	-2.87571700
H	-1.90546600	-0.48401200	-3.74377600



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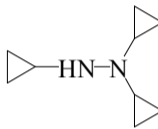
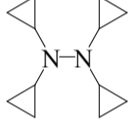
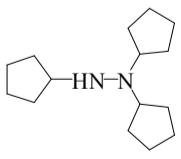
N	0.50444700	-0.09722100	-0.07977900
N	-0.81907100	-0.10137000	-0.60109300
C	-1.73760700	-1.11423300	-0.01110100
C	-3.13244000	-1.11062500	-0.68048700
C	-1.15581900	-2.53382100	-0.11873600
H	-1.90434100	-0.90842700	1.06535800
C	-4.06572000	-2.17983500	-0.08252700
H	-3.00447200	-1.28752300	-1.75888900
H	-3.62642900	-0.14071000	-0.57306500
C	-2.07285600	-3.59855900	0.50269500
H	-0.99944600	-2.76035700	-1.18333100
H	-0.17676100	-2.56977100	0.36019700
C	-3.46341800	-3.58772000	-0.14339700
H	-5.02950800	-2.15055900	-0.60813300
H	-4.27833000	-1.92409000	0.96696100
H	-1.60772300	-4.58807900	0.39950500
H	-2.17191900	-3.41353200	1.58355500
H	-4.12724000	-4.31030600	0.35000200
H	-3.37785900	-3.90379200	-1.19428800
C	-1.43716600	1.23403300	-0.84298800
C	-2.02851600	1.97211900	0.38457300
C	-0.51631700	2.17417700	-1.63680200
H	-2.27783800	1.02537700	-1.51538300
C	-2.77943400	3.24592000	-0.04305300
H	-1.22886400	2.25029400	1.08085400
H	-2.70831900	1.31191300	0.93815600
C	-1.25564400	3.45848700	-2.05501500
H	0.35976900	2.43923500	-1.03385200
H	-0.14579800	1.65437900	-2.52832900
C	-1.87250000	4.18574100	-0.85082700
H	-3.17656200	3.76315200	0.84085600
H	-3.65011300	2.96763100	-0.65718000
H	-0.56513900	4.12516200	-2.58887800
H	-2.05376500	3.20288900	-2.76896200
H	-2.43615700	5.06697400	-1.18557500
H	-1.06642400	4.55773600	-0.19990900
C	0.72884600	0.14864100	1.35739200
C	1.52124300	-0.95880200	2.09767100
C	1.34541600	1.52190000	1.74772900
H	-0.27792900	0.14031800	1.79237800
C	1.48231000	-0.75177800	3.62351900
H	2.56802100	-0.95356200	1.76347300
H	1.11589800	-1.94526600	1.84897500
C	1.27347200	1.74863400	3.26836100
H	2.39602400	1.56428800	1.43914100
H	0.83374600	2.33248700	1.21948900
C	2.00341200	0.63393100	4.03249800

H	0.78727000	-0.20727500	-1.35620900
C	-1.76328000	0.68309000	-0.32133400
C	-3.04003800	0.61850200	0.56065400
C	-1.78880900	2.22291900	-0.18464900
H	-1.99994100	0.39191200	-1.36107300
C	-3.28288200	2.11715900	0.23086200
H	-2.77151600	0.47937500	1.61445800
H	-3.81931300	-0.10234300	0.28927400
H	-1.15734800	2.54207500	0.65149400
H	-1.53535400	2.81334900	-1.06981900
H	-3.62738400	2.76058600	1.04681200
H	-3.95900100	2.24545100	-0.62176200
C	-0.77976300	-1.45885000	0.23911800
C	-0.83844700	-2.39467600	-1.01960200
C	0.30439400	-2.38938300	0.82998000
H	-1.70730200	-1.59642400	0.80586600
C	-0.19756800	-3.49927900	-0.13538100
H	-0.15109500	-2.07780200	-1.81419900
H	-1.81835800	-2.59103800	-1.46800300
H	1.30925200	-2.05973600	0.55451800
H	0.27666600	-2.57632800	1.90915700
H	0.55846200	-4.14060100	-0.59965500
H	-0.95688500	-4.13649400	0.33131200
C	1.72223500	0.84436700	0.16766700
C	2.96795400	-0.06409100	0.45172400
C	2.68026400	1.84040800	-0.53911300
H	1.34797800	1.26745300	1.10400300
C	3.86083400	1.18534000	0.22654700
H	3.11119200	-0.79945500	-0.35146400
H	3.02720500	-0.57843900	1.41731900
H	2.73460000	1.62712700	-1.61431900
H	2.48880600	2.91089300	-0.40533300
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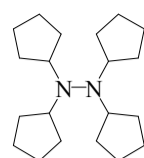


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N	-0.31048600	0.07926000	0.15695700
C	-1.18542700	1.27572900	0.10864800
C	-2.14992600	1.39448500	-1.09061400
C	-1.94232800	1.47312600	1.43458400
H	-0.47704100	2.11070400	0.02648800
C	-2.88730300	2.74531000	-1.07615200
H	-2.89597300	0.58691400	-1.05091500
H	-1.58460200	1.27604500	-2.02283200
C	-2.68814100	2.81953600	1.45254400
H	-2.67228800	0.66354200	1.58375500
H	-1.22993400	1.41374500	2.26704200
C	-3.63362300	2.96468700	0.24917200
H	-3.58688000	2.80201700	-1.92108600
H	-2.15884500	3.55775300	-1.22141900
H	-3.24757300	2.92488400	2.39169500
H	-1.95329300	3.63895100	1.43439300
H	-4.11253200	3.95307200	0.25932000
H	-4.44327200	2.22333400	0.33477800
C	-0.99030900	-1.23503300	0.12148400
C	-1.22918200	-1.87454500	-1.27251300
C	-0.30457400	-2.26180800	1.04548000
H	-1.98280400	-1.04605000	0.54960700
C	-2.07061600	-3.15841600	-1.15218400
H	-0.26916600	-2.14789700	-1.73666000
H	-1.71430900	-1.16364200	-1.94850900

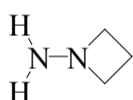
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H	0.44465500	-0.86542300	3.97374200	H	0.69583900	-2.49653700	0.65536600
H	1.70166300	2.72776000	3.52256200	H	-0.15995700	-1.80862300	2.03320800
H	0.21913800	1.77806900	3.58527700	C	-1.41323200	-4.17903100	-0.21135800
H	1.89612700	0.77632000	5.11625500	H	-2.22080800	-3.59844200	-2.14712200
H	3.08058200	0.69462500	3.81359000	H	-3.07140600	-2.90290500	-0.77145200
C	1.56189000	-0.37608400	-1.07451200	H	-0.59359400	-4.27908100	1.80252900
C	2.77723300	0.57749100	-1.00199200	H	-2.07643900	-3.33971600	1.66858700
C	2.08189300	-1.83745100	-1.14947600	H	-2.05277300	-5.06529000	-0.10403200
H	1.06515600	-0.18556500	-2.03179900	H	-0.46936900	-4.52636700	-0.65925500
C	3.72379600	0.38446200	-2.20022800	C	2.04067700	0.64658900	-0.20274600
H	3.34564500	0.38958500	-0.08074200	C	2.68105500	-0.36250600	0.76805500
H	2.43728000	1.61783100	-0.96160900	C	3.01484600	0.99523400	-1.34060500
C	3.03208200	-2.03906700	-2.34459100	H	1.83189700	1.56914700	0.35842300
H	2.60892700	-2.09926100	-0.22214800	C	4.02633900	0.14828100	1.31241300
H	1.23859700	-2.52527500	-1.24436100	H	2.84579000	-1.31304800	0.23441600
C	4.21684700	-1.06482700	-2.30601000	H	1.98702500	-0.56964900	1.58898400
H	4.57533500	1.07302000	-2.11309800	C	4.36796800	1.49553400	-0.80817500
H	3.19632700	0.65718600	-3.12710500	H	3.17920500	0.09715200	-1.95872200
H	3.39014400	-3.07745000	-2.36435000	H	2.55203100	1.74448800	-1.99433100
H	2.47140200	-1.88655100	-3.28003600	C	4.99919500	0.49811700	0.17564000
H	4.84885100	-1.19116300	-3.19545400	H	4.47214200	-0.60235600	1.97891700
H	4.84939900	-1.29679000	-1.43521000	H	3.85129400	1.04400200	1.92830900
				SCF energy= -462.0443551			
N	0.87264200	0.18342700	-0.79491700				
H	0.84759500	-0.16983000	-1.75741500	SCF energy= -578.75655			
N	-0.42027700	0.02126100	-0.18439900	N	-0.59672100	-0.30343000	0.25033900
C	-1.25478900	1.15104600	-0.53368200	N	0.79778800	0.06866700	0.11587200
C	-2.24379300	1.66843400	0.48281700	C	1.67088100	-1.08520100	0.14703300
C	-1.00093500	2.46281600	0.14839100	C	2.91942400	-1.01440900	0.99733200
H	-1.56529600	1.19747700	-1.58452300	C	1.75548800	-1.88375400	1.41518600
H	-2.26969900	1.17293200	1.44845300	H	1.76666700	-1.64106900	-0.79028500
H	-3.20852500	2.02178800	0.12690400	H	3.08242100	-0.10030400	1.56004200
H	-1.09831900	3.37203000	-0.43898900	H	3.82367400	-1.48799200	0.62237500
H	-0.20371100	2.48026300	0.88544800	H	1.84931900	-2.96376700	1.33445800
C	-1.03941200	-1.24159700	-0.52294600	H	1.14509500	-1.54591500	2.24727300
C	-0.73858600	-2.47118100	0.30122100	C	1.10485600	0.95023200	-0.98803900
C	-2.09905300	-1.81868600	0.37953200	C	0.85485000	2.43279700	-0.86475100
H	-1.18770500	-1.40576900	-1.59923000	C	2.26799800	1.90254000	-0.84657900
H	-0.08565400	-2.34558600	1.15931600	H	0.97203400	0.52205400	-1.98700200
H	-0.64051800	-3.42350500	-0.21419300	H	0.44590200	2.79102500	0.07354000
H	-2.94826200	-2.31220500	-0.08579500	H	0.50477900	2.96407600	-1.74680500
H	-2.33552400	-1.27106700	1.28586100	H	2.90225700	2.06072800	-1.71514900
C	1.95382600	-0.43671500	-0.07122000	H	2.79102200	1.91162100	0.10415800
C	3.31966000	0.17495000	-0.27626400	C	-1.24994700	0.57872700	1.20259700
C	2.59169300	0.35649800	1.03669000	C	-2.04302500	1.82834900	0.86387800
H	1.92310400	-1.52049900	0.05775300	C	-2.73713500	0.59919600	1.42438000
H	3.37772500	1.03458400	-0.93815400	H	-0.64353800	0.64714800	2.10121800
H	4.17907700	-0.48981300	-0.31162900	H	-2.22645300	2.05968400	-0.18196900
H	2.95064800	-0.18123800	1.91057600	H	-1.92159900	2.70475400	1.49722000
H	2.16683700	1.33423100	1.24359500	H	-3.09273100	0.61720600	2.45210500
				SCF energy= -698.0499611			
N	-0.65145700	-0.13004800	-0.70438000	H	-3.37712800	0.04611200	0.74550900
H	-0.96047800	0.81081800	-0.94434000	C	-1.29521800	-0.58142200	-0.97750600
N	0.41317600	-0.01787600	0.29267000	C	-1.03668900	-1.89828100	-1.67639900
C	1.39972500	-1.08533000	0.05275900	C	-2.34881400	-1.66645300	-0.97431400
C	2.48333200	-0.94912800	-1.04299100	H	-1.49494900	0.26713500	-1.63957400
C	2.20737600	-1.47123300	1.31555700	H	-0.34187600	-2.58543200	-1.20605900
				H	-1.01578700	-1.89801800	-2.76339200
				H	-3.24411600	-1.50875100	-1.57091400
				H	-2.50847900	-2.19088200	-0.03714700

H	0.79455400	-1.95677600	-0.22490100
C	3.37684800	-2.16767400	-0.76164100
H	3.06221600	-0.02796100	-0.89933700
H	2.06426400	-0.93216800	-2.05455600
C	3.44995200	-2.24617800	0.79001500
H	1.59585000	-2.05853600	2.00906900
H	2.51764300	-0.57119500	1.85968100
H	2.90250100	-3.07290800	-1.16423700
H	4.36659300	-2.09284000	-1.22662000
H	3.46530200	-3.28489700	1.13891300
H	4.37462300	-1.78180300	1.15298700
C	0.94389200	1.34978200	0.41495200
C	1.30357600	2.12952200	-0.90075500
C	-0.02348600	2.30438700	1.19386700
H	1.85880100	1.23720000	1.00361500
C	0.93251000	3.59595200	-0.61710100
H	0.71899000	1.74914000	-1.74722200
H	2.35624100	2.01175900	-1.17480100
C	-0.32856800	3.48934900	0.25699100
H	0.47859300	2.66642100	2.10000000
H	-0.91823000	1.77167200	1.52295700
H	1.73575500	4.08586200	-0.04812400
H	0.77888700	4.18267600	-1.53089100
H	-0.55874000	4.41454600	0.79803100
H	-1.19948300	3.26597600	-0.37712900
C	-1.80282700	-0.88555700	-0.19941300
C	-2.64859600	-0.31034900	0.95666800
C	-2.84206900	-1.10406600	-1.32052900
H	-1.41649300	-1.86282400	0.12049400
C	-3.91850500	-1.17752100	0.91545400
H	-2.90095700	0.73874400	0.73698000
H	-2.13196800	-0.33665700	1.92121800
C	-4.17843700	-1.43284700	-0.59824100
H	-2.52468900	-1.88172600	-2.02278400
H	-2.93710100	-0.17639400	-1.90276700
H	-3.73013800	-2.12817500	1.43190700
H	-4.77247400	-0.70865600	1.41746100
H	-4.49286500	-2.46724900	-0.77758800
H	-4.98756600	-0.79323400	-0.96960200



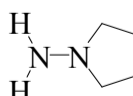
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N	-0.43668700	-0.10477200	0.03200900
N	0.97499600	-0.05858500	0.19036300
C	1.71999200	-1.12237300	-0.54245200
C	2.97974300	-1.63439400	0.24134600
C	0.91066500	-2.40463300	-0.82576400
H	2.05769900	-0.72150700	-1.51684400
C	2.94284000	-3.18289100	0.18173800
H	2.94991400	-1.27003100	1.27207100
H	3.90212900	-1.25493500	-0.21070500
C	1.97831900	-3.49749000	-0.97299600
H	0.26543300	-2.31518200	-1.70436100
H	0.26901200	-2.63083000	0.03166700
H	3.93740800	-3.62402400	0.04795700
H	2.53483300	-3.58936900	1.11654700
H	2.49383700	-3.40133500	-1.93960800
H	1.55958500	-4.50986300	-0.92570600
C	1.52743800	1.29392300	-0.03380900
C	0.95597400	2.35988300	0.92147700
C	3.04492500	1.45380800	0.19628600
H	1.32853900	1.60980700	-1.07801600
C	1.92292000	3.56373500	0.80648400
H	0.97209200	1.94814500	1.93884900
H	-0.07634300	2.63107500	0.69354200
C	3.24800600	2.98262700	0.23060900
H	3.65996400	0.97451400	-0.57109100
H	3.31190600	1.01165400	1.16407800
H	1.51553900	4.33319900	0.14010100
H	2.07442000	4.04361900	1.77989600
H	3.42150900	3.36202000	-0.78423400
H	4.12533600	3.26259100	0.82445400
C	-1.02215700	0.20892300	-1.27087100
C	-2.22073000	-0.66859900	-1.71677200
C	-1.51539000	1.67663800	-1.55909600
H	-0.22055300	0.00572000	-1.99284800
C	-2.74245800	0.05870700	-2.96153900
H	-3.00003300	-0.68239400	-0.94597200
H	-1.92822100	-1.70662300	-1.90625500
C	-2.69677500	1.55128700	-2.56058900
H	-0.69862800	2.28103900	-1.96960300
H	-1.83523600	2.16781800	-0.63739800
H	-2.06938300	-0.12918100	-3.81011600
H	-3.74383900	-0.26777900	-3.26518100
H	-2.58688800	2.21117100	-3.42864500
H	-3.63967900	1.82925000	-2.07221500
C	-1.18794600	-0.25121900	1.27803700
C	-2.36552400	0.71646700	1.55996100
C	-1.80038100	-1.66541700	1.56467500
H	-0.44433200	-0.06394100	2.05850200
C	-3.03292300	0.08944900	2.79217300
H	-3.07692400	0.73295200	0.72553700
H	-2.03057600	1.74506500	1.73241100
C	-3.02120500	-1.43109300	2.49669800
H	-1.05024500	-2.31902000	2.02456400
H	-2.10319200	-2.14434300	0.62917100
H	-2.43168000	0.30712000	3.68592700
H	-4.04101200	0.47688300	2.97999600
H	-2.97251100	-2.02596700	3.41582700
H	-3.95004100	-1.71784800	1.98750500



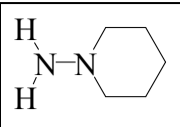
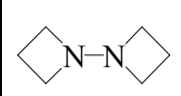
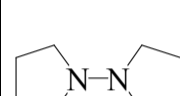
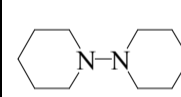
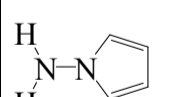
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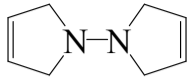
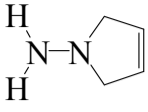
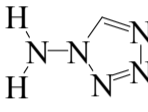
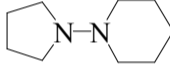
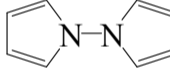
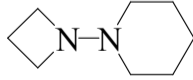
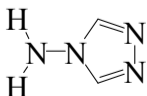
C	0.06614800	-0.43389300	1.04573100
C	0.06614800	-1.57368900	0.00000000
C	0.06614800	-0.43389300	-1.04573100
H	-0.57006800	-0.52396400	1.93359300
H	1.08904000	-0.15377900	1.34312300
H	-0.86081800	-2.15319400	0.00000000
H	0.92405500	-2.24990900	0.00000000
H	-0.57006800	-0.52396400	-1.93359300
H	1.08904000	-0.15377900	-1.34312300
N	-0.46127800	0.47798300	0.00000000
N	0.19278500	1.78663900	0.00000000
H	-0.20619500	2.27754200	-0.80481400
H	-0.20619500	2.27754200	0.80481400

