

NO₂ Bond Cleavage by MoL₃ Complexes

Miranda F. Shaw, Narges Mahdizadeh Ghohe, Alireza Ariafard,* Nigel J. Brookes,

Robert Stranger, and Brian F. Yates*

School of Chemistry, University of Tasmania, Hobart, Australia; School of Chemistry, Central

Tehran Branch, Islamic Azad University, Gharb, Tehran, Iran; School of Chemistry, Australian

National University, Canberra, Australia.

Supporting Information

Contents

1. M06 optimized geometries and total energies for all species discussed.
2. Potential energy surfaces for selected structures using B3LYP.
3. B3LYP optimized geometries and total energies for species shown in Section 3.
4. Comparison between solvated and gas-phase optimised geometries for selected structures.

1. M06 optimized geometries and total energies for all species.

NO₂

E (M06/BS2) = -205.038955 au
H (M06/BS2) = -205.026083 au
G (M06/BS2) = -205.053287 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -205.039870 au
N 0.00000 0.00000 0.31851
O 0.00000 1.09341 -0.13935
O 0.00000 -1.09341 -0.13935

1_Q

E (M06/BS2) = -236.026227 au
H (M06/BS2) = -235.94421 au
G (M06/BS2) = -235.986409 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -236.037364 au
N -1.35320 1.41890 0.00176
N 1.90583 0.46239 0.00177
N -0.55209 -1.88147 0.00154
H -0.71790 -2.44479 0.82799
H -0.71948 -2.44641 -0.82346
H -1.75978 1.84592 -0.82306
H -1.76144 1.84091 0.82833
H 2.47869 0.60187 -0.82294
H 2.47672 0.59937 0.82830
Mo -0.00001 0.00010 -0.00120

2_T

E (M06/BS2) = -441.153178 au
H (M06/BS2) = -441.055022 au
G (M06/BS2) = -441.104095 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -441.166616 au
Mo -0.50612 0.04568 0.05355
O 2.47204 0.66527 -0.13055
N 1.57212 -0.14031 -0.26074
O 1.73815 -1.29305 -0.67101
N -1.85717 -0.16490 -1.32959
H -2.15390 0.58893 -1.93998
H -2.11541 -1.05733 -1.73877
N -0.15483 1.87869 0.49374
H 0.81148 2.20266 0.52547
H -0.77865 2.50758 0.98795
N -0.58050 -1.27683 1.45255
H 0.19410 -1.91494 1.61473
H -1.23954 -1.29998 2.22236

3_T

E (M06/BS2) = -441.162537 au
H (M06/BS2) = -441.066715 au
G (M06/BS2) = -441.115181 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -441.1625368 au
Mo -0.31798 0.00010 -0.02505
N 1.79939 0.00076 -0.03220
O 2.97151 0.00006 -0.20181
O 1.30865 0.00088 1.21560
N -0.81113 1.62491 -0.92984
N -0.80830 -1.62564 -0.92969
N -1.91649 -0.00095 1.14983
H -0.34432 2.00886 -1.74334
H -1.65823 2.13521 -0.70794
H -0.34047 -2.00908 -1.74285
H -1.65493 -2.13695 -0.70834
H -1.83932 -0.00157 2.16050
H -2.89297 -0.00186 0.87739

4_T

E (M06/BS2) = -441.167434 au
H (M06/BS2) = -441.070517 au
G (M06/BS2) = -441.120359 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -441.167434 au
Mo 0.61966 -0.01151 0.00980
O -1.29154 0.49989 -0.39640
N -2.32390 -0.30468 -0.06043
O -3.36766 0.09430 -0.44760
N 0.05482 -1.40841 1.20373
N 2.05100 -0.62403 -1.14454

N	0.93697	1.79011	0.62319
H	-0.94380	-1.58511	1.30718
H	0.58149	-1.77293	1.99036
H	2.17850	-1.59560	-1.40953
H	2.56071	-0.02734	-1.78841
H	0.17248	2.46054	0.62085
H	1.66596	2.07945	1.26612

5_T

E (M06/BS2) = -441.178313 au
H (M06/BS2) = -441.081727 au
G (M06/BS2) = -441.130492 au
E (M06/BS2//M06/BS2, Solvent = DiethylEther) = -441.178313 au

Mo	-0.28664	-0.02033	0.03529
N	2.25472	0.34026	-0.37528
O	1.33376	1.23965	-0.27150
O	1.73831	-0.79969	-0.24233
N	-1.67943	1.32995	-0.14183
N	-1.14008	-1.27449	-1.16672
N	-0.19311	-0.58136	1.87666
H	-1.47821	2.31960	-0.03754
H	-2.67241	1.19095	-0.29944
H	-0.75225	-2.18137	-1.40382
H	-1.92678	-1.05354	-1.76710
H	0.58201	-1.09747	2.27843
H	-0.98454	-0.54416	2.50793

TS1_T

E (M06/BS2) = -441.150810 au
H (M06/BS2) = -441.054054 au
G (M06/BS2) = -441.101901 au
E (M06/BS2//M06/BS2, Solvent = DiethylEther) = -441.161870 au

Mo	-0.43698	-0.00814	0.03860
O	2.58468	0.82911	-0.19950
N	1.62094	0.11244	-0.20887
O	1.65530	-1.10702	-0.52246
N	-1.63701	-0.63254	-1.36011
H	-2.13771	-0.01720	-1.99259
H	-1.64217	-1.57942	-1.72537
N	-0.93103	1.84320	0.27293
H	-0.23127	2.55437	0.46537
H	-1.85965	2.20606	0.46382
N	-0.34772	-1.02257	1.67661
H	0.43394	-1.63480	1.89064
H	-1.06613	-1.06717	2.38874

TS2_T

E (M06/BS2) = -441.149283 au
H (M06/BS2) = -441.052996 au
G (M06/BS2) = -441.102470 au
E (M06/BS2//M06/BS2, Solvent = DiethylEther) = -441.159363 au

Mo	0.44654	-0.05273	0.00558
N	1.93261	-0.11161	-0.24543
O	3.11669	-0.10229	-0.31240
O	1.32877	1.02377	0.04236
N	1.37669	-0.90244	-1.46646
N	0.37667	-1.12405	1.60637
N	1.51189	1.56052	0.21396
H	1.12083	-1.77988	-1.90644
H	2.07977	-0.42613	-2.02135
H	0.46221	-1.60284	1.91886
H	1.15350	-1.30214	2.23114
H	1.07232	2.39518	0.59192
H	2.51607	1.60187	0.35269

TS3_T

E (M06/BS2) = -441.144431 au
H (M06/BS2) = -441.048118 au
G (M06/BS2) = -441.097451 au
E (M06/BS2//M06/BS2, Solvent = DiethylEther) = -441.156652 au

Mo	-0.55153	-0.02802	0.01404
N	2.42430	0.20272	0.14683
O	1.26283	0.82557	-0.17653
O	2.90425	-0.40527	-0.74507
N	-1.32527	1.74315	0.00255
N	-1.62882	-1.21498	-1.06331
N	-0.01986	-0.94866	1.62679
H	-0.70838	2.55000	-0.04430

H	-2.20982	1.99771	0.42874
H	-1.51505	-2.22379	-1.07738
H	-2.15411	-0.91950	-1.88035
H	0.91898	-0.83292	2.00160
H	-0.65628	-1.23255	2.36451

TS6_T

E (M06/BS2) = -441.148791 au
H (M06/BS2) = -441.053526 au
G (M06/BS2) = -441.101836 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -441.159024 au

Mo	0.32129	-0.06302	-0.02021
O	-0.97067	-0.38561	1.30553
N	-1.72832	-0.38925	-0.06572
O	-2.76106	0.18888	-0.08801
N	1.73125	0.76372	1.02186
N	1.18562	-1.61264	-0.78739
N	0.15166	1.52250	-1.12738
H	1.84653	0.56283	2.01168
H	2.14117	1.66934	0.81174
H	0.70565	-2.28400	-1.37568
H	2.18856	-1.74718	-0.81249
H	-0.64458	1.68332	-1.73365
H	0.74076	2.34603	-1.08234

TS7_T

E (M06/BS2) = -441.140477 au
H (M06/BS2) = -441.045687 au
G (M06/BS2) = -441.096099 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -441.151198 au

Mo	-0.58882	0.00207	0.00523
N	2.46088	-0.20655	0.10516
O	1.11321	0.51620	-0.43998
O	3.38356	0.21539	-0.45142
N	-1.66665	1.60936	-0.03133
N	-1.41291	-1.39178	-1.07134
N	-0.04776	-0.70234	1.72347
H	-1.24089	2.52939	-0.07356
H	-2.63413	1.68260	0.26473
H	-1.34446	-2.36932	-0.80827
H	-1.60771	-1.32006	-2.06507
H	0.89514	-0.53746	2.06695
H	-0.64642	-1.08560	2.44512

TS8_T

E (M06/BS2) = -441.148764 au
H (M06/BS2) = -441.053598 au
G (M06/BS2) = -441.100735 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -441.158914 au

Mo	0.22069	0.00448	0.05303
N	-2.15281	0.21040	0.39083
O	-1.00549	-0.02821	1.42240
O	-1.77849	-0.34888	-0.68363
N	2.00746	0.25919	0.72745
N	0.69317	-1.69174	-0.74573
N	0.26686	1.58390	-1.05900
H	2.44771	1.16022	0.88987
H	2.66744	-0.48972	0.91519
H	-0.00906	-2.24915	-1.21914
H	1.63065	-2.02674	-0.93120
H	-0.53822	1.82990	-1.62583
H	1.10141	2.07169	-1.36148

7_D

E (M06/BS2) = -311.327942 au
H (M06/BS2) = -311.240492 au
G (M06/BS2) = -311.283251 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -311.338207 au

Mo	0.07798	-0.03745	0.08730
O	0.34693	-0.49781	1.67569
N	-1.08641	1.52371	-0.06610
N	1.71203	0.22762	-0.93696
N	-1.22620	-1.16401	-0.82563
H	-2.09588	1.44067	-0.13652
H	-0.84753	2.41981	0.34316
H	2.62872	0.01629	-0.56162
H	1.78608	0.56310	-1.88991
H	-1.23485	-2.17537	-0.78160

H -2.08345 -0.81994 -1.24502

NO

E (M06/BS2) = -129.859213 au
H (M06/BS2) = -129.851360 au
G (M06/BS2) = -129.874644 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -129.859602 au
N 0.00000 0.00000 -0.60926
O 0.00000 0.00000 0.53310

2_S

E (M06/BS2) = -441.168497 au
H (M06/BS2) = -441.069414 au
G (M06/BS2) = -441.115430 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -441.181846 au
Mo 0.42535 0.01832 -0.00667
O -1.63400 -1.05257 -0.00807
N -1.50058 0.20006 -0.20539
O -2.40895 0.97433 -0.36236
N 1.35758 1.65230 -0.40435
H 1.74392 1.88067 -1.31634
H 1.35155 2.48217 0.18186
N 0.35724 -0.25084 1.88882
H 1.16256 -0.39549 2.49079
H -0.48820 -0.60740 2.33371
N 0.98234 -1.51860 -1.01138
H 1.95318 -1.75468 -1.19419
H 0.37958 -2.32960 -1.12591

3_S

E (M06/BS2) = -441.173767 au
H (M06/BS2) = -441.075161 au
G (M06/BS2) = -441.121525 au
E (M06/BS2//M06/2 Solvent =DiethylEther) = -441.184226 au
Mo 0.31539 -0.04715 0.00002
N -1.62967 0.01300 0.00002
O -2.79103 -0.25819 0.00025
O -1.19220 1.30325 -0.00103
N 0.77570 -1.00896 1.60401
N 0.77550 -1.01182 -1.60229
N 1.66355 1.33861 -0.00119
H 0.17686 -1.68220 2.07005
H 1.72207 -1.06281 1.96877
H 0.17652 -1.68587 -2.06700
H 1.72180 -1.06642 -1.96713
H 1.86324 1.89991 -0.82691
H 1.86313 1.90151 0.82346

4_S

E (M06/BS2) = -441.154571 au
H (M06/BS2) = -441.057697 au
G (M06/BS2) = -441.105392 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -441.164595 au
Mo 0.49715 0.10497 0.00214
O -1.35179 0.61122 0.16782
N -2.39577 -0.28634 -0.13089
O -3.44276 0.19137 0.06149
N 0.78076 -1.25156 -1.31201
N 1.83759 1.48791 -0.12958
N 1.03558 -1.12978 1.35208
H 0.70208 -1.15937 -2.32003
H 1.15126 -2.17516 -1.08114
H 1.58796 2.44869 -0.33866
H 2.84425 1.36971 -0.14339
H 1.15077 -0.94217 2.34326
H 1.23262 -2.11274 1.15796

5_S

E (M06/BS2) = -441.175913 au
H (M06/BS2) = -441.077329 au
G (M06/BS2) = -441.123065 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -441.185208 au
Mo 0.31438 -0.01352 -0.00007
N -2.24048 0.45372 -0.00066
O -1.25927 1.30304 -0.00108
O -1.73083 -0.69136 0.00062
N 1.65765 1.35353 -0.00130

N	0.58296	-1.05542	1.59189
N	0.58319	-1.05936	-1.58944
H	1.93296	1.87862	-0.82994
H	1.93244	1.88054	0.82629
H	-0.12043	-1.66961	1.99173
H	1.50429	-1.29150	1.95162
H	-0.12023	-1.67430	-1.98807
H	1.50459	-1.29654	-1.94828

6_S

E (M06/BS2) = -441.190667 au
H (M06/BS2) = -441.092802 au
G (M06/BS2) = -441.137413 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -441.201068 au

Mo	-0.14472	-0.00002	0.06013
N	1.81441	-0.00039	0.08063
O	1.32729	-1.09266	-0.60728
O	1.32787	1.09243	-0.60654
N	-1.34645	1.37582	-0.59079
N	-1.34740	-1.37500	-0.59099
N	-0.29671	-0.00022	1.96547
H	-1.04712	2.33484	-0.72805
H	-2.10973	1.15868	-1.22351
H	-1.04869	-2.33425	-0.72813
H	-2.11002	-1.15731	-1.22433
H	0.54045	-0.00059	2.53691
H	-1.15455	-0.00005	2.50207

8_S

E (M06/BS2) = -441.208915 au
H (M06/BS2) = -441.110704 au
G (M06/BS2) = -441.156634 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -441.216408 au

Mo	-0.31925	-0.09460	0.11134
O	-0.30583	-0.26511	1.78158
N	1.79630	-0.34410	0.13670
O	2.68381	0.33807	-0.16204
N	-0.24967	-1.70932	-1.01022
N	-2.05431	0.64850	-0.37509
N	0.32871	1.61877	-0.59341
H	0.24752	-2.55575	-0.76203
H	-0.58562	-1.74946	-1.96554
H	-2.86844	0.40063	0.17863
H	-2.23491	1.49193	-0.90534
H	-0.23973	2.45226	-0.66624
H	1.31879	1.85326	-0.61799

9_S

E (M06/BS2) = -441.208820 au
H (M06/BS2) = -441.110386 au
G (M06/BS2) = -441.155466 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -441.215550 au

Mo	0.13073	0.03903	0.11218
N	-1.83467	-0.70144	-0.05924
O	-0.15783	0.27559	1.74828
O	-2.02763	0.43862	-0.28949
N	0.21912	-1.76650	-0.75440
N	0.30732	1.65205	-1.00432
N	2.07918	-0.13662	0.02579
H	1.04423	-2.10436	-1.23537
H	-0.46107	-2.50511	-0.62984
H	-0.39328	2.37828	-1.07485
H	1.19200	1.94161	-1.39948
H	2.65563	0.62464	0.36837
H	2.55866	-1.02061	0.13433

TS4_S

E (M06/BS2) = -441.151650 au
H (M06/BS2) = -441.054730 au
G (M06/BS2) = -441.101638 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -441.161163 au

Mo	-0.47919	-0.10569	0.00062
N	2.48151	-0.18580	-0.54377
O	1.23153	-0.83939	-0.38488
O	2.99829	0.03589	0.47625
N	-2.01009	-1.23983	0.33265
N	-0.34236	1.30611	1.28798
N	-0.98010	1.16809	-1.32733

H	-1.91032	-2.18121	0.69829
H	-2.97477	-0.93558	0.40835
H	-0.63053	2.26502	1.08926
H	-0.08369	1.22445	2.26624
H	-1.23584	0.97874	-2.29195
H	-0.92004	2.17576	-1.17432

TS5_S

E (M06/BS2) = -441.155988 au
H (M06/BS2) = -441.059830 au
G (M06/BS2) = -441.103480 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -441.163739 au

Mo	-0.23978	0.08795	-0.01728
N	2.22635	-0.02176	-0.05030
O	1.61443	-0.14823	1.05369
O	1.53532	-0.50536	-1.01304
N	-1.34774	-1.00626	-1.12997
N	-1.20853	-0.69880	1.42426
N	-0.67565	1.94959	-0.21781
H	-1.10005	-1.25168	-2.08411
H	-2.14574	-1.56395	-0.82371
H	-0.89655	-0.63874	2.38947
H	-1.93782	-1.40673	1.33313
H	-0.92387	2.33356	-1.12377
H	-1.08400	2.50280	0.52636

TS9_S

E (M06/BS2) = -441.172496 au
H (M06/BS2) = -441.075075 au
G (M06/BS2) = -441.119587 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -441.182154 au

Mo	0.29057	0.02724	-0.01606
O	-1.04908	-1.06674	-0.84613
N	-1.65910	-0.17356	0.15258
O	-2.82457	0.00821	0.10045
N	1.10459	-0.73432	1.55127
N	1.89976	-0.31904	-1.03724
N	0.22019	1.95579	0.04978
H	0.66481	-0.81031	2.46034
H	2.07925	-1.01804	1.59471
H	2.63346	-0.96826	-0.75835
H	2.07526	-0.01597	-1.99096
H	1.02153	2.56939	0.14565
H	-0.64731	2.46488	0.17404

TS10_S

E (M06/BS2) = -441.146623 au
H (M06/BS2) = -441.050473 au
G (M06/BS2) = -441.098990 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -441.154351 au

Mo	0.48857	-0.09360	0.02003
N	-2.61382	-0.20295	0.56866
O	-1.02646	-0.90714	0.52097
O	-2.95299	0.00613	-0.48955
N	1.99056	-1.24362	-0.39963
N	0.16102	1.22791	-1.35149
N	1.03123	1.30232	1.23769
H	2.92951	-0.95420	-0.64934
H	1.88427	-2.24480	-0.51683
H	-0.17560	1.07008	-2.29465
H	0.43836	2.20357	-1.24479
H	0.91962	2.29339	1.02824
H	1.33623	1.18583	2.19798

TS11_S

E (M06/BS2) = -441.181952 au
H (M06/BS2) = -441.085226 au
G (M06/BS2) = -441.128836 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -441.192100 au

Mo	0.17501	-0.02695	0.02743
N	-1.75630	-0.38366	0.33147
O	-0.79484	0.18299	1.56681
O	-1.85044	0.57704	-0.44744
N	0.68171	1.57632	-0.93253
N	1.96977	-0.23735	0.71416
N	0.11506	-1.60759	-1.08356
H	0.02848	2.16142	-1.43607

H	1.60648	1.98832	-0.89221
H	2.28017	-0.96749	1.34608
H	2.69706	0.46309	0.61225
H	-0.73651	-2.13290	-1.24056
H	0.86403	-1.89451	-1.70321

10_T

E (M06/BS2) = -365.963201 au
H (M06/BS2) = -365.870340 au
G (M06/BS2) = -365.916010 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -365.971138 au

N	-1.13275	-0.90749	1.39320
N	-1.13809	-0.90129	-1.39396
N	-0.45710	1.99650	0.00313
H	-1.37582	2.42596	0.00479
H	0.26632	2.70370	0.00512
H	-1.00381	-0.77409	2.39016
H	-1.82115	-1.63825	1.23303
H	-1.00974	-0.76692	-2.39086
H	-1.82975	-1.62905	-1.23417
Mo	-0.18315	0.07259	0.00005
N	1.64766	-0.07372	-0.00063
O	2.75355	-0.52101	-0.00284

10_S

E (M06/BS2) = -366.014312 au
H (M06/BS2) = -365.920171 au
G (M06/BS2) = -365.964133 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -366.025106 au

