Electronic Supplementary Information

N-Methylcarbamoyl Azide: Spectroscopy, X-ray Structure and Decomposition via Methylcarbamoyl Nitrene

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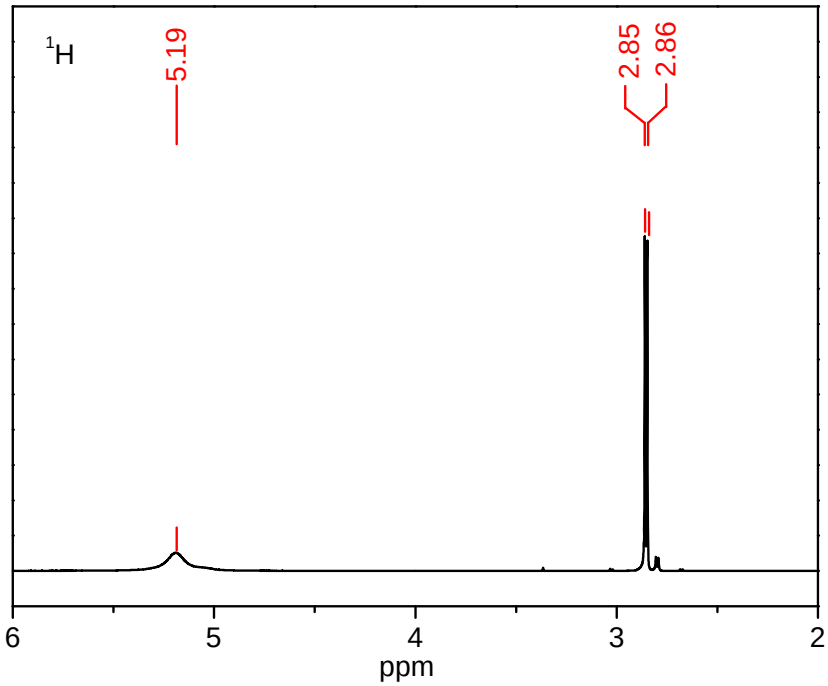

Figure S1. The ^{1}H NMR ($CDCl_3$) of $Me(H)NC(O)N_3$.

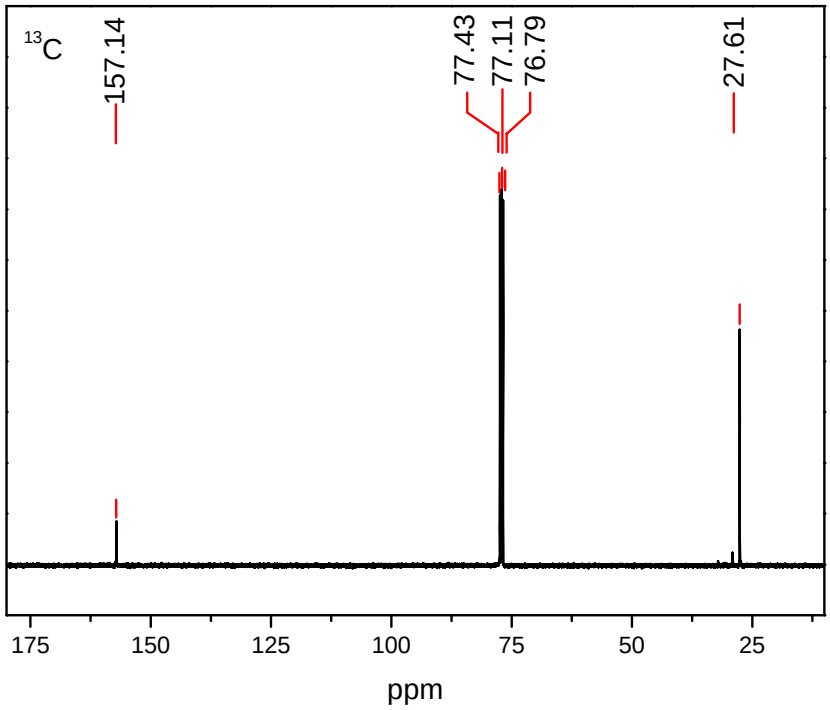

Figure S2. The ^{13}C NMR ($CDCl_3$) of $Me(H)NC(O)N_3$.

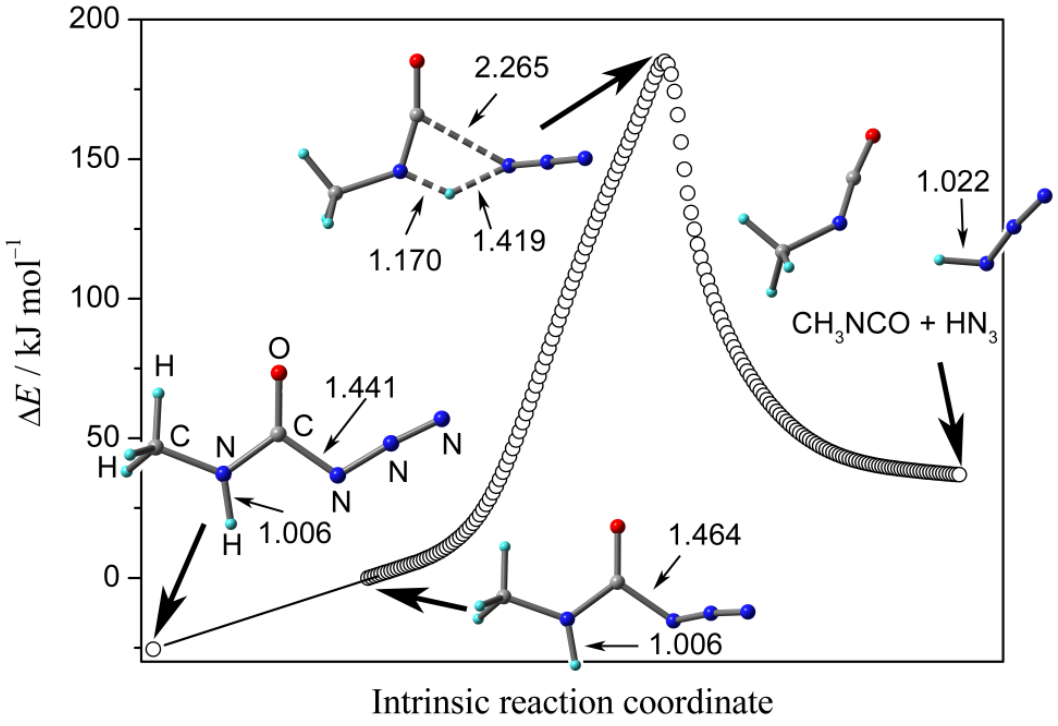

Figure S3. Calculated IRC for the decomposition of Me(H)NC(O)N_3 into CH_3NCO and HN_3 at the B3LYP/6-311++G(3df,3pd) level.

Table S1. Calculated[a] IR frequencies (cm^{-1}) of $Me(H)NC(O)N_3$.

syn-syn	*anti-syn*	*syn-anti*	*anti-anti*
3641 (46)	3648 (62)	3646 (25)	3618 (44)
3147 (1)	3131 (13)	3138 (8)	3126 (11)
3086 (22)	3100 (17)	3105 (14)	3098 (12)
3030 (55)	3036 (41)	3040 (36)	3037 (29)
2283 (585)	2286 (567)	2240 (509)	2252 (476)
1778 (319)	1773 (475)	1795 (553)	1795 (772)
1563 (255)	1523 (43)	1543 (164)	1526 (28)
1503 (26)	1492 (14)	1509 (33)	1501 (9)
1495 (66)	1477 (36)	1482 (18)	1476 (18)
1453 (19)	1463 (9)	1460 (10)	1467 (7)
1316 (298)	1342 (621)	1314 (274)	1330 (353)
1232 (351)	1308 (128)	1229 (253)	1296 (110)
1180 (32)	1196 (4)	1188 (11)	1191 (7)
1154 (11)	1154 (4)	1155 (5)	1149 (5)
1056 (40)	1046 (107)	1064 (29)	1044 (105)
911 (28)	872 (9)	875 (36)	830 (12)
762 (7)	742 (30)	745 (13)	746 (48)
746 (11)	662 (37)	721 (16)	660 (7)
594 (2)	596 (9)	591 (10)	589 (9)
520 (9)	578 (11)	544 (10)	571 (36)
499 (93)	502 (2)	474 (8)	519 (32)
450 (15)	472 (67)	333 (60)	503 (16)
288 (7)	259 (<1)	281 (15)	285 (3)
157 (3)	157 (1)	155 (5)	167 (1)
150 (1)	152 (1)	146 (5)	140 (1)
86 (4)	101 (3)	62 (4)	118 (1)
38 (<1)	47 (1)	49 (6)	78 (4)

[a] Calculation at the B3LYP/6-311++G(3df,3pd) level of theory, IR intensities (km mol^{-1}) in parentheses.

Table S2. Calculated[a] IR frequencies (cm^{-1}) for Me(H)NNCO with different theoretical methods.

B3LYP	B3PW91	M06-2X
3534 (10)	3555 (11)	3569 (16)
3116 (15)	3130 (14)	3150 (10)
3082 (20)	3093 (20)	3114 (14)
3003 (50)	3009 (48)	3031 (33)
2310 (977)	2340 (932)	2365 (1090)
1546 (7)	1550 (5)	1558 (5)
1510 (6)	1504 (9)	1519 (8)
1481 (10)	1474 (11)	1491 (11)
1452 (1)	1445 (<1)	1455 (1)
1407 (3)	1422 (6)	1442 (5)
1206 (30)	1206 (32)	1217 (32)
1152 (2)	1147 (2)	1157 (3)
1035 (5)	1057 (5)	1076 (6)
909 (44)	908 (34)	920 (28)
795 (55)	807 (71)	829 (80)
663 (23)	666 (21)	686 (23)
556 (23)	551 (21)	579 (24)
435 (1)	437 (1)	449 (1)
282 (6)	284 (6)	295 (3)
180 (9)	180 (8)	170 (10)
52 (3)	60 (3)	56(3)

[a] The 6-311++G(3df,3pd) basis set was used. IR intensities (km mol^{-1}) in parentheses.

