Electronic Supplementary Information (ESI) for

The decomposition of benzenesulfonyl azide: A matrix isolation and computational study

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Table S1. Calculated harmonic IR frequencies (unscaled, cm^{-1}) for $PhS(O)_2N_3$ with different theoretical methods.

B3LYP[a]	M06-2X[a]	MPW1PW91[a]	CBS-QB3
3215 (5)	3209 (6)	3236 (6)	3211 (5)
3214 (<1)	3205 (<1)	3235 (<1)	3210 (<1)
3199 (6)	3198 (<1)	3223 (4)	3195 (9)
3190 (7)	3192 (4)	3214 (6)	3186 (9)
3178 (<1)	3181 (<1)	3201 (<1)	3174 (<1)
2251 (554)	2348 (515)	2313 (552)	2248 (532)
1622 (2)	1661 (2)	1649 (3)	1627 (<1)
1621 (<1)	1658 (<1)	1647 (<1)	1626 (2)
1511 (4)	1519 (3)	1517 (3)	1509 (4)
1479 (21)	1488 (29)	1486 (27)	1479 (22)
1404 (152)	1450 (164)	1442 (152)	1381 (130)
1351 (12)	1342 (9)	1366 (9)	1347 (21)
1330 (2)	1326 (<1)	1341 (3)	1332 (1)
1269 (244)	1279 (267)	1308 (253)	1261 (224)
1204 (4)	1231 (268)	1223 (227)	1202 (2)
1189 (143)	1200 (7)	1204 (10)	1187 (<1)
1188 (<1)	1177 (<1)	1187 (<1)	1163 (216)
1104 (5)	1124 (36)	1116 (36)	1103 (6)
1094 (31)	1110 (5)	1110 (6)	1086 (33)
1041 (1)	1056 (1)	1052 (1)	1043 (3)
1024 (<1)	1038 (<1)	1026 (<1)	1019 (<1)
1006 (<1)	1016 (<1)	1009 (<1)	1015 (2)
1000 (2)	1005 (1)	998 (1)	995 (<1)
958 (<1)	967 (<1)	961 (<1)	951 (<1)
865 (<1)	874 (<1)	870 (<1)	860 (<1)
773 (15)	803 (121)	777 (19)	771 (17)
742 (122)	778 (25)	767 (132)	730 (104)
717 (11)	735 (44)	729 (26)	710 (13)
695 (32)	703 (39)	693 (37)	704 (33)
627 (<1)	635 (183)	624 (25)	628 (<1)
606 (259)	624 (36)	622 (199)	597 (280)
586 (8)	623 (7)	604 (12)	569 (10)
566 (86)	581 (93)	575 (86)	557 (86)
488 (9)	511 (4)	499 (4)	480 (15)
449 (2)	463 (2)	459 (2)	441 (2)
429 (<1)	449 (2)	442 (<1)	414 (2)
411 (<1)	409 (<1)	408 (<1)	412 (<1)
333 (<1)	342 (<1)	339 (<1)	324 (<1)
313 (1)	322 (2)	319 (1)	309 (<1)
268 (<1)	281 (<1)	274 (<1)	264 (1)

190 (<1)	191 (<1)	189 (<1)	191 (<1)
152 (<1)	159 (<1)	154 (<1)	151 (<1)
118 (<1)	119 (<1)	119 (<1)	118 (<1)
38 (<1)	38 (<1)	38 (<1)	40 (<1)
29 (<1)	30 (<1)	31 (<1)	29 (<1)

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

Table S2. Calculated harmonic IR frequencies (unscaled, cm^{-1}) for singlet and triplet $PhS(O)_2N$ with different theoretical methods.

$PhS(O)_2N$ (^1A)				$PhS(O)_2N$ (^3A)			
B3LYP[a]	M06-2X[a]	MPW1PW91[a]	CBS-QB3	B3LYP[a]	M06-2X[a]	MPW1PW91[a]	CBS-QB3
3221 (3)	3222 (6)	3242 (4)	3216 (3)	3215 (7)	3220 (7)	3236 (8)	3210 (7)
3214 (3)	3218 (2)	3235 (4)	3211 (3)	3214 (<1)	3218 (<1)	3235 (<1)	3209 (<1)
3200 (5)	3206 (<1)	3224 (3)	3196 (8)	3199 (5)	3208 (<1)	3223 (3)	3195 (7)
3191 (7)	3200 (5)	3215 (6)	3187 (9)	3191 (7)	3203 (4)	3215 (6)	3187 (9)
3178 (<1)	3185 (<1)	3202 (<1)	3175 (<1)	3178 (<1)	3189 (<1)	3201 (<1)	3175 (<1)
1621 (4)	1662 (2)	1648 (4)	1626 (2)	1618 (28)	1658 (<1)	1644 (24)	1622 (26)
1620 (<1)	1657 (3)	1646 (1)	1624 (3)	1611 (<1)	1657 (15)	1639 (<1)	1617 (<1)
1509 (3)	1520 (3)	1516 (3)	1506 (4)	1507 (<1)	1519 (<1)	1513 (<1)	1504 (<1)
1480 (19)	1492 (25)	1488 (22)	1480 (21)	1477 (18)	1492 (21)	1484 (20)	1477 (20)
1374 (131)	1440 (158)	1417 (145)	1352 (13)	1353 (2)	1427 (169)	1389 (131)	1350 (2)
1349 (29)	1345 (13)	1370 (17)	1338 (95)	1336 (148)	1347 (14)	1368 (25)	1332 (<1)
1334 (5)	1334 (2)	1341 (3)	1333 (49)	1331 (<1)	1334 (<1)	1338 (5)	1310 (138)
1204 (<1)	1205 (<1)	1204 (<1)	1201 (<1)	1204 (<1)	1230 (210)	1207 (62)	1201 (<1)
1189 (<1)	1182 (1)	1188 (<1)	1187 (<1)	1189 (<1)	1205 (18)	1197 (152)	1187 (<1)
1116 (129)	1157 (159)	1144 (152)	1110 (101)	1163 (206)	1185 (<1)	1188 (<1)	1140 (200)
1105 (4)	1112 (4)	1110 (5)	1103 (6)	1104 (4)	1123 (28)	1114 (24)	1103 (5)
1048 (11)	1085 (20)	1067 (22)	1047 (<1)	1090 (16)	1114 (3)	1110 (5)	1079 (12)
1028 (32)	1055 (5)	1049 (11)	1019 (3)	1040 (<1)	1057 (<1)	1051 (<1)	1042 (3)
1024 (<1)	1040 (<1)	1025 (<1)	1017 (<1)	1026 (<1)	1043 (<1)	1027 (<1)	1021 (<1)
1007 (<1)	1020 (<1)	1010 (<1)	994 (65)	1007 (<1)	1024 (<1)	1011 (<1)	1014 (5)
989 (13)	997 (12)	989 (18)	994 (6)	998 (3)	1005 (<1)	997 (1)	997 (<1)
962 (<1)	994 (7)	986 (3)	949 (1)	963 (<1)	977 (<1)	966 (<1)	956 (<1)
954 (15)	973 (2)	964 (2)	918 (20)	864 (<1)	882 (<1)	869 (<1)	860 (<1)
865 (<1)	877 (<1)	869 (<1)	858 (<1)	777 (30)	797 (12)	784 (19)	774 (33)
770 (49)	777 (46)	770 (51)	765 (50)	734 (16)	763 (60)	751 (34)	728 (16)
717 (15)	733 (25)	727 (20)	715 (13)	697 (3)	721 (11)	714 (9)	699 (32)
687 (21)	696 (26)	683 (21)	696 (27)	690 (30)	703 (30)	689 (28)	677 (6)
626 (<1)	623 (<1)	623 (<1)	628 (<1)	625 (<1)	622 (<1)	622 (<1)	627 (<1)
549 (116)	580 (105)	558 (112)	543 (118)	545 (81)	561 (100)	553 (86)	536 (82)
513 (25)	523 (40)	518 (28)	507 (23)	519 (36)	534 (39)	526 (37)	514 (38)
448 (8)	502 (15)	470 (8)	428 (9)	434 (8)	444 (9)	438 (8)	428 (9)
411 (<1)	416 (3)	410 (<1)	411 (<1)	412 (3)	425 (4)	418 (4)	410 (<1)