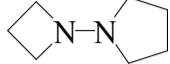
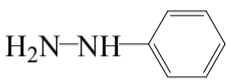
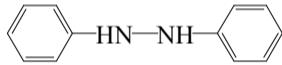
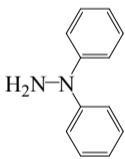
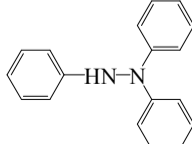


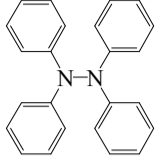
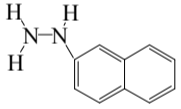
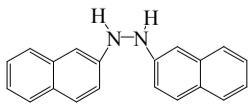
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C	-0.05183100	-1.14996600	0.54022600
C	-0.05155800	1.14970200	0.54062900
C	-1.23090800	0.77667200	-0.39670200
C	-1.23128200	-0.77625400	-0.39668100
H	0.48239600	-2.05773500	0.24110700
H	-0.40085200	-1.29740100	1.56944700

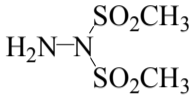


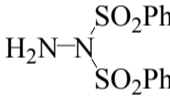


H	-0.40081300	1.29663300	1.56983500					
H	0.48279400	2.05759300	0.24206700		SCF energy= -307.2785449			
H	-2.17470900	1.19739200	-0.03232300		C	-0.30534300	-0.62231000	1.20966100
H	-1.06324200	1.16322400	-1.40579900		C	-0.30534300	-0.62231000	-1.20966100
H	-2.17516000	-1.19645000	-0.03187400		C	-0.30534300	0.91583000	-1.26228900
H	-1.06435900	-1.16292700	-1.40586000		C	-0.96250300	1.49729700	0.00000000
N	0.87600700	-0.00020100	0.57055000		C	-0.30534300	0.91583000	1.26228900
N	1.59067700	-0.00004200	-0.73186300		H	0.20945500	-1.04583200	-2.08238400
H	2.21999300	0.80378100	-0.67128600		H	-1.33784900	-0.99689700	1.24117900
H	2.22063300	-0.80333000	-0.67095100		H	0.20945500	-1.04583200	2.08238400
					SCF energy= -345.3168731			
C	-1.58142900	-1.04757700	-0.07376800		H	0.72689300	1.27792900	-1.34066900
C	-2.71386300	0.00043800	0.02938400		H	-0.83673500	1.24619400	-2.16538400
C	-1.58052200	1.04761200	-0.07246100		H	-0.89635300	2.59306300	0.00000000
H	-1.61675800	-1.93469800	0.56758100		H	-2.03579100	1.24786800	0.00000000
H	-1.39655700	-1.34550100	-1.11739800		H	0.72689300	1.27792900	1.34066900
H	-3.20660900	0.00003300	1.00535400		H	-0.83673500	1.24619400	2.16538400
H	-3.46610800	0.00130000	-0.76283000		H	-1.33784900	-0.99689700	-1.24117900
H	-1.61507400	1.93405700	0.56985800		N	0.29968200	-1.20819800	0.00000000
H	-1.39554400	1.34655400	-1.11580000	N	1.74033000	-0.87038800	0.00000000	
N	-0.62079300	-0.00065700	0.37006000	H	2.11589500	-1.37981400	0.80421600	
C	1.58050700	1.04760200	0.07246000	H	2.11589500	-1.37981400	-0.80421600	
C	1.58144300	-1.04758400	0.07376900					
C	2.71386300	0.00045000	-0.02947600	SCF energy= -424.0148683				
H	1.39566600	1.34654700	1.11581700	C	-1.58077400	1.06522500	-0.64884500	
H	1.61499600	1.93406300	-0.56981800	C	-1.58979800	-1.20047000	-0.40732600	
H	1.39670500	-1.34542300	1.11742000	C	-2.34406300	-0.69157500	0.85025200	
H	1.61665200	-1.93474600	-0.56752300	C	-2.30010700	0.85336500	0.70596100	
H	3.46606700	0.00129800	0.76279400	H	-1.02977800	2.00303600	-0.72691400	
H	3.20669700	0.00006000	-1.00539700	H	-2.30618500	1.04974400	-1.47136800	
N	0.62077500	-0.00065400	-0.36999000	H	-2.29179000	-1.39007400	-1.22831900	
				SCF energy= -502.6786501				
C	-1.08333500	-1.44253200	-0.68193100	H	-1.02845400	-2.12089500	-0.24230900	
C	-0.73271600	-2.90659500	-0.97700600	H	-3.36768800	-1.08172700	0.88215400	
C	-0.03305400	-3.56283100	0.22241400	H	-1.83845200	-1.01308500	1.76557300	
C	1.16149600	-2.71224300	0.67853800	H	-3.29652500	1.30947100	0.70630600	
C	0.73271600	-1.26078200	0.92991300	H	-1.72895500	1.30445000	1.52362900	
H	-0.74811700	-3.65762900	1.05402100	N	-0.70206800	-0.10611400	-0.87206700	
H	-1.48912700	-0.94878900	-1.56961100	C	1.39087900	-1.14901300	-0.28836400	
H	-1.64815000	-3.45399500	-1.23797100	C	1.28226400	1.15425800	-0.22852400	
H	1.60370500	-3.12501700	1.59515900	C	2.71248000	-0.73108300	0.37501800	
H	0.03787200	-1.23589500	1.79282700	H	1.49982800	-1.23569600	-1.38472100	
H	1.94105300	-2.72243300	-0.09510100	H	1.01865900	-2.10361700	0.09321300	
H	1.60307800	-0.64900100	1.19123600	C	2.64536200	0.82068800	0.40283400	
H	0.29241900	-4.58041300	-0.03000100	H	0.83305000	2.04645600	0.21638100	
H	-0.07103600	-2.93963200	-1.85322500	H	1.37682900	1.31896300	-1.31839200	
H	-1.86548700	-1.40895800	0.10486000	H	2.78336300	-1.13473200	1.39033600	
N	0.11695600	-0.70588900	-0.28339500	H	3.57297500	-1.10779500	-0.18771400	
C	1.08333500	1.44253200	-0.68193100	H	2.69716500	1.19314000	1.43103300	
C	-0.73271600	1.26078200	0.92991300	H	3.46212900	1.28952100	-0.15593200	
C	0.73271600	2.90659500	-0.97700600	N	0.46583600	-0.04467600	0.03507000	
H	1.86548700	1.40895800	0.10486000					
C	-1.16149600	2.71224300	0.67853800	SCF energy= -265.5468348				
H	-1.60307800	0.64900100	1.19123600	C	0.17671800	-1.13161700	-0.00019700	
H	0.07103600	2.93963200	-1.85322500	C	0.12898700	1.12299900	-0.00008900	
H	-1.60370500	3.12501700	1.59515900	C	1.45474300	0.73638100	0.00014800	
N	-0.11695600	0.70588900	-0.28339500	C	1.48516400	-0.69019000	0.00016900	
C	0.03305400	3.56283100	0.22241400	H	-0.33595900	2.09940700	-0.00012000	
H	-0.29241900	4.58041300	-0.03000100	H	2.30707200	1.40345800	0.00026600	
H	0.74811700	3.65762900	1.05402100	H	2.36528600	-1.31947600	0.00049500	
H	-1.94105300	2.72243300	-0.09510100	H	-0.25925600	-2.11964400	-0.00102000	
H	-0.03787200	1.23589500	1.79282700	N	-0.63799200	-0.02451600	-0.00039400	
				N	-2.03909300	-0.11689400	0.00003400	
				H	-2.40521100	0.34834400	0.82921100	

H	1.64815000	3.45399500	-1.23797100	H	-2.40600000	0.35234800	-0.82649300
H	1.48912700	0.94878900	-1.56961100				
							
		SCF energy=	-421.5571778			SCF energy=	-266.721356
C	0.04659400	1.44707200	-1.18245600	C	-0.00744600	0.09902100	1.18679200
C	-0.04659400	2.86021100	-0.66738100	C	-0.00744600	1.51468900	0.66775200
C	-0.04659400	2.86021100	0.66738100	C	-0.00744600	1.51468900	-0.66775200
C	0.04659400	1.44707200	1.18245600	C	-0.00744600	0.09902100	-1.18679200
H	-0.61985700	1.24083700	-2.02857200	H	0.69731700	-0.06799200	2.01285400
H	1.08179500	1.21478000	-1.50000700	H	-1.01578300	-0.19546500	1.53688800
H	-0.07825400	3.72973000	-1.31651700	H	-0.03025200	2.38672500	1.31391600
H	-0.07825400	3.72973000	1.31651700	H	-0.03025200	2.38672500	-1.31391600
H	-0.61985700	1.24083700	2.02857200	H	0.69731700	-0.06799200	-2.01285400
H	1.08179500	1.21478000	1.50000700	H	-1.01578300	-0.19546500	-1.53688800
N	-0.34464500	0.64225600	0.00000000	N	0.39350800	-0.68503600	0.00000000
C	-0.04659400	-1.44707200	-1.18245600	N	-0.29467400	-1.97920800	0.00000000
C	-0.04659400	-1.44707200	1.18245600	H	0.09215100	-2.48067700	-0.80362200
C	0.04659400	-2.86021100	-0.66738100	H	0.09215100	-2.48067700	0.80362200
H	0.61985700	-1.24083700	-2.02857200				
H	-1.08179500	-1.21478000	-1.50000700				
C	0.04659400	-2.86021100	0.66738100			SCF energy=	-313.6441448
H	0.61985700	-1.24083700	2.02857200	C	-0.27419300	1.07970000	0.00002400
H	-1.08179500	-1.21478000	1.50000700	H	0.03163800	2.11470300	-0.00009900
H	0.07825400	-3.72973000	-1.31651700	N	-1.50115900	0.60388300	0.00007900
H	0.07825400	-3.72973000	1.31651700	N	-1.37108100	-0.75715200	0.00008500
N	0.34464500	-0.64225600	0.00000000	N	-0.12761800	-1.10908900	-0.00003300
				N	0.58759400	0.04321400	-0.00038500
		SCF energy=	-463.3486232	N	1.98015000	0.10270400	0.00015500
C	1.80076500	0.57310500	-1.07705400	H	2.31891200	-0.38880500	0.82641900
C	3.25140200	0.24678300	-0.66230200	H	2.31940600	-0.38901100	-0.82577100
C	3.12659100	-0.40653700	0.74855000				
C	1.64299300	-0.24427400	1.11462000				
N	0.99678200	-0.28938400	-0.20732800			SCF energy=	-419.1955926
H	1.57665000	0.35072600	-2.12440400	C	-0.80196300	1.47909600	0.80195700
H	3.71468100	-0.44828500	-1.36971600	C	0.80205900	1.47906600	-0.80188100
H	3.78235200	0.06236600	1.48979400	C	0.50541800	2.79099400	-0.50540700
H	1.48262300	0.72031200	1.63180500	C	-0.50541800	2.79100900	0.50532300
H	1.26416200	-1.04308100	1.76079100	H	1.49540600	1.02588300	-1.49519200
H	3.38708300	-1.46889700	0.70090800	H	0.96240200	3.65866100	-0.96240400
H	3.86955500	1.15042500	-0.64191400	H	-0.96246600	3.65869100	0.96222800
H	1.58435800	1.64513400	-0.90749700	H	-1.49527700	1.02596900	1.49533800
C	-1.15645000	-1.29838000	-0.10105700	N	0.00000500	0.68834200	0.00001200
C	-0.93382400	1.05307600	0.48638300	C	0.80196300	-1.47909600	0.80195700
C	-2.62201400	-1.10355600	-0.50842900	C	-0.80205900	-1.47906600	-0.80188100
H	-1.11260300	-1.62525800	0.95879900	C	0.50541800	-2.79100900	0.50532300
H	-0.67987300	-2.07606100	-0.70464900	H	1.49527700	-1.02596900	1.49533800
C	-2.38603000	1.33799600	0.08247400	C	-0.50541800	-2.79099400	-0.50540700
H	-0.89711000	0.83261800	1.57204600	H	-1.49540600	-1.02588300	-1.49519200
H	-0.31194600	1.93769800	0.31051500	H	0.96246600	-3.65869100	0.96222800
C	-3.25308000	0.08033600	0.23902700	H	-0.96240200	-3.65866100	-0.96240400
H	-3.18044500	-2.02809900	-0.31053400	N	-0.00000500	-0.68834200	0.00001200
H	-2.66479800	-0.92132300	-1.59087400				
H	-2.78004700	2.15916200	0.69602500				
H	-2.40280200	1.67277400	-0.96347400			SCF energy=	-423.9953032
H	-4.27199700	0.26719800	-0.12423800	C	-1.14996900	-1.41159500	1.26200300
H	-3.33989100	-0.16860300	1.30780900	C	-1.14996900	0.12626000	1.20786900
N	-0.40279300	-0.06063100	-0.31045500	C	-1.14996900	0.12626000	-1.20786900
				C	-1.14996900	-1.41159500	-1.26200300
		SCF energy=	-297.6243821	C	-1.80254200	-1.99785200	0.00000000
C	-0.20796500	1.08367300	0.00009400	H	-2.18273300	0.50042300	1.22605500
C	-0.24518600	-1.08620300	0.00000900	H	-0.64831800	0.54828500	2.08604700
H	0.16066300	2.10076700	0.00014400	H	-0.11683900	-1.77171100	1.34458500
				H	-1.68300100	-1.74109500	2.16449600

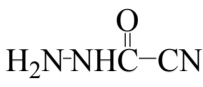
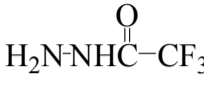
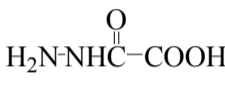
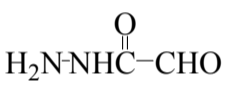
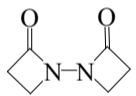
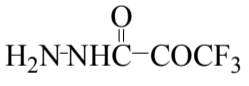
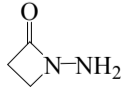
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N	0.61169100	-0.01880200	-0.00008000	H	-0.64831800	0.54828500	-2.08604700
N	2.01138800	-0.11546500	-0.00001500	H	-1.68300100	-1.74109500	-2.16449600
H	2.38181600	0.34216200	-0.83060400	H	-0.11683900	-1.77171100	-1.34458500
H	2.38177500	0.34202300	0.83067400	H	-2.87685500	-1.75363800	0.00000000
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N	-1.46399100	0.71387100	-0.00006600	N	-0.53260200	0.70964800	0.00000000
		SCF energy=	-384.6692346	C	1.67193700	1.10939100	-1.04583400
C	-1.89543600	1.04651600	0.10544800	C	1.67193700	1.10939100	1.04583400
C	-3.03272700	0.00022200	0.07845600	C	2.78235600	1.35474300	0.00000000
C	-1.89584300	-1.04654000	0.10689900	H	1.17913000	2.05002300	-1.33920000
H	-1.97402500	1.93588100	-0.52881800	H	1.90439100	0.51569000	-1.93697300
H	-1.64113800	1.34032000	1.13587400	H	1.17913000	2.05002300	1.33920000
H	-3.58708900	-0.00038200	-0.86381200	H	1.90439100	0.51569000	1.93697300
H	-3.73176400	0.00098900	0.91797800	H	3.25736500	2.33846400	0.00000000
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C	1.12206400	-1.15468600	-0.23382200	H	-2.56262700	-0.85987600	0.99503000
C	1.12149000	1.15475200	-0.23291600	H	-3.00481700	-0.95012200	-0.59825500
C	2.56041700	-0.77889000	0.16474200	N	-1.81810400	0.59623900	-0.18806500
H	0.76771100	-2.07788900	0.23632300	H	-2.05144300	1.53170700	0.12039300
C	2.56011300	0.77917400	0.16510400	C	-0.46098900	0.26495300	-0.07724800
H	1.02723600	1.26713900	-1.32900500	C	-0.01415300	-1.06730000	-0.08358300
H	2.80122300	-1.16575100	1.16009600	C	0.49394300	1.29917700	-0.00449200
H	2.80097100	1.16564900	1.16058400	C	1.35397100	-1.35027700	-0.01906000
H	1.02789500	-1.26615100	-1.32998500	H	-0.72733300	-1.88333000	-0.15187000
H	3.28851000	-1.19987400	-0.53628200	C	1.85284300	1.00397600	0.05628100
H	3.28793200	1.20076500	-0.53585100	H	0.16057900	2.33543500	-0.00021100
H	0.76698000	2.07744900	0.23808600	C	2.29747200	-0.32448600	0.05091200
		SCF energy=	-574.0987319	H	1.67845600	-2.38818500	-0.02632500
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H	0.42888900	-1.12229200	1.53248800	H	3.35857400	-0.55125600	0.10175300
N	-0.47452800	0.51023300	0.71989500			SCF energy=	-574.0928649
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C	-1.78177100	0.19617300	0.30264600	H	-0.23369400	2.76386600	0.90307600
C	-2.04549500	-0.88796600	-0.54879600	H	-0.62645700	2.70814500	-0.70471400
C	-2.84236200	1.02464300	0.70918800	N	-0.00247600	0.96616600	0.04242900
C	-3.35036700	-1.12685400	-0.98538300	C	-1.24372300	0.29933100	-0.00422200
H	-1.22782700	-1.52771400	-0.86280400	C	-2.40068400	0.90414800	0.52431700
C	-4.13968700	0.77673600	0.26214500	C	-1.37504000	-0.95677800	-0.63279200
H	-2.64681100	1.86634300	1.37159700	C	-3.64006300	0.26542500	0.44039900
C	-4.40611700	-0.30150500	-0.58821200	H	-2.33634500	1.87298200	1.01003300
H	-3.53906000	-1.97002200	-1.64567600	C	-2.61533900	-1.58712500	-0.70250700
H	-4.94711100	1.42874200	0.58654000	H	-0.50396900	-1.42954600	-1.07364700
H	-5.41838300	-0.49549000	-0.93154100	C	-3.75995900	-0.98586600	-0.16654700
C	1.78172400	-0.19603600	0.30267600	H	-4.51550700	0.75384700	0.86165400
C	2.04558300	0.88791700	-0.54898800	H	-2.68865900	-2.55299200	-1.19667000
C	2.84226600	-1.02451400	0.70939800	H	-4.72513000	-1.48050700	-0.22874200
C	3.35048800	1.12659200	-0.98557100	C	1.25762700	0.32170900	0.04923300
H	1.22797000	1.52769200	-0.86306200	C	1.43607100	-0.89664400	0.72970100
C	4.13961500	-0.77682200	0.26231800	C	2.36400200	0.91175300	-0.58617600
H	2.64664000	-1.86608500	1.37195000	C	2.68381300	-1.52093300	0.74337100
C	4.40617400	0.30124000	-0.58821600	H	0.60027600	-1.34849700	1.25467000
H	3.53927900	1.96961500	-1.64602400	C	3.60927900	0.28322500	-0.55596700
H	4.94694600	-1.42886400	0.58687800	H	2.23866700	1.86681700	-1.08295000
H	5.41845600	0.49510700	-0.93156200	C	3.78048100	-0.93930600	0.10046500
		SCF energy=	-805.1974238	H	2.79928900	-2.46142000	1.27690100
				H	4.45200300	0.75499900	-1.05587300