N	-1.39810	0.00612	1.57799
N	-0.39650	-1.68575	-0.98802
N	-0.39633	1.67908	-0.99858
H	-1.26267	1.98202	-1.43373
H	0.37625	2.24910	-1.32010
H	-1.46598	0.82766	2.17241
H	-1.46843	-0.81062	2.17865
H	0.37584	-2.25814	-1.30589
H	-1.26296	-1.99132	-1.42108
Mo	-0.26110	-0.00036	-0.04117
N	1.45729	0.00050	0.20387
O	2.60124	0.00209	0.53655

11_Q

E (M06/BS2) = -677.259060 au
H (M06/BS2) = -677.076444 au
G (M06/BS2) = -677.146164 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -677.273664 au

Mo	-2.34842	-0.03615	0.01898
H	-3.77979	-0.15464	-2.19771
H	-3.79081	1.41084	-1.66262
H	-3.16976	-2.41898	0.79105
H	-1.53032	-2.48098	0.50191
H	-3.20828	1.31453	2.11553
H	-1.57363	1.58080	1.93393
N	-3.59624	0.44910	-1.40234
N	-2.37904	-1.93744	0.37431
N	-2.41278	1.21613	1.49257
O	0.38091	-0.34899	0.91166
O	0.31080	0.39956	-1.10247
Mo	2.16640	0.03185	-0.03988
N	-0.41336	0.02274	-0.09348
H	2.73096	-0.90535	-2.45150
H	3.73730	-1.64846	-1.34606
H	3.33551	2.36192	0.27372
H	1.89644	2.60215	-0.55339
H	3.01039	-0.85551	2.31471
H	4.29488	-1.03168	1.28044
N	3.03563	-0.93032	-1.48496
N	2.46848	1.94143	-0.03890
N	3.31993	-0.76141	1.35341

11_D

E (M06/BS2) = -677.269683 au
H (M06/BS2) = -677.088359 au
G (M06/BS2) = -677.152146 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -677.2846987 au

N	-2.93249	-0.35309	1.65932
N	-3.15251	-1.29930	-0.89547
N	-2.62714	1.76256	-0.79852
H	-2.10351	2.61997	-0.67203
H	-3.55135	1.93203	-1.17436
H	-3.66397	-1.03917	1.80451
H	-2.50379	-0.09035	2.53946
H	-3.87342	-1.85924	-0.44797
H	-2.77156	-1.81834	-1.68279
O	-0.44181	0.58364	0.90989
O	-0.46459	-0.63761	-0.85039
N	0.45027	-0.07328	0.06291
Mo	-2.08104	0.07760	-0.03563
Mo	2.29767	-0.01666	-0.00999
N	2.58021	-1.77479	-0.77623
N	2.61379	0.10732	1.89853
N	3.03339	1.46848	-1.05172
H	3.01099	1.48069	-2.06739
H	3.02698	2.42637	-0.71328
H	3.53551	0.14812	2.32486
H	1.91681	-0.11560	2.60297
H	1.87747	-2.50808	-0.78423
H	3.49409	-2.16945	-0.98108

TS12_Q

E (M06/BS2) = -677.241927 au

H (M06/BS2) = -677.062518 au

G (M06/BS2) = -677.131077 au

E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -677.257536 au

N	-1.75559	-0.78244	-1.72611
N	-3.01234	1.58636	0.34108
N	-3.38767	-1.16295	0.55987
H	-3.43701	-2.15933	0.37187
H	-4.25059	-0.85815	0.99894
H	-2.49695	-1.32464	-2.15426
H	-1.16400	-0.34894	-2.42746
H	-2.63318	2.51973	0.23152
H	-4.00117	1.60521	0.55990
O	-0.30425	1.29024	-0.48269
O	-0.49985	-0.29428	1.19618
N	0.49346	0.72697	0.38228
Mo	-1.91427	0.01509	0.05019
Mo	2.18471	-0.09263	0.00660
N	2.78396	-0.70786	1.75332
N	3.10509	1.43062	-0.79449
N	1.48574	-1.42667	-1.22562
H	2.04327	-2.03533	-1.81413
H	0.49722	-1.65365	-1.31091
H	3.95995	1.39261	-1.33665
H	2.73968	2.37601	-0.77781
H	2.17102	-0.70093	2.56156
H	3.65773	-1.17176	1.97166

TS13_D

E (M06/BS2) = -677.267963 au

H (M06/BS2) = -677.088000 au

G (M06/BS2) = -677.151587 au

E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -677.282536 au

N	-2.82621	-0.85165	1.52623
N	-3.33540	-0.85493	-1.16773
N	-2.53355	1.93375	-0.25042
H	-1.98656	2.68357	0.15306
H	-3.42536	2.25296	-0.60460
H	-3.48365	-1.62060	1.48618
H	-2.38777	-0.78974	2.43750
H	-4.22882	-1.25867	-0.89742
H	-3.07191	-1.20454	-2.08544
O	-0.40196	0.46032	1.03365
O	-0.53290	-0.51074	-0.92844
N	0.48659	-0.04154	0.14958
Mo	-2.06905	0.06844	-0.01602
Mo	2.28942	-0.02541	-0.03076
N	2.43803	-1.55666	-1.20306
N	2.72606	-0.33452	1.83284
N	3.04668	1.62518	-0.76922
H	2.97666	1.86650	-1.75346
H	3.07897	2.48395	-0.22708
H	3.67645	-0.42166	2.18195
H	2.06943	-0.68691	2.52190

H	1.67618	-2.20667	-1.37108
H	3.31430	-1.93959	-1.54540

12_Q

E (M06/BS2) = -677.260906 au
H (M06/BS2) = -677.079355 au
G (M06/BS2) = -677.146343 au
E (M06/BS2//M06/BS2, Solvent = DiethylEther) = -677.275353 au

Mo	-1.88066	-0.00855	-0.00165
H	-4.18487	-1.15411	-0.59703
H	-4.24808	0.45864	-1.02835
H	-1.87140	-0.71744	2.53800
H	-0.80298	-1.66213	1.63571
H	-2.22955	2.44450	0.97604
H	-0.99443	2.47264	-0.15070
N	-3.71463	-0.25699	-0.54756
N	-1.57665	-0.99962	1.60940
N	-1.74747	1.92520	0.25073
Mo	1.76708	0.03472	-0.03938
H	3.48449	-1.74000	0.91050
H	4.11912	-0.25097	1.26567
H	3.66027	0.36552	-1.83693
H	2.21313	0.91008	-2.48872
H	0.79996	2.16754	1.24805
H	2.13165	1.56730	2.06246
N	3.28214	-0.74868	0.98285
N	2.66234	0.46577	-1.69563
N	1.55078	1.48688	1.23567
O	-0.24587	0.21118	-1.13660
N	-0.45971	-1.16852	-0.85723
O	0.58531	-1.57228	-0.07080

12_D

E (M06/BS2) = -677.260928 au
H (M06/BS2) = -677.079194 au
G (M06/BS2) = -677.141865 au
E (M06/BS2//M06/BS2, Solvent = DiethylEther) = -677.275101 au

Mo	1.92872	-0.00703	0.00775
H	4.26229	0.64875	-1.07894
H	4.28574	-0.98610	-0.69916
H	2.02818	1.96813	1.78415
H	0.90746	2.30193	0.56236
H	2.23279	-1.63016	2.11167
H	0.94933	-2.18030	1.18251
N	3.77869	-0.10955	-0.60284
N	1.69816	1.72439	0.85272
N	1.74890	-1.55356	1.21975
Mo	-1.84273	-0.02154	-0.04664
H	-4.00945	1.51449	-0.30536
H	-3.67766	1.31688	1.31967
H	-3.53198	-1.79312	-1.11538
H	-1.96146	-2.11131	-1.61523
H	-0.88383	-1.01249	2.25586
H	-2.32984	-0.23484	2.55880
N	-3.39752	1.05616	0.36975
N	-2.58226	-1.43354	-1.17527
N	-1.63200	-0.45798	1.84503
O	0.25446	-0.74561	-0.89122
N	0.47438	0.58778	-1.33783
O	-0.56720	1.33337	-0.79964

13_Q

E (M06/BS2) = -677.272346 au
H (M06/BS2) = -677.090799 au
G (M06/BS2) = -677.157769 au
E (M06/BS2//M06/BS2, Solvent = DiethylEther) = -677.283939 au

Mo	-1.70484	-0.06809	-0.00413
H	-2.40948	-1.30293	-2.21036
H	-3.82269	-0.81788	-1.47372
H	-1.79627	-2.26573	1.39379
H	-0.26457	-1.57373	1.62668
H	-4.07691	1.10057	0.25384
H	-3.10601	1.53395	1.53614
N	-2.80932	-0.81058	-1.41752
N	-1.17508	-1.49512	1.17402
N	-3.19354	0.93057	0.72442
Mo	1.70590	0.02123	0.00518

H	2.67535	-1.42980	-2.00914
H	3.65557	-1.71916	-0.71321
H	3.79437	1.39617	-0.76195
H	2.76239	2.42278	0.08110
H	1.72273	-0.44090	2.60444
H	2.49249	-1.70666	1.83409
N	2.75034	-1.36041	-0.99928
N	2.90324	1.48799	-0.28781
N	1.87693	-0.90855	1.71678
O	-0.06406	1.17992	0.75116
N	-0.47239	1.34670	-0.56585
O	0.05983	0.11786	-1.19465

13_D

E (M06/BS2) = -677.276482 au
H (M06/BS2) = -677.093656 au
G (M06/BS2) = -677.156314 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -677.287653 au

Mo	-1.67305	0.02367	0.00493
H	-2.61591	0.36301	2.43262
H	-3.93483	0.22640	1.42292
H	-1.67885	2.56604	-0.52642
H	-0.13042	1.97199	-0.90360
H	-4.03368	-0.80375	-0.90433
H	-2.94247	-0.77507	-2.16003
N	-2.92152	0.21440	1.47628
N	-1.05556	1.76625	-0.52366
N	-3.09618	-0.53581	-1.18564
Mo	1.71547	-0.08991	0.00979
H	1.81795	1.20625	2.27937
H	2.27834	2.25209	1.07152
H	4.04742	-1.15591	0.55425
H	3.33750	-1.97735	-0.71484
H	1.72906	1.18628	-2.32362
H	2.38067	2.20661	-1.18051
N	2.09304	1.27357	1.30190
N	3.18655	-1.32598	0.04936
N	1.91199	1.31324	-1.33273
O	0.06001	-0.90592	-1.01381
N	-0.49947	-1.53749	0.11890
O	0.01898	-0.67680	1.13927

TS14_Q

E (M06/BS2) = -677.242135 au
H (M06/BS2) = -677.062777 au
G (M06/BS2) = -677.129156 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -677.2773041 au

Mo	-1.68826	-0.05900	-0.02697
H	-2.39721	-1.29751	-2.22115
H	-3.80894	-0.82913	-1.45972
H	-1.82810	-2.25675	1.37147
H	-0.30023	-1.56166	1.63349
H	-4.02588	1.18743	0.18528
H	-3.10245	1.54104	1.51963
N	-2.79526	-0.79792	-1.43213
N	-1.20690	-1.48116	1.17385
N	-3.18578	0.94617	0.70100
Mo	1.68366	0.03919	-0.02313
H	2.62609	-1.46688	-1.99285
H	3.65918	-1.66167	-0.71026
H	3.78299	1.41328	-0.80923
H	2.74486	2.43981	0.02311
H	1.70168	-0.41388	2.58254
H	2.48007	-1.67428	1.81572
N	2.73927	-1.34155	-0.99267
N	2.90253	1.49659	-0.31538
N	1.85083	-0.88721	1.69691
O	-0.08418	1.23555	0.81590
N	-0.47638	1.46224	-0.41539
O	0.06706	-0.03151	-1.15930

TS15_D

E (M06/BS2) = -677.256096 au
H (M06/BS2) = -677.076685 au
G (M06/BS2) = -677.142354 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -677.282712 au

Mo	-1.72385	0.03214	0.05430
H	-2.42010	0.16307	2.59358
H	-3.84438	0.09463	1.71644
H	-1.75161	2.64450	-0.17587
H	-0.24652	2.08657	-0.75364
H	-4.13128	-0.84534	-0.70223
H	-3.17186	-0.61693	-2.05466
N	-2.82763	0.07833	1.66363
N	-1.15575	1.83877	-0.34989
N	-3.24512	-0.48253	-1.04780
Mo	1.70091	-0.00737	0.03037
H	2.77664	1.61325	1.84001
H	3.86378	0.39937	1.47668
H	3.83345	-1.55590	0.33596
H	2.90133	-2.14881	-0.92433
H	1.31783	1.15487	-2.23772
H	2.57001	1.97017	-1.50461
N	2.92489	0.76825	1.28831
N	2.97615	-1.42729	-0.20912
N	1.73080	1.41790	-1.34101
O	-0.12535	-0.73785	-1.25110
N	-0.46653	-1.49863	-0.20138
O	0.08894	-0.62002	1.02796

14_T

E (M06/BS2) = -365.962453 au
H (M06/BS2) = -365.870275 au
G (M06/BS2) = -365.916113 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -365.971711 au

Mo	-0.12034	0.00015	-0.01827
H	-2.28566	0.82449	1.29283
H	-2.28557	-0.82596	1.29159
H	-0.86004	2.07424	-1.51869
H	0.78974	2.11843	-1.23020
H	-0.86101	-2.07314	-1.51969
H	0.78899	-2.11713	-1.23247
N	-1.84040	-0.00042	0.89983
N	-0.08798	1.66064	-1.00789
N	-0.08867	-1.65962	-1.00923
O	1.90955	-0.00084	0.24587
N	1.23012	-0.00071	1.36261

14_S

E (M06/BS2) = -365.986889 au
H (M06/BS2) = -365.894264 au
G (M06/BS2) = -365.937697 au
E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -365.997199 au

Mo	0.05926	0.01143	-0.10040
H	1.28787	-1.69852	-1.72079
H	1.77228	-1.95109	-0.13522
H	1.57599	2.13436	0.37888
H	0.57211	2.46138	-0.91385
H	1.12528	0.11268	2.26999
H	-0.44718	-0.38882	2.44035
N	1.22991	-1.37173	-0.76435
N	0.86176	1.76582	-0.23798
N	0.35129	-0.36617	1.81687
O	-1.87082	-0.19709	0.33670
N	-1.50138	0.03304	-0.92829

1_QF

E (M06/BS1) = -1635.614125 au

H (M06/BS1) = -1634.746108 au

G (M06/BS1) = -1634.866424 au

E (M06/BS2//M06/BS2, Solvent=DiethylEther) = -1636.10083272 au

Mo	-0.29329	-1.21914	-0.03489
N	-2.30707	-1.0074	-0.12772
N	0.81739	-1.13013	-1.70570
N	0.74968	-1.21842	1.66318
C	1.62875	-0.09655	1.65372
C	3.00555	-0.24205	1.42946
C	1.10810	1.20132	1.74483
C	3.84042	0.86755	1.30854
H	3.42234	-1.24201	1.29920
C	1.91848	2.32712	1.59868
H	0.03135	1.32354	1.87975
C	3.28611	2.14567	1.39787
H	3.93069	3.01945	1.27636
C	-2.76707	0.28005	0.21525
C	-3.47820	1.12889	-0.65556
C	-2.44892	0.78086	1.48591
C	-3.84464	2.41672	-0.27675
H	-3.72555	0.79048	-1.66166
H	-1.93152	0.11937	2.18531
C	-3.47249	2.89267	0.98571
H	-3.74132	3.91049	1.27737
C	1.12688	0.22809	-1.93383
C	2.42728	0.76129	-1.98161
C	0.05016	1.13380	-1.99616
C	2.64480	2.13575	-2.03029
H	3.29147	0.10307	-1.92511
C	0.24855	2.51557	-2.00928
H	-0.96869	0.73708	-2.01979
C	1.55205	3.00566	-2.02689
H	1.72239	4.08468	-2.03712
C	-2.77045	2.08325	1.87501
C	-3.21582	-1.99299	-0.76906
C	1.58450	-2.24057	-2.31582
C	0.70125	-2.10356	2.84443
C	-4.60835	3.30310	-1.21627
H	-5.63028	3.48319	-0.85389
H	-4.12960	4.28719	-1.31699
H	-4.68470	2.86107	-2.21746
C	-2.39322	2.56959	3.24365
H	-3.01783	2.10462	4.01957
H	-1.34981	2.32060	3.48764
H	-2.51168	3.65643	3.33249
C	1.30451	3.69501	1.63337
H	0.46142	3.75838	0.92913
H	0.91104	3.94160	2.63006
H	2.03107	4.47054	1.35961
C	5.30247	0.67667	1.02738
H	5.78010	0.02943	1.77537
H	5.45832	0.19652	0.04911
H	5.84061	1.63288	1.01638
C	-0.92894	3.44361	-1.98569
H	-1.67937	3.16367	-2.73868
H	-1.43932	3.40720	-1.01012
H	-0.62790	4.48202	-2.17322
C	4.04459	2.67498	-2.06118
H	4.46274	2.66012	-3.07813
H	4.07956	3.71381	-1.70817
H	4.71501	2.08018	-1.42556
C	0.31390	-1.28420	4.07613
H	0.25339	-1.92439	4.96755
H	1.05517	-0.49737	4.27171
H	-0.66411	-0.80236	3.93070
C	2.03530	-2.80561	3.10282
H	2.82743	-2.09104	3.35849
H	1.93567	-3.50603	3.94419
H	2.35152	-3.37677	2.21786
C	-0.36198	-3.16393	2.58692
H	-1.34803	-2.70492	2.41638
H	-0.10609	-3.76911	1.70165
H	-0.44456	-3.84126	3.44830
C	-4.65458	-1.82432	-0.28266
H	-5.09159	-0.86774	-0.59180
H	-5.28054	-2.62911	-0.69187
H	-4.69873	-1.87959	0.81436
C	-2.75119	-3.38892	-0.35199

H	-1.71357	-3.58131	-0.66522
H	-2.80311	-3.50366	0.73937
H	-3.38503	-4.15902	-0.81403
C	-3.15777	-1.90194	-2.29797
H	-3.74680	-2.70856	-2.75870
H	-3.55213	-0.94897	-2.67252
H	-2.11771	-1.99104	-2.64699
C	0.73218	-3.50369	-2.19395
H	0.58245	-3.78404	-1.13707
H	-0.25377	-3.36193	-2.65814
H	1.22981	-4.34868	-2.68992
C	2.90998	-2.52585	-1.59637
H	3.33452	-3.47450	-1.95574
H	3.66739	-1.75113	-1.75908
H	2.74025	-2.61206	-0.51245
C	1.82064	-1.96048	-3.79794
H	2.43811	-1.06708	-3.95313
H	2.33084	-2.81047	-4.27167
H	0.86015	-1.80302	-4.30933

2_TF

E (M06/BS1) = -1840.671385 au

H (M06/BS1) = -1839.785716 au

G (M06/BS1) = -1839.909975 au

E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -1841.218844 au

N	2.48880	0.10196	-0.36602
N	0.25069	0.00046	1.96756
N	-0.19797	-1.66094	-1.18337
C	-1.53967	-1.18382	-1.23658
C	-2.61806	-1.97336	-0.81382
C	-1.80265	0.10483	-1.71387
C	-3.93095	-1.51850	-0.92832
H	-2.42197	-2.94656	-0.36593
C	-3.10344	0.59874	-1.79597
H	-0.96378	0.73115	-2.02038
C	-4.15910	-0.23178	-1.41995
H	-5.18404	0.14290	-1.48612
C	2.02811	1.35956	-0.86650
C	2.06397	2.51441	-0.07294
C	1.46956	1.44209	-2.14745
C	1.53907	3.72109	-0.53015
H	2.46318	2.44743	0.94062
H	1.44526	0.54111	-2.76350
C	0.95920	3.75998	-1.80140
H	0.52103	4.69526	-2.15785
C	-0.99804	0.66515	1.76732
C	-2.21199	0.01874	2.03876
C	-1.02573	1.97460	1.28232
C	-3.42624	0.67317	1.84738
H	-2.19490	-1.02168	2.36623
C	-2.22981	2.64709	1.06944
H	-0.08068	2.47095	1.07025
C	-3.41902	1.98410	1.35994
H	-4.37253	2.48941	1.18329
C	0.92429	2.63455	-2.62598
C	3.95836	-0.15171	-0.39656
C	0.77258	-0.03292	3.36492
C	0.15610	-2.74442	-2.14870
C	1.55605	4.93407	0.35277
H	2.56040	5.37580	0.41150
H	0.87441	5.71059	-0.01574
H	1.25814	4.68212	1.38112
C	0.32027	2.69668	-3.99769
H	-0.23224	1.77712	-4.23666
H	-0.36988	3.54362	-4.09541
H	1.09405	2.81458	-4.76927
C	-3.34846	1.98912	-2.30300
H	-2.49904	2.64805	-2.07215
H	-3.48533	2.00466	-3.39429
H	-4.25053	2.42796	-1.85599
C	-5.07494	-2.40655	-0.53384
H	-5.37170	-3.06488	-1.36301
H	-4.80768	-3.05561	0.31028
H	-5.96106	-1.82492	-0.24953
C	-2.22067	4.05776	0.55585
H	-1.98972	4.77615	1.35620
H	-1.45402	4.19078	-0.22238
H	-3.19249	4.34113	0.13185
C	-4.72468	-0.01555	2.14307