392 (4)	406 (1)	402 (3)	383 (4)	408 (<1)	410 (<1)	406 (<1)	406 (3)
378 (<1)	393 (1)	387 (1)	358 (2)	310 (<1)	320 (1)	316 (<1)	306 (<1)
309 (2)	319 (3)	316 (3)	305 (3)	283 (3)	303 (3)	291 (3)	277 (3)
263 (1)	279 (1)	267 (1)	258 (1)	242 (<1)	257 (1)	246 (1)	243 (1)
178 (1)	182 (2)	177 (2)	178 (2)	181 (1)	186 (<1)	180 (1)	183 (1)
130 (<1)	134 (<1)	130 (<1)	127 (<1)	113 (<1)	112 (<1)	112 (<1)	112 (<1)
48 (<1)	59 (<1)	51 (<1)	44 (<1)	52 (<1)	50 (<1)	50 (<1)	53 (<1)

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

Table S3. Calculated vertical transitions for $PhS(O)_2N_3$, $PhS(O)_2N$(singlet), $PhS(O)_2N$(triplet) and $PhNSO_2$ at the TD-B3LYP/6-311++G(3df,3pd) level.

$PhS(O)_2N_3$		$PhS(O)_2N$ (singlet)		$PhS(O)_2N$ (triplet)		$PhNSO_2$	
273 nm	f = 0.0167	513 nm	f = 0.0036	550 nm	f = 0.0007	306 nm	f = 0.0001
248 nm	f = 0.0106	292 nm	f = 0.0376	466 nm	f = 0.0011	281 nm	f = 0.3248
230 nm	f = 0.0428	280 nm	f = 0.0034	425 nm	f = 0.0540	275 nm	f = 0.0067
226 nm	f = 0.0085	269 nm	f = 0.0437	395 nm	f = 0.0060	258 nm	f = 0.0001
197 nm	f = 0.0319	246 nm	f = 0.0035	388 nm	f = 0.0002	249 nm	f = 0.0004

Table S4. Calculated harmonic IR frequencies (unscaled, cm^{-1}) for $PhNSO_2$ (c) with different theoretical methods.

B3LYP[a]	M06-2X[a]	MPW1PW91[a]	CBS-QB3
3227 (1)	3237 (<1)	3247 (2)	3222 (1)
3206 (4)	3219 (4)	3229 (4)	3202 (6)
3196 (12)	3205 (4)	3220 (10)	3191 (17)
3184 (8)	3199 (3)	3208 (7)	3180 (11)
3173 (<1)	3185 (<1)	3197 (<1)	3170 (<1)
1631 (1)	1669 (9)	1657 (3)	1636 (1)
1615 (5)	1655 (4)	1641 (5)	1619 (5)
1520 (37)	1539 (74)	1531 (59)	1519 (39)
1483 (7)	1495 (13)	1491 (9)	1484 (8)
1376 (258)	1443 (288)	1418 (298)	1359 (12)
1362 (60)	1417 (288)	1399 (134)	1353 (196)
1349 (88)	1355 (2)	1362 (24)	1324 (99)
1310 (65)	1312 (20)	1333 (32)	1305 (111)
1209 (22)	1249 (57)	1229 (87)	1206 (14)
1189 (73)	1207 (1)	1203 (10)	1184 (7)
1185 (4)	1177 (<1)	1184 (<1)	1177 (97)
1108 (9)	1118 (8)	1114 (10)	1107 (11)
1054 (1)	1080 (2)	1066 (1)	1053 (1)
1013 (13)	1055 (8)	1038 (12)	1016 (2)
1012 (<1)	1029 (<1)	1011 (<1)	1008 (<1)
999 (<1)	1015 (<1)	1001 (<1)	994 (21)

993 (7)	1001 (3)	991 (4)	989 (<1)
943 (4)	954 (4)	944 (4)	938 (5)
858 (<1)	872 (<1)	861 (<1)	853 (<1)
775 (59)	796 (31)	778 (9)	778 (52)
765 (8)	784 (37)	776 (63)	766 (8)
689 (18)	702 (21)	682 (16)	704 (29)
634 (<1)	635 (3)	634 (2)	634 (<1)
612 (8)	618 (4)	612 (7)	613 (9)
536 (39)	555 (48)	544 (42)	526 (39)
521 (6)	524 (4)	522 (6)	521 (7)
421 (<1)	441 (31)	420 (3)	421 (1)
368 (20)	418 (<1)	393 (20)	370 (18)
352 (1)	361 (1)	358 (1)	349 (2)
323 (7)	348 (5)	325 (7)	319 (8)
280 (<1)	270 (2)	281 (<1)	279 (<1)
146 (2)	153 (1)	148 (2)	149 (2)
103 (<1)	107 (<1)	103 (<1)	102 (<1)
27 (<1)	35 (<1)	23 (<1)	20 (<1)

