

Supplementary Data

Bio-mimetic self-assembled computationally designed catalysts of Mo and W for hydrogenation of CO₂/dehydrogenation of HCOOH inspired by the active site of formate dehydrogenase.

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1. Optimized geometrical coordinates for Mo-type I complexes including their thermochemical data and single point energies.

Name - CO₂\\SCF E(UB3LYP-D3BJ/BS1)=-188.5783129\\G=-188.587614\\ H=-188.563295\\SCF E(UB3LYP-D3BJ/BS2)=-188.6446057\\ ZeroPoint=0.011420

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16917217
O	0.00000000	0.00000000	-1.16917217

Name - H₂\\SCF E(UB3LYP-D3BJ/BS1)=-1.1760072\\G=-1.177351\\ H=-1.162558\\SCF E(UB3LYP-D3BJ/BS2)=-1.1771183\\ ZeroPoint=0.010145

H	0.00000000	0.00000000	0.37158204
H	0.00000000	0.00000000	-0.37158204

Name - HCOO-\\SCF E(UB3LYP-D3BJ/BS1)=-189.2978189\\G=-189.301031\\H=-189.273291\\SCF E(UB3LYP-D3BJ/BS2)=-189.3866915\\ ZeroPoint= 0.020613

C	0.00000000	0.33621916	0.00000000
H	-0.00069103	1.45956806	-0.00000000
O	1.13307499	-0.21681054	0.00000000
O	-1.13298861	-0.21779983	0.00000000

Name - HCOOH\\SCF E(UB3LYP-D3BJ/BS1)=-189.7709832\\G=-189.761557\\H=-189.733293\\SCF E(UB3LYP-D3BJ/BS2)=-189.839359\\ ZeroPoint=0.033516

C	0.12087010	0.37206753	-0.00000049
H	0.02913356	1.46797415	0.00000068
O	1.17868696	-0.22093457	-0.00000588
O	-1.04994872	-0.28565845	0.00000513
H	-1.78426004	0.35236484	0.00000820

Name - MoICF3\\SCF E(UB3LYP-D3BJ/BS1)=-3542.3397482\\G=-3542.205817\\H=-3542.102490\\SCF E(UB3LYP-D3BJ/BS2)=-3543.0664003\\ ZeroPoint=0.2036537

C	3.78256665	-2.44211120	-0.16462323
C	3.20471559	0.01597463	-0.22991040
Mo	-0.01004864	-0.02712636	0.76380756
S	1.51256773	1.69378895	1.45472315
S	1.47303772	-1.86475316	1.18608034
S	-1.75840222	1.58007004	0.25318216
C	-3.19825788	0.67656227	-0.08168695

S	-1.74874087	-1.61554031	0.12275394
C	-3.18953852	-0.69560026	-0.15470737
C	2.25872301	0.05812305	-1.38437022
N	0.88442787	0.08084346	-1.19885838
C	0.31629864	0.14315620	-2.40150363
N	1.27706439	0.16128071	-3.34495764
C	2.51043218	0.10935816	-2.72733434
H	1.11225625	0.20759958	-4.34326484
C	3.62858212	2.50830478	-0.08484609
H	3.43483452	0.11527354	-3.28117183
C	3.13544351	-1.29220908	0.60125038
C	3.13730461	1.27505521	0.66942716
C	-0.67016499	-0.14697257	2.78840059
C	-4.42980532	1.52041647	-0.36792050
C	-4.42810559	-1.52160452	-0.46329497
O	-1.01838490	-0.21494263	3.87199292
H	3.84601540	1.13653150	1.48981126
H	3.74706952	-1.15660836	1.49676648
F	-4.65908741	1.62908529	-1.69530009
F	-5.15959956	-0.99686473	-1.46847204
F	-5.23429464	-1.62389304	0.61613965
F	-4.11131264	-2.77748178	-0.83275494
F	3.78762278	3.55702367	0.74901433
F	2.78996046	2.90288197	-1.06638375
F	4.83070255	2.27696710	-0.66283038
F	3.86735562	-3.55440763	0.59362581
F	5.04429290	-2.12504618	-0.53947592
F	3.10865854	-2.77126519	-1.28726092
F	-4.29602995	2.77411163	0.10627498
F	-5.54375288	1.01002473	0.19668795
H	4.21477275	0.03071648	-0.64795408
H	-0.74147663	0.17247660	-2.60783402

Name - MoIPh\\SCF E(UB3LYP-D3BJ/BS1)=-2810.0415416\\G=-2809.714708\\
 H=-2809.615831\\SCF E(UB3LYP-D3BJ/BS2)=-2810.4480805\\
 ZeroPoint=0.3942488

C	-4.02815586	-2.93891245	0.74299638
C	-2.14677120	3.08465039	-0.76171096
C	-2.32785285	0.00008295	0.25417830
Mo	0.99811971	-0.00018367	0.76927453
C	-2.76696937	-2.48138933	0.34271848
S	-0.39682675	-1.75864385	1.57431053
C	-2.76709374	2.48149573	0.34254675
S	-0.39643376	1.75913891	1.57340090
S	2.62590030	-1.61660590	-0.09442014
C	4.06896077	-0.70836677	-0.52395932

S	2.62587136	1.61676987	-0.09379474
C	4.06896625	0.70872313	-0.52361323
C	-1.58025879	-0.00009110	-1.03348637
N	-0.19377345	-0.00028254	-1.05379375
C	0.19127776	-0.00045552	-2.32691507
N	-0.89795784	-0.00038010	-3.12269074
C	-2.02715926	-0.00015647	-2.32747068
H	1.20818932	-0.00059948	-2.68425990
H	-0.88166782	-0.00046657	-4.13467150
C	-2.77950659	4.11908343	-1.45028059
C	-4.02820982	2.93894022	0.74314672
C	-4.03955550	4.56798882	-1.04495684
C	-4.66207379	3.97597813	0.05530922
H	-5.63855192	4.32133310	0.38152675
H	-4.52912205	5.37595538	-1.58011747
H	-2.28711183	4.57691390	-2.30303533
H	-4.51474896	2.47701429	1.59783599
C	-4.66166948	-3.97615570	0.05515014
C	-2.14621607	-3.08467549	-0.76122457
C	-2.77859950	-4.11931854	-1.44979707
C	-4.03872134	-4.56830098	-1.04479676
H	-2.28587192	-4.57725321	-2.30230076
H	-4.52801208	-5.37643217	-1.57995826
H	-5.63820912	-4.32156718	0.38111601
H	-1.16236253	-2.75074735	-1.07311677
H	-3.02307043	-0.00007936	-2.73892033
C	-2.13787584	1.31234788	1.07103741
H	-2.66430378	1.16810402	2.01778615
C	-2.13810911	-1.31207042	1.07123799
H	-2.66487631	-1.16773735	2.01778038
H	-3.39413641	0.00013766	0.00092936
H	-4.51501982	-2.47688872	1.59744496
H	-1.16297559	2.75077540	-1.07385007
C	5.23554440	-1.39732098	-0.90722846
C	6.37766908	-0.70112064	-1.28078738
C	6.37769294	0.70179957	-1.28040978
C	5.23558548	1.39783646	-0.90649875
H	5.23317419	2.48331077	-0.90476536
H	7.27048444	1.24728959	-1.56922314
H	7.27044195	-1.24648388	-1.56989341
H	5.23309955	-2.48279604	-0.90605626
C	2.08034720	-0.00013443	2.56754598
O	2.69651119	-0.00009025	3.53290951

Name - MoICHNMe\\SCF E(UB3LYP-D3BJ/BS1)=-2725.296235\\G=-2724.979964\\
H=-2724.875216\\SCF E(UB3LYP-D3BJ/BS2)=-2725.6998157\\
ZeroPoint=0.3863461

N	4.44093736	-3.16720866	-0.51248959
C	3.16249819	0.03873561	0.16733534
Mo	-0.12469034	-0.05873057	-0.60788177

C	3.46644857	-2.44666633	-0.11562253
S	1.47927395	-1.46949937	-1.66235770
C	3.55139972	2.50909383	0.29241251
S	1.20999502	1.94084316	-0.89422858
S	-1.84918533	-1.58561033	0.09484115
C	-3.33495514	-0.68044383	0.27700392
S	-1.83703716	1.59411918	0.05167117
C	-3.33128748	0.70467147	0.22973780
C	2.30581361	-0.14787021	1.37798046
N	0.92746595	-0.29000712	1.27976307
C	0.45203857	-0.46445659	2.51039871
N	1.47104391	-0.44100430	3.39131307
C	2.65062772	-0.24472771	2.69934817
H	1.37924317	-0.55373649	4.39341442
H	3.60753170	-0.19853521	3.19305866
C	2.96581363	1.40726634	-0.54177363
H	3.47845980	1.37092624	-1.50538275
C	3.10899236	-1.16186400	-0.80595239
H	3.82571958	-0.97825493	-1.60811173
C	-1.01226157	0.13586666	-2.50420959
C	-4.54986026	-1.46230512	0.54194851
C	-4.57468770	1.48236229	0.34155974
N	-4.60940249	-2.72951012	0.37097564
N	-4.59668893	2.76015016	0.40828089
N	4.40183640	3.33274538	-0.18129831
C	4.68489856	-4.39647990	0.22874700
H	5.70682986	-4.38628339	0.62089668
H	4.61811436	-5.24953678	-0.45421498
H	3.98785421	-4.55616965	1.06221500
C	-5.86786321	-3.37053930	0.71038551
H	-6.63938871	-2.67460178	1.06660765
H	-5.69255991	-4.12621894	1.48381618
H	-6.25082450	-3.90418462	-0.16602490
C	-5.90639128	3.38045570	0.50396061
H	-5.95761569	3.97916475	1.41986696
H	-6.73950063	2.66439729	0.50344304
H	-6.03989164	4.07665166	-0.33110845
C	4.88763004	4.36156368	0.72753332
H	5.97783233	4.29529669	0.80141436
H	4.46102735	4.29751589	1.73761121
H	4.65957110	5.34858999	0.31219256
H	2.83450818	-2.72994016	0.73610530
H	-5.50683478	0.91066279	0.34670738
H	-5.41427676	-0.90922824	0.91897445
H	4.20157294	0.05042043	0.51974894
H	-0.58423834	-0.59348690	2.77798565
H	3.19378636	2.56082661	1.33012504
O	-1.51476762	0.24632920	-3.52596217

Name - MoICN\\SCF E(UB3LYP-D3BJ/BS1)=-2563.1630955\\G=-2563.045178\\
H=-2562.957902\\SCF E(UB3LYP-D3BJ/BS2)=-2563.5429609\\
ZeroPoint=0.1783433

N	-3.79099258	3.34422518	0.68518840
C	-3.11358811	0.00738318	0.14887370
Mo	0.16168677	-0.01202121	-0.63768441
C	-3.43736649	2.43355794	0.05434650
S	-1.27867617	1.74565270	-1.36546050
C	-3.47271303	-2.41723957	0.11462691
S	-1.27998058	-1.79961409	-1.28585663
S	1.86274340	1.62591617	0.03207088
C	3.27478296	0.69447858	0.40984823
S	1.85919550	-1.63055271	0.09489393
C	3.27223449	-0.68861451	0.44034176
C	-2.24730275	0.02645673	1.36136191
N	-0.86141187	0.02741069	1.26130348
C	-0.37077376	0.05268227	2.49917976
N	-1.38853880	0.06680418	3.37953794
C	-2.58160575	0.05019712	2.68702314
H	-1.28598976	0.09044476	4.38724112
H	-3.53871647	0.05865915	3.18219443
C	-2.97722491	-1.30009310	-0.68256365
H	-3.60173197	-1.21066656	-1.57624076
C	-2.97206116	1.28846985	-0.72085629
H	-3.61232348	1.18366826	-1.60174217
C	1.01555846	-0.04986960	-2.60408317
C	4.45870832	1.41749492	0.72958899
C	4.45030948	-1.40096816	0.80311712
N	5.41898564	2.02646277	0.98878228
N	5.40525550	-2.00157358	1.09888930
O	1.47478602	-0.06822906	-3.64527907
N	-3.85105291	-3.30551094	0.76286036
H	-4.15420458	0.01564431	0.48902703
H	0.67185789	0.06219837	2.77337347

Name - MoICOOMe\\SCF E(UB3LYP-D3BJ/BS1)=-3105.7517741\\G=-
3105.471151\\H=-3105.358458\\SCF E(UB3LYP-D3BJ/BS2)=-3106.2953613\\
ZeroPoint=0.3555156

C	3.97157009	2.20820571	0.44602685
C	3.26597022	-0.18536122	0.12027008
Mo	0.04545492	0.13901892	-0.78762155
S	1.57121260	-1.25738641	-1.97360936
S	1.52450047	2.02713210	-0.66755555
S	-1.74528014	-1.49043707	-0.59050413
C	-3.15806502	-0.60805183	-0.09979946
S	-1.63978832	1.63633316	0.22286714
C	-3.10692474	0.71497316	0.25960698
C	2.33661780	-0.46892878	1.25512681
N	0.96083902	-0.49095573	1.07098979

C	0.40621546	-0.86760640	2.22103863
N	1.37522302	-1.09371820	3.12882157
C	2.60185419	-0.85437079	2.54078731
O	4.40784806	3.27239492	-0.24048246
C	5.08428504	4.28891967	0.53460425
C	3.31358292	-2.63460812	-0.31066925
O	4.57569954	-2.75875143	0.12349033
O	2.45588138	-3.48070638	-0.14356907
H	3.53092734	-0.97424791	3.07337806
C	3.20859393	1.25069218	-0.45085750
C	3.12614198	-1.27475166	-0.98120496
C	-0.69261336	0.79128640	-2.66813150
C	-4.43106373	-1.39051534	-0.06540459
C	-4.31384654	1.44218649	0.76869322
O	-5.44805700	-0.69936633	-0.60000546
C	-6.75567737	-1.30349521	-0.47177515
H	-6.78440524	-2.25624884	-1.00364768
H	-7.44650044	-0.59275011	-0.92170390
H	-6.99297611	-1.45607476	0.58307750
O	-4.52779672	-2.52701634	0.36634540
O	-4.66277786	2.54360028	0.38009940
O	-4.93595549	0.74865177	1.73149019
C	-6.19153712	1.29941718	2.19229441
H	-6.88935591	1.38326884	1.35661469
H	-6.02961211	2.27977637	2.64430589
H	-6.56197500	0.59256498	2.93251270
O	-1.09851652	1.15524229	-3.67086630
H	5.35208938	5.06643014	-0.17882070
H	5.97903202	3.87323847	1.00203996
H	4.41433313	4.68532554	1.30029684
O	4.15421536	2.04798865	1.64113025
C	4.85874143	-3.94291228	0.90508434
H	5.91219683	-3.86976843	1.16989339
H	4.67242291	-4.84085476	0.31326277
H	4.23625239	-3.95011931	1.80238641
H	3.94313594	-1.13475256	-1.69331950
H	3.67043276	1.25900611	-1.44099773
H	4.28146560	-0.30723132	0.50617512
H	-0.64902550	-0.97157947	2.41623209
H	1.22231022	-1.38910307	4.08536892

Name - MoICycPyr\\SCF E(UB3LYP-D3BJ/BS1)=-2442.5532051\\G=-
 2442.327384\\H=-2442.249746\\SCF E(UB3LYP-D3BJ/BS2)=-2442.8727686\\
 ZeroPoint=0.2799677

C	4.11175587	-0.88232621	-1.25813746
C	2.91103020	0.95602158	0.00138450
Mo	-0.18969406	-0.39207616	-0.00151252
S	1.37198923	-0.77880122	1.76475670
S	1.37431578	-0.77731389	-1.76542477
S	-1.97214316	0.00912054	1.66376772
S	-1.97322507	0.01619119	-1.66322468
C	1.85184528	2.00749545	0.00130138
N	0.50313635	1.68224129	0.00024821
C	-0.18724952	2.81682112	0.00031375
N	0.66603612	3.86197612	0.00131307
C	1.95920041	3.37361389	0.00205726
H	0.39698271	4.83764171	0.00155237
C	4.11010240	-0.88383656	1.26033561
H	2.81878692	4.02415790	0.00289384
C	2.94659639	0.11789812	-1.30115469
C	2.94498920	0.11646219	1.30306293
C	-0.77467604	-2.38978517	-0.00370291
N	-5.54228040	0.12291873	0.00166194
C	4.08286948	-1.75226711	0.00056320
H	4.10060811	-1.50137685	2.16339504
H	5.04237022	-0.30248664	1.27853965
H	5.04398738	-0.30086928	-1.27440912
H	4.10349476	-1.49878103	-2.16194943
H	3.17722817	-2.36989339	-0.00039732
H	4.94013405	-2.43353807	0.00071763
H	3.87013269	1.49100716	0.00224829
H	-1.26145107	2.90716172	-0.00036929
H	3.09922318	0.81429416	2.13074918
H	3.10158184	0.81658194	-2.12798392
O	-1.12375227	-3.48364697	-0.00483733
C	-4.76444121	0.08428037	1.13251947
H	-5.20068323	0.09685295	2.11929066
C	-3.44016560	0.03108284	0.72136515
C	-3.44063959	0.03452542	-0.71976841
C	-4.76515183	0.08962852	-1.12987336
H	-5.20209332	0.10660660	-2.11626860
H	-6.55275980	0.15422989	0.00205516

Name - MoIiPr\\SCF E(UB3LYP-D3BJ/BS1)=-2666.065886\\G=-2665.612432\\
 H=-2665.506102\\SCF E(UB3LYP-D3BJ/BS2)=-2666.4285275\\zeropoint=
 0.523295

C	3.21246615	2.72043709	0.18930802
C	3.06165189	0.13923849	0.39543089

Mo	-0.10970878	-0.16945465	-0.75582321
S	1.43714882	-2.02322245	-0.66660008
S	1.48760111	1.44028479	-1.61908121
S	-1.87997310	-1.61579545	0.09626352
C	-3.30354954	-0.65716485	0.33864414
S	-1.89225406	1.46979398	-0.59373685
C	-3.31903754	0.68861963	0.00419205
C	2.04518818	0.25247533	1.48908987
N	0.68282986	0.28422181	1.22262448
C	0.04359411	0.46915326	2.37276684
N	0.94331390	0.56246313	3.37383598
C	2.21125870	0.43098622	2.83873264
H	0.72092303	0.70488872	4.35079937
C	4.10924383	-2.20699350	0.18484456
H	3.09694615	0.47653827	3.45084406
C	3.01669962	1.37195264	-0.54550165
C	3.08860522	-1.20369687	-0.40319382
C	-0.53708735	-0.68841725	-2.73671852
C	-4.53393002	-1.37461902	0.88321669
C	-4.55012116	1.56481090	0.21223776
H	3.43148410	-0.95448844	-1.41185791
H	3.84596052	1.25414852	-1.25208733
C	-4.21523506	-2.41055741	1.96860013
C	-4.49278148	2.22198008	1.60264657
C	-4.75509048	2.61638161	-0.88523685
H	-5.42456830	0.90962025	0.18461202
C	4.35054008	-3.39127571	-0.75575873
C	3.76116425	-2.69026511	1.59607591
H	5.04982851	-1.64050250	0.24532505
C	3.31381254	3.89010084	-0.79726922
C	4.47045675	2.70262141	1.07348741
H	2.33834627	2.88200496	0.83293898
C	-5.32538519	-2.01050286	-0.27301027
H	-5.16970089	-0.61846973	1.35049392
H	-3.66010902	-3.26221527	1.56613481
H	-5.14902318	-2.78897341	2.39669665
H	-3.62303904	-1.96928001	2.77647890
H	-4.72207501	-2.77457951	-0.77504379
H	-5.61107286	-1.26018688	-1.01678172
H	-6.23653396	-2.48740487	0.10319184
H	-5.39526374	2.81478758	1.78506554
H	-3.62592164	2.88774488	1.67487740
H	-4.40929667	1.46948050	2.39303211
H	-4.76297994	2.15744820	-1.87892216
H	-3.97078163	3.37796361	-0.86837368
H	-5.71584207	3.11887118	-0.73386483
H	4.16994630	3.75376637	-1.46946099
H	3.45996122	4.83131647	-0.25734796
H	2.41526378	3.98564178	-1.41064590
H	5.35335867	2.41789890	0.48863238
H	4.38580094	2.01544877	1.91808743
H	4.65157247	3.70214348	1.48215052

H	2.80263532	-3.21960581	1.60062129
H	3.69041403	-1.86401101	2.30767587
H	4.52918231	-3.38131534	1.95929024
H	3.46785703	-4.03531586	-0.81856595
H	5.18517170	-4.00151773	-0.39469507
H	4.59241033	-3.05138885	-1.76893816
H	4.03723317	0.18983510	0.88722517
H	-1.02508511	0.52876212	2.50434026
O	-0.73167319	-0.99091464	-3.82720119

Name - MoINH2\\SCF E(UB3LYP-D3BJ/BS1)=-2415.6743732\\G=-2415.475798\\
H=-2415.395834\\SCF E(UB3LYP-D3BJ/BS2)=-2416.0113116\\
ZeroPoint=0.2536753

C	-2.97234834	0.45938810	-0.02120883
Mo	0.23772694	-0.73381786	0.03025532
S	-1.35442786	-1.26015042	-1.73285284
S	-1.35895837	-1.11796446	1.82697402
S	2.05009433	-0.20799594	-1.60731640
C	3.34394034	0.49594338	-0.72167727
S	2.00764632	0.01818667	1.64324137
C	3.29553947	0.65519091	0.69356908
C	-1.95588615	1.55667818	-0.07953689
N	-0.58937579	1.30789285	-0.06412071
C	0.03249479	2.47854490	-0.12477741
N	-0.87854833	3.47477483	-0.17925282
C	-2.14037356	2.91397214	-0.15120125
H	-0.66510641	4.46258988	-0.23186203
H	-3.03677003	3.51192746	-0.18255732
C	-2.98067061	-0.30033784	1.32224888
H	-3.69128552	-1.12415874	1.22977264
C	-2.98791741	-0.43456659	-1.27965853
H	-3.67630590	-1.26059147	-1.09010034
C	0.72436349	-2.72971499	0.11893674
O	0.93772866	-3.86337650	0.16815838
H	-3.95100588	0.95049430	-0.04334351
H	1.09971648	2.63363088	-0.13257748
N	4.33873707	1.27937673	1.31778607
N	4.45008265	0.94558040	-1.39622690
N	-3.46170950	0.59863508	2.35701749
N	-3.50748408	0.34356741	-2.39081043
H	4.84945886	1.98321607	0.79658802
H	5.34213016	0.88716765	-0.91658677
H	-2.79723803	1.36616021	2.45335971
H	-2.86580355	1.11484023	-2.57379560
H	4.50295837	0.70577234	-2.37812031
H	4.23088744	1.48491467	2.30234264
H	-3.49926035	-0.23125542	-3.23051227
H	-3.45517369	0.11006016	3.24974788

Name - MoINHMe\\SCF E(UB3LYP-D3BJ/BS1)=-2572.9248884\\G=-2572.621627\\
H=-2572.527712\\SCF E(UB3LYP-D3BJ/BS2)=-2573.2888151\\
ZeroPoint=0.366283

C	2.94947608	0.11140168	0.67859021
Mo	-0.12196006	-0.15161768	-0.82089671
S	1.49801656	-1.96398779	-0.76895190
S	1.52418902	1.53791079	-1.42762900
S	-1.99351899	-1.64666214	-0.11480377
C	-3.33062098	-0.65088981	0.29254544
S	-1.93278727	1.56988753	-0.57079892
C	-3.26202771	0.78249230	0.18735455
C	1.82740270	0.25922082	1.65660243
N	0.49372977	0.21205380	1.27476376
C	-0.24162069	0.38340045	2.36574315
N	0.56495092	0.53942345	3.43919381
C	1.87654881	0.46464913	3.01222652
H	0.25491208	0.68386142	4.39141883
H	2.70870709	0.56341259	3.69040438
C	3.04309346	1.27731872	-0.33172774
H	3.85304624	1.04439491	-1.02792075
C	3.06356473	-1.30407590	0.06496220
H	3.81392544	-1.26311359	-0.72898103
C	-0.43997878	-0.50520543	-2.80307862
O	-0.56621535	-0.71024842	-3.93666155
H	3.87068077	0.20885092	1.26025276
H	-1.31885852	0.39746674	2.41369462
C	-4.69277746	-2.64930895	0.82120390
H	-5.69798593	-2.82912460	1.20335965
H	-4.58714200	-3.14025768	-0.15417579
H	-3.96660870	-3.09280566	1.50678955
C	-4.33224880	2.96880657	0.64637790
H	-4.31692310	3.33571003	-0.38305117
H	-5.25622326	3.29343205	1.12501273
H	-3.47822870	3.40537540	1.17806689
C	3.90511815	-3.54025195	0.59901480
H	3.07088692	-4.07942427	0.12966300
H	4.70753852	-3.45295948	-0.14077428
H	4.27773820	-4.14205915	1.43228462
N	-4.29635549	1.51672795	0.67384507
N	-4.49397286	-1.21203902	0.73390277
N	3.41364746	2.48032271	0.38772649
N	3.54989627	-2.20953754	1.08740935
H	-4.87953554	1.07689895	1.37463378
H	-5.33838634	-0.67629513	0.57095898
C	3.75420658	3.61549689	-0.46726000
H	2.93835887	3.93281954	-1.13102168
H	4.03822022	4.46559080	0.15889564

H	4.61404378	3.35404877	-1.09273230
H	2.63693883	2.73961212	0.99402093
H	2.82846250	-2.29686588	1.80187512

Name - MoI1CN\\SCF E(UB3LYP-D3BJ/BS1)=-2564.2907923\\G=-2564.160782\\
H=-2564.069344\\SCF E(UB3LYP-D3BJ/BS2)=-2564.6749984\\
ZeroPoint=0.1930227

C	-3.09900914	-0.03909838	-0.64052470
Mo	0.63441600	-0.01500355	-0.13266842
C	-3.33214316	2.34362451	-1.16823263
S	-0.85574565	1.81563111	-0.36874389
C	-3.34852311	-2.46045650	-0.91097840
S	-0.83067613	-1.87063606	-0.30844183
S	2.41873891	1.63152814	0.21166894
C	3.85530917	0.71665832	0.44578198
S	2.45876457	-1.61975946	0.17731114
C	3.87397846	-0.67500847	0.42606936
C	-3.41253765	0.02537658	0.82262924
N	-2.47291517	-0.00766789	1.84418596
C	-3.16532321	0.08205214	2.96675343
N	-4.50008797	0.17151105	2.72042828
C	-4.67468789	0.13604737	1.35754820
H	-2.75515096	0.08626987	3.96604864
H	-5.23153813	0.24903115	3.41517083
H	-5.64785464	0.18980366	0.89564778
C	-2.42164963	-1.35113077	-1.11826214
H	-2.21825875	-1.27505670	-2.19135893
C	-2.39794450	1.22239903	-1.21822759
H	-2.13917146	1.04507541	-2.26761614
H	-4.06441609	-0.05283494	-1.16015526
C	5.06482162	1.44198133	0.64657127
C	5.10349716	-1.37365000	0.59679762
C	0.86675907	-0.02526881	-2.16802234
O	0.96434567	-0.02911922	-3.30491792
H	0.43056196	0.02078882	1.98854597
H	-0.33090766	-0.00236935	1.84705577
N	6.10264063	-1.95750976	0.73729568
N	6.04683000	2.04767575	0.81279948
N	-4.08812646	-3.33892689	-0.73060842
N	-4.07921129	3.23249164	-1.11239398

Name - MoI1CycPyr\\SCF E(UB3LYP-D3BJ/BS1)=-2443.6868643\\G=-
2443.448874\\H=-2443.367143\\SCF E(UB3LYP-D3BJ/BS2)=-2444.0090652\\
ZeroPoint=0.2946786

C	-2.94721659	-2.29841900	1.26430937
C	-3.25231759	-0.13254847	-0.00003812
Mo	0.57629107	-0.13701891	0.00000249
S	-0.97062821	-0.38055638	-1.79621344
S	-0.97073615	-0.37990490	1.79625220
S	2.34979827	0.28491188	-1.67645469
S	2.34969466	0.28597582	1.67641981
C	-3.33058055	1.36632935	-0.00011684
N	-2.25641123	2.24353031	-0.00043789
C	-2.77439386	3.46045698	-0.00049836
N	-4.13223411	3.41766130	-0.00017510
C	-4.50181185	2.09033359	0.00009485
H	-4.75555679	4.21404434	-0.00024563
C	-2.94733881	-2.29856481	-1.26411579
H	-5.53568140	1.78212612	0.00038010
C	-2.71604173	-0.77757342	1.29467831
C	-2.71602324	-0.77777238	-1.29466349
C	1.05938259	-2.10005063	0.00045684
N	5.83309155	0.93849054	-0.00013832
C	-2.39792359	-2.96163020	0.00011043
H	-2.52283413	-2.75842429	-2.16127687
H	-4.03395416	-2.45537044	-1.30671742
H	-4.03381667	-2.45527185	1.30702031
H	-2.52259279	-2.75809313	2.16150602
H	-1.30654140	-2.91458569	0.00005774
H	-2.66159785	-4.02466919	0.00018797
H	-2.21833048	4.38681709	-0.00072781
H	-3.28913939	-0.35378337	-2.12377324
H	-3.28921765	-0.35359500	2.12374909
O	1.37214200	-3.20631506	0.00078511
C	5.07802580	0.79521531	-1.13347144
H	5.51068126	0.87535585	-2.11813671
C	3.77119947	0.55317699	-0.72614420
C	3.77115128	0.55365724	0.72601295
C	5.07795534	0.79595120	1.13324771
H	5.51055850	0.87670338	2.11788579
H	6.82715265	1.13030661	-0.00017384
H	-0.30876603	1.92316411	-0.00020953
H	0.46854095	1.96483727	0.00007168
H	-4.30584619	-0.45021550	0.00004061

Name - MoI1NH2\\SCF E(UB3LYP-D3BJ/BS1)=-2416.8022665\\G=-2416.591293
 \\H=-2416.509531\\SCF E(UB3LYP-D3BJ/BS2)=-2417.1441329\\
 ZeroPoint=0.2670006

C	2.98521068	0.49743059	0.54664443
Mo	-0.72114793	0.09558973	0.11722873

S	0.78516189	1.62262372	-0.97212897
S	0.78515098	-1.11269303	1.55014700
S	-2.57073537	0.99548731	-1.31900448
C	-3.99452801	0.13138495	-0.91624705
S	-2.54721592	-1.48148629	0.78809839
C	-3.96862731	-1.00830839	-0.04369444
C	3.37289048	-0.47225409	-0.53293427
N	2.49731485	-1.20699725	-1.32284487
C	3.25696705	-1.92394622	-2.13381085
N	4.57942275	-1.69410219	-1.91265554
C	4.66730512	-0.77013191	-0.89418410
H	2.90543168	-2.61327942	-2.88825330
H	5.35279075	-2.12083268	-2.40472431
H	5.61533998	-0.41271544	-0.52348700
C	2.32359424	-0.11163609	1.80150384
H	2.00916219	0.73126210	2.43218179
C	2.30199765	1.79998219	0.07506868
H	1.96304255	2.32686438	0.97775842
H	3.94235061	0.86828161	0.94651787
C	-1.02028559	1.42354846	1.55443816
O	-1.13463535	2.20743241	2.40112203
H	-0.45447548	-1.35389842	-1.46630731
H	0.29494729	-1.23367598	-1.33917006
N	-5.11979284	-1.70447873	0.15344128
H	-5.82467943	-1.69629298	-0.57397086
H	-5.06514946	-2.56538420	0.68216863
N	-5.18256864	0.50437526	-1.46463900
H	-5.20082587	1.35795274	-2.00779622
H	-6.03625746	0.30956036	-0.95442070
N	3.28141964	-0.99500774	2.47071394
H	4.10945813	-0.44237862	2.69303514
H	2.88320001	-1.27207981	3.36564375
N	3.25551097	2.58265401	-0.71482612
H	2.83827430	3.49172127	-0.90382212
H	4.06860774	2.76623943	-0.12676191

Name - MoI1CF3\\SCF E(UB3LYP-D3BJ/BS1)=-3543.4693374\\G=-3543.323327\\
 H=-3543.216112\\SCF E(UB3LYP-D3BJ/BS2)=-3544.1992991\\
 ZeroPoint=0.2180068

C	3.33638554	0.00829344	-0.24639128
Mo	-0.39793457	-0.00678577	-0.07833464
S	1.10174189	-1.84277822	-0.18807346
S	1.09551909	1.84018595	-0.07815277

S	-2.23239271	-1.60448445	0.05171567
C	-3.68923300	-0.69785899	0.15237689
S	-2.22796983	1.58852031	0.09290211
C	-3.68676510	0.68360130	0.18566736
C	3.52677808	-0.01568313	1.24322353
N	2.51076127	-0.05265856	2.18726059
C	3.11571668	-0.06217159	3.36351898
N	4.46817311	-0.03334798	3.22523482
C	4.74603909	-0.00384679	1.87826699
H	2.62819706	-0.08854776	4.32713223
H	5.14547689	-0.03313500	3.97646529
H	5.75414037	0.02278206	1.49569164
C	2.69206216	1.29243436	-0.82126049
H	2.51372552	1.14438215	-1.88994401
C	2.71764170	-1.26631502	-0.86669478
H	2.57230787	-1.09588623	-1.93744754
H	4.34454248	0.02406113	-0.67216476
C	-0.40223340	0.05253742	-2.11608168
O	-0.35937894	0.08589276	-3.25821766
H	-0.39409857	-0.09424573	2.05527044
H	0.37681441	-0.06625244	1.98727143
C	3.65753861	2.47275350	-0.73050201
C	3.68700754	-2.44383332	-0.77127987
F	3.18563333	3.54254435	-1.40390574
F	3.88857363	2.86883311	0.53832532
F	4.85660730	2.16217093	-1.27437882
F	4.90302720	-2.11250963	-1.26270812
F	3.87450822	-2.87277131	0.49399150
F	3.24622694	-3.49794307	-1.48913198
F	-4.70799862	2.78697779	0.60150116
F	-5.54524723	1.57841142	-0.98899081
F	-5.86410610	1.02682860	1.09407373
C	-4.95910528	1.51944805	0.22562754
F	-5.93969976	-1.03664141	-0.56004605
C	-4.96370950	-1.52903551	0.22912289
F	-5.44093158	-1.57709429	1.49028541
F	-4.75264636	-2.79972778	-0.15921287

Name - MoI1CHNMe\\SCF E(UB3LYP-D3BJ/BS1)=-2726.423238\\G=-
 2726.096484\\H= -2725.986830\\SCF E(UB3LYP-D3BJ/BS2)=-2726.8281959\\
 ZeroPoint=0.4000904

C	-3.20759888	0.02392226	-0.55545420
Mo	0.50126716	0.01856935	-0.16222748
C	-3.61499241	2.43336437	-0.92887028
S	-0.98484761	1.87491396	-0.26167855
C	-3.59081325	-2.35539098	-1.11239221

S	-0.98276932	-1.82850497	-0.34679411
S	2.35120547	1.59115309	-0.00029403
C	3.80636621	0.68375252	0.21066408
S	2.30911611	-1.59694205	0.16428950
C	3.78379611	-0.71009999	0.30343829
C	-3.51937837	-0.02851366	0.91258145
N	-2.58576186	-0.02149254	1.94127514
C	-3.28616355	-0.08210162	3.06150651
N	-4.62254626	-0.12817896	2.81206844
C	-4.78648582	-0.09444543	1.44529859
H	-2.88101380	-0.09473375	4.06307625
H	-5.35881147	-0.17850284	3.50345471
H	-5.75979442	-0.11888865	0.98087813
C	-2.54991977	-1.26198942	-1.12960150
H	-2.31229308	-1.05829576	-2.18103431
C	-2.56743538	1.35223756	-1.04432663
H	-2.35142803	1.22432321	-2.11209666
H	-4.18888834	0.03445720	-1.05024376
C	5.07653268	1.43260916	0.22019876
C	5.02126409	-1.47542773	0.54821716
C	0.58861023	0.04027173	-2.17735586
O	0.58737418	0.05059004	-3.32575640
H	0.39201980	-0.03413917	2.00729981
H	-0.36789342	-0.01005776	1.88839484
C	6.39142520	-3.34942828	0.65287467
H	6.23316696	-4.14160279	1.39252434
H	6.79110124	-3.83499577	-0.24362691
H	7.14096783	-2.64683754	1.04069195
C	6.45596540	3.29623742	0.38320585
H	6.45833807	4.08085673	-0.38111617
H	6.66949863	3.78944720	1.33734890
H	7.26264902	2.58463328	0.16224842
H	5.97940298	0.85430248	0.00318267
H	5.86391724	-0.90739689	0.95353345
N	5.11590224	-2.73229596	0.33445619
N	5.13731502	2.69057922	0.44115483
C	-4.63875799	-4.34881145	-0.53699445
H	-4.28950767	-5.32066462	-0.90003597
H	-5.05152919	-4.51420563	0.46334290
H	-5.44254684	-3.99294231	-1.19569602
H	-4.47007912	-2.12066520	-1.73093911
N	-3.51024791	-3.43377956	-0.44354999
N	-3.52914089	3.46296286	-0.18768053
C	-4.66539957	4.37318929	-0.19714453
H	-5.48059537	4.05599620	-0.86163807
H	-5.05835740	4.46905674	0.82010457
H	-4.32993945	5.36966378	-0.50194419
H	-4.50460435	2.23581828	-1.54561209

Name - MoI1COOMe\\SCF E(UB3LYP-D3BJ/BS1)=-3106.8674967\\G=-
 3106.572295\\H=-3106.457426\\SCF E(UB3LYP-D3BJ/BS2)=-3107.4175232\\
 ZeroPoint=0.3710651

C	-3.39583779	-0.00402299	0.01809673
Mo	0.34646547	-0.00172576	0.03051848
C	-3.75682441	2.45676583	-0.02388794
S	-1.14775116	1.81298349	0.35949781
C	-3.76662811	-2.36166446	-0.68569849
S	-1.14314513	-1.82980705	-0.23328833
S	2.19237651	1.57727606	0.34446214
C	3.63783541	0.66108489	0.19269004
S	2.18081957	-1.60348475	-0.19924128
C	3.63321920	-0.70470532	-0.01340763
C	-3.53755762	-0.22792106	1.49308626
N	-2.48762360	-0.37746090	2.38896707
C	-3.05098245	-0.55628409	3.57171914
N	-4.40840462	-0.53029898	3.48513458
C	-4.73388869	-0.32180226	2.16501226
H	-2.52976344	-0.70688058	4.50600024
H	-5.05874895	-0.64269284	4.25163275
H	-5.75528313	-0.25895985	1.82399960
C	-2.78580753	-1.19536898	-0.78013284
H	-2.65842073	-0.87399367	-1.81306633
C	-2.76595342	1.35869623	-0.39971788
H	-2.59927312	1.33289605	-1.47531344
H	-4.42158772	0.06269575	-0.37097879
C	4.91420616	1.44704352	0.25336079
C	4.90570154	-1.49328712	-0.09921060
C	0.22587862	0.33506943	-1.96766855
O	0.10815467	0.52532044	-3.09066091
H	0.46656418	-0.35179084	2.15412951
H	-0.30393944	-0.34153429	2.11848889
O	5.73965314	1.11542562	-0.74581777
O	5.75249537	-1.15487852	0.87992819
C	7.05631699	1.71477860	-0.70090314
H	7.58732525	1.30558814	-1.55828702
H	6.97728225	2.80056353	-0.77905721
H	7.55643849	1.44056201	0.23009992
C	7.06904704	-1.75154393	0.80913482
H	7.54786159	-1.48163898	-0.13424129
H	7.61809690	-1.33637460	1.65216001
H	6.99424000	-2.83703871	0.89522219
O	-4.67625807	-2.52937773	-1.66076957
C	-4.69034564	-1.70958449	-2.85133968
H	-4.85600333	-0.66105026	-2.59945614
H	-3.76400456	-1.83111446	-3.41641843