H	-5.15785	0.3334	3.09148
H	-5.46656	0.18248	1.35728
H	-4.59424	-1.10248	2.21934
C	-0.23165	-2.29285	-3.55810
H	0.07530	-3.05107	-4.29177
H	-1.31536	-2.14798	-3.65433
H	0.26389	-1.34508	-3.81504
C	-0.52768	-4.08004	-1.84015
H	-1.60801	-4.03841	-2.01986
H	-0.11464	-4.86052	-2.49504
H	-0.35661	-4.37987	-0.79786
C	1.66341	-2.96412	-2.11196
H	2.19906	-2.02248	-2.29514
H	1.99029	-3.37633	-1.14772
H	1.95415	-3.67979	-2.89272
C	4.45425	-0.09795	-1.84189
H	4.27798	0.88837	-2.29182
H	5.53512	-0.29224	-1.87337
H	3.95524	-0.85461	-2.46181
C	4.24343	-1.52550	0.18739
H	3.91289	-1.59923	1.23105
H	3.74911	-2.32322	-0.37907
H	5.32559	-1.71165	0.16134
C	4.71793	0.89380	0.42237
H	5.78998	0.65398	0.41480
H	4.60026	1.90371	0.01007
H	4.38101	0.90175	1.46815
C	2.21037	-0.53668	3.35038
H	2.28654	-1.57590	3.00594
H	2.83443	0.09541	2.70188
H	2.62687	-0.49513	4.36594
C	-0.07067	-0.93897	4.26355
H	0.38188	-0.99790	5.26377
H	-1.08968	-0.54949	4.38261
H	-0.13149	-1.95239	3.84662
C	0.77697	1.38796	3.93264
H	-0.23671	1.79977	4.01288
H	1.22017	1.38343	4.93805
H	1.37216	2.06044	3.29694
Mo	0.89497	-0.84457	0.29106
O	1.98903	-3.41705	1.30988
N	0.96810	-2.73611	1.20898
O	-0.12710	-3.13127	1.61889

3_TF

E (M06/BS1) = -1840.643902 au

H (M06/BS1) = -1839.759540 au

G (M06/BS1) = -1839.882763 au

E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -1841.194941 au

N	2.49527	-0.27970	-0.28594
N	0.05508	0.16835	1.69162
N	-0.38842	-1.40388	-1.24377
C	-1.78360	-1.21053	-0.99599
C	-2.49639	-2.07862	-0.16626
C	-2.46020	-0.15782	-1.62455
C	-3.87531	-1.93426	0.00615
H	-1.96026	-2.88106	0.34344
C	-3.83479	-0.00163	-1.47711
H	-1.88595	0.55410	-2.22181
C	-4.53003	-0.90884	-0.66996
H	-5.60916	-0.79016	-0.54341
C	2.25972	1.06326	-0.72963
C	2.57962	2.17017	0.07097
C	1.67938	1.28549	-1.97978
C	2.32173	3.46696	-0.36195
H	2.99848	2.01417	1.06474
H	1.42583	0.42573	-2.59925
C	1.74010	3.65526	-1.62097
H	1.52466	4.67070	-1.96169
C	-1.08535	0.93431	1.28564
C	-2.37061	0.61731	1.74792
C	-0.91182	2.06827	0.49355
C	-3.45059	1.44926	1.47227
H	-2.52348	-0.29342	2.32716
C	-1.98961	2.89495	0.16729
H	0.08988	2.32689	0.15708
C	-3.24385	2.58683	0.68277
H	-4.09225	3.23697	0.45434
C	1.40397	2.57704	-2.43540

C	3.93310	-0.74199	-0.25247
C	0.46972	0.39418	3.13151
C	-0.12156	-2.29002	-2.43026
C	2.57305	4.63612	0.54240
H	3.36518	4.42526	1.27103
H	2.85444	5.53408	-0.02148
H	1.66441	4.88405	1.11294
C	0.73663	2.77949	-3.76330
H	-0.30138	2.41438	-3.74354
H	0.70889	3.83940	-4.04315
H	1.25067	2.22975	-4.56316
C	-4.56186	1.10999	-2.17416
H	-3.87410	1.91008	-2.47726
H	-5.07303	0.75213	-3.07936
H	-5.32922	1.55461	-1.52625
C	-4.61822	-2.86377	0.92003
H	-4.50530	-3.91203	0.61215
H	-4.23679	-2.79407	1.94914
H	-5.69037	-2.63307	0.94446
C	-1.78275	4.07890	-0.73005
H	-0.89569	4.65882	-0.43868
H	-1.62076	3.76122	-1.77196
H	-2.65030	4.75037	-0.72108
C	-4.81254	1.15849	2.02929
H	-5.06346	1.85371	2.84325
H	-5.59440	1.26846	1.26562
H	-4.87670	0.14118	2.43493
C	-0.55362	-1.57458	-3.71214
H	-0.31551	-2.20583	-4.57939
H	-1.63214	-1.37700	-3.72611
H	-0.02773	-0.61658	-3.83336
C	-0.87028	-3.62068	-2.32114
H	-1.95833	-3.48849	-2.35040
H	-0.58867	-4.26207	-3.16797
H	-0.60422	-4.14120	-1.39216
C	1.36280	-2.60384	-2.52605
H	1.97462	-1.69390	-2.56759
H	1.69077	-3.21532	-1.67601
H	1.55491	-3.18132	-3.44031
C	4.70917	-0.07605	-1.38864
H	4.80973	1.00813	-1.25302
H	5.71920	-0.50549	-1.42413
H	4.22876	-0.26062	-2.35945
C	4.00967	-2.25075	-0.45570
H	3.36866	-2.79666	0.24695
H	3.74644	-2.53058	-1.48125
H	5.04243	-2.57895	-0.27626
C	4.59413	-0.40718	1.08396
H	5.65106	-0.70639	1.05095
H	4.56381	0.66732	1.30242
H	4.11445	-0.95696	1.90353
C	1.95882	0.12850	3.32404
H	2.22848	-0.92011	3.17556
H	2.55972	0.74936	2.64919
H	2.23345	0.39563	4.35362
C	-0.32299	-0.51553	4.06985
H	0.06628	-0.41989	5.09380
H	-1.38571	-0.24697	4.09553
H	-0.22363	-1.56325	3.75913
C	0.23636	1.86069	3.51078
H	-0.82174	2.14547	3.47944
H	0.59559	2.01966	4.53652
H	0.79639	2.53451	2.84541
Mo	0.79452	-1.06009	0.33396
O	2.35296	-3.14371	2.12008
N	1.29932	-2.53181	1.90810
O	0.59237	-2.97855	0.76906

4_TF

E (M06/BS1) = -1840.659018 au

H (M06/BS1) = -1839.774474 au

G (M06/BS1) = -1839.902551 au

E (M06/BS2//M06/BS2, Solvent = DiethylEther) = -1841.208071 au

N	-2.28427	0.62295	-0.09871
N	0.04529	-1.02943	-1.83585
N	-0.07872	-1.00409	1.69524
C	1.32577	-0.75595	1.63018
C	2.24911	-1.80406	1.54215
C	1.79711	0.56148	1.63130

C	3.62078	-1.54882	1.51377
H	1.88677	-2.83127	1.46963
C	3.16064	0.84154	1.58476
H	1.07388	1.37845	1.65781
C	4.06014	-0.22589	1.55146
H	5.13287	-0.02012	1.52322
C	-1.76091	1.91123	0.23380
C	-1.62482	2.93619	-0.71700
C	-1.35430	2.17163	1.54597
C	-1.12263	4.18653	-0.36476
H	-1.90733	2.75231	-1.75295
H	-1.46209	1.38489	2.29212
C	-0.69287	4.39769	0.94936
H	-0.27488	5.36859	1.22499
C	1.18960	-0.18221	-1.85832
C	2.49019	-0.68782	-1.69981
C	1.02390	1.19426	-2.03612
C	3.59572	0.15408	-1.73423
H	2.62680	-1.75705	-1.53468
C	2.11743	2.06632	-2.03197
H	0.01563	1.58066	-2.19354
C	3.39265	1.53015	-1.89332
H	4.25747	2.19822	-1.90238
C	-0.79457	3.39726	1.91315
C	-3.72882	0.53986	-0.46582
C	-0.15986	-1.93571	-3.01153
C	-0.60341	-1.51367	2.99747
C	-1.05629	5.29678	-1.37166
H	-1.87666	6.01312	-1.22287
H	-0.11966	5.86408	-1.28991
H	-1.13610	4.91644	-2.39757
C	-0.28898	3.60619	3.30971
H	-0.92675	3.10465	4.04932
H	0.72460	3.19155	3.42836
H	-0.23772	4.67064	3.56843
C	3.64460	2.26107	1.59237
H	2.88186	2.94159	1.18921
H	3.88323	2.60115	2.61070
H	4.55553	2.37800	0.98980
C	4.59414	-2.68400	1.39095
H	4.45552	-3.42795	2.18682
H	4.46162	-3.21550	0.43660
H	5.63217	-2.33188	1.43394
C	1.91104	3.54495	-2.16562
H	1.19860	3.78356	-2.96726
H	1.49604	3.96677	-1.23757
H	2.85214	4.06630	-2.37946
C	4.98875	-0.39083	-1.62737
H	5.45887	-0.47378	-2.61806
H	5.63054	0.26381	-1.02205
H	5.00009	-1.38961	-1.17347
C	-0.03258	-0.67197	4.14088
H	-0.45663	-1.01539	5.09453
H	1.05957	-0.75838	4.20678
H	-0.28481	0.39163	4.01867
C	-0.23828	-2.98330	3.22582
H	0.84007	-3.11335	3.37800
H	-0.74612	-3.35848	4.12554
H	-0.54704	-3.60475	2.37491
C	-2.12243	-1.37774	3.01223
H	-2.43734	-0.33548	2.86984
H	-2.58691	-1.99581	2.23411
H	-2.51184	-1.71735	3.98181
C	-4.56217	1.25272	0.59763
H	-4.31100	2.31925	0.66424
H	-5.62966	1.17373	0.35046
H	-4.40312	0.79823	1.58571
C	-4.14018	-0.92502	-0.50891
H	-3.61358	-1.47140	-1.30446
H	-3.94473	-1.42956	0.44603
H	-5.21604	-0.99644	-0.71672
C	-4.00527	1.15123	-1.84191
H	-5.02705	0.90261	-2.16133
H	-3.92201	2.24424	-1.83621
H	-3.30336	0.74815	-2.58751
C	-1.65752	-2.14163	-3.23402
H	-2.11972	-2.69089	-2.40714
H	-2.16222	-1.17017	-3.34659
H	-1.82081	-2.71978	-4.15416
C	0.51944	-3.28998	-2.79919

H	0.29530	-3.96255	-3.64034
H	1.61068	-3.18364	-2.74405
H	0.16059	-3.75958	-1.87544
C	0.39202	-1.27794	-4.27849
H	1.47987	-1.14231	-4.24112
H	0.16192	-1.91327	-5.14450
H	-0.07134	-0.29451	-4.44292
Mo	-0.91957	-0.80983	-0.09515
O	-1.42613	-2.79459	-0.27610
N	-2.38375	-3.39168	0.42149
O	-2.44966	-4.57059	0.18688

5_TF

E (M06/BS1) = -1840.661627 au

H (M06/BS1) = -1839.776386 au

G (M06/BS1) = -1839.899654 au

E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -1841.218462 au

Mo	0.82160	-0.93258	0.28750
N	-0.29640	-1.62374	-1.23330
N	0.21782	-0.14210	2.00785
N	2.49734	-0.09380	-0.32103
C	-1.58641	-1.02148	-1.29824
C	-2.74933	-1.72076	-0.94664
H	-2.66065	-2.72603	-0.53687
C	-4.00830	-1.13591	-1.07781
C	-4.09750	0.18889	-1.50932
H	-5.08084	0.65930	-1.59363
C	-2.95534	0.93159	-1.80728
C	-1.71164	0.30866	-1.71447
H	-0.81078	0.86710	-1.97262
C	-0.01964	-2.68361	-2.24779
C	-0.84288	-3.95842	-2.04018
H	-1.90665	-3.79968	-2.25154
H	-0.74323	-4.32937	-1.01197
H	-0.48491	-4.74062	-2.72476
C	-0.31455	-2.11870	-3.63973
H	-1.37466	-1.85933	-3.75688
H	-0.06175	-2.86278	-4.40806
H	0.28189	-1.21378	-3.82826
C	-0.93064	0.68089	1.79070
C	-2.22825	0.18005	1.97628
H	-2.35418	-0.86854	2.24692
C	-3.34094	0.99260	1.78410
C	-3.14890	2.31865	1.37904
H	-4.02272	2.95329	1.20776
C	0.66211	-0.29756	3.42308
C	0.80692	1.08466	4.06307
H	-0.15383	1.61190	4.12134
H	1.50699	1.71011	3.49003
H	1.19784	0.97970	5.08460
C	-0.32606	-1.13008	4.24063
H	-1.29734	-0.62722	4.33115
H	0.06543	-1.28397	5.25638
H	-0.48642	-2.11086	3.77579
C	2.19085	1.20901	-0.81952
C	2.33555	2.34926	-0.01728
H	2.71381	2.23698	1.00039
C	2.09908	4.80819	0.41349
H	1.47632	5.64577	0.07587
H	3.14057	5.15869	0.42828
H	1.82612	4.57778	1.45332
C	1.37777	3.71176	-1.74496
H	1.03686	4.68784	-2.09826
C	1.23560	2.59998	-2.57749
C	-1.87642	2.84105	1.17232
C	-0.77404	2.01038	1.38966
H	0.23473	2.40121	1.25962
C	1.65590	1.35584	-2.10471
H	1.53988	0.46415	-2.72429
C	3.93181	-0.50073	-0.29707
C	4.76219	0.43024	0.58905
H	4.79633	1.45288	0.19363
H	5.79562	0.06076	0.63977
H	4.36368	0.46487	1.61264
C	4.04800	-1.91529	0.25004
H	3.66350	-1.98543	1.27525
H	5.10527	-2.21202	0.26230
H	3.50128	-2.63766	-0.36635
C	1.45609	-3.05707	-2.18880

H	1.70883	-3.54194	-1.23754
H	2.08917	-2.16744	-2.31319
H	1.69282	-3.75948	-2.99933
C	-5.24127	-1.92880	-0.75372
H	-5.13771	-2.46030	0.20184
H	-5.43763	-2.69098	-1.52105
H	-6.13046	-1.28882	-0.69171
C	2.02673	-0.97435	3.44727
H	2.75145	-0.40414	2.84667
H	1.98126	-1.99773	3.05773
H	2.40092	-1.01912	4.47908
C	-4.72917	0.46477	1.98469
H	-4.71936	-0.58651	2.29760
H	-5.31221	0.53323	1.05484
H	-5.27191	1.03910	2.74828
C	-1.67572	4.26591	0.74575
H	-0.90978	4.33898	-0.04032
H	-1.33591	4.89380	1.58239
H	-2.60451	4.70490	0.35988
C	4.49393	-0.45816	-1.71869
H	4.43155	0.55184	-2.14523
H	3.94949	-1.14487	-2.38078
H	5.55154	-0.75583	-1.71384
C	1.94229	3.60651	-0.47109
C	-3.05000	2.36173	-2.25029
H	-3.92065	2.86362	-1.80737
H	-3.14854	2.44343	-3.34286
H	-2.15029	2.92333	-1.96132
C	0.64604	2.73295	-3.95050
H	0.03670	1.85724	-4.21361
H	1.43040	2.82005	-4.71555
H	0.01284	3.62524	-4.03061
N	0.28790	-3.59126	1.46322
O	1.24388	-2.82934	1.00992
O	-0.81927	-3.08615	1.45394

TS3_TF

E (M06/BS1) = -1840.651251 au

H (M06/BS1) = -1839.768632 au

G (M06/BS1) = -1839.892233 au

E (M06/BS2//M06/BS2, Solvent = DiethylEther) = -1841.199478 au

N	2.54814	-0.16370	-0.26947
N	0.09310	-0.30642	1.92417
N	-0.29753	-1.42509	-1.44230
C	-1.59245	-0.82698	-1.42137
C	-2.68418	-1.52002	-0.88868
C	-1.79887	0.46202	-1.93373
C	-3.96924	-0.97553	-0.91023
H	-2.51874	-2.49966	-0.43882
C	-3.06762	1.03416	-1.94804
H	-0.94179	1.01560	-2.32381
C	-4.14603	0.29443	-1.45171
H	-5.14622	0.73598	-1.46869
C	2.34053	1.20311	-0.61607
C	2.57330	2.23086	0.30694
C	1.79073	1.52942	-1.86421
C	2.26021	3.55519	0.00529
H	2.94944	1.97693	1.29921
H	1.61060	0.72638	-2.58099
C	1.70116	3.84434	-1.24036
H	1.42648	4.87603	-1.47276
C	-0.99387	0.59471	1.71965
C	-2.31308	0.21605	2.01897
C	-0.76600	1.87506	1.20712
C	-3.36772	1.10579	1.85464
H	-2.50508	-0.80227	2.36275
C	-1.81619	2.77359	0.99503
H	0.25775	2.17629	0.98210
C	-3.10324	2.38348	1.34440
H	-3.93299	3.08107	1.20174
C	1.45756	2.84511	-2.18525
C	3.94130	-0.69068	-0.27955
C	0.56178	-0.47214	3.33345
C	-0.08632	-2.45831	-2.49923
C	2.44677	4.62277	1.04226
H	3.50026	4.72633	1.33455
H	2.09831	5.59899	0.68415
H	1.88501	4.37937	1.95697
C	0.85333	3.18493	-3.51546

H	0.41161	2.30233	-3.99692
H	0.06982	3.94842	-3.41366
H	1.60537	3.59031	-4.20690
C	-3.28455	2.42595	-2.46183
H	-2.37690	2.83158	-2.92711
H	-4.09341	2.46511	-3.20389
H	-3.56904	3.10315	-1.64244
C	-5.11836	-1.75222	-0.33842
H	-5.29506	-2.68183	-0.89706
H	-4.91913	-2.04280	0.70317
H	-6.04898	-1.17094	-0.35318
C	-1.54298	4.11712	0.38619
H	-0.71051	4.63163	0.88727
H	-1.25867	4.01322	-0.67299
H	-2.42425	4.76955	0.43269
C	-4.77652	0.71099	2.18126
H	-4.81977	-0.26359	2.68287
H	-5.25911	1.45027	2.83480
H	-5.38824	0.64208	1.26897
C	-0.34447	-1.82037	-3.86614
H	-0.14922	-2.55126	-4.66350
H	-1.38408	-1.48234	-3.96567
H	0.31417	-0.95395	-4.02505
C	-0.98857	-3.68344	-2.33386
H	-2.04492	-3.43998	-2.50221
H	-0.70436	-4.44751	-3.07183
H	-0.88016	-4.10833	-1.32745
C	1.36060	-2.92647	-2.44772
H	2.05028	-2.07465	-2.52915
H	1.56241	-3.46605	-1.51347
H	1.56292	-3.60844	-3.28482
C	4.51246	-0.57474	-1.69305
H	4.52368	0.47003	-2.03228
H	5.54607	-0.94648	-1.71530
H	3.92346	-1.16263	-2.40920
C	3.92263	-2.14988	0.15180
H	3.53884	-2.26329	1.17375
H	3.29978	-2.76168	-0.51100
H	4.94435	-2.55161	0.12387
C	4.84526	0.08849	0.67824
H	5.84537	-0.36623	0.68460
H	4.96057	1.13607	0.37366
H	4.45601	0.06372	1.70536
C	1.89327	-1.21363	3.33921
H	1.79637	-2.23197	2.94739
H	2.63598	-0.67377	2.73258
H	2.27623	-1.27616	4.36694
C	-0.44032	-1.23509	4.20127
H	-0.02766	-1.36937	5.21152
H	-1.38622	-0.68825	4.30023
H	-0.64442	-2.22681	3.77890
C	0.79291	0.91299	3.94519
H	-0.13748	1.49109	4.01595
H	1.20189	0.80519	4.95936
H	1.51051	1.49236	3.34593
Mo	0.80178	-0.95821	0.16785
O	0.91440	-2.91907	0.79130
N	0.04366	-3.43422	1.67346
O	-0.90226	-3.96879	1.16522