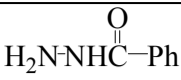
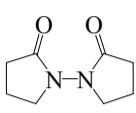
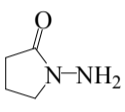
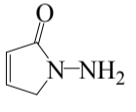
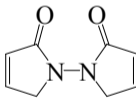
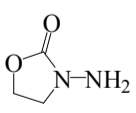
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N	0.51765800	-0.35667200	-0.22258900					
C	0.09930900	1.02431900	-0.10689400					
C	-0.66898900	1.58436400	-1.12986600					
C	0.44508400	1.79572800	1.01053800					
C	-1.08622000	2.91659900	-1.04242900					
H	-0.93138800	0.97030600	-1.98611300					
C	0.02847800	3.12468900	1.09590600					
H	1.04129900	1.34991800	1.80190200					
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H	-1.68136300	3.34877400	-1.84282000					
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H	-1.05991000	4.72426800	0.13568000					
C	1.92055900	-0.57303500	-0.11256300					
C	2.76395000	0.10287800	-1.01804000					
C	2.49601500	-1.46563700	0.80717000					
C	4.13771000	-0.11374700	-1.00157100					
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C	3.87969400	-1.68472200	0.80435100					
H	1.88199500	-1.96055700	1.55097600					
C	4.70923500	-1.01605900	-0.09364500					
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H	4.30432900	-2.37865200	1.52609800					
H	5.78188100	-1.18939600	-0.09002300					
C	-1.65908000	-1.24976000	0.32966800					
C	-2.56933100	-0.56880400	1.14267200					
C	-2.12218600	-1.96492900	-0.78277200					
C	-3.93486800	-0.60229400	0.84711200					
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C	-3.48853700	-2.00941800	-1.07016600					
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C	-4.39728900	-1.32414400	-0.25695900					
H	-4.63749200	-0.07145700	1.48441500					
H	-3.84274500	-2.57564300	-1.92812500					
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	C	-1.66943700	-0.21876600	-0.11066500	C	-0.94396700	1.41979300	-0.70305100
	C	1.85812200	-1.50355500	0.01835600	C	-1.57409400	0.84669200	-1.82061400
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	C	2.32150400	1.26422100	0.02857100	H	-0.90716200	3.13504700	0.61306800
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H	-2.27667100	1.85798300	-0.13250900	H	-3.05020500	1.08002500	-3.36028700	
C	3.38414900	0.38534100	0.06788600	H	-2.65420500	4.36667100	-0.61123700	
H	3.98746800	-1.70073100	0.09409100	H	-3.74424500	3.35801100	-2.61653700	
H	2.49570200	2.33850700	0.03239600	C	1.13225800	1.28006900	0.71013800	
H	0.03413400	2.73825200	-0.05042400	C	1.71814000	2.47761600	0.26243600	
H	4.40395700	0.75968600	0.10267500	C	1.67921900	0.63552500	1.83252900	
H	-0.77103700	-2.17116400	-0.05899700	C	2.79912800	3.03128700	0.94804300	
H	-2.97873700	-0.71555300	-0.23764600	H	1.33039400	2.97011400	-0.62333400	
H	-3.05191600	-1.70368200	-0.00801600	C	2.76997500	1.19173700	2.50175100	
N	-4.02332500	0.09113500	0.27169900	H	1.25596500	-0.30402700	2.17176800	
H	-4.85138900	-0.04655700	-0.30006400	C	3.33342300	2.39646100	2.07325300	
H	-4.24093000	-0.13801400	1.24333900	H	3.23627200	3.95861700	0.58580100	
	SCF energy= -881.4558315			H	3.17726600	0.67650000	3.36813900	
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	C	3.24442300	-1.94524400	-0.76408500	C	-1.13224500	-1.27982100	0.71033200
	C	2.92730100	-0.63707400	-0.30246700	C	-1.67932500	-0.63479700	1.83242800
	C	3.99003900	0.20283400	0.16618500	C	-1.71813800	-2.47747400	0.26303000
	C	5.31987800	-0.29561900	0.16197300	C	-2.77015800	-1.19069200	2.50173600
	C	5.59547300	-1.56955800	-0.29030400	H	-1.25611600	0.30489100	2.17133600
	H	0.80144800	-0.77742300	-0.68613900	C	-2.79927400	-3.03081100	0.94872800
	H	4.77263300	-3.40241800	-1.11369900	H	-1.33038600	-2.97039600	-0.62249900
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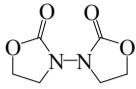
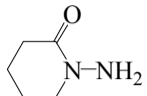
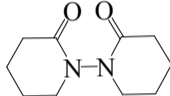
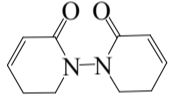
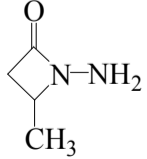
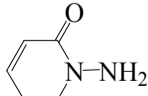
C	0.81654300	0.93992000	0.95924800	H	-2.66168500	2.92117000	-2.38407300
H	3.48010100	2.31854000	4.82808700	H	-3.31074700	5.30341200	-2.47962100
H	0.61623600	-0.66293500	2.41362600	H	-2.71198200	6.84928500	-0.61567200
H	2.04750600	0.40056300	4.10077200	N	0.85399700	-0.44503700	1.63028600
C	3.30378500	2.80927300	3.87307100	H	0.58754800	-1.08744600	2.37073100
C	2.84552800	4.06511500	1.40324700	C	2.15585400	-0.60930800	1.12139900
H	1.25599300	2.64831700	-0.26508700	C	2.52983100	-0.16984700	-0.13492200
C	3.64797500	4.66364600	2.35134100	C	3.87183300	-0.30885700	-0.58156200
C	3.87971400	4.03257600	3.60019100	C	4.84698000	-0.91115500	0.27972300
H	2.66928200	4.55133800	0.44607800	C	4.42757900	-1.34845800	1.56738000
H	4.10721100	5.62680900	2.14319300	C	3.12569100	-1.20174200	1.98186300
H	4.51307100	4.51590800	4.33942700	H	3.55021700	0.58969700	-2.52788300
N	-0.00049800	-1.10718300	0.00116400	H	1.79467500	0.28795800	-0.78936300
C	-1.19204400	-1.76610600	0.39616900	C	4.28517800	0.13019200	-1.87057300
C	-2.06600400	-1.18134400	1.29773500	C	6.18488800	-1.05145700	-0.17556000
C	-3.28040800	-1.81895700	1.66275000	H	5.15711600	-1.80742500	2.23122100
C	-3.60781400	-3.09238600	1.09279400	H	2.82625000	-1.53535500	2.97367900
C	-2.70257900	-3.65772700	0.15284400	C	6.55428400	-0.61661100	-1.43164800
C	-1.53834100	-3.01657400	-0.19771100	C	5.59222100	-0.02019700	-2.28499200
H	-3.94175500	-0.26924900	3.02791100	H	6.91767000	-1.51002000	0.48556300
H	-1.83409600	-0.21207600	1.72791100	H	7.58101000	-0.72909800	-1.76988700
C	-4.18552200	-1.23678300	2.59450800	H	5.88966300	0.32147100	-3.27334800
C	-4.81759100	-3.73213800	1.47209900	$\text{H}_2\text{N}-\text{NH}-\text{CHO}$ SCF energy= -225.2590187			
H	-2.95195000	-4.60967300	-0.31111500	N	-0.42220900	-0.42968900	0.00126400
H	-0.87899400	-3.45605800	-0.93897700	H	-0.31312400	-1.43734000	-0.00204500
C	-5.67330300	-3.14386900	2.38028000	N	-1.74400000	0.04034800	-0.00081600
C	-5.35121800	-1.88415100	2.94598900	H	-1.93577000	0.59087700	0.83259900
H	-5.06009600	-4.69766200	1.03279200	H	-1.93335600	0.59349700	-0.83326700
H	-6.59673000	-3.64213400	2.66356300	C	0.69666000	0.35335500	0.00044500
H	-6.03161300	-1.42649200	3.65975500	O	1.83934000	-0.07205600	-0.00059500
C	5.34818700	-1.89051600	-2.94574800	H	0.45103600	1.43467100	0.00166400
C	4.18352900	-1.24162400	-2.59362300	$\begin{array}{c} \text{CHO} \\ \diagdown \\ \text{H}_2\text{N}-\text{N} \\ \diagup \\ \text{CHO} \end{array}$ SCF energy= -338.6233812			
C	3.27788900	-1.82286100	-1.66179400	N	0.01149600	0.30461300	0.00016000
C	3.60368600	-3.09694600	-1.09240300	N	-0.61780800	1.56790000	-0.00012200
C	4.81240600	-3.73828400	-1.47237400	H	-1.22680900	1.61516500	-0.81711400
C	5.66865400	-3.15090800	-2.38063400	H	-1.22619400	1.61561300	0.81729200
H	1.83376600	-0.21395700	-1.72599900	C	1.41283500	0.30024600	0.00001100
H	6.02899600	-1.43354300	-3.65956000	O	2.09011900	-0.70475500	-0.00009600
H	3.94099000	-0.27358100	-3.02657900	H	1.80928300	1.32798900	0.00009600
C	2.06447600	-1.18367100	-1.29618400	C	-0.74708700	-0.86796500	0.00006700
C	2.69798600	-3.66132100	-0.15229400	O	-1.96222400	-0.85578100	-0.00005400
H	5.05367300	-4.70432600	-1.03352100	H	-0.12973700	-1.77575700	0.00020500
H	6.59125700	-3.65040400	-2.66443100	$\text{OHC}-\text{HN}-\text{NH}-\text{CHO}$ SCF energy= -338.6228798			
C	1.53478900	-3.01865000	0.19888100	N	-0.63758600	-0.47103900	-0.26272800
C	1.18997800	-1.76753100	-0.39455300	H	-0.86851100	-1.15066000	-0.98253300
H	2.94619000	-4.61375800	0.31127800	N	0.63757300	-0.47093500	0.26284500
H	0.87509800	-3.45738100	0.94028700	H	0.86838600	-1.14965000	0.98354200
$\begin{array}{c} \text{CHO} \\ \diagdown \\ \text{OHC}-\text{HN}-\text{N} \\ \diagup \\ \text{CHO} \end{array}$ SCF energy= -451.9782923				C	-1.65534300	0.27868000	0.28673400
N	0.52964200	0.05510300	0.15480500	O	-2.80496400	0.23083600	-0.10062600
N	-0.74912400	0.43447100	0.54529300	H	-1.29828900	0.92911700	1.10556200
H	-1.02382500	0.14848000	1.48246000	C	1.65537400	0.27845300	-0.28695100
C	1.51629600	1.05741900	0.08026500	O	2.80494100	0.23090800	0.10065800
O	2.66513200	0.84994300	-0.23230400	H	1.29849400	0.92826600	-1.10633800
H	1.10122400	2.04531100	0.33997900	$\begin{array}{c} \text{OHC} \quad \text{CHO} \\ \diagdown \quad \diagup \\ \text{N}-\text{N} \\ \diagup \quad \diagdown \\ \text{OHC} \quad \text{CHO} \end{array}$ SCF energy= -565.3208512			
C	0.81258100	-1.30734400	-0.07931500	N	-0.85427100	-0.03464600	-0.00022000
O	-0.02609400	-2.17215000	0.02021400	N	0.52682700	-0.22278500	-0.00038500
H	1.86328600	-1.47015200	-0.35214600	C	-1.68482400	-1.17596800	-0.00188100
C	-1.76766500	0.48541000	-0.40106000	$\text{H}_2\text{N}-\text{NH}-\text{SO}_2\text{CH}_3$ SCF energy= -699.8740914			
O	-2.93765000	0.56489900	-0.10461500				
H	-1.38269500	0.49489700	-1.43667100				

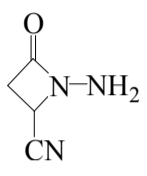
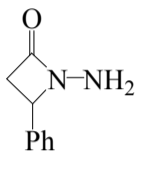
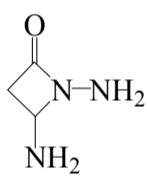
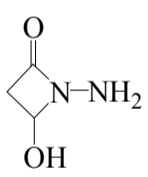
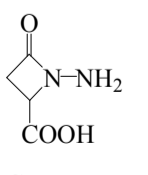
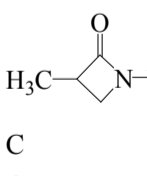
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O	-1.36564000	-0.88466300	-0.84703200	H	-1.09299600	-2.10699900	-0.00337100
O	-0.58218300	-0.29641800	1.52082000	C	-1.36864300	1.28450600	0.00178700
C	-0.61048200	1.62155100	-0.29241700	O	-0.65628500	2.25864200	0.00325600
H	0.18432100	2.13928600	0.24774900	H	-2.46608100	1.29518500	0.00165800
H	-0.53341000	1.77064400	-1.37170200	C	1.17190500	-0.17834000	-1.26786200
H	-1.58925600	1.94748900	0.06770000	O	2.35228600	-0.30152300	-1.44419600
N	1.07860000	-0.62024400	-0.40857200	H	0.42799200	-0.02810700	-2.07129000
H	1.09696400	-0.86194700	-1.39840600	C	1.17150500	-0.18276600	1.26737000
N	2.13617600	0.16255600	0.09180900	O	2.35178900	-0.30704400	1.44371400
H	2.81467500	-0.44302800	0.54470700	H	0.42731700	-0.03492400	2.07104300
H	2.58519800	0.71182400	-0.63724300				
 SCF energy= -1287.847166				 SCF energy= -891.6479733			
S	1.50349000	-0.24965900	0.16786000	S	1.12986100	-0.21451700	0.43863600
O	2.50451500	0.34050400	1.04871800	O	1.46839300	-1.64798800	0.46762400
O	1.11666900	-1.65868000	0.29259200	O	1.52792200	0.66495000	1.53670000
C	1.95385800	0.09416200	-1.54338600	C	-0.63510000	-0.05738100	0.13483200
H	1.14468500	-0.26058300	-2.18435500	C	-1.23535900	1.20006500	0.25433500
H	2.12113200	1.16825200	-1.64419900	C	-1.37426900	-1.19575800	-0.19391800
H	2.87949800	-0.45458100	-1.73479400	C	-2.60731600	1.31500300	0.02824700
N	0.02034400	0.62758900	0.43610100	H	-0.63742800	2.06374700	0.52720400
N	0.16605800	2.01771400	0.35043800	C	-2.74856000	-1.06707900	-0.41481800
H	-0.27111300	2.39759000	-0.48806500	H	-0.87979100	-2.15985700	-0.25741200
H	-0.25548400	2.44614300	1.17028500	C	-3.36138700	0.18424800	-0.30673100
S	-1.51566600	-0.03919400	-0.16477300	H	-3.08887100	2.28475200	0.11909200
O	-2.45234900	1.06918300	0.05244000	H	-3.33803900	-1.94478100	-0.66535300
O	-1.33166800	-0.59195900	-1.51195700	H	-4.43052000	0.27948600	-0.47761400
C	-1.87958600	-1.36767100	0.99080400	N	1.70975700	0.51136700	-1.03396400
H	-1.08781700	-2.11265200	0.91453900	H	1.30677900	-0.01868400	-1.81245500
H	-1.93707400	-0.93871700	1.99213600	N	3.12215000	0.54265800	-1.04217500
H	-2.84678700	-1.77226000	0.68044900	H	3.53739700	-0.26861400	-1.49348700
 SCF energy= -1287.852948				 SCF energy= -1671.408235			
S	-0.07870300	-2.01254800	-0.12654300	S	-1.00743200	-0.94779300	-0.83686600
O	-1.09538700	-2.91000600	0.43311300	O	-0.37262800	-0.22369900	-1.94134000
O	0.07870300	-1.80453000	-1.55909700	O	-1.26240400	-2.39098800	-0.93490300
S	0.07870300	2.01254800	-0.12654300	C	-2.53046900	-0.12295500	-0.38197500
O	1.09538700	2.91000600	0.43311300	C	-3.50514000	-0.85240000	0.30467000
O	-0.07870300	1.80453000	-1.55909700	C	-2.72340200	1.20926300	-0.75075600
C	1.54120600	-2.44076900	0.54996400	C	-4.70336300	-0.21962800	0.63743000
H	2.24948600	-1.65362700	0.28472400	H	-3.33371000	-1.89360300	0.55682300
H	1.45660700	-2.56832500	1.63129200	C	-3.92974400	1.82584300	-0.41414200
H	1.83019100	-3.38285600	0.07751500	H	-1.94405700	1.74564700	-1.27858000
C	-1.54120600	2.44076900	0.54996400	C	-4.91418500	1.11613600	0.27962000
H	-1.45660700	2.56832500	1.63129200	H	-5.47301400	-0.77197800	1.16923700
H	-1.83019100	3.38285600	0.07751500	H	-4.09613600	2.86266300	-0.69221500
H	-2.24948600	1.65362700	0.28472400	H	-5.84983500	1.60371300	0.54022800
N	0.48462500	0.49631300	0.60682900	N	0.00885700	-0.87159500	0.62652700
H	0.96769100	0.65400400	1.49143800	N	0.65443900	-2.04303100	1.02050600
N	-0.48462500	-0.49631300	0.60682900	H	0.00246400	-2.63805100	1.52453100
H	-0.96769100	-0.65400400	1.49143800	H	1.04005300	-2.55257800	0.22719200
 SCF energy= -1671.413734				 SCF energy= -1671.413734			
S	-1.25498100	1.04761900	-0.85671500	S	0.87906000	0.57323400	1.05419600
O	-0.44950100	1.83903500	0.06818600	O	0.10588500	1.65447400	0.44074500
O	-1.68076700	1.54044200	-2.16963800	O	1.08537600	0.50310700	2.49789700
C	-2.69834200	0.45032400	0.03378700	C	2.47968400	0.43767700	0.25311200
C	-2.62767700	0.29414300	1.42135500	C	2.61416800	0.85321000	-1.07502000
C	-3.86174900	0.15008500	-0.68154100	C	3.55870200	-0.06786300	0.98387200
C	-3.74900800	-0.18589400	2.10206300	C	3.86730400	0.75382700	-1.68210100
H	-1.71827400	0.55839400	1.95043700	H	1.75702200	1.23747800	-1.61632700
C	-4.97535500	-0.32670700	0.01311400	C	4.80522300	-0.16073700	0.36105000
H	-3.89499600	0.30861800	-1.75487300	H	3.41857700	-0.36898900	2.01624900
				C	4.95837300	0.24848000	-0.96731600