H	-5.52922072	-2.08050086	-3.43919179
O	5.14695621	2.30186946	1.08930477
O	5.12136207	-2.35344416	-0.93438234
O	-4.57175440	2.95279259	-0.97038156
C	-4.46209184	2.56413756	-2.35860199
H	-3.48823978	2.84808616	-2.76283872
H	-4.63366763	1.49335819	-2.47990695
H	-5.24742736	3.11982577	-2.86976120
O	-3.88063220	2.86979515	1.11559373
O	-3.79948957	-3.12163244	0.26571338

Name - MoI1Ph\\SCF E(UB3LYP-D3BJ/BS1)=-2811.1722959\\G=-2810.834052\\

H=-2810.730654\\SCF E(UB3LYP-D3BJ/BS2)=-2811.5825553\\

ZeroPoint=0.4083369

C	-3.35502880	2.88344319	-1.76318871
C	-2.88172108	-3.08053482	0.56391200
C	-2.28382483	0.00656849	-0.18178630
Mo	1.47842193	0.00030641	-0.11464289
C	-2.64381373	2.46478776	-0.63228404
S	-0.03210989	1.83488002	-0.05802386
C	-2.66166430	-2.44326197	-0.66612550
S	-0.03016916	-1.83268136	-0.18329344
S	3.30185815	1.60761912	0.07322314
C	4.78500173	0.70209103	0.21290336
S	3.30273560	-1.61760647	-0.01352722
C	4.78520675	-0.71962916	0.17519342
C	-2.46517714	-0.01835625	1.30581917
N	-1.44102198	-0.06910136	2.24373635
C	-2.03645282	-0.08304105	3.42514885
N	-3.39105975	-0.04297122	3.30058951
C	-3.67841643	-0.00197862	1.95514087
H	-1.54148720	-0.12001896	4.38492193
H	-4.06162570	-0.04350797	4.05750760
C	-3.82196798	-4.10511606	0.67048774
C	-3.40017961	-2.85335313	-1.78240730
C	-4.55721915	-4.50630384	-0.44835004
C	-4.34307321	-3.87813196	-1.67634282
H	-4.90575423	-4.18561074	-2.55271101
H	-5.28779851	-5.30504574	-0.36323117
H	-3.98080061	-4.59088698	1.62865510
H	-3.23509572	-2.36371052	-2.73830596
C	-4.30527555	3.90258103	-1.67093482
C	-2.89921222	3.08726671	0.59818379
C	-3.84684090	4.10656843	0.69107145
C	-4.55437712	4.51656530	-0.44226445
H	-4.03297905	4.58137778	1.64981612
H	-5.29062410	5.31116292	-0.36786751
H	-4.84638259	4.21695147	-2.55839094

H	-2.34985239	2.77900064	1.48098725
H	-4.68976204	0.03333625	1.58224737
C	-1.69349494	-1.28747492	-0.80706513
H	-1.54999779	-1.08857452	-1.87246201
C	-1.66981970	1.31273060	-0.76080189
H	-1.48638869	1.13611287	-1.82378131
H	-3.29996473	0.02095034	-0.59623801
H	-3.16283339	2.40448885	-2.71945068
H	-2.31084888	-2.77938450	1.43542493
C	6.01102068	1.39034393	0.34815434
C	7.19957199	0.69007850	0.45330952
C	7.19986706	-0.71799051	0.41640019
C	6.01181598	-1.41279503	0.27485816
H	6.00913951	-2.49735538	0.24223988
H	8.13546768	-1.26173084	0.49726034
H	8.13483902	1.22933552	0.56290213
H	6.00729644	2.47513816	0.37263697
C	1.41449827	0.07342515	-2.13274665
O	1.32711588	0.11599857	-3.27629173
H	1.54638843	-0.08323066	2.05787481
H	0.77941600	-0.07142548	2.00324932

Name - MoI1iPr\\SCF E(UB3LYP-D3BJ/BS1)=-2667.2010746\\G=-

2666.734633\\H=-2666.624715\\SCF E(UB3LYP-D3BJ/BS2)=-2667.5674797\\

ZeroPoint=0.5384343

C	3.20693668	-0.03705996	-0.21198939
Mo	-0.53457549	-0.01455555	-0.14894271
S	0.94451841	-1.85270905	-0.46767246
S	1.01205847	1.78340656	0.08366885
S	-2.40566797	-1.58601196	-0.20571379
C	-3.87030173	-0.71823652	0.06322220
S	-2.37094244	1.53413389	0.29475279
C	-3.85181403	0.65247959	0.31584000
C	3.34455660	-0.17240978	1.28107046
N	2.32236379	-0.45366408	2.17896656
C	2.87983085	-0.45346894	3.37879204
N	4.21011849	-0.18251265	3.30824325
C	4.52070971	0.00027111	1.97801051
H	2.37202508	-0.64034763	4.31420105
H	4.85246963	-0.12805368	4.08725048
H	5.52453301	0.21757241	1.64889741
C	2.65518852	1.34004386	-0.67070919

H	2.47894807	1.27969519	-1.75113940
C	2.61134395	-1.22802771	-1.00034180
H	2.44307432	-0.85881587	-2.01747773
H	4.23586926	-0.01986567	-0.57736270
C	-0.52026465	0.30219957	-2.13077737
O	-0.45531647	0.48561830	-3.26643822
H	-0.56461433	-0.33596190	1.97677822
H	0.20466442	-0.36473446	1.91465113
C	-5.13116814	1.45211627	0.53598828
H	-5.88316347	0.76021496	0.92326312
C	-5.16710143	-1.52036450	0.05911969
H	-5.97173848	-0.83416941	-0.21693708
C	-5.45439501	-2.04584995	1.47760441
H	-5.49444468	-1.22889964	2.20448555
H	-6.41232087	-2.57557583	1.50056341
H	-4.66989329	-2.74268666	1.79190643
C	-5.19165397	-2.66256753	-0.96333873
H	-4.95154006	-2.30268804	-1.96860424
H	-4.48214794	-3.45360672	-0.70583545
H	-6.19302807	-3.10378320	-0.98850305
C	-5.63931245	2.00248779	-0.80889517
H	-5.79687302	1.19775652	-1.53356010
H	-6.58743166	2.53203011	-0.66974297
H	-4.91355204	2.70492872	-1.23259354
C	-4.98921715	2.57442012	1.57139638
H	-4.59607059	2.19345073	2.51910780
H	-4.32395853	3.36798042	1.22036850
H	-5.97120888	3.01852815	1.76253745
C	3.63600035	2.51544873	-0.41881448
H	3.72523907	2.65146007	0.66680352
C	3.11629685	3.81924398	-1.03875501
H	2.14230317	4.10850073	-0.63849598
H	3.81851865	4.63693529	-0.84725573
H	3.01578415	3.71173257	-2.12585679
C	5.03630778	2.22570022	-0.98580006
H	5.57001738	1.44940923	-0.43262964
H	4.97639650	1.91540639	-2.03589185
H	5.64726318	3.13297798	-0.94215985
C	3.55341555	-2.45474745	-1.13903294
H	2.99840835	-3.16749127	-1.76197096
C	4.83278338	-2.08942420	-1.90526740
H	4.60676768	-1.54760829	-2.83013721
H	5.50551999	-1.46835982	-1.30432925
H	5.38172945	-2.99858673	-2.17199968
C	3.89520610	-3.16033408	0.17758221
H	2.99505173	-3.40623183	0.74841561
H	4.42860830	-4.09445730	-0.02869223
H	4.53657043	-2.53966614	0.80858268

Name - MoI1NHMe\\SCF E(UB3LYP-D3BJ/BS1)=-2574.0596707\\G=-
 2573.745433\\H=-2573.646359\\SCF E(UB3LYP-D3BJ/BS2)=-2574.4264815\\
 ZeroPoint=0.380777

C	3.05460422	0.09497302	-0.25985140
Mo	-0.67484446	0.04681063	-0.17382889
S	0.86066738	-1.73347505	-0.69667737
S	0.84187672	1.81183403	0.43878882
S	-2.57324634	-1.60889802	-0.33339049
C	-4.00045767	-0.81656192	0.15300965
S	-2.60449867	1.55242111	0.43753006
C	-4.03768691	0.63733969	0.34035069
C	3.29377929	-0.35502083	1.15387051
N	2.32913419	-0.66055476	2.10989515
C	2.99763527	-1.00482675	3.19658160
N	4.34395313	-0.94067346	3.00247193
C	4.54655344	-0.52776552	1.70454070
H	2.56341927	-1.30669601	4.13923412
H	5.05940874	-1.15745936	3.68339078
H	5.53404693	-0.39476256	1.29048751
C	2.46086467	1.51952135	-0.41152527
H	2.28095272	1.68602221	-1.47817646
C	2.47347487	-0.98203073	-1.21189924
H	2.28883654	-0.49908804	-2.17645598
H	4.06480064	0.22993857	-0.66630972
C	-0.53711576	0.63526657	-2.02675997
O	-0.34451468	0.98691623	-3.12606007
H	-0.78460763	-0.60082072	1.91667899
H	-0.02319210	-0.57327960	1.84177073
N	-5.13006459	-1.51403284	0.35903927
N	-5.23849697	1.23540316	0.43489431
H	-6.05373539	0.72995207	0.11067267
H	-5.90162048	-1.05628187	0.82756113
C	-5.22829240	-2.95701951	0.21576918
H	-4.99510696	-3.25670496	-0.80961237
H	-4.53282133	-3.46765973	0.89087251
H	-6.24907276	-3.25178891	0.45525515
C	-5.41404011	2.66196450	0.65021096
H	-4.95542304	2.96516536	1.59506708
H	-4.95441392	3.24216709	-0.15803968
H	-6.48269690	2.87031911	0.68322170
H	3.76460371	2.25364554	0.94106287
N	3.38348355	2.56222751	0.04690983
C	4.49884734	2.78866793	-0.87652716
H	5.16087467	3.55144221	-0.45726582
H	5.11223956	1.90030804	-1.09322211
H	4.11333660	3.16469004	-1.82944551
C	4.51908131	-1.72027929	-2.33059110

H	5.19559142	-2.57397307	-2.42725301
H	4.12813675	-1.48612088	-3.32574632
H	5.11805891	-0.85858996	-1.99721992
H	3.79724463	-2.34587808	-0.53679928
N	3.41062689	-2.08542773	-1.44371427

Name - TSCHNMe\\SCF E(UB3LYP-D3BJ/BS1)=-2726.4204848\\G=-
 2726.094926\\H=-2725.986408\\SCF E(UB3LYP-D3BJ/BS2)=-2726.8235486\\
 ZeroPoint=0.3985957

C	-3.24102719	0.00271352	-0.47310503
Mo	0.47381071	0.00127225	-0.29898666
C	-3.71003838	2.39074101	-0.90676813
S	-1.01751224	1.87820731	-0.49662991
C	-3.70990090	-2.38307584	-0.91813745
S	-1.01405050	-1.87049005	-0.54053282
S	2.29188647	1.59423500	-0.03318267
C	3.74591916	0.69619922	0.21845943
S	2.27535787	-1.59616931	0.06418835
C	3.73644890	-0.69933915	0.27373012
C	-3.34464173	-0.00691124	1.02408127
N	-2.28130398	-0.01932019	1.91806715
C	-2.79527023	-0.02532699	3.13857468
N	-4.14616510	-0.01759912	3.07735488
C	-4.51188942	-0.00599472	1.74853266
H	-2.23544187	-0.03468375	4.06149117
H	-4.77384256	-0.02005863	3.87116548
H	-5.54355979	0.00164523	1.43509233
C	-2.67177495	-1.30107593	-1.09972739
H	-2.58936161	-1.11458169	-2.17728499
C	-2.66675131	1.31277827	-1.08302830
H	-2.57040634	1.13443939	-2.16073030
H	-4.28389129	0.00610824	-0.81914220
C	5.00477343	1.45874346	0.31958309
C	4.97140738	-1.45683590	0.55024854
C	0.62140394	0.01563793	-2.35737348
O	0.64839346	0.02413982	-3.50390993
H	0.10221939	-0.01715541	1.61060367
H	-0.79365709	-0.01732075	1.65680384
C	6.35999980	-3.31649536	0.66726549
H	6.18562499	-4.12342614	1.38711119
H	6.79731447	-3.78140662	-0.22262754
H	7.08700361	-2.61247655	1.09363306
C	6.35150094	3.32107379	0.66576641
H	6.36761683	4.15847561	-0.04013103
H	6.52674667	3.74698816	1.65926807

H	7.17515226	2.63681828	0.42226179
H	5.92188781	0.90887547	0.08691325
H	5.79193458	-0.88819382	0.99819778
N	5.08939790	-2.70791059	0.31439436
N	5.04041193	2.69692948	0.63643843
C	-4.69415717	-4.34638907	-0.15659609
H	-4.39867088	-5.33248501	-0.52900939
H	-4.98216352	-4.47751954	0.89141042
H	-5.57076236	-4.00301687	-0.72278929
H	-4.65758844	-2.15750335	-1.43023982
N	-3.55580356	-3.44165173	-0.23058881
N	-3.56960048	3.44328126	-0.20714906
C	-4.71180287	4.34386222	-0.14236468
H	-5.57868705	4.00283840	-0.72471623
H	-5.01605000	4.46491911	0.90226537
H	-4.41390904	5.33413339	-0.50158812
H	-4.64936556	2.16757142	-1.43519225

Name - TSCycPyr\\SCF E(UB3LYP-D3BJ/BS1)=-2443.6847813\\G=-

2443.447536\\H=-2443.367308\\SCF E(UB3LYP-D3BJ/BS2)=-2444.0052812\\

ZeroPoint=0.2931536

C	-3.01119928	-2.28705816	1.26072081
C	-3.25138279	-0.11134858	-0.00024505
Mo	0.55266245	-0.09928710	0.00004401
S	-0.98892055	-0.42422184	-1.81131831
S	-0.98920291	-0.42377315	1.81124825
S	2.32298001	0.31941517	-1.67578042
S	2.32268452	0.31992718	1.67605463
C	-3.25811344	1.38855844	-0.00040780
N	-2.14590655	2.21850847	-0.00042666
C	-2.58120423	3.46966670	-0.00057749
N	-3.93183463	3.49055524	-0.00065722
C	-4.37789968	2.18546195	-0.00055149
H	-4.51006379	4.32120784	-0.00077166
C	-3.01103222	-2.28733622	-1.26069103
H	-5.42744211	1.93762161	-0.00058603
C	-2.74016113	-0.77352219	1.29761125
C	-2.73996617	-0.77381353	-1.29787691
C	1.06455936	-2.10592905	0.00035052
N	5.83700678	0.81294369	0.00036953
C	-2.46350392	-2.95787378	0.00012476

H	-2.60604786	-2.75708574	-2.16164410
H	-4.10139698	-2.42060119	-1.29078715
H	-4.10156610	-2.42033089	1.29070583
H	-2.60632670	-2.75660421	2.16183010
H	-1.37095345	-2.91485919	0.00018987
H	-2.73485179	-4.01895989	0.00022518
H	-1.96409720	4.35538917	-0.00062922
H	-3.31073505	-0.33731527	-2.12222871
H	-3.31106684	-0.33685186	2.12177709
O	1.38188883	-3.20881977	0.00051746
C	5.07477146	0.70225391	-1.13268792
H	5.51016923	0.76281408	-2.11762545
C	3.75917622	0.51676659	-0.72489162
C	3.75904798	0.51699358	0.72535776
C	5.07457068	0.70260963	1.13332754
H	5.50979563	0.76347640	2.11832279
H	6.83840577	0.95958859	0.00043569
H	-0.72381024	1.87005884	-0.00030462
H	0.18046322	1.78066809	-0.00024756
H	-4.31890239	-0.37578518	-0.00029591

Name - TSNHMe\\SCF E(UB3LYP-D3BJ/BS1)=-2574.0520446\\G=-2573.738774\\
H=-2573.641182\\SCF E(UB3LYP-D3BJ/BS2)=-2574.4166683\\
ZeroPoint=0.379241

C	3.07384121	0.05799801	-0.20956998
Mo	-0.62350339	0.04926846	-0.19938508
S	0.90180797	-1.76530475	-0.77107999
S	0.89892592	1.92174525	0.15756877
S	-2.48791944	-1.61428933	-0.23597262
C	-3.94140696	-0.79008222	0.14165055
S	-2.52501725	1.55874309	0.41453726
C	-3.96921653	0.63722393	0.34397479
C	3.08733449	-0.28261714	1.25040302
N	1.98166223	-0.49878982	2.06553015
C	2.42300617	-0.77890746	3.28194006
N	3.77288988	-0.75624473	3.29783094
C	4.20997412	-0.44611437	2.02691160
H	1.81036532	-0.99526982	4.14400642
H	4.35575406	-0.93909398	4.10474178
H	5.25723332	-0.36926862	1.78165560
C	2.54853308	1.47854416	-0.55520999
H	2.44692597	1.52640961	-1.64375545
C	2.58021202	-1.07865954	-1.14331942
H	2.53241932	-0.66044124	-2.15337685
H	4.13583752	0.12957233	-0.47021912

C	-0.63738712	0.55602106	-2.15228863
O	-0.53651133	0.85300653	-3.26972965
H	-0.31759167	-0.40620203	1.65371623
H	0.63817644	-0.43060701	1.75363267
N	-5.10748182	-1.48228325	0.23767365
N	-5.17514989	1.24803521	0.49188758
H	-5.97765664	0.77938212	0.08882270
H	-5.84540149	-1.05387090	0.78256079
C	-5.18921156	-2.92736338	0.10803064
H	-4.84773561	-3.24193383	-0.88137446
H	-4.57775858	-3.43956567	0.86089019
H	-6.23155387	-3.22000999	0.23415611
C	-5.32330764	2.68130376	0.67929301
H	-4.81833632	3.00200550	1.59394955
H	-4.90305048	3.24737722	-0.16106183
H	-6.38708790	2.90358265	0.76378012
H	3.76797099	2.34187392	0.80372595
N	3.48072644	2.53530246	-0.15522522
C	4.67661457	2.60252929	-0.99936630
H	5.33524371	3.38977227	-0.62250122
H	5.26584420	1.67370709	-1.05001420
H	4.38682310	2.86589506	-2.02144087
C	4.74596305	-1.93188267	-1.90317511
H	5.38308726	-2.82019629	-1.87872856
H	4.51942940	-1.70830394	-2.95037081
H	5.33372064	-1.09122975	-1.50323368
H	3.72799986	-2.46142244	-0.22181472
N	3.50079972	-2.21712827	-1.18515940

Name - TSCN\\SCF E(UB3LYP-D3BJ/BS1)=-2564.2897689\\G=-2564.157675\\
H=-2564.071503\\SCF E(UB3LYP-D3BJ/BS2)=-2564.6728435\\
ZeroPoint=0.1915398

C	3.12197822	0.00479616	-0.58193257
Mo	-0.60895382	0.00259851	-0.19850299
C	3.40560689	-2.39250347	-0.99696280
S	0.85885249	-1.85880464	-0.48925091
C	3.40916118	2.40910254	-0.94808962
S	0.85733220	1.86761355	-0.47352756
S	-2.39008704	-1.62586168	0.20156033
C	-3.81431045	-0.69892488	0.46267245
S	-2.39702313	1.62461966	0.19226668
C	-3.81780333	0.69308594	0.45681692
C	3.30334432	-0.00648000	0.90551056
N	2.28063136	-0.00712959	1.84549310
C	2.86119090	-0.01721088	3.03418225
N	4.21006556	-0.02288437	2.90599155
C	4.50936115	-0.01611975	1.56366893

H	2.35312311	-0.02059678	3.98677671
H	4.87755335	-0.03086007	3.66688056
H	5.52298760	-0.01850924	1.19573865
C	2.48557381	1.29807656	-1.16139568
H	2.35131725	1.17271448	-2.24077146
C	2.48095671	-1.27726639	-1.18169037
H	2.33708653	-1.13146580	-2.25734337
H	4.13246867	0.00689744	-1.00748056
C	-5.02722042	-1.41326288	0.68073491
C	-5.03492280	1.40324452	0.66457782
C	-0.91248010	0.00593125	-2.25762307
O	-1.04217523	0.00729414	-3.39048180
H	-0.19339271	-0.00351266	1.72931206
H	0.65036633	-0.00384624	1.68727216
N	-6.02411967	1.99636144	0.83393184
N	-6.01270886	-2.00986407	0.85915997
N	4.14539248	3.28910409	-0.76092793
N	4.14275961	-3.27618673	-0.83207705

Name - TSNH2\\SCF E(UB3LYP-D3BJ/BS1)=-2416.7971332\\G=-2416.587312
H=-2416.505439\\SCF E(UB3LYP-D3BJ/BS2)=-2417.1368849\\ ZeroPoint=
0.266142

C	3.01387342	0.64371234	0.17745822
Mo	-0.67595145	0.18507217	0.06760458
S	0.81555465	0.98737410	-1.67700445
S	0.82635687	-0.00696458	1.97002695
S	-2.50736710	0.16701275	-1.63791741
C	-3.92746212	-0.38832728	-0.84936869
S	-2.48862662	-0.82679101	1.45753184
C	-3.90521031	-0.88210432	0.48890562
C	3.21885391	-0.78392851	-0.23548891
N	2.22005395	-1.71985515	-0.47405684
C	2.80624256	-2.85766106	-0.81562176
N	4.14753294	-2.70400790	-0.80903240
C	4.42640996	-1.40273821	-0.44554584
H	2.30283922	-3.77927959	-1.06563558
H	4.82450916	-3.42205271	-1.03342256
H	5.43627058	-1.03295147	-0.36756780
C	2.41839991	0.85417708	1.58699356
H	2.19735604	1.92650434	1.67464172
C	2.38595055	1.56665677	-0.89168595
H	2.13251956	2.50745459	-0.38470107
H	4.03153741	1.04885868	0.28186379
C	-1.02310160	2.11997048	0.59239980
O	-1.14361966	3.22996451	0.88990600
H	-0.12760006	-1.59905721	-0.42773769

H	0.81776315	-1.57984350	-0.42378181
N	-5.06237586	-1.37417576	1.02531299
H	-5.72640450	-1.80679297	0.39281668
H	-4.99340530	-1.82922652	1.92657976
N	-5.11287718	-0.39865349	-1.53171081
H	-5.12275886	0.05288314	-2.43737653
H	-5.96360450	-0.26551491	-0.99586968
N	3.38855158	0.39203993	2.58402265
H	4.23450995	0.95165391	2.47313994
H	3.02515344	0.61984171	3.50732496
N	3.34962308	1.75099923	-1.98120471
H	2.95959241	2.42567187	-2.63636422
H	4.17865837	2.19603181	-1.58633351

Name - TSCF3\\SCF E(UB3LYP-D3BJ/BS1)=-3543.468166\\G=-3543.322604\\
H=-3543.217230\\SCF E(UB3LYP-D3BJ/BS2)= \\ZeroPoint=0.2165582

C	3.33568142	0.00651084	-0.17626108
Mo	-0.38131893	-0.00015741	-0.17186756
S	1.11354390	-1.85990860	-0.36723929
S	1.11358285	1.87033769	-0.20223475
S	-2.20398846	-1.60079323	-0.02814899
C	-3.65957900	-0.69965705	0.12402082
S	-2.20008776	1.58790857	0.09263927
C	-3.65664213	0.68069801	0.19211294
C	3.36698807	-0.01816492	1.32490662
N	2.26441805	-0.07422657	2.16552349
C	2.73034205	-0.08257670	3.40452144
N	4.08395381	-0.03543768	3.40308011
C	4.50475064	0.00537804	2.09317598
H	2.13549647	-0.11966652	4.30472837
H	4.67792479	-0.03089124	4.22251272
H	5.54754714	0.04657364	1.82170363
C	2.74885098	1.28692945	-0.82065434
H	2.64764796	1.11474733	-1.89571064
C	2.78871096	-1.26754372	-0.86211433
H	2.76134132	-1.08554324	-1.94007346
H	4.38529723	0.02391929	-0.48507520
C	-0.42885064	0.09746218	-2.24037806
O	-0.41090857	0.15376429	-3.38136074
H	-0.17156522	-0.08764684	1.78588500
H	0.67699811	-0.08215179	1.83815409
C	3.72613103	2.45278851	-0.68662439
C	3.75245120	-2.43808447	-0.67455582
F	3.30734179	3.52916657	-1.38330492

F	3.90277661	2.84600755	0.59217763
F	4.94549637	2.12081486	-1.17156178
F	5.00449329	-2.09956825	-1.06081203
F	3.83302722	-2.85678237	0.60560795
F	3.38555266	-3.50055651	-1.42055052
F	-4.66803480	2.77164910	0.68864704
F	-5.54614635	1.60269705	-0.90928571
F	-5.80937854	0.99793578	1.16682342
C	-4.92772825	1.51363693	0.28746301
F	-5.92850438	-1.02338645	-0.53356928
C	-4.93012392	-1.53460830	0.21470770
F	-5.37247530	-1.61724845	1.48698478
F	-4.72874080	-2.79434193	-0.21284650

Name - TsiPr\\SCF E (UB3LYP-D3BJ/BS1)=-2667.1983431\\G=-2666.732541\\
 H=-2666.624311\\SCF E (UB3LYP-D3BJ/BS2)=-2667.5627833\\
 ZeroPoint=0.5369041

C	3.21109998	-0.05621095	-0.14647050
Mo	-0.51972959	-0.03593522	-0.18650910
S	0.99837355	-1.91353735	-0.28107929
S	1.02368745	1.81154978	-0.35817526
S	-2.38467179	-1.58379020	0.07232851
C	-3.84707753	-0.67564223	0.18925394
S	-2.33620801	1.57445643	0.01919578
C	-3.82205846	0.71611446	0.20067607
C	3.19542341	-0.15966631	1.35516079
N	2.07716908	-0.08064001	2.17669276
C	2.49424948	-0.16242175	3.43112206
N	3.83986529	-0.28348410	3.46580831
C	4.30006656	-0.27991530	2.16598988
H	1.86778769	-0.14050479	4.31003755
H	4.40545825	-0.36354271	4.30101253
H	5.34875731	-0.36562940	1.93192774
C	2.79856580	1.33715068	-0.68136372
H	2.89213358	1.28966934	-1.77256986
C	2.57424337	-1.21548443	-0.96600008
H	2.29639555	-0.79323754	-1.93610600
H	4.27167936	-0.11999190	-0.40095236
C	-0.56189322	-0.13127240	-2.23719653
O	-0.52455023	-0.19734436	-3.38485695
H	-0.25982937	-0.00278716	1.73115751
H	0.64515841	-0.02435641	1.82552827
C	-5.09684367	1.54739731	0.29599367
H	-5.84287646	0.93821332	0.81256666
C	-5.14565182	-1.46309783	0.32839395

H	-5.95359087	-0.82336175	-0.03524457
C	-5.41281596	-1.76815899	1.81333245
H	-5.44056792	-0.85068856	2.40920950
H	-6.37137737	-2.28427859	1.93021586
H	-4.62528236	-2.41286057	2.21828976
C	-5.18729677	-2.74537191	-0.51162389
H	-4.96423344	-2.53950980	-1.56314540
H	-4.47245317	-3.48991364	-0.15095689
H	-6.18844593	-3.18421333	-0.45419451
C	-5.62636449	1.85229943	-1.11678591
H	-5.79804922	0.93247506	-1.68425510
H	-6.57066050	2.40362059	-1.05982942
H	-4.90574017	2.46390653	-1.67034207
C	-4.93798952	2.83570359	1.11248645
H	-4.52783018	2.62901305	2.10590006
H	-4.27975109	3.55272295	0.61435830
H	-5.91698567	3.30880221	1.23863380
C	3.71327831	2.48622063	-0.18408942
H	3.55477527	2.59859747	0.89620669
C	3.37511942	3.81585353	-0.87065061
H	2.34517491	4.12681315	-0.68449361
H	4.03988465	4.60744791	-0.51006001
H	3.51212451	3.73235014	-1.95581556
C	5.19934474	2.17050903	-0.42509593
H	5.56933114	1.35742207	0.20308912
H	5.37620473	1.90071943	-1.47316120
H	5.80547152	3.05473625	-0.20316279
C	3.54494109	-2.38621867	-1.26676790
H	2.94450959	-3.12979133	-1.80532578
C	4.66669778	-1.94114905	-2.21547899
H	4.26217818	-1.47275391	-3.11916976
H	5.34633844	-1.22545898	-1.73991034
H	5.26663674	-2.80479644	-2.52128576
C	4.12082528	-3.06392537	-0.02005249
H	3.33441485	-3.33695582	0.69016408
H	4.65449857	-3.97771070	-0.30199843
H	4.83048258	-2.41240263	0.49709658

Name - TSCOOMe\\SCF E(UB3LYP-D3BJ/BS1)=-3106.8654393\\G=-3106.571251\\
H=-3106.458161\\SCF E(UB3LYP-D3BJ/BS2)=-3107.4141785\\
ZeroPoint=0.3691602

C	-3.38852742	-0.02701636	0.09553119
Mo	0.32908639	0.00549315	-0.05837556
C	-3.80530643	2.42449218	0.21300548
S	-1.16321383	1.84076725	0.32844272
C	-3.82814183	-2.32080328	-0.76229104
S	-1.16763748	-1.80695588	-0.52030133

S	2.16129960	1.55501086	0.40136345
C	3.60928896	0.65092525	0.20851957
S	2.15743475	-1.58826260	-0.32259922
C	3.60746849	-0.70146510	-0.07371787
C	-3.35479147	-0.35817657	1.55652571
N	-2.21331676	-0.53701192	2.32686300
C	-2.61983777	-0.82440105	3.55327832
N	-3.97243640	-0.84007756	3.61206772
C	-4.45503310	-0.54751992	2.35650952
H	-1.98232817	-1.02229558	4.40180231
H	-4.52714140	-1.03531363	4.43569131
H	-5.51016865	-0.49828862	2.13946854
C	-2.85585049	-1.14644775	-0.85023868
H	-2.83462436	-0.73954208	-1.86008753
C	-2.82972467	1.37143054	-0.30386029
H	-2.76321219	1.39670286	-1.38938773
H	-4.45532691	0.04226393	-0.15601918
C	4.88420503	1.43168590	0.32907151
C	4.88050264	-1.48629423	-0.17968725
C	0.26073256	0.48065528	-2.06972650
O	0.17134023	0.74374196	-3.17934491
H	0.18209635	-0.43559027	1.85083952
H	-0.67844940	-0.45510844	1.95069224
O	5.72160110	1.15534386	-0.67739945
O	5.71428009	-1.19688495	0.82619890
C	7.03693254	1.75158511	-0.58400624
H	7.57731956	1.39366940	-1.45832982
H	6.95784652	2.84007224	-0.59914575
H	7.52782032	1.42349364	0.33439144
C	7.03227176	-1.78835752	0.74265989
H	7.52387509	-1.46868777	-0.17834096
H	7.56907493	-1.41796488	1.61399360
H	6.95789833	-2.87691968	0.77019518
O	-4.83484485	-2.39978836	-1.65092846
C	-4.97811325	-1.46802923	-2.74784287
H	-5.12172347	-0.45075126	-2.37876089
H	-4.11631331	-1.51999002	-3.41638183
H	-5.87276143	-1.79298196	-3.27783354
O	5.10740990	2.23988218	1.21270567
O	5.10769165	-2.30516052	-1.05260321
O	-4.64297185	3.02658098	-0.64848572
C	-4.59527717	2.77683365	-2.07168799
H	-3.62748366	3.07001702	-2.48411088
H	-4.80872027	1.72932274	-2.29210596
H	-5.37842013	3.40550576	-2.49411220
O	-3.89139477	2.71365710	1.39383298
O	-3.77205308	-3.16515164	0.11403116

Name - TSPH\\SCF E(UB3LYP-D3BJ/BS1)=-2811.1699125\\G=-2810.831743\\
H=-2810.730536\\SCF E(UB3LYP-D3BJ/BS2)=-2811.5784744\\
ZeroPoint=0.4070569

C	-3.54805091	2.86364345	-1.67833840
C	-2.85439333	-3.07443786	0.62387354
C	-2.29852662	0.00000493	-0.18292750
Mo	1.45673659	0.00002324	-0.19405113
C	-2.72436220	2.44840414	-0.62507377
S	-0.05855531	1.85815340	-0.36946103
C	-2.72437846	-2.44846993	-0.62477560
S	-0.05858756	-1.85815559	-0.36918857
S	3.26151525	1.61366386	0.05982405
C	4.74211562	0.71119810	0.23804359
S	3.26153917	-1.61358314	0.05950368
C	4.74212951	-0.71113406	0.23788758
C	-2.32252100	0.00008417	1.31448720
N	-1.21179366	-0.00005029	2.14857965
C	-1.65947487	0.00013640	3.39538691
N	-3.01268280	0.00037454	3.40780537
C	-3.44907010	0.00034835	2.10103604
H	-1.05115185	0.00009417	4.28730633
H	-3.59665793	0.00055185	4.23433660
C	-3.79137327	-4.09042994	0.81141606
C	-3.54773351	-2.86415123	-1.67812524
C	-4.61124084	-4.49696722	-0.24492981
C	-4.48574073	-3.88190513	-1.49167269
H	-5.11425981	-4.19398117	-2.32039998
H	-5.33856933	-5.28954883	-0.09747946
H	-3.88062010	-4.56617934	1.78351263
H	-3.45262738	-2.38468095	-2.64854534
C	-4.48614096	3.88133275	-1.49195738
C	-2.85414007	3.07473557	0.62341494
C	-3.79120113	4.09066799	0.81088573
C	-4.61139683	4.49676717	-0.24537243
H	-3.88026233	4.56670176	1.78285990
H	-5.33879285	5.28929754	-0.09798049
H	-5.11491878	4.19306753	-2.32061691
H	-2.21461886	2.77306685	1.44572403
H	-4.49569538	0.00050702	1.84260573
C	-1.76276636	-1.29919400	-0.84747422
H	-1.71350874	-1.09793976	-1.92048975
C	-1.76272978	1.29911683	-0.84764410
H	-1.71347045	1.09772349	-1.92063522
H	-3.35479266	0.00001476	-0.47925033
H	-3.45313338	2.38388427	-2.64863424
H	-2.21510656	-2.77245386	1.44624678
C	5.96636310	1.40194218	0.37940875

C	7.15230509	0.70439919	0.52267629
C	7.15231789	-0.70437899	0.52250951
C	5.96638437	-1.40190119	0.37907922
H	5.96307024	-2.48699876	0.37570681
H	8.08605924	-1.24604466	0.63353868
H	8.08603866	1.24605327	0.63383105
H	5.96304029	2.48704050	0.37628905
C	1.54690850	-0.00019203	-2.25807114
O	1.54725866	-0.00032677	-3.40420388
H	1.16508279	0.00023431	1.73493206
H	0.28094087	-0.00001601	1.81291715

2. Optimized geometrical coordinates for Mo-type II complexes including their thermochemical data and single point energies.