TS7_TF

E (M06/BS1) = -1840.643565 au

H (M06/BS1) = -1839.762431 au

G (M06/BS1) = -1839.890816 au

E (M06/BS2//M06/BS2, Solvent = DiethylEther) = -1841.196500 au

N	2.25858	0.93058	-0.24586
N	0.24833	-0.43098	1.91740
N	0.15395	-1.23133	-1.46674
C	-1.26356	-1.09892	-1.47146
C	-2.11489	-2.20605	-1.37324
C	-1.83500	0.17343	-1.58536
C	-3.50050	-2.05879	-1.45820
H	-1.69184	-3.19720	-1.21226
C	-3.21558	0.35034	-1.62510
H	-1.17834	1.04236	-1.63351
C	-4.03682	-0.77782	-1.58423
H	-5.12218	-0.65381	-1.62562
C	1.42195	2.04927	-0.55060
C	1.04493	2.95631	0.44781

C	0.92333	2.22814	-1.84486
C	0.18087	4.01509	0.17370
H	1.41963	2.80518	1.46239
H	1.20351	1.50996	-2.61815
C	-0.33065	4.14113	-1.12091
H	-1.03437	4.94802	-1.33855
C	-1.14235	-0.11026	1.87310
C	-2.11454	-1.12104	1.87534
C	-1.55621	1.22123	1.83943
C	-3.47031	-0.80887	1.87013
H	-1.79640	-2.16497	1.85890
C	-2.91063	1.56068	1.80552
H	-0.79993	2.00495	1.84270
C	-3.85235	0.53655	1.83047
H	-4.91628	0.78640	1.80145
C	0.03393	3.26226	-2.14179
C	3.73078	1.18025	-0.25285
C	0.80934	-0.78708	3.26104
C	0.77694	-1.97569	-2.60707
C	-0.18583	4.99482	1.24890
H	0.59594	5.75739	1.37375
H	-1.11984	5.52142	1.01580
H	-0.30762	4.50084	2.22260
C	-0.55190	3.37641	-3.51773
H	0.22808	3.47940	-4.28384
H	-1.13222	2.47575	-3.77108
H	-1.22332	4.23947	-3.59986
C	-3.79944	1.72836	-1.72765
H	-3.05874	2.49294	-1.45269
H	-4.14095	1.95001	-2.74935
H	-4.66916	1.84442	-1.06623
C	-4.38670	-3.26941	-1.40625
H	-4.29622	-3.87096	-2.32161
H	-4.12068	-3.92603	-0.56651
H	-5.44301	-2.99344	-1.29680
C	-3.31856	3.00374	1.75057
H	-3.02209	3.54264	2.66192
H	-2.83420	3.51926	0.90725
H	-4.40406	3.11472	1.63693
C	-4.51095	-1.88724	1.89558
H	-5.08031	-1.87414	2.83571
H	-5.23670	-1.75914	1.07986
H	-4.06033	-2.88245	1.79298
C	0.12082	-1.53879	-3.91631
H	0.62233	-2.03091	-4.76100
H	-0.94249	-1.80528	-3.95351
H	0.20779	-0.45001	-4.05047
C	0.66921	-3.49372	-2.43671
H	-0.35007	-3.85787	-2.60908
H	1.32173	-3.99631	-3.16501
H	0.98934	-3.78877	-1.42807
C	2.25847	-1.61502	-2.68401
H	2.39836	-0.52837	-2.75227
H	2.81410	-1.99924	-1.81720
H	2.70209	-2.07280	-3.57859
C	4.17214	1.64987	-1.63963
H	3.66549	2.57886	-1.93189
H	5.25358	1.84363	-1.63979
H	3.96431	0.88615	-2.40064
C	4.45924	-0.10777	0.09309
H	4.20234	-0.46143	1.10017
H	4.23224	-0.91212	-0.61662
H	5.54309	0.06790	0.06699
C	4.11118	2.24994	0.77226
H	5.20204	2.38069	0.77836
H	3.66131	3.22257	0.53639
H	3.79884	1.95913	1.78454
C	2.32728	-0.64470	3.23084
H	2.78731	-1.37672	2.55433
H	2.61431	0.36905	2.91438
H	2.73660	-0.81679	4.23547
C	0.45182	-2.22504	3.63571
H	0.94359	-2.50024	4.57982
H	-0.62949	-2.34630	3.77733
H	0.78840	-2.92158	2.85608
C	0.26853	0.17542	4.31766
H	-0.81816	0.08831	4.44076
H	0.73600	-0.04735	5.28654
H	0.50315	1.21692	4.05448
Mo	1.14288	-0.65198	0.16116

O	1.91913	-2.30087	0.51015
N	3.31004	-3.03679	0.44358
O	3.14493	-4.18833	0.69135

TS8_TF

E (M06/BS1) = -1840.654375 au

H (M06/BS1) = -1839.772789 au

G (M06/BS1) = -1839.898004 au

E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -1841.205926 au

Mo	0.91137	-1.04961	0.21273
N	-0.18782	-1.34997	-1.40451
N	0.08097	-0.42055	1.88578
N	2.53130	-0.00423	-0.20620
C	-1.51426	-0.82307	-1.40775
C	-2.61347	-1.63710	-1.12617
H	-2.44424	-2.66541	-0.80637
C	-3.91547	-1.14010	-1.21968
C	-4.10024	0.19789	-1.56215
H	-5.11533	0.59969	-1.62405
C	-3.01526	1.04942	-1.79110
C	-1.72917	0.52317	-1.72365
H	-0.86610	1.16340	-1.91259
C	0.16823	-2.20789	-2.58353
C	-0.53133	-3.56768	-2.52584
H	-1.61646	-3.47515	-2.65130
H	-0.32778	-4.06763	-1.56989
H	-0.15756	-4.20752	-3.33798
C	-0.22340	-1.48909	-3.87509
H	-1.30595	-1.32304	-3.94049
H	0.07678	-2.09885	-4.73832
H	0.27798	-0.51395	-3.95628
C	-1.07394	0.41440	1.74386
C	-2.36485	-0.11126	1.88484
H	-2.48881	-1.18274	2.04939
C	-3.48215	0.71573	1.79870
C	-3.29844	2.07931	1.54532
H	-4.17460	2.72930	1.47249
C	0.53392	-0.65170	3.29855
C	0.77024	0.69179	3.98970
H	-0.14542	1.29224	4.05468
H	1.53095	1.27869	3.45332
H	1.13340	0.51932	5.01228
C	-0.51124	-1.45565	4.07086
H	-1.44923	-0.89893	4.18677
H	-0.13110	-1.68444	5.07631
H	-0.72505	-2.39993	3.55290
C	2.17884	1.32943	-0.58958
C	2.23998	2.38767	0.32558
H	2.57653	2.18823	1.34383
C	1.87789	4.77796	0.98829
H	1.29069	5.64765	0.66876
H	2.90930	5.11806	1.15528
H	1.48898	4.44564	1.96173
C	1.32328	3.88705	-1.30938
H	0.97125	4.88402	-1.5839
C	1.26367	2.85937	-2.2514
C	-2.02945	2.62275	1.37217
C	-0.92375	1.77683	1.48081
H	0.08103	2.18281	1.37146
C	1.70218	1.58760	-1.87942
H	1.65041	0.76689	-2.5968
C	3.99254	-0.32338	-0.14796
C	4.69934	0.50949	0.92415
H	4.68486	1.58011	0.68677
H	5.75111	0.19996	0.99325
H	4.23705	0.36541	1.91109
C	4.19156	-1.79706	0.17666
H	3.76358	-2.06540	1.15000
H	5.26773	-2.01276	0.20768
H	3.73801	-2.44741	-0.57985
C	1.67305	-2.45071	-2.60414
H	1.98865	-3.04931	-1.74067
H	2.23055	-1.50434	-2.60657
H	1.94252	-3.00586	-3.51238
C	-5.07992	-2.03815	-0.92084
H	-5.04088	-2.40535	0.11487
H	-5.08320	-2.92419	-1.57021
H	-6.03754	-1.51982	-1.05635
C	1.84475	-1.42724	3.31362

H	2.63166	-0.88908	2.76401
H	1.73425	-2.42795	2.88073
H	2.18532	-1.53670	4.35181
C	-4.86583	0.15522	1.93244
H	-4.85362	-0.85040	2.37127
H	-5.34844	0.07732	0.94630
H	-5.50390	0.79371	2.55757
C	-1.83164	4.08716	1.10876
H	-1.09162	4.25078	0.31164
H	-1.45692	4.60918	2.00156
H	-2.76835	4.57527	0.81190
C	4.62989	-0.02245	-1.50527
H	4.52933	1.03717	-1.77369
H	4.17177	-0.62540	-2.30063
H	5.70170	-0.26096	-1.47302
C	1.82245	3.67095	-0.02247
C	-3.23212	2.50119	-2.09802
H	-3.90711	2.96183	-1.36272
H	-3.68581	2.64764	-3.08854
H	-2.28534	3.05793	-2.07609
C	0.73652	3.09792	-3.63569
H	1.53126	3.00568	-4.38871
H	0.29940	4.09883	-3.73392
H	-0.03870	2.36415	-3.90066
N	0.33062	-3.95508	1.08653
O	1.31821	-2.80651	0.61149
O	-0.78878	-3.55408	1.25670

7_Df

E (M06/BS1) = -1710.861713 au

H (M06/BS1) = -1709.987472 au

G (M06/BS1) = -1710.106861 au

E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -1711.380018 au

Mo	0.79384	-1.17584	0.67405
N	-0.35907	-1.66215	-0.87901
N	-0.01755	0.29194	1.73679
N	2.57211	-0.50774	0.04198
C	-1.74703	-1.33425	-0.80427
C	-2.58830	-1.97955	0.10763
H	-2.15677	-2.70337	0.80322
C	-3.95729	-1.71172	0.14222
C	-4.47631	-0.77540	-0.74957
H	-5.54603	-0.55294	-0.72732
C	-3.65592	-0.08416	-1.64428
C	-2.29332	-0.37449	-1.66223
H	-1.62685	0.16211	-2.34192
C	-0.05479	-2.77850	-1.83328
C	-0.83041	-4.04661	-1.47192
H	-1.91376	-3.90850	-1.57118
H	-0.61068	-4.35123	-0.43942
H	-0.53281	-4.86556	-2.14180
C	-0.39986	-2.35942	-3.26304
H	-1.47072	-2.15277	-3.37964
H	-0.13535	-3.16609	-3.96108
H	0.15783	-1.45721	-3.55376
C	-1.07339	1.08713	1.19587
C	-2.40488	0.92186	1.60121
H	-2.66021	0.11506	2.28812
C	-3.41385	1.73848	1.09806
C	-3.08446	2.72205	0.16032
H	-3.87638	3.35390	-0.25057
C	0.37003	0.58980	3.15251
C	0.43275	2.10237	3.36921
H	-0.54586	2.57803	3.22992
H	1.14319	2.56929	2.67045
H	0.76910	2.31236	4.39398
C	-0.61459	-0.04096	4.13912
H	-1.60012	0.43705	4.09451
H	-0.24076	0.06736	5.16737
H	-0.73252	-1.11297	3.92576
C	2.46546	0.72192	-0.68114
C	2.71181	1.94982	-0.05205
H	3.00155	1.95988	0.99911
C	2.71451	4.45550	0.00716
H	2.75172	5.30736	-0.68261
H	3.63456	4.45989	0.60578
H	1.87999	4.63150	0.70366
C	2.08938	3.13103	-2.04695
H	1.92668	4.07385	-2.57426

C	1.82585	1.92772	-2.70012
C	-1.77798	2.88430	-0.28838
C	-0.77833	2.07167	0.25148
H	0.25624	2.20644	-0.06040
C	2.02763	0.73175	-2.00828
H	1.82497	-0.21719	-2.50591
C	3.95426	-1.04255	0.24962
C	4.84999	-0.04975	0.99693
H	4.99713	0.87730	0.43023
H	5.83797	-0.50382	1.15326
H	4.43868	0.20407	1.98275
C	3.89534	-2.32876	1.06230
H	3.46771	-2.16100	2.05898
H	4.91286	-2.72084	1.19212
H	3.30013	-3.10388	0.56461
C	1.42918	-3.11177	-1.78427
H	1.72790	-3.49246	-0.79716
H	2.04292	-2.23779	-2.02522
H	1.65268	-3.89968	-2.51606
C	-4.83645	-2.39855	1.14573
H	-4.77321	-3.49196	1.06193
H	-5.88809	-2.11121	1.02189
H	-4.54038	-2.14315	2.17417
C	1.75722	0.01925	3.43497
H	2.49965	0.43117	2.73902
H	1.77139	-1.07668	3.36524
H	2.06332	0.28657	4.45535
C	-4.83519	1.57170	1.54731
H	-4.99577	0.59209	2.01499
H	-5.53274	1.65885	0.70255
H	-5.11905	2.34046	2.28055
C	-1.44493	3.88025	-1.35974
H	-0.53224	4.44512	-1.12411
H	-2.26143	4.59691	-1.51479
H	-1.26043	3.37610	-2.32179
C	4.60538	-1.33629	-1.10497
H	4.63196	-0.44094	-1.74001
H	4.07369	-2.12978	-1.64443
H	5.64143	-1.66976	-0.95439
C	2.53023	3.15751	-0.72187
C	-4.22704	0.94795	-2.57112
H	-5.18322	1.33664	-2.19608
H	-4.41141	0.53627	-3.57393
H	-3.54060	1.79790	-2.68829
C	1.31169	1.90109	-4.10919
H	1.96035	1.30530	-4.76568
H	1.23936	2.91045	-4.53199
H	0.31065	1.44737	-4.15569
O	0.77547	-2.59220	1.65269

2_SF

E (M06/BS1) = -1840.674788 au

H (M06/BS1) = -1839.788791 au

G (M06/BS1) = -1839.910327 au

E (M06/BS2//M06/BS2, Solvent = DiethylEther) = -1841.223669 au

N	2.49883	-0.22241	-0.08344
N	-0.03724	0.30105	1.75270
N	-0.24414	-1.56188	-1.12390
C	-1.64536	-1.32217	-0.96712
C	-2.40344	-2.15541	-0.14302
C	-2.26959	-0.28123	-1.66714
C	-3.78733	-1.98059	-0.03551
H	-1.90397	-2.96272	0.39743
C	-3.64583	-0.10792	-1.59539
H	-1.65556	0.39865	-2.26143
C	-4.38953	-0.97394	-0.78298
H	-5.47240	-0.84161	-0.71952
C	2.29047	1.05536	-0.70718
C	2.47839	2.26060	-0.01461
C	1.80645	1.12444	-2.01836
C	2.17737	3.49040	-0.59772
H	2.81318	2.23983	1.02170
H	1.68053	0.20011	-2.57915
C	1.68449	3.51731	-1.90429
H	1.43876	4.47715	-2.36421
C	-1.17929	1.02642	1.28677
C	-2.47323	0.70187	1.71717
C	-1.00182	2.11894	0.43803
C	-3.56370	1.47776	1.33785

H	-2.62408	-0.18009	2.34091
C	-2.08630	2.89004	0.01427
H	0.00667	2.38163	0.12029
C	-3.35382	2.57257	0.48987
H	-4.21055	3.17645	0.17957
C	1.49090	2.34080	-2.62627
C	3.93058	-0.64859	0.06308
C	0.39555	0.63742	3.16048
C	0.12582	-2.41374	-2.30954
C	2.29544	4.75149	0.20569
H	3.19490	4.75206	0.83428
H	2.32489	5.64063	-0.43576
H	1.43251	4.86366	0.88039
C	0.94173	2.36531	-4.02249
H	-0.09484	1.99701	-4.05248
H	0.93998	3.38067	-4.43682
H	1.52613	1.72480	-4.69654
C	-4.33130	0.96488	-2.38720
H	-3.61403	1.70069	-2.77233
H	-4.86627	0.54134	-3.24918
H	-5.07468	1.50120	-1.78233
C	-4.58836	-2.86137	0.87630
H	-4.46717	-3.92325	0.62361
H	-4.26404	-2.74652	1.92059
H	-5.65772	-2.62229	0.82983
C	-1.86219	4.02562	-0.94005
H	-1.12794	4.74491	-0.54932
H	-1.45667	3.66070	-1.89619
H	-2.79168	4.56845	-1.15159
C	-4.94656	1.15574	1.82056
H	-5.31281	1.91611	2.52470
H	-5.66337	1.12083	0.98810
H	-4.97971	0.18554	2.33151
C	-0.26171	-1.72013	-3.61529
H	0.05965	-2.34316	-4.46091
H	-1.34623	-1.58074	-3.69769
H	0.21958	-0.73781	-3.71647
C	-0.60513	-3.75517	-2.21662
H	-1.69354	-3.63762	-2.28295
H	-0.28610	-4.39060	-3.05436
H	-0.35489	-4.26515	-1.27806
C	1.61990	-2.69071	-2.30639
H	2.20394	-1.76650	-2.35465
H	1.90491	-3.24950	-1.40729
H	1.87517	-3.30131	-3.18242
C	4.62136	-0.59855	-1.30343
H	4.60657	0.41251	-1.73081
H	5.67271	-0.89732	-1.19233
H	4.15384	-1.28536	-2.02002
C	3.99865	-2.07189	0.59542
H	3.57050	-2.15261	1.60165
H	3.47551	-2.77843	-0.05958
H	5.05064	-2.38251	0.65065
C	4.71794	0.25425	1.01706
H	5.74421	-0.12775	1.10767
H	4.78386	1.28514	0.64875
H	4.27490	0.26166	2.02002
C	1.89257	0.41115	3.32737
H	2.17900	-0.62153	3.10474
H	2.46350	1.09249	2.68608
H	2.17083	0.61896	4.36970
C	-0.36464	-0.24853	4.14759
H	-0.01805	-0.04937	5.17204
H	-1.44233	-0.04590	4.11758
H	-0.19118	-1.30741	3.92144
C	0.12378	2.10946	3.47534
H	-0.94485	2.35587	3.46438
H	0.50871	2.32972	4.48026
H	0.63874	2.76957	2.76319
Mo	0.72848	-0.94243	0.43550
O	1.40469	-2.60485	2.51080
N	1.11069	-2.72641	1.29829
O	1.05954	-3.84302	0.76586