Table S3. Calculated[a] IR frequencies (cm^{-1}) for singlet Me(H)NC(O)N with different theoretical methods.

syn-singlet			*anti*-singlet		
B3LYP	B3PW91	M06-2X	B3LYP	B3PW91	M06-2X
3637 (50)	3660 (53)	3673 (70)	3627 (55)	3649 (57)	3660 (76)
3142 (3)	3154 (3)	3156 (2)	3134 (7)	3148 (6)	3166 (5)
3097 (17)	3110 (16)	3130 (9)	3105 (13)	3118 (12)	3140 (7)
3040 (41)	3046 (41)	3059 (31)	3037 (36)	3044 (35)	3063 (27)
1831 (443)	1869 (434)	1921 (483)	1835 (416)	1873 (410)	1927 (463)
1528 (3)	1525 (3)	1535 (5)	1541 (28)	1543 (33)	1548 (24)
1493 (7)	1490 (21)	1497 (7)	1502 (17)	1497 (20)	1509 (33)
1491 (17)	1485 (8)	1492 (27)	1496 (16)	1487 (11)	1499 (7)
1458 (14)	1450 (13)	1457 (11)	1466 (13)	1458 (12)	1470 (11)
1359 (22)	1373 (23)	1359 (22)	1310 (26)	1320 (26)	1307 (30)
1154 (<1)	1161 (41)	1171 (46)	1159 (2)	1169 (16)	1178 (19)
1145 (42)	1150 (<1)	1156 (<1)	1153 (12)	1157 (4)	1164 (4)
1133 (21)	1135 (17)	1134 (19)	1143 (21)	1143 (13)	1151 (15)
909 (7)	921 (8)	940 (9)	922 (10)	933 (11)	953 (14)
616 (20)	612 (19)	611 (22)	623 (14)	619 (11)	618 (7)
597 (1)	599 (1)	607 (<1)	581 (10)	585 (10)	610(15)
456 (19)	474 (18)	530 (18)	456 (12)	471 (11)	505 (9)
444 (91)	449 (91)	455 (92)	414 (106)	419 (107)	439 (112)
241 (4)	238 (5)	245 (5)	220 (4)	218 (5)	223 (5)
133 (3)	137 (2)	136 (3)	138 (4)	141(4)	148 (4)
57 (1)	62 (1)	60 (1)	78 (<1)	74 (<1)	100 (1)

[a] The 6-311++G(3df,3pd) basis set was used. IR intensities (km mol^{-1}) in parentheses.

Table S4. Calculated[a] IR frequencies (cm^{-1}) for triplet Me(H)NC(O)N with different theoretical methods.

syn-triplet			*anti*-triplet		
B3LYP	B3PW91	M06-2X	B3LYP	B3PW91	M06-2X
3624 (50)	3643 (50)	3677 (73)	3600 (45)	3623 (46)	3637 (57)
3144 (1)	3158 (<1)	3170 (6)	3137(4)	3147 (4)	3157 (5)
3096 (16)	3100 (15)	3123 (7)	3084 (18)	3099 (16)	3133 (12)
3030 (30)	3039 (33)	3059 (18)	3032 (38)	3038 (38)	3067 (31)
1645 (241)	1680 (259)	1752 (321)	1646 (316)	1675 (339)	1750 (445)
1543 (50)	1550 (58)	1547 (142)	1522 (13)	1519 (13)	1541 (22)
1500 (8)	1489 (7)	1515 (17)	1489 (7)	1480 (7)	1501 (7)
1483 (21)	1481 (18)	1489 (13)	1472 (4)	1465 (3)	1489 (1)
1450 (21)	1440 (18)	1461 (14)	1450 (2)	1449 (<1)	1475 (19)
1229 (55)	1238 (60)	1259 (46)	1350 (92)	1365 (91)	1376 (136)
1166 (3)	1163 (10)	1185 (5)	1162 (26)	1171 (20)	1195 (25)
1144 (8)	1140 (<1)	1159 (1)	1150 (<1)	1145 (<1)	1163 (<1)
1086 (5)	1104 (4)	1117 (6)	1063 (23)	1069 (25)	1081 (33)
894 (8)	901 (13)	921 (4)	851 (8)	862 (9)	867 (4)
687 (14)	689 (11)	701 (21)	686 (74)	688 (73)	697 (65)
625 (6)	627 (4)	637 (7)	567 (10)	570 (10)	580 (9)
467 (108)	486 (111)	415 (13)	522 (37)	525 (37)	512 (52)
401 (19)	400 (20)	383 (94)	467 (25)	463 (25)	492 (19)
263 (3)	266 (3)	253 (3)	273 (<1)	271 (<1)	306 (<1)
152 (1)	153 (1)	147 (3)	132 (1)	136 (1)	151 (1)
30 (<1)	33 (<1)	88 (5)	69 (<1)	70 (<1)	88 (<1)

[a] The 6-311++G(3df,3pd) basis set was used. IR intensities (km mol^{-1}) in parentheses.

Table S5. Calculated vertical transitions for $Me(H)NC(O)N_3$ at the TD-B3LYP/6-311++G(3df,3pd) level.

syn-syn		*anti-syn*		*syn-anti*		*anti-anti*	
energy	Oscillator strength	energy	Oscillator strength	energy	Oscillator strength	energy	Oscillator strength
257.37 nm	f = 0.0004	249.48 nm	f = 0.0005	263.30 nm	f = 0.0005	259.64 nm	f = 0.0019
233.92 nm	f = 0.0002	235.54 nm	f = 0.0005	239.61 nm	f = 0.0005	233.57 nm	f = 0.0013
227.80 nm	f = 0.0004	234.35 nm	f = 0.0004	230.19 nm	f = 0.0013	225.28 nm	f = 0.0039
225.64 nm	f = 0.0007	211.72 nm	f = 0.0933	225.17 nm	f = 0.0012	215.88 nm	f = 0.0156
202.58 nm	f = 0.1839	196.56 nm	f = 0.0001	211. 82 nm	f = 0.0573	205.36 nm	f = 0.0381
195.14 nm	f = 0.0005	194.60 nm	f = 0.1492	201.25 nm	f = 0.0517	198.12 nm	f = 0.0443
191.55 nm	f = 0.0962	183.41 nm	f = 0.0166	195.16 nm	f = 0.0009	194.23 nm	f = 0.0029
180.85 nm	f = 0.034	176.07 nm	f = 0.0030	186.15 nm	f = 0.0004	185.06 nm	f = 0.0018
176.25 nm	f = 0.0005	174.94 nm	f = 0.0121	181.01 nm	f = 0.0030	182.55 nm	f = 0.0023
172.09 nm	f = 0.0107			179.22 nm	f = 0.0089	174.59 nm	f = 0.0427

Table S6. Calculated vertical transitions for Me(H)NC(O)N at the TD-B3LYP/6-311++G(3df,3pd) level.

syn-singlet		*syn*-triplet		*anti*-singlet		*anti*-triplet	
energy	Oscillator strength	energy	Oscillator strength	energy	Oscillator strength	energy	Oscillator strength
591.69 nm	f = 0.0004	537.10 nm	f = 0.0193	581.05 nm	f = 0.0005	578.86 nm	f = 0.0149
276.05 nm	f = 0.0005	443.16 nm	f = 0.0042	225.65 nm	f = 0.0002	432.77 nm	f = 0.0085
229.41 nm	f = 0.0007	401.95 nm	f = 0.0003	212.21 nm	f = 0.0104	299.18 nm	f = 0.0045
212.27 nm	f = 0.0065	287.27 nm	f = 0.0053	203.02 nm	f = 0.0122	244.45 nm	f = 0.0118
202.31 nm	f = 0.0120	241.50 nm	f = 0.0107	198.81 nm	f = 0.0090	213.64 nm	f = 0.0182
199.84 nm	f = 0.0002	212.80 nm	f = 0.0416	184.18 nm	f = 0.0061	198.83 nm	f = 0.0001
184.24 nm	f = 0.0013	200.27 nm	f = 0.0003	180.29 nm	f = 0.0197	198.41 nm	f = 0.0003
179.51 nm	f = 0.0052	189.80 nm	f = 0.0001	179.04 nm	f = 0.0018	188.79 nm	f = 0.0002
178.59 nm	f = 0.0001			163.33 nm	f = 0.0930		
164.70 nm	f = 0.0175						

Table S7. Calculated vertical transitions for Me(H)NNCO at the TD-B3LYP/6-311++G(3df.3pd) level.

energy	Oscillator strength
274.38 nm	f = 0.0125
217.70 nm	f = 0.0016
202.87 nm	f = 0.0036
198.12 nm	f = 0.0065
192.50 nm	f = 0.0218
182.70 nm	f = 0.0472
173.08 nm	f =0.0470
165.84 nm	f = 0.0392
160.61 nm	f = 0.0056

Calculated absolute energies (in Hartrees), and the atomic coordinates (in angstroms) for all optimized structures.

***syn-syn* Me(H)NC(O)N_3**

B3LYP/6-311++G(3df,3pd)

Zero-point correction=	0.077731
Thermal correction to Energy=	0.085108
Thermal correction to Enthalpy=	0.086052
Thermal correction to Gibbs Free Energy=	0.045115
Sum of electronic and zero-point Energies=	-372.870139
Sum of electronic and thermal Energies=	-372.862762
Sum of electronic and thermal Enthalpies=	-372.861818
Sum of electronic and thermal Free Energies=	-372.902755

N	-1.43539900	-0.60082100	-0.01500700
H	-1.35786900	-1.60293100	0.01475800
C	-2.74150000	0.02682200	0.01148800
H	-2.61375900	1.08719900	-0.18476400
H	-3.38342600	-0.40231800	-0.75722900
H	-3.22368400	-0.09367500	0.98331200
C	-0.28584100	0.10904100	-0.00523400
O	-0.18458200	1.31460800	-0.00561500
N	0.83374000	-0.79756200	-0.00112000
N	1.93759800	-0.24286200	0.00260100
N	2.98112300	0.16691300	0.00657200

CBS-QB3

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.076995	E(Thermal)=	0.084374
E(SCF)=	-370.794514	DE(MP2)=	-1.352824
DE(CBS)=	-0.129203	DE(MP34)=	-0.017632
DE(CCSD)=	-0.042853	DE(Int)=	0.041765
DE(Empirical)=	-0.059409		
CBS-QB3 (0 K)=	-372.277674	CBS-QB3 Energy=	-372.270295
CBS-QB3 Enthalpy=	-372.269351	CBS-QB3 Free Energy=	-372.309925

N	-1.43671500	-0.60383700	-0.00033300
H	-1.35357900	-1.60781900	0.00023900
C	-2.74654900	0.02170100	0.00022700
H	-2.60026800	1.10034000	-0.00016200
H	-3.31694900	-0.25930600	-0.88960700
H	-3.31603900	-0.25878000	0.89082300
C	-0.28872500	0.11487800	-0.00011000
O	-0.18891600	1.32114100	-0.00010100
N	0.83335400	-0.79507100	-0.00001100

N	1.94128400	-0.24372200	0.00005100
N	2.99205000	0.16219700	0.00012200

B3LYP/aug-cc-pVTZ

Zero-point correction=			0.077636
Thermal correction to Energy=			0.085000
Thermal correction to Enthalpy=			0.085944
Thermal correction to Gibbs Free Energy=			0.045130
Sum of electronic and zero-point Energies=			-372.877826
Sum of electronic and thermal Energies=			-372.870462
Sum of electronic and thermal Enthalpies=			-372.869518
Sum of electronic and thermal Free Energies=			-372.910332
N	1.07642100	1.12324200	0.00000000
H	1.98278400	0.68855400	0.00000000
C	0.96493500	2.56841000	0.00000000
H	-0.09012000	2.82598200	0.00000000
H	1.43156800	2.99568600	0.88870500
H	1.43156800	2.99568600	-0.88870500
C	0.00000000	0.30631500	0.00000000
O	-1.16312000	0.64549800	0.00000000
N	0.44403400	-1.06462800	0.00000000
N	-0.47115900	-1.89507300	0.00000000
N	-1.22650300	-2.72329100	0.00000000