Name - MoIICH3CN\\SCF E(UB3LYP-D3BJ/BS1)= -2462.0082875\\G -
 2461.747026\\H=-2461.663244\\SCF E(UB3LYP-D3BJ/BS2)=-2462.3301686\\
 ZeroPoint= 0.319127

C	-4.11744471	0.99675454	-1.25727132
C	-3.03882768	-0.91705686	0.00003196
Mo	0.16548953	0.20952381	-0.00014366
S	-1.38959864	0.69043338	1.77211506
S	-1.38989872	0.69090159	-1.77192311
S	1.88872678	-0.38575895	1.67371888
S	1.88887051	-0.38636754	-1.67351800
C	-2.03991927	-2.02572128	-0.00013035
N	-0.67207611	-1.78234898	-0.00022172
C	-0.04964322	-2.95635990	-0.00033482
N	-0.96397739	-3.94784639	-0.00030579
C	-2.22586919	-3.38318340	-0.00017883
H	-0.75222387	-4.93743563	-0.00037456
C	-4.11723291	0.99653535	1.25786915
H	-3.12270678	-3.98119197	-0.00014274
C	-3.02181557	-0.07882763	-1.30359785
C	-3.02162509	-0.07908360	1.30382761
N	5.45704264	-0.63048508	0.00028192
C	-4.02687923	1.86350226	0.00036733
H	-4.06910686	1.60986879	2.16277313
H	-5.08807316	0.48116005	1.27065163
H	-5.08827483	0.48135908	-1.26997171
H	-4.06948884	1.61024556	-2.16207702

H	-3.07755595	2.41124028	0.00033322
H	-4.83230896	2.60570868	0.00050064
H	-4.02596270	-1.39862544	0.00005125
H	1.01702493	-3.10790157	-0.00042368
H	-3.23530979	-0.76923928	2.12470350
H	-3.23557054	-0.76881766	-2.12459497
C	4.67880130	-0.56300489	1.13116239
H	5.11419650	-0.59636096	2.11800158
C	3.35798805	-0.45000813	0.72127418
C	3.35804499	-0.45031655	-0.72092546
C	4.67888262	-0.56350238	-1.13068116
H	5.11434375	-0.59727787	-2.11747679
H	6.46521600	-0.69792737	0.00033216
N	0.88784896	2.26551074	-0.00027716
C	1.29810592	3.34912839	-0.00039486
C	1.81534067	4.70199378	-0.00054128
H	2.42719710	4.85896004	0.89216560
H	2.42648856	4.85903836	-0.89372029
H	0.98264931	5.41095104	-0.00018320

Name - MoIICH3SCH3\\SCF E(UB3LYP-D3BJ/BS1)=-2807.2791845\\G= -
2806.986003\\H=-2806.901755\\SCF E(UB3LYP-D3BJ/BS2)=-2807.6106748\\
ZeroPoint= 0.350505

C	-4.18374197	-0.75914572	1.40630652
C	-3.10014398	0.99012534	-0.06938583
Mo	0.09751895	-0.15172385	0.06511755
S	-1.46096478	-0.82690309	-1.63699212
S	-1.45695365	-0.40410919	1.87885213
S	1.83031053	0.23862982	-1.64504359
S	1.79966839	0.62439917	1.67672576
C	-2.09482859	2.08497507	-0.20125424
N	-0.72885075	1.83543851	-0.17418818
C	-0.09860477	2.99684940	-0.31194120
N	-1.00714945	3.98727816	-0.42748399
C	-2.27237843	3.43433913	-0.36010569
H	-0.79030366	4.96901268	-0.54326723
C	-4.18600701	-1.05670218	-1.09022223
H	-3.16555957	4.03398326	-0.42846685
C	-3.08615981	0.31238951	1.32455782
C	-3.08755878	0.00266695	-1.26390443
N	5.36978719	0.84161599	0.00180833
C	-4.09367117	-1.76904516	0.26050770
H	-4.14070724	-1.77256291	-1.91656555
H	-5.15573005	-0.54420308	-1.16197055
H	-5.15393095	-0.24477292	1.35733103
H	-4.13648739	-1.26089925	2.37757695
H	-3.14340556	-2.31169634	0.32384213
H	-4.89808974	-2.50698259	0.34926075
H	-4.08475501	1.47347274	-0.12697537
H	0.96902913	3.14101207	-0.33072261

H	-3.29829474	0.59028588	-2.16174196
H	-3.29696323	1.09530524	2.05830712
C	4.60456357	0.61753576	-1.11800206
H	5.04771156	0.55048731	-2.09965625
C	3.28475260	0.50854886	-0.70418527
C	3.27124857	0.67539000	0.72694973
C	4.58300340	0.87956172	1.12852901
H	5.00813166	1.03807503	2.10768509
H	6.37360087	0.95726160	-0.00217471
S	0.85457661	-2.63515735	0.36467922
C	2.65988908	-2.66084065	0.60779611
H	2.86951471	-2.17711616	1.56108347
H	2.99155808	-3.70070830	0.63402988
H	3.15366795	-2.11776132	-0.19807668
C	0.79072586	-3.39359009	-1.29032521
H	-0.25753765	-3.45893135	-1.58127331
H	1.33509859	-2.76675650	-1.99925831
H	1.22842233	-4.39252941	-1.23832397

Name - MoIIIMI\\SCF E(UB3LYP-D3BJ/BS1) ==-2555.5032737\\G= -
 2555.214602\\H=-2555.131537\\SCF E(UB3LYP-D3BJ/BS2)=-2555.8472178\\
 ZeroPoint=0.345728

C	4.14374267	-0.97364173	-1.25801141
C	3.13552182	0.97679554	-0.00039063
Mo	-0.11759292	-0.03974384	-0.00026198
S	1.42872622	-0.57685474	1.76454562
S	1.42872032	-0.57729377	-1.76533922
S	-1.81351520	0.64596412	1.67324288
S	-1.81349652	0.64481268	-1.67387994
C	2.18153146	2.12444527	-0.00015053
N	0.80581419	1.93646162	-0.00095895
C	0.23266840	3.13432438	0.00033410
N	1.18627722	4.08943541	0.00187858
C	2.42395906	3.47336209	0.00150238
H	1.01545122	5.08679671	0.00254242
C	4.14375275	-0.97359859	1.25760425
H	3.34439250	4.03448381	0.00228252
C	3.08582514	0.13929785	-1.30354285
C	3.08598830	0.13944732	1.30295058
N	-5.37419243	1.02649809	-0.00052804
C	4.02451113	-1.83662951	-0.00018889
H	4.07301036	-1.58559144	2.16204154
H	5.13249313	-0.49330957	1.27161913
H	5.13244668	-0.49326927	-1.27198093
H	4.07311370	-1.58572274	-2.16239005
H	3.05715788	-2.35198013	-0.00017661
H	4.80384055	-2.60629754	-0.00021070
H	4.14087503	1.41953547	-0.00049515

H	-0.82711503	3.32897372	-0.00018571
H	3.32353611	0.82111491	2.12442047
H	3.32344150	0.82080621	-2.12513640
C	-4.59786479	0.93365940	1.13027360
H	-5.03207744	0.98002119	2.11716306
C	-3.28090511	0.77930699	0.72075637
C	-3.28087215	0.77893770	-0.72146565
C	-4.59777889	0.93334215	-1.13117869
H	-5.03179933	0.97929806	-2.11817199
H	-6.37929111	1.12922846	-0.00057065
N	-0.87841496	-2.11768455	0.00049958
C	-0.12615789	-3.28180732	0.00054279
C	-2.15834533	-2.48024988	0.00120235
C	-0.97389813	-4.35457653	0.00130914
H	0.95079691	-3.24967296	-0.00006368
H	-3.00679947	-1.81456323	0.00146856
H	-0.79348489	-5.41732360	0.00149736
H	-3.11579646	-4.35260840	0.00234883
N	-2.25124354	-3.82631365	0.00176747

Name - MoIINH2CH3\\SCF E(UB3LYP-D3BJ/BS1) ==-2425.1331547\\G= -
 2424.848398\\H= -2424.768058\\SCF E(UB3LYP-D3BJ/BS2)=-2425.4423805\\
 ZeroPoint= 0.340198

C	4.14093634	-0.97273785	-1.25581008
C	2.99332636	0.90195688	0.00062805
Mo	-0.17585180	-0.34207626	-0.00078573
S	1.40367383	-0.75948291	1.77646371
S	1.40517078	-0.75973572	-1.77640090
S	-1.91813359	0.15913866	1.67366791
S	-1.91871634	0.16571004	-1.67196945
C	1.95697772	1.97702508	0.00033322
N	0.59711306	1.69265460	-0.00018016
C	-0.05941467	2.84728040	-0.00038353
N	0.82455068	3.86694110	0.00000407
C	2.10242367	3.33985190	0.00044634
H	0.58371946	4.84981288	-0.00005738
C	4.13988430	-0.97294836	1.25778752
H	2.98107722	3.96443084	0.00074724
C	3.00872237	0.06405948	-1.30365507
C	3.00773125	0.06395054	1.30485431
N	-5.49611206	0.25905648	0.00153847
C	4.07724745	-1.84287141	0.00089190
H	4.11395927	-1.58694829	2.16320890
H	5.09295439	-0.42516359	1.26872195
H	5.09397201	-0.42487911	-1.26582225
H	4.11583128	-1.58659126	-2.16135231
H	3.14479925	-2.41894585	0.00044897
H	4.90504750	-2.56009689	0.00118169
H	3.96293694	1.41831029	0.00099869
H	-1.13017593	2.96719109	-0.00083195

H	3.19983785	0.76220591	2.12413309
H	3.20129226	0.76237077	-2.12277803
C	-4.71499473	0.22828239	1.13235092
H	-5.15145880	0.23573469	2.11927842
C	-3.39061173	0.18150853	0.72192060
C	-3.39083708	0.18457962	-0.71966426
C	-4.71531241	0.23322364	-1.12958507
H	-5.15201266	0.24484547	-2.11636758
H	-6.50611040	0.28425004	0.00172915
N	-0.67739005	-2.56026624	-0.00169806
H	-0.20202066	-2.95907119	-0.81079845
H	-0.20859780	-2.95815749	0.81167002
C	-2.09097860	-3.00001720	-0.00706558
H	-2.59161692	-2.60336567	0.87567808
H	-2.58455764	-2.60439980	-0.89422988
H	-2.16274863	-4.09197444	-0.00668412

Name - MoIINH3\\SCF E(UB3LYP-D3BJ/BS1)=-2385.8235738\\G=-

2385.565734\\H=-2385.488644\\SCF E(UB3LYP-D3BJ/BS2)=-2386.12479\\

ZeroPoint= 0.311325

C	-4.03097784	-1.15395522	1.25832361
C	-2.95742377	0.75880339	-0.00467290
Mo	0.26044948	-0.33127119	0.00435643
S	-1.29769979	-0.85094475	-1.76196793
S	-1.30220551	-0.83751195	1.76895958
S	2.00860686	0.14173241	-1.68075076
S	2.01147250	0.17733885	1.67493823
C	-1.97160546	1.88113151	-0.00784685
N	-0.59832504	1.66439815	-0.00575956
C	-0.00019774	2.85071852	-0.00923679
N	-0.93371527	3.82482069	-0.01362101
C	-2.18363572	3.23497632	-0.01275053
H	-0.74184289	4.81844412	-0.01684523
C	-4.02784846	-1.16359860	-1.25563446
H	-3.09204895	3.81535676	-0.01547433
C	-2.93760029	-0.07605433	1.30118467
C	-2.93429203	-0.08610716	-1.30401068
N	5.56055902	-0.29741436	-0.00096236
C	-3.93667846	-2.02591866	0.00477660
H	-3.97667297	-1.77979655	-2.15849529
H	-5.00028745	-0.65115547	-1.27135008
H	-5.00342620	-0.64139180	1.26760945
H	-3.98210825	-1.76319562	2.16601484
H	-2.98497990	-2.56962753	0.00797065
H	-4.73924608	-2.77126604	0.00666333
H	-3.94877740	1.23208050	-0.00766860
H	1.06328878	3.02444237	-0.00872489
H	-3.14785817	0.59899968	-2.12913137
H	-3.15298067	0.61525627	2.12064643
C	4.78290256	-0.22456496	-1.13186505

H	5.21515804	-0.29149940	-2.11841306
C	3.46614298	-0.06867022	-0.72367666
C	3.46749973	-0.05243578	0.72006414
C	4.78492073	-0.19898671	1.12941463
H	5.21888486	-0.24391768	2.11645469
H	6.56098258	-0.43988794	-0.00022296
N	1.03167484	-2.44861908	0.01912524
H	0.72382345	-2.96304362	0.84284930
H	0.72619947	-2.97192607	-0.79987066
H	2.05163612	-2.44864136	0.02025720

Name - MoIIPH2CH3\\SCF E(UB3LYP-D3BJ/BS1) =-2711.7231508\\G= -
2711.450480\\H= -2711.367969\\SCF E(UB3LYP-D3BJ/BS2)=-2712.0450906
ZeroPoint= 0.329464

C	-4.07153782	-0.94221466	1.34940371
C	-3.05511572	0.86993886	-0.09546188
Mo	0.19842657	-0.09217144	0.08921639
S	-1.29604205	-0.85192171	-1.64313600
S	-1.37311708	-0.47210735	1.86083052
S	1.93601260	0.10617575	-1.66039287
S	1.95094175	0.71466472	1.62184368
C	-2.11952211	2.02882708	-0.20679667
N	-0.74016359	1.87297997	-0.16228229
C	-0.19220475	3.07618077	-0.28682096
N	-1.16499577	4.00366655	-0.41137492
C	-2.38906082	3.36362307	-0.36266138
H	-1.01539932	4.99842055	-0.52235483
C	-4.01666550	-1.22126929	-1.14878495
H	-3.32066522	3.90051517	-0.44047025
C	-3.02472094	0.18054671	1.29222787
C	-2.96924516	-0.10727572	-1.29546798
N	5.52206154	0.26807708	-0.00883006
C	-3.91317409	-1.93822260	0.19870788
H	-3.91974784	-1.92827495	-1.97839043
H	-5.01000218	-0.75845402	-1.23539971
H	-5.06450676	-0.47492099	1.28724742
H	-4.01566594	-1.44807077	2.31808971
H	-2.93823246	-2.43381482	0.27483669
H	-4.68144084	-2.71564854	0.26895470
H	-4.06622515	1.29384365	-0.16350171
H	0.86317766	3.29526185	-0.29119210
H	-3.19300376	0.47546219	-2.19344439
H	-3.27820840	0.94446179	2.03269492
C	4.73590007	0.07194869	-1.11911060
H	5.16798042	-0.13363624	-2.08641996
C	3.41318401	0.19190405	-0.71878724
C	3.42032654	0.46459392	0.69664477
C	4.74605344	0.50371378	1.10131414
H	5.18685688	0.67028429	2.07216271
H	6.53107322	0.21565385	-0.00313776

H	0.90211583	-3.00564064	1.70986249
H	2.54798800	-2.45292861	0.43093102
P	1.13862936	-2.41712289	0.45037761
C	0.66783346	-3.75217388	-0.71956694
H	1.17322577	-4.68947323	-0.47780531
H	-0.41447993	-3.88963302	-0.67280368
H	0.93646145	-3.43813608	-1.73056515

Name - MoIIPH3\\SCF E(UB3LYP-D3BJ/BS1) =-2672.3904323\\G=-
2672.145003\\H=-2672.066373\\SCF E(UB3LYP-D3BJ/BS2)=-2672.7037711
ZeroPoint=0.299811

C	4.06926360	-1.08510917	-1.25545420
C	3.00676416	0.83612808	0.00349325
Mo	-0.20351190	-0.25397031	-0.00333516
S	1.33941972	-0.77067799	1.76327470
S	1.34456144	-0.76598268	-1.76534588
S	-1.95944624	0.21038544	1.67168295
S	-1.96187714	0.23629004	-1.66661260
C	2.02762629	1.96351049	0.00379714
N	0.65561403	1.74820511	0.00191222
C	0.05756717	2.93414816	0.00238828
N	0.99184284	3.90774524	0.00465299
C	2.24155834	3.31712278	0.00550897
H	0.80086090	4.90161085	0.00552990
C	4.06568357	-1.08878055	1.25984923
H	3.15031209	3.89701150	0.00706362
C	2.98138257	-0.00171478	-1.30002989
C	2.97767141	-0.00553425	1.30450917
N	-5.53731407	0.07046535	0.00380809
C	3.97142960	-1.95309847	0.00080535
H	4.01055947	-1.70320376	2.16360202
H	5.04014810	-0.58052327	1.27587060
H	5.04373725	-0.57677007	-1.26716716
H	4.01675605	-1.69688396	-2.16115119
H	3.01826434	-2.49442627	-0.00129714
H	4.77149190	-2.70101031	0.00083715
H	4.00143264	1.30211383	0.00551727
H	-1.00599749	3.10856377	0.00122529
H	3.19003351	0.67937356	2.13011906
H	3.19577152	0.68547077	-2.12322844
C	-4.75588128	0.08287223	1.13444801
H	-5.19131306	0.05438753	2.12140316
C	-3.43199738	0.13008629	0.72365548
C	-3.43307793	0.14211916	-0.71780797
C	-4.75749046	0.10194892	-1.12756654
H	-5.19429017	0.08974641	-2.11425449
H	-6.54627950	0.01544259	0.00404982
H	-0.80965425	-3.48459621	-1.09533023
H	-0.81173972	-3.49191722	1.06257222
H	-2.52023855	-2.72539133	-0.01531111
P	-1.11392514	-2.63330571	-0.01374340

Name - MoIIPy\\SCF E(UB3LYP-D3BJ/BS1) =-2577.5657977\\G=-
 2577.260486\\H=-2577.175734\\SCF E(UB3LYP-D3BJ/BS2)=-2577.9106767\\
 ZeroPoint=0.363443

C	-3.91032468	1.80537145	-1.22567342
C	-3.39382664	-0.35545449	-0.01587084
Mo	0.00668787	-0.17365094	-0.01808530
S	-1.37211493	0.69018936	1.78137524
S	-1.35911492	0.80385108	-1.73121890
S	1.51548954	-1.06429613	1.73601334
S	1.51975830	-1.31573293	-1.60234046
C	-2.74419745	-1.69954626	-0.03996920
N	-1.36292636	-1.85862548	-0.03821979
C	-1.10477381	-3.16219633	-0.05800504
N	-2.26517568	-3.84975290	-0.07144415
C	-3.31132501	-2.94664805	-0.06144404
H	-2.34831692	-4.85808113	-0.08818487
C	-3.91331984	1.75089526	1.28856080
H	-4.34210569	-3.26184526	-0.07080371
C	-3.14085588	0.47801840	-1.29717244
C	-3.15222061	0.41665279	1.30605417
N	5.08312574	-1.55169895	0.09872467
C	-3.59132390	2.58852983	0.04954027
H	-3.69906785	2.30800939	2.20575281
H	-4.98815477	1.52013111	1.29699133
H	-4.98367337	1.56928137	-1.24521972
H	-3.69748434	2.40243299	-2.11763735
H	-2.52913853	2.85863730	0.05660754
H	-4.16588774	3.52078825	0.06898760
H	-4.47574298	-0.54560842	-0.02695141
H	-0.12667991	-3.61381294	-0.06308730
H	-3.55083064	-0.20698610	2.11094486
H	-3.51803646	-0.10951051	-2.13892361
C	4.30514627	-1.36816132	1.21745392
H	4.73861260	-1.33200006	2.20516025
C	2.98876848	-1.25051563	0.79728376
C	2.99098347	-1.36488953	-0.64177721
C	4.30636649	-1.55058328	-1.03679448
H	4.74155855	-1.67225121	-2.01685567
H	6.08895272	-1.64570029	0.10692823
C	1.66525160	2.30116916	1.06311602
C	1.90867605	2.05200258	-1.22710211
C	2.50895017	3.40399569	1.07386122
H	1.21657326	1.92941354	1.97488397
C	2.76213618	3.14579678	-1.29686934
H	1.65277502	1.48086223	-2.11028829
H	2.71825119	3.90677989	2.01106370
H	3.17432391	3.44062778	-2.25499969

N	1.36375383	1.63177324	-0.06773920
C	3.07224667	3.83628863	-0.12637853
H	3.73930561	4.69176408	-0.14818504

Name - MoIIPyNH2\\SCF E(UB3LYP-D3BJ/BS1)= -2632.9439393\\G=-
2632.625633\\H=-2632.535911\\SCF E(UB3LYP-D3BJ/BS2)=-2633.3076015
ZeroPoint=0.379710

C	-3.65383624	2.34722695	-1.25365835
C	-3.53421353	0.15203400	-0.00067037
Mo	-0.14636842	-0.27163843	-0.00104582
S	-1.34222243	0.86110236	1.76614813
S	-1.34067114	0.86998943	-1.76219230
S	1.12503926	-1.57349017	1.67887941
S	1.12387605	-1.58339640	-1.67312520
C	-3.13764286	-1.28711209	-0.00322023
N	-1.80761610	-1.68937187	-0.00361388
C	-1.78653193	-3.01741085	-0.00595620
N	-3.05130783	-3.48825549	-0.00708207
C	-3.91951255	-2.41272672	-0.00541212
H	-3.31229998	-4.46591472	-0.00885398
C	-3.65423873	2.34239952	1.26093676
H	-4.99004377	-2.53926413	-0.00601740
C	-3.14505863	0.89853731	-1.30199971
C	-3.14604361	0.89332709	1.30396223
N	4.51503237	-2.73914716	0.00510169
C	-3.18919799	3.08245898	0.00513544
H	-3.33943473	2.86938205	2.16688494
H	-4.75309793	2.31049873	1.27352100
H	-4.75267397	2.31500597	-1.26661497
H	-3.33895486	2.87776906	-2.15749708
H	-2.09534666	3.15157045	0.00543147
H	-3.58170790	4.10504752	0.00704670
H	-4.63274058	0.16110949	-0.00115583
H	-0.90470247	-3.63632751	-0.00694067
H	-3.64276485	0.36751933	2.12418016
H	-3.64044209	0.37571037	-2.12493502
C	3.77916495	-2.46751417	1.13517310
H	4.19271302	-2.60495997	2.12257339
C	2.53222821	-2.02069930	0.72545020
C	2.53163374	-2.02536943	-0.71800848
C	3.77808725	-2.47494694	-1.12605437
H	4.19077459	-2.61868580	-2.11291686
H	5.47569032	-3.05160932	0.00565507
C	2.01108491	1.71638671	1.15190507
C	2.01569653	1.70889235	-1.15758008
C	3.01767377	2.65517044	1.19997885
H	1.58974111	1.31760317	2.06588776
C	3.02252564	2.64729627	-1.20777550
H	1.59803163	1.30407818	-2.07061838
H	3.38847996	3.00372348	2.15777648
H	3.39721937	2.98962850	-2.16630880

N	1.49339287	1.23286168	-0.00228966
C	3.56311103	3.15638248	-0.00445355
N	4.57630010	4.05379055	-0.00532112
H	4.82789608	4.51454047	-0.86789809
H	4.82459983	4.51996579	0.85528307

Name - MoII1CH3CN\\SCF E(UB3LYP-D3BJ/BS1)=-2463.1387567\\G=-
2462.864301\\H=-2462.777127\\SCF E(UB3LYP-D3BJ/BS2)=-2463.4636893
ZeroPoint=0.334357

C	-3.10097279	2.07352593	-1.26250650
C	-3.27975955	-0.10635686	0.00040061
Mo	0.55460700	0.15932616	-0.00059247
S	-1.01954259	0.27321025	1.80019015
S	-1.02044045	0.26998819	-1.80085708
S	2.30139811	-0.34437893	1.67983131
S	2.29999279	-0.35040839	-1.68033251
C	-3.25726379	-1.60727964	0.00131290
N	-2.12618382	-2.41077647	0.00226699
C	-2.55878544	-3.66055303	0.00274254
N	-3.91614480	-3.71015438	0.00216412
C	-4.37541909	-2.41064108	0.00125464
H	-4.48361918	-4.54730304	0.00233640
C	-3.10081914	2.07513138	1.26036216
H	-5.42806775	-2.17432959	0.00066339
C	-2.78375605	0.56905925	-1.29639595
C	-2.78327637	0.57079418	1.29608137
N	5.59637422	-1.68709968	0.00074552
C	-2.57358866	2.76041977	-0.00152281
H	-2.70737510	2.55766774	2.16006264
H	-4.19482840	2.17738223	1.29379961
H	-4.19496391	2.17594031	-1.29599991
H	-2.70751879	2.55483545	-2.16286281
H	-1.48132180	2.74126867	-0.00163541
H	-2.87378442	3.81414746	-0.00221394
H	-1.94041172	-4.54650309	0.00345589
H	-3.33898345	0.11571208	2.12069472
H	-3.34004275	0.11308610	-2.12012761
C	4.87880274	-1.39490250	1.13268304
H	5.28466700	-1.55970205	2.11854303
C	3.64961612	-0.89382124	0.72354776
C	3.64897224	-0.89650680	-0.72321353
C	4.87778123	-1.39915149	-1.13161143
H	5.28279793	-1.56754637	-2.11721180
H	6.53385050	-2.06664802	0.00102555
H	-0.30445651	-1.82070047	0.00215867
H	0.48630254	-1.83166053	0.00193515
H	-4.35234997	0.14017924	0.00046829
N	0.97144518	2.23079161	-0.00243230
C	1.18831890	3.36907313	-0.00156712
C	1.44826494	4.79230586	0.00071292
H	1.57979948	5.14134283	-1.02726500

H	0.60151490	5.31276395	0.45723055
H	2.35564404	4.99788160	0.57562229

Name - MoII1CH3SCH3\\SCF E(UB3LYP-D3BJ/BS1)=-2808.4080182\\G=-
 2808.103487\\H=-2808.014669\\SCF E(UB3LYP-D3BJ/BS2)=-2808.7409305\\
 ZeroPoint=0.364695

C	2.95629954	-2.29242652	-1.26355050
C	3.36749761	-0.15486897	0.00007272
Mo	-0.46963257	0.19690491	-0.00002763
S	1.04553711	-0.32590459	1.77423930
S	1.04569651	-0.32566950	-1.77427536
S	-2.12123640	0.91710499	1.69010695
S	-2.12129803	0.91717085	-1.69018450
C	3.55280855	1.33368422	0.00007481
N	2.54552956	2.28546825	0.00056525
C	3.14031723	3.46738862	0.00037458
N	4.48952650	3.32904416	-0.00021726
C	4.76875013	1.97919941	-0.00036586
H	5.16546628	4.08139099	-0.00047906
C	2.95632221	-2.29242516	1.26369071
H	5.77961713	1.60263186	-0.00079559
C	2.78781042	-0.76340084	-1.29481392
C	2.78775266	-0.76340076	1.29492595
N	-5.66682782	1.25306652	0.00004144
C	2.36063045	-2.91405608	0.00007543
H	2.51223259	-2.73379142	2.16093822
H	4.03393582	-2.50537239	1.29938451
H	4.03390493	-2.50541737	-1.29926816
H	2.51217705	-2.73378751	-2.16078517
H	1.27991072	-2.75417816	0.00009502
H	2.52547703	-3.99672516	0.00006161
H	2.64542860	4.42745848	0.00062437
H	3.37322010	-0.36078455	2.12595001
H	3.37338808	-0.36084542	-2.12578953
C	-4.89398983	1.16896787	1.13128237
H	-5.32900413	1.21129998	2.11771640
C	-3.57516464	1.02512067	0.72354432
C	-3.57518888	1.02513097	-0.72354997
C	-4.89402652	1.16900578	-1.13123346
H	-5.32907949	1.21139227	-2.11764794
H	-6.67315366	1.34985272	0.00006444
H	0.80902660	2.00157680	0.00018120
H	0.00598502	2.09193091	-0.00035380
H	4.39786073	-0.54081538	0.00009200
S	-1.77455623	-1.96594399	-0.00012735
C	-1.28219263	-3.00442480	1.40959675
H	-1.53505573	-2.44530836	2.31083156
H	-1.85819785	-3.93146731	1.37228563

H	-0.21291100	-3.20879173	1.39191950
C	-1.28176910	-3.00445833	-1.40970983
H	-0.21233169	-3.20800759	-1.39219421
H	-1.85711358	-3.93189171	-1.37199906
H	-1.53524416	-2.44574912	-2.31102677

Name - MoIII1MI\\SCF E(UB3LYP-D3BJ/BS1)=-2556.634687\\G=-

2556.333630\\H=-2556.246331\\SCF E(UB3LYP-D3BJ/BS2)=-2556.9814799\\

ZeroPoint=0.360880

C	3.09678083	1.91878588	1.39494601
C	3.31200411	-0.22486176	0.08979427
Mo	-0.53846703	0.04382173	0.02954552
S	1.09435859	0.02424455	-1.75733408
S	0.99885109	0.12992343	1.83252500
S	-2.15316752	-0.67812576	-1.65610595
S	-2.37676552	-0.33639864	1.68463256
C	3.32054156	-1.72614729	0.04654790
N	2.23296450	-2.56043333	0.26307136
C	2.68187363	-3.79511008	0.10977106
N	4.00637231	-3.80617700	-0.19455206
C	4.42822871	-2.49453530	-0.23490818
H	4.57711784	-4.62570552	-0.35290188
C	3.04952236	1.97981885	-1.13142714
H	5.45103680	-2.22757514	-0.45087937
C	2.78314129	0.41419801	1.38881447
C	2.81013457	0.46123722	-1.20146776
N	-5.39956060	-2.21131302	-0.04093472
C	2.53955646	2.62626948	0.15922313
H	2.60421992	2.46273113	-2.00676747
H	4.13562630	2.13784343	-1.19718192
H	4.19043952	2.02606171	1.41800998
H	2.71082743	2.37575283	2.31139598
H	1.44983123	2.59200094	0.19093969
H	2.82543597	3.68389706	0.17580587
H	2.09870507	-4.69940408	0.20847035
H	3.41906523	0.05856966	-2.01605568
H	3.31012193	-0.06317217	2.21952021
C	-4.63266231	-1.96204238	-1.14800850
H	-4.94059391	-2.27419492	-2.13397150
C	-3.49867021	-1.28263500	-0.71919211
C	-3.60107007	-1.13112947	0.71145776
C	-4.79449451	-1.72166990	1.09558528
H	-5.25065186	-1.83188855	2.06718431
H	-6.29152278	-2.68664292	-0.05624406
H	0.27186905	-2.00387591	0.19706684
H	-0.50473575	-2.02886874	0.18657516
H	4.37828966	0.04754327	0.10912280
N	-0.91080144	2.14554798	-0.12023960
C	-0.72935394	2.89868811	-1.20627221

C	-1.28481454	2.99603219	0.91133728
H	-0.41568678	2.54184277	-2.17281711
C	-1.32814021	4.27223679	0.42805149
H	-1.49004504	2.62518924	1.90170202
H	-0.91647985	4.95741322	-1.55976115
H	-1.57053924	5.21187290	0.89715681
N	-0.97963306	4.18537362	-0.90767048

Name - MoII1NH2CH3\\SCF E(UB3LYP-D3BJ/BS1)=-2426.2648383\\G=-
2425.967854\\H=-2425.883250\\SCF E(UB3LYP-D3BJ/BS2)= -2426.5692055
ZeroPoint=0.355130

C	3.04186588	2.30979888	1.26327189
C	3.31722672	0.14682764	-0.00007538
Mo	-0.54001540	0.12843654	-0.00010081
S	1.02513073	0.44106563	-1.79094459
S	1.02522509	0.44075743	1.79095209
S	-2.25273666	-0.44256005	-1.68374696
S	-2.25223626	-0.44375529	1.68315846
C	3.40153258	-1.35177282	-0.00008778
N	2.33458926	-2.23741029	-0.00079640
C	2.85925142	-3.45157813	-0.00048601
N	4.21635360	-3.39949461	0.00036431
C	4.57700049	-2.06942745	0.00067566
H	4.84469354	-4.19186783	0.00068019
C	3.04183169	2.30989405	-1.26326560
H	5.60898525	-1.75498173	0.00134581
C	2.78244951	0.79378216	1.29556386
C	2.78242258	0.79387688	-1.29564056
N	-5.75608372	-1.08212516	0.00014782
C	2.49461442	2.97714384	0.00003761
H	2.62670740	2.77688834	-2.16129944
H	4.13076976	2.45493569	-1.29997499
H	4.13080661	2.45484123	1.29994498
H	2.62677473	2.77673361	2.16135071
H	1.40238878	2.92568896	0.00004361
H	2.75775347	4.04043472	0.00007004
H	2.30858539	-4.38108364	-0.00090295
H	3.35140054	0.35998897	-2.12246985
H	3.35152527	0.35985523	2.12230652
C	-4.99287304	-0.93961732	-1.13158423
H	-5.42362039	-1.01650698	-2.11775465
C	-3.68930361	-0.69262743	-0.72276813
C	-3.68904783	-0.69318389	0.72250017
C	-4.99246184	-0.94056888	1.13165622
H	-5.42278127	-1.01824101	2.11795387
H	-6.75088779	-1.26303008	0.00026373
H	0.46997100	-1.80926401	-0.00020451
H	-0.31523868	-1.87587242	-0.00065206
H	4.37164410	0.46230649	-0.00007482
N	-1.12436831	2.26203366	-0.00068689
H	-0.66937824	2.67911048	0.81139159

H	-0.67353852	2.67719708	-0.81606932
C	-2.55670536	2.64416033	0.00257431
H	-3.03910413	2.23154035	-0.88236582
H	-3.03425309	2.23448069	0.89149063
H	-2.65894093	3.73311533	0.00102254

Name - MoII1NH3\\SCF E(UB3LYP-D3BJ/BS1)=-2386.9548614\\G=-

2386.683293\\H=-2386.603333\\SCF E(UB3LYP-D3BJ/BS2)=-2387.2498799\\

ZeroPoint=0.326642

C	-2.76899134	-2.49607427	1.25873535
C	-3.22143713	-0.35922888	0.00062383
Mo	0.60956460	0.02398558	0.00002374
S	-0.91014359	-0.47725712	-1.78440497
S	-0.90844755	-0.48463035	1.78375078
S	2.32101581	0.59153804	-1.68722511
S	2.32217847	0.58136033	1.68986675
C	-3.41993880	1.12884421	0.00225322
N	-2.42395878	2.09402720	0.00818722
C	-3.03923901	3.26495661	0.00687739
N	-4.38801140	3.10918884	0.00042220
C	-4.64627840	1.75543553	-0.00246771
H	-5.07489683	3.85130621	-0.00172877
C	-2.76877382	-2.49250447	-1.26395117
H	-5.65139098	1.36347247	-0.00750063
C	-2.63479707	-0.96358376	1.29433468
C	-2.63546300	-0.95986628	-1.29520174
N	5.87290304	0.30788838	-0.00084636
C	-2.15998421	-3.11033151	-0.00343453
H	-2.32036138	-2.92198716	-2.16473055
H	-3.84194732	-2.72858201	-1.29499554
H	-3.84226437	-2.73181654	1.28880612
H	-2.32097231	-2.92836271	2.15836479
H	-1.07647667	-2.95574225	-0.00307202
H	-2.32540363	-4.19322491	-0.00500692
H	-2.56073641	4.23356146	0.01040624
H	-3.23646898	-0.57312550	-2.12300872
H	-3.23482183	-0.57876153	2.12374943
C	5.09842674	0.36035874	-1.13188175
H	5.53448265	0.32902407	-2.11818855
C	3.77370653	0.44522213	-0.72439829
C	3.77421876	0.44072378	0.72512699
C	5.09921383	0.35313413	1.13108139
H	5.53601705	0.31561086	2.11684071
H	6.88033201	0.22096781	-0.00148608
H	-0.55204611	1.86623060	0.00588046
H	0.22975718	1.99225211	0.00488323
H	-4.24830478	-0.75503449	0.00029783
N	1.47396855	-1.99604585	-0.00600019
H	2.49363534	-1.95446046	-0.00614705

H	1.18446977	-2.52378699	0.81634560
H	1.18374604	-2.51903566	-0.83103220

Name - MoII1PH2CH3\\SCF E(UB3LYP-D3BJ/BS1)=-2712.858476\\G=-
2712.572890\\H=-2712.487081\\SCF E(UB3LYP-D3BJ/BS2)=-2713.1817849
ZeroPoint=0.344089

C	-2.71710796	2.55094148	-0.89785260
C	-3.32218316	0.30015543	0.07686447
Mo	0.50337123	-0.19557167	0.04227575
S	-1.01874654	0.08635468	1.86346555
S	-0.99929011	0.47817935	-1.67449874
S	2.19307013	-0.94354660	1.66692709
S	2.23162960	-0.62331139	-1.67819559
C	-3.60388573	-1.16119484	-0.12216491
N	-2.66908683	-2.18506184	-0.15986196
C	-3.35187622	-3.30001904	-0.35936145
N	-4.68471997	-3.05285373	-0.45308591
C	-4.86110196	-1.69459844	-0.30260033
H	-5.41191552	-3.74032967	-0.59899695
C	-2.79200875	2.22703608	1.60751255
H	-5.83718850	-1.23601511	-0.33440746
C	-2.68506366	1.02882955	-1.12552721
C	-2.72120084	0.69943828	1.44048982
N	5.77088227	-0.97137383	0.02344922
C	-2.12356847	2.96807552	0.44909350
H	-2.34635555	2.51762468	2.56341776
H	-3.85471095	2.50434106	1.64926241
H	-3.77134874	2.85953507	-0.93209754
H	-2.20872494	3.06057556	-1.72185786
H	-1.05125366	2.75952617	0.46258714
H	-2.23528330	4.04946231	0.58240385
H	-2.93521746	-4.29365957	-0.44122498
H	-3.33999004	0.23189879	2.21150447
H	-3.30001410	0.79561039	-1.99917909
C	4.98296064	-1.03074104	1.14364400
H	5.40673487	-1.14595578	2.12910644
C	3.66320198	-0.91260193	0.72693487
C	3.68134892	-0.77391493	-0.71302015
C	5.01040795	-0.81429357	-1.10934482
H	5.46092717	-0.74239122	-2.08696435
H	6.78050346	-1.02500209	0.03141660
H	-0.66934562	-2.15140044	-0.14298015
H	0.09241622	-2.29104787	-0.17026899
H	-4.32497175	0.75207822	0.11923704
H	2.96351360	1.89432708	0.34685967
H	1.24890154	2.77364951	1.34833566
P	1.56714585	2.01481311	0.20679868
C	1.37976525	3.19200228	-1.18402806
H	0.32688059	3.45447262	-1.29522755
H	1.97309270	4.09084262	-1.00140312
H	1.72030505	2.70119116	-2.09760518

Name - MoII1PH3\\SCF E(UB3LYP-D3BJ/BS1)=-2673.5233387\\G=-
 2673.265422\\H=-2673.182924\\SCF E(UB3LYP-D3BJ/BS2)=-2673.8383956\\
 ZeroPoint=0.314675

C	-2.79329513	-2.44008499	1.26238569
C	-3.28384321	-0.31201439	0.00038036
Mo	0.54563397	0.06959758	0.00020854
S	-0.97382803	-0.37851953	-1.78172519
S	-0.97324430	-0.38150234	1.78195488
S	2.27444989	0.60468156	-1.67928170
S	2.27525275	0.59982367	1.68036706
C	-3.50850650	1.17242617	0.00089559
N	-2.53023653	2.15563160	0.00363578
C	-3.16966659	3.31336222	0.00273478
N	-4.51600615	3.13233484	-0.00041115
C	-4.74751551	1.77398358	-0.00163581
H	-5.21722824	3.86085152	-0.00163708
C	-2.79292780	-2.43875978	-1.26400240
H	-5.74471128	1.36216339	-0.00407783
C	-2.68703268	-0.90545705	1.29376994
C	-2.68715279	-0.90406721	-1.29373776
N	5.83442772	0.71952115	-0.00011152
C	-2.18256712	-3.04846534	-0.00103844
H	-2.33189737	-2.86070231	-2.16185703
H	-3.86191740	-2.69121859	-1.30226041
H	-3.86235796	-2.69233145	1.29999926
H	-2.33265737	-2.86312092	2.15992723
H	-1.10159517	-2.88430616	-0.00073418
H	-2.33526617	-4.13298553	-0.00165121
H	-2.71109846	4.29170485	0.00429421
H	-3.29156864	-0.52812639	-2.12396401
H	-3.29108369	-0.53015670	2.12455250
C	5.05992472	0.68802390	-1.13193540
H	5.49735478	0.70275442	-2.11796797
C	3.73416543	0.63426124	-0.72330677
C	3.73451014	0.63210650	0.72379861
C	5.06046637	0.68465027	1.13196920
H	5.49835339	0.69648876	2.11783825
H	6.84501884	0.75401447	-0.00030446
H	-0.57664656	2.02258469	0.00275074
H	0.19512831	2.13615293	0.00226823
H	-4.30325972	-0.72673568	0.00018991
H	2.94045713	-2.19229326	-0.00334844
H	1.25303108	-3.03581676	1.08526460
H	1.25196205	-3.03362833	-1.09208071
P	1.53230795	-2.18948861	-0.00269721

Name - MoII1Py\\SCF E(UB3LYP-D3BJ/BS1)= -2578.6984785\\G=-
 2578.381000\\H=-2578.291957\\SCF E(UB3LYP-D3BJ/BS2)=-2579.0389727\\
 ZeroPoint=0.378309

C	2.90911149	2.13446437	1.26286206
C	3.38620800	-0.00143720	0.00013097
Mo	-0.46747217	-0.18520436	0.00007854
S	1.09929368	0.05376669	-1.79849695
S	1.09914146	0.05395290	1.79862939
S	-2.14802597	-0.87345579	-1.67991355
S	-2.14841958	-0.87309627	1.68005177
C	3.56301752	-1.49263535	0.00006493
N	2.54818198	-2.43963395	0.00048078
C	3.14555250	-3.61943065	0.00020255
N	4.49814390	-3.48812571	-0.00033339
C	4.77910494	-2.13888965	-0.00049664
H	5.17216301	-4.24183914	-0.00059407
C	2.90904749	2.13451645	-1.26253081
H	5.79073949	-1.76395394	-0.00093674
C	2.80208921	0.60087015	1.29639898
C	2.80211765	0.60091788	-1.29613790
N	-5.29530628	-2.54128376	-0.00018034
C	2.29839523	2.74441237	0.00019386
H	2.44705223	2.55697625	-2.15994737
H	3.97826924	2.38707548	-1.30250153
H	3.97834985	2.38695885	1.30277562
H	2.44719819	2.55691791	2.16032410
H	1.21999027	2.58242765	0.00022699
H	2.45584785	3.82867430	0.00020838
H	2.65227594	-4.58074726	0.00041173
H	3.41688279	0.22662402	-2.11952291
H	3.41675029	0.22648025	2.11981734
C	-4.60888943	-2.17893101	-1.13198161
H	-4.99461359	-2.38560280	-2.11811929
C	-3.43877162	-1.55353959	-0.72256498
C	-3.43895900	-1.55337715	0.72252317
C	-4.60917184	-2.17868941	1.13174405
H	-4.99516887	-2.38516449	2.11781599
H	-6.19284032	-3.00717292	-0.00024807
H	0.58772940	-2.08650626	0.00028762
H	-0.18791524	-2.19854392	0.00035540
H	4.41590101	0.38743424	0.00015598
C	-1.25810931	2.58041807	1.16168176
C	-1.25756101	2.58036525	-1.16206752
C	-1.57520155	3.93075901	1.19945043
H	-1.11293284	2.00870045	2.06813522
C	-1.57464827	3.93070235	-1.20004520
H	-1.11191774	2.00860985	-2.06842241
H	-1.68986157	4.42349489	2.15778726
H	-1.68886662	4.42339255	-2.15845805
N	-1.09714105	1.91222534	-0.00014017
C	-1.73389016	4.62330859	-0.00035092
H	-1.97683572	5.68056632	-0.00043179