3_SF

E (M06/BS1) = -1840.670795 au

H (M06/BS1) = -1839.784762 au

G (M06/BS1) = -1839.905463 au

E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -1841.222416 au

N	2.50671	-0.25522	-0.21588
N	0.07327	-0.00611	1.68017
N	-0.39873	-1.20729	-1.35039
C	-1.79626	-1.04772	-1.09143
C	-2.51605	-1.98497	-0.34604
C	-2.47040	0.05934	-1.62117
C	-3.89242	-1.84435	-0.15055
H	-1.98771	-2.83867	0.08325
C	-3.84360	0.21092	-1.45564
H	-1.89500	0.81835	-2.15571
C	-4.54219	-0.75627	-0.72600
H	-5.61915	-0.63921	-0.58078
C	2.30093	1.10966	-0.60855
C	2.56795	2.17223	0.26868
C	1.76704	1.41113	-1.86344
C	2.30332	3.49186	-0.08987
H	2.94466	1.96374	1.27014
H	1.55696	0.59610	-2.55299
C	1.76378	3.75410	-1.35253
H	1.53817	4.78536	-1.63410
C	-1.05009	0.83210	1.37943
C	-2.33513	0.49618	1.82376
C	-0.86449	2.02639	0.68478
C	-3.41163	1.35131	1.60688
H	-2.49935	-0.46275	2.31569
C	-1.93520	2.88606	0.43011
H	0.13494	2.29675	0.35050
C	-3.19454	2.54670	0.91400
H	-4.03990	3.21206	0.72158
C	1.48096	2.72302	-2.24540
C	3.93483	-0.72238	-0.23491
C	0.52586	0.04799	3.11900
C	-0.12072	-1.95740	-2.62412
C	2.49581	4.59780	0.90456
H	3.32896	4.39167	1.58775
H	2.68401	5.56039	0.41324
H	1.59304	4.72067	1.52321
C	0.84971	2.99440	-3.57882
H	-0.19091	2.63568	-3.60165
H	0.83387	4.06670	-3.80845
H	1.38006	2.48037	-4.39174
C	-4.56561	1.37820	-2.06049
H	-3.87877	2.20686	-2.27739
H	-5.05487	1.10091	-3.00543
H	-5.35194	1.75491	-1.39227
C	-4.63851	-2.84160	0.68625
H	-4.51319	-3.86485	0.30718
H	-4.27173	-2.84288	1.72347
H	-5.71291	-2.62101	0.71299
C	-1.71666	4.13563	-0.37128
H	-0.98338	4.80308	0.10445
H	-1.31899	3.89789	-1.37007
H	-2.64934	4.69831	-0.50331
C	-4.77932	1.00604	2.11690
H	-4.95851	1.44459	3.10938
H	-5.56418	1.38779	1.45038
H	-4.91164	-0.07959	2.20897
C	-0.48807	-1.08455	-3.82744
H	-0.22981	-1.61170	-4.75652
H	-1.56266	-0.86694	-3.85338
H	0.05477	-0.12932	-3.81424
C	-0.91069	-3.26617	-2.70988
H	-1.99364	-3.09608	-2.74075
H	-0.63018	-3.79633	-3.63090
H	-0.68299	-3.91916	-1.85837
C	1.35852	-2.30582	-2.71174
H	1.99181	-1.41592	-2.64444
H	1.64908	-3.01164	-1.92201
H	1.56300	-2.79530	-3.67332
C	4.50751	-0.54638	-1.64462
H	4.44071	0.49621	-1.98166
H	5.56835	-0.83151	-1.64732
H	3.98963	-1.18143	-2.37415
C	4.01954	-2.19300	0.14650
H	3.73745	-2.36536	1.19122
H	3.39258	-2.82595	-0.49517
H	5.05766	-2.53035	0.02562
C	4.82407	0.06551	0.73260
H	5.83857	-0.35537	0.70850
H	4.90183	1.12302	0.45393

H	4.45902	-0.00346	1.76498
C	2.00755	-0.30139	3.22416
H	2.22688	-1.34228	2.96118
H	2.60486	0.36232	2.58934
H	2.33305	-0.15960	4.26364
C	-0.28001	-0.94053	3.96240
H	0.14714	-1.00566	4.97327
H	-1.32702	-0.63180	4.06427
H	-0.25123	-1.94314	3.51398
C	0.36243	1.46684	3.67009
H	-0.68410	1.79420	3.68802
H	0.74386	1.49650	4.69941
H	0.93836	2.18613	3.06904
Mo	0.79003	-1.13530	0.25037
O	1.76134	-3.44326	2.14991
N	1.23433	-2.74854	1.30667
O	0.45493	-3.27374	0.37771

4_SF

E (M06/BS1) = -1840.666915 au

H (M06/BS1) = -1839.783130 au

G (M06/BS1) = -1839.909465 au

E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -1841.216318 au

N	2.54747	-0.22524	-0.26038
N	0.09951	-0.11172	1.74876
N	-0.39309	-1.34181	-1.29348
C	-1.75229	-0.92101	-1.16923
C	-2.70363	-1.76684	-0.59767
C	-2.15073	0.33170	-1.64917
C	-4.05033	-1.39786	-0.54144
H	-2.38136	-2.72557	-0.18832
C	-3.48548	0.72100	-1.60274
H	-1.39136	1.00729	-2.04982
C	-4.42486	-0.16293	-1.06147
H	-5.47585	0.13481	-1.02493
C	2.35177	1.13908	-0.64249
C	2.65557	2.19632	0.22613
C	1.74306	1.45147	-1.86594
C	2.35348	3.51834	-0.09674
H	3.08970	1.97717	1.20165
H	1.51284	0.64143	-2.55883
C	1.73593	3.78911	-1.31833
H	1.48166	4.82099	-1.57203
C	-0.99733	0.77979	1.53814
C	-2.30064	0.41868	1.90173
C	-0.77441	2.03501	0.97209
C	-3.35911	1.30467	1.72621
H	-2.48343	-0.57953	2.30292
C	-1.82545	2.92999	0.76201
H	0.24030	2.31104	0.68696
C	-3.10479	2.56014	1.16307
H	-3.93612	3.25329	1.01060
C	1.41717	2.76408	-2.21035
C	3.96068	-0.71799	-0.25274
C	0.66243	-0.12010	3.13873
C	-0.09354	-2.13716	-2.53278
C	2.61161	4.60631	0.90318
H	3.65120	4.59812	1.25622
H	2.40160	5.59883	0.48660
H	1.97258	4.47456	1.79011
C	0.70235	3.05996	-3.49588
H	0.97535	2.34801	-4.28530
H	-0.38972	2.99298	-3.36802
H	0.92149	4.07201	-3.85783
C	-3.92410	2.04962	-2.14355
H	-3.08001	2.74435	-2.24372
H	-4.38569	1.94580	-3.13614
H	-4.67201	2.51900	-1.48970
C	-5.05647	-2.32359	0.07628
H	-5.18930	-3.23506	-0.52305
H	-4.73581	-2.64799	1.07651
H	-6.03836	-1.84393	0.17527
C	-1.56332	4.24616	0.09100
H	-0.80410	4.83391	0.62713
H	-1.17197	4.09548	-0.92734
H	-2.47485	4.85284	0.01890
C	-4.75458	0.92998	2.12773
H	-5.04348	1.40629	3.07568
H	-5.48416	1.25058	1.37077

H	-4.85778	-0.15466	2.25672
C	-0.44905	-1.33895	-3.7858
H	-0.18349	-1.92089	-4.67909
H	-1.52138	-1.11407	-3.83595
H	0.10285	-0.38921	-3.82381
C	-0.88020	-3.44878	-2.52486
H	-1.96262	-3.27845	-2.55855
H	-0.60512	-4.04389	-3.40682
H	-0.64594	-4.03999	-1.62890
C	1.38944	-2.47782	-2.56882
H	2.00675	-1.57264	-2.58477
H	1.68108	-3.09417	-1.70616
H	1.61266	-3.05783	-3.47412
C	4.54799	-0.59921	-1.66228
H	4.50573	0.43628	-2.02629
H	5.60231	-0.90897	-1.65819
H	4.01436	-1.23831	-2.37681
C	3.98951	-2.17845	0.17649
H	3.62061	-2.31524	1.20056
H	3.38602	-2.81333	-0.48189
H	5.02482	-2.54427	0.14100
C	4.86946	0.07634	0.69370
H	5.86698	-0.38431	0.70603
H	4.99321	1.11616	0.36835
H	4.49185	0.07721	1.72512
C	1.93428	-0.95808	3.15467
H	1.73521	-2.01277	2.92205
H	2.67035	-0.56820	2.43925
H	2.38913	-0.92276	4.15329
C	-0.33887	-0.74515	4.11005
H	0.12279	-0.84460	5.10271
H	-1.23865	-0.12798	4.21919
H	-0.63935	-1.74496	3.76706
C	1.00027	1.29877	3.59456
H	0.10845	1.93645	3.63663
H	1.44178	1.26827	4.60024
H	1.72502	1.77016	2.91564
Mo	0.81260	-1.07964	0.21488
O	1.02400	-3.03284	0.75542
N	-0.08983	-3.55273	1.30047
O	0.04482	-4.70092	1.61202

5_SF

E (M06/BS1) = -1840.672702 au

H (M06/BS1) = -1839.786664 au

G (M06/BS1) = -1839.906941 au

E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -1841.220426 au

Mo	-0.64148	-1.03699	-0.48190
N	0.34745	-1.45268	1.16574
N	-0.03409	0.40628	-1.67666
N	-2.46019	-0.44625	0.06086
C	1.73718	-1.24051	0.90628
C	2.43254	-2.05258	0.00268
H	1.90048	-2.85098	-0.51895
C	3.80453	-1.87765	-0.21018
C	4.47498	-0.91359	0.53416
H	5.55356	-0.79433	0.40320
C	3.80136	-0.07583	1.43293
C	2.43086	-0.23484	1.59415
H	1.87370	0.42876	2.25925
C	0.07818	-2.37437	2.32549
C	0.86049	-3.68383	2.19679
H	1.94495	-3.52121	2.21754
H	0.59928	-4.20858	1.27017
H	0.60638	-4.33457	3.04500
C	0.49236	-1.68407	3.62812
H	1.57158	-1.49180	3.66088
H	0.24076	-2.33076	4.47993
H	-0.03064	-0.72680	3.76109
C	1.07976	1.14199	-1.16333
C	2.37672	0.95189	-1.66108
H	2.56220	0.14537	-2.37095
C	3.42491	1.76637	-1.24828
C	3.16941	2.77338	-0.30868
H	3.99134	3.41450	0.02102
C	-0.48728	0.85360	-3.04510
C	-0.37072	2.37701	-3.16721
H	0.66507	2.73017	-3.09141
H	-0.96461	2.88065	-2.39012

H	-0.75927	2.68496	-4.14753
C	0.36241	0.18802	-4.12978
H	1.40272	0.53329	-4.10142
H	-0.03971	0.43909	-5.12193
H	0.34526	-0.90259	-4.01516
C	-2.38818	0.83900	0.70612
C	-2.73524	2.02871	0.04413
H	-3.11955	1.98595	-0.97298
C	-2.91354	4.52882	-0.10892
H	-2.26494	5.36681	0.17712
H	-3.94841	4.83644	0.09815
H	-2.82858	4.38900	-1.19449
C	-2.00855	3.34413	1.92162
H	-1.83618	4.31988	2.38188
C	-1.66687	2.18707	2.61585
C	1.90184	2.95380	0.23414
C	0.85975	2.13806	-0.21262
H	-0.15339	2.30566	0.15075
C	-1.87335	0.95012	2.00062
H	-1.59409	0.04419	2.53196
C	-3.84556	-1.00390	-0.10620
C	-4.76099	-0.10490	-0.94434
H	-4.94939	0.86155	-0.46215
H	-5.73267	-0.60292	-1.06767
H	-4.34782	0.07022	-1.94528
C	-3.78193	-2.36233	-0.78768
H	-3.40438	-2.28122	-1.81360
H	-4.79311	-2.78869	-0.83274
H	-3.1438	-3.06427	-0.23962
C	-1.40186	-2.71667	2.41179
H	-1.74405	-3.25272	1.51960
H	-2.01948	-1.82362	2.54097
H	-1.56743	-3.36736	3.28097
C	4.52425	-2.70759	-1.23051
H	4.34367	-2.32426	-2.24582
H	4.18434	-3.75115	-1.21996
H	5.6086	-2.69889	-1.06612
C	-1.95372	0.51022	-3.28707
H	-2.59305	1.02280	-2.56250
H	-2.15548	-0.56330	-3.24236
H	-2.23752	0.86225	-4.28816
C	4.81242	1.57137	-1.78225
H	4.84057	0.80260	-2.56460
H	5.50252	1.25529	-0.98606
H	5.21556	2.50129	-2.20593
C	1.63177	3.99600	1.27873
H	1.22662	3.53846	2.19406
H	0.88039	4.72324	0.93779
H	2.54110	4.54782	1.54753
C	-4.49688	-1.17180	1.26992
H	-4.52951	-0.22196	1.82042
H	-3.96278	-1.91030	1.87933
H	-5.53115	-1.52271	1.14855
C	-2.55262	3.27675	0.63546
C	4.55634	0.95554	2.21702
H	5.27591	1.49411	1.58530
H	5.13044	0.49351	3.03292
H	3.88020	1.69526	2.66485
C	-1.05374	2.24994	3.98421
H	-0.01976	1.87236	3.97397
H	-1.60793	1.63309	4.70485
H	-1.02839	3.27691	4.36880
N	-0.89902	-3.31828	-1.88134
O	-0.68499	-3.21137	-0.62867
O	-1.04544	-2.14541	-2.33545

6_SF

E (M06/BS1) = -1840.651929 au

H (M06/BS1) = -1839.766697 au

G (M06/BS1) = -1839.884823 au

E (M06/BS2//M06/BS2, Solvent=DiethylEther) = -1841.206106 au

N	2.47665	-0.46957	-0.31563
N	0.17316	0.16742	1.69056
N	-0.46198	-1.34897	-1.08467
C	-1.86736	-1.11432	-0.89879
C	-2.70747	-1.94455	-0.15737
C	-2.41658	-0.00292	-1.55038
C	-4.08094	-1.69484	-0.08992
H	-2.28153	-2.78291	0.39111

C	-3.78301	0.25378	-1.51385
H	-1.75140	0.67601	-2.08714
C	-4.60561	-0.60903	-0.78465
H	-5.67939	-0.41073	-0.73634
C	2.25615	0.86295	-0.78530
C	2.71196	1.96762	-0.04269
C	1.59536	1.11453	-1.98724
C	2.52935	3.27188	-0.48735
H	3.21203	1.79965	0.91153
H	1.23535	0.27434	-2.57645
C	1.86052	3.48383	-1.69910
H	1.69775	4.50579	-2.05011
C	-0.93380	0.98703	1.27565
C	-2.22727	0.68266	1.71706
C	-0.71709	2.14143	0.52717
C	-3.28765	1.54521	1.45288
H	-2.40541	-0.24751	2.25742
C	-1.77065	3.00685	0.22843
H	0.29168	2.38567	0.20491
C	-3.03989	2.70713	0.71538
H	-3.86925	3.38483	0.49727
C	1.37736	2.41663	-2.44911
C	3.92470	-0.92170	-0.32429
C	0.62450	0.44319	3.11307
C	-0.21559	-2.26434	-2.26678
C	2.96457	4.43742	0.35057
H	3.67620	4.13434	1.12823
H	3.43434	5.22205	-0.25641
H	2.10190	4.89765	0.85621
C	0.61259	2.64291	-3.71978
H	-0.44700	2.36816	-3.59797
H	0.64620	3.69455	-4.02956
H	1.00415	2.03260	-4.54475
C	-4.36692	1.42742	-2.24287
H	-3.59051	2.14839	-2.53151
H	-4.88489	1.11459	-3.16078
H	-5.10531	1.95582	-1.62405
C	-4.95989	-2.58168	0.74264
H	-4.92351	-3.62564	0.40280
H	-4.63887	-2.58182	1.79457
H	-6.00673	-2.25476	0.71199
C	-1.52709	4.22049	-0.61873
H	-0.57110	4.70113	-0.36985
H	-1.47666	3.95361	-1.68587
H	-2.32676	4.96281	-0.50397
C	-4.66812	1.24994	1.96026
H	-4.89752	1.83634	2.86168
H	-5.43077	1.50071	1.21039
H	-4.78553	0.18915	2.21561
C	-0.67060	-1.60255	-3.56931
H	-0.44830	-2.27909	-4.40577
H	-1.74855	-1.40469	-3.57443
H	-0.14767	-0.65513	-3.75554
C	-0.96695	-3.59003	-2.10261
H	-2.05441	-3.45848	-2.13248
H	-0.68844	-4.25978	-2.92791
H	-0.69867	-4.07719	-1.15658
C	1.26185	-2.59602	-2.37807
H	1.88187	-1.70285	-2.50149
H	1.61334	-3.14368	-1.49254
H	1.42083	-3.25232	-3.24430
C	4.72336	-0.12454	-1.36178
H	4.82682	0.93596	-1.10542
H	5.73251	-0.55208	-1.42941
H	4.26108	-0.19336	-2.35650
C	4.06593	-2.39102	-0.73749
H	3.46860	-3.06713	-0.12076
H	3.80025	-2.53847	-1.79066
H	5.11976	-2.68090	-0.62576
C	4.58287	-0.74839	1.04523
H	5.63079	-1.07653	0.99417
H	4.58686	0.30057	1.36748
H	4.07317	-1.35121	1.80437
C	2.03953	-0.07154	3.34036
H	2.11295	-1.15936	3.25464
H	2.74658	0.38939	2.64146
H	2.35048	0.20046	4.35767
C	-0.32099	-0.22865	4.10882
H	0.09066	-0.12231	5.12229
H	-1.31357	0.23618	4.10555

H	-0.42292	-1.29766	3.88697
C	0.64383	1.95334	3.36310
H	-0.35297	2.40507	3.29528
H	1.02705	2.13284	4.37640
H	1.30758	2.46597	2.65209
Mo	0.77721	-1.24275	0.49560
O	1.95273	-2.64140	1.29115
N	0.79129	-2.57528	2.00783
O	-0.17095	-2.96229	1.10027

TS4_SF

E (M06/BS1) = -1840.661864 au

H (M06/BS1) = -1839.778935 au

G (M06/BS1) = -1839.901280 au

E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -1841.211445 au

N	2.57102	-0.27644	-0.21000
N	0.10248	-0.03996	1.76078
N	-0.35433	-1.43623	-1.21089
C	-1.69386	-0.94551	-1.17878
C	-2.69939	-1.68463	-0.55265
C	-2.02359	0.26245	-1.80385
C	-4.02823	-1.25541	-0.57736
H	-2.43462	-2.61556	-0.04682
C	-3.33888	0.71638	-1.83035
H	-1.22806	0.85163	-2.26570
C	-4.33288	-0.06384	-1.23061
H	-5.37030	0.27995	-1.26168
C	2.37000	1.06738	-0.65730
C	2.66615	2.16389	0.16102
C	1.77006	1.31393	-1.89989
C	2.36669	3.46881	-0.23336
H	3.09293	1.99053	1.14951
H	1.53906	0.46303	-2.54037
C	1.75481	3.67390	-1.46966
H	1.49660	4.69072	-1.77610
C	-1.00989	0.81984	1.50143
C	-2.30335	0.48436	1.92095
C	-0.80261	2.03897	0.85733
C	-3.36473	1.36408	1.72765
H	-2.47788	-0.48841	2.38492
C	-1.85670	2.92480	0.62693
H	0.20535	2.29991	0.53573
C	-3.12536	2.58472	1.08628
H	-3.95759	3.27631	0.92897
C	1.44524	2.60458	-2.31374
C	3.97842	-0.78116	-0.22026
C	0.66281	0.06786	3.15327
C	-0.06058	-2.36185	-2.35879
C	2.62626	4.61158	0.70294
H	3.64780	4.58422	1.10403
H	2.47956	5.58049	0.21058
H	1.94413	4.57187	1.56601
C	0.76686	2.84685	-3.63010
H	0.56471	1.90721	-4.15970
H	-0.19269	3.36694	-3.49323
H	1.37734	3.47885	-4.28935
C	-3.68649	2.03337	-2.45560
H	-2.89264	2.38628	-3.12673
H	-4.62088	1.97910	-3.02957
H	-3.82701	2.80148	-1.67920
C	-5.09020	-2.06870	0.10226
H	-5.14213	-3.08749	-0.30551
H	-4.88553	-2.17096	1.17805
H	-6.08184	-1.61218	-0.00778
C	-1.60337	4.20360	-0.11576
H	-0.80869	4.79867	0.35649
H	-1.26780	3.99632	-1.14393
H	-2.50534	4.82595	-0.17348
C	-4.75397	1.00521	2.16160
H	-4.75795	0.14410	2.84125
H	-5.24817	1.84365	2.67019
H	-5.37628	0.74275	1.29282
C	-0.19250	-1.62640	-3.69212
H	-0.00647	-2.32693	-4.51808
H	-1.19784	-1.20743	-3.82461
H	0.53576	-0.80829	-3.77741
C	-1.01128	-3.55904	-2.35314
H	-2.04870	-3.26175	-2.54768
H	-0.70840	-4.26175	-3.14201