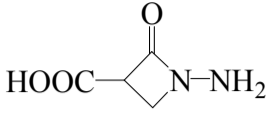
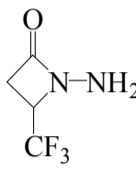
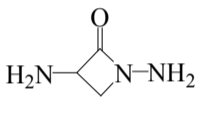
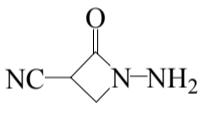
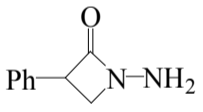
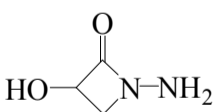
O	1.22931400	2.11413900	1.41306200	H	4.37627100	-4.91654500	0.75398900
O	-0.55097200	0.36083100	1.98611500	C	-3.31408400	-0.79924800	0.17525500
S	-2.11518700	1.17199500	-1.31065700	C	-4.42566700	-0.02188000	0.51254400
O	-1.51892200	2.03184600	-2.32536800	C	-3.31352200	-1.64810400	-0.93645900
O	-3.25751100	0.30004400	-1.58712900	C	-5.56527700	-0.09617500	-0.29163200
S	-1.03036500	-1.73048300	-1.22386200	H	-4.39493600	0.61122100	1.39325200
O	-1.29801200	-1.87695500	-2.64915400	C	-4.46018300	-1.70991400	-1.72977600
O	0.18371200	-2.30693100	-0.62823400	H	-2.43455000	-2.23718700	-1.17438900
C	-2.45766300	2.17194800	0.13182200	C	-5.58132700	-0.93692900	-1.40862000
C	-1.76560500	3.37400900	0.29592600	H	-6.43973500	0.49785900	-0.04105400
C	-3.45137600	1.75456800	1.02113600	H	-4.47726300	-2.36393600	-2.59705300
C	-2.07830400	4.17481400	1.39608800	H	-6.47139600	-0.99318100	-2.02977500
H	-1.00549600	3.67080300	-0.41890500	N	-0.85957500	0.41149700	0.29152200
C	-3.75419300	2.56957200	2.11060600	H	-1.27282200	0.55194200	-0.63222400
H	-3.97570100	0.81983800	0.85414200				
C	-3.06764000	3.77468400	2.29812700	$\text{H}_2\text{N}-\overset{\text{O}}{\parallel}{\text{NHC}}-\text{OH}$		SCF energy=	-244.5119438
H	-1.54604300	5.10987200	1.54477000	S	0.01266300	0.49191100	0.07117300
H	-4.52707400	2.26590200	2.81124600	O	0.19164600	1.84460600	-0.46884800
H	-3.30741000	4.40487300	3.15064500	O	0.11179900	0.24008600	1.51995500
C	-2.46584600	-2.29920000	-0.30262700	C	1.11988400	-0.76378500	-0.71754200
C	-3.48848600	-2.92036500	-1.02065000	H	0.53451300	-1.69141300	-0.72107500
C	-2.50165800	-2.17788000	1.08813500	H	1.32832800	-0.42072600	-1.73170900
C	-4.57294800	-3.44926500	-0.31753200	H	1.32832800	-0.42072600	-1.73170900
H	-3.43561700	-2.97310900	-2.10240300	N	-1.50664700	-0.00211000	-0.55054600
C	-3.59673700	-2.70566000	1.77441400	H	-2.11896200	0.81904500	-0.55036500
H	-1.71528700	-1.65526600	1.62189000	N	-2.01126000	-1.16743000	0.06976700
C	-4.62695500	-3.34369100	1.07505900	H	-2.52034400	-0.96513500	0.92904800
H	-5.37770300	-3.93555400	-0.86171800	H	-2.60476300	-1.65531800	-0.59426200
H	-3.64392500	-2.61375000	2.85615500	O	2.31692100	-0.84969100	-0.01529700
H	-5.47521500	-3.75389300	1.61683900	H	2.12174200	-1.06753800	0.91381900
C	3.06422100	0.34796200	-1.33816100				
C	4.11027900	1.23232500	-1.06542600	$\text{H}_2\text{N}-\overset{\text{O}}{\parallel}{\text{NHC}}-\text{OCH}_3$		SCF energy=	-283.8182668
C	3.25991800	-1.03302700	-1.43537200	S	0.44429700	-0.55009900	0.13518300
C	5.39333400	0.71176300	-0.88214300	O	0.63353200	-1.90707700	-0.39245100
H	3.91734800	2.29849800	-1.01384800	O	0.10073000	-0.30691300	1.53842400
C	4.54655700	-1.53514200	-1.24103500	C	-0.79160100	0.37392100	-0.91829500
H	2.42616200	-1.69329500	-1.65096900	H	-0.60036800	1.43875600	-0.72811200
C	5.60970700	-0.66621400	-0.96990200	H	-0.54273600	0.09977500	-1.94725900
H	6.22176800	1.38479800	-0.67863000	N	1.93629300	0.20576600	-0.18419600
H	4.71911400	-2.60548200	-1.31013400	H	2.41436500	-0.20492700	-0.98421300
H	6.61104600	-1.06583000	-0.83154900	N	2.00770100	1.59691800	0.00873900
C	1.98757200	-0.36861700	1.87488700	H	2.76733400	1.80901200	0.65000300
C	1.72006700	-1.73291700	2.01556100	H	2.13906800	2.09647300	-0.86767400
C	3.19578900	0.19189200	2.29606400	O	-2.09750700	-0.00432500	-0.66744700
C	2.69688600	-2.55150700	2.58233800	C	-2.74439800	0.66228800	0.42626600
H	0.78272500	-2.15225000	1.67327500	H	-3.77947300	0.31676000	0.40962800
C	4.16075600	-0.64070500	2.86731600	H	-2.27541400	0.40530800	1.37994500
H	3.36445400	1.25755500	2.19106200	H	-2.71753200	1.75089400	0.27691600
C	3.91278500	-2.00799600	3.01021600				
H	2.50358600	-3.61497600	2.69198700	$\text{H}_2\text{N}-\overset{\text{O}}{\parallel}{\text{NHC}}-\text{Cl}$		SCF energy=	-628.8593645
H	5.10239900	-0.21592700	3.20384300	N	1.10269800	0.58909300	-0.00038200
H	4.66530700	-2.65144200	3.45859000	H	1.57732500	1.48420800	0.00014100
				N	1.93821800	-0.53339800	0.00018900
$\text{H}_2\text{N}-\overset{\text{O}}{\parallel}{\text{NHC}}-\text{NH}_2$		SCF energy=	-224.6414173	H	1.75966500	-1.09918200	0.82726200
S	0.00189000	0.47252900	0.07291200	H	1.76019700	-1.09960800	-0.82670300
O	0.36567200	1.61797500	-0.77938400	C	-0.25577900	0.65145800	0.00003600
O	0.07344600	0.55832500	1.53475400	O	-0.91567200	1.65447300	0.00012400
C	1.03031200	-1.00196500	-0.43338700	Cl	-1.03079700	-0.98940100	-0.00003300
H	0.55120000	-1.86324400	0.03771700				
H	0.93984200	-1.06139300	-1.52186600	$\text{H}_2\text{N}-\overset{\text{O}}{\parallel}{\text{NHC}}-\text{CH}_3$		SCF energy=	-208.5702564
N	-1.61552100	0.14363200	-0.36478100	N	-0.68245900	-0.64403700	0.00028100
H	-1.79996800	0.41420300	-1.32976000	H	-0.77178100	-1.65679700	0.00010600
N	-2.13852900	-1.08378400	0.08748200	N	-1.81564500	0.18047100	-0.00015200
H	-3.00981300	-0.91283300	0.58164700				
H	-2.29003300	-1.73986700	-0.67499600				

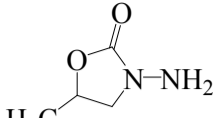
N	2.39955800	-0.89671500	-0.03899600	H	-2.38019200	0.00915800	-0.83001200
H	2.50211300	-0.84315200	0.97153800	H	-2.38032300	0.00974200	0.82973500
H	2.86305200	-0.09471100	-0.45944900	C	0.60371400	-0.15382000	-0.00006300
 <chem>H2N-NHC(=O)CN</chem>				O	1.54964600	-0.93523900	-0.00009300
SCF energy= -261.4873197				C	0.76487800	1.35225300	-0.00000700
S	-0.29282600	0.52921800	0.07266700	H	0.28976700	1.79829700	0.87983100
O	-0.09069000	1.69058200	-0.79385600	H	1.83272500	1.57695000	-0.00096600
O	-0.18315100	0.58961200	1.52309000	H	0.28780900	1.79892800	-0.87842600
C	0.81818000	-0.84362200	-0.49123600	 <chem>H2N-NHC(=O)CF3</chem>			
H	0.44041100	-1.75021500	-0.00830500	SCF energy= -581.6437251			
H	0.70662200	-0.91757400	-1.57740200	S	-0.96622500	0.55754800	0.07154600
N	-1.84268200	-0.02696000	-0.33019000	O	-0.99260900	1.78222800	-0.72995400
H	-2.10859000	0.23748900	-1.27733400	O	-0.88433400	0.56481200	1.52560900
N	-2.18998600	-1.30765600	0.13423700	C	0.35933100	-0.54736100	-0.55841200
H	-3.02940400	-1.24305000	0.70382900	H	0.09479900	-1.56085800	-0.24676000
H	-2.33385400	-1.96158800	-0.63149900	H	0.34821700	-0.46263600	-1.64739200
C	2.20875300	-0.60745300	-0.13649000	N	-2.39007500	-0.25086600	-0.37878200
N	3.32397700	-0.43219100	0.13317000	H	-2.69063200	0.00685800	-1.31732500
 <chem>H2N-NHC(=O)COOH</chem>				N	-2.50179300	-1.59599600	0.01459100
SCF energy= -357.8531505				H	-3.34187800	-1.71456200	0.57424600
S	0.64117200	-0.50515900	-0.17713800	H	-2.52071300	-2.22444600	-0.78508000
O	0.29745800	-1.01935200	-1.50603800	C	1.76149300	-0.23312200	-0.05864000
O	0.76813400	-1.36804500	0.98996400	F	2.64804100	-1.01143500	-0.73873100
C	-0.53010700	0.85584700	0.24043700	F	2.11115800	1.05113500	-0.27047200
H	-0.30075600	1.14560400	1.26893100	F	1.91896600	-0.49864600	1.24964600
H	-0.33451000	1.67833400	-0.44880500	 <chem>H2N-NHC(=O)CHO</chem>			
N	2.13129900	0.28701100	-0.41274600	SCF energy= -282.5761004			
H	2.20787500	0.63857100	-1.36666200	S	-0.41454900	0.54192700	0.04433500
N	2.53397900	1.14318800	0.63024300	O	-0.21933100	1.64894400	-0.89626500
H	3.46850900	0.88351000	0.93282800	O	-0.45554100	0.74694900	1.49093300
H	2.51323600	2.12140100	0.35168300	C	0.84994000	-0.74316200	-0.25416800
C	-1.98442100	0.45575000	0.08935200	H	0.47287500	-1.63468300	0.26324300
O	-2.75415300	0.99957500	-0.67047500	H	0.93225000	-0.92098000	-1.32907100
O	-2.32624900	-0.54994400	0.91700400	N	-1.89044300	-0.15297000	-0.43671900
H	-3.26441400	-0.76371600	0.75138600	H	-2.05937000	-0.00659900	-1.43104500
 				N	-2.17315300	-1.42346300	0.09826100
SCF energy= -493.447131				H	-3.07384100	-1.39533200	0.56811900
C	1.61100200	-1.01027200	-1.01773700	H	-2.17249800	-2.14590400	-0.61799300
C	2.72510200	-0.35067200	-0.15655000	C	2.20300700	-0.35830000	0.32491300
H	1.37398900	-2.04511100	-0.75380400	O	3.23305700	-0.51734600	-0.29101400
H	1.71198800	-0.90189800	-2.10195400	H	2.19536500	0.04809600	1.35288800
H	3.19314100	-1.00622200	0.58173600	 <chem>H2N-NHC(=O)COCF3</chem>			
H	3.49131100	0.19645200	-0.71142500	SCF energy= -619.7130922			
N	0.67901700	-0.03050800	-0.41122700	S	1.46427200	0.44991500	-0.32664700
C	1.61828700	0.54658300	0.44058200	O	1.85992800	1.85767500	-0.36840600
O	1.53041900	1.40635800	1.28316200	O	0.93282000	-0.25394600	-1.48785600
C	-1.61126400	1.01082000	-1.01716300	C	0.24278100	0.20299800	1.03888000
C	-2.72514900	0.35054400	-0.15624800	H	0.28807200	-0.86253100	1.27689100
H	-1.37441400	2.04564100	-0.75292600	H	0.57718300	0.82552900	1.87116500
H	-1.71222600	0.90283700	-2.10144600	N	2.86004500	-0.35838900	0.20114200
H	-3.19359400	1.00549900	0.58232500	H	3.45488300	0.25036100	0.76134600
H	-3.49117400	-0.19653600	-0.71148000	N	2.68905000	-1.68910400	0.61833800
N	-0.67900400	0.03105400	-0.41102200	H	3.28558100	-2.29585800	0.06253500
C	-1.61815100	-0.54683300	0.44035700	H	2.89032900	-1.80518900	1.60845700
O	-1.53017800	-1.40704500	1.28249700	C	-1.15008700	0.64465500	0.63380800
 				O	-1.58171100	1.74849400	0.85944000
SCF energy= -302.6734254				C	-2.08901100	-0.38091400	-0.07841200
C	0.20210200	-1.47177400	0.00015900	F	-3.26317700	-0.43895500	0.58292100
C	1.47535200	-0.57491000	0.00002600	F	-2.33389500	-0.00130300	-1.34062300
				F	-1.56720000	-1.62604500	-0.09579500

H	0.05061400	-2.08055900	0.89805200				
H	0.05089300	-2.08134300	-0.89724100			SCF energy= -400.3561237	
H	2.09841000	-0.64239100	0.89542400	S	-1.46470600	0.31085300	0.45012000
H	2.09832900	-0.64267500	-0.89541500	O	-1.35456900	1.74111200	0.76782600
N	-0.57302200	-0.22212800	-0.00050900	O	-1.30617200	-0.72465200	1.46923800
N	-1.95399700	-0.03489100	0.00015900	C	-0.33611500	-0.09449600	-0.95003300
H	-2.22311200	0.49998700	0.82559000	H	-0.67679100	-1.07193800	-1.30236700
H	-2.22394000	0.49972500	-0.82515400	H	-0.54231200	0.66466800	-1.71053600
C	0.50707000	0.63148600	-0.00012200	N	-3.04192100	0.17167300	-0.19562900
O	0.59134900	1.84219600	0.00010200	H	-3.32198400	1.03706200	-0.65533800
		SCF energy= -572.1556086		N	-3.33385800	-1.03751300	-0.85576000
C	-1.50176400	0.93720500	1.12313600	H	-4.18311100	-1.43426400	-0.46349400
C	-2.88413300	0.83437200	0.43890300	H	-3.43679500	-0.91096600	-1.86010300
C	-2.86741700	-0.53160800	-0.27742400	C	1.11198600	-0.10605900	-0.54328800
H	-1.08023100	1.94482800	1.07697200	C	1.89267900	1.05232100	-0.66601900
H	-1.52835900	0.61325800	2.17361500	C	1.69863000	-1.27404900	-0.03453500
H	-2.98113400	1.63747700	-0.29881100	C	3.23800700	1.04242400	-0.29244800
H	-3.70373600	0.93433100	1.15586100	H	1.44303300	1.96590900	-1.04741800
H	-3.27831500	-1.33606600	0.34720400	C	3.04327200	-1.28380600	0.33965400
H	-3.40942300	-0.54396700	-1.22639700	H	1.09649100	-2.17172600	0.07909200
N	-0.68775900	0.01861900	0.32396000	C	3.81668600	-0.12638200	0.20996500
C	-1.38889700	-0.82091900	-0.51516100	H	3.83214300	1.94698900	-0.39262700
O	-0.88921000	-1.65068300	-1.25945600	H	3.48607100	-2.19479800	0.73376900
C	1.45252600	-1.10053300	0.90621100	H	4.86406000	-0.13508900	0.50055100
C	2.84870600	0.35473600	-0.46144200			SCF energy= -342.0283	
C	2.90608900	-0.61018800	0.73998800	C	0.70251300	-1.32427500	0.16100300
H	1.24568200	-2.00644600	0.32391800	C	1.83578900	-0.32729400	-0.16125400
H	1.17822600	-1.27841400	1.95098700	C	1.20560800	1.05593200	0.10209100
H	3.04736800	-0.15921500	-1.41091700	H	0.72766000	-2.22282800	-0.46263600
H	3.53906700	1.19973800	-0.39389100	H	0.70426700	-1.64041200	1.21489700
H	3.59968100	-1.44199300	0.58928400	H	2.11635100	-0.41792800	-1.21641500
H	3.21989500	-0.07037800	1.64050700	H	2.72977800	-0.51576700	0.43965900
N	0.68666000	0.03039400	0.36457600	H	1.39639600	1.41274300	1.12286500
C	1.40408200	0.83698600	-0.50820400	H	1.53980700	1.84015700	-0.58284200
O	0.93218800	1.74611500	-1.16856000	N	-0.49174600	-0.53264400	-0.12791300
		SCF energy= -340.8012825		N	-1.76743800	-1.10352600	0.05291500
C	0.75184400	-1.31414300	0.00398600	H	-2.32325300	-0.42513800	0.57916400
C	1.82757200	-0.25957300	0.01513500	H	-2.21220100	-1.18067200	-0.86266500
C	1.28204000	0.96579100	-0.00009300	C	-0.29481700	0.82233900	-0.03422000
H	0.83231900	-1.98637000	-0.86241400	O	-1.19488500	1.65535400	-0.01409500
H	0.76895500	-1.93893700	0.90905600			SCF energy= -569.7031238	
H	2.88397500	-0.50551600	0.02817500	C	1.53484800	-0.99334600	-1.02072000
H	1.78447000	1.92520900	0.00462200	C	2.87750700	-0.63642600	-0.44379600
N	-0.45459600	-0.51168000	-0.05677400	C	2.77543200	0.40612400	0.39368500
N	-1.72611900	-1.09076800	0.02960100	H	1.53014500	-0.97535700	-2.11939800
H	-2.21267900	-0.67886200	0.82751700	H	1.19616800	-1.98320300	-0.68565700
H	-2.25696600	-0.82513000	-0.80043600	H	3.78049600	-1.17935400	-0.70170800
C	-0.20376900	0.84647800	-0.01650000	H	3.55849900	0.88540000	0.96776900
O	-1.06015000	1.72442900	0.00856700	N	0.68401600	0.05490300	-0.46659000
		SCF energy= -377.9504615		C	1.35754900	0.84121100	0.47610400
C	0.75283700	-1.28112600	0.16461400	O	0.83977000	1.70122100	1.17138200
C	1.79546900	-0.18750800	-0.10192700	C	-1.53496800	0.99361700	-1.02032700
H	0.89944200	-2.17008300	-0.45408300	C	-2.87763900	0.63609100	-0.44392500
H	0.71483500	-1.58315900	1.22154500	H	-1.52980000	0.97618500	-2.11898600
H	2.63353200	-0.18863400	0.59638900	H	-1.19661400	1.98338700	-0.68460400
C	-0.26791200	0.80495300	-0.03453900	C	-2.77541100	-0.40633900	0.39371800
O	-1.12976500	1.65243000	0.03793300	H	-3.55870800	-0.88596900	0.96719900
				N	-0.68406400	-0.05475000	-0.46646700
				C	-1.35749700	-0.84116500	0.47627300
				O	-0.83951100	-1.70114200	1.17144300