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

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

$PhSO_2N_3$

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

Zero-point correction= 0.114005
Thermal correction to Energy= 0.124273
Thermal correction to Enthalpy= 0.125217
Thermal correction to Gibbs Free Energy= 0.076276
Sum of electronic and zero-point Energies= -944.558782
Sum of electronic and thermal Energies= -944.548514
Sum of electronic and thermal Enthalpies= -944.547570
Sum of electronic and thermal Free Energies= -944.596511

C	2.45876900	1.24955000	0.71913600
C	1.14151600	0.84148800	0.88829200
C	0.67275700	-0.23707400	0.14491200
C	1.49016900	-0.91404400	-0.75606300
C	2.80319900	-0.49424400	-0.91378800
C	3.28553400	0.58579600	-0.18013800
H	2.83868700	2.08163200	1.29534100
H	0.49099500	1.33469800	1.59512900
H	1.10341800	-1.75752100	-1.30846000
H	3.45121600	-1.01353600	-1.60601100
H	4.31059800	0.90645000	-0.30629700
S	-1.00751800	-0.76379600	0.34483000
O	-1.10668800	-2.15433200	0.03990000
O	-1.53491600	-0.20049800	1.55389400
N	-1.80162800	-0.00910000	-0.99296400
N	-2.19143800	1.14653100	-0.78836500
N	-2.58599900	2.19382900	-0.69744900

M06-2X

Zero-point correction= 0.115394
Thermal correction to Energy= 0.125470
Thermal correction to Enthalpy= 0.126415
Thermal correction to Gibbs Free Energy= 0.077887
Sum of electronic and zero-point Energies= -944.308354
Sum of electronic and thermal Energies= -944.298278
Sum of electronic and thermal Enthalpies= -944.297334
Sum of electronic and thermal Free Energies= -944.345861

C	2.40424600	1.21909900	0.71540600
C	1.08290900	0.82693800	0.87424400

C	0.62498300	-0.27009200	0.15872100
C	1.44664300	-0.98349300	-0.70315900
C	2.76418400	-0.58147500	-0.84845300
C	3.23920100	0.51828600	-0.14351800
H	2.78110200	2.06736300	1.26849400
H	0.41899900	1.34370600	1.55253600
H	1.05460500	-1.84023400	-1.23248600
H	3.42163200	-1.12887500	-1.50843600
H	4.26858800	0.82645200	-0.26075000
S	-1.06143700	-0.75332600	0.32043900
O	-1.19230600	-2.13440500	0.02062400
O	-1.59005400	-0.17190000	1.51169000
N	-1.79207400	0.01903600	-1.01079100
N	-2.00151600	1.22415800	-0.80458600
N	-2.21727300	2.30818700	-0.68810100

MPW1PW91

Zero-point correction=	0.115270
Thermal correction to Energy=	0.125433
Thermal correction to Enthalpy=	0.126377
Thermal correction to Gibbs Free Energy=	0.077694
Sum of electronic and zero-point Energies=	-944.420255
Sum of electronic and thermal Energies=	-944.410092
Sum of electronic and thermal Enthalpies=	-944.409147
Sum of electronic and thermal Free Energies=	-944.457831

C	2.43507900	1.22957100	0.72596600
C	1.11968200	0.82703000	0.89132100
C	0.65146600	-0.24684200	0.14809300
C	1.46573500	-0.92594300	-0.74807800
C	2.77713400	-0.51229000	-0.90153400
C	3.25909800	0.56383200	-0.16870100
H	2.81716800	2.06029000	1.30276500
H	0.46623000	1.31989400	1.59640600
H	1.07415100	-1.76830000	-1.29956700
H	3.42607000	-1.03413100	-1.59102900
H	4.28573500	0.88077100	-0.29211200
S	-1.01967600	-0.75827000	0.33598400
O	-1.12699400	-2.14080100	0.02974300
O	-1.54351200	-0.19678100	1.53916800
N	-1.79124600	-0.00205800	-0.98443200
N	-2.12283700	1.16760500	-0.78887800
N	-2.46301000	2.22906800	-0.70181800

CBS-QB3

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.112431 E(Thermal)= 0.122849
E(SCF)= -940.791088 DE(MP2)= -2.195954
DE(CBS)= -0.213777 DE(MP34)= -0.021687
DE(CCSD)= -0.079143 DE(Int)= 0.069843
DE(Empirical)= -0.094086
CBS-QB3 (0 K)= -943.213460 CBS-QB3 Energy= -943.203042
CBS-QB3 Enthalpy= -943.202098 CBS-QB3 Free Energy= -943.251272

C	2.47222900	1.27516600	0.69775600
C	1.15264400	0.86696400	0.87417000
C	0.68579200	-0.22410300	0.14276100
C	1.50489500	-0.91906800	-0.74719100
C	2.81995600	-0.49801200	-0.91260300
C	3.30103500	0.59698800	-0.19413800
H	2.85273300	2.11774600	1.26272600
H	0.49841800	1.36816600	1.57543400
H	1.11676000	-1.77434100	-1.28465900
H	3.47072000	-1.02816000	-1.59772600
H	4.32785600	0.91804500	-0.32585800
S	-0.99780400	-0.75862500	0.36087400
O	-1.08723500	-2.16223800	0.08723700
O	-1.53100300	-0.15178400	1.55392000
N	-1.79129500	-0.03280200	-1.01959700
N	-2.23666200	1.10509100	-0.80418100
N	-2.68276300	2.13644300	-0.70446400

$PhSO_2N(^1A)$

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

Zero-point correction= 0.102974
Thermal correction to Energy= 0.111319
Thermal correction to Enthalpy= 0.112263
Thermal correction to Gibbs Free Energy= 0.068966
Sum of electronic and zero-point Energies= -834.951446
Sum of electronic and thermal Energies= -834.943101
Sum of electronic and thermal Enthalpies= -834.942157
Sum of electronic and thermal Free Energies= -834.985455

C	2.42287900	1.12716300	0.05487700
C	1.03766500	1.22785900	0.02756100
C	0.28280400	0.06057600	-0.03273300
C	0.88009600	-1.19831600	-0.07468400
C	2.26301100	-1.28116200	-0.04212900