H	-0.96987	-4.08168	-1.38895
C	1.36016	-2.88831	-2.21876
H	2.08142	-2.06295	-2.17185
H	1.46652	-3.51522	-1.32190
H	1.61691	-3.50873	-3.08774
C	4.52535	-0.74145	-1.65065
H	4.51438	0.28108	-2.05120
H	5.56543	-1.09557	-1.66675
H	3.94308	-1.37888	-2.32830
C	4.00703	-2.21350	0.29668
H	3.65066	-2.27561	1.33279
H	3.39359	-2.88602	-0.31401
H	5.03998	-2.58673	0.27165
C	4.91562	0.05922	0.65464
H	5.91770	-0.39140	0.64544
H	5.01466	1.08573	0.28191
H	4.57781	0.09761	1.69871
C	1.99161	-0.67416	3.22832
H	1.86893	-1.74881	3.04268
H	2.70920	-0.26512	2.50482
H	2.42162	-0.55619	4.23177
C	-0.29694	-0.55900	4.16507
H	0.16331	-0.54398	5.16336
H	-1.24171	-0.00561	4.22560
H	-0.51439	-1.60269	3.89924
C	0.90357	1.53186	3.52150
H	-0.03086	2.10485	3.56053
H	1.37734	1.58790	4.51118
H	1.56970	2.01372	2.79282
Mo	0.84062	-1.11197	0.30509
O	0.87836	-2.90838	1.15386
N	-0.12198	-3.50724	1.83726
O	-0.83872	-4.18052	1.15287

TS9_SF

E (M06/BS1) = -1840.649433 au

H (M06/BS1) = -1839.765672 au

G (M06/BS1) = -1839.885078 au

E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -1841.203867 au

N	2.52510	-0.04880	-0.12482
N	0.00313	0.41000	1.61164
N	-0.13133	-1.6532	-0.93561
C	-1.53877	-1.42625	-0.79639
C	-2.31086	-2.23002	0.04328
C	-2.16809	-0.44533	-1.57326
C	-3.70370	-2.10754	0.07025
H	-1.81482	-2.96118	0.68389
C	-3.54997	-0.31039	-1.57048
H	-1.55276	0.20253	-2.20057
C	-4.30443	-1.16409	-0.75600
H	-5.39288	-1.06511	-0.74805
C	2.04441	1.13847	-0.76950
C	2.20433	2.39234	-0.15431
C	1.41836	1.09106	-2.01534
C	1.78873	3.56497	-0.77190
H	2.66588	2.44185	0.83386
H	1.26777	0.12463	-2.49430
C	1.17160	3.48072	-2.02633
H	0.82663	4.39599	-2.51344
C	-1.22446	1.00881	1.18453
C	-2.45391	0.58132	1.70295
C	-1.19739	2.08381	0.30132
C	-3.63275	1.24098	1.36830
H	-2.48975	-0.29896	2.34502
C	-2.36993	2.74542	-0.06753
H	-0.24258	2.41627	-0.09523
C	-3.57335	2.32917	0.49106
H	-4.49829	2.84548	0.22096
C	0.96380	2.25404	-2.64922
C	4.03895	-0.20543	-0.11891
C	0.43239	0.81039	3.00486
C	0.17964	-2.74352	-1.94356
C	1.91480	4.88691	-0.07497
H	2.70401	4.87061	0.68671
H	2.13431	5.69859	-0.77987
H	0.97496	5.14829	0.43558
C	0.24651	2.16331	-3.96368
H	-0.75975	1.73238	-3.83834
H	0.12412	3.15054	-4.42572

H	0.77910	1.51739	-4.67421
C	-4.23079	0.71116	-2.43130
H	-3.51344	1.43505	-2.84028
H	-4.74885	0.24102	-3.27943
H	-4.98745	1.27131	-1.86381
C	-4.51628	-2.96369	0.99601
H	-4.38718	-4.03314	0.78061
H	-4.21026	-2.81428	2.04184
H	-5.58620	-2.73185	0.92438
C	-2.31041	3.86462	-1.06484
H	-1.63298	4.66627	-0.73711
H	-1.92272	3.50693	-2.03167
H	-3.29975	4.30593	-1.23910
C	-4.95159	0.80002	1.93042
H	-5.34475	1.52992	2.65237
H	-5.70723	0.69599	1.13875
H	-4.86884	-0.16505	2.44575
C	-0.67274	-2.55698	-3.20256
H	-0.36401	-3.30786	-3.94242
H	-1.74445	-2.69486	-3.01648
H	-0.52151	-1.56353	-3.64867
C	-0.11012	-4.12350	-1.35127
H	-1.17921	-4.25145	-1.14169
H	0.18268	-4.90158	-2.07048
H	0.45471	-4.28318	-0.42505
C	1.63473	-2.68218	-2.38081
H	1.87504	-1.72584	-2.86250
H	2.31886	-2.84057	-1.54738
H	1.81629	-3.47806	-3.11552
C	4.75191	0.98459	-0.77449
H	4.63132	1.92216	-0.22142
H	5.82507	0.75524	-0.80042
H	4.42073	1.14892	-1.80829
C	4.44169	-1.42805	-0.94586
H	4.06280	-2.36033	-0.52003
H	4.07515	-1.33365	-1.97698
H	5.53765	-1.49773	-0.98342
C	4.59847	-0.34017	1.29757
H	5.67739	-0.54035	1.23833
H	4.46726	0.58867	1.86753
H	4.13412	-1.15835	1.85663
C	1.91648	0.52206	3.19371
H	2.15808	-0.54484	3.10695
H	2.51955	1.08274	2.47098
H	2.21712	0.83551	4.20228
C	-0.35706	0.02555	4.05360
H	0.07366	0.20870	5.04808
H	-1.40817	0.33400	4.08657
H	-0.30481	-1.05171	3.84800
C	0.22692	2.31217	3.20681
H	-0.82973	2.60246	3.16364
H	0.61234	2.59217	4.19680
H	0.77513	2.89016	2.44882
Mo	0.90716	-1.01647	0.62239
O	2.40274	-3.25890	0.61958
N	2.28579	-2.39694	1.46380
O	0.63953	-2.31967	1.90783

TS16_SF

E (M06/BS1) = -1840.648350 au

H (M06/BS1) = -1839.767470 au

G (M06/BS1) = -1839.893047 au

E (M06/BS2//M06/BS2, Solvent =DiethylEther) = -1841.203198 au

N	2.57850	-0.22109	-0.26143
N	0.12436	-0.22261	1.77745
N	-0.31431	-1.27831	-1.33985
C	-1.64697	-0.77403	-1.28672
C	-2.69056	-1.54691	-0.77540
C	-1.94337	0.49564	-1.79995
C	-4.01448	-1.10487	-0.81889
H	-2.46498	-2.51821	-0.33165
C	-3.25288	0.96334	-1.84914
H	-1.12371	1.12479	-2.15496
C	-4.28173	0.14377	-1.37203
H	-5.31366	0.50232	-1.41498
C	2.33603	1.14632	-0.60869
C	2.60700	2.18689	0.28788
C	1.72817	1.46917	-1.82995
C	2.27316	3.50939	-0.00458

H	3.04257	1.95393	1.25939
H	1.50307	0.66423	-2.53067
C	1.65519	3.79157	-1.22177
H	1.36807	4.82079	-1.45025
C	-1.00919	0.62872	1.60486
C	-2.29223	0.22065	1.99352
C	-0.84431	1.90685	1.07007
C	-3.37858	1.08493	1.89335
H	-2.43499	-0.79502	2.36800
C	-1.92366	2.78166	0.93344
H	0.1513	2.22382	0.75748
C	-3.17781	2.36667	1.36943
H	-4.03004	3.04615	1.28187
C	1.38024	2.78214	-2.14730
C	4.00049	-0.67957	-0.29728
C	0.70346	-0.21742	3.16333
C	-0.05515	-2.19199	-2.50336
C	2.50650	4.58143	1.01875
H	3.55389	4.60893	1.34736
H	2.24622	5.57403	0.63179
H	1.89526	4.40293	1.91651
C	0.73383	3.11430	-3.46025
H	0.22766	2.24400	-3.89803
H	-0.00709	3.91746	-3.34928
H	1.47388	3.46181	-4.19513
C	-3.56527	2.33146	-2.37740
H	-2.70734	2.76868	-2.90460
H	-4.41718	2.31458	-3.07042
H	-3.83327	3.01642	-1.55878
C	-5.10729	-1.96753	-0.25943
H	-5.12463	-2.95826	-0.73399
H	-4.96624	-2.13463	0.81893
H	-6.09546	-1.51107	-0.39822
C	-1.71431	4.12800	0.30484
H	-0.90003	4.68357	0.79164
H	-1.43110	4.02375	-0.75468
H	-2.62139	4.74418	0.35047
C	-4.75486	0.65052	2.29964
H	-5.25157	1.40969	2.91871
H	-5.39251	0.49157	1.41655
H	-4.73448	-0.28858	2.86678
C	-0.50908	-1.54261	-3.81109
H	-0.25002	-2.19685	-4.65522
H	-1.59334	-1.37711	-3.83445
H	-0.01252	-0.57429	-3.96659
C	-0.77308	-3.53118	-2.32652
H	-1.86305	-3.41253	-2.34264
H	-0.49896	-4.21203	-3.14503
H	-0.48108	-4.00213	-1.37703
C	1.43833	-2.47049	-2.60654
H	2.00923	-1.54220	-2.72510
H	1.80897	-3.00961	-1.72393
H	1.63623	-3.10851	-3.47849
C	4.55584	-0.52582	-1.71542
H	4.48808	0.51521	-2.05900
H	5.61486	-0.81834	-1.73877
H	4.01550	-1.16102	-2.42833
C	4.08107	-2.14458	0.11361
H	3.70792	-2.30620	1.13270
H	3.51005	-2.79253	-0.56066
H	5.12973	-2.47003	0.08152
C	4.89998	0.12600	0.64778
H	5.91387	-0.29679	0.62869
H	4.97704	1.17698	0.34499
H	4.54088	0.08783	1.68526
C	2.00058	-1.01755	3.17625
H	1.82494	-2.07809	2.95670
H	2.71618	-0.61820	2.44400
H	2.46588	-0.94923	4.16871
C	-0.26265	-0.86169	4.15877
H	0.21542	-0.92599	5.14670
H	-1.18256	-0.27522	4.27025
H	-0.52986	-1.87805	3.83766
C	1.00795	1.21167	3.61473
H	0.10092	1.82699	3.66480
H	1.46050	1.19387	4.61599
H	1.71334	1.69967	2.92804
Mo	0.88914	-1.16066	0.22566
O	0.94759	-2.88447	0.75496
N	-0.52731	-3.47950	1.65937

O -0.78321 -4.54032 1.28902

11_DF

E (M06/BS1) = -3476.311685 au

H (M06/BS1) = -3474.557849 au

G (M06/BS1) = -3474.770081 au

E (M06/BS2//M06/BS2, Solvent = DiethylEther) = -3477.350042 au

O 0.38081 -1.08363 0.02212
O 0.43516 0.91044 -0.67231
N -0.49054 -0.05747 -0.39360
Mo -2.40676 -0.14616 -0.18000
N -2.85394 -2.05273 -0.60335
N -3.15995 1.03978 -1.59879
N -2.90723 0.50748 1.64941
C -3.91779 -2.51086 0.23682
C -4.54015 0.80845 -1.89634
C -3.84294 1.57954 1.71162
C -5.21718 -2.00650 0.07404
C -3.70500 -3.44758 1.25816
C -1.50575 -4.14855 -0.87215
C -1.43511 -2.36219 -2.57939
C -3.49040 -3.72296 -2.32283
C -5.54493 1.58557 -1.31059
C -4.90848 -0.17587 -2.81923
C -1.63562 1.25181 -3.54232
C -1.67055 3.00399 -1.72823
C -3.51444 2.84285 -3.33597
C -3.42614 2.90439 1.53016
C -5.19599 1.33514 1.96986
C -3.65782 -0.82010 3.65673
C -2.05027 1.04226 3.91114
C -1.36969 -1.04912 2.72734
C -6.26501 -2.38700 0.91079
H -5.40505 -1.29861 -0.72999
H -2.70024 -3.82762 1.44025
C -4.74430 -3.86867 2.08943
H -2.13372 -4.84752 -0.30716
H -0.95390 -4.73735 -1.61986
H -0.77630 -3.68764 -0.19121
H -1.97082 -1.55807 -3.10188
H -0.56151 -1.92873 -2.08251
H -1.07931 -3.08264 -3.32983
H -3.09709 -4.43325 -3.06409
H -4.15540 -4.27795 -1.64804
H -4.09260 -2.97202 -2.85265
C -6.88800 1.38559 -1.62778
H -5.26064 2.37707 -0.61633
C -6.24678 -0.42100 -3.12896
H -4.12613 -0.78180 -3.27921
H -0.88636 0.64770 -3.02207
H -2.25821 0.58797 -4.15995
H -1.11282 1.94528 -4.21733
H -1.15424 3.70791 -2.39894
H -2.33456 3.58303 -1.07009
H -0.91881 2.49745 -1.11450
H -4.15367 3.44577 -2.67741
H -2.95580 3.53273 -3.98365
H -4.16066 2.22960 -3.97644
C -4.32827 3.96384 1.59753
H -2.37316 3.09665 1.31714
C -6.11132 2.38202 2.09291
H -5.54169 0.30271 2.05006
H -3.27165 -1.32228 4.55669
H -4.45232 -0.13625 3.97937
H -4.09186 -1.57973 2.99719
H -2.88305 1.70342 4.18431
H -1.65016 0.60743 4.83874
H -1.26572 1.65302 3.45135
H -1.68663 -1.87877 2.07700
H -0.50894 -0.56122 2.25280
H -1.03480 -1.48654 3.67932
C -6.01790 -3.32920 1.91138
C -7.63608 -1.80539 0.72137
C -4.46100 -4.82041 3.21430
C -7.22506 0.36993 -2.52644
C -7.95602 2.26549 -1.04678
C -6.62356 -1.55152 -4.03969
C -5.66655 3.68927 1.90002
C -3.87955 5.37129 1.33347

C	-7.54534	2.08492	2.42228
H	-6.83057	-3.64096	2.57170
H	-8.31332	-2.51742	0.22803
H	-8.09575	-1.54475	1.68502
H	-7.60036	-0.89913	0.09979
H	-3.82164	-5.65251	2.89210
H	-3.93302	-4.30977	4.03403
H	-5.38435	-5.24090	3.63093
H	-8.27731	0.19505	-2.76483
H	-8.39080	2.92000	-1.81477
H	-8.78400	1.67646	-0.62709
H	-7.55419	2.90484	-0.25077
H	-5.86130	-1.72467	-4.81039
H	-6.72832	-2.48957	-3.47293
H	-7.58211	-1.36822	-4.54109
H	-6.37858	4.51480	1.97754
H	-2.79403	5.47697	1.45346
H	-4.12420	5.67856	0.30592
H	-4.36918	6.08678	2.00662
H	-7.91572	1.22724	1.84255
H	-7.66711	1.82983	3.48470
H	-8.19772	2.94228	2.21323
Mo	2.10208	-0.09522	-0.05630
N	3.03834	0.69720	-1.70271
N	3.22680	-1.77666	-0.07308
N	2.57617	0.81789	1.63117
C	4.02428	1.67863	-1.39592
C	4.51731	-1.80986	-0.69615
C	3.82424	0.41334	2.22421
C	5.38554	1.40088	-1.56770
C	3.65440	2.95564	-0.94801
C	3.70994	0.63775	-4.10653
C	1.78848	2.03363	-3.38942
C	1.62788	-0.45782	-3.35536
C	5.65952	-1.63430	0.09072
C	4.68510	-2.09844	-2.05290
C	2.01745	-3.78892	-0.86875
C	1.86726	-3.13662	1.55475
C	3.93708	-4.08670	0.67582
C	3.86958	-0.62145	3.16333
C	4.99879	1.09448	1.90948
C	2.81907	3.09240	2.65356
C	1.49809	1.33454	3.81092
C	0.64034	2.41473	1.73964
C	6.35936	2.36717	-1.31006
H	5.68214	0.41021	-1.91323
H	2.59324	3.17667	-0.81120
C	4.60791	3.93497	-0.67280
H	4.30976	-0.26443	-3.93260
H	3.30310	0.59154	-5.12670
H	4.37338	1.51009	-4.05254
H	0.94409	2.14722	-2.69953
H	2.45174	2.90231	-3.28569
H	1.40268	2.03096	-4.41950
H	1.17498	-0.38611	-4.35466
H	2.17087	-1.41030	-3.30280
H	0.81088	-0.48598	-2.62899
C	6.94065	-1.75473	-0.44742
H	5.53653	-1.44719	1.15544
C	5.95450	-2.19816	-2.62385
H	3.80932	-2.24851	-2.68186
H	1.15644	-3.17248	-1.15256
H	2.67942	-3.89466	-1.73878
H	1.65258	-4.79287	-0.60550
H	1.44485	-4.13917	1.71510
H	2.46008	-2.88512	2.44434
H	1.03373	-2.43464	1.47025
H	4.54206	-3.66056	1.48778
H	3.52447	-5.04237	1.02763
H	4.59760	-4.29964	-0.17329
C	5.06629	-0.99241	3.77008
H	2.94565	-1.14073	3.41711
C	6.20912	0.75885	2.52089
H	4.96756	1.90613	1.18253
H	2.26100	3.88750	3.16634
H	3.68750	2.84112	3.27294
H	3.17828	3.48780	1.69512
H	2.38113	1.05611	4.39808
H	0.94855	2.09728	4.37995
H	0.85465	0.45069	3.71138

H	0.87754	2.88033	0.77445
H	-0.10509	1.63169	1.55876
H	0.17950	3.18037	2.37984
C	5.95808	3.62356	-0.85500
C	7.81066	2.06765	-1.54882
C	4.20224	5.29828	-0.19186
C	7.07472	-2.02576	-1.80983
C	8.16013	-1.63402	0.42087
C	6.11345	-2.47036	-4.09153
C	6.22820	-0.28213	3.44687
C	5.10947	-2.14671	4.72763
C	7.46443	1.48015	2.13264
H	6.71471	4.38384	-0.64334
H	8.14397	2.45764	-2.52144
H	8.45121	2.52840	-0.78440
H	7.99917	0.98553	-1.55285
H	3.11110	5.39365	-0.12314
H	4.62037	5.51386	0.80174
H	4.56546	6.08544	-0.86648
H	8.07348	-2.12039	-2.24442
H	8.73754	-2.56921	0.42703
H	8.84016	-0.84814	0.06044
H	7.89262	-1.39991	1.45931
H	5.18689	-2.86025	-4.53176
H	6.37584	-1.55447	-4.64166
H	6.91324	-3.19752	-4.28320
H	7.17132	-0.55313	3.92815
H	4.13484	-2.31158	5.20393
H	5.37863	-3.07913	4.21004
H	5.85494	-1.99199	5.51788
H	7.80523	1.14842	1.13957
H	7.30626	2.56517	2.06741
H	8.27880	1.29004	2.84296
C	-2.51276	-0.07061	2.96949
C	-2.49815	2.01359	-2.54356
C	2.54839	0.73219	-3.11167
C	2.76337	-3.16858	0.31433
C	-2.33252	-3.06390	-1.57049
C	1.88551	1.89624	2.44212