O	1.06956800	1.05329000	0.07515100	H	-3.78085200	1.17861700	-0.70188700
H	2.16866100	-0.22048900	-1.13117500				
N	-0.45401900	-0.55642000	-0.21686600			SCF energy=	-643.9981224
N	-1.71149900	-1.13607200	0.04277600	C	-1.36364200	1.10650400	0.89015100
H	-2.20055000	-0.55663700	0.72832700	C	-2.81641900	0.66850300	0.64793800
H	-2.25808800	-1.09723500	-0.81594500	H	-1.07541600	1.97209800	0.28390700
				H	-1.15920300	1.30574200	1.94610500
		SCF energy=	-381.3514083	H	-3.26769200	0.22349000	1.54077500
C	-0.41716700	-1.48891800	0.10759000	C	-1.46627900	-0.82746700	-0.46671100
C	-1.74926500	-0.86264700	-0.30190600	O	-1.11891600	-1.73277700	-1.18043300
C	-1.90846400	0.51684600	0.34186200	O	-2.73820000	-0.35789000	-0.36939700
C	-0.77240600	1.43562700	-0.12263000	H	-3.45573500	1.46676900	0.26865600
H	-2.87866100	0.96035000	0.08727700	N	-0.66962600	-0.10229500	0.43172200
H	-1.79278900	-0.76676600	-1.39592400	C	1.57815400	-0.87304300	1.16387900
H	-2.56045600	-1.53822700	-0.00467000	C	2.90957700	-0.65180400	0.42395000
H	-0.45193000	-1.81260300	1.15944000	H	1.30124800	-1.92888100	1.22071600
H	-0.19542900	-2.37619900	-0.49335300	H	1.57633400	-0.44128800	2.17490400
H	-0.92698400	1.72523600	-1.17204300	H	3.14357300	-1.48452600	-0.24642300
H	-0.73251600	2.36698200	0.45088300	H	3.75504900	-0.45656900	1.08462200
H	-1.88439700	0.41572000	1.43640300	N	0.68998300	-0.14343600	0.27037700
N	0.70136000	-0.55453700	-0.06658000	C	1.36410900	0.73813500	-0.55775800
N	1.97728900	-1.15594600	0.08090800	O	0.88228500	1.57264900	-1.28699000
H	2.50027300	-0.97569500	-0.77761100	O	2.70062500	0.53030800	-0.38776100
H	2.47595000	-0.63607000	0.80598900				
C	0.61857900	0.81576500	-0.04645200			SCF energy=	-650.803788
O	1.63359200	1.51382600	-0.00843300	C	1.44508300	-1.40588800	-0.83164200
				C	1.91185400	-1.73312100	0.59633500
		SCF energy=	-648.346827	C	2.73434900	-0.57208100	1.18161700
C	0.97058900	2.83155100	0.40399700	C	1.97968200	0.77318100	1.02451500
C	-0.13893300	3.48431500	0.02849800	H	2.95867400	-0.74978100	2.24053400
C	-1.35975200	2.73669000	-0.43730100	H	1.03911100	-1.92883400	1.23428600
C	-0.97058900	1.38656900	-1.04092200	H	2.50701500	-2.65575100	0.57752600
H	-0.18505500	4.57015200	0.09497100	H	2.30785100	-1.23972100	-1.48616500
H	1.85453100	3.33913700	0.77721100	H	0.87894400	-2.22677100	-1.27958700
H	-2.03881100	2.58099300	0.41423700	H	1.09387300	0.77577600	1.66466000
H	-0.53162900	1.53104800	-2.04081500	H	2.61105100	1.62259800	1.29763100
N	-0.00791600	0.69259600	-0.16942400	H	3.69732800	-0.50472600	0.65745300
C	1.04619500	1.34748300	0.44121300	N	0.65854000	-0.14022100	-0.94184300
O	1.97332200	0.75034700	0.98536600	C	1.59844300	0.90101800	-0.44007000
H	-1.91400700	3.31886100	-1.18326000	O	2.23866800	1.52591200	-1.25118200
H	-1.84846000	0.74523600	-1.13220500	N	-0.57792900	-0.20173700	-0.16797400
C	0.97058900	-1.38656900	-1.04092200	C	-3.46871300	0.02124100	0.03713600
C	-0.97058900	-2.83155100	0.40399700	H	-4.43920300	0.02607400	0.54745900
C	1.35975200	-2.73669000	-0.43730100	H	-3.66355300	0.23618200	-1.02279000
H	0.53162900	-1.53104800	-2.04081500	C	-1.43433100	-1.34048700	-0.54928100
H	1.84846000	-0.74523600	-1.13220500	H	-0.90959300	-2.26684800	-0.30253500
C	0.13893300	-3.48431500	0.02849800	H	-1.57496400	-1.31908800	-1.64084900
H	-1.85453100	-3.33913700	0.77721100	C	-2.78231000	-1.33563800	0.17157900
H	1.91400700	-3.31886100	-1.18326000	H	-3.39363700	-2.14035100	-0.25463700
H	2.03881100	-2.58099300	0.41423700	H	-2.63420800	-1.57308200	1.23412300
H	0.18505500	-4.57015200	0.09497100	C	-2.55265800	1.09537600	0.62769800
N	0.00791600	-0.69259600	-0.16942400	H	-2.51933300	1.00030500	1.72296800
C	-1.04619500	-1.34748300	0.44121300	H	-2.90311500	2.10879800	0.41229800
O	-1.97332200	-0.75034700	0.98536600	C	-1.11616600	1.03122900	0.12697600
				O	-0.42765700	2.05158100	0.06332900
		SCF energy=	-341.9991435				
C	-1.01058700	-0.20952700	0.45022400			SCF energy=	-380.1244108
H	-1.23343400	-0.04698500	1.51347000	C	0.76105600	1.42113700	0.09275200
N	0.17452600	0.56936400	0.02726700	C	1.88188600	0.69225600	-0.00887200
				C	1.82276500	-0.79716300	-0.21807200

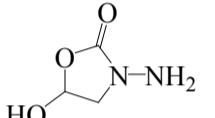
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H	0.63770200	2.32214300	-0.77554300	H	0.76974300	2.49931600	0.21925500
C	1.02627400	-0.50675100	-0.08639600	H	1.92453800	-1.01347400	-1.29356600
O	2.22019100	-0.58087800	-0.29537400	H	0.52846400	-1.41291600	1.41547200
C	-0.13422900	-1.47937200	0.21465400	N	-0.62893000	-0.55985800	-0.13429500
H	0.03355700	-2.10932800	1.09219500	N	-1.88940800	-1.19962200	-0.01508100
H	-0.43200600	-2.09705500	-0.63757700	H	-2.48245600	-0.59581400	0.55920800
C	-2.25515400	-0.01036300	-0.39890800	H	-2.32018900	-1.20023600	-0.94022300
H	-3.05441900	-0.68728200	-0.07349800	C	-0.59153200	0.81662800	-0.01529200
H	-2.62399700	1.01773500	-0.30573600	O	-1.61940900	1.49802800	-0.01911000
H	-2.04332200	-0.20634500	-1.45698700	H	2.66415900	-1.29474400	0.27916500
							
SCF energy= -394.9325129				SCF energy= -533.7812412			
C	0.67758000	0.22989500	0.63972000	C	-0.63922300	-0.78210600	-0.27632500
H	0.81828600	0.07600600	1.71581700	H	-0.69682800	-1.56442900	-1.04332500
N	-0.41911700	-0.57806300	0.07824900	N	-1.65001600	0.27499300	-0.50815300
N	-0.59817100	-1.95337600	0.16658100	N	-1.89021400	0.97947300	-1.69046600
H	-1.46486800	-2.15524500	0.66410800	H	-2.84205200	0.78581300	-2.00383200
H	-0.65406500	-2.35446600	-0.76808000	H	-1.81627300	1.97956700	-1.50997000
C	-1.27123300	0.48690400	-0.15700100	C	-2.49998300	-0.11562600	0.50538700
O	-2.42403200	0.53628200	-0.51645600	O	-3.63050100	0.22385800	0.78796600
C	-0.18183200	1.48945500	0.28327800	C	-1.47458200	-1.15444700	0.99857900
H	-0.45842100	2.10749400	1.14025500	H	-1.85590700	-2.17865500	1.02493300
H	0.21617700	2.10887200	-0.52285700	H	-0.99747800	-0.90620000	1.94976400
C	1.96573100	0.08874400	-0.04781600	C	0.78835700	-0.32485000	-0.10685400
N	2.98781100	-0.01754700	-0.58864200	C	1.83533400	-1.08796900	-0.63879200
							
SCF energy= -358.0445592				SCF energy= -377.9223905			
C	-1.02505700	-0.28585600	0.45968200	C	-1.03542800	-0.24869900	0.42729000
H	-1.44635000	-0.20449900	1.47313200	H	-1.42925200	-0.09716700	1.44032700
N	0.15898300	0.56531000	0.29218400	N	0.14261800	0.57609200	0.15139100
N	0.18590400	1.94561200	0.09103400	N	0.23769100	1.96529400	0.09742600
H	0.83484500	2.37117600	0.75096300	H	0.94961300	2.28470500	0.75359200
H	0.51474700	2.14364800	-0.85422500	H	0.51832700	2.25051400	-0.84032300
C	1.02824000	-0.45585300	-0.03429000	C	1.01714900	-0.47314600	-0.05303000
O	2.18530700	-0.45676000	-0.39443100	O	2.20071900	-0.51138300	-0.30783200
C	-0.07831700	-1.50047500	0.23436900	C	-0.12333800	-1.48223700	0.21627800
H	0.10076500	-2.13778600	1.10428400	H	0.03191400	-2.12006500	1.08986100
H	-0.33051900	-2.09971300	-0.64379100	H	-0.40654600	-2.07966800	-0.65332700
N	-1.99423200	-0.08907800	-0.60802800	O	-2.06606700	-0.17133000	-0.52702800
H	-2.75623700	-0.76080800	-0.52492200	H	-2.55372700	0.65818000	-0.39619500
H	-2.40349200	0.84226200	-0.53489100				
				SCF energy= -491.2990105			
C	-0.07640600	-1.37190900	-0.23871800	C	0.36837500	0.29502900	0.67966700
C	-1.10334400	-0.21641700	-0.46667800	H	0.63999200	0.32225000	1.73915400
H	0.13568500	-2.00772600	-1.10533300	N	-0.81492900	-0.50451200	0.37767300
H	-0.26638600	-1.99190400	0.64544700				
H	-1.42370700	-0.14203500	-1.51203400				
N	0.92900800	-0.32413100	-0.01428700				
N	2.27941900	-0.44621400	0.31406500				
H	2.84295400	0.01775800	-0.39797200				
H	2.45359900	0.01832000	1.20524100				
C	0.07810300	0.74384500	-0.17433700				
O	0.24551800	1.94427200	-0.08993300				
C	-2.29333500	-0.11945700	0.48189600				

H	-2.79471900	0.84784800	0.36704300	N	-0.96052100	-1.88597600	0.45591400
H	-3.02534800	-0.90983500	0.27802500	H	-1.81915900	-2.10586300	0.95733200
H	-1.97532400	-0.21055300	1.52762900	H	-1.01540200	-2.27641200	-0.48479200
				C	-1.58360800	0.52564500	-0.12229400
		SCF energy=	-491.2975331	O	-2.70347400	0.56585300	-0.57839300
C	0.60374700	-1.24471000	-0.65100400	C	-0.44674300	1.53385900	0.16806700
C	-0.43567300	-0.09437800	-0.74158100	H	-0.67625600	2.27805400	0.93385900
H	0.92794300	-1.65381300	-1.61306200	H	-0.05033300	2.01700600	-0.72812600
H	0.33691300	-2.04201500	0.04712800	C	1.57410800	-0.05386600	-0.17308900
H	-0.68725700	0.23274900	-1.75225400	O	1.53122900	-0.61010600	-1.24821900
N	1.53827400	-0.25794700	-0.08539100	O	2.72470300	0.36341700	0.40588500
N	2.84428900	-0.43521600	0.36053400	H	3.45685700	0.14106500	-0.20082700
H	3.46507700	0.20263900	-0.13590200				
H	2.89634700	-0.22742300	1.35754600			SCF energy=	-639.8246364
C	0.68069900	0.80818000	-0.09314800	C	0.10381300	0.18139100	0.67666700
O	0.77839800	1.96175900	0.25572200	H	0.26390200	-0.03145100	1.73934400
C	-1.66767000	-0.23854700	0.11181900	N	-1.01027400	-0.56668700	0.08384500
O	-1.75729500	-0.93000300	1.10511600	N	-1.29691300	-1.92510900	0.21972300
O	-2.68106500	0.53298100	-0.34438100	H	-2.21882400	-2.02844700	0.64404100
H	-3.42389000	0.43883400	0.28237500	H	-1.31656300	-2.36108800	-0.70092000
				C	-1.83291800	0.53638000	-0.07895600
		SCF energy=	-358.0372344	O	-2.99837100	0.63274600	-0.38632800
C	-0.06320400	-1.39122600	-0.18084800	C	-0.70098200	1.48063200	0.38085400
C	-1.11636000	-0.26680300	-0.43892600	H	-0.94867700	2.07280300	1.26445900
H	0.14045800	-2.07172600	-1.01456800	H	-0.29611400	2.12220500	-0.40445100
H	-0.23594400	-1.94459800	0.74729000	C	1.43513600	0.02015400	-0.04261900
H	-1.45229100	-0.24048800	-1.48676000	F	1.34504300	0.27717900	-1.36769900
N	0.92907200	-0.31201600	-0.04569900	F	2.35165500	0.87623300	0.47683700
N	2.27785600	-0.38821900	0.30226900	F	1.92810800	-1.23171900	0.09169600
H	2.83782000	0.06806500	-0.41698400				
H	2.42725800	0.10604400	1.18224000			SCF energy=	-394.9320246
C	0.04655400	0.72626000	-0.18363200	C	0.17397700	-1.35629200	-0.33450800
O	0.16027900	1.93300200	-0.09964300	C	-0.79174000	-0.17259400	-0.67359000
N	-2.17076300	-0.14514700	0.55330600	H	0.48951200	-1.94956800	-1.19833500
H	-2.46747400	0.82618200	0.63240500	H	-0.15429100	-2.00626100	0.48129500
H	-2.98716100	-0.69920500	0.30482000	H	-0.98166900	-0.05325900	-1.74458000
				N	1.14954900	-0.33611200	0.07377700
		SCF energy=	-533.777606	N	2.46646400	-0.50692000	0.48794100
C	-1.49558700	-0.17828800	-1.40658700	H	3.09075100	0.00801900	-0.13206800
C	-0.57306500	-0.84943200	-0.33196600	H	2.57773200	-0.14483100	1.43435800
H	-1.98155500	-0.87560000	-2.09857100	C	0.37725300	0.76585900	-0.18640200
H	-1.05027500	0.65522600	-1.95829300	O	0.56304000	1.95500300	-0.10225500
H	-0.57804400	-1.94081800	-0.41641900	C	-2.03557600	-0.10372500	0.07494000
N	-2.36162100	0.24044100	-0.29351200	N	-3.02599200	-0.05605500	0.68038600
N	-3.65923700	0.75305000	-0.34286200				
H	-4.28986700	0.11761500	0.14702100			SCF energy=	-377.906454
H	-3.68525000	1.65187600	0.13717400	C	-0.13242800	-1.37050000	-0.18990900
C	-1.64800600	-0.38843500	0.70032700	C	-1.13808500	-0.19091900	-0.40883700
O	-1.85519800	-0.53154100	1.88647500	H	0.06834700	-2.00720000	-1.05933600
C	0.83518400	-0.33960700	-0.16446400	H	-0.34887400	-1.97703800	0.69548800
C	1.92035000	-1.22459500	-0.21805600	H	-1.48675400	-0.10387900	-1.44525500
C	1.09296300	1.02428300	0.04820100	N	0.88844000	-0.33700900	0.03311700
C	3.23156700	-0.76250300	-0.07030500	N	2.26387800	-0.48003000	0.21173300
H	1.73792500	-2.28563900	-0.37505000	H	2.75177400	0.07743600	-0.48931600
C	2.40026000	1.48940000	0.19447600	H	2.52180100	-0.12393200	1.13209200
H	0.26503900	1.72765900	0.10938300	C	0.06535300	0.75247200	-0.11956100
C	3.47580700	0.59687300	0.13480000	O	0.26483200	1.94678000	-0.07298500
H	4.05907700	-1.46613800	-0.11424100	O	-2.18507400	-0.04706600	0.51997300
H	2.57975400	2.54850500	0.36160200	H	-2.97962700	-0.49014500	0.18631100
H	4.49393900	0.95902300	0.25165800				



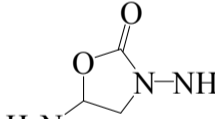
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H	0.15079800	1.55349800	-1.49453700
H	1.96299100	-0.01423900	-1.41645200
C	-0.67842700	-0.79668800	-0.00740000
O	-1.58371000	-1.58588200	0.15393300
O	0.58131700	-1.13685900	-0.40047100
N	-0.73532400	0.57512400	0.15966600
N	-1.97403500	1.24184000	0.20038000
H	-2.64282800	0.72199100	-0.37150400
H	-2.31948300	1.20744100	1.15818200
C	2.38654700	0.07020400	0.70424300
H	2.97400100	-0.85322900	0.72360200
H	3.07645800	0.91806200	0.61292800
H	1.84786000	0.16050000	1.65421200