***anti-syn* Me(H)NC(O)N_3**

B3LYP/6-311++G(3df,3pd)

Zero-point correction=			0.077727
Thermal correction to Energy=			0.085076
Thermal correction to Enthalpy=			0.086020
Thermal correction to Gibbs Free Energy=			0.045271
Sum of electronic and zero-point Energies=			-372.867036
Sum of electronic and thermal Energies=			-372.859687
Sum of electronic and thermal Enthalpies=			-372.858743
Sum of electronic and thermal Free Energies=			-372.899492
N	1.62038300	0.35455500	-0.03017800
H	2.17991300	1.18858900	0.01843900
C	2.27492300	-0.94303300	0.01737500
H	1.87170700	-1.60873300	-0.74244800
H	3.33383100	-0.79584200	-0.18098900
H	2.16589800	-1.42160200	0.99169000
C	0.28852600	0.59070300	-0.00505100
O	-0.22395400	1.68795700	0.01437300
N	-0.45042500	-0.64154900	-0.01299200
N	-1.67784500	-0.49552200	-0.00281400

N	-2.79788700	-0.46778200	0.00660900

CBS-QB3

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.077036	E(Thermal)=	0.084400
E(SCF)=	-370.791188	DE(MP2)=	-1.353476
DE(CBS)=	-0.129210	DE(MP34)=	-0.017450
DE(CCSD)=	-0.042836	DE(Int)=	0.041771
DE(Empirical)=	-0.059393		
CBS-QB3 (0 K)=	-372.274746	CBS-QB3 Energy=	-372.267382
CBS-QB3 Enthalpy=	-372.266438	CBS-QB3 Free Energy=	-372.307203

N	1.62421400	0.35111300	-0.04877500
H	2.17844600	1.19040100	0.02055500
C	2.29368800	-0.93947400	0.02800300
H	1.68231000	-1.69958800	-0.45398300
H	3.24721200	-0.87485100	-0.49887400
H	2.48201600	-1.24751700	1.06216800
C	0.28884400	0.59042800	-0.00712800
O	-0.22127400	1.68848400	0.02380300
N	-0.45729000	-0.64307900	-0.01989800
N	-1.68606300	-0.49470700	-0.00489400
N	-2.81157300	-0.46790300	0.00991900

B3LYP/aug-cc-pVTZ

Zero-point correction=	0.077660
Thermal correction to Energy=	0.084991
Thermal correction to Enthalpy=	0.085935
Thermal correction to Gibbs Free Energy=	0.045312
Sum of electronic and zero-point Energies=	-372.874754
Sum of electronic and thermal Energies=	-372.867423
Sum of electronic and thermal Enthalpies=	-372.866479
Sum of electronic and thermal Free Energies=	-372.907102

N	1.62051200	0.35432600	-0.02933300
H	2.17975100	1.18813300	0.01786000
C	2.27613400	-0.94304200	0.01693400
H	1.87338900	-1.60847600	-0.74367800
H	3.33507300	-0.79420500	-0.18119200
H	2.16745500	-1.42273000	0.99101800
C	0.28839700	0.59039700	-0.00491800
O	-0.22445500	1.68949700	0.01400400
N	-0.45066400	-0.64223500	-0.01270100
N	-1.67835100	-0.49487200	-0.00272300
N	-2.79824300	-0.46905100	0.00645100

***syn-anti* Me(H)NC(O)N_3**

B3LYP/6-311++G(3df,3pd)

Zero-point correction=	0.077196
Thermal correction to Energy=	0.084760
Thermal correction to Enthalpy=	0.085704
Thermal correction to Gibbs Free Energy=	0.044243
Sum of electronic and zero-point Energies=	-372.860348
Sum of electronic and thermal Energies=	-372.852785
Sum of electronic and thermal Enthalpies=	-372.851840
Sum of electronic and thermal Free Energies=	-372.893302

N	-0.77633600	-0.68670800	-0.01422400
H	-0.09841200	-1.41694200	0.11292100
C	-2.18634300	-1.04566000	0.00498900
H	-2.71805400	-0.49959400	-0.77068400
H	-2.27429100	-2.11236900	-0.18545500
H	-2.64787700	-0.81268500	0.96540900
C	-0.40100600	0.61891300	0.00228500
O	-1.16541000	1.54851300	-0.02224900
N	1.01783100	0.88408900	0.03942100
N	1.80293900	-0.06178700	0.00266500
N	2.61070900	-0.84788500	-0.02612500

CBS-QB3

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.076498	E(Thermal)=	0.084039
E(SCF)=	-370.778300	DE(MP2)=	-1.359672
DE(CBS)=	-0.129662	DE(MP34)=	-0.015336
DE(CCSD)=	-0.043772	DE(Int)=	0.042013
DE(Empirical)=	-0.059262		
CBS-QB3 (0 K)=	-372.267493	CBS-QB3 Energy=	-372.259953
CBS-QB3 Enthalpy=	-372.259008	CBS-QB3 Free Energy=	-372.300677

N	-0.78294700	-0.68017000	-0.00345700
H	-0.09023700	-1.40951100	0.04401300
C	-2.18604200	-1.06998700	0.00145100
H	-2.78181700	-0.16681500	-0.11194100
H	-2.39979300	-1.74694200	-0.82934300
H	-2.45825600	-1.55814700	0.94168300
C	-0.40784200	0.63083700	0.00145900
O	-1.15815900	1.57242200	-0.01097300
N	1.01915600	0.88382800	0.01821700
N	1.80069200	-0.06935800	0.00146900
N	2.61433900	-0.85759400	-0.01252800

B3LYP/aug-cc-pVTZ

Zero-point correction=	0.077112
Thermal correction to Energy=	0.084665
Thermal correction to Enthalpy=	0.085609
Thermal correction to Gibbs Free Energy=	0.044245
Sum of electronic and zero-point Energies=	-372.868032
Sum of electronic and thermal Energies=	-372.860480
Sum of electronic and thermal Enthalpies=	-372.859536
Sum of electronic and thermal Free Energies=	-372.900899

N	-0.77717900	-0.68692800	-0.01383600
H	-0.09974000	-1.41713200	0.11217100
C	-2.18748200	-1.04616700	0.00497800
H	-2.71915600	-0.50029600	-0.77113700
H	-2.27477200	-2.11316200	-0.18537700
H	-2.64953200	-0.81314400	0.96538400
C	-0.40097200	0.61895200	0.00222400
O	-1.16564700	1.55009900	-0.02172300
N	1.01859800	0.88366300	0.03854000
N	1.80360200	-0.06240000	0.00244900
N	2.61199500	-0.84773000	-0.02579200

anti-anti **Me(H)NC(O)N_3**

B3LYP/6-311++G(3df,3pd)

Zero-point correction=	0.077712
Thermal correction to Energy=	0.084921
Thermal correction to Enthalpy=	0.085865
Thermal correction to Gibbs Free Energy=	0.045839
Sum of electronic and zero-point Energies=	-372.854027
Sum of electronic and thermal Energies=	-372.846818
Sum of electronic and thermal Enthalpies=	-372.845874
Sum of electronic and thermal Free Energies=	-372.885900

N	0.99669200	0.84129500	-0.27018400
H	1.91016400	1.09476200	-0.61074300
C	0.12719500	1.91435800	0.19459700
H	-0.30310200	1.67180600	1.16478300
H	0.72507100	2.81496600	0.31226100
H	-0.67993600	2.12943800	-0.50663700
C	0.90324200	-0.48956200	0.00700500
O	1.80410300	-1.27457300	-0.13417000
N	-0.36272300	-0.94650300	0.53858900
N	-1.40132300	-0.52488900	0.03093500
N	-2.41373800	-0.23607000	-0.37018700

CBS-QB3

Temperature=	298.150000 Pressure=		1.000000
E(ZPE)=	0.076850 E(Thermal)=		0.084167
E(SCF)=	-370.772078 DE(MP2)=		-1.361157
DE(CBS)=	-0.129479 DE(MP34)=		-0.015369
DE(CCSD)=	-0.043808 DE(Int)=		0.042039
DE(Empirical)=	-0.059220		
CBS-QB3 (0 K)=	-372.262222 CBS-QB3 Energy=		-372.254904
CBS-QB3 Enthalpy=	-372.253960 CBS-QB3 Free Energy=		-372.294369
N	1.01854400	0.82230600	-0.28182500
H	1.93528100	1.05270700	-0.63465700
C	0.17987200	1.91797900	0.19660800
H	-0.17358600	1.72746200	1.21222400
H	0.78171200	2.82639700	0.21570100
H	-0.68310600	2.09626600	-0.45081800
C	0.89518900	-0.50731900	0.00792300
O	1.76906200	-1.32101500	-0.13797700
N	-0.38385100	-0.91344400	0.56617100
N	-1.41505800	-0.49743800	0.03176000
N	-2.42865800	-0.21123500	-0.38265100

B3LYP/aug-cc-pVTZ

Zero-point correction=			0.077624
Thermal correction to Energy=			0.084831
Thermal correction to Enthalpy=			0.085775
Thermal correction to Gibbs Free Energy=			0.045759
Sum of electronic and zero-point Energies=			-372.861535
Sum of electronic and thermal Energies=			-372.854328
Sum of electronic and thermal Enthalpies=			-372.853384
Sum of electronic and thermal Free Energies=			-372.893400
N	1.00224300	0.83803800	-0.26746800
H	1.91582400	1.08605200	-0.61061000
C	0.13735600	1.91692500	0.19283700
H	-0.29607300	1.67944300	1.16309300
H	0.74018400	2.81472400	0.30892200
H	-0.66734500	2.13452000	-0.51077300
C	0.90057300	-0.49264500	0.00755000
O	1.79854800	-1.28333600	-0.13509800
N	-0.36757500	-0.94508100	0.53905900
N	-1.40462200	-0.51956800	0.03048400
N	-2.41698100	-0.22963600	-0.36952900

CH_3(H)NNCO

B3LYP/6-311++G(3df,3pd)

Zero-point correction=			0.067675

Thermal correction to Energy=			0.073195
Thermal correction to Enthalpy=			0.074139
Thermal correction to Gibbs Free Energy=			0.038538
Sum of electronic and zero-point Energies=			-263.329742
Sum of electronic and thermal Energies=			-263.324222
Sum of electronic and thermal Enthalpies=			-263.323278
Sum of electronic and thermal Free Energies=			-263.358879
N	1.12575400	-0.56323600	-0.31162200
C	1.79009500	0.68885000	0.06235000
H	2.81620400	0.63435700	-0.29878200
H	1.29520100	1.52054300	-0.43729900
H	1.79302800	0.87231000	1.14123000
H	1.63899500	-1.34474700	0.07531900
N	-0.16016500	-0.67105900	0.26538800
C	-1.18457000	-0.07818800	0.02070200
O	-2.24196300	0.41170300	-0.08189200