2. Potential energy surfaces for selected structures using B3LYP.

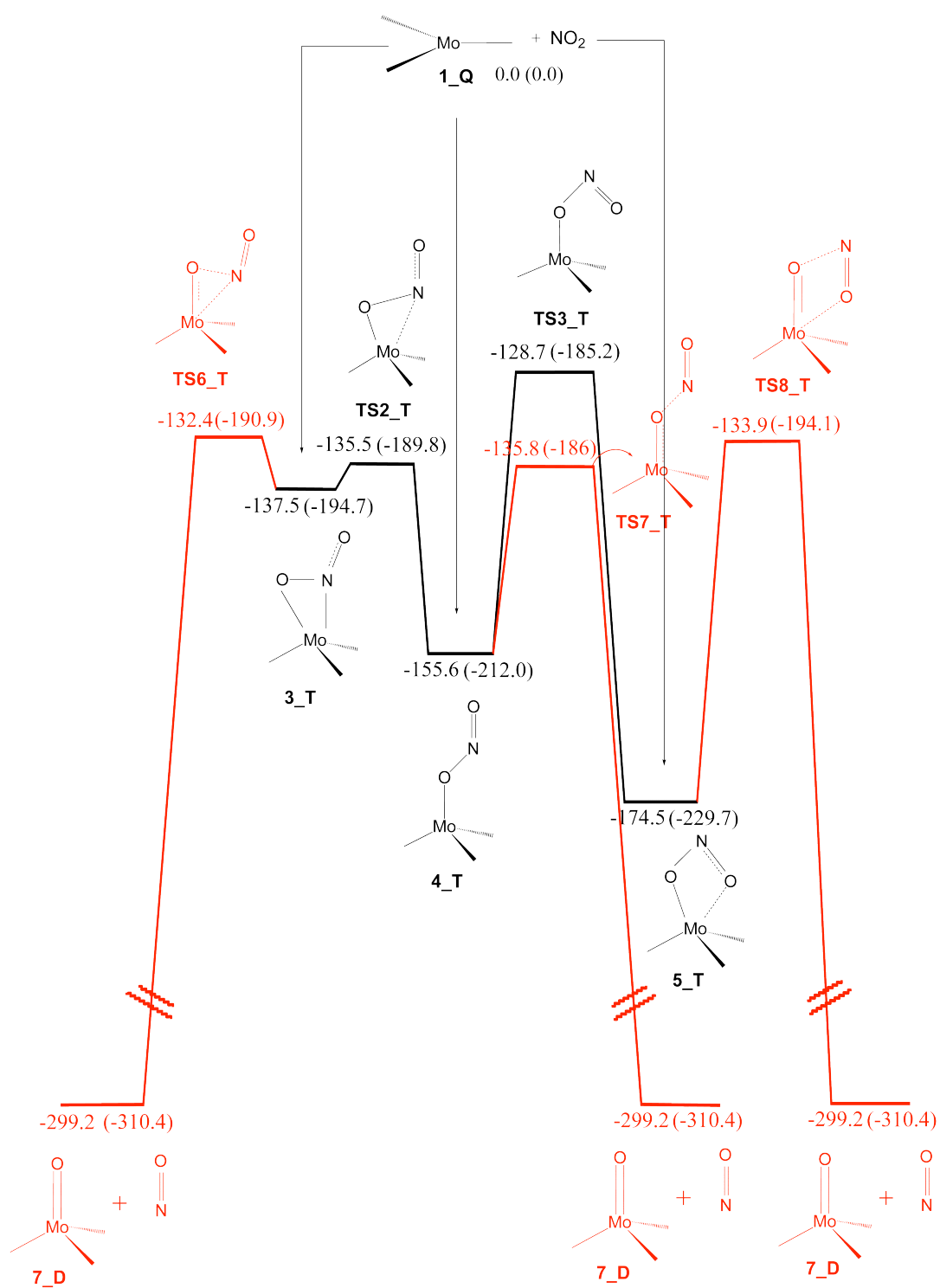


Figure S1: Relative Gibbs free energies for the model ligand, triplet pathways from the B3LYP/BS2(solvent=Et₂O)//B3LYP/BS2 level of theory (kJ mol⁻¹, uncorrected energies in parentheses).

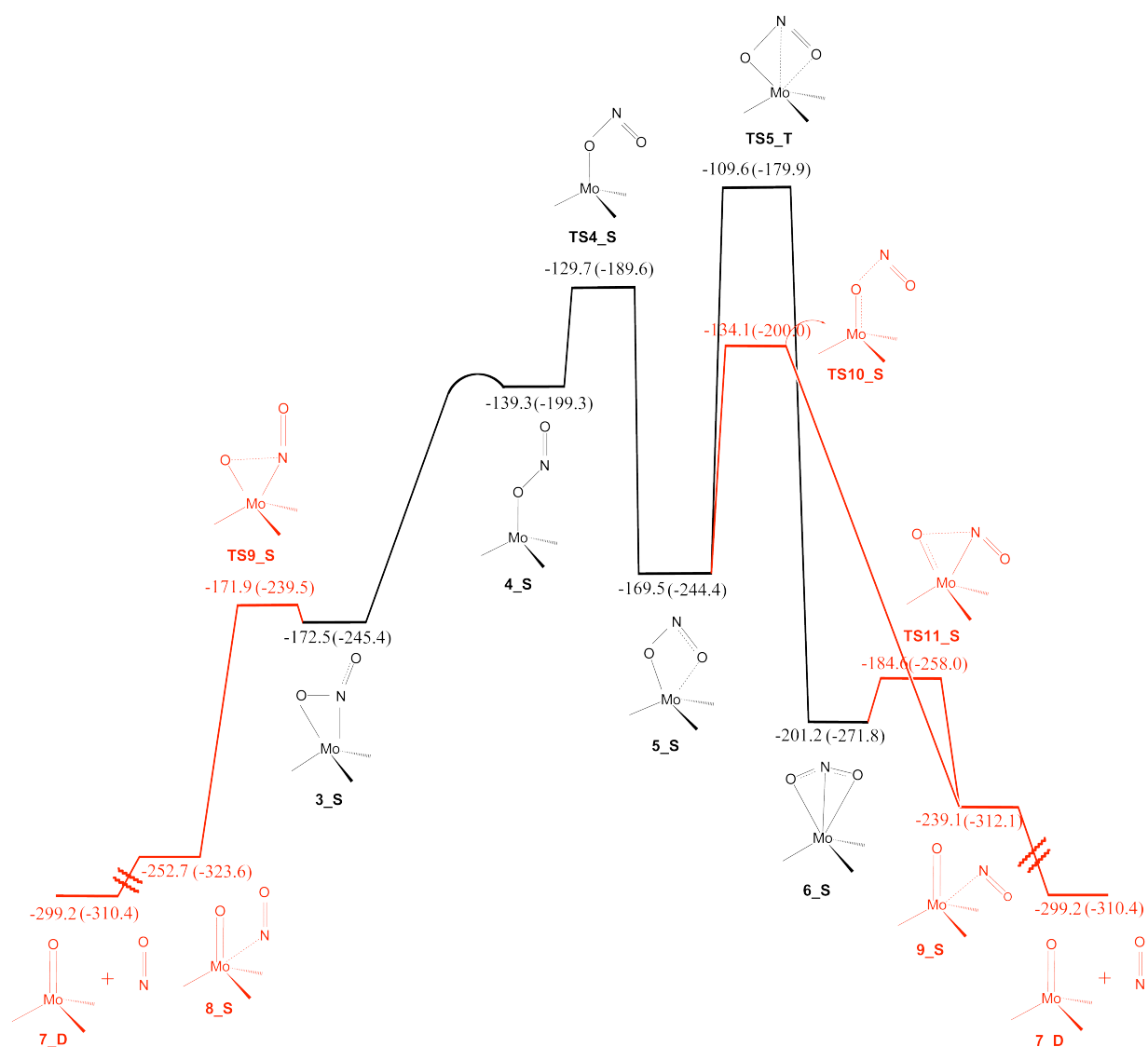


Figure S2: Relative Gibbs free energies for the model ligand, singlet pathways from the B3LYP/BS2(solvent=Et₂O)//B3LYP/BS2 level of theory (kJ mol⁻¹, uncorrected energies in parentheses).

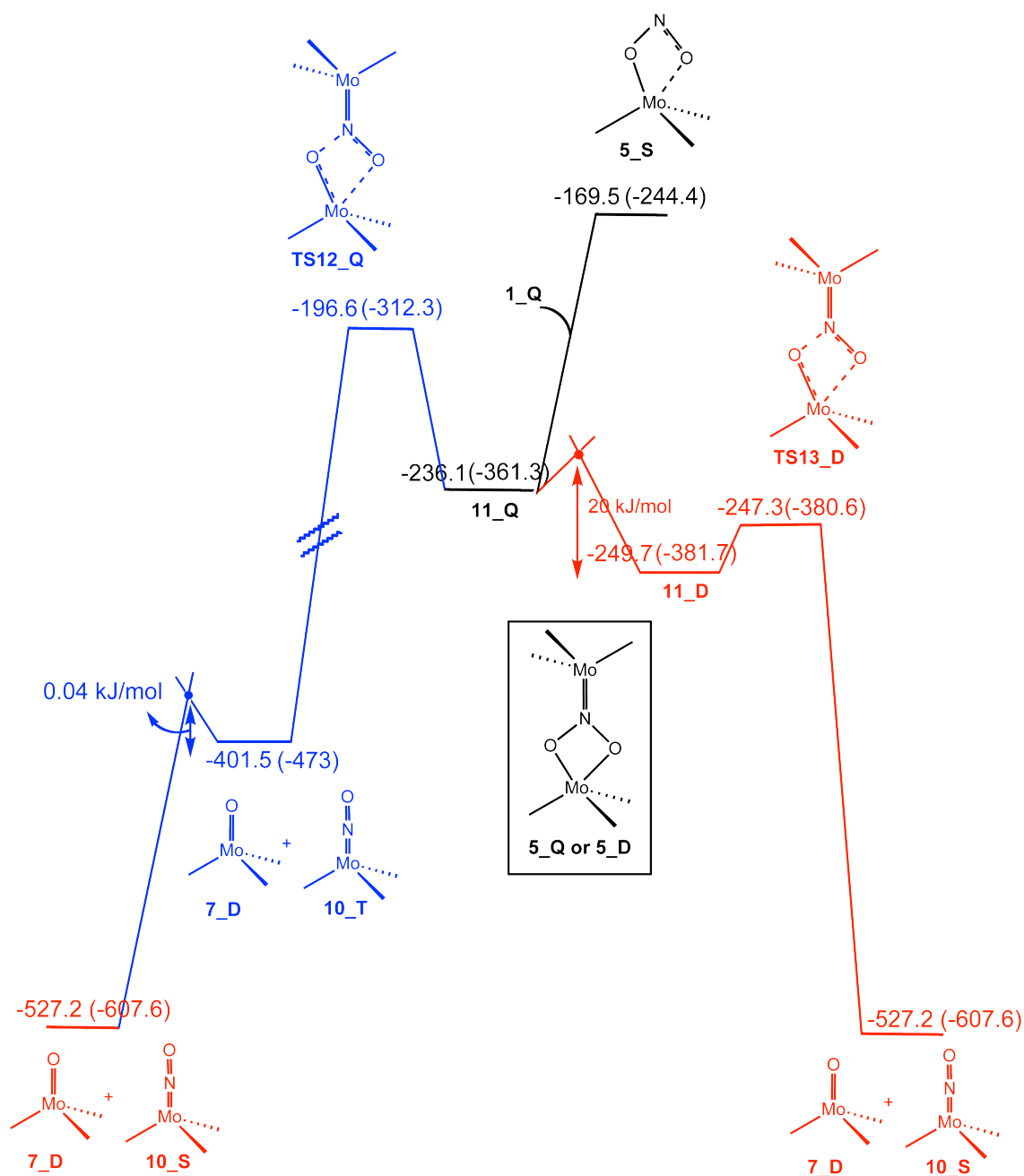


Figure S3: Relative Gibbs free energies for the model ligand, binuclear pathways from the B3LYP/BS2(solvent=Et₂O)//B3LYP/BS2 level of theory (kJ mol⁻¹, uncorrected energies in parentheses).

3. B3LYP optimized geometries and total energies for selected species shown in Section 3.

1_Q

E (B3LYP/BS2) = -236.209561 au
H (B3LYP/BS2) = -236.127559 au
G(B3LYP/BS2) = -236.169813 au
E(B3LYP/BS2//B3LYP/BS2, Solvent = DiethylEther) = -236.221116 au

N	1.81597500	0.76272100	0.00022300
N	-0.24702200	-1.95392500	-0.00030900
N	-1.56882700	1.19082200	0.00000300
H	-2.03472400	1.54451300	0.82775500
H	-2.03461300	1.54462500	-0.82776400
H	2.35507800	0.98975000	-0.82749000
H	2.35499200	0.98944500	0.82808000
H	-0.32103600	-2.53401700	-0.82815200
H	-0.32117500	-2.53421800	0.82738600
Mo	0.00001400	0.00006100	0.00001800

3_T

E (B3LYP/BS2) = -441.442137 au
H (B3LYP/BS2) = -441.346504 au
G(B3LYP/BS2) = -441.395280 au
E(B3LYP/BS2//B3LYP/BS2, Solvent = DiethylEther) = -441.442137 au

Mo	-0.32973300	0.00009800	-0.02842800
N	1.81298500	0.00078700	-0.03050200
O	2.99310800	-0.00000800	-0.19210200
O	1.30736700	0.00111200	1.22488500
N	-0.80688200	1.63433400	-0.95028900
N	-0.80395000	-1.63522200	-0.94987600
N	-1.90560600	-0.00093300	1.18714800
H	-0.32665500	2.01048900	-1.75928900
H	-1.64615700	2.16029000	-0.73929700
H	-0.32267200	-2.01096300	-1.75844300
H	-1.64271000	-2.16219100	-0.73936800
H	-1.80477100	-0.00129100	2.19577000
H	-2.88789400	-0.00203200	0.93696000

TS2_T

E (B3LYP/BS2) = -441.429063 au
H (B3LYP/BS2) = -441.333307 au
G(B3LYP/BS2) = -441.383306 au
E(B3LYP/BS2//B3LYP/BS2, Solvent = DiethylEther) = -441.440256 au

Mo	-0.45568800	0.05226300	0.02663400
N	2.06937600	0.11744500	0.24256700
O	3.25046700	-0.01496000	0.19556600
O	1.34554900	-0.79665900	-0.43560200
N	-1.33349000	-0.01132000	1.76406600
N	-0.69051400	1.73140200	-0.91708100
N	-1.42414900	-1.37171900	-0.91213900
H	-1.11162500	0.56976600	2.56476000
H	-1.97428100	-0.75068400	2.02703700
H	-0.02833300	2.49867300	-0.86291700
H	-1.50878100	1.99947200	-1.44988600
H	-0.93484700	-1.91662900	-1.61550300
H	-2.41990800	-1.36335300	-1.10371200

4_T

E (B3LYP/BS2) = -441.448717 au
H (B3LYP/BS2) = -441.352098 au
G(B3LYP/BS2) = -441.402171 au
E(B3LYP/BS2//B3LYP/BS2, Solvent = DiethylEther) = -441.448717 au

Mo	0.61685600	-0.00911600	0.01518400
O	-1.28099200	0.47257700	-0.42154100
N	-2.36208500	-0.29090100	-0.03146400
O	-3.39319400	0.12793400	-0.43960600
N	0.09173200	-1.44883900	1.20033500
N	2.02746800	-0.60868100	-1.19818800
N	0.97728400	1.79039100	0.65306500
H	-0.89817600	-1.63845500	1.33753000
H	0.64957500	-1.84054100	1.95094000
H	2.13087100	-1.57445600	-1.49178300
H	2.49809100	-0.00113900	-1.86093100
H	0.23115000	2.47890300	0.67739400
H	1.73324200	2.06067100	1.27206300

TS3_T

E (B3LYP/BS2) = -441.426432 au
H (B3LYP/BS2) = -441.330394 au
G(B3LYP/BS2) = -441.379811 au
E(B3LYP/BS2//B3LYP/BS2, Solvent = DiethylEther) = -441.438529 au

Mo	-0.55715700	-0.02242300	0.01395100
N	2.51154300	0.17735000	0.19229700
O	1.28093500	0.76340400	-0.04959000
O	2.99961200	-0.32419200	-0.76203100
N	-1.32190200	1.76808300	0.07179300
N	-1.60974000	-1.10153100	-1.21930600
N	-0.17813400	-1.10400600	1.58681900
H	-0.70420900	2.57285800	0.11874200
H	-2.23447100	2.00076300	0.44731600
H	-1.50704300	-2.10645100	-1.31733000
H	-2.06107000	-0.72327700	-2.04600800
H	0.72721800	-1.05011000	2.04466600
H	-0.87656200	-1.44496200	2.23841600

5_T

E (B3LYP/BS2) = -441.455451 au
H (B3LYP/BS2) = -441.359106 au
G(B3LYP/BS2) = -441.409375 au
E(B3LYP/BS2//B3LYP/BS2, Solvent = DiethylEther) = -441.455451 au

Mo	-0.28208600	-0.02105800	0.01898400
N	2.28229800	0.40811000	-0.22902100
O	1.30402500	1.27909800	-0.23097800
O	1.79945600	-0.74854900	-0.08083700
N	-1.75490900	1.27387700	-0.12105200
N	-0.91648700	-1.23762400	-1.35694900
N	-0.40016400	-0.68455100	1.83646700
H	-1.59458400	2.27465100	-0.07135500
H	-2.74774900	1.08652400	-0.21192400
H	-0.45442300	-2.10076200	-1.61827700
H	-1.69527500	-1.03654600	-1.97220200
H	0.26213900	-1.32885800	2.25241600
H	-1.22552700	-0.57365900	2.41240800

3TS_T

E (B3LYP/BS2) = -441.431469 au
H (B3LYP/BS2) = -441.336490 au
G(B3LYP/BS2) = -441.383497 au
E(B3LYP/BS2//B3LYP/BS2, Solvent = DiethylEther) = -441.441887 au

Mo	0.24687800	0.00636700	0.03378600
N	-2.29085000	-0.11683700	0.47770200
O	-0.93258200	-0.31125200	1.39747400
O	-1.82903300	0.02095200	-0.68859900
N	2.02100600	0.04719400	0.79279200
N	0.64504100	-1.51897100	-1.10570400
N	0.28577200	1.79049100	-0.74975800
H	2.29161600	0.60830100	1.59514700
H	2.83648400	-0.39807900	0.38351900
H	-0.00980600	-1.83895000	-1.80956400
H	1.38874800	-2.19186300	-0.96281900
H	-0.53746300	2.17222500	-1.19856400
H	1.12767800	2.29020300	-1.00294900

7_D

E (B3LYP/BS2) = -311.541013 au
H (B3LYP/BS2) = -311.453521 au
G(B3LYP/BS2) = -311.496121 au
E(B3LYP/BS2//B3LYP/BS2, Solvent = DiethylEther) = -311.551569 au

Mo	0.06398300	-0.05056500	0.08438800
O	0.27426300	-0.54912800	1.68830200
N	-0.93353900	1.63307900	-0.04948700
N	1.73861300	0.14821800	-0.90955200
N	-1.29193100	-1.09759900	-0.86366900
H	-1.94777600	1.65507300	-0.01732900
H	-0.56338000	2.50530700	0.31157100
H	2.62681500	-0.18509500	-0.55535900
H	1.85134900	0.55710500	-1.82934100
H	-1.40097800	-2.10040100	-0.77946100
H	-2.03942100	-0.70111700	-1.42186400

NO

E (B3LYP/BS2) = -129.934267 au

H (B3LYP/BS2) = -129.926508 au
G(B3LYP/BS2) = -129.949800 au
E(B3LYP/BS2//B3LYP/BS2, Solvent = DiethylEther) = -129.934639 au
N 0.00000000 0.00000000 -0.61196800
O 0.00000000 0.00000000 0.53547200

TS7_T

E (B3LYP/BS2) = -441.428283 au
H (B3LYP/BS2) = -441.333498 au
G(B3LYP/BS2) = -441.384073 au
E(B3LYP/BS2//B3LYP/BS2, Solvent = DiethylEther) = -441.438824 au
Mo -0.58959900 0.00223800 0.00830800
N 2.50609700 -0.24533900 0.08772400
O 1.15366400 0.53690300 -0.34909900
O 3.43279400 0.24259000 -0.41127700
N -1.49300300 1.69513800 0.34449900
N -1.57595700 -1.02077800 -1.34013800
N -0.16764300 -1.17243000 1.50310000
H -0.96698000 2.54939900 0.49408700
H -2.44132200 1.79869200 0.68817700
H -1.50217700 -2.03114900 -1.39590900
H -1.84202800 -0.65059600 -2.24710300
H 0.76859900 -1.18317700 1.89622900
H -0.83106300 -1.60922300 2.13230900