SCF energy= -453.2025395

C	0.43735000	1.23418700	-0.41567800
C	1.44499500	0.07656100	-0.40716900
H	0.76774100	2.04487200	0.23796600
H	0.26175300	1.62489000	-1.42696600
H	2.06452200	0.00877400	-1.30615300
C	-0.65024700	-0.80303400	-0.01530300
O	-1.52923700	-1.61905500	0.14375400
O	0.63776600	-1.11780800	-0.38750900
N	-0.73964400	0.56185900	0.10638400
N	-1.97309500	1.22626000	0.17231600
H	-2.64308600	0.73202200	-0.41920800
H	-2.31897200	1.16657500	1.12918300
O	2.22617900	0.17171700	0.74950100
H	2.78696800	-0.61908000	0.81721500



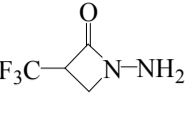
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H	0.75714500	2.05224700	0.20642800
H	0.23322100	1.61718900	-1.44684500
H	1.99707700	-0.00858600	-1.37266500
C	-0.66475900	-0.79859300	-0.01027300
O	-1.55346000	-1.60306800	0.16001800
O	0.60877300	-1.12738400	-0.39941700
N	-0.74246800	0.56842500	0.11076200
N	-1.97187400	1.23900000	0.19225100
H	-2.65095900	0.74828800	-0.39211700
H	-2.30691400	1.17555800	1.15282600
N	2.24283200	0.07270800	0.76446100
H	2.84565700	-0.74795600	0.79554500
H	2.83426100	0.90141700	0.79577200



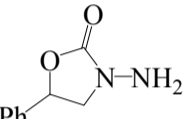
SCF energy= -417.2766603

C	-1.08858500	-0.08791300	0.38217200
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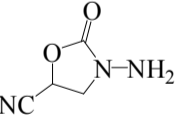
SCF energy= -639.821782

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C	-0.19535600	-0.12396100	-0.74002900
H	1.02004900	-1.92163900	-1.32322400
H	0.40232600	-1.99988600	0.36263200
H	-0.42950200	0.02230300	-1.79713000
N	1.74279600	-0.35500900	-0.02503100
N	3.05320600	-0.56892700	0.39025600
H	3.69185300	-0.05731100	-0.21785000
H	3.16974100	-0.22422500	1.34273700
C	0.99065200	0.76985700	-0.25156100
O	1.21160900	1.95298700	-0.13800900
C	-1.47663100	-0.04017500	0.05490700
F	-2.11413000	1.13152400	-0.15002800
F	-2.33649200	-1.03395500	-0.29862000
F	-1.26314700	-0.16222700	1.38885200



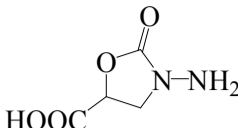
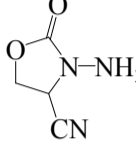
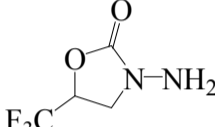
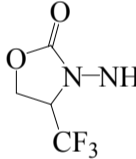
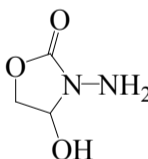
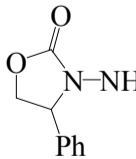
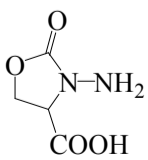
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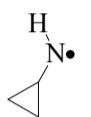
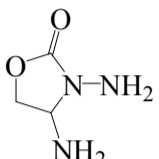
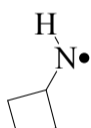
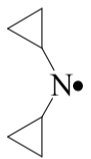
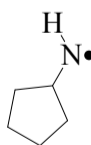
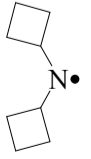
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C	-0.27331900	0.65467700	-0.92898000
H	-0.53322300	1.86307400	0.90849200
H	-1.71119200	2.24742900	-0.37756700
H	-0.14113300	1.23074100	-1.84868200
C	-2.10919100	-0.62754500	-0.35989200
O	-2.94122400	-1.50736400	-0.39673600
O	-1.10509500	-0.48246100	-1.27516400
N	-2.00581000	0.38228400	0.57361400
N	-3.08773300	0.69990000	1.41525000
H	-3.95603600	0.46777800	0.92900500
H	-3.03873900	0.09617100	2.23463900
C	1.08140100	0.21522600	-0.40582800
C	2.14074700	1.13378800	-0.42800200
C	1.30108000	-1.06545500	0.11350400
C	3.39509700	0.78560300	0.07630500
H	1.98744600	2.12716300	-0.84717100
C	2.55825100	-1.41565500	0.61560400
H	0.49769000	-1.79529100	0.10918700
C	3.60657600	-0.49265600	0.60221500
H	4.20743500	1.50741900	0.04964800
H	2.71727800	-2.41497800	1.01259800
H	4.58365200	-0.76860200	0.99015400

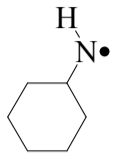
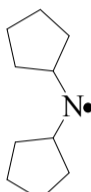


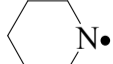
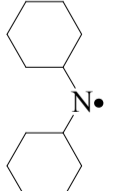


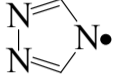
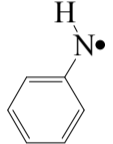
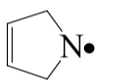
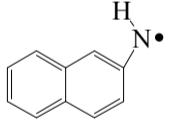
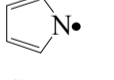
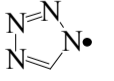
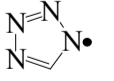
SCF energy= -470.2040549

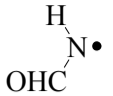
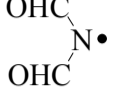
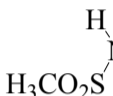
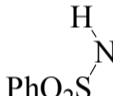
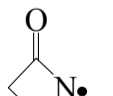

C	0.12777400	1.17691800	-0.68399300
C	1.10157500	-0.02215100	-0.77560800
H	0.57790700	2.05770300	-0.22230600
H	-0.26840300	1.44548700	-1.67291800
H	1.55513500	-0.12363500	-1.76432900
C	-0.90783700	-0.78716000	0.04089100
O	-1.78251700	-1.55200800	0.36487600
O	0.27240800	-1.18036500	-0.55523700
N	-0.89881400	0.58730600	0.16138900
N	-2.09049000	1.29849500	0.38720300
H	-2.86904300	0.76491500	-0.00379500
H	-2.24027300	1.35482000	1.39335800
C	2.17510800	0.03529900	0.23558200
N	3.03870900	0.10595000	1.00735900

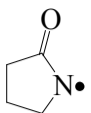
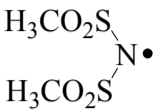
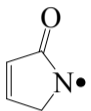
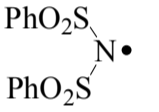
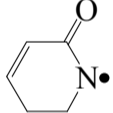
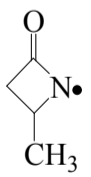
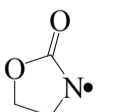
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C	1.19996800	-0.23055700	-0.08915200	C	-0.12286400	1.26178600	-0.50459700
O	2.36491000	0.09723300	-0.13586500	C	0.74846500	0.02288700	-0.82717300
O	0.76678600	-1.51778900	0.03237700	H	0.39589100	2.00550200	0.10459900
N	0.09764200	0.60957400	-0.12580300	H	-0.49513900	1.74651700	-1.41780900
N	0.25759700	1.97844600	0.16876600	H	1.19227500	0.07322500	-1.82347100
H	1.07022800	2.08670900	0.77939600	C	-1.30397500	-0.71809000	-0.12779600
H	0.47894400	2.46301200	-0.69927400	O	-2.23982100	-1.45652100	0.06509600
C	-0.68044500	-1.52663700	0.02790900	O	-0.15953900	-1.08162200	-0.79356400
H	-1.01914400	-1.80355300	-0.97746200	N	-1.19654200	0.61172600	0.23152700
H	-1.01457800	-2.27353900	0.74990800	N	-2.33861900	1.35535300	0.57876100
C	-2.39000900	0.38285000	-0.25127500	H	-3.14598700	0.95637900	0.09584100
H	-3.23669400	-0.19376700	0.14057600	H	-2.50143900	1.23462600	1.57727600
H	-2.56102000	1.43863100	-0.01903000	C	1.85904800	-0.18118000	0.20357800
H	-2.35912700	0.26526000	-1.34071500	O	1.83766900	-0.94503700	1.13589900
	SCF energy= -470.2059831	O	2.89236900	-0.65549800	-0.06903400		
C	0.79250000	0.22490500	0.50655600	H	3.57105700	0.52323600	0.62030600
H	0.82128600	0.10593800	1.60014400		SCF energy= -715.0984264		
C	-1.43946900	0.11701600	-0.15421500	C	-0.45088300	1.21323900	-0.65073300
O	-2.55003700	-0.33577400	-0.28875400	C	0.49891300	0.00983800	-0.84488400
O	-1.15372300	1.44429200	-0.01610800	H	-0.00022600	2.02405300	-0.07270700
N	-0.25450300	-0.60831400	-0.07786400	H	-0.79710300	1.61572100	-1.61137200
N	-0.28694900	-1.97445600	0.26216800	H	0.90803300	-0.05267300	-1.85588800
H	-1.18168400	-2.17203300	0.71375500	C	-1.50708800	-0.79482200	-0.05071800
H	-0.25660200	-2.51616600	-0.59979000	O	-2.37224200	-1.58389800	0.24228900
C	0.27038900	1.62281700	0.08967000	O	-0.29783000	-1.15656600	-0.60896100
H	0.66595300	1.92143600	-0.88536600	N	-1.53319600	0.57307200	0.07746300
H	0.46860000	2.39606800	0.83207700	N	-2.72698100	1.27178900	0.31407400
C	2.13030200	-0.06732200	-0.02403200	H	-3.49249200	0.78080700	-0.15071500
N	3.19719400	-0.27264100	-0.43141900	H	-2.91870400	1.24805900	1.31467000
	SCF energy= -715.0988178	C	1.69002600	0.01208000	0.11788900		
C	0.23900800	-0.20556600	-0.58754900	F	1.31127600	0.08397300	1.41095900
H	0.35287800	-0.00753600	-1.66183300	F	2.44654600	-1.09077800	-0.03204100
C	-1.98377200	-0.16431600	0.13323100	F	2.47512200	1.09032700	-0.14121900
O	-3.09578200	0.26388200	0.33165000		SCF energy= -453.2022301		
O	-1.67899100	-1.48150800	-0.02268800	C	-1.17536000	0.17687200	0.36892200
N	-0.82641100	0.59124900	-0.01309300	H	-1.72839900	0.54431300	1.24044000
N	-0.93377200	1.95253400	-0.37307500	C	1.03948500	-0.44002500	-0.05622800
H	-1.88275200	2.10564900	-0.71939200	O	2.19164200	-0.32112700	-0.40332900
H	-0.83393700	2.51079400	0.47372200	O	0.32538900	-1.59483600	-0.10792500
C	-0.27143300	-1.63636400	-0.28661800	N	0.22058600	0.56101500	0.45843600
H	0.20161900	-2.06325200	0.60122500	N	0.53902400	1.91817500	0.24938300
H	-0.15429200	-2.31591100	-1.13111600	H	1.12064200	2.23119400	1.02488600
C	1.60183600	0.05816500	0.05576800	H	1.10896300	1.99079000	-0.59548400
F	2.51008300	-0.82057800	-0.44622600	C	-1.02655700	-1.34844700	0.34328100
F	2.05526100	1.30038400	-0.19755200	H	-1.71524900	-1.80968400	-0.36549900
F	1.58155700	-0.10277500	1.39709900	H	-1.14439900	-1.78787400	1.33795700
	SCF energy= -609.0578622	O	-1.79672900	0.61136200	-0.82489500		
C	0.45627000	0.47007000	-0.54269800	H	-1.74666500	1.58333800	-0.84369100
H	0.55478800	0.64076700	-1.62544900		SCF energy= -566.5735073		
C	2.62041700	-0.02688200	0.19633600	C	0.47398800	0.25098600	0.48369000
O	3.67986300	-0.60968800	0.26728400				
O	2.46358100	1.31143900	0.40007100				
N	1.39131600	-0.58021600	-0.12863100				

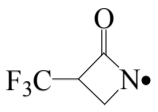
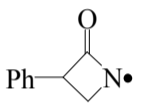
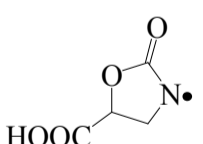
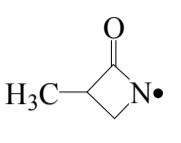
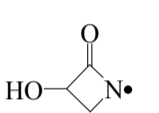
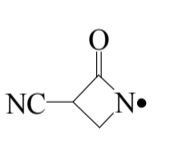
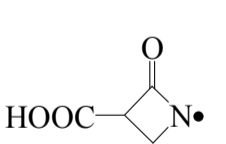
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H	2.29531600	-1.98504700	-1.19019500	C	-1.77078300	0.17456900	-0.12657100
H	1.17672200	-2.54915800	-0.13593300	O	-2.90486000	-0.23850300	-0.20484400
C	1.06559200	1.64764600	0.24936000	O	-1.42621900	1.49766100	-0.15753700
H	0.61975100	1.73375900	1.24542200	N	-0.62486800	-0.57826900	0.04442700
H	0.99904100	2.60430700	-0.27081400	N	-0.71151000	-1.90050800	0.52932500
C	-0.99543000	0.18841700	-0.21819400	H	-1.67235000	-2.04493000	0.84519200
C	-1.98779100	0.47037100	-1.16403400	H	-0.55105200	-2.52853700	-0.25747500
C	-1.37470700	-0.32404600	1.03109200	C	0.00574600	1.62276700	-0.06411200
C	-3.33735100	0.25566000	-0.86825300	H	0.40399000	1.81754700	-1.06537900
H	-1.70377700	0.85214100	-2.14254300	H	0.23924400	2.45534200	0.59931400
C	-2.72066200	-0.54499600	1.32712500	C	1.80667700	-0.18816100	-0.10317300
H	-0.61165200	-0.56089400	1.76878400	O	1.96778000	-1.03362600	-0.95081400
C	-3.70688400	-0.25269700	0.37872300	O	2.81674800	0.52542400	0.45081900
H	-4.09554400	0.47779800	-1.61473700	H	3.65154800	0.22664100	0.04190000
H	-3.00056600	-0.94734200	2.29745400				
H	-4.75470900	-0.42596100	0.60982000				
Radicals:							
							
			SCF energy= -172.6156708			SCF energy= -433.3202183	
N	1.58537200	0.00018700	-0.10098600	C	-1.10367200	-0.08187300	0.36746500
H	1.46045300	-0.00034400	-1.12261500	H	-1.20249100	0.05704200	1.46062600
C	0.32905100	-0.00053900	0.49158700	C	1.18811300	-0.23464100	-0.08178900
C	-0.87268800	0.74394100	-0.13815900	O	2.35234600	0.09183600	-0.13250700
C	-0.87318300	-0.74376000	-0.13872800	O	0.74815700	-1.52103400	0.02282000
H	0.35452800	-0.00115700	1.57918900	N	0.08892200	0.60641800	-0.09705400
H	-0.68280600	1.26825100	-1.07130000	N	0.22088500	1.98159900	0.15955300
H	-1.52264700	1.27472100	0.55310600	H	0.98885300	2.12518200	0.81857300
H	-1.52334600	-1.27385800	0.55275100	H	0.48658700	2.44030000	-0.71018500
H	-0.68286300	-1.26677100	-1.07242800	C	-0.69933600	-1.52722600	0.02525800
				H	-1.05567000	-1.78770800	-0.97613500
			SCF energy= -211.9309725	H	-1.02746100	-2.26864200	0.75581900
N	1.94286800	0.00013300	-0.08616600	N	-2.28145200	0.35957200	-0.36598000
H	1.86775600	-0.00131300	-1.11564600	H	-3.11898800	-0.07030500	0.02645200
C	0.61303600	-0.00011500	0.42104700	H	-2.38397200	1.36703400	-0.23888200
C	-0.41240600	1.08287400	-0.08045700				
C	-0.41261200	-1.08287100	-0.08030800			SCF energy= -289.3408299	
H	0.64867200	0.00012400	1.51687500	N	-0.07192700	-0.00046800	0.88714500
C	-1.52075100	0.00010800	-0.04741800	C	1.32025600	-0.00036700	0.71035700
H	-0.17666900	1.39599500	-1.10468400	C	2.04409800	-0.74757900	-0.42188300
H	-0.52612400	1.97285200	0.54626500	C	2.04377800	0.74804900	-0.42113600
H	-0.17704000	-1.39606000	-1.10456900	H	1.84772600	-0.00055800	1.66125400
H	-0.52652900	-1.97281700	0.54642800	H	1.42438000	-1.26418300	-1.15012500
H	-2.25076300	0.00010200	-0.86283700	H	2.95427700	-1.27655500	-0.15070200
H	-2.06298200	0.00021400	0.90414600	H	2.95370500	1.27739400	-0.14976000
			SCF energy= -251.2821131	H	1.42376800	1.26495000	-1.14891500
N	-2.23494800	0.00002500	0.03330800	C	-0.89606300	-0.00011400	-0.24526600
H	-2.27488900	-0.00005300	-0.99917500	C	-2.23059700	-0.74627700	-0.11754000
C	-0.84258700	0.00005200	0.38546000	C	-2.23033500	0.74656200	-0.11731700
C	-0.02948400	-1.20303300	-0.16410500	H	-0.45781000	-0.00012300	-1.24578900
C	-0.02943100	1.20297300	-0.16433700	H	-2.39202400	-1.25891800	0.82562500
H	-0.77248100	0.00017800	1.48278900	H	-2.58311700	-1.27322400	-1.00081700
C	1.44642500	-0.77967500	0.02469200	H	-2.58279900	1.27410300	-1.00024600
H	-0.26262800	-1.32911200	-1.23131900	H	-2.39144100	1.25874900	0.82616600
H	-0.28163200	-2.14139900	0.34024000				
C	1.44640200	0.77968400	0.02496500			SCF energy= -367.9779224	
H	-0.28169600	2.14151500	0.33962400	N	0.00002000	-0.00017100	0.62946900
				C	-1.17176700	0.25244900	-0.14870600
				C	-2.08696400	-0.99852800	-0.45702400