Name - MoII1PyNH2\\SCF E(UB3LYP-D3BJ/BS1)=-2634.0784772\\G=-
2633.744636\\H=-2633.654848\\SCF E(UB3LYP-D3BJ/BS2)=-2634.4446093
ZeroPoint=0.394519

C	2.58517482	2.39882001	1.26387132
C	3.40487748	0.37124556	0.00019483
Mo	-0.39790141	-0.37701033	0.00018552
S	1.14013091	0.04313545	-1.79339998
S	1.13991401	0.04333951	1.79366093
S	-1.92403265	-1.35584282	-1.68223455
S	-1.92515973	-1.35489526	1.68247400
C	3.82712716	-1.06969640	0.00006984
N	2.98479299	-2.17303400	0.00060602
C	3.77259586	-3.23508012	0.00019656
N	5.08473310	-2.87939050	-0.00059398
C	5.13482591	-1.50214060	-0.00067887
H	5.87568291	-3.50928689	-0.00102410
C	2.58495008	2.39893442	-1.26322993
H	6.06891918	-0.96220969	-0.00123286
C	2.72792377	0.86809870	1.29584767
C	2.72788566	0.86822751	-1.29540103
N	-4.58353434	-3.73330977	-0.00017997
C	1.88675555	2.90439085	0.00040860
H	2.05719572	2.73933918	-2.15936701
H	3.59888111	2.82174892	-1.30755958
H	3.59916313	2.82151159	1.30803322
H	2.05764027	2.73920882	2.16014436
H	0.84833187	2.57330422	0.00050828
H	1.87087341	4.00000736	0.00045534
H	3.44848878	-4.26589604	0.00043647
H	3.39501516	0.59867083	-2.11911646
H	3.39494545	0.59830509	2.11957083
C	-4.00139723	-3.21603833	-1.13140423
H	-4.32451273	-3.50990226	-2.11806517
C	-3.01594494	-2.32880895	-0.72142746
C	-3.01646140	-2.32838754	0.72145471
C	-4.00220550	-3.21537645	1.13119584
H	-4.32603789	-3.50870940	2.11777936
H	-5.34083257	-4.40267402	-0.00026367
H	0.92734423	-2.15616362	0.00060967
H	0.18543604	-2.38415969	0.00068511
H	4.35566359	0.92599167	0.00022292
C	-1.55917205	2.22457025	1.16034929
C	-1.55861555	2.22443663	-1.16095751
C	-2.03190016	3.51371840	1.20646683
H	-1.35032745	1.67999805	2.07140524
C	-2.03135526	3.51357027	-1.20744295
H	-1.34928480	1.67976373	-2.07184049
H	-2.20805518	3.99152589	2.16377507
H	-2.20707725	3.99126238	-2.16488856

N	-1.31092936	1.56451598	-0.00020684
C	-2.27976374	4.21275326	-0.00058800
N	-2.72628127	5.48127827	-0.00076201
H	-2.91606014	5.96053289	-0.86832506
H	-2.91644486	5.96063015	0.86666343

Name - TSCH3CN\\SCF E(UB3LYP-D3BJ/BS1)= -2463.1382691\\G=-2462.865057\\H=-2462.779116\\SCF E(UB3LYP-D3BJ/BS2)=-2463.4620247\\ZeroPoint=0.332430

C	3.13864827	2.07112929	1.25935607
C	3.28475539	-0.11395668	0.00002204
Mo	-0.52905139	0.12038667	0.00001529
S	1.03926297	0.29611489	-1.81078160
S	1.03924501	0.29620521	1.81079658
S	-2.27236384	-0.38794338	-1.67986249
S	-2.27246563	-0.38771881	1.67989037
C	3.21390639	-1.61240364	0.00003349
N	2.05530166	-2.37601670	0.00010074
C	2.42774066	-3.64603553	0.00006785
N	3.77840031	-3.74484145	-0.00001590
C	4.29294012	-2.46526364	-0.00003868
H	4.31040673	-4.60541489	-0.00005339
C	3.13864340	2.07109379	-1.25937923
H	5.35438813	-2.27369505	-0.00010046
C	2.80378290	0.57092147	1.29838942
C	2.80378958	0.57088229	-1.29836939
N	-5.63592900	-1.55079093	-0.00001906
C	2.61044951	2.76004107	-0.00002029
H	2.75590608	2.55718559	-2.16170726
H	4.23388984	2.16278105	-1.28517779
H	4.23389538	2.16280955	1.28514621
H	2.75591898	2.55724976	2.16167210
H	1.51741648	2.74118332	-0.00001717
H	2.91272372	3.81314680	-0.00003570
H	1.76801184	-4.50100854	0.00010322
H	3.36038350	0.10998561	-2.11917723
H	3.36036155	0.11004358	2.11921803
C	-4.90339615	-1.29738446	-1.13204762
H	-5.31708769	-1.44182768	-2.11788708
C	-3.65024606	-0.85942989	-0.72303645
C	-3.65029221	-0.85933152	0.72304020
C	-4.90346845	-1.29722825	1.13202597
H	-5.31722592	-1.44154062	2.11785689
H	-6.59268506	-1.87829319	-0.00002792
H	0.53686041	-1.85853129	0.00009375
H	-0.30897538	-1.77436699	0.00013530
H	4.36402030	0.09946508	0.00002387
N	-0.97624903	2.21450424	-0.00006612
C	-1.19327439	3.35267665	-0.00009156
C	-1.45435166	4.77642780	-0.00012082
H	-0.50378948	5.31746521	-0.00031227

H	-2.02593146	5.04384681	-0.89325312
H	-2.02561684	5.04393061	0.89318810

Name - TSCH3SCH3\\SCF E(UB3LYP-D3BJ/BS1)= -2808.4080172\\G=-
2808.102092\\H=-2808.015767\\SCF E(UB3LYP-D3BJ/BS2)=-2808.7407888\\
ZeroPoint=0.364413

C	-2.96395672	2.29066350	-1.26325865
C	-3.36755019	0.15152268	-0.00002497
Mo	0.46728446	-0.19818048	-0.00003898
S	-1.04663978	0.32999459	1.77465775
S	-1.04655811	0.33070930	-1.77457715
S	2.11895125	-0.91839681	1.68991402
S	2.11914999	-0.91734426	-1.69031455
C	-3.54550986	-1.33780395	-0.00018135
N	-2.53320230	-2.28422592	-0.00068573
C	-3.11988822	-3.47031344	-0.00063925
N	-4.46936735	-3.33943147	-0.00013976
C	-4.75701529	-1.99125839	0.00014797
H	-5.14075914	-4.09590865	-0.00001157
C	-2.96379140	2.29038576	1.26369204
H	-5.77017111	-1.62099142	0.00054934
C	-2.79017384	0.76225305	-1.29496764
C	-2.79015147	0.76194796	1.29506061
N	5.66559055	-1.24636307	-0.00007726
C	-2.36983441	2.91407702	0.00024428
H	-2.52143036	2.73308138	2.16113303
H	-4.04210872	2.49985028	1.29906117
H	-4.04229633	2.50004749	-1.29841458
H	-2.52176275	2.73359804	-2.16066395
H	-1.28857696	2.75762498	0.00013895
H	-2.53822112	3.99620480	0.00038083
H	-2.61842573	-4.42688808	-0.00094459
H	-3.37476418	0.35750615	2.12580536
H	-3.37469534	0.35791637	-2.12582744
C	4.89242137	-1.16430802	1.13114228
H	5.32746211	-1.20596046	2.11759925
C	3.57331801	-1.02324614	0.72336064
C	3.57340841	-1.02277705	-0.72364783
C	4.89256305	-1.16357049	-1.13134697
H	5.32773374	-1.20459099	-2.11777296
H	6.67209721	-1.34104622	-0.00004228
H	-0.83240730	-1.99864600	-0.00062654
H	-0.02161358	-2.07807811	-0.00057129
H	-4.39969698	0.53257576	0.00003206
S	1.77525177	1.96748513	0.00049149
C	1.28138181	3.00592678	1.40966074
H	1.53445592	2.44753026	2.31129715
H	1.85605071	3.93381026	1.37255287
H	0.21178594	3.20876606	1.39152719
C	1.28199745	3.00608511	-1.40877846
H	0.21253726	3.20964962	-1.39059694

H	1.85727799	3.93359497	-1.37181673
H	1.53464111	2.44740345	-2.31035749

Name - TSIMI\\SCF E(UB3LYP-D3BJ/BS1)=-2556.6326175\\G=-2556.332642
 \\H=-2556.246777\\SCF E(UB3LYP-D3BJ/BS2)=-2556.9777781\\

ZeroPoint=0.359067

C	3.13062698	1.97265961	1.31994842
C	3.33373187	-0.18939273	0.03409060
Mo	-0.48814727	-0.04688647	0.00786777
S	1.10794932	0.10953683	-1.81320818
S	1.06023571	0.15881015	1.82454424
S	-2.14892092	-0.70648814	-1.66300355
S	-2.26456747	-0.52140080	1.69462793
C	3.29721145	-1.68889342	0.01953468
N	2.15801703	-2.48120530	0.06068930
C	2.55224121	-3.74496490	0.03074264
N	3.90152646	-3.81183588	-0.02667191
C	4.38982623	-2.52144241	-0.03371098
H	4.45097666	-4.66100822	-0.05723720
C	3.10008623	2.00780396	-1.19897881
H	5.44627971	-2.30832782	-0.07364191
C	2.82725841	0.46642156	1.33778979
C	2.83881505	0.49314590	-1.26241719
N	-5.50023499	-1.98345057	-0.03775792
C	2.56501201	2.66050548	0.07729959
H	2.67788803	2.48744456	-2.08721304
H	4.18901275	2.15521153	-1.24127747
H	4.22369545	2.08991833	1.33465514
H	2.74636061	2.43667099	2.23336190
H	1.47495653	2.60185675	0.09747634
H	2.83015546	3.72361155	0.08642201
H	1.90786220	-4.61104663	0.04817897
H	3.43922865	0.07569773	-2.07580937
H	3.38410256	0.00463896	2.15790992
C	-4.73833779	-1.75043457	-1.15268763
H	-5.10059401	-1.97484239	-2.14404383
C	-3.53174267	-1.21130125	-0.72265838
C	-3.58568985	-1.12832606	0.71650160
C	-4.82356259	-1.61826338	1.10422993
H	-5.26596884	-1.73388392	2.08156607
H	-6.43518599	-2.36716867	-0.05214910
H	0.72946753	-2.03706528	0.06796788
H	-0.16033714	-1.92059902	0.08179457
H	4.40765871	0.04885536	0.04461142
N	-0.95256338	2.09404495	-0.05311116
C	-0.81566393	2.89387635	-1.10858901
C	-1.33145203	2.89263371	1.01502371
H	-0.50764019	2.58638876	-2.09414489
C	-1.42501183	4.18647164	0.58553253
H	-1.50641327	2.47647971	1.99334434

H	-1.07094516	4.96136201	-1.38013147
H	-1.68781576	5.09898059	1.09570328
N	-1.09900199	4.16326552	-0.75815770

Name - TSNH2CH3\\SCF E(UB3LYP-D3BJ/BS1)=-2426.2640694\\G=-

2425.957890\\H=-2425.876191\\SCF E(UB3LYP-D3BJ/BS2)=-2426.5744782\\

ZeroPoint=0.354257

C	3.10003615	-2.29494043	-1.26097070
C	3.31884439	-0.12394116	-0.00009195
Mo	-0.51780126	-0.10334546	-0.00002906
S	1.04054609	-0.47763918	1.79668124
S	1.04083254	-0.47818099	-1.79719440
S	-2.23004338	0.46311810	1.68296496
S	-2.22965041	0.46082319	-1.68290209
C	3.33844343	1.37572507	-0.00010844
N	2.23251072	2.21226595	-0.00019567
C	2.68234217	3.45746274	-0.00000025
N	4.03544159	3.46944800	0.00022458
C	4.46840220	2.15998474	0.00017561
H	4.62118273	4.29446519	0.00036096
C	3.09949621	-2.29478936	1.26113756
H	5.51570205	1.90227879	0.00030759
C	2.80483166	-0.78583478	-1.29753834
C	2.80461043	-0.78560574	1.29736021
N	-5.75594105	0.97959979	-0.00104500
C	2.55865867	-2.97081433	0.00000339
H	2.70005711	-2.77067852	2.16156070
H	4.19160753	-2.41649284	1.29057275
H	4.19218170	-2.41651317	-1.28986571
H	2.70105894	-2.77101794	-2.16149622
H	1.46534294	-2.92955638	-0.00030943
H	2.83463376	-4.03084084	0.00016201
H	2.07626213	4.35105385	0.00000256
H	3.36788152	-0.33963532	2.12169333
H	3.36823291	-0.33989598	-2.12180283
C	-4.98743503	0.86458134	1.13073433
H	-5.42055232	0.92695232	2.11693924
C	-3.67602187	0.66361171	0.72207300
C	-3.67579196	0.66267622	-0.72273837
C	-4.98709534	0.86311183	-1.13227448
H	-5.41976025	0.92411970	-2.11876361
H	-6.75611405	1.12706253	-0.00132742
H	0.72872340	1.81592610	-0.00034531
H	-0.13541462	1.76827180	-0.00067142
H	4.38518508	-0.39462290	0.00002881
N	-1.12506575	-2.26319952	-0.00023325
H	-0.67276314	-2.67588964	-0.81568574
H	-0.66782528	-2.67756712	0.81158581
C	-2.55640275	-2.64119231	0.00384410
H	-3.03314475	-2.22857905	0.89226575
H	-3.03900782	-2.22578327	-0.88011412

H	-2.66890264	-3.72949873	0.00243876
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Name - TSNH3\\SCF E(UB3LYP-D3BJ/BS1)=-2386.9543745\\G=-
2386.684125\\H=-2386.605419\\SCF E(UB3LYP-D3BJ/BS2)= -2387.2478683
ZeroPoint=0.324644

C	2.82362496	-2.48153307	-1.25826426
C	3.22096099	-0.33366064	-0.00008786
Mo	-0.59364258	0.02643162	0.00012465
S	0.91779881	-0.51267031	1.78885540
S	0.91741692	-0.51517854	-1.78841181
S	-2.30348710	0.59225872	1.68769684
S	-2.30365214	0.58696108	-1.68896860
C	3.36113586	1.16022573	-0.00084011
N	2.32765788	2.08560977	-0.00204131
C	2.88038283	3.28861739	-0.00218297
N	4.23010507	3.18871100	-0.00116717
C	4.55255418	1.84797644	-0.00032232
H	4.88210489	3.96222655	-0.00107076
C	2.82357981	-2.48009257	1.26065065
H	5.57479204	1.50401995	0.00056607
C	2.65346625	-0.95299152	-1.29611527
C	2.65364338	-0.95147985	1.29674443
N	-5.85322151	0.25971067	0.00001321
C	2.22105294	-3.10646729	0.00153953
H	2.38996962	-2.92084550	2.16319022
H	3.90190826	-2.69264216	1.28478399
H	3.90197480	-2.69401334	-1.28210330
H	2.39009012	-2.92337315	-2.16030908
H	1.13546694	-2.96282317	0.00141392
H	2.40014275	-4.18715678	0.00216942
H	2.35105972	4.22972257	-0.00297459
H	3.24879099	-0.55232854	2.12290322
H	3.24840367	-0.55469545	-2.12283902
C	-5.07890480	0.32134816	1.13122316
H	-5.51457379	0.28192067	2.11747021
C	-3.75569310	0.42663914	0.72416033
C	-3.75574706	0.42433122	-0.72479289
C	-5.07899899	0.31771643	-1.13142900
H	-5.51472698	0.27513767	-2.11751861
H	-6.85921397	0.15862113	0.00021630
H	0.76967293	1.83581526	-0.00187856
H	-0.08800952	1.87560381	-0.00152184
H	4.26199330	-0.68957891	0.00006192
N	-1.48126179	-2.00932526	0.00250298
H	-2.50044282	-1.96368080	0.00298469
H	-1.19292212	-2.53608580	-0.82048828
H	-1.19201763	-2.53462753	0.82610510

Name - TSPH2CH3\\SCF E(UB3LYP-D3BJ/BS1)=-2712.8561112\\G=-
 2712.570051\\H=-2712.486847\\SCF E(UB3LYP-D3BJ/BS2)= -2713.1773824\\
 ZeroPoint=0.342923

C	-2.80444563	2.54644058	-0.90581079
C	-3.32232587	0.27118983	0.05794477
Mo	0.47415597	-0.21694447	0.03346761
S	-1.04224344	0.11995252	1.87394367
S	-1.00116234	0.55669219	-1.68503996
S	2.15251112	-0.98877750	1.65664151
S	2.21366920	-0.61940792	-1.68565822
C	-3.51421721	-1.20358337	-0.13869670
N	-2.51623899	-2.16296051	-0.23561805
C	-3.10449497	-3.33806062	-0.40316929
N	-4.44650221	-3.18593666	-0.41893321
C	-4.72470879	-1.84512150	-0.25324652
H	-5.12422016	-3.92896540	-0.53148032
C	-2.86771289	2.21709392	1.59196804
H	-5.73466972	-1.46770368	-0.23052694
C	-2.71184834	1.02868140	-1.14143582
C	-2.75169496	0.69227308	1.43001361
N	5.74703733	-0.90152459	0.04713751
C	-2.21114758	2.97452082	0.43745125
H	-2.43855559	2.51897263	2.55182567
H	-3.93789688	2.46644140	1.62384758
H	-3.86981577	2.81625692	-0.92667664
H	-2.32379898	3.07711926	-1.73301444
H	-1.13487355	2.78211262	0.44528576
H	-2.34262347	4.05326740	0.57398628
H	-2.60314279	-4.28772204	-0.51317190
H	-3.37241026	0.21088949	2.19096172
H	-3.31653707	0.77486786	-2.01660184
C	4.94925354	-0.99739951	1.15814195
H	5.36619455	-1.11541527	2.14625667
C	3.63108025	-0.90636893	0.72998330
C	3.65904710	-0.74595617	-0.70710874
C	4.99228118	-0.74653385	-1.09062164
H	5.45015254	-0.64797256	-2.06256479
H	6.75741598	-0.92800294	0.06467491
H	-1.06810750	-1.99754489	-0.19205527
H	-0.15546003	-2.01458606	-0.18671878
H	-4.35020453	0.66164341	0.09234977
H	2.96812402	1.92741140	0.39708890
H	1.25772593	2.80405956	1.38520640
P	1.57084204	2.03779423	0.24471943
C	1.40476687	3.23716644	-1.13449139
H	0.35331065	3.50611271	-1.24829411
H	2.00114176	4.13255052	-0.94625559
H	1.74360789	2.75251290	-2.05238250

Name - TSPH3\\SCF E(UB3LYP-D3BJ/BS1)=-2673.5220534\\G=-
 2673.265263\\H=-2673.184395\\SCF E(UB3LYP-D3BJ/BS2)=-2673.8354587\\
 ZeroPoint=0.312621

C	2.86411548	2.42545599	1.26071639
C	3.28317241	0.28139010	-0.00004327
Mo	-0.52315743	-0.08248184	-0.00008628
S	0.98441651	0.42581843	-1.79203412
S	0.98450642	0.42498705	1.79203183
S	-2.25123225	-0.61713657	-1.68056040
S	-2.25096890	-0.61837519	1.68021789
C	3.43196105	-1.21170528	-0.00020737
N	2.40468350	-2.14444629	-0.00066806
C	2.96237886	-3.34547618	-0.00056861
N	4.31037465	-3.23670622	-0.00007844
C	4.62597548	-1.89426896	0.00014961
H	4.96657064	-4.00681281	0.00008075
C	2.86424730	2.42583844	-1.26012910
H	5.64635485	-1.54503694	0.00054196
C	2.71118432	0.89528404	1.29620393
C	2.71118896	0.89569090	-1.29609954
N	-5.81450955	-0.64924098	0.00010670
C	2.26161165	3.04811268	0.00035623
H	2.42309580	2.86221568	-2.16098449
H	3.94040989	2.64796377	-1.28861822
H	3.94025914	2.64764748	1.28941184
H	2.42282330	2.86151848	2.16165526
H	1.17717466	2.90253888	0.00026800
H	2.43572145	4.12942259	0.00053413
H	2.43663548	-4.28844741	-0.00083648
H	3.31002594	0.50402755	-2.12314414
H	3.31009487	0.50343030	2.12310502
C	-5.03886515	-0.63395697	-1.13175583
H	-5.47667348	-0.63532127	-2.11778653
C	-3.71221931	-0.61264344	-0.72342614
C	-3.71210298	-0.61318263	0.72332366
C	-5.03868537	-0.63480254	1.13185259
H	-5.47633316	-0.63688799	2.11795340
H	-6.82551644	-0.65687801	0.00018688
H	0.89108796	-1.92320928	-0.00068395
H	0.01185783	-1.93390142	-0.00078640
H	4.32172412	0.64419224	0.00001017
H	-2.94609239	2.22679380	0.00098349
H	-1.26874706	3.07283461	1.08437622
H	-1.26941181	3.07297933	-1.08330064
P	-1.53690765	2.21525373	0.00056118

Name - TSPy\\SCF E(UB3LYP-D3BJ/BS1)=-2578.6973592\\G=-2578.381331\\H=-
 2578.293567\\SCF E(UB3LYP-D3BJ/BS2)= -2579.0435681\\
 ZeroPoint=0.376252

C	2.89677443	2.22903301	1.25922780
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C	3.40735344	0.09749862	-0.00001776
Mo	-0.39835845	-0.27515968	-0.00005398
S	1.13042348	0.12315927	-1.81454399
S	1.13043097	0.12308453	1.81450394
S	-2.05469825	-1.01094940	-1.68015220
S	-2.05444434	-1.01132752	1.68002582
C	3.57461517	-1.39378861	-0.00002093
N	2.55125898	-2.33175600	-0.00008331
C	3.11751661	-3.52818811	-0.00004276
N	4.46613298	-3.41245492	0.00004167
C	4.77335073	-2.06781645	0.00005467
H	5.12688606	-4.17846130	0.00008940
C	2.89678777	2.22906001	-1.25922025
H	5.79163983	-1.71242791	0.00011913
C	2.82101296	0.69396443	1.29933569
C	2.82102086	0.69399258	-1.29936088
N	-5.35561540	-2.35179225	0.00006108
C	2.25983828	2.81868642	0.00000694
H	2.43568398	2.64310996	-2.16086850
H	3.96045675	2.50608692	-1.28580833
H	3.96044125	2.50606747	1.28583608
H	2.43565477	2.64305973	2.16087834
H	1.18685193	2.61563538	0.00000067
H	2.37869521	3.90783140	0.00001778
H	2.59905009	-4.47529823	-0.00007012
H	3.45076601	0.33508845	-2.11824693
H	3.45076824	0.33505125	2.11821052
C	-4.63734572	-2.05618156	-1.13170728
H	-5.04217888	-2.22237370	-2.11788120
C	-3.41190694	-1.54743663	-0.72238158
C	-3.41178929	-1.54760753	0.72235008
C	-4.63716145	-2.05645336	1.13177001
H	-5.04182675	-2.22286588	2.11797572
H	-6.29405844	-2.72804393	0.00009476
H	1.00703335	-2.07615279	-0.00012788
H	0.14007379	-2.11007072	-0.00019030
H	4.43854715	0.48097386	-0.00001432
C	-1.36773984	2.47765524	1.15973068
C	-1.36768388	2.47778593	-1.15956819
C	-1.76925447	3.80610909	1.19948965
H	-1.18865029	1.91505897	2.06609587
C	-1.76919051	3.80624514	-1.19919841
H	-1.18855319	1.91529210	-2.06598867
H	-1.91435414	4.29064515	2.15806719
H	-1.91423838	4.29088947	-2.15772907
N	-1.16683677	1.81966889	0.00004929
C	-1.97235347	4.48765336	0.00017910
H	-2.28266950	5.52721128	0.00022951

Name - TSPyNH2\\SCF E(UB3LYP-D3BJ/BS1)=-2634.0761417\\G=-
2633.745974\\H=-2633.654189\\SCF E(UB3LYP-D3BJ/BS2)=-2634.4327577
ZeroPoint=0.392663

C	2.64478355	2.44041240	1.25891302
C	3.42395892	0.39149352	0.00010315
Mo	-0.31531807	-0.44529555	0.00011315
S	1.16969000	0.11742697	-1.81797848
S	1.16958297	0.11742018	1.81806277
S	-1.83513624	-1.42857373	-1.68198895
S	-1.83604082	-1.42775147	1.68225817
C	3.77248485	-1.06749828	0.00003558
N	2.87262714	-2.12485408	0.00022110
C	3.57692652	-3.24616980	0.00006160
N	4.89964625	-2.96600594	-0.00021322
C	5.04239440	-1.59371707	-0.00022923
H	5.64828513	-3.64650159	-0.00038186
C	2.64474259	2.44050083	-1.25854708
H	6.01030571	-1.11815042	-0.00042260
C	2.76707001	0.90850409	1.30023506
C	2.76707472	0.90859649	-1.30000004
N	-4.73976704	-3.49921640	-0.00022424
C	1.93576628	2.94230688	0.00021276
H	2.13418198	2.79104590	-2.16052044
H	3.66355241	2.85342017	-1.28459108
H	3.66361104	2.85328593	1.28494374
H	2.13427950	2.79091413	2.16093609
H	0.89928021	2.59948458	0.00022315
H	1.91149379	4.03775169	0.00025257
H	3.17469170	-4.24801507	0.00012847
H	3.44122208	0.63585951	-2.11689402
H	3.44114468	0.63564514	2.11714667
C	-4.10594384	-3.04638339	-1.13141097
H	-4.45994932	-3.30230957	-2.11806444
C	-3.03061546	-2.27006696	-0.72138160
C	-3.03103907	-2.26968929	0.72138757
C	-4.10661711	-3.04577787	1.13113799
H	-4.46123366	-3.30121627	2.11769817
H	-5.56660450	-4.08059934	-0.00032270
H	1.38442852	-2.06158368	0.00030052
H	0.48962303	-2.17225484	0.00034988
H	4.40056552	0.89789548	0.00013574
C	-1.57570812	2.17352789	1.15656533
C	-1.57528067	2.17350801	-1.15690945
C	-2.08406209	3.45136370	1.20511517
H	-1.35083322	1.63515692	2.06810298
C	-2.08364386	3.45133499	-1.20566394
H	-1.35002582	1.63512928	-2.06834891
H	-2.27160779	3.92470606	2.16275639
H	-2.27085832	3.92465439	-2.16338136
N	-1.31139297	1.51945358	-0.00011791

C	-2.35340870	4.14208486	-0.00033002
N	-2.86269585	5.39157394	-0.00042762
H	-2.94683248	5.90454270	-0.86558726
H	-2.94711627	5.90455720	0.86469561

3. Optimized geometrical coordinates for Mo-type III complexes including their thermochemical data and single point energies.

(R₁123R₂ = Cyclohexyl group, R₃45R₄ = Imidazole ring: L₁ = CO)

Name - MoIIICl\\SCF E(UB3LYP-D3BJ/BS1)=-2902.1395419\\G=-

2901.924074\\H=-2901.844561\\SCF E(UB3LYP-D3BJ/BS2)=-2902.491585

\\ZeroPoint=0.270335

C	4.27869085	-0.78902475	-1.25866777
C	2.96199011	0.96775754	0.00000226
Mo	-0.04576008	-0.57267362	-0.00000993
S	1.53994363	-0.84529838	1.77254033
S	1.53995787	-0.84530440	-1.77254046
S	-1.85060191	-0.37001008	1.66494840
S	-1.85061269	-0.36998743	-1.66494679
C	1.84619650	1.95920478	-0.00000044
N	0.50387445	1.57990909	-0.00000566
C	-0.20385471	2.70067647	-0.00000494
N	0.60681426	3.77998863	0.00002689
C	1.91199089	3.32568790	0.00000268
H	0.30463353	4.74693953	0.00004468
C	4.27868169	-0.78902561	1.25868149
H	2.75115927	4.00235373	0.00000886
C	3.05402604	0.13718977	-1.30342622
C	3.05401747	0.13719008	1.30343198
C	-0.41071545	-2.60884386	-0.00001120
N	-5.41265901	-0.55012975	0.00001023
C	4.30224060	-1.65885291	0.00000672
H	4.30843287	-1.40449971	2.16264929
H	5.17358138	-0.15157651	1.27391952
H	5.17359014	-0.15157496	-1.27389854
H	4.30844919	-1.40449802	-2.16263589
H	3.43505050	-2.32941414	0.00000325
H	5.19854905	-2.28782389	0.00000989
H	3.88234975	1.56722006	0.00000446
H	3.16988689	0.84725593	2.12698522
H	3.16989785	0.84725469	-2.12697991
O	-0.62591864	-3.73691489	-0.00000627
C	-4.63583248	-0.52270830	1.13137869
H	-5.07247151	-0.54335195	2.11778460
C	-3.31094377	-0.46757532	0.72114012
C	-3.31094826	-0.46756392	-0.72113064

C	-4.63583948	-0.52268727	-1.13136247
H	-5.07248454	-0.54331301	-2.11776606
H	-6.42229904	-0.60471252	0.00001284
Cl	-1.90602653	2.83353136	-0.00000944

Name - MoIIIme\\SCF E(UB3LYP-D3BJ/BS1)=-2481.8862587\\G=-

2481.632426\\H=-2481.554335\\SCF E(UB3LYP-D3BJ/BS2)=-2482.2134358

\\ZeroPoint=0.307602

C	4.17168719	-0.91617614	-1.25823335
C	2.95173252	0.91253400	0.00045375
Mo	-0.13343147	-0.44268727	-0.00026606
S	1.43398584	-0.82022811	1.77228564
S	1.43433017	-0.81924436	-1.77267250
S	-1.93315437	-0.17652406	1.66876449
S	-1.93336008	-0.17451179	-1.66845997
C	1.88681473	1.95934320	0.00059846
N	0.52749673	1.65535525	0.00030730
C	-0.14933665	2.80941488	0.00036010
N	0.73809677	3.83108030	0.00075650
C	2.02156861	3.31983959	0.00088613
H	0.48419245	4.81072865	0.00088854
C	4.17144148	-0.91690858	1.25831196
H	2.89440267	3.95239704	0.00122107
C	3.00069643	0.07686232	-1.30227521
C	3.00045150	0.07611450	1.30270321
C	-0.59097217	-2.47645192	-0.00098759
N	-5.50080190	-0.23650358	0.00028454
C	4.14565275	-1.78681386	-0.00021604
H	4.16768864	-1.53300900	2.16244552
H	5.10081986	-0.33068932	1.27278671
H	5.10106253	-0.32994014	-1.27218333
H	4.16811760	-1.53175081	-2.16272524
H	3.24083198	-2.40585824	-0.00048424
H	5.00416891	-2.46654433	-0.00032937
H	3.90429683	1.45958042	0.00069339
H	3.15528546	0.77813804	2.12682267
H	3.15567154	0.77936016	-2.12596424
O	-0.85241405	-3.59380657	-0.00139073
C	-4.72293377	-0.23607398	1.13146991
H	-5.15971130	-0.24212147	2.11803599
C	-3.39721219	-0.22483916	0.72111870
C	-3.39728528	-0.22388026	-0.72071887
C	-4.72305109	-0.23456693	-1.13096585
H	-5.15991769	-0.23935314	-2.11749943
H	-6.51162755	-0.25416989	0.00032319
C	-1.62076565	3.00343930	-0.00045245
H	-2.06830354	2.54087765	-0.88348089
H	-2.07019093	2.53370281	0.87776650
H	-1.85664954	4.06955680	0.00354574

Name - MoIIINMe\\SCF E(UB3LYP-D3BJ/BS1)=-2576.5434451\\G=-
 2576.247497\\H=-2576.162408\\SCF E(UB3LYP-D3BJ/BS2)=-2576.8952871
 \\ZeroPoint=0.353455

C	-4.21834674	-1.17266407	1.30351990
C	-3.04436850	0.77438594	0.19073256
Mo	0.03111153	-0.54167743	-0.11622074
S	-1.62263815	-0.72143046	-1.83174896
S	-1.46420027	-1.12065763	1.70463984
S	1.93675073	-0.07064428	-1.57042500
S	1.74892007	-1.03373909	1.61743046
C	-1.98571423	1.83081241	0.21330090
N	-0.60223778	1.58363216	0.15006293
C	0.00015751	2.79020532	0.08904421
N	-0.94631282	3.76569885	0.11085710
C	-2.19719509	3.17444337	0.18088538
H	-0.75764341	4.75782739	0.13565222
C	-4.33149886	-0.92375794	-1.19385199
H	-3.10559684	3.75451570	0.18829086
C	-3.04203395	-0.18905398	1.39901610
C	-3.17179973	0.08175327	-1.18753133
C	0.28215994	-2.56867821	-0.47852118
N	5.35060287	-1.20851955	0.02790332
C	-4.24152263	-1.91604358	-0.03342350
H	-4.36479768	-1.44257775	-2.15660239
H	-5.26453882	-0.35000956	-1.10549460
H	-5.14682830	-0.59424523	1.41022192
H	-4.17946994	-1.87371644	2.14270212
H	-3.33062597	-2.51849482	-0.13394540
H	-5.09227725	-2.60475445	-0.06441505
H	-3.99076283	1.32308420	0.29339399
H	-3.37252257	0.86877432	-1.92045364
H	-3.16266246	0.42753901	2.29425957
O	0.40389075	-3.69130465	-0.68409686
C	4.65194143	-0.72312398	-1.04919902
H	5.13963811	-0.49770313	-1.98485430
C	3.32185583	-0.62124196	-0.66496800
C	3.23674227	-1.06759406	0.70311330
C	4.51654992	-1.43218592	1.09556382
H	4.88881057	-1.81593030	2.03271334
H	6.34470234	-1.39345247	0.02943701
N	1.33808744	3.07017542	-0.05541521
C	1.67906206	4.46716300	-0.32250643
H	1.51130301	5.11715448	0.54960624
H	2.73852106	4.51363981	-0.58043732
H	1.10466884	4.84665439	-1.17066112
C	2.27458884	2.43199336	0.87345960
H	3.25389453	2.34366982	0.39913632
H	2.37648568	3.02749681	1.79241321
H	1.92612705	1.43957468	1.13907866

Name - MoIIINO2\\SCF E(UB3LYP-D3BJ/BS1)=-2647.0395895\\G=-
 2646.814519\\H=-2646.731535\\SCF E(UB3LYP-D3BJ/BS2)=-2647.4270648
 \\ZeroPoint=0.282082

C	-4.23732536	-1.03573414	1.25543789
C	-3.03309644	0.80460618	0.00011302
Mo	0.06167783	-0.56460741	-0.00012450
S	-1.50738286	-0.87696784	-1.80160385
S	-1.50716600	-0.87701284	1.80166579
S	1.86136153	-0.50169307	-1.67106633
S	1.86095116	-0.50206171	1.67096362
C	-1.97216463	1.85606985	0.00001087
N	-0.61560549	1.60115270	-0.00008931
C	-0.02467546	2.79723106	-0.00005065
N	-0.93362093	3.79738722	0.00004878
C	-2.16730213	3.22830459	0.00005280
H	-0.70005211	4.78523290	0.00005138
C	-4.23749210	-1.03577528	-1.25500054
H	-3.07381247	3.81224568	-0.00005158
C	-3.08263257	-0.02441336	1.30728052
C	-3.08285492	-0.02443492	-1.30701582
C	0.28723553	-2.61173957	-0.00054668
N	5.39372769	-0.93217701	0.00043486
C	-4.18628412	-1.90813073	0.00022312
H	-4.22805251	-1.64673096	-2.16226369
H	-5.17700079	-0.46601913	-1.25995320
H	-5.17682710	-0.46597146	1.26047867
H	-4.22777854	-1.64666907	2.16271283
H	-3.26414948	-2.50183142	0.00017803
H	-5.02575506	-2.61092461	0.00028640
H	-3.98168162	1.35713553	0.00019130
H	-3.26217348	0.68191983	-2.12236492
H	-3.26186965	0.68199280	2.12260457
O	0.38723195	-3.75481205	-0.00088027
C	4.62360635	-0.84707539	-1.13143901
H	5.05833877	-0.90052405	-2.11734942
C	3.30598896	-0.68976943	-0.72225943
C	3.30576855	-0.68997715	0.72252064
C	4.62331851	-0.84721634	1.13205647
H	5.05774426	-0.90078049	2.11809800
H	6.39767785	-1.05585817	0.00056906
N	1.36390707	3.10261748	-0.00004900
O	1.65591115	4.31030552	-0.00045652
O	2.17676969	2.18194731	0.00033397

Name - MoIIItBu\\SCF E(UB3LYP-D3BJ/BS1)=-2599.8407693\\G=-
 2599.506605\\H=-2599.419059\\SCF E(UB3LYP-D3BJ/BS2)=-2600.1931753
 \\ZeroPoint=0.392764

C	4.27803116	-1.23864671	-1.20909662
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C	3.08624842	0.71413741	-0.10750222
Mo	0.00058106	-0.58906222	0.04538512
S	1.57023939	-0.78100293	1.85370334
S	1.54890345	-1.06060013	-1.77419677
S	-1.89558673	-0.52735980	1.63213347
S	-1.69613751	-0.99016934	-1.67771633
C	2.03513441	1.77804148	-0.18364898
N	0.64741977	1.58315949	-0.09401677
C	0.07289828	2.80110397	-0.15691577
N	1.05005026	3.73007421	-0.30354776
C	2.27800507	3.11413719	-0.31780654
H	0.89505660	4.72552272	-0.37882723
C	4.29029840	-1.03180256	1.29043994
H	3.19986968	3.66358816	-0.42016940
C	3.14050770	-0.21569205	-1.34073461
C	3.15035473	-0.00407647	1.26168364
C	-0.06581371	-2.64868259	0.25888494
N	-5.23735389	-1.66912441	-0.11631745
C	4.21804590	-2.00497551	0.11296550
H	4.28060608	-1.56409766	2.24620862
H	5.23798236	-0.47765997	1.24034505
H	5.22809399	-0.68834942	-1.26061690
H	4.25696590	-1.92160467	-2.06360355
H	3.28540408	-2.57985142	0.16526441
H	5.04442380	-2.72125062	0.16854479
H	4.03725102	1.26242025	-0.15215966
H	3.34370050	0.76837399	2.01211254
H	3.33774917	0.42539872	-2.20497309
O	-0.06505314	-3.78938053	0.38058019
C	-4.55905017	-1.30733558	1.02326650
H	-5.04759450	-1.27476142	1.98448179
C	-3.24998018	-1.03487962	0.65538888
C	-3.15681508	-1.25086984	-0.77001925
C	-4.41358780	-1.65121420	-1.20927053
H	-4.77053884	-1.91037617	-2.19384523
H	-6.21602416	-1.92330340	-0.14236360
C	-1.37268713	3.22617237	0.02891528
C	-1.70255706	3.16258092	1.53658083
H	-1.60392589	2.14451255	1.91741134
H	-1.03750953	3.81846395	2.10735068
H	-2.73407661	3.49214377	1.69944250
C	-1.55970585	4.67954119	-0.45188612
H	-0.99065990	5.39618710	0.14957486
H	-1.27966132	4.79748607	-1.50349614
H	-2.61484012	4.94682344	-0.35187924
C	-2.34153740	2.33651928	-0.76165374
H	-2.08605836	2.31976722	-1.82512355
H	-2.34057934	1.31564723	-0.39202211
H	-3.35586235	2.73357521	-0.65562537