M06-2X

Zero-point correction=			0.068636
Thermal correction to Energy=			0.074091
Thermal correction to Enthalpy=			0.075035
Thermal correction to Gibbs Free Energy=			0.039589
Sum of electronic and zero-point Energies=			-263.214171
Sum of electronic and thermal Energies=			-263.208716
Sum of electronic and thermal Enthalpies=			-263.207772
Sum of electronic and thermal Free Energies=			-263.243218
N	1.14540400	-0.57034800	-0.29344100
C	1.70158300	0.73292200	0.06330500
H	2.74373400	0.74549200	-0.24768400
H	1.16833300	1.50571500	-0.48757500
H	1.63322900	0.94496300	1.13317000
H	1.68790100	-1.30262400	0.14509800
N	-0.15024200	-0.73491400	0.22518300
C	-1.15311200	-0.09846600	0.01998900
O	-2.18626900	0.42956900	-0.07062000

B3PW91

Zero-point correction=			0.067944
Thermal correction to Energy=			0.073437
Thermal correction to Enthalpy=			0.074382
Thermal correction to Gibbs Free Energy=			0.038944
Sum of electronic and zero-point Energies=			-263.221882
Sum of electronic and thermal Energies=			-263.216389
Sum of electronic and thermal Enthalpies=			-263.215444

Sum of electronic and thermal Free Energies=			-263.250882
N	1.13538500	-0.56756800	-0.29353700
C	1.75753900	0.70385600	0.05979500
H	2.79585200	0.66558300	-0.26966500
H	1.25931600	1.51003900	-0.47943800
H	1.72498200	0.92110600	1.13314900
H	1.65684100	-1.32757800	0.12308200
N	-0.15416700	-0.69143400	0.23815100
C	-1.17292500	-0.08361700	0.01482400
O	-2.22665100	0.41530400	-0.07089300

CBS-QB3

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.066997	E(Thermal)=	0.072546
E(SCF)=	-261.859533	DE(MP2)=	-0.951087
DE(CBS)=	-0.091651	DE(MP34)=	-0.024414
DE(CCSD)=	-0.028687	DE(Int)=	0.030125
DE(Empirical)=	-0.043890		
CBS-QB3 (0 K)=	-262.902140	CBS-QB3 Energy=	-262.896590
CBS-QB3 Enthalpy=	-262.895646	CBS-QB3 Free Energy=	-262.931390
N	-1.11168100	-0.55798800	-0.32805400
H	-1.60490300	-1.36351300	0.04227900
C	-1.83825300	0.65917900	0.06080800
H	-1.36320300	1.52537500	-0.40431500
H	-2.85274700	0.57335700	-0.33458400
H	-1.88087400	0.81723800	1.14596400
N	0.16084300	-0.62197600	0.29824100
C	1.20232500	-0.06863700	0.01946000
O	2.27164500	0.39550500	-0.09028200

B3LYP/aug-cc-pVTZ

Zero-point correction=			0.067559
Thermal correction to Energy=			0.073083
Thermal correction to Enthalpy=			0.074028
Thermal correction to Gibbs Free Energy=			0.038457
Sum of electronic and zero-point Energies=			-263.334493
Sum of electronic and thermal Energies=			-263.328969
Sum of electronic and thermal Enthalpies=			-263.328024
Sum of electronic and thermal Free Energies=			-263.363595
N	1.13178400	-0.56554000	-0.30627000
C	1.77931200	0.69721500	0.06232700
H	2.80939200	0.65009800	-0.28912200
H	1.27976400	1.51851100	-0.45019200
H	1.77012500	0.89102700	1.13955000

H	1.64842200	-1.33924500	0.09108300
N	-0.16013200	-0.68324100	0.25612600
C	-1.18123100	-0.08196200	0.01873100
O	-2.23721900	0.41619500	-0.07833300

***syn*-singlet Me(H)NC(O)N**

B3LYP/6-311++G(3df,3pd)

Zero-point correction=	0.065985
Thermal correction to Energy=	0.071797
Thermal correction to Enthalpy=	0.072741
Thermal correction to Gibbs Free Energy=	0.036727
Sum of electronic and zero-point Energies=	-263.263886
Sum of electronic and thermal Energies=	-263.258074
Sum of electronic and thermal Enthalpies=	-263.257130
Sum of electronic and thermal Free Energies=	-263.293143

N	-0.82998000	-0.46633100	0.00000000
H	-1.81697400	-0.27233700	0.00000000
C	-0.36093300	-1.84531900	0.00000000
H	0.72553000	-1.83957400	0.00000000
H	-0.70657100	-2.37190500	0.88913600
H	-0.70657100	-2.37190500	-0.88913600
C	0.00000000	0.57113600	0.00000000
O	1.29433800	0.60687200	0.00000000
N	0.01790500	1.84430800	0.00000000

M06-2X

Zero-point correction=	0.066807
Thermal correction to Energy=	0.072524
Thermal correction to Enthalpy=	0.073468
Thermal correction to Gibbs Free Energy=	0.037693
Sum of electronic and zero-point Energies=	-263.146772
Sum of electronic and thermal Energies=	-263.141054
Sum of electronic and thermal Enthalpies=	-263.140110
Sum of electronic and thermal Free Energies=	-263.175886

N	-0.87200500	-0.42757700	0.00000000
H	-1.84944900	-0.19148100	0.00000000
C	-0.44740500	-1.81793500	0.00000000
H	0.63863300	-1.83683000	0.00000000
H	-0.80796300	-2.33039900	0.88910700
H	-0.80796300	-2.33039900	-0.88910700
C	0.00000000	0.56578500	0.00000000
O	1.30072600	0.56046200	0.00000000
N	0.17277100	1.81590700	0.00000000

B3PW91

Zero-point correction=	0.066296
Thermal correction to Energy=	0.072071
Thermal correction to Enthalpy=	0.073015
Thermal correction to Gibbs Free Energy=	0.037159
Sum of electronic and zero-point Energies=	-263.156196
Sum of electronic and thermal Energies=	-263.150422
Sum of electronic and thermal Enthalpies=	-263.149477
Sum of electronic and thermal Free Energies=	-263.185334

N	-0.84034700	-0.45764300	0.00000000
H	-1.82418300	-0.25113500	0.00000000
C	-0.38759600	-1.83439800	0.00000000
H	0.70007900	-1.83904000	0.00000000
H	-0.73670200	-2.36009000	0.88959700
H	-0.73670200	-2.36009000	-0.88959700
C	0.00000000	0.56641800	0.00000000
O	1.29428800	0.59688700	0.00000000
N	0.06445800	1.83523300	0.00000000

CBS-QB3

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.065211	E(Thermal)=	0.071129
E(SCF)=	-261.787786	DE(MP2)=	-0.949104
DE(CBS)=	-0.092396	DE(MP34)=	-0.033676
DE(CCSD)=	-0.032388	DE(Int)=	0.030261
DE(Empirical)=	-0.043633		
CBS-QB3 (0 K)=	-262.843509	CBS-QB3 Energy=	-262.837592
CBS-QB3 Enthalpy=	-262.836647	CBS-QB3 Free Energy=	-262.873449

N	0.70344400	-0.64570700	-0.00010700
H	0.83386200	-1.64477100	0.00007800
C	1.86116400	0.24168100	0.00004900
H	1.50333500	1.27031600	-0.00002100
H	2.47260000	0.08600200	0.89198200
H	2.47284300	0.08596600	-0.89170900
C	-0.54586700	-0.17923300	-0.00001800
O	-0.97211700	1.04415400	-0.00002600
N	-1.76022600	-0.57221200	0.00006300

B3LYP/aug-cc-pVTZ

Zero-point correction=	0.065945
Thermal correction to Energy=	0.071737
Thermal correction to Enthalpy=	0.072681
Thermal correction to Gibbs Free Energy=	0.036793
Sum of electronic and zero-point Energies=	-263.269478

Sum of electronic and thermal Energies=			-263.263687
Sum of electronic and thermal Enthalpies=			-263.262742
Sum of electronic and thermal Free Energies=			-263.298630
N	-0.83189000	-0.46529400	0.00000000
H	-1.81799000	-0.26887000	0.00000000
C	-0.36606900	-1.84575200	0.00000000
H	0.72063000	-1.84233300	0.00000000
H	-0.71318100	-2.37166000	0.88916900
H	-0.71318100	-2.37166000	-0.88916900
C	0.00000000	0.57090700	0.00000000
O	1.29720800	0.60618700	0.00000000
N	0.02367200	1.84445000	0.00000000

***syn*-triplet Me(H)NC(O)N**

B3LYP/6-311++G(3df,3pd)

Zero-point correction=			0.065292
Thermal correction to Energy=			0.071092
Thermal correction to Enthalpy=			0.072036
Thermal correction to Gibbs Free Energy=			0.034481
Sum of electronic and zero-point Energies=			-263.280640
Sum of electronic and thermal Energies=			-263.274839
Sum of electronic and thermal Enthalpies=			-263.273895
Sum of electronic and thermal Free Energies=			-263.311450
N	-0.56743800	-0.61990900	-0.01355100
H	-0.53862100	-1.62539100	0.03023000
C	-1.84744100	0.06430400	0.00460400
H	-1.70215100	1.07693700	-0.36100200
H	-2.55262300	-0.45512000	-0.64166700
H	-2.26080700	0.11552000	1.01395900
C	0.61816600	0.03891900	-0.00056900
O	0.76540600	1.25416300	-0.00056200
N	1.75409600	-0.77503200	0.00480400

M06-2X

Zero-point correction=			0.066198
Thermal correction to Energy=			0.071939
Thermal correction to Enthalpy=			0.072883
Thermal correction to Gibbs Free Energy=			0.036219
Sum of electronic and zero-point Energies=			-263.164437
Sum of electronic and thermal Energies=			-263.158697
Sum of electronic and thermal Enthalpies=			-263.157752
Sum of electronic and thermal Free Energies=			-263.194416
N	-0.54473400	-0.64324200	-0.01272800
H	-0.50033700	-1.64705000	0.02414100

C	-1.81991400	0.04508300	0.00452000
H	-1.85264500	0.77949300	-0.79755600
H	-2.61384200	-0.68122300	-0.13555500
H	-1.96646900	0.56603900	0.95006600
C	0.61090800	0.05580800	-0.00138000
O	0.69880000	1.26438600	-0.00030600
N	1.77286700	-0.74785700	0.00451500

B3PW91

Zero-point correction=	0.065566
Thermal correction to Energy=	0.071335
Thermal correction to Enthalpy=	0.072279
Thermal correction to Gibbs Free Energy=	0.034874
Sum of electronic and zero-point Energies=	-263.173504
Sum of electronic and thermal Energies=	-263.167735
Sum of electronic and thermal Enthalpies=	-263.166791
Sum of electronic and thermal Free Energies=	-263.204196