C	3.03242500	-0.12158100	0.02155300
H	3.02316400	2.02490400	0.10189100
H	0.54437500	2.18755500	0.05316800
H	0.26449700	-2.08348400	-0.13750900
H	2.74179700	-2.24986500	-0.07187700
H	4.11126500	-0.19390800	0.04208500
S	-1.47626400	0.16187600	-0.07194500
O	-1.85331100	1.53978700	-0.11099400
O	-2.04806800	-0.79327000	0.96971600
N	-2.19530200	-1.01922800	-0.77615300

M06-2X

Zero-point correction= 0.104339
Thermal correction to Energy= 0.112471
Thermal correction to Enthalpy= 0.113415
Thermal correction to Gibbs Free Energy= 0.070668
Sum of electronic and zero-point Energies= -834.738206
Sum of electronic and thermal Energies= -834.730073
Sum of electronic and thermal Enthalpies= -834.729129
Sum of electronic and thermal Free Energies= -834.771876

C	2.41924100	1.12062200	0.04324900
C	1.03664000	1.23185700	0.01723900
C	0.28236200	0.06959100	-0.03353700
C	0.86121300	-1.19324400	-0.06434600
C	2.24088600	-1.28618600	-0.03200300
C	3.01583400	-0.13176100	0.02015200
H	3.02757200	2.01263300	0.08074300
H	0.54363700	2.19254400	0.03674200
H	0.22952700	-2.06905800	-0.11601800
H	2.71390300	-2.25721200	-0.05253800
H	4.09362100	-0.21199600	0.04043700
S	-1.46503900	0.17477000	-0.07425100
O	-1.84508600	1.54322300	-0.06018700
O	-2.02942900	-0.83231200	0.91334100
N	-2.18693800	-1.00225400	-0.76158500

MPW1PW91

Zero-point correction= 0.103970
Thermal correction to Energy= 0.112231
Thermal correction to Enthalpy= 0.113175
Thermal correction to Gibbs Free Energy= 0.070077
Sum of electronic and zero-point Energies= -834.840961
Sum of electronic and thermal Energies= -834.832701

Sum of electronic and thermal Enthalpies= -834.831756
Sum of electronic and thermal Free Energies= -834.874854

C	2.41334600	1.12204000	0.05686400
C	1.03230500	1.22672800	0.02823100
C	0.27818300	0.06401500	-0.03395900
C	0.86801800	-1.19376500	-0.07743400
C	2.24672200	-1.28062000	-0.04300700
C	3.01662700	-0.12573300	0.02290000
H	3.01704800	2.01740100	0.10534900
H	0.53810100	2.18644200	0.05458200
H	0.24496700	-2.07413000	-0.14354600
H	2.72337600	-2.25034500	-0.07359500
H	4.09529700	-0.20125100	0.04473200
S	-1.46536600	0.16643500	-0.07468500
O	-1.84238800	1.53682400	-0.10801400
O	-2.03567900	-0.79699700	0.95036900
N	-2.18280200	-1.01938500	-0.75042700

CBS-QB3

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.101463 E(Thermal)= 0.109968
E(SCF)= -831.783753 DE(MP2)= -1.789948
DE(CBS)= -0.177104 DE(MP34)= -0.037186
DE(CCSD)= -0.068376 DE(Int)= 0.058217
DE(Empirical)= -0.078322
CBS-QB3 (0 K)= -833.775009 CBS-QB3 Energy= -833.766503
CBS-QB3 Enthalpy= -833.765559 CBS-QB3 Free Energy= -833.809224

C	2.42781900	1.13070800	0.05591500
C	1.03934700	1.23170800	0.03065500
C	0.28434300	0.06096600	-0.02914300
C	0.88122300	-1.20108300	-0.07556800
C	2.26758000	-1.28373900	-0.04498500
C	3.03834400	-0.12126800	0.02008800
H	3.02992400	2.03012900	0.10327100
H	0.54302400	2.19251200	0.05758400
H	0.26257200	-2.08659800	-0.14096200
H	2.74802500	-2.25421800	-0.07773800
H	4.11964000	-0.19367100	0.03918200
S	-1.48362400	0.16065900	-0.07088800
O	-1.85730400	1.54620600	-0.11831300
O	-2.04689500	-0.79651600	0.98736000
N	-2.19479400	-1.02285400	-0.79161100

$PhSO_2N(^3A)$

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

Zero-point correction=	0.102296
Thermal correction to Energy=	0.110842
Thermal correction to Enthalpy=	0.111786
Thermal correction to Gibbs Free Energy=	0.067059
Sum of electronic and zero-point Energies=	-834.975107
Sum of electronic and thermal Energies=	-834.966562
Sum of electronic and thermal Enthalpies=	-834.965617
Sum of electronic and thermal Free Energies=	-835.010344

C	-2.31697100	1.20892700	-0.00085700
C	-0.93055500	1.21756300	-0.02886300
C	-0.24938800	0.00009700	-0.04771400
C	-0.93042900	-1.21747500	-0.02892700
C	-2.31683100	-1.20900400	-0.00086800
C	-3.00700900	-0.00007000	0.01536100
H	-2.85932500	2.14399800	0.00501400
H	-0.37640200	2.14421100	-0.05329700
H	-0.37619800	-2.14407100	-0.05350900
H	-2.85908700	-2.14413100	0.00504200
H	-4.08829200	-0.00013200	0.03779300
S	1.51471900	0.00009500	-0.06697200
O	1.99697100	1.25346300	-0.58362700
O	1.99698000	-1.25260000	-0.58529400
N	1.83989800	-0.00121900	1.57615600

M06-2X

Zero-point correction=	0.103719
Thermal correction to Energy=	0.112104
Thermal correction to Enthalpy=	0.113048
Thermal correction to Gibbs Free Energy=	0.068596
Sum of electronic and zero-point Energies=	-834.759664
Sum of electronic and thermal Energies=	-834.751279
Sum of electronic and thermal Enthalpies=	-834.750335
Sum of electronic and thermal Free Energies=	-834.794787

C	-2.30532200	1.20768800	0.00099300
C	-0.92055900	1.21614400	-0.03870500
C	-0.24845000	0.00002900	-0.06076500
C	-0.92051900	-1.21611400	-0.03871300
C	-2.30527800	-1.20771000	0.00100100
C	-2.99208300	-0.00002100	0.02280300