Name - MoIIII1Cl\\SCF E(UB3LYP-D3BJ/BS1)=-2903.2771924\\G=-
 2903.051478\\H=-2902.965990\\SCF E(UB3LYP-D3BJ/BS2)=-2903.6315316
 \\ZeroPoint=0.284788

C	-2.39192674	-2.99100555	1.28470269
C	-3.04188683	-0.91462545	0.00683740
Mo	0.75135967	-0.31461886	0.00151030
S	-0.75397554	-0.78021043	-1.78802786
S	-0.74344133	-0.78016754	1.79630179
S	2.44354813	0.34774043	-1.68064953
S	2.45691610	0.34706949	1.67185924
C	-3.35829216	0.55074175	-0.00910221
N	-2.42613047	1.57959141	0.06055272
C	-3.12678850	2.68586110	0.00748188
N	-4.46049005	2.46046198	-0.09226700
C	-4.62099742	1.08816194	-0.10268738
H	-5.19011404	3.15991003	-0.14534838
C	-2.38219156	-3.00699176	-1.24575000
H	-5.59542096	0.63084478	-0.17342983
C	-2.40593472	-1.45249797	1.30475676
C	-2.40523555	-1.46914922	-1.28508330
C	1.52198479	-2.17987033	-0.00418727
N	5.83691819	1.39030601	-0.01893418
C	-1.74150420	-3.56664320	0.02552943
H	-1.88139639	-3.39471805	-2.13750445
H	-3.42809720	-3.33967812	-1.29486728
H	-3.43972214	-3.31834676	1.32866919
H	-1.90022036	-3.37049710	2.18501399
H	-0.67122412	-3.35017730	0.02890359
H	-1.83552628	-4.65779956	0.03176035
H	-3.04166134	-1.15138609	-2.11537138
H	-3.03641989	-1.11906623	2.13347072
O	2.00182456	-3.22447155	-0.00831444
C	5.09846709	1.16303282	-1.14903614
H	5.51534718	1.29082292	-2.13548923
C	3.82894312	0.77483589	-0.73631471
C	3.83509772	0.77435176	0.71605910
C	5.10783567	1.16235324	1.11774759
H	5.53352214	1.28968633	2.10048428
H	6.80413112	1.68942020	-0.02297341
H	-0.38035969	1.61492930	0.01993569
H	0.37090254	1.78492199	-0.00452125
H	-4.03192049	-1.39486915	0.00908919
Cl	-2.46881110	4.28064769	0.05719640

Name - MoIIII1Me\\SCF E(UB3LYP-D3BJ/BS1)=-2483.0169177\\G=-
 2482.754932\\H=-2482.668002\\SCF E(UB3LYP-D3BJ/BS2)=-2483.346952
 \\ZeroPoint=0.321926

C	-2.72596539	-2.63607665	1.26640887
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C	-3.17178807	-0.49425194	0.00090493
Mo	0.64893497	-0.24779890	-0.00036510
S	-0.87928871	-0.59692743	-1.79602690
S	-0.87836231	-0.59423162	1.79666762
S	2.39301728	0.28271813	-1.67719688
S	2.39311112	0.28452869	1.67581958
C	-3.33911377	0.99673501	-0.00033945
N	-2.31442712	1.93179148	0.00004943
C	-2.88670909	3.12792264	-0.00507176
N	-4.24421291	3.00201118	-0.00904171
C	-4.54578085	1.65530322	-0.00564500
H	-4.90829167	3.76469320	-0.01530880
C	-2.72654258	-2.63805682	-1.26158599
H	-5.56242734	1.29405542	-0.01136181
C	-2.59465402	-1.10353036	1.29566322
C	-2.59530536	-1.10556438	-1.29325901
C	1.25903518	-2.17720308	0.00087331
N	5.83952963	1.11101634	-0.00116864
C	-2.13296883	-3.26138231	0.00276414
H	-2.27345466	-3.06995336	-2.15867690
H	-3.80057940	-2.86614843	-1.30269365
H	-3.79999062	-2.86407232	1.30834277
H	-2.27248896	-3.06659917	2.16396152
H	-1.04764483	-3.13734539	0.00242622
H	-2.32202521	-4.34019172	0.00364627
H	-3.19467978	-0.72007069	-2.12263403
H	-3.19353810	-0.71677553	2.12481312
O	1.64411870	-3.26037433	0.00155476
C	5.09248545	0.92934542	-1.13439532
H	5.52064107	1.03044983	-2.11911311
C	3.79960617	0.62167863	-0.72691777
C	3.79963726	0.62244093	0.72513145
C	5.09253625	0.93053823	1.13225691
H	5.52070584	1.03268169	2.11686307
H	6.82300565	1.35118694	-0.00130909
H	-0.38331297	1.73954573	-0.00080937
H	0.39343507	1.82743324	-0.00218875
H	-4.20358757	-0.87700768	0.00142175
C	-2.18113699	4.43928128	0.01137559
H	-2.31029841	4.94900874	0.97289517
H	-1.11371790	4.28117509	-0.15310162
H	-2.56184588	5.10426688	-0.77034975

Name - MoIII1NMe\\SCF E(UB3LYP-D3BJ/BS1)=-2577.6818541\\G=-
 2577.375314\\H=-2577.284047\\SCF E(UB3LYP-D3BJ/BS2)=-2578.0368321
 \\ZeroPoint=0.368630

C	-2.10962446	-3.31263315	1.26680057
C	-2.86112355	-1.27600260	-0.03220931
Mo	0.86341535	-0.45037571	0.00512325
S	-0.54953911	-1.07859706	-1.80474043

S	-0.61318741	-0.99642028	1.79689504
S	2.51058538	0.35039014	-1.66379717
S	2.45577103	0.42387973	1.68750528
C	-3.27797099	0.16659528	-0.04261975
N	-2.44809157	1.27443166	-0.22091909
C	-3.23992616	2.34118316	-0.15271068
N	-4.53496972	1.97412592	0.08008613
C	-4.56696676	0.58779666	0.14366199
H	-5.33023277	2.59083050	0.16164525
C	-2.09572690	-3.34360356	-1.26107372
H	-5.48380583	0.04749272	0.32007691
C	-2.21589954	-1.77778051	1.27779726
C	-2.18671175	-1.80800404	-1.31210865
N	5.70052344	1.87405957	0.03393357
C	-1.42290615	-3.85734218	0.01315832
H	-1.58020474	-3.71614580	-2.15104306
H	-3.12481247	-3.72621032	-1.30219452
H	-3.13632049	-3.70173997	1.30833279
H	-1.60058319	-3.65773278	2.17144742
H	-0.36717488	-3.57562609	0.01476946
H	-1.45131042	-4.95220805	0.02674156
H	-2.82395489	-1.52180198	-2.15339363
H	-2.88383159	-1.48013890	2.09072725
C	5.02218872	1.52542234	-1.10399250
H	5.43936447	1.68671450	-2.08540739
C	3.80802809	0.97915920	-0.70527442
C	3.78360405	1.01134906	0.74624529
C	4.98448026	1.57565662	1.16185478
H	5.36772684	1.78049462	2.14897806
H	6.61962961	2.29857747	0.03997534
H	-0.49625911	1.27490709	-0.08886070
H	0.24887612	1.50179396	-0.02753322
H	-3.81925874	-1.81774263	-0.03440030
N	-2.86114270	3.65856517	-0.36017540
C	-1.41764021	3.89019265	-0.31389808
H	-1.22909169	4.93603645	-0.56241915
H	-0.98869492	3.68018546	0.67648734
H	-0.91427514	3.26354259	-1.05019933
C	-3.63348228	4.65852945	0.38419470
H	-3.52568322	4.54703200	1.47270849
H	-3.28258331	5.65103738	0.09777308
H	-4.69364635	4.60175917	0.12737927
C	1.79129787	-2.25489535	0.06450280
O	2.34633077	-3.26066652	0.09912267

Name - MoIII1NO2\\SCF E(UB3LYP-D3BJ/BS1)=-2648.1870675\\G=-
2647.948710\\H=-2647.863556\\SCF E(UB3LYP-D3BJ/BS2)=-2648.5780947
\\ZeroPoint=0.296748

C	-2.07110852	-3.27007893	1.26738748
C	-2.89295719	-1.25286624	0.00048167

Mo	0.85055112	-0.35693503	0.00003636
S	-0.62003025	-0.92026330	-1.79096631
S	-0.61934470	-0.91998638	1.79152775
S	2.49503385	0.42629582	-1.67682007
S	2.49591949	0.42619827	1.67605554
C	-3.32410344	0.18191172	-0.00055709
N	-2.49669856	1.26876397	0.00294391
C	-3.30097190	2.31755448	0.00004749
N	-4.61618340	1.97322146	-0.00532961
C	-4.65201006	0.61461946	-0.00564635
H	-5.39894919	2.61791441	-0.00826530
C	-2.07052042	-3.27111538	-1.26475163
H	-5.57995284	0.06393383	-0.00931998
C	-2.21281564	-1.73835857	1.29780974
C	-2.21276955	-1.73947708	-1.29647065
C	1.76085344	-2.16003567	-0.00038517
N	5.78580565	1.73895206	-0.00124427
C	-1.38406910	-3.78560369	0.00168880
H	-1.54298930	-3.61283603	-2.15971527
H	-3.08739601	-3.68369608	-1.31386399
H	-3.08812184	-3.68234239	1.31628597
H	-1.54411578	-3.61126913	2.16287058
H	-0.33377542	-3.48824524	0.00185244
H	-1.39393010	-4.88070294	0.00211350
H	-2.87187439	-1.46792326	-2.12536696
H	-2.87164595	-1.46575429	2.12657955
O	2.32044494	-3.16376905	-0.00066893
C	5.07281523	1.45321259	-1.13454573
H	5.48217348	1.61452407	-2.11921499
C	3.83720115	0.96380394	-0.72712706
C	3.83759730	0.96375145	0.72566986
C	5.07342768	1.45313288	1.13243781
H	5.48333439	1.61438473	2.11688846
H	6.72510421	2.11701650	-0.00148585
H	-0.38868549	1.47972316	0.00114792
H	0.33976793	1.71651472	-0.00030993
H	-3.83850934	-1.81395720	0.00068036
N	-2.88847825	3.67167779	0.00221700
O	-3.78047217	4.53546331	-0.00099993
O	-1.67664368	3.91918864	0.00723157

Name - MoIIII1tBu\\SCF E(UB3LYP-D3BJ/BS1)=-2600.9827776\\G=-

2600.637409\\H=-2600.544638\\SCF E(UB3LYP-D3BJ/BS2)=-2601.3378002

\\ZeroPoint=0.407729

C	-1.80085429	-3.60850708	1.26325640
C	-2.71258887	-1.61811010	-0.00009138
Mo	0.94516881	-0.50916015	0.00000775
S	-0.45687323	-1.20657992	-1.80021598
S	-0.45702846	-1.20657510	1.80014601
S	2.50159163	0.43917441	-1.67676948

S	2.50147183	0.43918356	1.67686626
C	-3.20031996	-0.19948609	0.00005367
N	-2.40260887	0.93240508	-0.00057019
C	-3.21418199	1.98335660	-0.00001738
N	-4.51234289	1.56618121	0.00090106
C	-4.52036141	0.18597968	0.00092482
H	-5.32740776	2.16398093	0.00136192
C	-1.80090489	-3.60838783	-1.26359642
H	-5.43703471	-0.38296745	0.00155225
C	-2.01567061	-2.08556989	1.29476005
C	-2.01564508	-2.08543022	-1.29495698
C	1.99520916	-2.24748153	0.00004432
N	5.58988005	2.17825512	0.00016700
C	-1.08131667	-4.08303118	-0.00020609
H	-1.26393237	-3.92744315	-2.16162789
H	-2.79660494	-4.07121715	-1.30326592
H	-2.79653524	-4.07137743	1.30293640
H	-1.26382922	-3.92761661	2.16123767
H	-0.05176883	-3.71733032	-0.00021494
H	-1.02248301	-5.17671833	-0.00025690
H	-2.68754573	-1.84384342	-2.12311981
H	-2.68763604	-1.84410991	2.12290591
O	2.62151764	-3.21118641	0.00006669
C	4.92056849	1.80036747	-1.13320404
H	5.30493583	2.01492252	-2.11782433
C	3.76070097	1.15130974	-0.72596878
C	3.76064431	1.15131487	0.72615771
C	4.92048283	1.80037754	1.13348280
H	5.30476739	2.01493949	2.11813392
H	6.47291871	2.67356676	0.00019929
H	-0.53565680	1.13264285	-0.00016025
H	0.20590443	1.39916290	0.00008026
H	-3.63555851	-2.21733031	-0.00012922
C	-2.76866521	3.42755913	-0.00025254
C	-1.91740646	3.68729508	1.25972645
H	-2.49952897	3.50257056	2.16843651
H	-1.03635673	3.04037849	1.28030861
H	-1.57973548	4.72886900	1.27401834
C	-3.98030409	4.37246574	-0.00030233
H	-3.63463241	5.41006959	-0.00042552
H	-4.60377887	4.22776722	-0.88906398
H	-4.60369836	4.22798092	0.88854978
C	-1.91755013	3.68693188	-1.26039478
H	-1.03638052	3.04017810	-1.28076808
H	-2.49968683	3.50172260	-2.16899605
H	-1.58006924	4.72855989	-1.27513406

Name - TSC1\\SCF E(UB3LYP-D3BJ/BS1)=-2903.2704949\\G=-2903.045319
 \\H=-2902.961418\\SCF E(UB3LYP-D3BJ/BS2)=-2903.622859 \\ZeroPoint=
 0.283450

C	-2.57613975	-2.93279689	1.26055955
C	-3.08695892	-0.80676205	0.00003439
Mo	0.68596301	-0.29606898	0.00000999
S	-0.80542950	-0.82573337	-1.81217557
S	-0.80538337	-0.82587803	1.81221899
S	2.39340185	0.32618418	-1.67529977
S	2.39352967	0.32567171	1.67531744
C	-3.27174830	0.68037901	0.00002395
N	-2.25611366	1.63036464	0.00017650
C	-2.83073444	2.81715094	0.00005770
N	-4.17274533	2.70248158	-0.00015294
C	-4.46833527	1.35192855	-0.00017356
H	-4.83700159	3.46793590	-0.00027771
C	-2.57609417	-2.93276517	-1.26055398
H	-5.48566489	0.99480662	-0.00032791
C	-2.49651236	-1.39755927	1.29925595
C	-2.49651518	-1.39752392	-1.29920500
C	1.45446522	-2.23632771	-0.00024177
N	5.85344011	1.12048273	0.00001986
C	-1.94862090	-3.52958340	0.00000682
H	-2.11553828	-3.34729533	-2.16177528
H	-3.64121183	-3.20160983	-1.29039480
H	-3.64126513	-3.20161799	1.29034679
H	-2.11563002	-3.34736524	2.16178677
H	-0.87001924	-3.35092155	0.00003328
H	-2.08606363	-4.61611995	-0.00001207
H	-3.12001912	-1.03719799	-2.12207739
H	-3.11999310	-1.03723246	2.12214536
O	1.91052618	-3.28861778	-0.00041337
C	5.10318401	0.94412143	-1.13292903
H	5.53172638	1.04154565	-2.11795240
C	3.80900952	0.64468850	-0.72489613
C	3.80906260	0.64445618	0.72491239
C	5.10326988	0.94375532	1.13295747
H	5.53187460	1.04086517	2.11798464
H	6.83882239	1.35117454	0.00002187
H	-0.89917183	1.45979582	0.00017782
H	0.05038271	1.47456443	0.00012160
H	-4.11596801	-1.19428007	0.00002865
Cl	-1.99728668	4.31238872	0.00017202

Name - TSMe\\SCF E(UB3LYP-D3BJ/BS1)=-2483.0156879\\G=-2482.754707\\H=-2482.669409\\SCF E(UB3LYP-D3BJ/BS2)=-2483.3443714\\ZeroPoint= 0.319972

C	-2.82246132	-2.60061994	1.25582669
C	-3.18035073	-0.43816587	-0.00207038
Mo	0.62048742	-0.23655756	0.00004761
S	-0.90123270	-0.62958446	-1.81016518
S	-0.90388815	-0.63100554	1.80791040
S	2.36711281	0.27877322	-1.67456225
S	2.36391597	0.28048131	1.67728509
C	-3.27053920	1.05889004	0.00150282

N	-2.20341579	1.94707169	-0.01045704
C	-2.69895390	3.17932276	0.00415233
N	-4.05488196	3.11869322	0.02556488
C	-4.43193060	1.79011870	0.02316397
H	-4.67588508	3.91741677	0.04194028
C	-2.82357291	-2.59624336	-1.26648448
H	-5.46664276	1.48646932	0.04245334
C	-2.63371433	-1.07469162	1.29414880
C	-2.63291629	-1.07040468	-1.29980475
C	1.23310621	-2.20556937	0.00139514
N	5.84163390	0.98965746	0.00431542
C	-2.24187347	-3.23940045	-0.00669905
H	-2.39416735	-3.04279859	-2.16795017
H	-3.90546715	-2.78632926	-1.29753722
H	-3.90414181	-2.79184375	1.28746933
H	-2.39168496	-3.04971482	2.15538137
H	-1.15324513	-3.13895848	-0.00716928
H	-2.45700418	-4.31330858	-0.00839260
H	-3.22352664	-0.66244452	-2.12482473
H	-3.22617584	-0.67023314	2.11954313
O	1.60751509	-3.29082555	0.00228962
C	5.08892845	0.83179063	-1.12938357
H	5.52075336	0.91869105	-2.11391733
C	3.78683374	0.56564202	-0.72271679
C	3.78543426	0.56647317	0.72786262
C	5.08673377	0.83309656	1.13674382
H	5.51666255	0.92108066	2.12201205
H	6.83223620	1.19730204	0.00515927
H	-0.70391245	1.67403562	-0.00700977
H	0.17950532	1.64979787	-0.00097994
H	-4.23114842	-0.76348654	-0.00281260
C	-1.91295991	4.44157294	-0.03109016
H	-2.33340420	5.18235419	0.65466216
H	-0.87917866	4.24079970	0.25603979
H	-1.91262749	4.87573401	-1.03711723

Name - TSNMe\\SCF E(UB3LYP-D3BJ/BS1)=-2577.6807481\\G=-

2577.375522\\H=-2577.285889\\SCF E(UB3LYP-D3BJ/BS2)=-2578.0342044

\\ZeroPoint=0.366222

C	-2.26943219	-3.25294507	1.28961539
C	-2.90511536	-1.19022204	-0.02990299
Mo	0.80948632	-0.46338971	0.00371425
S	-0.59700405	-1.13106134	-1.81411382
S	-0.65636552	-1.02023083	1.81397123
S	2.46779796	0.28766586	-1.67160442
S	2.41390714	0.40053144	1.67653931
C	-3.22563983	0.27605982	-0.05876498
N	-2.32060109	1.33573704	-0.18214411
C	-3.03688910	2.46241432	-0.15292680
N	-4.35872423	2.17137612	-0.00122877

C	-4.48643851	0.78921303	0.05183784
H	-5.11535992	2.83845331	0.04364445
C	-2.24773205	-3.31202893	-1.23157895
H	-5.44601506	0.31145495	0.16899582
C	-2.29594050	-1.71488177	1.28917776
C	-2.26320452	-1.77517748	-1.30522324
N	5.72149511	1.69571733	0.00980427
C	-1.59420821	-3.83713559	0.04777763
H	-1.75476007	-3.71993607	-2.11874570
H	-3.29370706	-3.64746724	-1.26202032
H	-3.31420219	-3.59223857	1.31969169
H	-1.78923982	-3.61471342	2.20342148
H	-0.52913875	-3.58898361	0.05061693
H	-1.66060284	-4.93013007	0.07304250
H	-2.89330684	-1.47150471	-2.14586497
H	-2.95473001	-1.37723832	2.09403619
C	5.02873665	1.36172970	-1.12398520
H	5.45167578	1.49470454	-2.10725056
C	3.79366189	0.86937636	-0.71915799
C	3.77024916	0.91849319	0.73031761
C	4.99226624	1.43838078	1.14059801
H	5.38355209	1.63792616	2.12571087
H	6.65656073	2.08308481	0.01176543
H	-0.77839479	1.21497359	-0.11182150
H	0.08459252	1.30705487	-0.05916074
H	-3.89880551	-1.66288895	-0.02996927
N	-2.55790154	3.74352139	-0.32007971
C	-1.10956544	3.89197518	-0.16960554
H	-0.84911711	4.93158010	-0.37200431
H	-0.76330493	3.62949288	0.83971643
H	-0.58944122	3.26178024	-0.89191836
C	-3.34005393	4.80501852	0.32292378
H	-3.36335345	4.70267454	1.41657969
H	-2.88999794	5.76526738	0.06931355
H	-4.36516364	4.81546123	-0.05455181
C	1.72262317	-2.31348626	0.08050793
O	2.25383540	-3.33026096	0.12374671

Name - TSNO2\\SCF E(UB3LYP-D3BJ/BS1)=-2648.1741405\\G=-

2647.939079\\H=-2647.851888\\SCF E(UB3LYP-D3BJ/BS2)=-2648.5623495

\\ZeroPoint=0.295310

C	-2.32466401	-3.20357214	1.26012841
C	-2.96435230	-1.11651113	0.00008888
Mo	0.75972162	-0.35588447	-0.00000081
S	-0.69604032	-0.98303421	-1.81896653
S	-0.69597603	-0.98285339	1.81905223
S	2.42017751	0.37406438	-1.67407969
S	2.42018546	0.37466284	1.67387026
C	-3.22958762	0.35580151	0.00004286
N	-2.29921760	1.36485279	-0.00000589

C	-2.96588357	2.51428113	-0.00000247
N	-4.29456992	2.29788961	0.00004455
C	-4.48610280	0.95016442	0.00007400
H	-5.00326466	3.02609513	0.00006360
C	-2.32473045	-3.20368363	-1.25978940
H	-5.47051756	0.50966882	0.00011443
C	-2.34074169	-1.66634634	1.30357420
C	-2.34079447	-1.66646182	-1.30337250
C	1.65658516	-2.26510722	0.00023336
N	5.81287063	1.42379582	-0.00032373
C	-1.65782246	-3.75689138	0.00017625
H	-1.84069212	-3.58830935	-2.16172936
H	-3.37063516	-3.53943144	-1.28687512
H	-3.37056512	-3.53932343	1.28730069
H	-1.84057540	-3.58811364	2.16207729
H	-0.59373181	-3.50607024	0.00013540
H	-1.72226961	-4.85008674	0.00022760
H	-2.99243781	-1.34947954	-2.12217051
H	-2.99235363	-1.34929732	2.12237155
O	2.17603135	-3.28656192	0.00039097
C	5.07746764	1.19218247	-1.13320121
H	5.49777802	1.32016837	-2.11829672
C	3.80891154	0.79874883	-0.72478150
C	3.80891665	0.79901915	0.72440393
C	5.07747245	1.19260880	1.13265554
H	5.49780157	1.32095955	2.11769562
H	6.77926587	1.72399384	-0.00038456
H	-1.01631189	1.27404149	-0.00006601
H	-0.01169391	1.31941013	-0.00011293
H	-3.97099362	-1.55704956	0.00012957
N	-2.38966078	3.81066058	-0.00003434
O	-3.17181761	4.76816384	-0.00001466
O	-1.15854594	3.88949188	-0.00007796

Name - TStBu\\SCF E (UB3LYP-D3BJ/BS1)=-2600.9821457\\G=-

2600.638744\\H=-2600.546772\\SCF E (UB3LYP-D3BJ/BS2)=-2601.3359903

\\ZeroPoint=0.405474

C	1.91511884	-3.58389806	-1.26126150
C	2.75739489	-1.56250083	0.00003347
Mo	-0.89750644	-0.50550221	-0.00000105
S	0.49565567	-1.23006493	1.81021194
S	0.49574700	-1.22988719	-1.81020607
S	-2.46421766	0.41977973	1.67596532
S	-2.46411240	0.42002286	-1.67595172
C	3.18514866	-0.12497777	0.00005622
N	2.34499122	0.97790667	0.00009129
C	3.10364039	2.07045582	0.00005049
N	4.41199066	1.70472047	-0.00001982
C	4.48263610	0.32549736	-0.00001194
H	5.19910178	2.33920471	-0.00003659

C	1.91516064	-3.58396236	1.26121922
H	5.42378988	-0.20126718	-0.00005384
C	2.08000959	-2.05512259	-1.29700935
C	2.07998790	-2.05518427	1.29704027
C	-1.94963597	-2.27833312	-0.00015087
N	-5.64047574	1.99951888	0.00003045
C	1.20262709	-4.07446184	-0.00002136
H	1.39388455	-3.92134651	2.16170803
H	2.92454579	-4.01716010	1.29252912
H	2.92448391	-4.01713577	-1.29265568
H	1.39378114	-3.92120303	-2.16174444
H	0.16609761	-3.72682834	0.00000581
H	1.16582389	-5.16910982	-0.00005087
H	2.74888527	-1.79497013	2.12206574
H	2.74895047	-1.79491229	-2.12200078
O	-2.56406319	-3.24818869	-0.00023712
C	-4.95228853	1.65452100	1.13315701
H	-5.34698441	1.84847388	2.11801657
C	-3.76222573	1.06342000	0.72544420
C	-3.76218074	1.06352888	-0.72541497
C	-4.95221717	1.65469037	-1.13310915
H	-5.34685444	1.84879469	-2.11796234
H	-6.54756863	2.44876494	0.00003631
H	0.78927394	1.04055780	0.00011364
H	-0.05499786	1.23238360	0.00011508
H	3.70574903	-2.11993524	0.00002916
C	2.58990598	3.49017736	0.00002972
C	1.72750039	3.70715888	-1.26084145
H	2.31600561	3.54315953	-2.16917611
H	0.87280398	3.02531016	-1.27724741
H	1.34792851	4.73389788	-1.27727821
C	3.75877171	4.48751188	0.00000494
H	3.36546132	5.50780296	0.00002799
H	4.38750702	4.37119209	0.88909307
H	4.38745387	4.37121377	-0.88912372
C	1.72750921	3.70722339	1.26089358
H	0.87290050	3.02526957	1.27742767
H	2.31606452	3.54343493	2.16923395
H	1.34780479	4.73391567	1.27719279

(R₁123R₂ = Cyclohexyl group, R₃45R₄ = Imidazole ring: L1 = Pyridine)

Name - MoIIICl\\SCF E(UB3LYP-D3BJ/BS1)=-3037.1504599\\G=-
 3036.855659\\H=-3036.769000\\SCF E(UB3LYP-D3BJ/BS2)=-
 3037.5279724\\ZeroPoint=0.353659

C	-4.20093281	1.21794136	-1.25660461
C	-3.27082646	-0.77235131	-0.00000098
Mo	0.01137022	0.10882817	-0.00002188

S	-1.51045229	0.68744737	1.77936564
S	-1.51051237	0.68745032	-1.77944563
S	1.69618822	-0.53592874	1.67718809
S	1.69614088	-0.53592563	-1.67713271
C	-2.37142071	-1.96368880	0.00000303
N	-0.97678105	-1.86724818	-0.00004858
C	-0.51487032	-3.11166735	0.00001273
N	-1.53154085	-4.00006988	0.00007571
C	-2.71478019	-3.28764947	0.00006931
H	-1.43052438	-5.00782734	0.00009645
C	-4.20088948	1.21794718	1.25666341
H	-3.67529530	-3.77675015	0.00006005
C	-3.19545751	0.05770070	-1.30541403
C	-3.19542356	0.05769993	1.30542001
N	5.24783534	-0.93248412	-0.00005173
C	-4.03733599	2.07501053	0.00002506
H	-4.10492832	1.82437613	2.16239816
H	-5.21059897	0.78345605	1.26648541
H	-5.21064092	0.78344511	-1.26638555
H	-4.10501182	1.82437336	-2.16234111
H	-3.04517346	2.54061259	0.00000718
H	-4.77732386	2.88244003	0.00003453
H	-4.29075101	-1.18072850	0.00001206
H	-3.47041815	-0.61597865	2.12164101
H	-3.47050209	-0.61597177	-2.12162430
C	4.47331962	-0.83185694	1.13088793
H	4.90670621	-0.88585661	2.11770887
C	3.15836276	-0.66138795	0.72160052
C	3.15834323	-0.66138146	-0.72160885
C	4.47329145	-0.83184963	-1.13094724
H	4.90662068	-0.88580779	-2.11779630
H	6.25211833	-1.04440033	-0.00006393
C	1.09998205	2.84855221	1.15789679
C	1.09993176	2.84857020	-1.15785407
C	1.58626315	4.14880975	1.19890346
H	0.90408942	2.29528010	2.06691836
C	1.58622357	4.14882372	-1.19886133
H	0.90397995	2.29533453	-2.06688506
H	1.76547826	4.62131289	2.15782408
H	1.76541412	4.62133452	-2.15778268
N	0.85566957	2.20304206	0.00002252
C	1.83572929	4.81534481	0.00002146
H	2.21851106	5.83050911	0.00002206
Cl	1.11561941	-3.61286552	-0.00001632

Name - MoIIIme\\SCF E(UB3LYP-D3BJ/BS1)=-2616.8977135\\G=-
 2616.566531\\H=-2616.478447\\SCF E(UB3LYP-D3BJ/BS2)=-
 2617.2502343\\ZeroPoint=0.390897

C	-3.99962509	1.63684515	-1.24479663
C	-3.34177498	-0.46492017	0.00531530
Mo	0.02147494	-0.05623779	-0.00226380
S	-1.39579377	0.74237708	1.77776558
S	-1.40437649	0.75866916	-1.76713586
S	1.63337635	-0.85208301	1.70542682
S	1.62598492	-0.92037382	-1.65707462
C	-2.60811228	-1.76568033	-0.00070372
N	-1.21576132	-1.86352096	-0.00389141
C	-0.89782603	-3.16411546	-0.01260900
N	-2.04173929	-3.88818812	-0.01108764
C	-3.12442216	-3.03113460	-0.00511200
H	-2.07967249	-4.89910219	-0.01394913
C	-3.99202299	1.63198584	1.26871735
H	-4.14198557	-3.38665293	0.00045671
C	-3.15813982	0.35283932	-1.29727843
C	-3.15252192	0.34632153	1.31085187
N	5.16842071	-1.39740071	0.02227007
C	-3.71854463	2.46157657	0.01275298
H	-3.81167681	2.21854063	2.17478350
H	-5.05131151	1.33829403	1.28189914
H	-5.05856567	1.34170080	-1.25205873
H	-3.82602296	2.22731155	-2.14960777
H	-2.67216828	2.78786851	0.01009892
H	-4.34212212	3.36202568	0.01644613
H	-4.40812655	-0.72998081	0.00670504
H	-3.51171210	-0.28565442	2.12783339
H	-3.51888688	-0.27571998	-2.11623613
C	4.40093066	-1.24427340	1.15309348
H	4.83642534	-1.28746410	2.13955290
C	3.09057639	-1.04415023	0.74500493
C	3.08536412	-1.07876377	-0.69791156
C	4.39267018	-1.29951912	-1.10746430
H	4.81993958	-1.38732820	-2.09457131
H	6.16888754	-1.53912195	0.02170479
C	1.48811886	2.53104522	1.13150499
C	1.52135304	2.48832230	-1.18246205
C	2.16753389	3.74232129	1.16021105
H	1.19538053	2.03159295	2.04561992
C	2.20230204	3.69783819	-1.23674000
H	1.25466436	1.95530804	-2.08564903
H	2.40270298	4.19993579	2.11428785
H	2.46548306	4.11943854	-2.20003039
N	1.16464401	1.90885518	-0.01924361
C	2.53434449	4.34013315	-0.04471223
H	3.06921704	5.28404580	-0.05445204
C	0.45075614	-3.78293087	-0.04950801

H	0.87326021	-3.72433751	-1.05662387
H	1.12687064	-3.25401178	0.62383808
H	0.38570790	-4.83279297	0.24606485

Name - MoIIINMe2\\SCF E(UB3LYP-D3BJ/BS1)=-2711.5537494\\G=-
 2711.178739\\H=-2711.086151\\SCF E(UB3LYP-D3BJ/BS2)=-
 2711.9308192\\ZeroPoint= 0.436929

C	3.61828003	-2.41935955	-1.37684959
C	3.35357447	-0.30575282	-0.00607492
Mo	-0.01993680	-0.06273261	0.02807366
S	1.22317924	-1.23511272	1.68427633
S	1.24646224	-1.02092916	-1.83818464
S	-1.52523878	1.30702649	1.38187619
S	-1.60576981	0.39050841	-1.84334044
C	2.88316169	1.11094103	0.08247802
N	1.53930141	1.53218818	0.01529215
C	1.55392650	2.87684617	0.15401399
N	2.83588114	3.29542949	0.32872658
C	3.67637703	2.19562776	0.28853756
H	3.12936711	4.25973516	0.38943339
C	3.60376365	-2.56065361	1.12869999
H	4.74349012	2.28505189	0.41116819
C	3.03603511	-0.99797063	-1.35168743
C	3.02196578	-1.14478432	1.24926085
N	-5.12840363	1.21388500	-0.24172264
C	3.17646745	-3.24803866	-0.16949418
H	3.31604261	-3.15226183	2.00327134
H	4.69937137	-2.47345275	1.14602590
H	4.71458760	-2.33442400	-1.37118072
H	3.34099042	-2.91132369	-2.31434936
H	2.08580890	-3.36285602	-0.18310114
H	3.61193140	-4.25163057	-0.22295613
H	4.45029168	-0.23598154	0.00791716
H	3.48406108	-0.63708141	2.10109571
H	3.52441895	-0.40313302	-2.12870724
C	-4.31940953	1.45999776	0.84280600
H	-4.72620491	1.78782289	1.78707922
C	-3.01543711	1.19066750	0.45726216
C	-3.05302668	0.76649579	-0.92034990
C	-4.38223075	0.78812651	-1.31567363
H	-4.84399768	0.54126781	-2.25945265
H	-6.13358988	1.31486601	-0.24329557
C	-2.29669760	-1.94259956	1.26076832
C	-1.29918025	-2.90121959	-0.59496943
C	-3.13632096	-3.03910541	1.42564261
H	-2.33523053	-1.09739990	1.93493593

C	-2.09980340	-4.03055065	-0.49204873
H	-0.55098805	-2.80300438	-1.37166240
H	-3.84724441	-3.04520746	2.24407612
H	-1.98092785	-4.83415996	-1.21003519
N	-1.39190297	-1.86640518	0.26543349
C	-3.04217069	-4.10443164	0.53398934
H	-3.68461757	-4.97288959	0.63598080
N	0.49746780	3.75375271	0.18252122
C	-0.49986518	3.66182357	-0.88598662
H	-1.45223968	4.05661821	-0.52544101
H	-0.18286080	4.24620552	-1.76262012
H	-0.64898210	2.62907733	-1.18590605
C	0.81853878	5.13697527	0.53106179
H	1.39491153	5.64881701	-0.25496603
H	-0.11937470	5.67750164	0.66961608
H	1.37610880	5.17856276	1.46986811

Name - MoIIINO2\\SCF E(UB3LYP-D3BJ/BS1)= -2782.0493279\\G=-
 2781.745001\\H= -2781.654818\\SCF E(UB3LYP-D3BJ/BS2)=-2782.4623196
 \\ZeroPoint= 0.365388

C	-3.91389855	1.96919532	-1.25708706
C	-3.35737534	-0.15489457	-0.00159223
Mo	0.02766157	0.11830423	-0.00086606
S	-1.37310659	0.94343731	1.78701397
S	-1.37235404	0.94407383	-1.78953632
S	1.63203986	-0.68383964	1.68397762
S	1.63334778	-0.67096892	-1.69086093
C	-2.68650476	-1.48867298	-0.00064498
N	-1.31848003	-1.69244581	-0.00194280
C	-1.15363387	-3.01965235	0.00142334
N	-2.34337256	-3.66208049	0.00480633
C	-3.32033501	-2.71974905	0.00338974
H	-2.44843839	-4.67134488	0.00759873
C	-3.91426292	1.96936615	1.25385484
H	-4.36869949	-2.97207471	0.00523069
C	-3.13870316	0.64399194	-1.30986833
C	-3.13939554	0.64400981	1.30685364
N	5.17183458	-1.11574815	-0.00384602
C	-3.58998219	2.78065133	-0.00162263
H	-3.71041795	2.54656957	2.16064075
H	-4.98679237	1.72899209	1.25960568
H	-4.98638877	1.72864918	-1.26303755
H	-3.70996406	2.54638233	-2.16386343
H	-2.52727077	3.04890659	-0.00150903
H	-4.16323062	3.71373926	-0.00175794
H	-4.43233204	-0.38016013	-0.00189791
H	-3.54185114	0.03092938	2.11786271

H	-3.54073143	0.03089451	-2.12107007
C	4.39886569	-1.01252464	1.12710475
H	4.83161627	-1.07307827	2.11377502
C	3.08500898	-0.82984235	0.71939289
C	3.08555125	-0.82398102	-0.72637481
C	4.39981931	-1.00327752	-1.13448166
H	4.83333173	-1.05575644	-2.12128063
H	6.17489132	-1.23986629	-0.00393718
C	1.50011470	2.66650855	1.16308116
C	1.49436768	2.67610391	-1.15196101
C	2.17327612	3.88037359	1.20715392
H	1.22720079	2.14647336	2.07110910
C	2.16729581	3.89031106	-1.18925508
H	1.21681207	2.16373949	-2.06292905
H	2.42201863	4.31632499	2.16782504
H	2.41119865	4.33431627	-2.14747776
N	1.15963620	2.06776420	0.00390065
C	2.51643932	4.50785516	0.01067713
H	3.04630575	5.45457583	0.01327411
N	0.04347547	-3.79089150	0.00087256
O	-0.11167513	-5.02658204	0.01275962
O	1.12924798	-3.22229953	-0.01127126

Name - MoIIItBu\\SCF E(UB3LYP-D3BJ/BS1)= -2734.8488147\\G=-
 2734.434332\\H= -2734.340273\\SCF E(UB3LYP-D3BJ/BS2)=-
 2735.2261602\\ZeroPoint= 0.476641

C	2.79093185	-3.42583143	-1.24674609
C	3.11128834	-1.27542129	0.05457976
Mo	-0.06110911	-0.14091022	-0.00923373
S	0.85954449	-1.48094668	1.81281361
S	0.88072797	-1.46828638	-1.75805536
S	-1.38449323	0.86548717	1.80366313
S	-1.36627930	1.30125689	-1.53793298
C	3.04526747	0.21981999	0.08587902
N	1.88903432	1.01881255	0.02155740
C	2.30050250	2.30618950	0.05082453
N	3.65328019	2.32033137	0.15198979
C	4.13473603	1.03607391	0.16957630
H	4.21794013	3.15687106	0.19136320
C	2.74630517	-3.47634748	1.26160647
H	5.18681376	0.81203257	0.24162374
C	2.61446798	-1.90032618	-1.26882555
C	2.58539044	-1.95094545	1.34046777
N	-4.75244978	2.23795312	0.27275280
C	2.14163860	-4.06077165	-0.01572628
H	2.30754960	-3.93701726	2.15210908
H	3.82257708	-3.70073975	1.28190306