N	0.56772800	-0.61532400	0.00012500
H	0.53623100	-1.62133400	0.00001800
C	1.84237800	0.06293200	-0.00005500
H	1.65249000	1.13355600	-0.00169500
H	2.42166700	-0.19322700	0.88894600
H	2.42264200	-0.19586900	-0.88763000
C	-0.61554200	0.04216800	0.00002900
O	-0.76876100	1.25323500	0.00000800
N	-1.74543700	-0.78176200	-0.00006000

CBS-QB3

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.064735	E(Thermal)=	0.070480
E(SCF)=	-261.866804	DE(MP2)=	-0.876508
DE(CBS)=	-0.088959	DE(MP34)=	-0.041551
DE(CCSD)=	-0.026785	DE(Int)=	0.027960
DE(Empirical)=	-0.041927		
CBS-QB3 (0 K)=	-262.849840	CBS-QB3 Energy=	-262.844094
CBS-QB3 Enthalpy=	-262.843150	CBS-QB3 Free Energy=	-262.880056

N	-0.57028700	-0.62035100	-0.00005500
H	-0.54214500	-1.62869100	0.00010100
C	-1.85236400	0.06516400	0.00001900
H	-1.65630800	1.13593800	-0.00115300
H	-2.43339700	-0.19199300	-0.88993800
H	-2.43241900	-0.19016100	0.89115800
C	0.61983700	0.04008600	-0.00000200
O	0.77146700	1.25629800	-0.00000500

N	1.75424400	-0.78064600	0.00002200

B3LYP/aug-cc-pVTZ

Zero-point correction=			0.065185
Thermal correction to Energy=			0.071008
Thermal correction to Enthalpy=			0.071952
Thermal correction to Gibbs Free Energy=			0.034059
Sum of electronic and zero-point Energies=			-263.285742
Sum of electronic and thermal Energies=			-263.279920
Sum of electronic and thermal Enthalpies=			-263.278976
Sum of electronic and thermal Free Energies=			-263.316869
N	-0.56796600	-0.61975700	-0.01288600
H	-0.53929200	-1.62484700	0.03021100
C	-1.84841500	0.06436300	0.00461700
H	-1.70306600	1.07719600	-0.36100200
H	-2.55317200	-0.45554400	-0.64207300
H	-2.26230100	0.11558600	1.01401000
C	0.61837200	0.03874500	-0.00040800
O	0.76662200	1.25536700	-0.00062200
N	1.75441100	-0.77652400	0.00411100

***anti*-singlet Me(H)NC(O)N**

B3LYP/6-311++G(3df,3pd)

Zero-point correction=			0.065924
Thermal correction to Energy=			0.071745
Thermal correction to Enthalpy=			0.072689
Thermal correction to Gibbs Free Energy=			0.036854
Sum of electronic and zero-point Energies=			-263.264309
Sum of electronic and thermal Energies=			-263.258487
Sum of electronic and thermal Enthalpies=			-263.257543
Sum of electronic and thermal Free Energies=			-263.293378
N	-0.70829400	-0.57746600	-0.05106700
H	-0.75097100	-1.57632500	0.06812400
C	-1.92547400	0.21851400	0.02247300
H	-1.73325700	1.19909700	-0.40691900
H	-2.70789800	-0.26066400	-0.56142400
H	-2.26944700	0.34597000	1.04990600
C	0.50057000	-0.02919400	-0.00901700
O	1.67815100	-0.56703400	0.02183800
N	1.07769200	1.10493500	-0.00680900

M06-2X

Zero-point correction=			0.066929
Thermal correction to Energy=			0.072601

Thermal correction to Enthalpy=			0.073545
Thermal correction to Gibbs Free Energy=			0.038182
Sum of electronic and zero-point Energies=			-263.146723
Sum of electronic and thermal Energies=			-263.141052
Sum of electronic and thermal Enthalpies=			-263.140108
Sum of electronic and thermal Free Energies=			-263.175470
N	-0.72593200	-0.57674500	-0.03993800
H	-0.77402700	-1.57762700	0.05440200
C	-1.92766400	0.23750100	0.01772200
H	-1.66690000	1.25051800	-0.27740800
H	-2.66746700	-0.14548800	-0.67975700
H	-2.34835400	0.26007800	1.02155300
C	0.47756000	-0.03361800	-0.00744300
O	1.67372800	-0.54191700	0.01757500
N	1.12129600	1.05168200	-0.00592900

B3PW91

Zero-point correction=			0.066216
Thermal correction to Energy=			0.072022
Thermal correction to Enthalpy=			0.072966
Thermal correction to Gibbs Free Energy=			0.037145
Sum of electronic and zero-point Energies=			-263.156556
Sum of electronic and thermal Energies=			-263.150750
Sum of electronic and thermal Enthalpies=			-263.149806
Sum of electronic and thermal Free Energies=			-263.185627
N	-0.71565000	-0.57301100	-0.04724300
H	-0.76227900	-1.57197500	0.06384200
C	-1.92358400	0.22465500	0.02078800
H	-1.70882200	1.22258300	-0.35691100
H	-2.69276200	-0.21789900	-0.61011500
H	-2.30074400	0.31045100	1.04187500
C	0.49166300	-0.03047000	-0.00821800
O	1.67211500	-0.56157300	0.02013300
N	1.09839500	1.08505500	-0.00635300

CBS-QB3

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.065260	E(Thermal)=	0.071074
E(SCF)=	-261.787861	DE(MP2)=	-0.949505
DE(CBS)=	-0.092274	DE(MP34)=	-0.033510
DE(CCSD)=	-0.032520	DE(Int)=	0.030238
DE(Empirical)=	-0.043611		
CBS-QB3 (0 K)=	-262.843783	CBS-QB3 Energy=	-262.837970
CBS-QB3 Enthalpy=	-262.837026	CBS-QB3 Free Energy=	-262.872707

N	-0.70581100	-0.58669500	-0.06818100
H	-0.74766100	-1.58153700	0.09339600
C	-1.91992200	0.21625500	0.02946800
H	-1.74990000	1.17510900	-0.46151900
H	-2.73169400	-0.29143800	-0.49165300
H	-2.21455700	0.39948700	1.06729800
C	0.50586400	-0.03077600	-0.01283900
O	1.68250900	-0.56806200	0.02892600
N	1.05839400	1.11955100	-0.00877600

B3LYP/aug-cc-pVTZ

Zero-point correction=	0.065856
Thermal correction to Energy=	0.071682
Thermal correction to Enthalpy=	0.072626
Thermal correction to Gibbs Free Energy=	0.036757
Sum of electronic and zero-point Energies=	-263.269897
Sum of electronic and thermal Energies=	-263.264071
Sum of electronic and thermal Enthalpies=	-263.263127
Sum of electronic and thermal Free Energies=	-263.298996

N	-0.70980700	-0.57695300	-0.04887200
H	-0.75257400	-1.57587500	0.06604000
C	-1.92775000	0.21904400	0.02150600
H	-1.73467300	1.19932300	-0.40865700
H	-2.70900800	-0.26170300	-0.56306100
H	-2.27312700	0.34748500	1.04852200
C	0.49919400	-0.02884400	-0.00838700
O	1.68035700	-0.56670400	0.02078000
N	1.08093000	1.10312400	-0.00652800

***anti*-triplet Me(H)NC(O)N**

B3LYP/6-311++G(3df,3pd)

Zero-point correction=	0.065433
Thermal correction to Energy=	0.071113
Thermal correction to Enthalpy=	0.072057
Thermal correction to Gibbs Free Energy=	0.035301
Sum of electronic and zero-point Energies=	-263.277310
Sum of electronic and thermal Energies=	-263.271629
Sum of electronic and thermal Enthalpies=	-263.270685
Sum of electronic and thermal Free Energies=	-263.307442

N	-0.62157500	-0.56528100	0.00000000
H	-1.62937600	-0.52251700	0.00000000
C	0.02831200	-1.86466900	0.00000000
H	1.10599200	-1.72739600	0.00000000
H	-0.24679500	-2.43646200	0.88716300

H	-0.24679500	-2.43646200	-0.88716300
C	0.00000000	0.63816600	0.00000000
O	-0.57112100	1.72469400	0.00000000
N	1.39529900	0.66304000	0.00000000

M06-2X

Zero-point correction=	0.066654
Thermal correction to Energy=	0.072184
Thermal correction to Enthalpy=	0.073128
Thermal correction to Gibbs Free Energy=	0.036868
Sum of electronic and zero-point Energies=	-263.160713
Sum of electronic and thermal Energies=	-263.155184
Sum of electronic and thermal Enthalpies=	-263.154239
Sum of electronic and thermal Free Energies=	-263.190499

N	-0.56489100	-0.61696900	0.00007800
H	-0.53278200	-1.62459700	0.00002400
C	-1.85107600	0.05191200	-0.00003300
H	-1.69566100	1.12670400	-0.00053100
H	-2.42475900	-0.21266100	-0.88676000
H	-2.42456100	-0.21188600	0.88705600
C	0.64650700	-0.01718600	0.00000200
O	1.71417200	-0.59279300	-0.00003600
N	0.64943400	1.39645900	0.00002000

B3PW91

Zero-point correction=	0.065679
Thermal correction to Energy=	0.071348
Thermal correction to Enthalpy=	0.072292
Thermal correction to Gibbs Free Energy=	0.035582
Sum of electronic and zero-point Energies=	-263.170199
Sum of electronic and thermal Energies=	-263.164529
Sum of electronic and thermal Enthalpies=	-263.163585
Sum of electronic and thermal Free Energies=	-263.200296

N	-0.57509600	-0.61126100	0.00017000
H	-0.55026300	-1.61904400	0.00015600
C	-1.85480300	0.06229000	-0.00006700
H	-1.69401300	1.13804400	-0.00091700
H	-2.43374700	-0.19880500	-0.88783000
H	-2.43346200	-0.19745500	0.88828300
C	0.63642700	-0.01325100	-0.00010500
O	1.71063800	-0.60078800	-0.00004600
N	0.68033100	1.38116500	0.00007300

CBS-QB3

Temperature=	298.150000 Pressure=		1.000000
E(ZPE)=	0.064798 E(Thermal)=		0.070506
E(SCF)=	-261.863018 DE(MP2)=		-0.875247
DE(CBS)=	-0.088969 DE(MP34)=		-0.042432
DE(CCSD)=	-0.027363 DE(Int)=		0.027881
DE(Empirical)=	-0.042083		
CBS-QB3 (0 K)=	-262.846433 CBS-QB3 Energy=		-262.840725
CBS-QB3 Enthalpy=	-262.839781 CBS-QB3 Free Energy=		-262.876667
N	-0.62521200	-0.56605900	0.00000000
H	-1.63472100	-0.52288800	0.00000000
C	0.02740100	-1.86718900	0.00000000
H	1.10739900	-1.72587600	0.00000000
H	-0.24473700	-2.44139000	0.89005000
H	-0.24473700	-2.44139000	-0.89005000
C	0.00000000	0.64054400	0.00000000
O	-0.56946900	1.72930500	0.00000000
N	1.39780400	0.65991200	0.00000000