H	-2.84859900	2.14141800	0.01138200
H	-0.35999200	2.13954300	-0.06817500
H	-0.35992500	-2.13949600	-0.06820800
H	-2.84852300	-2.14145900	0.01140100
H	-4.07260400	-0.00004100	0.05354400
S	1.50625900	0.00003100	-0.07462300
O	1.98858800	1.24850100	-0.57291100
O	1.98858600	-1.24818400	-0.57355400
N	1.81791000	-0.00044300	1.58658100

MPW1PW91

Zero-point correction= 0.103259
Thermal correction to Energy= 0.111737
Thermal correction to Enthalpy= 0.112681
Thermal correction to Gibbs Free Energy= 0.068095
Sum of electronic and zero-point Energies= -834.866753
Sum of electronic and thermal Energies= -834.858274
Sum of electronic and thermal Enthalpies= -834.857330
Sum of electronic and thermal Free Energies= -834.901917

C	-2.30445100	1.20610800	-0.00020500
C	-0.92160900	1.21461000	-0.03172600
C	-0.24486100	0.00002600	-0.05145600
C	-0.92158300	-1.21458400	-0.03202200
C	-2.30442200	-1.20612300	-0.00048600
C	-2.99176300	-0.00001700	0.01775200
H	-2.84732300	2.14090000	0.00680900
H	-0.36412800	2.13968900	-0.05833200
H	-0.36408600	-2.13964600	-0.05887500
H	-2.84727300	-2.14092900	0.00631100
H	-4.07308100	-0.00003300	0.04252100
S	1.50555600	0.00003200	-0.06906300
O	1.98591800	1.24794800	-0.57767200
O	1.98592500	-1.24755800	-0.57847600
N	1.82348400	-0.00053400	1.57208800

CBS-QB3

Temperature= 298.150000 Pressure=1.000000
E(ZPE)= 0.100955 E(Thermal)= 0.109607
E(SCF)= -831.871380 DE(MP2)= -1.713471
DE(CBS)= -0.172195 DE(MP34)= -0.048023
DE(CCSD)= -0.062913 DE(Int)= 0.054860
DE(Empirical)= -0.074271
CBS-QB3 (0 K)= -833.786438 CBS-QB3 Energy-833.777786

CBS-QB3 Enthalpy= -833.776842 CBS-QB3 Free Energy= -833.821752

C	-2.32164300	1.21227100	-0.00073400
C	-0.93193800	1.22099100	-0.02821100
C	-0.25136800	0.00001800	-0.04224400
C	-0.93192100	-1.22097100	-0.02854100
C	-2.32162400	-1.21228000	-0.00105400
C	-3.01281600	-0.00001100	0.01521700
H	-2.86572800	2.14914900	0.00340200
H	-0.37381100	2.14793000	-0.05547400
H	-0.37378500	-2.14789800	-0.05607100
H	-2.86569700	-2.14916700	0.00283300
H	-4.09658000	-0.00002300	0.03664200
S	1.52099900	0.00002600	-0.06805800
O	1.99690400	1.26215700	-0.58823400
O	1.99690900	-1.26182500	-0.58892100
N	1.84528200	-0.00045100	1.58403500

$PhNSO_2$

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

Zero-point correction= 0.104218
Thermal correction to Energy= 0.112550
Thermal correction to Enthalpy= 0.113495
Thermal correction to Gibbs Free Energy= 0.069377
Sum of electronic and zero-point Energies= -835.056309
Sum of electronic and thermal Energies= -835.047976
Sum of electronic and thermal Enthalpies= -835.047032
Sum of electronic and thermal Free Energies= -835.091150

C	2.30834700	-1.32489200	0.00047100
C	0.95588700	-1.01158100	0.00072400
C	0.56078300	0.32950100	0.00034400
C	1.52912200	1.33820100	-0.00030800
C	2.87614800	1.01070100	-0.00055400
C	3.27174100	-0.32240500	-0.00016100
H	2.60880400	-2.36381700	0.00077500
H	0.21734500	-1.79750000	0.00117000
H	1.20437700	2.36868200	-0.00061100
H	3.61651600	1.79888400	-0.00105800
H	4.32221400	-0.57838300	-0.00035300
N	-0.77212900	0.80183300	0.00063300
S	-2.04491500	0.00939700	-0.00012100
O	-2.09624300	-1.42918800	-0.00118200
O	-3.26099200	0.76566300	0.00049200

M06-2X

Zero-point correction=	0.105782
Thermal correction to Energy=	0.113922
Thermal correction to Enthalpy=	0.114866
Thermal correction to Gibbs Free Energy=	0.071358
Sum of electronic and zero-point Energies=	-834.841927
Sum of electronic and thermal Energies=	-834.833787
Sum of electronic and thermal Enthalpies=	-834.832843
Sum of electronic and thermal Free Energies=	-834.876351

C	-2.28235000	1.31209300	-0.15044700
C	-0.93688100	0.98788200	-0.23441200
C	-0.54746600	-0.34306000	-0.10900300
C	-1.50312800	-1.33650300	0.08890500
C	-2.84252400	-0.99814200	0.17899300
C	-3.23709300	0.32744800	0.05963900
H	-2.58338000	2.34523200	-0.25085100
H	-0.20116300	1.76094300	-0.39321200
H	-1.17506600	-2.36274700	0.16801500
H	-3.57915300	-1.77317800	0.33655500
H	-4.28297400	0.59093200	0.12567500
N	0.78924700	-0.80821200	-0.21406300
S	2.01920700	-0.00883000	0.02903500
O	2.00046700	1.37034000	0.39040600
O	3.26032500	-0.67792900	-0.13469900

MPW1PW91

Zero-point correction=	0.105199
Thermal correction to Energy=	0.113481
Thermal correction to Enthalpy=	0.114425
Thermal correction to Gibbs Free Energy=	0.070296
Sum of electronic and zero-point Energies=	-834.945071
Sum of electronic and thermal Energies=	-834.936789
Sum of electronic and thermal Enthalpies=	-834.935845
Sum of electronic and thermal Free Energies=	-834.979974

C	2.29452900	1.32190700	-0.00036800
C	0.94619200	1.00688200	-0.00065400
C	0.55532400	-0.33104500	-0.00029600
C	1.52210600	-1.33517600	0.00033600
C	2.86506900	-1.00635000	0.00062400
C	3.25726900	0.32397700	0.00028100
H	2.59287700	2.36147700	-0.00065600