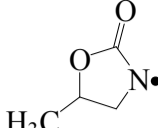
H	-0.26231700	1.32865300	-1.23165700	C	-2.38966800	0.89038200	0.56693400
H	1.83292400	-1.16271100	0.97620000	H	-0.94565500	0.77152900	-1.09639300
H	2.08334100	-1.19555400	-0.76375100	C	-3.32124100	-0.10017700	-0.18126000
H	1.83235900	1.16238000	0.97683300	H	-1.95373900	-1.76236500	0.31602300
H	2.08370500	1.19592100	-0.76297900	H	-1.98191200	-1.45940600	-1.44471600
				H	-2.34081100	0.67805000	1.64024300
		SCF energy=	-290.6029365	H	-2.55255600	1.96372300	0.42008200
N	2.49486300	-0.00017600	0.01131500	H	-4.14429100	-0.54616400	0.38603100
H	2.54488500	-0.00050400	-1.02096500	H	-3.72719300	0.32991800	-1.10369000
C	1.09048800	-0.00050800	0.35036600	C	1.17180500	-0.25262900	-0.14874900
C	0.37326400	1.26776500	-0.17820000	C	2.08678200	0.99854400	-0.45701100
C	0.37228800	-1.26821900	-0.17816400	C	2.38983400	-0.89036500	0.56686300
H	1.02067100	-0.00028300	1.44806400	H	0.94574800	-0.77170400	-1.09644700
C	-1.11570000	1.26971800	0.20654500	C	3.32121200	0.10043100	-0.18126000
H	0.47191300	1.29858500	-1.27463700	H	1.95337000	1.76229600	0.31609300
H	0.87435700	2.16100400	0.21379100	H	1.98164600	1.45948700	-1.44466400
C	-1.11667600	-1.26924700	0.20644200	H	2.34091000	-0.67812500	1.64018500
H	0.47101300	-1.29893000	-1.27462500	H	2.55295500	-1.96365700	0.41991700
H	0.87274400	-2.16184300	0.21379000	H	4.14418800	0.54654500	0.38603800
C	-1.83154600	0.00054600	-0.28157300	H	3.72724400	-0.32956700	-1.10370400
H	-1.60056300	2.16409900	-0.20622800				
H	-1.20665900	1.34268300	1.30046100			SCF energy=	-446.6792669
H	-1.60230300	-2.16317100	-0.20641600	N	0.00118800	0.14155600	-0.68735300
H	-1.20778800	-1.34226800	1.30035900	C	-1.20043000	-0.08318400	0.07079700
H	-2.87596700	0.00090500	0.05669000	C	-2.05312500	1.21385100	0.19103800
H	-1.85905300	0.00062800	-1.38198000	C	-2.18371600	-1.04492800	-0.62679000
		SCF energy=	-172.6078838	H	-0.98733900	-0.45407600	1.09134100
C	-0.05055500	-0.09765300	1.03852600	C	-3.48507600	0.71718700	0.51412400
C	-0.05055500	1.05092200	0.00000000	H	-2.02251700	1.72507900	-0.77887300
C	-0.05055500	-0.09765300	-1.03852600	H	-1.65412100	1.90525300	0.94142200
H	0.69383200	-0.08625900	1.84592300	C	-3.53375700	-0.77653800	0.06945700
H	-1.03435400	-0.28326400	1.49888900	H	-1.86420700	-2.09134300	-0.56287800
H	0.87445200	1.63515700	0.00000000	H	-2.22403600	-0.77635000	-1.69016900
H	-0.90546900	1.73445200	0.00000000	H	-3.69710100	0.80870100	1.58574300
H	0.69383200	-0.08625900	-1.84592300	H	-4.23438700	1.32383100	-0.00660600
H	-1.03435400	-0.28326400	-1.49888900	H	-3.64434400	-1.42869700	0.94467500
N	0.23172100	-1.10918100	0.00000000	H	-4.38234100	-0.98954800	-0.59010500
		SCF energy=	-211.9658305	C	1.21568300	0.18870500	0.08054800
C	0.28481300	-0.71424100	-0.98441000	C	1.93976600	-1.18976900	0.10543000
C	-0.28481300	0.71424100	-0.98441000	C	2.29057100	1.10328700	-0.53845600
C	0.00000000	1.17187800	0.46278900	H	1.02672300	0.49001200	1.12888600
C	0.00000000	-1.17187800	0.46278900	C	3.38053700	-0.84592000	0.54032600
H	-0.16960500	-1.36644700	-1.73786300	H	1.92130500	-1.60017100	-0.91211500
H	1.36695500	-0.69472200	-1.16845400	H	1.44723400	-1.91226000	0.76570400
H	-1.36695500	0.69472200	-1.16845400	C	3.62935900	0.62122100	0.07105800
H	0.16960500	1.36644700	-1.73786300	H	2.09083300	2.16479900	-0.35387100
H	1.00095900	1.63468200	0.53981700	H	2.27332600	0.95207100	-1.62494200
H	-0.70573100	1.91834600	0.85137200	H	3.47339900	-0.91849800	1.63078800
H	0.70573100	-1.91834600	0.85137200	H	4.10552900	-1.54885400	0.11490900
H	-1.00095900	-1.63468200	0.53981700	H	3.92080500	1.24950500	0.92098800
N	0.00000000	0.00000000	1.32710200	H	4.44405500	0.68618800	-0.65862000
		SCF energy=	-251.2903774			SCF energy=	-525.3416511
C	-0.03147900	-0.83664500	1.19366100	N	0.00004400	-0.00039400	0.86159900
C	-0.03147900	0.71188300	1.26143800	C	1.20814300	-0.14991000	0.07959400
C	0.60825400	1.30814100	0.00000000	C	1.84814900	1.24867700	-0.14192300
C	-0.03147900	0.71188300	-1.26143800	C	2.20193200	-1.07936700	0.80014900
C	-0.03147900	-0.83664500	-1.19366100	H	0.98721100	-0.56920900	-0.92177200

H	0.50668900	2.40139900	0.00000000	C	3.18347100	1.14223100	-0.89667400
H	-1.06891000	1.05995500	1.35529300	H	2.00760400	1.71177400	0.84154700
H	0.49916400	1.03234400	2.16717900	H	1.14802000	1.89226000	-0.68986400
H	1.01887200	-1.18566300	1.19850000	C	3.53875600	-1.18431100	0.04943000
H	-0.52904900	-1.25831800	2.07399700	H	2.36547400	-0.68456100	1.81275500
H	-1.06891000	1.05995500	-1.35529300	H	1.74881700	-2.07164600	0.92062500
H	0.49916400	1.03234400	-2.16717900	C	4.16570600	0.19887600	-0.18475800
H	-0.52904900	-1.25831800	-2.07399700	H	3.62426100	2.14240600	-1.00378000
H	1.01887200	-1.18566300	-1.19850000	H	2.99757500	0.77197800	-1.91626300
H	1.68663900	1.09008500	0.00000000	H	4.23054200	-1.82617100	0.61057200
N	-0.70393100	-1.30568900	0.00000000	H	3.37677000	-1.67719600	-0.92163900
				SCF energy= -241.6180315			
C	1.02966000	-0.36984200	-0.00001200	H	5.09089900	0.10515000	-0.76864600
C	-1.03549300	-0.35375200	0.00004800	H	4.44856500	0.63684300	0.78454200
H	-2.08022700	-0.63936300	0.00045100	C	-1.20813900	0.14948300	0.07971300
N	-0.00958200	-1.20672400	-0.00003100	C	-1.84856100	-1.24890900	-0.14201100
N	-0.63448300	1.01226000	-0.00023100	C	-2.20162500	1.07907600	0.80048700
N	0.65058000	1.00208700	0.00021500	H	-0.98715600	0.56885700	-0.92163000
H	2.06961700	-0.67243200	-0.00033900	C	-3.18381500	-1.14196100	-0.89679700
				SCF energy= -287.0097134			
N	2.35788800	-0.13674200	-0.00081100	H	-2.00822800	-1.71201400	0.84140200
H	2.77722100	0.80061600	-0.00177800	H	-1.14862300	-1.89263400	-0.68999700
C	1.02088100	-0.02937000	0.00082400	C	-3.53832900	1.18464800	0.04961200
C	0.24948400	-1.23952300	0.00054700	H	-2.36539200	0.68408100	1.81295000
C	0.30217100	1.21469700	0.00036000	H	-1.74805100	2.07111900	0.92118600
C	-1.13434900	-1.20115300	-0.00028700	C	-4.16570400	-0.19828300	-0.18482300
H	0.79399600	-2.17932900	0.00144500	H	-3.62512500	-2.14190900	-1.00386600
C	-1.08261300	1.23583600	0.00007400	H	-2.99778000	-0.77175000	-1.91636600
H	0.86859400	2.14418700	0.00075700	H	-4.23005700	1.82665900	0.61067900
C	-1.81111800	0.03228500	-0.00044800	H	-3.37595100	1.67767100	-0.92132700
H	-1.70313000	-2.12770700	-0.00019600	H	-5.09086000	-0.10420500	-0.76872000
H	-1.61102300	2.18618900	0.00040900	H	-4.44872200	-0.63625100	0.78443500
H	-2.89760300	0.05660200	-0.00137500				
				SCF energy= -210.7378303			
C	-1.05449300	-1.13678000	0.00033700	C	0.00002100	-0.39645700	1.17057000
C	0.26353500	-0.63632300	0.00015400	C	0.00002100	1.02992800	0.66795000
C	-2.18892400	-0.27604900	0.00009100	C	0.00002100	1.02992800	-0.66795000
C	1.39887600	-1.49722600	-0.00007800	C	0.00002100	-0.39645700	-1.17057000
C	0.47545300	0.78583900	0.00017600	H	0.87581400	-0.63874100	1.79799800
C	-1.93971700	1.15640900	-0.00020800	H	-0.87611300	-0.63870400	1.79764000
C	2.67915500	-0.98004400	-0.00015600	H	-0.00018700	1.90131400	1.31596900
H	1.23901800	-2.57288300	-0.00025100	H	-0.00018700	1.90131400	-1.31596900
C	1.79559900	1.28319200	0.00002100	H	0.87581400	-0.63874100	-1.79799800
C	-0.66997500	1.65284500	0.00015200	H	-0.87611300	-0.63870400	-1.79764000
H	-2.79587400	1.82803100	-0.00065700	N	0.00006700	-1.26419800	0.00000000
C	2.88122400	0.41972400	-0.00010300				
H	3.53620200	-1.64825800	-0.00034300	SCF energy= -209.5529339			
H	1.95398400	2.35945600	0.00004200	C	-0.43313100	-1.06256300	-0.00004900
H	-0.50246400	2.72805600	0.00022600	C	-0.41648700	1.06899400	-0.00021600
H	3.89198800	0.81892700	-0.00010700	C	0.98017600	-0.68987100	-0.00040700
H	-1.23697400	-2.20802700	0.00061900	H	-0.83765700	-2.06999700	0.00089600
N	-3.40155400	-0.83366400	-0.00022700	C	0.99027000	0.67542800	0.00039600
H	-4.11940400	-0.09917700	-0.00023800	H	1.84272700	1.34322400	0.00023600
				SCF energy= -257.6119794			
C	-0.00040400	1.07524800	0.00000700	N	-1.24944400	0.00897200	0.00008800
H	-0.00076200	2.15715700	0.00006500	H	1.82273600	-1.37000800	0.00014700
N	1.13966200	0.29707100	-0.00001000	H	-0.80667100	2.08204500	-0.00023500
N	0.78926900	-0.91134300	-0.00000100				
N	-0.78863000	-0.91189100	0.00001900	C	-0.00040400	1.07524800	0.00000700
N	-1.13984700	0.29635800	-0.00002400	H	-0.00076200	2.15715700	0.00006500

	SCF energy= -169.2376545				SCF energy= -282.5841122		
N	-1.17435400	-0.10130700	-0.04976700	N	-0.01932700	0.62511700	-0.27188300
H	-1.13357200	-1.09307500	0.22598000	C	-1.00881600	-0.32003100	0.02169000
C	0.07976900	0.42768900	0.04111800	O	-2.18574000	-0.03142200	0.06502100
O	1.09134800	-0.28600400	-0.02041900	H	-0.62160700	-1.33851100	0.20492800
H	0.14465300	1.52411800	0.03903100	C	1.28555200	0.44864700	0.15693400
				O	1.85147800	-0.61108700	-0.06166000
				H	1.77057200	1.33106300	0.59961200
	SCF energy= -643.8618321				SCF energy= -835.6471871		
S	0.11623300	0.11232300	0.01354200	S	1.48666800	-0.00000200	0.10142600
O	0.45833000	0.56316200	1.36791900	O	1.95088700	-1.27873800	0.66495300
O	0.44039100	0.93311900	-1.15789900	O	1.95091700	1.27858700	0.66518800
C	-1.65825700	-0.24017400	-0.02620700	C	-0.30098400	0.00000300	0.04977200
H	-1.92067700	-0.66213100	-0.99916400	C	-0.97818600	1.22147600	0.02778200
H	-1.91064600	-0.91827100	0.79232100	C	-0.97818500	-1.22147800	0.02779100
H	-2.16431100	0.71839400	0.11364300	C	-2.37332300	1.21337100	-0.02378500
N	0.94611700	-1.33554600	-0.19780300	H	-0.42327400	2.15329800	0.06282600
H	0.27285600	-2.11554900	-0.26177400	C	-2.37331700	-1.21336800	-0.02381800
				H	-0.42326700	-2.15329300	0.06285300
				C	-3.06796500	0.00000100	-0.05158000
				H	-2.91601300	2.15437500	-0.03759300
				H	-2.91600700	-2.15437200	-0.03765200
				H	-4.15404200	0.00000200	-0.08966000
				N	1.90357800	0.00017600	-1.53333200
				H	2.93820100	-0.00003300	-1.52836700
	SCF energy= -246.6524288				SCF energy= -825.4745231		
C	0.20210200	-1.47177400	0.00015900	N	-0.00003700	-1.07465900	-0.00010700
C	1.47535200	-0.57491000	0.00002600	C	1.19915500	-0.43346600	-0.11464700
H	0.05061400	-2.08055900	0.89805200	C	2.34405900	-1.16631700	0.24776300
H	0.05089300	-2.08134300	-0.89724100	C	3.64355000	-0.61922100	0.16531500
H	2.09841000	-0.64239100	0.89542400	C	3.81173400	0.70858800	-0.35494300
H	2.09832900	-0.64267500	-0.89541500	C	2.64973600	1.42249100	-0.77967900
N	-0.57302200	-0.22212800	-0.00050900	C	1.39348600	0.88840800	-0.66177800
N	-1.95399700	-0.03489100	0.00015900	H	4.67258400	-2.35490200	0.96001700
H	-2.22311200	0.49998700	0.82559000	H	2.20148800	-2.17737000	0.61979500
H	-2.22394000	0.49972500	-0.82515400	C	4.79951500	-1.34832500	0.56811100
				C	5.11601200	1.25121100	-0.44952200
				H	2.77899300	2.40984300	-1.21878700
				H	0.53568100	1.44029900	-1.03094600
				C	6.21842800	0.52010000	-0.04600800
				C	6.05707000	-0.79111300	0.46605900
				H	5.24017500	2.25661000	-0.84633400
				H	7.21381900	0.94988100	-0.12198900
				H	6.93049500	-1.35747300	0.77870000
				C	-6.05709300	-0.79111100	-0.46599200
				C	-4.79953700	-1.34834000	-0.56804800
				C	-3.64356200	-0.61923000	-0.16529500
				C	-3.81173800	0.70859600	0.35494200
				C	-5.11598500	1.25122700	0.44952400
				C	-6.21842800	0.52010500	0.04604000
				H	-2.20148800	-2.17734400	-0.61985200
				H	-6.93052100	-1.35747600	-0.77861100
				H	-4.67262100	-2.35492600	-0.95993400
				C	-2.34408500	-1.16630600	-0.24778600
				C	-2.64970600	1.42251000	0.77965100
				H	-5.24014900	2.25663600	0.84630700

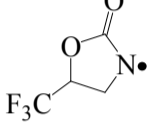
C	0.50707000	0.63148600	-0.00012200	H	-7.21380800	0.94990900	0.12202300
O	0.59134900	1.84219600	0.00010200	C	-1.39346700	0.88845100	0.66176400
				C	-1.19910100	-0.43347300	0.11464300
			SCF energy= -286.0072042	H	-2.77897700	2.40986500	1.21874800
C	1.26665800	-0.84484400	0.10603100	H	-0.53567800	1.44036500	1.03092600
C	1.41100900	0.67322200	-0.18006100				
C	0.00579000	1.20337400	0.13810500				SCF energy= -1231.839118
H	1.89616600	-1.49243000	-0.51669500	N	0.05072900	0.86287400	-0.00045400
H	1.53780500	-1.08466000	1.15170100	S	1.42922600	-0.14032100	-0.00005200
H	1.65178600	0.82895900	-1.23803300	O	1.46407500	-0.87508900	1.27147600
H	2.20393700	1.13820200	0.41275600	O	1.46425500	-0.87536500	-1.27131500
H	-0.07696700	1.56568000	1.17192100	S	-1.54381200	0.22732200	0.00003200
H	-0.34455800	2.00711300	-0.51535000	O	-2.09636900	0.68591400	1.27577300
N	-0.12076100	-1.21510700	-0.05621900	O	-2.09699300	0.68569600	-1.27564600
C	-0.88029600	-0.03795300	-0.00540500	C	2.70573100	1.12166700	-0.00000800
O	-2.10522600	-0.05248800	-0.05309800	H	2.59509500	1.72615200	-0.90161800
				H	2.59642300	1.72465800	0.90276200
			SCF energy= -284.7824943	H	3.65973600	0.58807400	-0.00116200
C	-1.34509300	-0.72487200	0.00006700	C	-1.49474800	-1.57527700	0.00011800
C	-1.31104200	0.78871700	-0.00001200	H	-0.98737800	-1.91662600	0.90364800
C	-0.03367400	1.19312300	0.00000200	H	-2.54326900	-1.88515000	0.00056500
H	-1.85914300	-1.15110700	0.87633600	H	-0.98797400	-1.91682700	-0.90365700
H	-1.85941500	-1.15124200	-0.87599300				
H	-2.19901300	1.41313200	-0.00012700				SCF energy= -1615.394374
H	0.35852300	2.20267700	-0.00005200	N	-0.33064900	-1.10819700	0.00071700
N	0.03074000	-1.18012900	-0.00011200	S	-0.77158000	0.54586000	0.00027800
C	0.83302300	-0.01506200	-0.00000500	O	-0.33555300	1.12231800	1.27831400
O	2.06057400	-0.06299900	0.00003900	O	-0.33539900	1.12230200	-1.27767400
				C	-2.55180300	0.39351400	0.00009100
			SCF energy= -324.1061191	C	-3.22505200	0.33616900	1.22279400
C	1.78637700	0.00791000	-0.10898500	C	-3.22461000	0.33510600	-1.22281900
C	0.98902600	1.27567600	0.00826500	C	-4.61546400	0.21467400	1.21369700
C	-0.35433400	1.26315900	0.02539800	H	-2.67200100	0.39452200	2.15447700
C	0.92657000	-1.22182200	0.28666400	C	-4.61501800	0.21357500	-1.21412700
H	1.53058300	2.21861100	0.06943400	H	-2.67125300	0.39270800	-2.15436400
H	2.13905600	-0.11138300	-1.14426000	C	-5.30697600	0.15129000	-0.00031300
H	2.68180900	0.04433800	0.52364400	H	-5.15688600	0.17148000	2.15442800
H	0.79026200	-1.21022600	1.38126200	H	-5.15607900	0.16949900	-2.15502600
H	1.43119400	-2.15171200	0.01053000	H	-6.38953500	0.05658500	-0.00045800
H	-0.95279500	2.16610500	0.10817700	S	1.31233900	-1.63473300	0.00014700
N	-0.35742000	-1.15705900	-0.37904100	O	1.42062200	-2.33949100	1.28030500
C	-1.10654100	-0.01624500	-0.05801800	O	1.41943400	-2.33897900	-1.28046900
O	-2.32059500	-0.08854800	0.09807000	C	2.45848700	-0.25995000	-0.00007000
				C	2.90364900	0.24766100	-1.22374500
			SCF energy= -285.9773259	C	2.90449500	0.24734400	1.22342900
C	0.88101000	0.02197900	0.44903900	C	3.82242400	1.29740200	-1.21448600
H	1.09676500	0.02287200	1.52872600	H	2.54160700	-0.17386000	-2.15496700
N	-0.11991600	-1.04266400	0.17616800	C	3.82322000	1.29712900	1.21379600
C	-1.10554600	-0.04385000	-0.04683600	H	2.54322600	-0.17443700	2.15483700
O	-2.29991400	-0.18205800	-0.21415700	C	4.27882000	1.82039900	-0.00043900
C	-0.13066300	1.13185400	0.04791700	H	4.18091300	1.70485700	-2.15541600
H	-0.37860400	1.89101400	0.79624800	H	4.18230200	1.70440800	2.15457700
H	0.07061800	1.61879200	-0.91244200	H	4.99425900	2.63850900	-0.00057800
C	2.17821200	-0.14604400	-0.33809300				
H	2.85911100	0.68553500	-0.12300900				SCF energy= -321.9350159
H	2.67247700	-1.08435100	-0.06592800	C	-1.30817600	-0.77331500	0.06458200
				C	-1.30051600	0.76742100	-0.05271900
				H	-1.66497800	-1.11786800	1.05055100
				H	-1.93748800	-1.27958700	-0.67863300
				H	-1.67951500	1.11904800	-1.01798900