B3LYP/aug-cc-pVTZ

Zero-point correction=	0.065332
Thermal correction to Energy=	0.071027
Thermal correction to Enthalpy=	0.071972
Thermal correction to Gibbs Free Energy=	0.035144
Sum of electronic and zero-point Energies=	-263.282392
Sum of electronic and thermal Energies=	-263.276696
Sum of electronic and thermal Enthalpies=	-263.275752
Sum of electronic and thermal Free Energies=	-263.312580

N	-0.62135000	-0.56593100	0.00000000
H	-1.62882500	-0.52314900	0.00000000
C	0.02848800	-1.86585700	0.00000000
H	1.10634700	-1.72882700	0.00000000
H	-0.24628300	-2.43752700	0.88738600
H	-0.24628300	-2.43752700	-0.88738600
C	0.00000000	0.63814600	0.00000000
O	-0.57225300	1.72579800	0.00000000
N	1.39594100	0.66406100	0.00000000

CH_3NCO

B3LYP/6-311++G(3df,3pd)

Zero-point correction=	0.050556
Thermal correction to Energy=	0.055283
Thermal correction to Enthalpy=	0.056227
Thermal correction to Gibbs Free Energy=	0.022958
Sum of electronic and zero-point Energies=	-208.020477

Sum of electronic and thermal Energies=			-208.015750
Sum of electronic and thermal Enthalpies=			-208.014806
Sum of electronic and thermal Free Energies=			-208.048075
C	1.32776600	1.12646700	0.00000000
H	1.25822900	2.21122300	0.00000000
H	1.88021800	0.81601500	0.88743100
H	1.88021800	0.81601500	-0.88743100
N	0.00000000	0.57225100	0.00000000
C	-0.55447000	-0.48750500	0.00000000
O	-1.20730500	-1.46034700	0.00000000

CBS-QB3

Zero-point correction=			0.050573
Thermal correction to Energy=			0.055275
Thermal correction to Enthalpy=			0.056220
Thermal correction to Gibbs Free Energy=			0.023213
Sum of electronic and zero-point Energies=			-207.999144
Sum of electronic and thermal Energies=			-207.994441
Sum of electronic and thermal Enthalpies=			-207.993497
Sum of electronic and thermal Free Energies=			-208.026503
C	1.33754100	1.11626200	0.00000000
H	1.27999100	2.20448100	0.00000000
H	1.88853100	0.79916300	0.88963900
H	1.88853100	0.79916300	-0.88963900
N	0.00000000	0.57710300	0.00000000
C	-0.55839000	-0.48375900	0.00000000
O	-1.21649500	-1.45469400	0.00000000

B3LYP/aug-cc-pVTZ

Zero-point correction=			0.050499
Thermal correction to Energy=			0.055217
Thermal correction to Enthalpy=			0.056161
Thermal correction to Gibbs Free Energy=			0.023034
Sum of electronic and zero-point Energies=			-208.024229
Sum of electronic and thermal Energies=			-208.019511
Sum of electronic and thermal Enthalpies=			-208.018567
Sum of electronic and thermal Free Energies=			-208.051694
C	1.32783600	1.12853700	0.00000000
H	1.25632300	2.21337800	0.00000000
H	1.87988100	0.81798000	0.88772200
H	1.87988100	0.81798000	-0.88772200
N	0.00000000	0.57223700	0.00000000
C	-0.55394200	-0.48789600	0.00000000
O	-1.20743100	-1.46235500	0.00000000

HN_3

B3LYP/6-311++G(3df,3pd)

Zero-point correction=			0.021447
Thermal correction to Energy=			0.024651
Thermal correction to Enthalpy=			0.025596
Thermal correction to Gibbs Free Energy=			-0.001514
Sum of electronic and zero-point Energies=			-164.828789
Sum of electronic and thermal Energies=			-164.825585
Sum of electronic and thermal Enthalpies=			-164.824640
Sum of electronic and thermal Free Energies=			-164.851750
N	0.08051300	-1.12125700	0.00000000
H	1.05426500	-1.41739000	0.00000000
N	0.00000000	0.11115200	0.00000000
N	-0.23112300	1.21258900	0.00000000

CBS-QB3

Zero-point correction=			0.021374
Thermal correction to Energy=			0.024595
Thermal correction to Enthalpy=			0.025539
Thermal correction to Gibbs Free Energy=			-0.001608
Sum of electronic and zero-point Energies=			-164.809164
Sum of electronic and thermal Energies=			-164.805943
Sum of electronic and thermal Enthalpies=			-164.804999
Sum of electronic and thermal Free Energies=			-164.832146
N	0.10298300	-1.12297600	0.00000000
H	1.08597000	-1.39324200	0.00000000
N	0.00000000	0.11035900	0.00000000
N	-0.25812200	1.21165200	0.00000000

B3LYP/aug-cc-pVTZ

Zero-point correction=			0.021429
Thermal correction to Energy=			0.024634
Thermal correction to Enthalpy=			0.025578
Thermal correction to Gibbs Free Energy=			-0.001533
Sum of electronic and zero-point Energies=			-164.833036
Sum of electronic and thermal Energies=			-164.829832
Sum of electronic and thermal Enthalpies=			-164.828888
Sum of electronic and thermal Free Energies=			-164.855999
N	0.08406300	-1.12118700	0.00000000
H	1.05868700	-1.41369800	0.00000000
N	0.00000000	0.11126100	0.00000000
N	-0.23530400	1.21188200	0.00000000

TS1

B3LYP/6-311++G(3df,3pd)

Zero-point correction=	0.077386
Thermal correction to Energy=	0.083975
Thermal correction to Enthalpy=	0.084920
Thermal correction to Gibbs Free Energy=	0.046021
Sum of electronic and zero-point Energies=	-372.857120
Sum of electronic and thermal Energies=	-372.850530
Sum of electronic and thermal Enthalpies=	-372.849586
Sum of electronic and thermal Free Energies=	-372.888485

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.00542500
C	1.27044700	0.00000000	-0.70872100
H	1.13453100	-0.45413500	-1.68639200
H	1.65626700	1.01131300	-0.84877900
H	1.99153100	-0.58314800	-0.14091400
C	-1.16116800	0.28567800	-0.63041700
O	-1.29305500	0.50956000	-1.80321100
N	-2.29655800	0.35950900	0.29414700
N	-2.74779800	-0.70882500	0.69729800
N	-3.24920400	-1.62842100	1.11579000

CBS-QB3

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.076600	E(Thermal)=	0.083228
E(SCF)=	-370.775200	DE(MP2)=	-1.359246
DE(CBS)=	-0.129428	DE(MP34)=	-0.015957
DE(CCSD)=	-0.043657	DE(Int)=	0.042004
DE(Empirical)=	-0.059241		
CBS-QB3 (0 K)=	-372.264124	CBS-QB3 Energy=	-372.257497
CBS-QB3 Enthalpy=	-372.256552	CBS-QB3 Free Energy=	-372.295610

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.00757800
C	1.27406200	0.00000000	-0.70645800
H	1.06743700	-0.06996500	-1.77250300
H	1.83739400	0.91897400	-0.51791400
H	1.87396200	-0.85869800	-0.39849800
C	-1.17151000	0.26955800	-0.62950600
O	-1.32259700	0.48343400	-1.80243600
N	-2.29760400	0.33796600	0.31245000
N	-2.71402700	-0.73323900	0.75509100
N	-3.19083700	-1.65218900	1.21509700

B3LYP/aug-cc-pVTZ

Zero-point correction=			0.077250
Thermal correction to Energy=			0.083860
Thermal correction to Enthalpy=			0.084805
Thermal correction to Gibbs Free Energy=			0.045835
Sum of electronic and zero-point Energies=			-372.864820
Sum of electronic and thermal Energies=			-372.858210
Sum of electronic and thermal Enthalpies=			-372.857266
Sum of electronic and thermal Free Energies=			-372.896236
N	1.02800400	-0.64194600	0.22231000
H	0.62447000	-1.37910800	0.77335100
C	2.42405200	-0.73814200	-0.17712700
H	2.56901500	-0.19719700	-1.10857200
H	3.09069600	-0.31334400	0.57565500
H	2.67508700	-1.78535300	-0.32876000
C	0.34252300	0.51891800	0.12098500
O	0.76132200	1.55004900	-0.33544900
N	-1.00399600	0.42885500	0.69533300
N	-1.84595700	-0.16767900	0.02933300
N	-2.69937800	-0.67780800	-0.50286600

TS2

B3LYP/6-311++G(3df,3pd)

Zero-point correction=			0.077050
Thermal correction to Energy=			0.083397
Thermal correction to Enthalpy=			0.084341
Thermal correction to Gibbs Free Energy=			0.046436
Sum of electronic and zero-point Energies=			-372.840456
Sum of electronic and thermal Energies=			-372.834109
Sum of electronic and thermal Enthalpies=			-372.833165
Sum of electronic and thermal Free Energies=			-372.871070
N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.01480900
C	1.39388100	0.00000000	-0.48224300
H	1.39410800	0.10376800	-1.56635500
H	1.89676400	0.86868500	-0.06356300
H	1.94720500	-0.90335400	-0.21253200
C	-0.71993500	-1.15633600	-0.42069400
O	-0.42546100	-2.30002100	-0.18726100
N	-1.85349500	-0.77382300	-1.17981800
N	-2.54570500	-1.72361100	-1.59319500
N	-3.24159300	-2.49058700	-2.01565500

CBS-QB3

Temperature=	298.150000	Pressure=	1.000000

E(ZPE)=	0.076295	E(Thermal)=	0.082683
E(SCF)=	-370.766339	DE(MP2)=	-1.351980
DE(CBS)=	-0.128330	DE(MP34)=	-0.018766
DE(CCSD)=	-0.043184	DE(Int)=	0.041679
DE(Empirical)=	-0.059258		
CBS-QB3 (0 K)=	-372.249883	CBS-QB3 Energy=	-372.243495
CBS-QB3 Enthalpy=	-372.242551	CBS-QB3 Free Energy=	-372.280549

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.01710300
C	1.39942900	0.00000000	-0.47323200
H	1.40638200	0.09116700	-1.56125700
H	1.89707900	0.87916800	-0.06275900
H	1.95822100	-0.89980900	-0.19008500
C	-0.70317100	-1.17340100	-0.41006900
O	-0.39482000	-2.31256200	-0.16623900
N	-1.84115400	-0.80764700	-1.17724400
N	-2.52684700	-1.76657300	-1.58755600
N	-3.22422100	-2.53854900	-2.01244400

B3LYP/aug-cc-pVTZ

Zero-point correction=	0.076928
Thermal correction to Energy=	0.083286
Thermal correction to Enthalpy=	0.084231
Thermal correction to Gibbs Free Energy=	0.046301
Sum of electronic and zero-point Energies=	-372.848160
Sum of electronic and thermal Energies=	-372.841802
Sum of electronic and thermal Enthalpies=	-372.840857
Sum of electronic and thermal Free Energies=	-372.878787