H	0.20518700	1.79104000	-0.00114100
H	1.19750700	-2.36590900	0.00056800
H	3.60664000	-1.79339800	0.00111300
H	4.30726700	0.58194000	0.00050800
N	-0.77114000	-0.80119600	-0.00069000
S	-2.03409600	-0.00963000	-0.00037900
O	-2.08049900	1.42015000	0.00116600
O	-3.24561400	-0.75688400	0.00020600

CBS-QB3

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.102935 E(Thermal)= 0.111355
E(SCF)= -831.889103 DE(MP2)= -1.796569
DE(CBS)= -0.177509 DE(MP34)= -0.024840
DE(CCSD)= -0.066145 DE(Int)= 0.058387
DE(Empirical)= -0.078590
CBS-QB3 (0 K)= -833.871434 CBS-QB3 Energy= -833.863014
CBS-QB3 Enthalpy= -833.862070 CBS-QB3 Free Energy= -833.906583

C	2.30874800	1.32769800	-0.00039000
C	0.95349300	1.01309700	-0.00058200
C	0.55844800	-0.33187000	-0.00020900
C	1.53082000	-1.34153200	0.00033900
C	2.88038200	-1.01266600	0.00053800
C	3.27520100	0.32390400	0.00017500
H	2.60892100	2.36924100	-0.00068600
H	0.21310800	1.80039400	-0.00099900
H	1.20361900	-2.37362500	0.00059000
H	3.62313200	-1.80189700	0.00096800
H	4.32775300	0.58173400	0.00032700
N	-0.77431800	-0.81671200	-0.00047300
S	-2.04658300	-0.00819300	-0.00003500
O	-2.08499800	1.43873400	0.00079000
O	-3.27169300	-0.76367900	-0.00023400

PhN_3

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

Zero-point correction= 0.103241
Thermal correction to Energy= 0.110215
Thermal correction to Enthalpy= 0.111159
Thermal correction to Gibbs Free Energy= 0.071337
Sum of electronic and zero-point Energies= -395.871569
Sum of electronic and thermal Energies= -395.864595
Sum of electronic and thermal Enthalpies= -395.863650

Sum of electronic and thermal Free Energies= -395.903473

C	2.20003300	-0.88254400	-0.00005800
C	0.87935600	-1.30490600	0.00018100
C	-0.14852200	-0.36236900	0.00012800
C	0.15211100	1.00043000	0.00019400
C	1.47925500	1.40943100	0.00004100
C	2.50798200	0.47461100	-0.00025700
H	2.99306400	-1.61799600	0.00024200
H	0.62695700	-2.35568700	0.00039300
H	-0.64105800	1.73626800	0.00036200
H	1.70705200	2.46707600	0.00006400
H	3.53884700	0.79983100	-0.00032900
N	-1.46938000	-0.87664600	-0.00019500
N	-2.41072900	-0.08790600	-0.00013600
N	-3.35505500	0.53063500	0.00003100

CBS-QB3

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.102213 E(Thermal)= 0.109248
E(SCF)= -393.507379 DE(MP2)= -1.535630
DE(CBS)= -0.143410 DE(MP34)= -0.019269
DE(CCSD)= -0.062120 DE(Int)= 0.048376
DE(Empirical)= -0.064440
CBS-QB3 (0 K)= -395.181658 CBS-QB3 Energy= -395.174624
CBS-QB3 Enthalpy= -395.173680 CBS-QB3 Free Energy= -395.213618

C	2.20480300	-0.88588600	-0.00008900
C	0.88062300	-1.30714700	0.00017100
C	-0.14906600	-0.36176300	0.00013300
C	0.15454700	1.00378500	0.00020700
C	1.48474900	1.41244400	0.00004100
C	2.51443000	0.47396700	-0.00022800
H	2.99877800	-1.62388500	0.00016100
H	0.62345100	-2.35913400	0.00035000
H	-0.63996000	1.74183300	0.00035900
H	1.71429700	2.47216800	0.00004000
H	3.54805300	0.79878000	-0.00034800
N	-1.47191100	-0.87800600	-0.00014900
N	-2.41546700	-0.08588600	-0.00010100
N	-3.36764000	0.52929700	-0.00003200

PhN

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

Zero-point correction= 0.090890
Thermal correction to Energy= 0.096199
Thermal correction to Enthalpy= 0.097143
Thermal correction to Gibbs Free Energy= 0.061045
Sum of electronic and zero-point Energies= -286.312037
Sum of electronic and thermal Energies= -286.306729
Sum of electronic and thermal Enthalpies= -286.305784
Sum of electronic and thermal Free Energies= -286.341882

C	1.04125200	-1.21181800	0.00000500
C	-0.33546500	-1.22870600	0.00000700
C	-1.06904700	-0.00000100	-0.00004200
C	-0.33546600	1.22870600	0.00000400
C	1.04125100	1.21181900	0.00000800
C	1.73913500	0.00000000	-0.00001000
H	1.58734100	-2.14592800	0.00001400
H	-0.88819800	-2.15736500	0.00002300
H	-0.88820000	2.15736300	0.00002000
H	1.58734000	2.14592900	0.00001700
H	2.82044200	0.00000100	-0.00000400
N	-2.38695700	0.00000000	0.00001400

CBS-QB3

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.090036 E(Thermal)= 0.095373
E(SCF)= -284.628171 DE(MP2)= -1.000896
DE(CBS)= -0.100416 DE(MP34)= -0.068360
DE(CCSD)= -0.055711 DE(Int)= 0.031764
DE(Empirical)= -0.051399
CBS-QB3 (0 K)= -285.783153 CBS-QB3 Energy= -285.777816
CBS-QB3 Enthalpy= -285.776872 CBS-QB3 Free Energy= -285.813017

C	1.04420700	-1.21438400	0.00000400
C	-0.33597200	-1.23059800	0.00000700
C	-1.07166300	-0.00000100	-0.00004000
C	-0.33597300	1.23059800	0.00000400
C	1.04420600	1.21438500	0.00000700
C	1.74370000	0.00000000	-0.00000800
H	1.59128000	-2.15085100	0.00001300
H	-0.89078400	-2.16088800	0.00002300
H	-0.89078600	2.16088700	0.00002100
H	1.59127800	2.15085200	0.00001600
H	2.82756400	0.00000100	-0.00000300