H	3.86952731	-3.63753858	-1.23402094
H	2.39132866	-3.85490794	-2.17070082
H	1.06206275	-3.87077501	-0.03095120
H	2.28345898	-5.14665510	-0.03539989
H	4.18693887	-1.50044372	0.05731136
H	3.20460312	-1.57562190	2.16037264
H	3.23251231	-1.48018799	-2.06780302
C	-4.02574007	1.82342602	1.36023606
H	-4.44443636	1.82844212	2.35484935
C	-2.77249888	1.43798283	0.90284606
C	-2.76526336	1.62928534	-0.53003433
C	-4.01039763	2.12725810	-0.88089772
H	-4.41960988	2.39905224	-1.84167986
H	-5.70993592	2.55897847	0.31034985
C	-2.33239817	-2.19671348	0.94739631
C	-2.44398690	-1.81602099	-1.32920732
C	-3.41307712	-3.06839922	0.89627453
H	-1.83348632	-1.98249671	1.88196656
C	-3.52953940	-2.67272661	-1.46246521
H	-2.03788177	-1.29503405	-2.18536623
H	-3.75944948	-3.54024733	1.80867382
H	-3.96966152	-2.82555018	-2.44124011
N	-1.84767957	-1.57483694	-0.14503172
C	-4.02959462	-3.31219211	-0.32967777
H	-4.87915533	-3.98349882	-0.40019412
C	1.55747433	3.62089515	-0.13804175
C	1.25295018	3.78839008	-1.64322974
H	0.59218389	2.99775222	-2.00052295
H	0.75742104	4.75076502	-1.81010613
H	2.17753374	3.77240666	-2.22924115
C	0.26396713	3.69633559	0.68301247
H	-0.45953353	2.95208318	0.36672843
H	0.46551180	3.55064948	1.74802459
H	-0.17997144	4.68804932	0.54872408
C	2.45652584	4.79632632	0.30303659
H	2.77214826	4.69750915	1.34650005
H	3.34425124	4.90766172	-0.32839273
H	1.88434818	5.72297220	0.21093893

Name - MoIIII1Cl\\SCF E(UB3LYP-D3BJ/BS1)= -3038.2890849\\G=-
3037.985491\\H= -3037.891042\\SCF E(UB3LYP-D3BJ/BS2)=-
3038.6611054\\ZeroPoint= 0.368448

C	1.76281928	-3.23819315	-1.26369638
C	2.94752007	-1.40168146	-0.00008036
Mo	-0.63203540	0.08140611	-0.00005580

S	0.78196968	-0.65477169	1.79160625
S	0.78180490	-0.65491376	-1.79170179
S	-1.97384262	1.30418388	1.67998741
S	-1.97430390	1.30397341	-1.67999566
C	3.62688001	-0.06416907	-0.00000999
N	2.98684882	1.17093131	-0.00044465
C	3.94937487	2.05975478	-0.00014449
N	5.18514360	1.50007775	0.00047247
C	4.98879264	0.13198300	0.00058307
H	6.07152157	1.98885572	0.00077732
C	1.76270239	-3.23820050	1.26346863
H	5.81639008	-0.56008236	0.00102619
C	2.18950139	-1.76128781	-1.29631390
C	2.18948381	-1.76132460	1.29614178
N	-4.15709657	4.11871559	0.00015007
C	0.98243647	-3.60405010	-0.00015157
H	1.18155439	-3.47447355	2.15989152
H	2.68000710	-3.84244983	1.30704360
H	2.68016501	-3.84238656	-1.30717339
H	1.18177817	-3.47450537	-2.16017839
H	0.02331254	-3.08613392	-0.00020401
H	0.76238098	-4.67729435	-0.00016107
H	2.89427959	-1.62045303	2.12033043
H	2.89425528	-1.62030488	-2.12051873
C	-3.67879226	3.50765944	1.13200155
H	-3.94472532	3.85532549	2.11808436
C	-2.86732283	2.45807978	0.72276350
C	-2.86753394	2.45798692	-0.72265807
C	-3.67912275	3.50751145	-1.13177665
H	-3.94535169	3.85506223	-2.11782016
H	-4.77878538	4.91616559	0.00019207
H	0.95698553	1.55158334	-0.00029619
H	0.27870973	1.92862775	-0.00025999
H	3.78205750	-2.11940310	-0.00008821
C	-2.29984301	-2.25201332	-1.16231979
C	-2.29947857	-2.25205252	1.16267862
C	-3.05756816	-3.41361917	-1.19966909
H	-1.96777502	-1.76419757	-2.06866650
C	-3.05719725	-3.41365752	1.20022388
H	-1.96710917	-1.76427224	2.06893337
H	-3.33250989	-3.83841685	-2.15792480
H	-3.33184187	-3.83848719	2.15855081
N	-1.92196092	-1.67853046	0.00013006
C	-3.44267637	-4.01038551	0.00032790
H	-4.03134263	-4.92154514	0.00040351
Cl	3.72006363	3.77069273	-0.00048854

Name - MoIIII1Me\\SCF E(UB3LYP-D3BJ/BS1)= -2618.0282459\\G=-
 2617.686307\\H= -2617.593515\\SCF E(UB3LYP-D3BJ/BS2)=-
 2618.3765793\\ZeroPoint= 0.405391

C	2.49724238	2.68074586	1.26220886
C	3.26542503	0.63009449	0.00006635
Mo	-0.51475482	-0.11022325	0.00007941
S	0.99279182	0.37223703	-1.80065465
S	0.99267917	0.37237689	1.80073531
S	-2.07352208	-1.04125929	-1.68025815
S	-2.07403715	-1.04084944	1.68035215
C	3.63938065	-0.82346606	-0.00000115
N	2.75571543	-1.89281286	0.00050789
C	3.48957967	-2.99711054	0.00026751
N	4.81539524	-2.68335550	-0.00037437
C	4.92678956	-1.30756590	-0.00056795
H	5.57751132	-3.34805687	-0.00064552
C	2.49714722	2.68079193	-1.26198006
H	5.88313616	-0.80826806	-0.00099251
C	2.60420661	1.14715766	1.29637601
C	2.60419012	1.14721021	-1.29622233
N	-4.93782661	-3.15870876	-0.00018503
C	1.80531038	3.19846964	0.00015021
H	1.98274048	3.03529902	-2.16030484
H	3.52080060	3.07995175	-1.29949829
H	3.52091787	3.07985371	1.29965460
H	1.98292828	3.03524830	2.16058895
H	0.76032427	2.88515748	0.00019112
H	1.80785813	4.29413751	0.00016897
H	3.26544975	0.86199483	-2.11924908
H	3.26540698	0.86184046	2.11941428
C	-4.31294718	-2.69807372	-1.13194542
H	-4.66309681	-2.96058249	-2.11808636
C	-3.24878778	-1.90568847	-0.72257431
C	-3.24902798	-1.90550383	0.72249755
C	-4.31332849	-2.69777217	1.13168898
H	-4.66382711	-2.96004113	2.11776951
H	-5.75421070	-3.75531073	-0.00024801
H	0.83530282	-1.82825515	0.00035049
H	0.07335419	-2.03680087	0.00029258
H	4.23324640	1.15446865	0.00007537
C	-1.71636665	2.50821570	1.16137794
C	-1.71613981	2.50813813	-1.16166380
C	-2.24077864	3.79239431	1.19939480
H	-1.48352354	1.96620714	2.06785073
C	-2.24055576	3.79231161	-1.19986519
H	-1.48310088	1.96607242	-2.06805211
H	-2.43037911	4.26146919	2.15778222
H	-2.42997871	4.26132046	-2.15831995
N	-1.45402987	1.87275787	-0.00009671
C	-2.50654867	4.45147691	-0.00028322

H	-2.91203439	5.45765702	-0.00035485
C	2.97475510	-4.39552961	0.00032766
H	2.35362514	-4.58136969	0.88239779
H	2.35897219	-4.58359507	-0.88505176
H	3.79963721	-5.11204628	0.00365945

Name - MoIIII1NMe2\\SCF E(UB3LYP-D3BJ/BS1)= -2712.6939798\\G=-
 2712.308099\\H= -2712.209647\\SCF E(UB3LYP-D3BJ/BS2)=-2713.0742273
 \\ZeroPoint= 0.451934

C	0.83681673	-3.67782319	-1.22519405
C	2.40041984	-2.15403260	0.05676217
Mo	-0.69012891	0.12474691	0.01435263
S	0.40425806	-0.97885332	1.82985642
S	0.50523352	-0.93996100	-1.78025791
S	-1.73134539	1.63853824	1.68491001
S	-1.60070829	1.67299428	-1.67262462
C	3.37095743	-1.00774002	0.05737072
N	3.05599651	0.34386183	0.20355467
C	4.20809585	1.00190571	0.13466841
N	5.25036914	0.14210975	-0.06823799
C	4.72302206	-1.14252462	-0.11069552
H	6.22754588	0.38539046	-0.14128485
C	0.82782420	-3.69093716	1.29749194
H	5.34828777	-2.00821334	-0.26336208
C	1.59913635	-2.34247874	-1.25107371
C	1.56794022	-2.34354333	1.34205543
N	-3.20154505	4.86992407	-0.02813535
C	-0.01586083	-3.85456105	0.03229008
H	0.21070033	-3.80385602	2.19402163
H	1.58851841	-4.48392946	1.32892595
H	1.58637970	-4.48120437	-1.26343334
H	0.22354766	-3.76989763	-2.12670185
H	-0.82491093	-3.12207980	0.03534512
H	-0.48434689	-4.84497728	0.02470332
H	2.27481259	-2.35790876	2.17639202
H	2.33499565	-2.37888786	-2.05933304
C	-2.91167294	4.15850225	1.11108506
H	-3.13762790	4.54679357	2.09197498
C	-2.32841314	2.96320789	0.71527720
C	-2.27042768	2.97728521	-0.72842003
C	-2.82066205	4.18108888	-1.15058318
H	-2.96546577	4.58552409	-2.14027036
H	-3.63932890	5.78138871	-0.03734782
H	1.24643697	1.04661244	0.10359100
H	0.66492724	1.57816029	0.06780697
H	3.04913264	-3.04343140	0.06396189
C	-2.85830533	-1.72168648	-1.23238055

C	-2.97559427	-1.68614696	1.08722246
C	-3.89137631	-2.64523501	-1.30862414
H	-2.36285848	-1.35252879	-2.12013296
C	-4.01124381	-2.60965426	1.08761845
H	-2.57621695	-1.28554002	2.00916610
H	-4.21948792	-2.99757828	-2.27951283
H	-4.43515140	-2.93357386	2.03089292
N	-2.40312386	-1.24782365	-0.05359476
C	-4.47930458	-3.10263411	-0.12998024
H	-5.28558372	-3.82798026	-0.15951478
N	4.37938616	2.36706573	0.31489522
C	3.13974891	3.14122375	0.23999183
H	3.37185539	4.18507641	0.45791004
H	2.66627747	3.08410620	-0.75097308
H	2.42851598	2.78200649	0.98398482
C	5.48265022	2.96581621	-0.44342159
H	5.34444912	2.87317383	-1.53036598
H	5.54423867	4.02473088	-0.18810351
H	6.43667948	2.50960385	-0.16943010

Name - MoIII1NO2\\SCF E(UB3LYP-D3BJ/BS1)= -2783.1998504\\G=-

2782.883494\\H= -2782.788484\\SCF E(UB3LYP-D3BJ/BS2)=-

2783.616253\\ZeroPoint= 0.380633

C	1.10730805	-3.54520914	-1.26464179
C	2.58491888	-1.94214553	-0.00006582
Mo	-0.70500125	0.11985462	-0.00001797
S	0.58476278	-0.82642083	1.79065941
S	0.58466847	-0.82642417	-1.79073109
S	-1.83989676	1.53474603	1.67946512
S	-1.84004982	1.53470236	-1.67946655
C	3.46889341	-0.73316949	0.00001546
N	3.04587524	0.56612712	-0.00015739
C	4.15005014	1.29178100	-0.00003625
N	5.27980714	0.53411324	0.00031284
C	4.86533492	-0.76096682	0.00032731
H	6.23093992	0.88540659	0.00048746
C	1.10721452	-3.54524428	1.26439807
H	5.56069285	-1.58633981	0.00053578
C	1.77740494	-2.16174220	-1.29842926
C	1.77737617	-2.16181028	1.29827843
N	-3.53045483	4.66910690	0.00004429
C	0.27848337	-3.77600553	-0.00015657
H	0.49264015	-3.67788451	2.15967905
H	1.90973007	-4.29479512	1.31113029
H	1.90985885	-4.29472532	-1.31132286
H	0.49281160	-3.67785769	-2.15997495
H	-0.58150611	-3.10710804	-0.00018747
H	-0.11621005	-4.79788583	-0.00018194
H	2.49633244	-2.14421493	2.12208295

H	2.49635729	-2.14404407	-2.12223476
C	-3.15875161	3.98855818	1.13203890
H	-3.36368283	4.37541721	2.11805396
C	-2.52954301	2.82053602	0.72297169
C	-2.52961455	2.82051642	-0.72294077
C	-3.15886914	3.98852300	-1.13197305
H	-3.36390671	4.37535496	-2.11797663
H	-4.01128098	5.55886079	0.00005642
H	1.06783003	1.33535696	-0.00011627
H	0.47346445	1.82697108	-0.00000808
H	3.28625790	-2.78925989	-0.00008025
C	-2.71586681	-1.92088917	-1.16262496
C	-2.71569446	-1.92095304	1.16277559
C	-3.64735244	-2.94830217	-1.19989289
H	-2.31147794	-1.49134343	-2.06903246
C	-3.64717749	-2.94836598	1.20012528
H	-2.31116243	-1.49146122	2.06914463
H	-3.98604266	-3.32418470	-2.15811271
H	-3.98572807	-3.32429859	2.15837489
N	-2.25217407	-1.41439238	0.00005478
C	-4.12200801	-3.47661224	0.00013701
H	-4.84676577	-4.28388167	0.00016834
N	4.20079873	2.70530601	-0.00013794
O	5.32515527	3.23357278	-0.00017274
O	3.13478711	3.33387099	0.00002087

Name - MoIIII1tBu\\SCF E(UB3LYP-D3BJ/BS1)= -2735.9947138\\G=-
 2735.570407\\H=-2735.471269\\SCF E(UB3LYP-D3BJ/BS2)=-
 2736.37476\\ZeroPoint=0.490467

C	-0.04710400	-3.86752829	-1.26017065
C	1.80091218	-2.68680796	0.00006879
Mo	-0.75615207	0.18630372	-0.00001914
S	0.13790816	-1.12064766	1.80418918
S	0.13806552	-1.12062629	-1.80403400
S	-1.39938417	1.88304031	1.68043644
S	-1.39993732	1.88286460	-1.68070251
C	2.95746413	-1.73049770	-0.00013894
N	2.85919520	-0.34882886	0.00061129
C	4.09384513	0.13591756	0.00003132
N	4.99246487	-0.88923250	-0.00110862
C	4.28815820	-2.07782977	-0.00121088
H	5.99855110	-0.79420171	-0.00179158
C	-0.04678294	-3.86755955	1.26062181
H	4.78249900	-3.03679046	-0.00196568
C	0.96113449	-2.70729091	-1.29649066

C	0.96130446	-2.70718387	1.29672877
N	-2.18922074	5.35659702	-0.00011916
C	-0.91314703	-3.85827733	0.00033611
H	-0.66821896	-3.84440421	2.16093320
H	0.52982528	-4.80312872	1.29241000
H	0.52940230	-4.80315253	-1.29216506
H	-0.66876372	-3.84426161	-2.16032537
H	-1.55208600	-2.97337339	0.00044696
H	-1.57673066	-4.73012839	0.00039695
H	1.66164838	-2.87845516	2.11902672
H	1.66137292	-2.87876336	-2.11883517
C	-2.01526918	4.59995368	1.13166271
H	-2.10960587	5.02722325	2.11782924
C	-1.72449624	3.30540524	0.72242591
C	-1.72475053	3.30534029	-0.72270880
C	-2.01567609	4.59984456	-1.13192439
H	-2.11035837	5.02705637	-2.11808287
H	-2.41990621	6.34104191	-0.00011932
H	1.36351516	0.67541768	0.00019261
H	0.86704036	1.30566551	-0.00029783
H	2.27156167	-3.68177967	0.00006506
C	-3.31483488	-1.15318928	-1.16121258
C	-3.31498302	-1.15280797	1.16125932
C	-4.51825795	-1.84333535	-1.19971218
H	-2.79699361	-0.86976212	-2.06768928
C	-4.51841794	-1.84293035	1.19983124
H	-2.79725627	-0.86908562	2.06770936
H	-4.95629311	-2.09679754	-2.15804134
H	-4.95658380	-2.09606682	2.15818678
N	-2.71804605	-0.81231167	0.00000527
C	-5.13353171	-2.19875305	0.00007855
H	-6.07228634	-2.74241161	0.00010760
C	4.44715979	1.60457790	0.00029464
C	3.84454007	2.26114056	-1.25882036
H	4.25062528	1.80702258	-2.16853709
H	2.75677942	2.14995593	-1.27674968
H	4.08162117	3.33011958	-1.27299609
C	3.84397490	2.26090211	1.25923934
H	2.75621072	2.14975744	1.27668038
H	4.24966197	1.80661651	2.16904998
H	4.08108615	3.32986990	1.27368095
C	5.97111797	1.79716154	0.00070010
H	6.43282570	1.35387364	-0.88799605
H	6.20554243	2.86548024	0.00093261
H	6.43235404	1.35353054	0.88946570

Name - TSC1\\SCF E(UB3LYP-D3BJ/BS1)=-3038.2840261\\G=-3037.976813\\H=-3037.889221\\SCF E(UB3LYP-D3BJ/BS2)=-3038.6617307 \\ZeroPoint=0.366921
C -1.94996959 -3.20511160 1.25844683

C	-3.03658951	-1.30398880	0.00001436
Mo	0.49735491	0.15338850	0.00004986
S	-0.85195139	-0.68290829	-1.81839012
S	-0.85194404	-0.68296843	1.81843407
S	1.88170890	1.31761390	-1.67906669
S	1.88195191	1.31739911	1.67917812
C	-3.60382506	0.08299551	0.00002945
N	-2.86822218	1.26384970	-0.00001508
C	-3.73225822	2.25877222	-0.00000616
N	-5.00014219	1.80051703	0.00003129
C	-4.93416819	0.41935507	0.00005133
H	-5.84058888	2.36670926	0.00002574
C	-1.94999049	-3.20507000	-1.25848811
H	-5.82355170	-0.19025990	0.00007746
C	-2.30893326	-1.71089331	1.30164452
C	-2.30893968	-1.71084745	-1.30163256
N	4.67452845	3.53223471	-0.00002195
C	-1.17046340	-3.58888836	-0.00003385
H	-1.39270534	-3.47272654	-2.16102175
H	-2.89237250	-3.77093021	-1.28245548
H	-2.89234613	-3.77098025	1.28241757
H	-1.39266399	-3.47278934	2.16096170
H	-0.20006668	-3.08804960	-0.00003540
H	-0.97436127	-4.66673207	-0.00005165
H	-3.01812478	-1.54643951	-2.11764727
H	-3.01811406	-1.54651784	2.11766912
C	4.06782466	3.04664333	-1.13171452
H	4.40902375	3.32059541	-2.11793896
C	3.03407580	2.21505651	-0.72209591
C	3.03418922	2.21495775	0.72214786
C	4.06800498	3.04648452	1.13170756
H	4.40936272	3.32031093	2.11791186
H	5.47037606	4.15568331	-0.00004361
H	-1.47216381	1.41855830	0.00007790
H	-0.57242701	1.67349487	0.00016719
H	-3.92733049	-1.94907782	0.00000773
C	2.20691120	-2.24308310	1.15879674
C	2.20697418	-2.24292827	-1.15893162
C	2.95220521	-3.41424820	1.19938192
H	1.88143073	-1.74958509	2.06512978
C	2.95227527	-3.41408562	-1.19963202
H	1.88154495	-1.74930740	-2.06521620
H	3.22275474	-3.84220413	2.15776340
H	3.22288327	-3.84191010	-2.15805552
N	1.83533048	-1.66448870	-0.00003922
C	3.33102307	-4.01582858	-0.00015489
H	3.90988407	-4.93347290	-0.00019973
Cl	-3.32212558	3.92274084	-0.00005852

Name - TSMe\\SCF E (UB3LYP-D3BJ/BS1)=-2618.0280123\\G=-2617.687349\\H=-2617.594763\\SCF E (UB3LYP-D3BJ/BS2)=-2618.3823817\\ZeroPoint=0.403734

C	-2.51730203	2.70917592	-1.25582047
C	-3.28124434	0.65302825	0.00244191
Mo	0.45682405	-0.16790255	0.00090564
S	-1.01340999	0.40765793	1.81309099
S	-1.01611836	0.40702244	-1.81045852
S	2.00845984	-1.10887609	1.68037613
S	2.00183899	-1.11346517	-1.68014204
C	-3.63074882	-0.80586618	0.00029293
N	-2.72811372	-1.86094425	0.00731146
C	-3.42885163	-2.98748174	-0.00333698
N	-4.75787442	-2.69971122	-0.01722759
C	-4.90164775	-1.32581987	-0.01454118
H	-5.50609097	-3.38023689	-0.02956474
C	-2.51823022	2.70734406	1.26331063
H	-5.86973724	-0.85018298	-0.02747028
C	-2.62649962	1.17604193	-1.29575001
C	-2.62601588	1.17403181	1.30097861
N	5.06712384	-2.93251067	-0.00390142
C	-1.81602360	3.21857633	0.00437099
H	-2.01060314	3.06252101	2.16512368
H	-3.54128598	3.10905118	1.29098836
H	-3.54001652	3.11174346	-1.28390367
H	-2.00859438	3.06510121	-2.15673005
H	-0.77436951	2.89067435	0.00461652
H	-1.80548263	4.31417714	0.00514006
H	-3.29173525	0.89080385	2.12108322
H	-3.29356716	0.89499075	-2.11550149
C	4.40331036	-2.53155881	1.12877315
H	4.78067444	-2.75541837	2.11443395
C	3.26669047	-1.84622825	0.72094305
C	3.26362086	-1.84839913	-0.72385164
C	4.39847386	-2.53505492	-1.13472181
H	4.77149661	-2.76168193	-2.12140273
H	5.94047299	-3.44212886	-0.00502805
H	-1.10710406	-1.79679386	0.00586764
H	-0.27460784	-1.94967256	0.00344307
H	-4.25741449	1.16095730	0.00305458
C	1.74362263	2.44154128	-1.16211172
C	1.74648775	2.44264504	1.15793594
C	2.29905564	3.71315839	-1.20276229
H	1.49752642	1.90391792	-2.06793180
C	2.30189249	3.71433421	1.19603760
H	1.50282495	1.90583116	2.06489122
H	2.49894336	4.17697438	-2.16173029
H	2.50402241	4.17910062	2.15407530
N	1.46760316	1.81267368	-0.00145439
C	2.58230431	4.36653694	-0.00402162
H	3.01230009	5.36258339	-0.00501068
C	-2.87127118	-4.36694624	0.01940685
H	-3.33918997	-4.99350862	-0.74593320

H	-1.79620789	-4.33004630	-0.16594906
H	-3.03810391	-4.84518265	0.99099658

Name - TSNMe2\\SCF E(UB3LYP-D3BJ/BS1)=-2712.6934341\\G=-
 2712.308995\\H=-2712.211513\\SCF E(UB3LYP-D3BJ/BS2)=-2713.0725301
 \\ZeroPoint=0.449986

C	-0.89224438	-3.70584967	1.24278790
C	-2.41931223	-2.15237493	-0.04728572
Mo	0.63465728	0.12313922	-0.01352324
S	-0.41490675	-1.02526157	-1.83878072
S	-0.50309182	-0.98195502	1.79833845
S	1.65490996	1.63635478	-1.68965352
S	1.54921443	1.67679097	1.66691448
C	-3.35138879	-0.97520775	-0.05817179
N	-2.99174031	0.37151198	-0.16719852
C	-4.12261915	1.07527653	-0.12840989
N	-5.19260158	0.24329391	0.01892075
C	-4.71070932	-1.05972163	0.05649273
H	-6.16329117	0.51770925	0.06342981
C	-0.86884958	-3.72590186	-1.27452357
H	-5.37044194	-1.90558636	0.16748415
C	-1.62920212	-2.35659162	1.26535911
C	-1.59194148	-2.36999742	-1.33268848
N	3.29892498	4.79020683	0.00932446
C	-0.02925361	-3.88850055	-0.00654686
H	-0.25319171	-3.85317953	-2.17003418
H	-1.63809104	-4.51102447	-1.29886386
H	-1.65531876	-4.49704682	1.26786643
H	-0.29192495	-3.81168746	2.15138834
H	0.78178482	-3.15663577	-0.00587382
H	0.43576669	-4.88048330	0.00605022
H	-2.30346726	-2.38737742	-2.16305794
H	-2.37048310	-2.37866373	2.06918022
C	2.96662163	4.09308068	-1.12680406
H	3.20472764	4.46873274	-2.10977768
C	2.32821922	2.92780115	-0.72535891
C	2.28139665	2.94487850	0.71814127
C	2.89320890	4.12011364	1.13533211
H	3.06573327	4.51719375	2.12358284
H	3.78145990	5.67874595	0.01488894
H	-1.46380941	0.91964018	-0.10183978
H	-0.77067298	1.40000758	-0.06132483
H	-3.09795387	-3.01881309	-0.05212754
C	2.86640673	-1.69770147	1.22350617
C	2.95289919	-1.68782215	-1.09493109
C	3.90927731	-2.61107228	1.29805690
H	2.38034207	-1.32132486	2.11373275
C	3.99798257	-2.60150606	-1.09952346
H	2.53721241	-1.30137493	-2.01601015
H	4.25344843	-2.94919367	2.26854966

H	4.41301364	-2.93212034	-2.04452865
N	2.39119875	-1.24149323	0.04689410
C	4.48646532	-3.07643936	0.11719415
H	5.30015545	-3.79365147	0.14441511
N	-4.24027563	2.44264716	-0.28579262
C	-2.98800999	3.18645451	-0.13910696
H	-3.19226860	4.24186152	-0.32424861
H	-2.55089199	3.08087388	0.86389790
H	-2.25897998	2.84405835	-0.87435426
C	-5.38199483	3.06228555	0.39521932
H	-5.32975170	2.95017122	1.48722942
H	-5.39355397	4.12521637	0.15153170
H	-6.32342677	2.63684942	0.04022005

Name - TSNO2\\SCF E(UB3LYP-D3BJ/BS1)=-2783.1890256\\G=-2782.874729\\H=-2782.780104\\SCF E(UB3LYP-D3BJ/BS2)=-2783.6027824\\ZeroPoint=0.378818

C	-1.28951692	-3.57575820	1.25831267
C	-2.67192769	-1.88122954	0.00010289
Mo	0.57110681	0.13860322	0.00045637
S	-0.63445517	-0.89947651	-1.82436688
S	-0.63441453	-0.89957071	1.82480338
S	1.72613694	1.52516240	-1.67625627
S	1.73063256	1.52240283	1.67729242
C	-3.43814234	-0.59692305	-0.00018911
N	-2.90781965	0.66845394	0.00029320
C	-3.92724198	1.51946483	-0.00045871
N	-5.10488991	0.86286797	-0.00141969
C	-4.82293753	-0.46936613	-0.00125034
H	-6.02017846	1.30399832	-0.00206816
C	-1.28933959	-3.57583099	-1.25784242
H	-5.59759767	-1.22011469	-0.00189979
C	-1.88949360	-2.16129952	1.30569547
C	-1.88934085	-2.16139102	-1.30538071
N	3.88083315	4.36596844	-0.00026608
C	-0.45671069	-3.82350611	0.00029809
H	-0.69621362	-3.74774549	-2.16065024
H	-2.12554227	-4.28906726	-1.28078408
H	-2.12575457	-4.28895392	1.28115203
H	-0.69654620	-3.74766872	2.16122470
H	0.41568662	-3.16743201	0.00032237
H	-0.08333581	-4.85331572	0.00036785
H	-2.62004107	-2.12190151	-2.11797416
H	-2.62023234	-2.12167218	2.11824246
C	3.41068457	3.74720182	-1.13187577
H	3.67158713	4.09828208	-2.11815854
C	2.61527781	2.68562649	-0.72169454
C	2.61737083	2.68437309	0.72216787
C	3.41401930	3.74518524	1.13173873
H	3.67780774	4.09467518	2.11781788
H	4.49345481	5.17021398	-0.00047550

H	-1.63126320	1.01853395	0.00088232
H	-0.73589454	1.41437488	0.00139166
H	-3.45218176	-2.65545915	0.00013372
C	2.64489132	-1.96988551	1.15819994
C	2.64573174	-1.96809535	-1.15886706
C	3.57019103	-3.00493748	1.19896434
H	2.24227960	-1.53678869	2.06484673
C	3.57111970	-3.00305037	-1.20053751
H	2.24376839	-1.53360824	-2.06513968
H	3.90631953	-3.38445004	2.15699144
H	3.90800674	-3.38105169	-2.15889455
N	2.18562272	-1.45807964	-0.00010979
C	4.04220306	-3.53579416	-0.00102599
H	4.76177253	-4.34797045	-0.00138271
N	-3.82579236	2.93207505	-0.00030766
O	-4.88639530	3.56965241	-0.00113173
O	-2.69429108	3.42682172	0.00061271

Name - TStBu\\SCF E(UB3LYP-D3BJ/BS1)=-2735.9933439\\G=-2735.572886\\H=-2735.471031\\SCF E(UB3LYP-D3BJ/BS2)=-2736.3659919\\ZeroPoint=0.489012

C	0.01056331	-3.87625183	1.25813165
C	-1.80786344	-2.64837345	-0.00048418
Mo	0.74242049	0.18250852	-0.00047768
S	-0.11895026	-1.13230520	-1.81979494
S	-0.11976071	-1.13231457	1.81934711
S	1.39615899	1.87403779	-1.67972215
S	1.39119492	1.87444159	1.67869748
C	-2.94793553	-1.67094468	-0.00024232
N	-2.85715348	-0.28186152	-0.00123008
C	-4.09614510	0.20100021	-0.00028230
N	-4.98337195	-0.83226904	0.00131427
C	-4.27646602	-2.01612098	0.00133246
H	-5.99030958	-0.73729914	0.00228688
C	0.01057566	-3.87613239	-1.25916793
H	-4.76564879	-2.97759533	0.00238675
C	-0.97390915	-2.69588632	1.29909646
C	-0.97381483	-2.69568684	-1.29998608
N	2.40257431	5.29187240	0.00097385
C	0.87914004	-3.87573653	-0.00051250
H	0.62945262	-3.86963443	-2.16144208
H	-0.58348301	-4.80099372	-1.28370702
H	-0.58339942	-4.80118380	1.28257737
H	0.62944667	-3.86976612	2.16039827
H	1.52742714	-2.99681433	-0.00046782
H	1.53292466	-4.75494319	-0.00056635
H	-1.68208225	-2.86015403	-2.11687565
H	-1.68232289	-2.86074678	2.11578597
C	2.18490005	4.54664769	-1.13115650
H	2.30724182	4.96720634	-2.11716228

C	1.81515797	3.27227305	-0.72221980
C	1.81289111	3.27240431	0.72226387
C	2.18129933	4.54688623	1.13236321
H	2.30055498	4.96742233	2.11875740
H	2.69264369	6.26039038	0.00137410
H	-1.47093249	0.55664363	-0.00161986
H	-0.88016426	1.16197685	-0.00210652
H	-2.30677616	-3.62933297	-0.00063948
C	3.32456624	-1.16358896	1.16104944
C	3.32575850	-1.16371500	-1.15917529
C	4.52583615	-1.85826562	1.20128570
H	2.80721170	-0.87733819	2.06719838
C	4.52701525	-1.85847154	-1.19811094
H	2.80942061	-0.87744542	-2.06590001
H	4.96273260	-2.11312603	2.15985258
H	4.96485755	-2.11349873	-2.15620144
N	2.72948263	-0.82054935	0.00061448
C	5.14041357	-2.21634702	0.00192390
H	6.07727214	-2.76339594	0.00242945
C	-4.53302213	1.64689817	-0.00038265
C	-5.37887480	1.91709242	1.26201798
H	-6.27780566	1.29274577	1.28453836
H	-4.79987508	1.71776533	2.16933007
H	-5.69603613	2.96463650	1.27855535
C	-3.31257867	2.57712079	-0.00436887
H	-2.68899756	2.42266062	0.88057984
H	-2.69270401	2.41998460	-0.89146320
H	-3.65323146	3.61684174	-0.00519066
C	-5.38565748	1.91512669	-1.25863270
H	-6.28471137	1.29078571	-1.27552305
H	-5.70295925	2.96262807	-1.27497141
H	-4.81151485	1.71455088	-2.16875441

4. Optimized geometries of final catalyst MoIIIItBu, MoIIIIiPr and WIIIIItBu along with their thermochemical data and single point energies.

MoIIIIiPr

Name-MoIIIIiPr\\SCF E(UB3LYP-D3BJ/BS1)=-2560.5303876\\G=-2560.225030\\H=-2560.137862\\ZeroPoint=0.364643

C	4.42394257	-0.53065664	-1.25840454
C	2.95710905	1.10742662	-0.00000415
Mo	0.09560849	-0.67660070	0.00009932
S	1.69938956	-0.81859552	1.77418761
S	1.69921177	-0.81842342	-1.77427135
S	-1.72142127	-0.68216334	1.67046737
S	-1.72122579	-0.68202802	-1.67027451
C	1.75384140	1.99162944	0.00009063
N	0.44956814	1.49918069	0.00010236

C	-0.38395793	2.54504415	0.00015097
N	0.35183639	3.68263910	0.00015051
C	1.69438066	3.35738167	0.00011288
H	-0.03721478	4.61694813	0.00028657
C	4.42406645	-0.53078138	1.25809821
H	2.46924295	4.10707665	0.00009503
C	3.12462708	0.28701363	-1.30240032
C	3.12475639	0.28688948	1.30229296
C	-0.04484782	-2.75701334	0.00012809
N	-5.25046788	-1.19687742	-0.00018385
C	4.52133734	-1.39597428	-0.00020061
H	4.50729298	-1.14098011	2.16240957
H	5.26139967	0.18071766	1.27217920
H	5.26127666	0.18084212	-1.27249761
H	4.50708587	-1.14076884	-2.16278260
H	3.71297389	-2.13662862	-0.00020054
H	5.46715559	-1.94778965	-0.00027178
H	3.82162807	1.78498169	-0.00000632
H	3.17934265	1.00428448	2.12609202
H	3.17914885	1.00450192	-2.12612160
O	-0.12702745	-3.90152241	0.00014853
C	-4.48002032	-1.09743757	1.13122197
H	-4.91296864	-1.15785436	2.11758120
C	-3.16546722	-0.92068213	0.72160268
C	-3.16536597	-0.92065200	-0.72163447
C	-4.47987193	-1.09739407	-1.13145483
H	-4.91265386	-1.15776205	-2.11789081
H	-6.25124313	-1.34214364	-0.00025348
C	-1.88043071	2.52827259	0.00010148
C	-2.43874619	3.18505927	1.27199585
H	-2.04655735	2.69665614	2.16887795
H	-2.17985769	4.24852013	1.31713035
H	-3.52964991	3.10091609	1.28358387
C	-2.43865517	3.18378625	-1.27249804
H	-2.17983842	4.24722168	-1.31862107
H	-2.04634252	2.69453348	-2.16885750
H	-3.52955249	3.09955064	-1.28411696
H	-2.17201657	1.47988304	0.00060301

Name-MoIIIIiPr\\SCF E(UB3LYP-D3BJ/BS1)=-2561.6594904\\G=-2561.342948\\H=-2561.250782\\ZeroPoint=0.379340

C	2.02054056	-3.44258167	-1.20978691
C	2.84237665	-1.37180051	-0.02744123
Mo	-0.86243627	-0.41673401	-0.01616866
S	0.60718598	-0.95909126	1.78444608
S	0.53049376	-1.15367622	-1.80218092
S	-2.42630647	0.54894433	1.64436303
S	-2.51716632	0.33085128	-1.70078384
C	3.26453766	0.06746556	-0.05709911
N	2.43076661	1.15037343	-0.28073949
C	3.17992652	2.24191322	-0.19030004

N	4.47194301	1.90163198	0.08109336
C	4.54242534	0.52515468	0.16464416
H	5.24557945	2.54368440	0.18738541
C	2.01374437	-3.35198104	1.31668244
H	5.46926367	0.00865427	0.36051337
C	2.15234115	-1.91194765	-1.29533341
C	2.17736487	-1.82279000	1.29135086
C	-1.82405814	-2.19322232	0.12521293
N	-5.69786803	1.90800365	-0.03574006
C	1.32139551	-3.90510003	0.06980002
H	1.48386168	-3.65538538	2.22431598
H	3.02534488	-3.77618625	1.37935541
H	3.03918794	-3.85365161	-1.23162597
H	1.50279685	-3.82216126	-2.09544217
H	0.27520895	-3.59080941	0.05332947
H	1.31578245	-4.99962567	0.11020202
H	2.85287064	-1.53199076	2.10048730
H	2.79386697	-1.66015722	-2.14434214
O	-2.40290449	-3.18287735	0.20797022
C	-4.96764008	1.66303355	1.09639581
H	-5.34162025	1.90899542	2.07766117
C	-3.76820512	1.08764217	0.69284076
C	-3.80832346	0.99175345	-0.75547600
C	-5.03018953	1.51305822	-1.16440485
H	-5.45847586	1.62903825	-2.14743077
H	-6.61896591	2.32817519	-0.03804260
H	0.52107921	1.32141496	-0.19883211
H	-0.22314327	1.55841224	-0.14376645
H	3.78998276	-1.93115514	-0.01597744
C	2.66671306	3.64928221	-0.29899178
C	3.77297575	4.65474849	-0.63635336
H	3.34257032	5.65054382	-0.77469557
H	4.50678311	4.72483377	0.17488573
H	4.30130097	4.38060601	-1.55473790
C	1.92860277	4.04646209	0.99326172
H	1.11510319	3.34881385	1.21234180
H	2.61816459	4.04687657	1.84449741
H	1.50452273	5.05109490	0.89572572
H	1.93612507	3.64677045	-1.11630406

Name-MoIII2iPr\\SCF E(UB3LYP-D3BJ/BS1)=-2561.6765924\\G=-
2561.355598\\H=-2561.264551\\ZeroPoint= 0.382928

C	1.35829915	-3.60577149	-1.10676412
C	2.65680251	-1.75026376	0.00407551
Mo	-0.81247096	-0.00955297	-0.00185585
S	0.59513084	-0.81346666	1.81871121
S	0.45606217	-1.02719734	-1.76413066
S	-2.43479558	0.70457352	1.66413098
S	-2.37050951	1.02516095	-1.68590368
C	3.34748581	-0.42804786	-0.09284001