N	1.53282900	-0.45378200	-0.50096700
H	1.87360600	-0.10239200	-1.38958800
C	2.53883300	-0.18727100	0.54437400
H	2.21861700	-0.65840100	1.47283200
H	3.47417700	-0.65134900	0.23933600
H	2.70559300	0.87779000	0.72644600
C	0.28935000	0.19239300	-0.23857300
O	0.11965100	1.37743400	-0.09589400
N	-0.74897000	-0.76860900	-0.15385300
N	-1.87783300	-0.29323200	0.07576500
N	-2.93435400	0.01335900	0.27667200

TS3

B3LYP/6-311++G(3df,3pd)

Zero-point correction=	0.077154
Thermal correction to Energy=	0.083460

Thermal correction to Enthalpy=	0.084404		
Thermal correction to Gibbs Free Energy=	0.046534		
Sum of electronic and zero-point Energies=	-372.839753		
Sum of electronic and thermal Energies=	-372.833447		
Sum of electronic and thermal Enthalpies=	-372.832503		
Sum of electronic and thermal Free Energies=	-372.870373		
N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.01518200
C	1.40003900	0.00000000	-0.47018400
H	1.41325700	0.08188200	-1.55598900
H	1.89613000	0.87726700	-0.06127600
H	1.94906700	-0.89783600	-0.17746200
C	-0.71285400	-1.17979200	-0.41501600
O	-0.40177000	-2.30764700	-0.15862100
N	-1.86420400	-0.93074600	-1.19441900
N	-2.14675200	0.25752900	-1.42699700
N	-2.52787700	1.26917200	-1.71815600

CBS-QB3

Temperature=	298.150000 Pressure=		1.000000
E(ZPE)=	0.076648 E(Thermal)=		0.083229
E(SCF)=	-370.771062 DE(MP2)=		-1.360862
DE(CBS)=	-0.129548 DE(MP34)=		-0.015606
DE(CCSD)=	-0.043668 DE(Int)=		0.042059
DE(Empirical)=	-0.059230		
CBS-QB3 (0 K)=	-372.261269 CBS-QB3 Energy=		-372.254688
CBS-QB3 Enthalpy=	-372.253744 CBS-QB3 Free Energy=		-372.292440
N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.01746700
C	1.40580700	0.00000000	-0.46089000
H	1.42644300	0.06550800	-1.55053700
H	1.89648100	0.88873300	-0.06280200
H	1.95954800	-0.89326300	-0.15184400
C	-0.69824800	-1.19735500	-0.40492200
O	-0.37971900	-2.31928300	-0.12785400
N	-1.84522600	-0.96421600	-1.20217400
N	-2.12407800	0.22528200	-1.45014200
N	-2.50581800	1.23697500	-1.75877100

B3LYP/aug-cc-pVTZ

Zero-point correction=	0.077033
Thermal correction to Energy=	0.083352
Thermal correction to Enthalpy=	0.084296
Thermal correction to Gibbs Free Energy=	0.046396

Sum of electronic and zero-point Energies=			-372.847423
Sum of electronic and thermal Energies=			-372.841104
Sum of electronic and thermal Enthalpies=			-372.840159
Sum of electronic and thermal Free Energies=			-372.878059
N	-0.75970700	-0.64595700	0.53172200
H	-1.14479700	-0.56695000	1.46747300
C	-1.75691100	-1.30614100	-0.33530600
H	-1.32430200	-1.46460400	-1.32221500
H	-1.98633200	-2.28013000	0.09144300
H	-2.67864000	-0.72958600	-0.44285800
C	-0.45499900	0.69097100	0.09276900
O	-1.24778300	1.58286900	-0.02799800
N	0.90509600	0.91690600	-0.21583600
N	1.68724400	-0.03819900	-0.06540300
N	2.50848000	-0.79427300	0.01885500

TS4

B3LYP/6-311++G(3df,3pd)

Zero-point correction=			0.077371
Thermal correction to Energy=			0.083961
Thermal correction to Enthalpy=			0.084905
Thermal correction to Gibbs Free Energy=			0.045857
Sum of electronic and zero-point Energies=			-372.853562
Sum of electronic and thermal Energies=			-372.846972
Sum of electronic and thermal Enthalpies=			-372.846028
Sum of electronic and thermal Free Energies=			-372.885077
N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.00737800
C	1.27632400	0.00000000	-0.69837100
H	1.22682200	0.63858300	-1.57680200
H	2.03526700	0.39795600	-0.02896400
H	1.58093200	-1.00227300	-1.00584300
C	-1.23809900	-0.01304600	-0.54632400
O	-2.26870100	0.01848900	0.07201900
N	-1.23472100	0.02428100	-2.00914000
N	-1.02786300	-1.03427100	-2.59271300
N	-0.86382200	-1.95327100	-3.22627400

CBS-QB3

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.076648	E(Thermal)=	0.083229
E(SCF)=	-370.771062	DE(MP2)=	-1.360862
DE(CBS)=	-0.129548	DE(MP34)=	-0.015606
DE(CCSD)=	-0.043668	DE(Int)=	0.042059

DE(Empirical)=	-0.059230		
CBS-QB3 (0 K)=	-372.261269 CBS-QB3 Energy=		-372.254688
CBS-QB3 Enthalpy=	-372.253744 CBS-QB3 Free Energy=		-372.292440
N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.00887200
C	1.27696900	0.00000000	-0.70448200
H	1.29127400	0.76720200	-1.47966800
H	2.06412100	0.22210700	0.01583900
H	1.49776200	-0.96932200	-1.16210200
C	-1.23843700	0.06878000	-0.55117100
O	-2.27182000	0.14357500	0.05859400
N	-1.21281000	0.12960200	-2.01822800
N	-1.03380300	-0.93001900	-2.61677000
N	-0.88967600	-1.84453500	-3.27009600

B3LYP/aug-cc-pVTZ

Zero-point correction=	0.077285		
Thermal correction to Energy=	0.083866		
Thermal correction to Enthalpy=	0.084810		
Thermal correction to Gibbs Free Energy=	0.045878		
Sum of electronic and zero-point Energies=	-372.861164		
Sum of electronic and thermal Energies=	-372.854582		
Sum of electronic and thermal Enthalpies=	-372.853638		
Sum of electronic and thermal Free Energies=	-372.892571		
N	1.38007600	0.35656400	-0.22461100
H	2.25116800	0.13988400	-0.68091200
C	1.07706900	1.74740500	0.07782900
H	0.61908900	1.83128200	1.06063100
H	2.00909000	2.30783000	0.08556600
H	0.41251400	2.19748300	-0.66248800
C	0.61960700	-0.73036300	0.04443000
O	0.93204600	-1.86977100	-0.18689200
N	-0.62587400	-0.41887200	0.74793000
N	-1.55471600	0.00954100	0.07082900
N	-2.47495500	0.39268700	-0.45717800

TS5

B3LYP/6-311++G(3df,3pd)

Zero-point correction=	0.073074		
Thermal correction to Energy=	0.081193		
Thermal correction to Enthalpy=	0.082137		
Thermal correction to Gibbs Free Energy=	0.039557		
Sum of electronic and zero-point Energies=	-372.809931		
Sum of electronic and thermal Energies=	-372.801813		

Sum of electronic and thermal Enthalpies=			-372.800869
Sum of electronic and thermal Free Energies=			-372.843449
N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.00306700
C	1.26619900	0.00000000	-0.71209700
H	1.05112800	0.00017600	-1.77753000
H	1.85089300	0.88870700	-0.47294400
H	1.85083700	-0.88883300	-0.47323900
C	-1.17723200	-0.00092600	-0.65757900
O	-1.32587400	-0.00148800	-1.89614900
N	-2.42558900	-0.00138700	-0.19343400
N	-2.44945700	-0.00060400	1.60823200
N	-3.09199300	-0.00050600	2.49748100

CBS-QB3

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.072385	E(Thermal)=	0.080501
E(SCF)=	-370.745816	DE(MP2)=	-1.317475
DE(CBS)=	-0.126197	DE(MP34)=	-0.038485
DE(CCSD)=	-0.045425	DE(Int)=	0.041503
DE(Empirical)=	-0.059225		
CBS-QB3 (0 K)=	-372.218735	CBS-QB3 Energy=	-372.210619
CBS-QB3 Enthalpy=	-372.209674	CBS-QB3 Free Energy=	-372.252108

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.00501300
C	1.26552900	0.00000000	-0.71736100
H	1.04107000	-0.00117200	-1.78357900
H	1.85283200	0.89221200	-0.48382600
H	1.85386100	-0.89108800	-0.48210000
C	-1.17882400	-0.00150000	-0.66310900
O	-1.32399200	-0.00239800	-1.90313500
N	-2.42855300	-0.00230000	-0.19318700
N	-2.45401700	-0.00102800	1.60125400
N	-3.12432700	-0.00071300	2.47650100

B3LYP/aug-cc-pVTZ

Zero-point correction=	0.073054
Thermal correction to Energy=	0.081129
Thermal correction to Enthalpy=	0.082073
Thermal correction to Gibbs Free Energy=	0.039813
Sum of electronic and zero-point Energies=	-372.818426
Sum of electronic and thermal Energies=	-372.810351
Sum of electronic and thermal Enthalpies=	-372.809407
Sum of electronic and thermal Free Energies=	-372.851667

N	0.91938300	-0.73625500	0.00000400
H	0.26498500	-1.49599500	0.00001500
C	2.34389900	-1.02264900	-0.00000300
H	2.87533000	-0.07428400	-0.00002600
H	2.63090600	-1.58522900	0.88904200
H	2.63088800	-1.58526200	-0.88903200
C	0.45586000	0.53025400	0.00000200
O	1.15167400	1.56799000	-0.00000400
N	-0.79318400	0.99372000	0.00000500
N	-1.98675300	-0.35170700	0.00000200
N	-3.05574000	-0.59844000	-0.00000600

TS6

B3LYP/6-311++G(3df,3pd)

Zero-point correction=	0.064406
Thermal correction to Energy=	0.069805
Thermal correction to Enthalpy=	0.070749
Thermal correction to Gibbs Free Energy=	0.035758
Sum of electronic and zero-point Energies=	-263.247277
Sum of electronic and thermal Energies=	-263.241878
Sum of electronic and thermal Enthalpies=	-263.240934
Sum of electronic and thermal Free Energies=	-263.275925

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.01051600
C	1.28532400	0.00000000	-0.68525900
H	1.10565600	0.00922700	-1.75653400
H	1.89629300	0.86304100	-0.41222700
H	1.82890400	-0.91042900	-0.43466300
C	-1.12388000	0.57297300	-0.58829600
O	-1.68007500	0.19112600	-1.63576100
N	-1.62731600	1.58991200	-0.00618400