N	-2.39422600	0.00000000	0.00001300

Ph

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

Zero-point correction= 0.087139
Thermal correction to Energy= 0.091514
Thermal correction to Enthalpy= 0.092458
Thermal correction to Gibbs Free Energy= 0.059106
Sum of electronic and zero-point Energies= -231.552966
Sum of electronic and thermal Energies= -231.548591
Sum of electronic and thermal Enthalpies= -231.547647
Sum of electronic and thermal Free Energies= -231.580998

C	-1.20879900	-0.62960900	-0.00000100
C	-1.22145800	0.76939400	0.00000000
C	0.00000100	1.39088200	0.00000100
C	1.22145900	0.76939300	-0.00000100
C	1.20879800	-0.62961000	0.00000000
C	-0.00000100	-1.31914800	0.00000000
H	-2.14535400	-1.17268900	-0.00000100
H	-2.15317300	1.31910300	0.00000100
H	2.15317500	1.31910100	0.00000000
H	2.14535300	-1.17269100	0.00000100
H	-0.00000100	-2.40064000	0.00000100

CBS-QB3

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.086138 E(Thermal)= 0.090554
E(SCF)= -230.132111 DE(MP2)= -0.855797
DE(CBS)= -0.082877 DE(MP34)= -0.054500
DE(CCSD)= -0.053278 DE(Int)= 0.027317
DE(Empirical)= -0.043195
CBS-QB3 (0 K)= -231.108302 CBS-QB3 Energy= -231.103886
CBS-QB3 Enthalpy= -231.102942 CBS-QB3 Free Energy= -231.136358

C	0.63154500	-1.21205500	0.00000000
C	-0.77105200	-1.22400800	0.00000000
C	-1.39588400	0.00000000	0.00000000
C	-0.77105200	1.22400800	0.00000000
C	0.63154500	1.21205500	0.00000000
C	1.32233900	0.00000000	0.00000000
H	1.17624500	-2.15067900	0.00000000
H	-1.32177800	-2.15813400	0.00000000
H	-1.32177700	2.15813400	0.00000000

H	1.17624500	2.15067800	0.00000000
H	2.40642000	0.00000000	0.00000000

SO_2

B3LYP/6-311+G(3df)

Zero-point correction= 0.007007
Thermal correction to Energy= 0.010077
Thermal correction to Enthalpy= 0.011021
Thermal correction to Gibbs Free Energy= -0.017154
Sum of electronic and zero-point Energies= -548.708946
Sum of electronic and thermal Energies= -548.705877
Sum of electronic and thermal Enthalpies= -548.704932
Sum of electronic and thermal Free Energies= -548.733107

S	0.00000000	0.00000000	0.36335600
O	0.00000000	1.23915800	-0.36335600
O	0.00000000	-1.23915800	-0.36335600

CBS-QB3

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.006796 E(Thermal)= 0.009878
E(SCF)= -547.289602 DE(MP2)= -0.659534
DE(CBS)= -0.069166 DE(MP34)= -0.001836
DE(CCSD)= -0.017073 DE(Int)= 0.021826
DE(Empirical)= -0.029068
CBS-QB3 (0 K)= -548.037656 CBS-QB3 Energy= -548.034573
CBS-QB3 Enthalpy= -548.033629 CBS-QB3 Free Energy= -548.061834

S	0.00000000	0.00000000	0.36431600
O	0.00000000	1.24533100	-0.36431600
O	0.00000000	-1.24533100	-0.36431600

O_2SN

B3LYP/6-311+G(3df)

Zero-point correction= 0.011125
Thermal correction to Energy= 0.014882
Thermal correction to Enthalpy= 0.015827
Thermal correction to Gibbs Free Energy= -0.016028
Sum of electronic and zero-point Energies= -603.354202
Sum of electronic and thermal Energies= -603.350444
Sum of electronic and thermal Enthalpies= -603.349500
Sum of electronic and thermal Free Energies= -603.381355

S	0.00000000	0.01322800	0.00000000

O	1.24900200	-0.68288800	0.00000000
O	-1.24893600	-0.68300900	0.00000000
N	-0.00007600	1.53079000	0.00000000

CBS-QB3

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.010787 E(Thermal)= 0.014577
E(SCF)= -601.652040 DE(MP2)= -0.817506
DE(CBS)= -0.086152 DE(MP34)= -0.012450
DE(CCSD)= -0.029827 DE(Int)= 0.026580
DE(Empirical)= -0.036372
CBS-QB3 (0 K)= -602.596980 CBS-QB3 Energy= -602.593190
CBS-QB3 Enthalpy= -602.592246 CBS-QB3 Free Energy= -602.624165

TS1

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

Zero-point correction= 0.107247
Thermal correction to Energy= 0.118991
Thermal correction to Enthalpy= 0.119935
Thermal correction to Gibbs Free Energy= 0.067527
Sum of electronic and zero-point Energies= -943.903807
Sum of electronic and thermal Energies= -943.892062
Sum of electronic and thermal Enthalpies= -943.891118
Sum of electronic and thermal Free Energies= -943.943526

N	2.08081900	-0.02696300	-0.83929900
N	2.58384900	1.56466800	-0.08657500
N	3.30975800	2.42183900	-0.10005300
O	1.14556300	-1.98016400	-1.05319100
S	0.89065700	-0.88194200	0.20340500
O	1.20633500	-1.20762900	1.77023300
C	-0.84962300	-0.21783300	0.06581100
C	-1.42187100	-0.15798600	-1.20154800
C	-1.49027900	0.18849100	1.23133800
C	-2.72344200	0.34708900	-1.29856400
H	-0.87629500	-0.50836000	-2.06983200
C	-2.79219400	0.69102800	1.11180900
H	-0.99429200	0.09596200	2.19055600
C	-3.40181100	0.77108400	-0.14708400
H	-3.20481700	0.40357400	-2.26858600
H	-3.32532500	1.01325800	1.99941400
H	-4.41063900	1.16094100	-0.23143700

CBS-QB3

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.108404 E(Thermal)= 0.119500
E(SCF)= -940.754768 DE(MP2)= -2.151481
DE(CBS)= -0.210339 DE(MP34)= -0.045662
DE(CCSD)= -0.080558 DE(Int)= 0.069422
DE(Empirical)= -0.094017
CBS-QB3 (0 K)= -943.158999 CBS-QB3 Energy= -943.147903
CBS-QB3 Enthalpy= -943.146959 CBS-QB3 Free Energy= -943.197773