N	2.73323887	0.81820323	-0.10720757
C	3.64190240	1.79734057	-0.19340485
N	4.84175877	1.19781844	-0.23529609
C	4.68760571	-0.17672405	-0.17538312
H	5.72671735	1.68657927	-0.29990339
C	1.46426476	-3.46797954	1.40931693
H	5.52997105	-0.84830073	-0.19473472
C	1.83988672	-2.15166920	-1.24431035
C	1.93646554	-2.00680832	1.34776795
C	-2.17393816	-1.74295019	-0.18237703
N	-5.90198815	1.55787506	0.01674685
C	0.61364366	-3.86765340	0.20365298
H	0.92127882	-3.63643418	2.34366132
H	2.36218243	-4.10161902	1.43901276
H	2.25078253	-4.24599242	-1.14279696
H	0.73958932	-3.86985603	-1.96917508
H	-0.32567322	-3.30927533	0.21843707
H	0.35020998	-4.92866976	0.27024158
H	2.67920494	-1.85048826	2.13483029
H	2.51747907	-2.08957241	-2.10055027
O	-2.98497903	-2.52740617	-0.37403669
C	-5.15554936	1.29823701	1.13286819
H	-5.59214149	1.28834551	2.11960711
C	-3.84986463	1.07357837	0.71111018
C	-3.82991983	1.20069852	-0.72649937
C	-5.12335068	1.50023582	-1.11996632
H	-5.54494205	1.67306591	-2.09803534
H	-6.89270618	1.75882766	0.02348185
H	1.71654891	0.98548754	-0.05149869
H	0.15957189	1.45615652	-0.06426779
H	3.48350483	-2.47477921	0.00905697
C	3.34602535	3.26404833	-0.21791588
C	4.62078084	4.09595507	-0.38360803
H	4.35644107	5.15454638	-0.43836998
H	5.29337383	3.96046008	0.47017240
H	5.15997483	3.83386237	-1.29905559
C	2.56249031	3.66523357	1.04580368
H	1.62858904	3.10285624	1.13305072
H	3.16310579	3.48625980	1.94314196
H	2.31794217	4.72987285	0.99813975
H	2.69915378	3.43197975	-1.08799278

Name-MoIII3iPr\\SCF E(UB3LYP-D3BJ/BS1)=-2750.2769268\\G=-
 2749.943871\\H=-2749.845449\\ZeroPoint=0.398894

C	-1.85318987	3.62044212	-1.35851252
C	-2.50056155	1.77884756	0.25697876
Mo	1.14111586	0.78421820	-0.07951644

S	-0.03790495	1.69933414	1.77526854
S	-0.51686449	1.16676950	-1.74359662
S	2.75000040	-0.13298050	1.53597384
S	2.36996559	-0.52684065	-1.76505692
C	-2.73079204	0.32130538	0.50937223
N	-3.25313651	-0.54525997	-0.44670905
C	-3.37590480	-1.78730980	0.04473399
N	-2.98475331	-1.71890306	1.32248729
C	-2.56476574	-0.43644652	1.63213748
H	-2.88910029	-2.52333721	1.93083684
C	-1.55862636	3.96300674	1.11642638
H	-2.17964625	-0.18958464	2.60566005
C	-2.01339603	2.10347888	-1.17107963
C	-1.69047217	2.45552357	1.37922113
C	2.19259408	2.47056828	-0.44186280
N	4.76360179	-3.10395305	-0.03678670
C	-1.00056308	4.27414013	-0.27205427
H	-0.94518602	4.41750694	1.89920326
H	-2.56491540	4.39448070	1.20462291
H	-2.86230598	4.05334290	-1.32960427
H	-1.44710099	3.82204543	-2.35355834
H	0.03347365	3.92604012	-0.34699348
H	-0.97866263	5.35788080	-0.42589921
H	-2.24182327	2.31261992	2.31255432
H	-2.78150804	1.76613577	-1.87256600
O	2.79066482	3.43114220	-0.64916045
C	4.40914534	-2.37446020	1.06596595
H	4.79362368	-2.60457192	2.04695294
C	3.52494664	-1.39080883	0.63791182
C	3.36020356	-1.56194496	-0.79693003
C	4.15378710	-2.64033801	-1.17131442
H	4.31555407	-3.10237726	-2.13231076
H	5.39121527	-3.89819615	-0.01402036
H	-3.47889735	-0.30732367	-1.40545675
H	0.17576474	-1.03618061	0.27868981
H	-3.48635770	2.26691939	0.31304701
C	-3.87554231	-2.98600920	-0.69441441
C	-5.39729752	-2.87971484	-0.90783905
H	-5.74260817	-3.73710823	-1.49203239
H	-5.92113670	-2.88044403	0.05298748
H	-5.66180344	-1.96601637	-1.44767866
C	-3.48607479	-4.28361356	0.02093229
H	-2.40324710	-4.34905965	0.15606135
H	-3.97126137	-4.35678092	1.00052594
H	-3.81404569	-5.13733490	-0.57686897
H	-3.38401496	-2.96008027	-1.67327761
C	-0.10601935	-2.15464509	0.34229288
O	-0.51489578	-2.63741608	-0.73269586
O	0.03287710	-2.65392333	1.47468864

Name-MoIII4iPr\\SCF E(UB3LYP-D3BJ/BS1)=-2560.9603832\\G=-
2560.641313\\H=-2560.553889\\ZeroPoint= 0.378545

C	1.73062137	-3.52597728	-1.15431889
C	2.77516895	-1.53097048	-0.01095589
Mo	-0.85269332	-0.25926049	-0.02761094
S	0.59970037	-0.89864531	1.80826369
S	0.51033834	-1.07682347	-1.78631207
S	-2.54117772	0.36948536	1.64171942
S	-2.34417192	0.85840310	-1.66691579
C	3.31552466	-0.13832515	-0.08696547
N	2.57848939	1.04237991	-0.11447064
C	3.38202345	2.11439424	-0.16179401
N	4.63412544	1.63892690	-0.17092687
C	4.62202320	0.25549710	-0.12671497
H	5.46347887	2.22085757	-0.20679546
C	1.80572387	-3.40645629	1.36870623
H	5.52920855	-0.32557594	-0.12425649
C	2.02773457	-2.02149348	-1.26872484
C	2.09124787	-1.89698220	1.32543332
C	-1.92368184	-1.93538674	-0.14701195
N	-5.79858438	1.76395040	-0.00649935
C	1.02730027	-3.90369149	0.15053288
H	1.28107675	-3.65383559	2.29557247
H	2.77958843	-3.91324675	1.40403157
H	2.69955942	-4.04051417	-1.20110960
H	1.15128983	-3.85406420	-2.02168966
H	0.01454983	-3.49490753	0.16585090
H	0.92155053	-4.99209882	0.20271171
H	2.79835348	-1.65117169	2.12158715
H	2.68901777	-1.85676264	-2.12353337
O	-2.56046665	-2.88953222	-0.23315395
C	-5.14064071	1.32629597	1.10230277
H	-5.60684182	1.30671373	2.07485751
C	-3.85503993	0.96773729	0.69741716
C	-3.77242771	1.19948475	-0.72967347
C	-5.00159784	1.69447478	-1.12827530
H	-5.36795057	1.99149285	-2.09823571
H	-6.75474380	2.09672350	-0.00755274
H	1.57042246	1.11293188	-0.08019015
H	3.68081276	-2.15273919	-0.00700587
C	2.93597715	3.54170712	-0.18508260
C	4.12919222	4.50001203	-0.22707682
H	3.76349650	5.52775141	-0.28309447
H	4.74006567	4.40689360	0.67697670
H	4.76351159	4.31908127	-1.10012356
C	2.01416280	3.82803113	1.01515383
H	1.13529395	3.17604284	1.01961713
H	2.55455621	3.68811837	1.95632779

H	1.66692965	4.86316242	0.96349064
H	2.35051397	3.66472225	-1.10506325

Name-MoIII5iPr\\SCF E(UB3LYP-D3BJ/BS1)=-2562.1389904\\G=-
2561.818262\\H= -2561.716529\\ZeroPoint=0.392711

C	-2.33692652	3.53846894	-0.84754537
C	-2.90907434	1.18412432	-0.10611164
Mo	0.72724075	0.47375383	-0.03476872
S	-0.77770310	0.77134760	1.81718834
S	-0.54272196	1.57967199	-1.73566482
S	2.21450887	-0.73230677	1.52398683
S	2.49421449	0.07403657	-1.71076472
C	-2.91405073	-0.27333558	-0.45492035
N	-2.92690511	-1.29127739	0.49032043
C	-2.91698249	-2.49719430	-0.09517528
N	-2.94236054	-2.26684653	-1.41460443
C	-2.93270073	-0.90494070	-1.66609046
H	-2.93930269	-2.99421510	-2.12033035
C	-2.47574990	3.00392012	1.60246019
H	-2.94227198	-0.51522290	-2.66947704
C	-2.26612699	2.04847158	-1.21108945
C	-2.42198479	1.49358084	1.32479763
C	1.60932867	2.21783795	0.45739175
N	5.68335932	-1.54101074	-0.10527503
C	-1.76051092	3.83391045	0.53700751
H	-2.07067957	3.20268501	2.59823341
H	-3.53636625	3.28854899	1.62364425
H	-3.39723066	3.82487052	-0.86307089
H	-1.83440713	4.12646471	-1.62021211
H	-0.68660007	3.62316134	0.55111131
H	-1.87524081	4.89862272	0.76414178
H	-3.10928293	1.00645679	2.02311292
H	-2.83905885	1.88841928	-2.12845715
O	2.11561926	3.20920464	0.73732401
C	4.86795968	-1.55149051	0.99346089
H	5.19906431	-1.93976507	1.94353631
C	3.65369086	-0.99706840	0.60465838
C	3.77695148	-0.64360618	-0.79937932
C	5.06000839	-0.99888422	-1.19736338
H	5.55836326	-0.90926796	-2.14951644
H	6.63396787	-1.89020240	-0.10958760
H	-0.20725700	-1.30694692	-0.95083259
H	-3.95983675	1.51227742	-0.09653114
C	-2.79061327	-3.80777617	0.60911971
C	-1.30891636	-4.05572728	0.96302812
H	-1.22363305	-4.98083579	1.53976806

H	-0.70964663	-4.15620519	0.05300009
H	-0.90028573	-3.23504890	1.55979646
C	-3.37818909	-4.95567082	-0.21787188
H	-4.42766344	-4.77485263	-0.46638300
H	-2.81835709	-5.10094903	-1.14808415
H	-3.31363486	-5.88341858	0.35571546
H	-2.85223696	-1.16641674	1.49320141
H	-3.35647363	-3.70893011	1.54187298
H	-0.10910133	-1.57829524	-0.25023704

Name-MoIII6iPr\\SCF E(UB3LYP-D3BJ/BS1)=-2751.4605851\\G=-
2751.114971\\H=-2751.013088\\ZeroPoint=0.413601

C	-1.17810559	4.06772605	-1.00300681
C	-2.18634386	1.75857547	-0.71849834
Mo	1.19431911	0.45888637	-0.00794276
S	-0.57553838	0.86762265	1.51554784
S	0.51727812	1.97009546	-1.74785217
S	2.09935182	-1.20922806	1.59289311
S	3.15143216	-0.09963028	-1.38217117
C	-2.31787200	0.35864297	-1.24427550
N	-2.78369037	-0.69346429	-0.47102831
C	-2.78990675	-1.78504630	-1.23378382
N	-2.36818980	-1.46149316	-2.48211469
C	-2.05979804	-0.11453282	-2.50874729
H	-2.26977799	-2.10594534	-3.25539951
C	-1.92221664	3.30745539	1.27316360
H	-1.69532025	0.36553261	-3.40149554
C	-1.21321240	2.62849703	-1.53800936
C	-1.98868503	1.84568239	0.80628205
C	2.24124908	1.93699118	0.87506055
N	5.64454141	-2.48209499	0.47141593
C	-0.89221463	4.12971661	0.49793382
H	-1.72646563	3.34049617	2.34870636
H	-2.91896697	3.74136656	1.11507036
H	-2.16457131	4.51047665	-1.19783452
H	-0.44732756	4.65237356	-1.56880146
H	0.11700180	3.75673218	0.70275387
H	-0.92020735	5.17048563	0.83695047
H	-2.84855167	1.36902481	1.28198756
H	-1.57872187	2.65085483	-2.56854906
O	2.83359499	2.78226475	1.37926946
C	4.63255059	-2.46560771	1.40051522
H	4.69967564	-3.02662833	2.31914816
C	3.63410758	-1.64047313	0.90475096
C	4.09080989	-1.15000148	-0.38160985
C	5.35034363	-1.69891251	-0.60780857

H	6.03233578	-1.59020436	-1.43632834
H	6.50504447	-3.00462950	0.57742791
H	-0.07816747	-0.87017715	-1.18713747
H	-3.15945110	2.25378967	-0.87043453
C	-3.12010491	-3.16828739	-0.75626466
C	-1.95396679	-3.71939526	0.08750682
H	-2.20732958	-4.71018317	0.47746450
H	-1.04834479	-3.80999230	-0.52189138
H	-1.73662036	-3.06103665	0.93270286
C	-3.47270126	-4.11430969	-1.90850903
H	-4.29819045	-3.72484947	-2.51202168
H	-2.61133244	-4.27835631	-2.56605047
H	-3.77066988	-5.08769206	-1.50971293
H	-3.13543687	-0.85811543	1.01170823
H	-3.99270047	-3.06907182	-0.10019079
H	0.22603772	-1.38485728	-0.71742398
O	-5.31812557	-1.27406027	3.15863249
O	-3.41211534	-1.06181628	2.00604300
C	-4.72562715	-1.05213132	2.11128948
H	-5.25901926	-0.82365303	1.17285998

Name-MoIII21iPr\\SCF E(UB3LYP-D3BJ/BS1)=-2750.9919448\\G=-
2750.655125\\H=-2750.554520\\ZeroPoint=0.404140

C	-0.96706988	4.23255095	-0.40293981
C	-2.18936153	2.03559600	-0.14549894
Mo	0.99962390	0.14006138	-0.23058619
S	-0.26932050	0.81992849	1.66924698
S	0.33217007	2.05177826	-1.58957649
S	2.06077696	-1.67754285	1.11604541
S	2.73948847	-0.34085373	-1.91636294
C	-2.63395616	0.75110482	-0.78237829
N	-3.15487485	-0.32029885	-0.06947895
C	-3.48203491	-1.26710696	-0.95046327
N	-3.21531796	-0.82449625	-2.20423552
C	-2.67924269	0.44566356	-2.11945900
H	-3.36711897	-1.34777654	-3.05581162
C	-1.44556627	3.32277814	1.89043533
H	-2.36899075	0.98818884	-2.99632885
C	-1.25083385	2.86549116	-1.04548617
C	-1.71720211	1.92329741	1.31579934
C	2.61099406	1.47752563	0.62051054
N	5.78807693	-2.11764736	-0.14261398
C	-0.45307203	4.11092715	1.03271501
H	-1.09028250	3.23349107	2.92135362
H	-2.40193731	3.86339466	1.92463574
H	-1.90957694	4.79880871	-0.39692082
H	-0.26256334	4.79105806	-1.02630625

H	0.51864944	3.60338183	1.03471024
H	-0.29845292	5.10776544	1.45985663
H	-2.52077138	1.45519743	1.89146734
H	-1.77576379	3.03838834	-1.98972027
O	3.42882589	2.15690710	1.03846523
C	4.82410242	-2.31148480	0.82113986
H	5.04295337	-2.83878159	1.73700333
C	3.65227645	-1.72728252	0.36639564
C	3.94067945	-1.15640919	-0.92751450
C	5.27527683	-1.41643471	-1.20525292
H	5.88376705	-1.15801217	-2.05832894
H	6.74617959	-2.42956523	-0.06862646
H	-3.00870347	-0.79479784	1.39518939
H	-0.16887708	-0.96797296	-0.89664871
H	-3.08992516	2.66746357	-0.06210894
C	-4.05631942	-2.61557093	-0.61616173
C	-4.26583449	-3.47744384	-1.86518611
H	-4.64753335	-4.45998559	-1.57547001
H	-4.99665284	-3.02175599	-2.54285878
H	-3.33180873	-3.62941536	-2.41547893
C	-5.36123066	-2.46507868	0.18369689
H	-5.19654447	-1.90503888	1.10731615
H	-6.11856072	-1.94064511	-0.40873199
H	-5.75371544	-3.45191501	0.44790942
H	-3.32539390	-3.12083146	0.02842950
O	-2.83414132	-1.24916773	2.32315019
C	-1.74725789	-1.99464124	2.21453980
O	-1.25432332	-2.59949226	3.15904203
H	-1.32658337	-2.04595636	1.20013152

Name-MoIII22iPr\\SCF E(UB3LYP-D3BJ/BS1)=-2561.1936981\\G=-
2560.887953\\H=-2560.795581\\ZeroPoint= 0.368804

C	-1.37096228	3.30765420	-1.71210416
C	-2.40928083	1.79379658	0.03513453
Mo	0.85932421	-0.08828513	0.11214485
S	-0.03569143	1.52467905	1.70945770
S	-0.41299834	0.67747675	-1.74092673
S	2.61837674	-0.52620781	1.78004825
S	2.13569337	-1.68536015	-1.36285445
C	-2.97034963	0.44541623	0.37266520
N	-3.73911136	-0.26017400	-0.54639343
C	-4.11607668	-1.37711116	0.06134005
N	-3.63501020	-1.41072212	1.33910906
C	-2.90393501	-0.25742425	1.55017662
H	-3.76899373	-2.16223772	2.00193468
C	-1.17518797	3.87688151	0.73068439

H	-2.39853879	-0.06505403	2.48136416
C	-1.78781411	1.86862978	-1.37240518
C	-1.55036673	2.44198567	1.13631646
C	2.38888245	1.40236740	-0.58350211
N	5.86199199	-1.86300371	-0.02798202
C	-0.48390554	3.93243609	-0.63326903
H	-0.54659101	4.32541385	1.50569982
H	-2.10217056	4.46679720	0.68594232
H	-2.29171842	3.90109551	-1.80344292
H	-0.87832830	3.33075134	-2.68891692
H	0.47135500	3.39895545	-0.58231131
H	-0.25664410	4.97161336	-0.89560653
H	-2.16642826	2.48592078	2.03986082
H	-2.55641434	1.54777867	-2.07939597
O	3.21269315	2.10125866	-0.95781328
C	5.25885922	-1.30028340	1.06749798
H	5.81873270	-1.04919758	1.95538795
C	3.91075194	-1.15306666	0.76988886
C	3.70851358	-1.64450020	-0.57122565
C	4.94213919	-2.07417959	-1.03260459
H	5.23345530	-2.50470308	-1.97839123
H	6.84725515	-2.07582452	-0.09643089
H	-0.19280300	-1.38832828	0.61988509
H	-3.27274846	2.47682946	-0.04493527
C	-4.92279203	-2.48771907	-0.54229606
C	-6.13371969	-2.85298840	0.33039022
H	-6.73807620	-3.62210395	-0.16066356
H	-5.81407472	-3.25112546	1.30018395
H	-6.76920579	-1.98115216	0.51417926
C	-4.04412000	-3.72290373	-0.80979621
H	-3.19006244	-3.46833146	-1.44517733
H	-3.65862560	-4.13523017	0.12921810
H	-4.62447131	-4.50543140	-1.30942282
H	-5.28305866	-2.10458218	-1.50261826

Name-MoIII23iPr\\SCF E (UB3LYP-D3BJ/BS1)=-2749.7997596\\G=-
2749.481082\\H=-2749.382491\\ZeroPoint= 0.384750

C	-1.76172900	3.63889000	-1.36551200
C	-2.45621500	1.79045100	0.22881700
Mo	1.17829500	0.74606100	-0.07608300
S	-0.00390900	1.66765400	1.76904900
S	-0.44156900	1.18589100	-1.74428500
S	2.75739400	-0.20164300	1.55502500
S	2.42113200	-0.56974800	-1.75506900
C	-2.76756500	0.33705700	0.43390100
N	-3.44267400	-0.39604500	-0.53430600
C	-3.60112400	-1.61562700	-0.03611400
N	-3.09116900	-1.68326400	1.22819200
C	-2.53900900	-0.45479000	1.53303200
H	-2.97707700	-2.52449500	1.77650700

C	-1.48881500	3.95148600	1.12164600
H	-2.03488800	-0.27910300	2.46823300
C	-1.94397200	2.12462400	-1.18494000
C	-1.64756000	2.44173700	1.36239100
C	2.24992200	2.42010400	-0.40904900
N	4.77710600	-3.17551200	-0.00776600
C	-0.91727200	4.27404900	-0.25993300
H	-0.87315500	4.39027100	1.91225700
H	-2.48893300	4.39777600	1.20908100
H	-2.76564800	4.08516000	-1.34879700
H	-1.33697400	3.84781200	-2.35186400
H	0.11453900	3.91769300	-0.32819500
H	-0.88325900	5.35976400	-0.39995900
H	-2.20454400	2.29159800	2.29157300
H	-2.69873100	1.77103600	-1.88966000
O	2.86009900	3.37782500	-0.60057600
C	4.41201200	-2.44913100	1.09323300
H	4.77978800	-2.68751000	2.07871600
C	3.53954000	-1.45745500	0.65812400
C	3.39337400	-1.61884800	-0.77841800
C	4.18470500	-2.69974300	-1.14814500
H	4.35669100	-3.15734100	-2.10954200
H	5.39707400	-3.97527200	0.01916700
H	0.16404700	-1.06301300	0.26810800
H	-3.41870100	2.32832800	0.27064200
C	-4.29485500	-2.76036500	-0.71646500
C	-5.80705300	-2.72984700	-0.42682400
H	-6.31785100	-3.52940200	-0.97349000
H	-5.99744900	-2.87297500	0.64246300
H	-6.24640200	-1.77358300	-0.72612500
C	-3.68868700	-4.11828800	-0.33623500
H	-2.61042000	-4.13673100	-0.51606200
H	-3.86459000	-4.34879100	0.72112900
H	-4.15516500	-4.91450200	-0.92403900
H	-4.15138700	-2.60147500	-1.79087200
C	-0.12129300	-2.17953600	0.30941800
O	-0.52288300	-2.64334900	-0.77779500
O	0.01611200	-2.70436800	1.43140700

Name-TS12\\SCF E(UB3LYP-D3BJ/BS1)=-2561.6585738\\G=-2561.342815\\H=-2561.252596\\ZeroPoint=0.377275

C	-2.16968659	-3.27945391	1.37047736
C	-2.88699809	-1.29161783	-0.01721671
Mo	0.82198621	-0.42641404	-0.01338845
S	-0.58024308	-1.19290613	-1.80028104
S	-0.63725645	-0.97026790	1.80743045
S	2.47230819	0.28037720	-1.71348924
S	2.41290391	0.52043037	1.62932453
C	-3.23453161	0.16489209	-0.09707026
N	-2.33424097	1.21788536	-0.15168607

C	-3.03024655	2.34966106	-0.19568730
N	-4.35659795	2.06013648	-0.17274039
C	-4.50432375	0.68797090	-0.11194333
H	-5.10572621	2.73881108	-0.20358925
C	-2.14365507	-3.42419572	-1.14812723
H	-5.47355567	0.21565537	-0.08560369
C	-2.25384643	-1.74462805	1.31641675
C	-2.21887716	-1.89289219	-1.27238167
C	1.77223504	-2.25001440	0.12798784
N	5.72231316	1.75250937	-0.08301890
C	-1.47363542	-3.88123242	0.14862854
H	-1.63312108	-3.84173789	-2.02073680
H	-3.17600424	-3.80015842	-1.16878131
H	-3.20111461	-3.65588434	1.41478613
H	-1.67547729	-3.59086452	2.29526987
H	-0.41846118	-3.59511814	0.14239190
H	-1.50073304	-4.97436176	0.21157867
H	-2.85825174	-1.64169465	-2.12323342
H	-2.91898383	-1.40337772	2.11453380
O	2.33154321	-3.24949835	0.20697079
C	5.03166409	1.37457040	-1.20360053
H	5.45521121	1.47026340	-2.19092179
C	3.79612440	0.89753347	-0.78147258
C	3.77060548	1.00222140	0.66521818
C	4.99162034	1.53826859	1.05628501
H	5.38194615	1.77600055	2.03325799
H	6.65692152	2.14084565	-0.09465893
H	-0.79495879	1.21215529	-0.14602517
H	0.06896153	1.35274204	-0.14743426
H	-3.86488738	-1.79522829	-0.00161442
C	-2.43856063	3.72947085	-0.23052980
C	-1.62216699	3.98881972	1.04866809
H	-1.15370626	4.97670750	1.00049645
H	-2.27100324	3.95840725	1.93055285
H	-0.83486689	3.24067347	1.17552129
C	-3.50380183	4.80998166	-0.44080727
H	-4.07359438	4.64365438	-1.36045968
H	-4.20597807	4.84193531	0.40014623
H	-3.02667713	5.79095645	-0.51166814
H	-1.74694210	3.75300557	-1.08196792

Name-TS23\\SCF E(UB3LYP-D3BJ/BS1)=-2750.2555602\\G=-2749.931026\\H=-2749.828073\\ZeroPoint=0.394709

C	-1.55342219	3.70918597	-1.47125325
C	-2.37971350	2.00044167	0.19460857
Mo	0.96153316	0.33136553	0.01741236
S	0.06349473	1.75743885	1.75376338
S	-0.43192694	1.15184429	-1.78282327
S	2.61516303	-0.48035776	1.66782794
S	2.21770601	-1.02391862	-1.61953517

C	-2.77873869	0.59137550	0.49868673
N	-3.33596312	-0.26276312	-0.44624700
C	-3.63322142	-1.45474470	0.09288140
N	-3.29761954	-1.36570399	1.38669930
C	-2.76320815	-0.11832350	1.66416660
H	-3.37877100	-2.12770536	2.04944069
C	-1.24508845	4.10787090	0.98888957
H	-2.40334762	0.13585113	2.64549819
C	-1.85075076	2.21876806	-1.24006243
C	-1.51608027	2.62927576	1.30633914
C	2.36717949	1.95880810	-0.42332531
N	5.68660709	-2.16174892	-0.14069859
C	-0.63837550	4.30432664	-0.40087878
H	-0.60214603	4.53357541	1.76426706
H	-2.20598041	4.63909882	1.03844804
H	-2.51429857	4.24239536	-1.45462657
H	-1.13048677	3.84155776	-2.47093952
H	0.34783275	3.83117590	-0.44740795
H	-0.49002281	5.37213060	-0.59365463
H	-2.09513900	2.57754925	2.23315426
H	-2.64911981	1.93490976	-1.93313291
O	3.11449467	2.79315561	-0.65485576
C	5.11069017	-1.66557830	1.00281163
H	5.62983753	-1.67925918	1.94848730
C	3.84879588	-1.19900659	0.66155512
C	3.67820633	-1.43036459	-0.75406054
C	4.84357957	-2.02775920	-1.21531316
H	5.12841615	-2.35761234	-2.20232503
H	6.61348834	-2.56297158	-0.18681617
H	-3.46725639	-0.05104984	-1.42836519
H	-0.18194200	-0.96912720	0.35356517
H	-3.30848082	2.59285071	0.21817642
C	-4.24821888	-2.61933851	-0.61524619
C	-5.72115183	-2.31544370	-0.94965591
H	-6.14697002	-3.15413641	-1.50720826
H	-6.30239621	-2.17641802	-0.03290043
H	-5.81374584	-1.41320814	-1.56069133
C	-4.10754077	-3.91075214	0.19731523
H	-3.06202781	-4.13457256	0.42659020
H	-4.66637585	-3.84955043	1.13758042
H	-4.51719261	-4.74364728	-0.37890204
H	-3.69440040	-2.72852345	-1.55412092
C	-0.57678683	-2.68972900	0.16331152
O	-0.95065338	-2.72736886	-0.96168894
O	-0.32546040	-3.08495371	1.25328751

Name-TS5,6\\SCF E(UB3LYP-D3BJ/BS1)=-2751.4593624\\G=-2751.107567\\H=-2751.015782\\ZeroPoint=0.409831

C	-1.13440979	4.06356367	-1.00706924
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C	-2.16865544	1.77106336	-0.69448321
Mo	1.21435645	0.44293248	-0.00689051
S	-0.54474424	0.86893010	1.52665017
S	0.52503439	1.93739938	-1.75744278
S	2.13093501	-1.20497223	1.60662476
S	3.15611847	-0.13969728	-1.39398719
C	-2.32162552	0.37249343	-1.21531602
N	-2.80651037	-0.67583915	-0.44778997
C	-2.83026239	-1.77881274	-1.19823780
N	-2.39937917	-1.45999764	-2.43804002
C	-2.06901709	-0.11807641	-2.47137640
H	-2.30661602	-2.10995727	-3.20799039
C	-1.86067798	3.32803014	1.28277563
H	-1.69069638	0.34916743	-3.36470893
C	-1.19323802	2.62160392	-1.53209216
C	-1.95121370	1.86373302	0.82797018
C	2.27572849	1.92671220	0.84808865
N	5.65593021	-2.51105099	0.46334632
C	-0.83037839	4.13253173	0.48987817
H	-1.65176771	3.36538645	2.35559910
H	-2.85398747	3.77278039	1.13359864
H	-2.11757236	4.51689723	-1.19383927
H	-0.40312994	4.63472835	-1.58570806
H	0.17676950	3.74993266	0.68599875
H	-0.84279235	5.17590148	0.82155530
H	-2.81130516	1.40212536	1.31770980
H	-1.57114856	2.64205710	-2.55815129
O	2.87704015	2.77453576	1.33683459
C	4.65488756	-2.47672561	1.40346731
H	4.72965178	-3.02539765	2.32892217
C	3.65497273	-1.65343710	0.90742901
C	4.09982502	-1.18276783	-0.39086734
C	5.35400458	-1.74137376	-0.62329830
H	6.02723457	-1.64790342	-1.46077885
H	6.51475234	-3.03699577	0.56679608
H	-0.06320369	-0.90717009	-1.16609188
H	-3.13808409	2.27473160	-0.83926061
C	-3.19441832	-3.14931260	-0.71267132
C	-2.09727815	-3.67169510	0.23556757
H	-2.37543323	-4.65840927	0.61798391
H	-1.14289376	-3.76222204	-0.29386012
H	-1.96068420	-2.99834656	1.08541772
C	-3.44904374	-4.12144637	-1.86857179
H	-4.22758029	-3.75210671	-2.54289248
H	-2.53712529	-4.29256174	-2.45164751
H	-3.77195578	-5.08703007	-1.47110208
H	-3.16790228	-0.73386129	0.78649184
H	-4.11813497	-3.03970909	-0.13263707
H	0.21342980	-1.41058137	-0.66898169
O	-5.44715306	-1.24444678	3.01835571
O	-3.52332281	-0.88799058	1.91805273
C	-4.81445497	-1.03166701	1.98176450

H	-5.34156161	-0.94625400	1.01115587
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Name-TS2,21\\SCF E (UB3LYP-D3BJ/BS1)=-2750.9913206\\G=-2750.650040\\H=-2750.557554\\ZeroPoint=0.400639

C	-0.94952112	4.21116760	-0.55034629
C	-2.19775288	2.02935482	-0.29538086
Mo	0.98103353	0.10544717	-0.23653828
S	-0.38530755	0.78094356	1.59488980
S	0.37297011	2.00496355	-1.65013568
S	2.00456001	-1.72192780	1.12992088
S	2.82013344	-0.30905683	-1.82864978
C	-2.60266946	0.72512107	-0.91442765
N	-3.12775323	-0.33866894	-0.19182941
C	-3.37943087	-1.33870011	-1.03609916
N	-3.06535331	-0.93542682	-2.28760697
C	-2.57400390	0.35513041	-2.23287948
H	-3.14885122	-1.50628843	-3.11893160
C	-1.48186991	3.33927289	1.74296219
H	-2.23569170	0.86948125	-3.11603273
C	-1.22342656	2.83634533	-1.17946121
C	-1.77435168	1.93855714	1.18316634
C	2.53507150	1.45011971	0.70926299
N	5.82194549	-1.98862348	0.11187132
C	-0.46298932	4.10320943	0.89574964
H	-1.14814249	3.25513527	2.78142641
H	-2.42935933	3.89634257	1.75393946
H	-1.88949884	4.78137526	-0.56912835
H	-0.23066615	4.75809057	-1.16745091
H	0.50277248	3.58556256	0.92254914
H	-0.30544026	5.10357681	1.31335944
H	-2.60777367	1.50953710	1.74525308
H	-1.71623300	2.99518577	-2.14343852
O	3.32256638	2.13363322	1.17575358
C	4.80665712	-2.23910130	1.00822730
H	4.98888232	-2.77109156	1.92938432
C	3.64303389	-1.69686377	0.48660158
C	3.98940735	-1.09354790	-0.77801878
C	5.34943762	-1.29163315	-0.97148676
H	6.00017953	-0.99256351	-1.77883931
H	6.78608046	-2.26013852	0.24429129
H	-3.29224933	-0.51687802	1.09420327
H	-0.13025615	-1.01687123	-0.97167781
H	-3.10209318	2.65932379	-0.25910528
C	-3.85015003	-2.70830290	-0.65594825
C	-2.66586376	-3.69330183	-0.65420876
H	-2.99221379	-4.67157452	-0.28803228
H	-2.27010383	-3.82156519	-1.66722538
H	-1.85439120	-3.33473955	-0.01430585
C	-4.98283436	-3.19740250	-1.56898200
H	-5.82839468	-2.50326318	-1.56197524
H	-4.63726052	-3.30752861	-2.60292905

H	-5.33656046	-4.17593091	-1.23161643
H	-4.22847074	-2.62097120	0.36717536
O	-3.45460865	-0.74901967	2.23761317
C	-2.54323725	-1.58166275	2.65841179
O	-2.42357744	-1.94738010	3.83037361
H	-1.86532220	-1.96715341	1.87748796

Name-TS22,23SCF E (UB3LYP-D3BJ/BS1)=-2749.7775958\\G=-2749.464066\\H=-2749.364323\\ZeroPoint=0.380689

C	-1.24545649	3.69441280	-1.48498606
C	-2.24192521	2.02811707	0.13965203
Mo	1.04480623	0.19312923	0.02015491
S	0.14740279	1.62574577	1.76397994
S	-0.25651543	1.09290755	-1.75911021
S	2.71671985	-0.51337892	1.68010581
S	2.26027652	-1.32242279	-1.55766958
C	-2.81432833	0.66228531	0.37678655
N	-3.64691293	0.06571194	-0.56356789
C	-4.03989361	-1.08768361	-0.03882674
N	-3.51560048	-1.24352004	1.21259806
C	-2.72288559	-0.14404432	1.48466923
H	-3.60196873	-2.06481341	1.79526154
C	-1.00394642	4.04984982	0.99486701
H	-2.16003072	-0.05995733	2.39880285
C	-1.64224081	2.22614483	-1.26626860
C	-1.37261794	2.58461101	1.28131276
C	2.54758269	1.70898456	-0.48904140
N	5.85342286	-2.10164630	-0.09926129
C	-0.34080162	4.22877031	-0.37256598
H	-0.36095831	4.43027962	1.79404105
H	-1.93239946	4.63826044	1.02086672
H	-2.17273266	4.28432038	-1.50443481
H	-0.77331416	3.80945308	-2.46528378
H	0.61924306	3.70168577	-0.38883136
H	-0.12577692	5.28884240	-0.54650734
H	-1.97812642	2.55022141	2.19222517
H	-2.41998124	1.95856451	-1.98528084
O	3.36638439	2.45705244	-0.77115772
C	5.27221898	-1.56026581	1.01765498
H	5.81214396	-1.46309429	1.94692321
C	3.97111721	-1.21118416	0.67916319
C	3.77887322	-1.55764509	-0.70850567
C	4.97026717	-2.10593405	-1.15634222
H	5.25419081	-2.48986514	-2.12402171
H	6.80555323	-2.43716000	-0.14534223
H	-0.08423788	-1.10513482	0.37341452
H	-3.10511351	2.71590495	0.12824925
C	-4.98640771	-2.06691090	-0.67069748
C	-6.44045119	-1.74819408	-0.27495716
H	-7.13372509	-2.42120648	-0.79012948

H	-6.58316188	-1.87342321	0.80394642
H	-6.70264826	-0.71850134	-0.53584335
C	-4.63436311	-3.52297119	-0.33540920
H	-3.60738993	-3.76398828	-0.62256121
H	-4.74756546	-3.72376847	0.73642223
H	-5.30877935	-4.20214364	-0.86561507
H	-4.88906494	-1.92271175	-1.75218089
C	-0.95441516	-2.63973958	0.23406500
O	-1.28075137	-2.62231791	-0.90537396
O	-0.83694303	-3.04026641	1.34411593

WIIItBu

Name-WIIItBu\\SCF E(UB3LYP-D3BJ/BS1)=-2600.1382683\\G= -

2599.803247\\H=-2599.716311\\ZeroPoint= 0.393205

C	4.33178567	-1.05762737	-1.24152175
C	3.07359388	0.83929938	-0.12242350
S	1.63622215	-0.76596572	1.79921760
S	1.58493875	-1.00946178	-1.74204252
S	-1.87499204	-0.42699665	1.60646891
S	-1.65025786	-0.85766186	-1.70049220
C	1.98309482	1.86113839	-0.19061488
N	0.60065821	1.62082243	-0.08555871
C	-0.00992572	2.82703302	-0.15398040
N	0.94092354	3.77824928	-0.31940256
C	2.18510565	3.20072959	-0.33966175
H	0.75625141	4.76810857	-0.39969568
C	4.36291230	-0.84900444	1.26313765
H	3.08984519	3.77507807	-0.45619055
C	3.14913162	-0.08540955	-1.35523267
C	3.17534836	0.12309231	1.24166809
C	-0.19242201	-2.57886910	0.27110371
N	-5.19678072	-1.62644762	-0.15613302
C	4.32993337	-1.82259288	0.08328110
H	4.38390369	-1.38461069	2.21696721
H	5.28168653	-0.24873827	1.21104623
H	5.25469142	-0.46520089	-1.31300269
H	4.32618270	-1.74462067	-2.09312073
H	3.43082696	-2.44740053	0.14648615
H	5.19451800	-2.49283348	0.12868806
H	4.00175231	1.42476501	-0.17431020
H	3.32082055	0.89480354	2.00283158
H	3.29820878	0.55943180	-2.22582954
O	-0.32027295	-3.71822064	0.39828324
C	-4.52288575	-1.27066776	0.98784150
H	-5.01156967	-1.25547488	1.94959826
C	-3.21819800	-0.97712689	0.62363347
C	-3.11808959	-1.17123062	-0.79910730

C	-4.36610693	-1.57895032	-1.24736288
H	-4.71603157	-1.83171652	-2.23626500
H	-6.16871757	-1.90271467	-0.18653924
C	-1.45773221	3.24657787	0.04804936
C	-1.76378060	3.20284670	1.56154195
H	-1.65672918	2.19175446	1.95673667
H	-1.09208486	3.86966866	2.11140689
H	-2.79364148	3.53227012	1.73474075
C	-1.65556491	4.69706922	-0.44161644
H	-1.08784380	5.42304549	0.14967905
H	-1.38763875	4.80955301	-1.49693329
H	-2.71140796	4.95747517	-0.33301165
C	-2.44326247	2.36019638	-0.72358763
H	-2.20496479	2.34012300	-1.79065246
H	-2.44480098	1.34153409	-0.35273325
H	-3.45241901	2.76598520	-0.60222311
W	0.03169646	-0.57270995	0.06205954