CBS-QB3

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.063737	E(Thermal)=	0.069139
E(SCF)=	-261.772578	DE(MP2)=	-0.919836
DE(CBS)=	-0.090536	DE(MP34)=	-0.044575
DE(CCSD)=	-0.044884	DE(Int)=	0.029766
DE(Empirical)=	-0.043792		
CBS-QB3 (0 K)=	-262.822699	CBS-QB3 Energy=	-262.817297
CBS-QB3 Enthalpy=	-262.816353	CBS-QB3 Free Energy=	-262.851316

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.24712200
N	1.13248500	0.00000000	-0.81890000

N	-1.13362100	0.01811800	-0.59034400
C	2.06445500	1.12224000	-0.79317100
H	2.01281600	1.58517500	0.19120200
H	3.08181200	0.75568700	-0.94847100
H	1.83483000	1.87068100	-1.55893800
H	1.03966000	-0.52030300	-1.68228700

B3LYP/aug-cc-pVTZ

Zero-point correction=	0.064309
Thermal correction to Energy=	0.069720
Thermal correction to Enthalpy=	0.070665
Thermal correction to Gibbs Free Energy=	0.035645
Sum of electronic and zero-point Energies=	-263.252258
Sum of electronic and thermal Energies=	-263.246846
Sum of electronic and thermal Enthalpies=	-263.245902
Sum of electronic and thermal Free Energies=	-263.280922

N	0.65970300	-0.34576800	-0.46960900
H	0.75314200	-1.22155600	-0.96406100
C	1.81333400	0.15333900	0.26682500
H	1.54107800	1.09283600	0.73972100
H	2.15055000	-0.55252900	1.02910200
H	2.63209400	0.34075100	-0.42754300
C	-0.63635900	-0.02596400	-0.07449100
O	-1.14040700	1.11552400	-0.05507900
N	-1.37619700	-0.98965200	0.31381000

TS7

B3LYP/6-311++G(3df,3pd)

Zero-point correction=	0.073053
Thermal correction to Energy=	0.080935
Thermal correction to Enthalpy=	0.081879
Thermal correction to Gibbs Free Energy=	0.040180
Sum of electronic and zero-point Energies=	-372.809025
Sum of electronic and thermal Energies=	-372.801143
Sum of electronic and thermal Enthalpies=	-372.800199
Sum of electronic and thermal Free Energies=	-372.841898

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.00871000
C	1.29478400	0.00000000	-0.66446500
H	1.13436800	0.15958500	-1.72786300
H	1.89039800	0.82356300	-0.27310600
H	1.84443700	-0.93354800	-0.51942400
C	-1.09539100	-0.68250200	-0.63419100
O	-1.56576600	-0.41063300	-1.71235500

N	-1.22368500	-1.64383700	0.27556200
N	-2.74043900	-2.50026000	-0.15574000
N	-3.42312200	-3.35131700	-0.06838000

CBS-QB3

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.072323	E(Thermal)=	0.080215
E(SCF)=	-370.745039	DE(MP2)=	-1.320734
DE(CBS)=	-0.126086	DE(MP34)=	-0.035417
DE(CCSD)=	-0.045644	DE(Int)=	0.041503
DE(Empirical)=	-0.059134		
CBS-QB3 (0 K)=	-372.218228	CBS-QB3 Energy=	-372.210336
CBS-QB3 Enthalpy=	-372.209392	CBS-QB3 Free Energy=	-372.251103

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.01072200
C	1.29777400	0.00000000	-0.66378600
H	1.12862900	0.10022000	-1.73580100
H	1.87324100	0.86191800	-0.31896600
H	1.87435700	-0.91239800	-0.47307400
C	-1.09315400	-0.69920700	-0.63526800
O	-1.56438000	-0.43765200	-1.71524800
N	-1.20303500	-1.65928700	0.28286100
N	-2.68404100	-2.56286800	-0.10684300
N	-3.30499000	-3.45726800	0.05139000

B3LYP/ aug-cc-pVTZ

Zero-point correction=	0.072971
Thermal correction to Energy=	0.080857
Thermal correction to Enthalpy=	0.081801
Thermal correction to Gibbs Free Energy=	0.040094
Sum of electronic and zero-point Energies=	-372.817431
Sum of electronic and thermal Energies=	-372.809544
Sum of electronic and thermal Enthalpies=	-372.808600
Sum of electronic and thermal Free Energies=	-372.850308

N	-1.54176300	-0.36363700	-0.50143400
H	-1.44844000	-1.21115300	-1.03987900
C	-2.62399100	-0.30858300	0.47060300
H	-2.68732200	0.70661400	0.85508000
H	-3.55956400	-0.55186200	-0.03157000
H	-2.47940800	-1.00097000	1.30408300
C	-0.32022000	0.33763800	-0.20915500
O	-0.21269100	1.53061900	-0.04550800
N	0.44827900	-0.74136000	-0.08780200
N	2.12603900	-0.11691600	0.01808700

N	3.18766400	-0.25836000	0.24367200

TS8

B3LYP/6-311++G(3df,3pd)

Zero-point correction=	0.070609
Thermal correction to Energy=	0.078531
Thermal correction to Enthalpy=	0.079475
Thermal correction to Gibbs Free Energy=	0.036770
Sum of electronic and zero-point Energies=	-372.796790
Sum of electronic and thermal Energies=	-372.788868
Sum of electronic and thermal Enthalpies=	-372.787923
Sum of electronic and thermal Free Energies=	-372.830629

N	1.16730700	-0.48559900	0.05180400
H	0.13768300	-0.94147300	0.37052600
C	2.52557600	-0.97510400	-0.21535100
H	3.17984400	-0.15670200	-0.50639500
H	2.91712100	-1.44905000	0.68223200
H	2.48405000	-1.70530900	-1.02021900
C	0.81707300	0.73076600	0.03809100
O	0.81599800	1.88028300	-0.07033300
N	-1.07640700	-0.30077900	0.73158700
N	-2.08328700	-0.28636700	0.05982400
N	-3.05083800	-0.25921300	-0.54320300

CBS-QB3

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.069946	E(Thermal)=	0.077852
E(SCF)=	-370.680052	DE(MP2)=	-1.388953
DE(CBS)=	-0.131197	DE(MP34)=	-0.002588
DE(CCSD)=	-0.047186	DE(Int)=	0.043254
DE(Empirical)=	-0.058532		
CBS-QB3 (0 K)=	-372.195309	CBS-QB3 Energy=	-372.187402
CBS-QB3 Enthalpy=	-372.186458	CBS-QB3 Free Energy=	-372.228987

N	1.16594500	-0.49495900	0.04889300
H	0.11929900	-0.95286400	0.37963700
C	2.53668000	-0.95807200	-0.21425000
H	3.17465600	-0.12849700	-0.52089300
H	2.94301400	-1.41129000	0.69101500
H	2.50999300	-1.70330500	-1.00968200
C	0.79979600	0.72060400	0.04167000
O	0.81153100	1.87349900	-0.07018600
N	-1.06175800	-0.29708800	0.72060300
N	-2.08100600	-0.28535300	0.05743600
N	-3.06004800	-0.26077500	-0.53309000

B3LYP/aug-cc-pVTZ

Zero-point correction=	0.070523
Thermal correction to Energy=	0.078442
Thermal correction to Enthalpy=	0.079386
Thermal correction to Gibbs Free Energy=	0.036707
Sum of electronic and zero-point Energies=	-372.804688
Sum of electronic and thermal Energies=	-372.796770
Sum of electronic and thermal Enthalpies=	-372.795826
Sum of electronic and thermal Free Energies=	-372.838504

N	1.16887800	-0.48667900	0.05156200
H	0.13610600	-0.94324500	0.36852700
C	2.52905200	-0.97270200	-0.21462300
H	3.18161800	-0.15216600	-0.50417200
H	2.92051500	-1.44669700	0.68325300
H	2.48983100	-1.70249300	-1.02029300
C	0.81660200	0.72928000	0.03817900
O	0.81480600	1.88044300	-0.06936700
N	-1.07479500	-0.30190000	0.72647200
N	-2.08455200	-0.28691800	0.05868200
N	-3.05530900	-0.25856100	-0.53867500

CASPT2(8,8)/6-311+G** Calculated energies (in Hartrees) of Me(H)NC(O)N.

syn-singlet Me(H)NC(O)N (CSS)

CASPT2 Energy: -262.598958384636 u.a

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22220000	0.9376470
22022000	-0.2270802
22200200	-0.1090922
22a2b000	-0.0601058
22b2a000	0.0601058
22baab00	-0.0561257
22abba00	-0.0561257
20220020	-0.0533506

N	-0.059626	0.129600	-0.122610
C	-1.298970	0.682099	0.016099
C	0.468096	-0.743188	0.919629
O	-1.932753	0.680517	1.117703
N	-1.921207	1.302551	-0.997399
H	-0.107853	-1.669584	1.014649
H	1.508093	-0.983061	0.671771
H	0.446348	-0.218886	1.875062
H	0.246942	-0.019291	-1.072894

anti-singlet Me(H)NC(O)N (CSS)

CASPT2 Energy: -262.599788785962 u.a.

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22220000	0.9368714
22022000	-0.2298671
22200200	-0.1094002
22a2b000	-0.0607932
22b2a000	0.0607932
22abba00	-0.0560281
22baab00	-0.0560281
20220020	-0.0530291

N	-0.107174	-0.075044	-0.020557
C	-1.188031	0.634207	0.347325
C	0.336178	0.001807	-1.410850
O	-1.648402	0.897753	1.536797
N	-2.175239	1.249435	-0.193945
H	0.823102	0.954612	-1.640760
H	1.026082	-0.819667	-1.604145
H	-0.533426	-0.119347	-2.058943
H	0.595829	-0.167305	0.699968

syn-triplet Me(H)NC(O)N (T)

CASPT2 Energy: -262.61559462 u.a.

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222aa000	0.9723652
220aa200	-0.1162440
2220aa00	-0.0665902
22a2a000	-0.0545118
22abaa00	-0.0533169
2202aa00	0.0527310

N	-0.108279	0.094570	-0.117360
C	-1.327354	0.667648	0.074780
C	0.474103	-0.747526	0.918129
O	-1.955192	0.665307	1.125417
N	-1.839909	1.333416	-1.064446
H	-0.085561	-1.679424	1.044019
H	1.504762	-0.973017	0.643415
H	0.465611	-0.207043	1.865187
H	0.220889	0.006830	-1.067129

***anti*-triplet Me(H)NC(O)N (T)**

CASPT2 Energy: -262.61425330 u.a.

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222aa000	0.9720080
202aa200	-0.0966843
2a22a000	0.0567186
2220aa00	0.0540110

N	-0.114650	-0.198844	-0.076099
C	-1.027524	0.806968	-0.191150
C	-0.064215	-1.131731	1.044452
O	-1.241696	1.462562	-1.205549
N	-1.750555	1.131367	0.980634
H	-0.824480	-1.915519	0.967533
H	0.924255	-1.592104	1.069148
H	-0.209767	-0.588491	1.978511
H	0.292582	-0.483616	-0.956850