TS6_T

E (B3LYP/BS2) = -441.430362 au
H (B3LYP/BS2) = -441.335053 au
G(B3LYP/BS2) = -441.382962 au
E(B3LYP/BS2//B3LYP/BS2, Solvent = DiethylEther) = -441.440709 au
Mo 0.31822900 -0.05740600 -0.02911700
O -1.03572100 -0.45742100 1.27835900
N -1.73562000 -0.30893000 -0.09267300
O -2.81799000 0.18234600 -0.10458200
N 1.72937900 0.63094400 1.13215500
N 1.18383000 -1.57562800 -0.87500000
N 0.26767200 1.59938400 -1.05867400
H 1.74084600 0.41304300 2.12435700
H 2.26980600 1.47329000 0.96158900
H 0.77490800 -2.11599300 -1.62808900
H 2.16029700 -1.80448200 -0.74193300
H -0.47300100 1.82794200 -1.71053200
H 0.87436600 2.39745400 -0.91334300

3_S

E (B3LYP/BS2) = -441.450788 au
H (B3LYP/BS2) = -441.352262 au
G(B3LYP/BS2) = -441.397935 au
E(B3LYP/BS2//B3LYP/BS2, Solvent = DiethylEther) = -441.4614508 au
Mo 0.31539900 -0.04715200 0.00002600
N -1.62967800 0.01300000 0.00002600
O -2.79103900 -0.25819100 0.00025900
O -1.19220400 1.30325300 -0.00103700
N 0.77570500 -1.00896000 1.60401700
N 0.77550000 -1.01182500 -1.60229900
N 1.66355000 1.33861100 -0.00119200
H 0.17686600 -1.68220900 2.07005000
H 1.72207900 -1.06281700 1.96877900
H 0.17652200 -1.68587100 -2.06700000
H 1.72180100 -1.06642700 -1.96713600
H 1.86324600 1.89991400 -0.82691500
H 1.86313400 1.90151500 0.82346800

4_S

E (B3LYP/BS2) = -441.433263 au
H (B3LYP/BS2) = -441.335746 au
G(B3LYP/BS2) = -441.385313 au
E(B3LYP/BS2//B3LYP/BS2, Solvent = DiethylEther) = -441.443905 au
Mo 0.49915400 0.05445500 -0.00325400
O -1.34384200 0.55344400 0.32039100
N -2.38964600 -0.34328500 -0.09237400
O -3.44613700 0.15821600 -0.01402300
N 0.86361800 -1.24582000 -1.38252700
N 1.59656400 1.62962200 -0.23602500
N 1.17340600 -0.95369900 1.47551000
H 0.55401100 -1.19209200 -2.34850100

H	1.60538400	-1.94012900	-1.30589000
H	1.29346200	2.41602200	-0.80567400
H	2.60181500	1.67518500	-0.10074400
H	1.42121800	-0.57481700	2.38557800
H	1.17190000	-1.97227000	1.50885800

TS4_S

E (B3LYP/BS2) = -441.430273 au
H (B3LYP/BS2) = -441.334010 au
G(B3LYP/BS2) = -441.382386 au
E(B3LYP/BS2//B3LYP/BS2, Solvent = DiethylEther) = -441.4401778 au

Mo	-0.46579100	-0.07840900	0.00829500
N	2.60097800	-0.48204600	-0.36759500
O	1.22733200	-0.91167600	-0.33902300
O	2.85175400	0.36827800	0.39934000
N	-1.88845200	-1.28594100	0.53283400
N	-0.41685300	1.47144300	1.13955300
N	-1.04292500	0.93562300	-1.50961500
H	-1.68714200	-2.17920600	0.97077900
H	-2.87590700	-1.06859400	0.61027500
H	-0.77455100	2.38337100	0.85325200
H	-0.14493100	1.50752300	2.11741400
H	-1.32589900	0.56827400	-2.41314100
H	-1.03027100	1.95541800	-1.53576300

4_S

E (B3LYP/BS2) = -441.451668 au
H (B3LYP/BS2) = -441.353077 au
G(B3LYP/BS2) = -441.398026 au
E(B3LYP/BS2//B3LYP/BS2, Solvent = DiethylEther) = -441.461084 au

Mo	0.31044100	-0.01359900	-0.00003100
N	-2.25806200	0.44984100	-0.00016100
O	-1.26339000	1.30457400	-0.00041400
O	-1.74072000	-0.69986600	0.00031300
N	1.66988200	1.34735200	-0.00056700
N	0.59663600	-1.04924200	1.60292700
N	0.59647700	-1.05076100	-1.60204300
H	1.95400300	1.86681400	-0.82940300
H	1.95387900	1.86753000	0.82786200
H	-0.09626300	-1.66811900	2.01158000
H	1.52244500	-1.27056800	1.95962500
H	-0.09649600	-1.66996700	-2.01007100
H	1.52224600	-1.27250900	-1.95857900

TS5_S

E (B3LYP/BS2) = -441.428091 au
H (B3LYP/BS2) = -441.331368 au
G(B3LYP/BS2) = -441.376240 au
E(B3LYP/BS2//B3LYP/BS2, Solvent = DiethylEther) = -441.436486 au

Mo	-0.24969300	-0.03397700	-0.01106800
N	2.12956600	-0.18263100	0.37705300
O	1.78988900	0.59263600	-0.56549600
O	1.22108300	-0.15594200	1.36664400
N	-1.85997900	-0.32356600	1.02315700
N	-0.88570100	1.67145300	-0.62568200
N	-0.28792100	-1.44975500	-1.31742100
H	-1.83474100	-0.63720300	1.98935300
H	-2.82200600	-0.13673700	0.74786800
H	-0.46267100	2.17172700	-1.39920800
H	-1.50349300	2.27155400	-0.08856500
H	-0.59531700	-2.39100900	-1.09651300
H	-0.05418400	-1.35333800	-2.29702400

6_S

E (B3LYP/BS2) = -441.4608994 au
H (B3LYP/BS2) = -441.363444 au
G(B3LYP/BS2) = -441.408942 au
E(B3LYP/BS2//B3LYP/BS2, Solvent = DiethylEther) = -441.4714846 au

Mo	-0.14769900	-0.00020600	0.05537800
N	1.83344600	-0.00393300	0.10198300
O	1.34359700	-1.10339200	-0.60225700
O	1.35025100	1.09982600	-0.59654100
N	-1.34663900	1.38948700	-0.59765500
N	-1.35578900	-1.38192900	-0.59774400
N	-0.32132600	-0.00038800	1.96862000
H	-1.05386000	2.35293700	-0.71058800
H	-2.10014500	1.17926100	-1.24382400

H	-1.07022400	-2.34775700	-0.70894900
H	-2.10792000	-1.16753300	-1.24412100
H	0.50450700	-0.00556300	2.55488000
H	-1.18760900	0.00317600	2.49068000

4TS_S

E (B3LYP/BS2) = -441.432852 au
H (B3LYP/BS2) = -441.336364 au
G(B3LYP/BS2) = -441.382654 au
E(B3LYP/BS2//B3LYP/BS2, Solvent =DiethylEther) = -441.444152 au

Mo	0.45968000	-0.03656400	-0.00351500
N	-2.24526300	0.39368500	-0.13871900
O	-1.26172700	-0.55425000	-0.67225500
O	-3.25232400	-0.13686000	0.15014000
N	1.37989600	-1.66140800	0.48512400
N	1.46516800	0.83956200	-1.37756300
N	0.62807200	1.26935900	1.41308500
H	2.38794600	-1.78244900	0.48418300
H	0.94954400	-2.38113500	1.06145400
H	1.90538000	0.37065900	-2.16422400
H	1.44211900	1.84524000	-1.53572100
H	1.47461100	1.81592300	1.55823900
H	0.05112500	1.30792000	2.24714900

7_S

E (B3LYP/BS2) = -441.479946 au
H (B3LYP/BS2) = -441.381758 au
G(B3LYP/BS2) = -441.427069 au
E(B3LYP/BS2//B3LYP/BS2, Solvent =DiethylEther) = -441.486834 au

Mo	-0.13602000	-0.04522500	0.10990600
N	1.82159000	0.72798800	-0.02766000
O	0.15001300	-0.33849000	1.75326500
O	2.05940000	-0.40489700	-0.28147300
N	-0.27486300	-1.63270900	-1.05878700
N	-2.09289100	0.13088300	0.03668500
N	-0.22661100	1.78442600	-0.73509500
H	0.43689700	-2.34699500	-1.13310500
H	-1.15376600	-1.93214200	-1.45778100
H	-2.57000700	1.01924000	0.10625700
H	-2.67138700	-0.61273800	0.41192300
H	0.44058200	2.52763500	-0.57827100
H	-1.03535000	2.11741200	-1.24538800

TS10_S

E (B3LYP/BS2) = -441.455955 au
H (B3LYP/BS2) = -441.359404 au
G(B3LYP/BS2) = -441.402905 au
E(B3LYP/BS2//B3LYP/BS2, Solvent =DiethylEther) = -441.466257 au

Mo	0.17374900	-0.03408100	0.01072400
N	-1.77550600	-0.38887800	0.28900200
O	-0.84088400	-0.00282700	1.57527300
O	-1.82193200	0.67242600	-0.39191300
N	0.71710700	1.63870900	-0.81607000
N	1.93841400	-0.27334600	0.78148000
N	0.14933400	-1.52353900	-1.22879900
H	0.08157800	2.27188000	-1.28108900
H	1.64750200	2.03005000	-0.73163500
H	2.20470600	-1.03449000	1.39678800
H	2.65136000	0.44847200	0.79811600
H	-0.68921000	-2.05901800	-1.41423800
H	0.90372000	-1.75290400	-1.86451700

TS9_S

E (B3LYP/BS2) = -441.449481 au
H (B3LYP/BS2) = -441.352205 au
G(B3LYP/BS2) = -441.398643 au
E(B3LYP/BS2//B3LYP/BS2, Solvent =DiethylEther) = -441.459191 au

Mo	0.29722800	-0.00764100	0.01675600
O	-1.05366000	0.28928100	-1.34831500
N	-1.65293100	0.02349600	0.02581000
O	-2.82944600	-0.01372400	0.14226800
N	0.61361700	-1.78593300	0.72754700
N	1.88215600	0.16326600	-1.09233300
N	0.71555500	1.40684100	1.27703700
H	-0.09612900	-2.34961400	1.17940700
H	1.53403800	-2.19136900	0.85865800
H	2.22990900	-0.56603800	-1.70990700

H	2.29113300	1.05237900	-1.36974700
H	1.65806500	1.72229900	1.48018100
H	0.05547300	1.79513300	1.93963100

8_S

E (B3LYP/BS2) = -441.483564 au

H (B3LYP/BS2) = -441.385444 au

G(B3LYP/BS2) = -441.431469 au

E(B3LYP/BS2//B3LYP/BS2, Solvent =DiethylEther) = -441.491233 au

Mo	-0.31925300	-0.09418600	0.10874400
O	-0.32492700	-0.28489200	1.79204400
N	1.79910300	-0.33857900	0.14308900
O	2.69450700	0.34578100	-0.15303700
N	-0.22755000	-1.71367100	-1.02334500
N	-2.06695200	0.63920800	-0.38079800
N	0.32258300	1.63647100	-0.58512800
H	0.27309500	-2.55498000	-0.76636800
H	-0.54008100	-1.75325100	-1.98619700
H	-2.88011700	0.39435000	0.17491400
H	-2.24835700	1.47597500	-0.92043100
H	-0.25279700	2.46551000	-0.64858000
H	1.30993400	1.87707600	-0.60937200

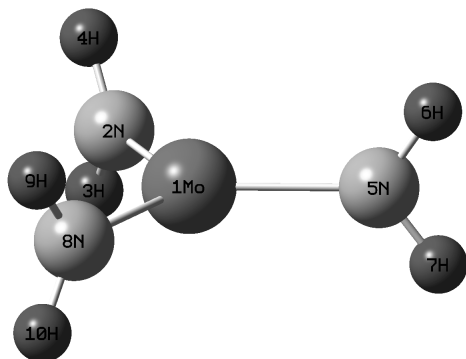
4. Comparison between solvated and gas-phase optimised geometries for selected structures.

M06/BS1 level of theory:

Energy differences between gas-phase and solvated structures for selected complexes:

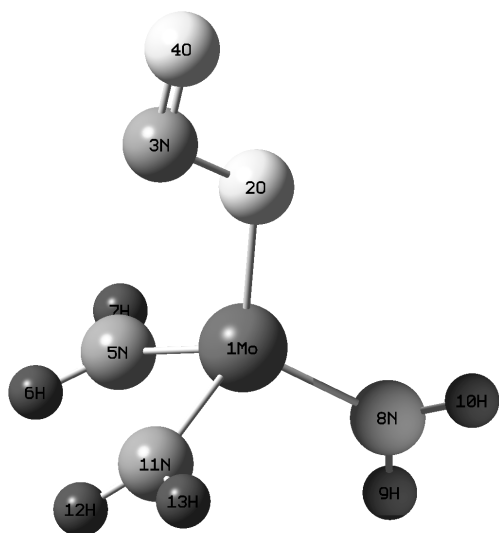
	Gas-phase		Solvent		
	Energy (Hartrees)	Energy (kJ/mol)	Energy (Hartrees)	Energy (kJ/mol)	E(solvent)-E(gas) (kJ/mol)
1_Q	-235.920207597	-619408.505046	-235.932271841	-619440.179719	-31.7
4_T	-440.983754620	-1157802.84775	-440.998100351	-1157840.51247	-37.7
4_S	-440.983310266	-1157801.6811	-440.995986637	-1157834.96292	-33.3
7_D	-311.186801779	-817020.948071	-311.198331547	-817051.219477	-30.3
TS7_T	-440.965108782	-1157753.89311	-440.977304445	-1157785.91282	-32.0

1_Q
(D_{3h})

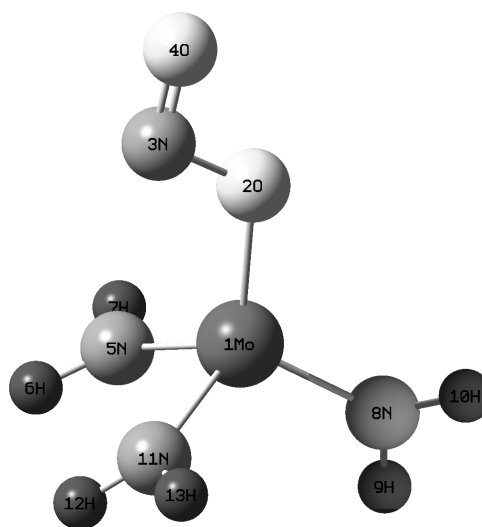


Bond lengths	gas	solvent
1Mo-5N	1.972	1.978
1Mo-2N	1.971	1.980
1Mo-8N	1.971	1.981

4_S



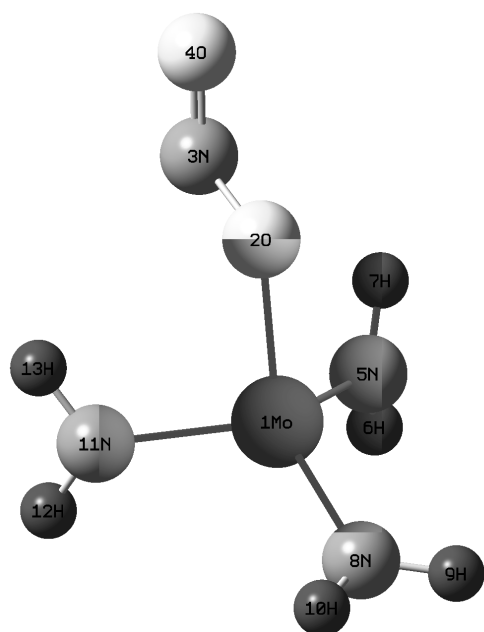
Gas-phase optimised geometry



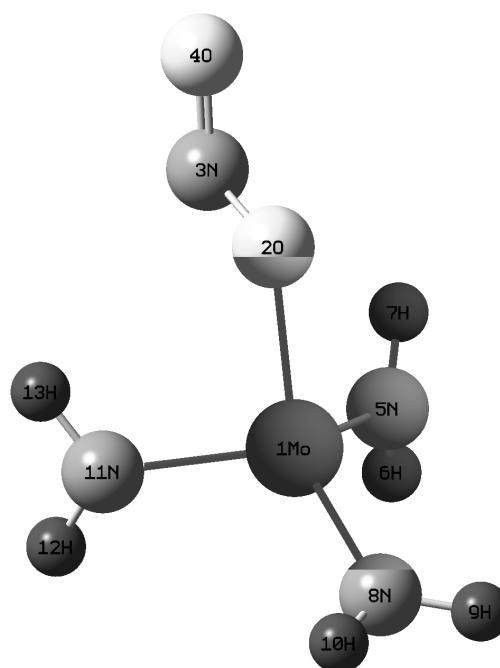
Solvent optimised geometry

Bond lengths	gas	solvent
1Mo-5N	1.910	1.897
1Mo-11N	1.923	1.932
1Mo-8N	1.941	1.951
1Mo-2O	1.958	1.990
2O-3N	1.393	1.361
3N-4O	1.179	1.191
Bond angles		
1Mo-2O-3N	118.77	123.01
2O-3N-4O	111.69	112.17
Dihedral angles		
2O-1Mo-5N-7H	70.56	75.34
2O-1Mo-2N-12H	123.59	122.83
2O-1Mo-8N-10H	32.26	53.01

4_T



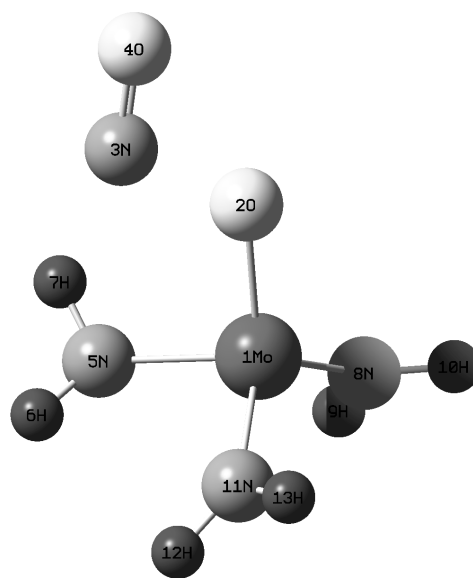
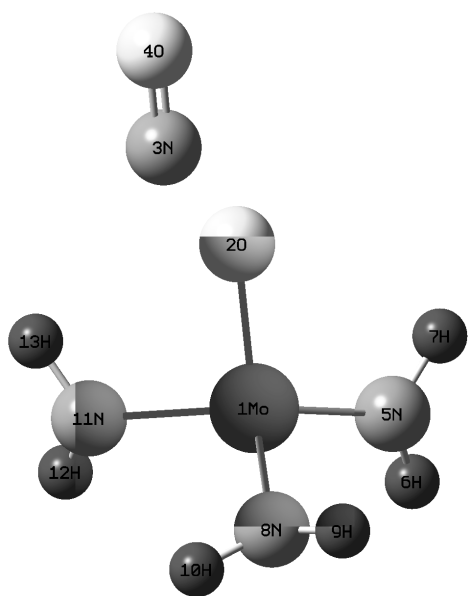
Gas-phase optimised geometry



Solvent optimised geometry

Bond lengths	gas	solvent
1Mo-5N	1.938	1.939
1Mo-11N	1.938	1.939
1Mo-8N	1.951	1.951
1Mo-2O	2.026	2.067
2O-3N	1.357	1.336
3N-4O	1.191	1.200
Bond angles		
1Mo-2O-3N	119.58	119.21
2O-3N-4O	112.64	113.00
Dihedral angles		
2O-1Mo-5N-7H	-4.73	-4.22
2O-1Mo-2N-12H	157.62	155.68
2O-1Mo-8N-10H	79.07	79.07

TS7_T



Gas-phase optimised geometry

Solvent optimised geometry

Bond lengths	gas	solvent
1Mo-5N	1.947	1.948
1Mo-11N	1.946	1.958
1Mo-8N	1.961	1.953
1Mo-2O	1.830	1.851
2O-3N	1.725	1.625
3N-4O	1.161	1.174
Bond angles		
1Mo-2O-3N	121.37	122.39
2O-3N-4O	109.34	109.58
Dihedral angles		
2O-1Mo-5N-7H	4.86	25.82
2O-1Mo-2N-12H	143.54	124.15
2O-1Mo-8N-10H	89.39	69.99