N	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.89775100
N	0.56028700	0.00000000	2.84196000
O	-0.95782100	-0.24753800	-1.87747900
S	-1.50755800	-0.23253000	-0.50864000
O	-2.26995700	-1.33045500	0.02303700
C	-2.48141000	1.24439700	-0.30358700
C	-1.99533600	2.44952700	-0.81529900
C	-3.70721500	1.17445700	0.35492700
C	-2.75544500	3.60201400	-0.65801800
H	-1.04204800	2.47347800	-1.32730900
C	-4.45826200	2.33830100	0.50709400
H	-4.06016300	0.22279000	0.72970500
C	-3.98406000	3.54699500	0.00321700
H	-2.39170300	4.54339500	-1.05263000
H	-5.41425800	2.29717900	1.01562800
H	-4.57238200	4.44955500	0.12255500

TS2
B3LYP/6-311++G(3df,3pd)
Zero-point correction= 0.109683
Thermal correction to Energy= 0.120665
Thermal correction to Enthalpy= 0.121609
Thermal correction to Gibbs Free Energy= 0.071516
Sum of electronic and zero-point Energies= -944.497829
Sum of electronic and thermal Energies= -944.486847
Sum of electronic and thermal Enthalpies= -944.485903
Sum of electronic and thermal Free Energies= -944.535996

N	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.83685700
N	0.54265700	0.00000000	2.78724400
O	-2.27182900	-1.22711400	-0.25174100
S	-1.54991400	0.00393300	-0.45360300
O	-2.26621500	1.23809900	-0.25102300

C	-0.68293500	0.00184600	-2.03482500
C	-0.40942500	-1.21982300	-2.65848100
C	-0.40144800	1.22184600	-2.65820900
C	0.12954000	-1.21311200	-3.93348100
H	-0.63611400	-2.14140900	-2.14324500
C	0.13751100	1.21186900	-3.93321000
H	-0.62193900	2.14481500	-2.14277500
C	0.40259100	-0.00140300	-4.56614800
H	0.34030400	-2.14693300	-4.43543200
H	0.35454400	2.14439800	-4.43489000
H	0.82667800	-0.00268700	-5.56129700

CBS-QB3

Temperature= 298.150000	Pressure= 1.000000
E(ZPE)= 0.108225	E(Thermal)= 0.119341
E(SCF)= -940.747174	DE(MP2)= -2.159818
DE(CBS)= -0.210718	DE(MP34)= -0.038708
DE(CCSD)= -0.080835	DE(Int)= 0.069428
DE(Empirical)= -0.093927	
CBS-QB3 (0 K)= -943.153527	CBS-QB3 Energy= -943.142412
CBS-QB3 Enthalpy= -943.141468	CBS-QB3 Free Energy= -943.191879

TS3

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

Zero-point correction=	0.099503
Thermal correction to Energy=	0.108241
Thermal correction to Enthalpy=	0.109185
Thermal correction to Gibbs Free Energy=	0.064862
Sum of electronic and zero-point Energies=	-834.408159
Sum of electronic and thermal Energies=	-834.399421
Sum of electronic and thermal Enthalpies=	-834.398477
Sum of electronic and thermal Free Energies=	-834.442800

S	1.56905400	0.06670300	-0.00886700
O	2.32884200	-1.01966600	-1.01333600
O	2.00423900	1.64184700	-0.08541000
N	1.56310300	-0.84194400	1.53459300
C	-0.30357400	0.02226400	-0.02879500
C	-0.94198700	-1.22282500	-0.07585800
C	-0.98282100	1.24197600	0.01076600
C	-2.33990800	-1.23532100	-0.09658900
H	-0.36226800	-2.13744700	-0.09495700
C	-2.37794000	1.20638000	-0.00912500
H	-0.42076600	2.16832600	0.04158400

C	-3.05087800	-0.02750000	-0.06039900
H	-2.86913800	-2.18046600	-0.13676400
H	-2.94087700	2.13277400	0.01043000
H	-4.13554300	-0.04412500	-0.07059600

CBS-QB3

TS4

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

Zero-point correction= 0.099705
Thermal correction to Energy= 0.108007
Thermal correction to Enthalpy= 0.108951
Thermal correction to Gibbs Free Energy= 0.065191
Sum of electronic and zero-point Energies= -834.706495
Sum of electronic and thermal Energies= -834.698193
Sum of electronic and thermal Enthalpies= -834.697249
Sum of electronic and thermal Free Energies= -834.741009

S	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.46756600
O	1.23684700	0.00000000	-0.78994700
N	-1.17855100	-1.01349000	-0.64566200
C	-1.49694500	0.67023100	-0.81892100
C	-2.58325500	1.14723200	0.00459600
C	-1.39010500	1.14849600	-2.17742200
C	-3.49074000	2.04287900	-0.51987200
H	-2.65628500	0.79710600	1.02818800
C	-2.32145600	2.04438500	-2.65774800
H	-0.56765200	0.79922600	-2.79165500
C	-3.37946400	2.49901600	-1.84745400
H	-4.30076500	2.40360500	0.10783900
H	-2.23004000	2.40604000	-3.67809200
H	-4.10392100	3.20343100	-2.24314800

CBS-QB3

Temperature= 298.150000 Pressure= 1.000000
E(ZPE)= 0.098276 E(Thermal)= 0.106595
E(SCF)= -831.808495 DE(MP2)= -1.699034
DE(CBS)= -0.174645 DE(MP34)= -0.064835
DE(CCSD)= -0.076364 DE(Int)= 0.054065
DE(Empirical)= -0.079299

CBS-QB3 (0 K)= -833.750329 CBS-QB3 Energy= -833.742011

CBS-QB3 Enthalpy= -833.741067 CBS-QB3 Free Energy= -833.784822

S	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.44581600
O	1.22040600	0.00000000	-0.77515500
N	-1.15714400	-1.00782300	-0.63612700
C	-1.50679400	0.63124400	-0.82638400
C	-2.59770000	1.10697600	-0.00698600
C	-1.40333700	1.10979700	-2.18578800
C	-3.48893600	2.01691800	-0.52444400
H	-2.68238300	0.74463800	1.00886400
C	-2.31969700	2.01983400	-2.65714600
H	-0.59232300	0.74928600	-2.80443500
C	-3.36884600	2.48477100	-1.84480100
H	-4.29621400	2.37834800	0.10233400
H	-2.22578600	2.38326200	-3.67412400
H	-4.08190900	3.20008500	-2.23464100