H	-1.03182200	1.58961000	-0.92720900	O	2.57672200	-0.21792300	0.32892500
H	-2.23837300	0.47967100	1.33376000	C	0.44676000	1.13404700	-0.02194100
N	0.62064100	0.43222200	-0.53414600	H	0.74763600	1.92836800	-0.71005600
C	1.61335900	-0.06162900	-0.05340000	H	0.15265900	1.56195400	0.94022500
O	2.62622200	-0.56888200	0.28489500	C	-1.86548600	-0.06673900	-0.00219500
N	-2.06117900	-0.90145800	-0.25035400	N	-2.92709200	-0.13331800	0.46299100
H	-1.37676700	-1.32956600	-0.86715600				
H	-2.62161500	-1.60274000	0.22030000				
							
			SCF energy= -583.7987224				
C	0.98449900	-1.52791800	-0.10474200				
C	0.23368800	-0.28028500	-0.63194100				
H	1.21496000	-2.31864400	-0.82807200				
H	0.55271800	-1.99525900	0.79061500				
H	0.13068500	-0.22925300	-1.71972500				
N	2.17969100	-0.73325600	0.24724500				
C	1.49333600	0.45358400	-0.10775500				
O	1.84837400	1.60560000	-0.01123300				
C	-1.10048800	0.06585400	-0.00874400				
F	-1.53641700	1.27870800	-0.40536800				
F	-2.04556400	-0.84473700	-0.35904600				
F	-1.04128700	0.07311000	1.34612800				
							
			SCF energy= -477.7567714				
C	-1.91040800	-0.85875900	-1.15057700				
C	-1.05019200	-0.73475100	0.14343300				
H	-2.28803400	-1.84890800	-1.43455900				
H	-1.45554600	-0.39762900	-2.03931400				
H	-1.16009900	-1.61974200	0.78047800				
N	-2.97291700	0.00839600	-0.60227100				
C	-2.13391800	0.31121400	0.50394300				
O	-2.28488700	1.15014500	1.36528400				
C	0.39800900	-0.32384400	0.06809500				
C	1.39992300	-1.17646900	0.55203800				
C	0.77649100	0.90214800	-0.50196900				
C	2.74849700	-0.82103400	0.46162100				
H	1.12284200	-2.12657400	1.00401800				
C	2.12227300	1.26018900	-0.59333500				
H	0.01717000	1.59128100	-0.86603100				
C	3.11346400	0.39842600	-0.11310100				
H	3.51069600	-1.49576000	0.84287800				
H	2.39644600	2.21567300	-1.03297700				
H	4.16120800	0.67900900	-0.18175900				
							
			SCF energy= -510.5545048				
C	-0.40045800	1.43369100	-0.36311200				
C	0.37015700	0.12715100	-0.66071100				
H	0.00429900	1.92929300	0.53621300				
H	-0.36715300	2.16823200	-1.17655800				
H	0.57350800	-0.02090600	-1.72533500				
C	-1.75929000	-0.34270000	0.08677500				
O	-2.69221000	-1.00722500	0.46455000				
O	-0.53429800	-0.90080800	-0.22940800				
N	-1.75651600	1.05236100	-0.09171700				
C	1.66449300	-0.01769800	0.14229400				
O	1.87054100	0.51237500	1.21085500				
O	2.54414900	-0.82078600	-0.48497200				
H	3.33008300	-0.91424700	0.08803400				
							
			SCF energy= -285.975158				
C	-0.22694700	1.43618600	-0.03176500				
C	-0.66417800	0.03424500	0.47355700				
H	-0.30145700	2.29203100	0.65064900				
H	-0.66567200	1.73108200	-0.99678800				
H	-0.79066300	0.00435600	1.56286000				
N	1.17519200	0.99897200	-0.21448000				
C	0.77528800	-0.33632100	0.07562900				
O	1.41403000	-1.36183700	-0.03395800				
C	-1.80162200	-0.70625700	-0.22443800				
H	-1.82074600	-1.75716800	0.08386200				
H	-2.76963200	-0.25835400	0.02891400				
H	-1.68565700	-0.67717500	-1.31437200				
							
			SCF energy= -321.8888971				
C	-0.53764200	1.32782800	-0.07550200				
C	-0.69688600	-0.11033200	0.45305500				
H	-0.85838100	2.16616500	0.55280400				
H	-0.96231100	1.45112000	-1.08228600				
H	-0.88117000	-0.16770700	1.53463800				
N	0.93650000	1.19245600	-0.13107200				
C	0.80863400	-0.20127000	0.08371100				
O	1.60927200	-1.09880100	-0.06413900				
O	-1.58816300	-0.90805600	-0.28787000				
H	-1.46714700	-1.83927000	-0.03916200				
							
			SCF energy= -338.9084654				
C	-0.45264900	-1.47448300	-0.04256800				
C	0.30020500	-0.26679300	0.59200500				
H	-0.71634600	-2.30341000	0.62490900				
H	0.01458600	-1.88991100	-0.94551700				
H	0.30881200	-0.28067600	1.68753500				
N	-1.62122700	-0.64583800	-0.38974400				
C	-0.93504400	0.51408400	0.04031600				
O	-1.25701800	1.67529700	-0.02772900				
C	1.61604200	0.08336900	0.08202100				
N	2.66090800	0.35077600	-0.34964700				
							
			SCF energy= -435.2758308				
C	0.97053300	-1.40127900	-0.29916900				
C	0.05817700	-0.20879400	-0.64852800				
H	1.29189100	-2.06772700	-1.10753000				
H	0.58333200	-2.01058700	0.53034600				
H	-0.01408700	0.03757800	-1.71162700				
N	2.05994100	-0.51575200	0.16021300				
C	1.19678600	0.59983500	0.04904200				
O	1.34928400	1.74316700	0.40638800				
C	-1.29808500	-0.14748400	0.01027700				
O	-1.66872200	-0.87976700	0.90310600				
O	-2.05026000	0.85144600	-0.49782600				
H	-2.88760200	0.87857400	0.00425000				



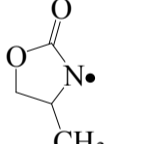
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H	0.85505000	1.56980200	1.03321400
H	0.79452500	2.14916000	-0.62925300
H	1.24993100	-0.05710100	-1.51401200
C	-1.22253000	-0.17898800	0.01345300
O	-2.31736200	-0.66528900	0.17633500
O	-0.10217400	-0.92687800	-0.23830000
N	-0.93071400	1.20177600	0.06899400
C	2.23715500	-0.59554900	0.33149300
H	2.50525600	-1.59920000	-0.01274000
H	3.10151900	0.06215800	0.17799500
H	2.02011200	-0.64330000	1.40455200



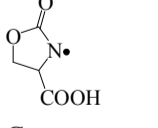
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C	-0.53557600	1.52541700	-0.20057400
C	0.15717400	0.24827300	-0.74626200
H	0.02847100	2.03384600	0.59268500
H	-0.69614000	2.27788800	-0.98770200
H	0.45762600	0.32907100	-1.79460600
C	-1.95521300	-0.25523000	0.01527500
O	-2.91901100	-0.93523800	0.26019200
O	-0.83494700	-0.76128300	-0.62565500
N	-1.81289600	1.11285200	0.30656300
C	1.39740300	-0.15324300	0.05474000
F	1.12048600	-0.30930100	1.36682300
F	1.93949500	-1.29748500	-0.39621900
F	2.33438100	0.82346400	-0.05634700



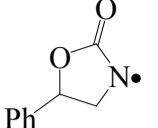
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H	1.14077900	-0.14955400	1.49481600
C	-1.22114400	-0.24484700	-0.03064400
O	-2.34865500	-0.67497200	-0.09599900
O	-0.93170900	1.09724900	-0.05548800
N	-0.05396300	-1.02780400	0.09293800
C	0.49188300	1.27529900	-0.01804900
H	0.83751000	1.56387000	-1.01803000
H	0.72235800	2.07334800	0.69112100
C	2.35025000	-0.53748300	-0.24452400
H	3.14217400	0.17154400	0.02319300
H	2.64178800	-1.53336400	0.10112900
H	2.26090900	-0.56360700	-1.33589500



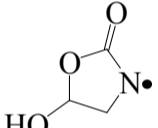
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C	0.35789700	0.04645600	0.56665400
H	0.50359000	-0.19586600	1.63398500
C	-1.78011600	-0.36912700	-0.12644600
O	-2.79159500	-0.96244700	-0.41406200
O	-1.73678500	0.97798100	0.10842800
N	-0.50858100	-0.97180300	0.02340500
C	-0.38616500	1.38626800	0.37489700
H	-0.00124400	1.94345900	-0.48259600



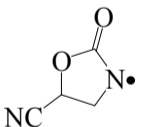
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C	-1.13194600	1.44241700	0.09721600
C	-0.27331900	0.65467700	-0.92898000
H	-0.53322300	1.86307400	0.90849200
H	-1.71119200	2.24742900	-0.37756700
H	-0.14113300	1.23074100	-1.84868200
C	-2.10919100	-0.62754500	-0.35989200
O	-2.94122400	-1.50736400	-0.39673600
O	-1.10509500	-0.48246100	-1.27516400
N	-2.00581000	0.38228400	0.57361400
N	-3.08773300	0.69990000	1.41525000
H	-3.95603600	0.46777800	0.92900500
H	-3.03873900	0.09617100	2.23463900
C	1.08140100	0.21522600	-0.40582800
C	2.14074700	1.13378800	-0.42800200
C	1.30108000	-1.06545500	0.11350400
C	3.39509700	0.78560300	0.07630500
H	1.98744600	2.12716300	-0.84717100
C	2.55825100	-1.41565500	0.61560400
H	0.49769000	-1.79529100	0.10918700
C	3.60657600	-0.49265600	0.60221500
H	4.20743500	1.50741900	0.04964800
H	2.71727800	-2.41497800	1.01259800
H	4.58365200	-0.76860200	0.99015400



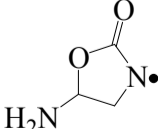
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C	-0.63987300	1.27706600	0.14097700
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H	-1.24387700	1.74250100	-0.64796300
H	-0.70760200	1.93109800	1.02511900
H	-1.57629700	-0.31057700	1.40914200
C	1.15823900	-0.11826600	-0.02765000
O	2.27367000	-0.54349300	-0.20986300
O	0.13546100	-0.89642600	0.47551000
N	0.73833900	1.20513300	-0.26202000
O	-1.91220200	-0.59124400	-0.61300800
H	-2.15450100	-1.52217100	-0.47579000



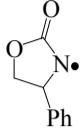
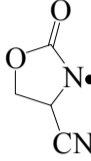
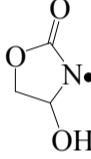
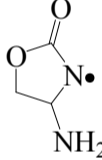
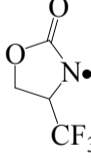
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C	-0.09747800	1.41979100	-0.00659700
C	-0.72469500	0.12883900	0.60978400
H	-0.57587600	1.70141700	-0.95835100
H	-0.17591800	2.29400100	0.65174100
H	-0.89449100	0.23711800	1.68702700
C	1.44142200	-0.27171500	-0.06850000
O	2.44660100	-0.90010800	-0.28170000
O	0.28591700	-0.86447600	0.41212300
N	1.27777200	1.11255100	-0.26183800
C	-1.98359600	-0.27880500	-0.02588900
N	-2.99602600	-0.55605400	-0.52053100



SCF energy= -377.307593

C	-0.61840200	1.29246000	0.16509700
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H	-0.38699400	2.01938200	1.26419600	C	-1.08011500	-0.15008100	0.46911000
C	1.74230000	-0.01654500	-0.09229600	H	-1.24635100	1.80892000	-0.57134900
O	2.13906000	0.76665000	-0.92373600	H	-0.60180700	1.92153300	1.07140900
O	2.45611100	-1.05338700	0.37756200	H	-1.53677200	-0.26308600	1.46099600
H	3.30689600	-1.07703800	-0.10180600	C	1.15904200	-0.12314700	-0.04080600
				O	2.27323600	-0.55059100	-0.22768500
		SCF energy=	-553.0404196	O	0.15476700	-0.87551500	0.52363000
C	-0.62627500	0.49141800	0.37952600	N	0.73082800	1.19059000	-0.32394900
H	-0.73260000	1.20912100	1.21641800	N	-1.86734300	-0.67461100	-0.62884500
C	-2.73991900	-0.34410500	0.15895400	H	-2.12246400	-1.64645100	-0.46192400
O	-3.76630200	-0.91996700	0.43128300	H	-2.72417900	-0.13930700	-0.75754500
O	-2.67848800	0.69614400	-0.73591600				
N	-1.47378300	-0.62776000	0.71350000			SCF energy=	-414.1857078
C	-1.31178700	1.11063100	-0.87133400	C	0.71782500	0.01195700	0.48928900
H	-0.89887400	0.69666700	-1.79755300	H	0.73124400	0.03031800	1.59483700
H	-1.27797300	2.20108100	-0.90485900	C	-1.46757800	-0.31259500	-0.06264000
C	0.84032200	0.15712300	0.21899500	O	-2.54819700	-0.83918100	-0.14268500
C	1.81063400	1.12167400	0.52221600	O	-1.28158100	1.04721700	-0.10267300
C	1.24691500	-1.09136000	-0.27143300	N	-0.24140200	-1.00384600	0.10112700
C	3.16719300	0.84897400	0.32917000	C	0.11593200	1.34602100	-0.04131400
H	1.50712100	2.08969000	0.91694200	H	0.48457900	1.58572700	-1.04326300
C	2.60302700	-1.36619900	-0.45883400	H	0.26889500	2.19189300	0.62996500
H	0.50161200	-1.85195900	-0.48793800	C	2.07985100	-0.26871000	0.02480400
C	3.56609800	-0.39678700	-0.16211600	N	3.16673500	-0.44362000	-0.34105700
H	3.90960700	1.60521900	0.57026300				
H	2.90758000	-2.33996500	-0.83346500			SCF energy=	-397.177884
H	4.62109500	-0.61317600	-0.30810800	C	1.03977600	-0.16478900	0.36721100
				H	1.11222500	-0.23771500	1.47151600
		SCF energy=	-377.3059924	C	-1.19755800	-0.22158000	-0.03688600
C	1.04187400	-0.14054200	0.38711000	O	-2.33399900	-0.62601500	-0.04074700
H	1.13413000	-0.18613300	1.48443000	O	-0.86877100	1.11087400	-0.02986800
C	-1.20546200	-0.23708600	-0.04023200	N	-0.03854100	-1.03172000	-0.03088700
O	-2.33843200	-0.65725300	-0.05361800	C	0.56247700	1.24389900	-0.04032700
O	-0.90331900	1.10313000	-0.03184800	H	0.90845900	1.48347000	-1.05047800
N	-0.04200400	-1.03043200	0.00027400	H	0.84422500	2.03329000	0.65727300
C	0.52306900	1.25628900	-0.03398800	O	2.26483200	-0.46061400	-0.24306300
H	0.86186700	1.51066600	-1.04478000	H	2.48020900	-1.39614000	-0.09267000
H	0.79426500	2.05562900	0.65674600				
N	2.32776000	-0.44531800	-0.19004100			SCF energy=	-659.0798073
H	2.74096300	-1.27467400	0.23008600	C	0.10466200	0.11462000	0.55370700
H	2.24560300	-0.61421900	-1.19172100	H	0.21932900	0.11683000	1.65127900
				C	-2.06189700	-0.31190300	-0.00516400
				O	-3.11570400	-0.88861900	-0.10771100
				O	-1.93605500	1.05198400	-0.07639700
				N	-0.81251900	-0.93907600	0.21120800
				C	-0.55974100	1.42670600	0.06441200
				H	-0.17588000	1.75055800	-0.90762600
				H	-0.49184600	2.24580500	0.78137700
				C	1.50161400	-0.13960500	-0.01452700
				F	1.48463600	-0.25288100	-1.35897500
				F	2.30950200	0.90709500	0.29660900
				F	2.05500400	-1.25260200	0.49334500