Name-WIIItBu\\SCF E(UB3LYP-D3BJ/BS1)=-2601.2756892\\G=-

2600.930668\\H=-2600.837370\\ZeroPoint=0.408090

C	2.23528989	-3.40475903	-1.27300506
C	2.88154057	-1.31668231	0.00682483
S	0.59677342	-1.19296411	1.78577295
S	0.60638923	-1.17153288	-1.78453569
S	-2.45029830	0.15945645	1.66043860
S	-2.44067650	0.18185117	-1.65829477
C	3.16545153	0.15817427	0.01815926
N	2.22803012	1.18655755	-0.00040966
C	2.90518620	2.32973625	0.01565970
N	4.24498783	2.07301639	0.04511965
C	4.42409306	0.70683018	0.04618608
H	4.97589928	2.77169093	0.06027255
C	2.22488164	-3.42316300	1.25165911
H	5.40364606	0.25499232	0.06701559
C	2.25872364	-1.86772439	-1.29133556
C	2.24995292	-1.88657861	1.29276564
C	-1.72934987	-2.59811586	-0.01558759
N	-4.73898082	2.90169916	0.01283669
C	1.57784462	-3.97868315	-0.01747547
H	1.72754282	-3.81074825	2.14562816
H	3.27032820	-3.75842276	1.29601067
H	3.28138828	-3.73846634	-1.31344789
H	1.74571751	-3.77974196	-2.17658964
H	0.50889882	-3.75231649	-0.02037856
H	1.66297402	-5.07056852	-0.02500620
H	2.88058662	-1.56854618	2.12704867
H	2.89357894	-1.53635357	-2.11720006
O	-2.21074527	-3.65022013	-0.02401939

C	-4.23646354	2.31041573	1.14328156
H	-4.52292569	2.63872699	2.13002808
C	-3.36479387	1.31292248	0.72909921
C	-3.36053934	1.32272143	-0.71678017
C	-4.22982550	2.32577070	-1.12253817
H	-4.51061098	2.66740907	-2.10638574
H	-5.39185790	3.67455439	0.01619119
H	-0.37504103	1.16648775	0.01696930
H	3.88085249	-1.77758841	0.00712652
C	2.35732626	3.73791625	-0.01125595
C	0.82337510	3.72148803	0.01963847
H	0.41108467	3.20426125	-0.85089263
H	0.44633675	3.22963388	0.92063744
H	0.45241800	4.75092467	0.01149553
C	2.83337961	4.43642144	-1.30310292
H	2.43911572	5.45703497	-1.34189910
H	3.92560242	4.49455874	-1.34846395
H	2.48216424	3.89763804	-2.18893473
C	2.88436831	4.51130678	1.21562558
H	2.57134895	4.02727607	2.14623785
H	3.97731795	4.57431293	1.21307331
H	2.48966209	5.53230900	1.20866689
W	-0.91735326	-0.76366208	-0.00103640
H	0.40816214	1.01783134	0.00780966

Name-WIII2tBu\\SCF E(UB3LYP-D3BJ/BS1)=-2601.2966939\\G=-

2600.948619\\H=-2600.854993\\ZeroPoint=0.411423

C	2.37867359	-3.29861574	-1.26214805
C	3.03375658	-1.21806256	0.01023498
S	0.74851120	-1.06730530	1.79123994
S	0.76109924	-1.03525380	-1.77927337
S	-2.52190864	-0.06401044	1.65432555
S	-2.46571123	0.03097148	-1.67696018
C	3.27549150	0.25784565	0.01275140
N	2.29590148	1.24384517	0.02171098
C	2.84478954	2.46424466	0.00937324
N	4.17437553	2.27973552	-0.00516280
C	4.46686424	0.92609277	-0.00340740
H	4.85523943	3.02906544	-0.01714316
C	2.38405063	-3.31038867	1.26135201
H	5.48006026	0.55998297	-0.01479460
C	2.40127308	-1.76247024	-1.29060238
C	2.39813133	-1.77462614	1.30397563
C	-1.57145411	-2.66853629	-0.04930750
N	-5.09955488	2.43596201	0.01622048
C	1.72652493	-3.86660717	-0.00154321
H	1.89396321	-3.69638350	2.15981935
H	3.43052902	-3.64459181	1.29683412

H	3.42345420	-3.63690594	-1.30649087
H	1.88256675	-3.67350475	-2.16203212
H	0.66074208	-3.62861424	0.00293092
H	1.80265123	-4.95919446	-0.00730475
H	3.03614241	-1.45603651	2.13241572
H	3.04514360	-1.44099726	-2.11340545
O	-2.05061978	-3.71627376	-0.08307280
C	-4.54302575	1.87884376	1.14146698
H	-4.88042311	2.14703867	2.13064076
C	-3.55188251	1.00409485	0.72178130
C	-3.52577085	1.04716936	-0.71965496
C	-4.50189797	1.94709257	-1.12034415
H	-4.80582154	2.27350670	-2.10284142
H	-5.83572527	3.12844775	0.02402765
H	1.27612107	1.07683019	0.03091706
H	-0.33142731	1.02628323	0.03895227
H	4.04377134	-1.65121335	0.00956496
C	2.08615053	3.76348950	0.00733890
C	1.18585491	3.80171616	-1.24643306
H	1.78411199	3.73492037	-2.15998149
H	0.46289313	2.98062148	-1.24116683
H	0.63240782	4.74512908	-1.26151057
C	3.06550369	4.94615923	-0.01403089
H	2.49593260	5.87878558	-0.01494745
H	3.71352584	4.94804575	0.86851531
H	3.69230715	4.93355216	-0.91168647
C	1.21364022	3.82383292	1.27950782
H	0.49175221	3.00209201	1.30462525
H	1.83179846	3.77406824	2.18079563
H	0.65940534	4.76683657	1.28955066
W	-0.82274472	-0.67300611	0.00280733

Name-WIII3tBu\\SCF E (UB3LYP-D3BJ/BS1)=-2789.8953535\\G= -
2789.533739\\H=-2789.434345\\ZeroPoint=0.427404

C	-0.79720299	3.92585670	-1.33078548
C	-1.92249779	2.39498141	0.35008980
S	0.45680603	1.58443223	1.77116122
S	-0.29251091	1.15037246	-1.65457495
S	2.75743268	-0.77957078	1.44018097
S	2.05436864	-1.15801282	-1.77367779
C	-2.56557282	1.07413752	0.64139840
N	-3.35206929	0.38739716	-0.28028806
C	-3.80985260	-0.76334321	0.23679889
N	-3.36095496	-0.80122355	1.49770864
C	-2.58029525	0.30841769	1.77014470
H	-3.47355197	-1.59219491	2.11982234
C	-0.34518360	4.20902889	1.13294380
H	-2.10131928	0.43784348	2.72425541

C	-1.40123225	2.53365285	-1.09447860
C	-0.90481625	2.81062474	1.42730350
C	2.76966440	1.84346560	-0.59469641
N	3.20466658	-4.43663168	0.06694633
C	0.23088031	4.33328514	-0.27677610
H	0.40217989	4.47034694	1.88717916
H	-1.17781167	4.91643452	1.24636812
H	-1.63287694	4.63832308	-1.30799284
H	-0.36860022	3.96970470	-2.33590858
H	1.12680095	3.71491036	-0.36791382
H	0.54752855	5.36593345	-0.45559553
H	-1.43026535	2.83866290	2.38521588
H	-2.25164134	2.42789766	-1.77272824
O	3.57124048	2.63102984	-0.87641995
C	3.26338393	-3.55902251	1.11825383
H	3.57005866	-3.87355220	2.10331893
C	2.85905134	-2.32114960	0.63864860
C	2.55060466	-2.48693497	-0.76555752
C	2.78022933	-3.81873784	-1.08071021
H	2.66615261	-4.35923257	-2.00706995
H	3.43204611	-5.42045205	0.13328607
H	-3.53650716	0.68302763	-1.23147061
H	0.07108416	-1.07803833	0.36658256
H	-2.71320006	3.15863655	0.42188541
C	-4.68223412	-1.77655103	-0.45248737
C	-6.15272006	-1.32359915	-0.31295659
H	-6.80064156	-2.05144088	-0.81016830
H	-6.44490560	-1.26010277	0.73920865
H	-6.30857922	-0.34597362	-0.77819928
C	-4.48991963	-3.15367705	0.20657409
H	-3.44437013	-3.46861559	0.15839947
H	-4.81108105	-3.15007634	1.25310644
H	-5.10288536	-3.88721687	-0.32339860
C	-0.57231571	-2.01640922	0.60052192
O	-1.09369548	-2.52822465	-0.40894549
O	-0.61600338	-2.31377675	1.80678922
C	-4.29287140	-1.84894457	-1.94039668
H	-4.47545655	-0.90006054	-2.45468803
H	-3.23927579	-2.11482218	-2.05696956
H	-4.90335626	-2.61231159	-2.42984869
W	1.38954737	0.48901787	-0.11541975

Name-WIII5tBu\\SCF E(UB3LYP-D3BJ/BS1)= -2601.7531749\\G=-
2601.394147\\H=-2601.300917\\ZeroPoint=0.421547

C	-1.62684765	-3.99039285	0.76086520
C	-2.64219300	-1.74542123	0.18348906
S	-0.66061393	-0.87540603	-1.74937445
S	-0.16355313	-1.79135666	1.69054357

S	1.91113700	1.28513156	-1.43399192
S	2.54270370	0.17751785	1.63160953
C	-2.90041094	-0.33480103	0.61655377
N	-3.10273277	0.71533410	-0.26932317
C	-3.27949807	1.87487197	0.38313457
N	-3.24102899	1.56977858	1.68708995
C	-2.99968923	0.21699867	1.86210450
H	-3.34335888	2.24717880	2.43391512
C	-1.95368543	-3.35586328	-1.64758918
H	-2.92110249	-0.22269466	2.84169688
C	-1.80576192	-2.53378420	1.21110681
C	-2.15922448	-1.88056362	-1.27220350
C	2.05949226	-1.83348566	-0.67611933
N	5.34622187	2.45604342	0.10283725
C	-1.06222138	-4.10231691	-0.65533506
H	-1.55764751	-3.42022789	-2.66461398
H	-2.94757486	-3.82264560	-1.65931450
H	-2.61804284	-4.46289586	0.79144472
H	-0.99677271	-4.51927346	1.48092756
H	-0.04327660	-3.70192041	-0.68623641
H	-0.99627823	-5.15589908	-0.94461163
H	-2.93204641	-1.47069441	-1.92885763
H	-2.35171990	-2.52523802	2.15779472
O	2.76341629	-2.65450436	-1.07523492
C	4.45387439	2.46441077	-0.94458710
H	4.65273177	3.01414349	-1.85114397
C	3.37709424	1.67740701	-0.57159058
C	3.65288141	1.18544675	0.75546203
C	4.89015115	1.69052126	1.13886794
H	5.45818080	1.56247746	2.04692586
H	6.23137268	2.94654402	0.10233751
H	-0.45275064	0.96505203	1.07449002
H	-3.61428710	-2.26215871	0.18180589
C	-3.38227263	3.23478811	-0.24849125
C	-1.98765366	3.59108148	-0.81648021
H	-2.03548086	4.57560513	-1.29066859
H	-1.23846264	3.62327011	-0.01994444
H	-1.66620482	2.86162690	-1.56578108
C	-3.80057594	4.27093263	0.80471498
H	-4.77241484	4.02487712	1.24326718
H	-3.06069417	4.35290869	1.60752549
H	-3.88024669	5.24985617	0.32576574
H	-3.03981840	0.65278484	-1.27838701
H	-0.30756641	1.40086300	0.46635312
C	-4.41922861	3.18870226	-1.38734105
H	-5.40572901	2.90682818	-1.00830030
H	-4.49157155	4.18016324	-1.84238248
H	-4.13022253	2.48067798	-2.17005841
W	0.84832801	-0.40376550	0.01234790

Name-WIII6tBu\\SCF E(UB3LYP-D3BJ/BS1)=-2791.0757778\\G=-

2790.701703\\H=-2790.598391\\ZeroPoint=0.442587

C	-1.01351019	4.06493251	-1.25664003
C	-2.12006203	1.82301206	-0.82896842
S	-0.52361966	1.03929612	1.45845686
S	0.61241444	1.86665410	-1.81971083
S	1.91329431	-1.35967636	1.57491675
S	3.06966589	-0.30882746	-1.36218801
C	-2.30660995	0.39993018	-1.27283035
N	-2.79296713	-0.60704422	-0.45008664
C	-2.80597384	-1.73670713	-1.16106197
N	-2.37586111	-1.47354926	-2.42150239
C	-2.04957097	-0.13665472	-2.51212678
H	-2.26876937	-2.15611891	-3.15962129
C	-1.78785261	3.48748969	1.05954090
H	-1.66386566	0.29222045	-3.42170504
C	-1.10320803	2.59560572	-1.69285659
C	-1.91822897	2.00389997	0.68374133
C	2.39592926	1.72745062	0.88014533
N	5.51973893	-2.64986882	0.62850984
C	-0.72390472	4.21450565	0.23720354
H	-1.59166645	3.57845326	2.13172159
H	-2.76612702	3.95056688	0.87273913
H	-1.98181952	4.53188883	-1.48365558
H	-0.26038065	4.58089268	-1.85874583
H	0.26903183	3.81151749	0.46769555
H	-0.70847496	5.27507551	0.50843291
H	-2.78643457	1.59325536	1.19838958
H	-1.45057958	2.56096359	-2.72868542
O	3.09650818	2.48709244	1.39312379
C	4.46609764	-2.61885887	1.51320712
H	4.49291308	-3.16740374	2.44165603
C	3.49287168	-1.79981960	0.96543718
C	3.99863409	-1.32916820	-0.29829767
C	5.26322130	-1.87725013	-0.47131525
H	5.97675434	-1.77497759	-1.27404084
H	6.37633883	-3.16638448	0.77777313
H	-0.15535486	-0.80097783	-1.15345971
H	-3.06959490	2.35028255	-1.01705046
C	-3.18875918	-3.10888610	-0.65712392
C	-2.29764025	-3.45706955	0.55407769
H	-2.54317889	-4.46102516	0.91475404
H	-1.23859624	-3.43946853	0.27594172
H	-2.44899112	-2.75283137	1.37506370
C	-2.97680195	-4.15954206	-1.75931672
H	-3.59757891	-3.95541342	-2.63820361
H	-1.92908295	-4.20695289	-2.07396862
H	-3.25588706	-5.14483014	-1.37649327
H	-3.26651167	-0.56168826	1.02458850
H	0.10847335	-1.33245702	-0.66920866
O	-5.39031985	0.02939847	3.20258095

O	-3.58443012	-0.56517487	2.02607843
C	-4.80164390	-0.06786551	2.13524912
H	-5.25111417	0.25903429	1.18261369
C	-4.67223481	-3.10608370	-0.23597981
H	-4.85445185	-2.39134636	0.56891883
H	-5.31698260	-2.84676904	-1.08161071
H	-4.95581292	-4.10136193	0.12058805
W	1.19533390	0.40089049	-0.00153031

Name-WIII21tBu\\SCF E(UB3LYP-D3BJ/BS1)=-2790.611823\\G=-

2790.248665\\H=-2790.144942\\ZeroPoint=0.432523

C	-0.72141821	4.29128569	-0.68268123
C	-2.05207153	2.16660514	-0.34235569
S	-0.24565458	0.98132346	1.59785536
S	0.53215903	1.98808569	-1.65763497
S	1.86950412	-1.86994051	1.08049726
S	2.80413854	-0.45029711	-1.81501312
C	-2.52838031	0.86910204	-0.93163947
N	-3.15180910	-0.14295096	-0.20941365
C	-3.49656403	-1.10029635	-1.07512291
N	-3.12588348	-0.72225304	-2.32469673
C	-2.51673156	0.51255297	-2.25606853
H	-3.27010606	-1.26110308	-3.16732123
C	-1.31116964	3.54339857	1.64052295
H	-2.12542432	0.99892849	-3.13326096
C	-1.04230664	2.89950640	-1.24864021
C	-1.63591936	2.12866019	1.13654802
C	2.69474389	1.10467580	0.76825230
N	5.69140969	-2.34123168	0.12481407
C	-0.25924564	4.23785828	0.77418644
H	-0.99229130	3.49544066	2.68598999
H	-2.24281347	4.12564927	1.61507798
H	-1.63843267	4.89456889	-0.74527764
H	0.02628324	4.77968733	-1.31455058
H	0.68984693	3.69284101	0.83987119
H	-0.07715081	5.25152051	1.14700568
H	-2.47102808	1.73449365	1.71918635
H	-1.51333831	3.03173846	-2.22662843
O	3.61826745	1.52164110	1.31381110
C	4.64935415	-2.54690785	1.00295136
H	4.78680198	-3.10588385	1.91593812
C	3.52764048	-1.93057133	0.47499751
C	3.92520848	-1.32666991	-0.77149608
C	5.27244310	-1.59707773	-0.95151160
H	5.95064320	-1.31959957	-1.74393460
H	6.63513302	-2.67373921	0.26237103
H	-3.27609252	-0.30478773	1.31273389
H	-0.13906101	-0.95689633	-0.89208407
H	-2.92612137	2.83961053	-0.33176186
C	-4.17630999	-2.41418983	-0.75840407

C	-4.63771440	-3.10091573	-2.05571277
H	-5.16186991	-4.02722178	-1.80499733
H	-5.32522734	-2.46740730	-2.62530552
H	-3.79173175	-3.36669659	-2.69855336
C	-5.40180167	-2.15795934	0.13967562
H	-5.11436537	-1.69642747	1.08661584
H	-6.12204604	-1.50236293	-0.36005588
H	-5.89850410	-3.10800683	0.36089504
O	-3.38501257	-0.38923400	2.36013511
C	-2.41084785	-1.10565648	2.89023504
O	-2.30364991	-1.29184230	4.09613247
H	-1.70258217	-1.53295334	2.16716585
C	-3.18077457	-3.34171011	-0.03051494
H	-2.28019135	-3.49793616	-0.63252775
H	-2.88162183	-2.92344329	0.93204320
H	-3.64762318	-4.31514446	0.15201500
W	1.04898504	0.13187534	-0.18171362

Name-WIII22tBu\\SCF E(UB3LYP-D3BJ/BS1)=-2600.8137767\\G=-

2600.480964\\H=-2600.386313\\ZeroPoint=0.397120

C	-1.24582779	3.40579618	-1.77563603
C	-2.27842627	2.01606811	0.07536056
S	0.14019006	1.69760048	1.66370151
S	-0.37976403	0.75338363	-1.71417539
S	2.67290347	-0.45829216	1.74234372
S	1.92720234	-1.89045168	-1.20546617
C	-2.87041644	0.70542660	0.50052206
N	-3.60810186	-0.07296386	-0.38256097
C	-4.01560816	-1.13467422	0.29921118
N	-3.58402507	-1.05782392	1.59460689
C	-2.85373519	0.10564509	1.73545687
H	-3.73894663	-1.75261578	2.31238550
C	-0.91498257	4.06646400	0.62732238
H	-2.38240214	0.37182601	2.66666407
C	-1.71057490	2.00447950	-1.35418033
C	-1.34799706	2.67288152	1.11042068
C	2.45392635	1.16311354	-0.75963997
N	5.74224081	-2.10534645	-0.13185409
C	-0.28076787	4.02862713	-0.76463840
H	-0.23206855	4.51202488	1.35671841
H	-1.81112957	4.70293773	0.59486068
H	-2.14148186	4.03826377	-1.85151160
H	-0.79889100	3.36421489	-2.77361698
H	0.64780453	3.44743223	-0.73052214
H	-0.01338644	5.04252076	-1.08181401
H	-1.92035216	2.78852836	2.03577004
H	-2.50976835	1.67521651	-2.02173609
O	3.33658089	1.68985944	-1.27961605

C	5.23735901	-1.41535148	0.94237476
H	5.86795666	-1.10407902	1.76115820
C	3.88001483	-1.24023654	0.72191949
C	3.56499244	-1.84498804	-0.54636664
C	4.74479991	-2.36810098	-1.04741429
H	4.95128877	-2.89875380	-1.96431556
H	6.71173354	-2.36500011	-0.24518758
H	-0.23510887	-1.21437695	0.73346791
H	-3.11656091	2.73051330	-0.00239651
C	-4.80223111	-2.31122303	-0.22800144
C	-6.03500940	-2.55876189	0.66501654
H	-6.61284111	-3.40451185	0.27819074
H	-5.74767324	-2.79566637	1.69462293
H	-6.68649231	-1.67916384	0.68628996
C	-3.89932101	-3.56396951	-0.21213036
H	-3.01005204	-3.40951630	-0.83194172
H	-3.56945419	-3.80288509	0.80400043
H	-4.44596524	-4.42878963	-0.60301025
C	-5.26095928	-2.03190206	-1.66549283
H	-5.90689061	-1.15026612	-1.71223207
H	-4.40889053	-1.86257671	-2.32904658
H	-5.82498016	-2.89079018	-2.04265135
W	0.89771873	-0.00827068	0.11100480

Name-WIII23tBu\\SCF E(UB3LYP-D3BJ/BS1)=-2789.4177454\\G=-
2789.070718\\H=-2788.971303\\ZeroPoint=0.412868

C	-0.89882006	3.90005850	-1.33644086
C	-1.96238902	2.33631845	0.36047716
S	0.44735180	1.60102179	1.76776222
S	-0.28157127	1.15823117	-1.64335652
S	2.71895823	-0.77082758	1.47358203
S	2.13869394	-1.10857248	-1.76962922
C	-2.59893744	1.00365845	0.62749319
N	-3.43466721	0.40725317	-0.30622059
C	-3.83287966	-0.74192927	0.22448885
N	-3.32303250	-0.88170161	1.48379419
C	-2.52001173	0.20995257	1.74612069
H	-3.36871214	-1.71562244	2.05216968
C	-0.42653965	4.19821167	1.12616127
H	-1.97477320	0.29956532	2.67030035
C	-1.45294804	2.49188503	-1.08317857
C	-0.95181541	2.78642791	1.42554116
C	2.74179955	1.89976674	-0.54284308
N	3.26388877	-4.40243522	0.06511126
C	0.12724411	4.34085612	-0.29202250
H	0.32534784	4.48008617	1.86908832
H	-1.27417595	4.88578717	1.25169795
H	-1.75638794	4.58631757	-1.30657301

H	-0.47994604	3.95969826	-2.34545778
H	1.04007276	3.74904338	-0.39439091
H	0.41152706	5.38296285	-0.47262982
H	-1.46783101	2.80024765	2.38929043
H	-2.30254750	2.31752353	-1.74515012
O	3.52610536	2.71602521	-0.79743505
C	3.27283240	-3.53861848	1.12981716
H	3.54459723	-3.86388586	2.12166412
C	2.87458149	-2.29822679	0.65204048
C	2.61959904	-2.44704043	-0.76385884
C	2.87550418	-3.77166251	-1.08892928
H	2.80175877	-4.30012857	-2.02626683
H	3.49816554	-5.38474967	0.12643946
H	0.04471064	-1.11528100	0.32406481
H	-2.75784895	3.09817059	0.42745851
C	-4.75340816	-1.75230692	-0.42141983
C	-6.21439392	-1.28775152	-0.24018822
H	-6.90043825	-2.00544810	-0.70296045
H	-6.46985080	-1.20572760	0.82134329
H	-6.37382693	-0.31064003	-0.70630910
C	-4.57195504	-3.13566005	0.22842958
H	-3.53243435	-3.47020797	0.15910282
H	-4.86689403	-3.13128170	1.28342752
H	-5.20442586	-3.86744112	-0.28310425
C	-0.55260007	-2.09660719	0.46440263
O	-1.10839676	-2.50693068	-0.57500548
O	-0.52768443	-2.55177548	1.62362459
C	-4.42496570	-1.84864456	-1.92144150
H	-4.54676861	-0.88108229	-2.41439014
H	-3.39321466	-2.17948120	-2.07097214
H	-5.09442512	-2.56829941	-2.40371194
W	1.39135812	0.51013155	-0.11289230

Name=TS5,6\\SCF E (UB3LYP-D3BJ/BS1)=-2791.0743879\\G=-2790.703440\\H=-2790.600838\\ZeroPoint=0.438989

C	-0.98802200	4.05191700	-1.25730500
C	-2.11548400	1.82693700	-0.80212700
S	-0.50012200	1.02586900	1.46527800
S	0.59922200	1.82748100	-1.83820800
S	1.94342400	-1.35560700	1.58224100
S	3.07943900	-0.32091900	-1.36822200
C	-2.32196200	0.40612200	-1.24180700
N	-2.82139500	-0.59874000	-0.42301400
C	-2.85684600	-1.73814800	-1.12262000
N	-2.42520500	-1.47782900	-2.37640600
C	-2.07872900	-0.14574400	-2.47397700
H	-2.32932300	-2.16445100	-3.11301500
C	-1.73245400	3.49439100	1.07310500

H	-1.68741700	0.27191400	-3.38598400
C	-1.10240700	2.58230200	-1.68616000
C	-1.88825600	2.01086800	0.70731200
C	2.40577800	1.73573200	0.85176900
N	5.53369300	-2.66850200	0.60615300
C	-0.67304500	4.20485400	0.23094200
H	-1.51838800	3.58693900	2.14164500
H	-2.70778300	3.96871900	0.89973500
H	-1.95405500	4.52964800	-1.47108500
H	-0.23831800	4.55532400	-1.87399400
H	0.31903400	3.79284900	0.44817500
H	-0.64189200	5.26645600	0.49655100
H	-2.75357800	1.61330400	1.23691500
H	-1.46808800	2.54834200	-2.71568100
O	3.10138400	2.50886300	1.35093300
C	4.48817600	-2.62964000	1.50054200
H	4.52098600	-3.17554900	2.43033000
C	3.51400400	-1.80781300	0.95913300
C	4.01086600	-1.34378400	-0.31071900
C	5.27155200	-1.89851700	-0.49348800
H	5.97807200	-1.80251500	-1.30314400
H	6.38869500	-3.18958700	0.74902600
H	-0.14147800	-0.83962200	-1.14158600
H	-3.06307600	2.36079800	-0.97903000
C	-3.26572000	-3.09680300	-0.60809900
C	-2.39639000	-3.44089200	0.62019400
H	-2.65911000	-4.43903100	0.98399300
H	-1.33320300	-3.43669900	0.35828700
H	-2.55581500	-2.72762300	1.43174100
C	-3.05108500	-4.15917000	-1.69811400
H	-3.65773500	-3.95603900	-2.58696700
H	-1.99966900	-4.22181000	-1.99704500
H	-3.34793200	-5.13644300	-1.30876400
H	-3.22403000	-0.52427700	0.80428000
H	0.11110700	-1.36155700	-0.64267500
O	-5.38573400	0.12338200	3.13681800
O	-3.59502300	-0.50872700	1.94216800
C	-4.78409600	0.00562000	2.06761400
H	-5.24595300	0.34974400	1.12190700
C	-4.75557600	-3.06540100	-0.20958300
H	-4.93737800	-2.33909900	0.58504500
H	-5.38327000	-2.80654200	-1.06787600
H	-5.05700000	-4.05294700	0.15303000
W	1.21052300	0.38879600	-0.00591100

Name-TS2,21\\SCF E(UB3LYP-D3BJ/BS1)=-2790.6109361\\G=-2790.251507\\H=-2790.147787\\ZeroPoint=0.428989

C	-0.71822900	4.26661100	-0.79224400
C	-2.04593200	2.14735300	-0.41359400
S	-0.26499100	1.00386200	1.57365500
S	0.55220100	1.94447500	-1.69724700
S	1.87815900	-1.83118800	1.16168000
S	2.82512800	-0.49809100	-1.77261100
C	-2.50233200	0.83269800	-0.97795700
N	-3.12564100	-0.17325500	-0.24654500
C	-3.43801300	-1.16868000	-1.08462200
N	-3.04760400	-0.81460000	-2.32984500
C	-2.46082600	0.43222000	-2.28707400
H	-3.16181200	-1.38168900	-3.15888400
C	-1.32390300	3.57231600	1.54225900
H	-2.05841600	0.89712900	-3.17048900
C	-1.02898800	2.86089900	-1.32808000
C	-1.64481500	2.14574700	1.07067400
C	2.68860700	1.13532200	0.76734600
N	5.70427300	-2.32762800	0.23626400
C	-0.26634500	4.24816200	0.66856500
H	-1.01388000	3.54894800	2.59117100
H	-2.25599800	4.15256700	1.49564100
H	-1.63703800	4.86464200	-0.87536900
H	0.03210700	4.74256500	-1.43036500
H	0.68336300	3.70706800	0.75397500
H	-0.08930200	5.27064600	1.01896300
H	-2.48702900	1.76803300	1.65349900
H	-1.49097100	2.96840400	-2.31342000
O	3.60331000	1.57445200	1.30997500
C	4.65849200	-2.50766000	1.11560400
H	4.79232100	-3.03896200	2.04548500
C	3.53863800	-1.90842600	0.56442400
C	3.94142400	-1.34196300	-0.69781600
C	5.28964500	-1.61655700	-0.86374600
H	5.97108200	-1.36244200	-1.66120200
H	6.64774600	-2.65471100	0.38798200
H	-3.32808700	-0.21946800	1.06254500
H	-0.12337800	-0.98506000	-0.86103800
H	-2.92499800	2.81300000	-0.43026900
C	-4.09311700	-2.48572100	-0.73760600
C	-4.48852400	-3.23366900	-2.02264400
H	-4.99232700	-4.16563300	-1.75270400
H	-5.17581800	-2.64396500	-2.63761900
H	-3.61308300	-3.49592100	-2.62622400
C	-5.35604400	-2.22792000	0.10686500
H	-5.11504800	-1.71439300	1.03970000
H	-6.07795400	-1.61978200	-0.44739000
H	-5.82957000	-3.18315100	0.35397900
O	-3.55127200	-0.22954400	2.21327500
C	-2.66929200	-0.90996800	2.89391600
O	-2.67716600	-1.01620600	4.12184600
H	-1.89145500	-1.40585300	2.29031600
C	-3.09456600	-3.35167100	0.05936700

H	-2.17388200	-3.50988200	-0.51072400
H	-2.83302500	-2.88251100	1.00950300
H	-3.54271100	-4.32752000	0.27198300
W	1.05688800	0.12428700	-0.17065400

Name-TS22,23\\SCF E (UB3LYP-D3BJ/BS1)=-2789.3978313\\G=-

2789.055592\\H=-2788.955186\\ZeroPoint=0.409125

C	-0.96174000	3.98163300	-1.31789100
C	-1.94809100	2.37420100	0.38718100
S	0.53300400	1.75712000	1.76216700
S	-0.28131900	1.26102000	-1.67122700
S	2.85830900	-0.71071100	1.40117300
S	2.10134000	-1.13057100	-1.81635600
C	-2.53586800	1.01789000	0.65163600
N	-3.42097200	0.43486600	-0.24564300
C	-3.75133600	-0.74630000	0.26029500
N	-3.13995600	-0.92810700	1.46871400
C	-2.35448800	0.17991100	1.72419600
H	-3.16495400	-1.76828200	2.02929500
C	-0.48010000	4.29150800	1.13204100
H	-1.73275100	0.24268900	2.60083400
C	-1.46950700	2.55479100	-1.06746700
C	-0.93557400	2.85686200	1.43973500
C	2.78059700	1.91084000	-0.57179500
N	3.04171300	-4.44446800	0.12487300
C	0.07146500	4.43794200	-0.28699900
H	0.25785000	4.61072000	1.87408300
H	-1.35490000	4.94764600	1.24565100
H	-1.83365100	4.64914900	-1.26506100
H	-0.56352400	4.05943200	-2.33426500
H	0.98629300	3.84680100	-0.39004700
H	0.34541200	5.48206800	-0.47402400
H	-1.44486900	2.85181900	2.40799400
H	-2.33322400	2.37243400	-1.70976000
O	3.58827100	2.70488600	-0.80457100
C	3.18533000	-3.53276100	1.14203300
H	3.47729900	-3.83682300	2.13531600
C	2.86886700	-2.28463900	0.62735900
C	2.52291800	-2.47010100	-0.76327000
C	2.63980400	-3.82461900	-1.03496200
H	2.46793700	-4.38320600	-1.94201200
H	3.18943500	-5.43953600	0.22209500
H	0.23984800	-0.86542400	0.32683100
H	-2.77189800	3.10345800	0.47272200
C	-4.70038300	-1.74610400	-0.36129700
C	-6.14963500	-1.26079600	-0.14378000
H	-6.85738000	-1.96753100	-0.59043600
H	-6.37714700	-1.17669800	0.92397900
H	-6.30573400	-0.28074900	-0.60434300

C	-4.52639300	-3.13257000	0.28210800
H	-3.49983700	-3.49664800	0.17331200
H	-4.78054000	-3.12173500	1.34766800
H	-5.19436000	-3.84903400	-0.20524100
C	-0.59107500	-2.46511300	0.41674800
O	-1.02035200	-2.55678200	-0.68332900
O	-0.36977300	-2.74622300	1.54639900
C	-4.41296200	-1.84589000	-1.87024900
H	-4.52132000	-0.87296100	-2.35572200
H	-3.39504300	-2.20460800	-2.05029900
H	-5.11347700	-2.54519700	-2.33833900
W	1.33023700	0.46461200	-0.10932000

MoIIIItBu

Name-MoIII2tBu\\SCF E(UB3LYP-D3BJ/BS1)=-2601.0002075\\G=-

2600.652171\\H=-2600.558942\\ZeroPoint=0.410864

C	-1.05101802	3.70484370	-1.24948282
C	-2.46562660	2.01332296	-0.01929387
Mo	0.88926888	0.06228607	0.04512076
S	-0.43819524	1.06289772	1.82865469
S	-0.35558695	1.02627102	-1.76517845
S	2.52769599	-0.57696795	1.72082172
S	2.31091570	-1.23851453	-1.57180741
C	-3.23769075	0.73331973	-0.03856884
N	-2.70117850	-0.54579549	0.04198795
C	-3.66515555	-1.47338451	-0.00973984
N	-4.82440967	-0.80665520	-0.12216825
C	-4.58852227	0.55768561	-0.14144776
H	-5.73439285	-1.24794252	-0.17857659
C	-1.15260544	3.73232694	1.26984096
H	-5.38782181	1.27543976	-0.22470448
C	-1.63890178	2.28444704	-1.29629531
C	-1.71500201	2.30281627	1.30062084
C	2.33921965	1.68286754	-0.35515026
N	5.88041603	-1.77732256	0.05049825
C	-0.28265441	3.99610614	0.04107330
H	-0.59595568	3.92484938	2.19143980
H	-2.00819095	4.42261194	1.25887874
H	-1.89507237	4.40452448	-1.32474743
H	-0.41978683	3.86903035	-2.12750987
H	0.61541011	3.37533185	0.09251276
H	0.05426704	5.03823592	0.03973745
H	-2.45572083	2.23822036	2.10236662
H	-2.33195873	2.22421094	-2.14024510
O	3.17843377	2.39328006	-0.67385861
C	5.19336838	-1.36438733	1.15855515

H	5.66981396	-1.27527560	2.12263664
C	3.88434574	-1.11584481	0.76173009
C	3.79965435	-1.38912619	-0.65267660
C	5.05966425	-1.79583360	-1.05780689
H	5.43200372	-2.09142862	-2.02643226
H	6.85983242	-2.02747052	0.04297144
H	-1.69678176	-0.76756518	0.12186636
H	-0.17236682	-1.33388469	0.11506839
H	-3.24436864	2.78847374	-0.05158517
C	-3.45348034	-2.96128814	0.04498404
C	-4.80557635	-3.68699899	-0.00386999
H	-4.63159985	-4.76508781	0.03736573
H	-5.43876878	-3.41461840	0.84658506
H	-5.34589901	-3.46913698	-0.93073576
C	-2.71847453	-3.30342006	1.35822050
H	-1.74336517	-2.80989694	1.40742236
H	-3.30843524	-2.99860995	2.22766879
H	-2.55798934	-4.38424192	1.40835337
C	-2.58782245	-3.37546983	-1.16460242
H	-3.08398798	-3.12021118	-2.10569177
H	-1.61130743	-2.88303839	-1.13945828
H	-2.42771889	-4.45723772	-1.13800593

Name-MoIII3tBu\\SCF E(UB3LYP-D3BJ/BS1)= -2789.6001773\\G=-2789.239730\\H=-2789.139425\\ZeroPoint=0.426980

C	-1.19118730	3.86595557	-1.38995054
C	-2.06917315	2.21090761	0.31727866
Mo	1.36903394	0.65680767	-0.09926051
S	0.40769103	1.79271823	1.75798754
S	-0.28955930	1.20945507	-1.71455991
S	2.90984914	-0.40897438	1.49541403
S	2.31433876	-0.89266149	-1.76290802
C	-2.52582547	0.81985120	0.62826178
N	-3.24792852	0.04374742	-0.27395856
C	-3.56207801	-1.14922345	0.25493641
N	-3.08181285	-1.13105078	1.50501665
C	-2.42641335	0.06174098	1.75803737
H	-3.09053057	-1.92633540	2.13216454
C	-0.76587351	4.24352933	1.06208863
H	-1.94429962	0.24911060	2.70108844
C	-1.58792512	2.40277574	-1.13691770
C	-1.12108340	2.78484405	1.38671451
C	2.63798858	2.14897985	-0.59190308
N	4.36708258	-3.72625083	0.00087506
C	-0.21308006	4.41536177	-0.35233777
H	-0.06312968	4.62324119	1.80880490
H	-1.68947101	4.82982844	1.16151430
H	-2.11679004	4.45641800	-1.35499441
H	-0.78848803	3.96315178	-2.40191756

H	0.75201029	3.90890401	-0.43979122
H	-0.02846416	5.47636677	-0.54946220
H	-1.65292539	2.76059302	2.34155079
H	-2.42650579	2.17249468	-1.80020496
O	3.36176704	2.99701623	-0.87549052
C	4.18156182	-2.90047105	1.07726597
H	4.57314605	-3.14214646	2.05265969
C	3.43797782	-1.81295964	0.63446458
C	3.18025165	-2.02221162	-0.78175029
C	3.78150818	-3.22656688	-1.13059469
H	3.82318743	-3.75197897	-2.07142588
H	4.86374375	-4.60786201	0.04086988
H	-3.48089631	0.31264920	-1.22212815
H	0.15668281	-0.98130861	0.38530246
H	-2.96033084	2.85477947	0.38378606
C	-4.34558736	-2.25027105	-0.40671684
C	-5.84940450	-1.96604341	-0.19127866
H	-6.43495606	-2.75918087	-0.66549854
H	-6.09496968	-1.94261539	0.87431511
H	-6.13655618	-1.00949409	-0.63734325
C	-3.97139361	-3.60233180	0.22589008
H	-2.89900140	-3.79456495	0.13804363
H	-4.25491691	-3.64702308	1.28232512
H	-4.51408977	-4.39636156	-0.29352761
C	-0.27557107	-2.04353644	0.52181565
O	-0.72652496	-2.54745675	-0.52675121
O	-0.22210297	-2.47172232	1.68974075
C	-4.02595214	-2.26779282	-1.91269004
H	-4.34278803	-1.34302853	-2.40610363
H	-2.95613411	-2.41017618	-2.08467890
H	-4.56900789	-3.09302770	-2.38055380

Name-MoIII5tBu\\SCF E(UB3LYP-D3BJ/BS1)=-2601.109447\\G=-
2601.102447\\H=-2601.009628\\ZeroPoint=0.421111

C	-1.58081575	-4.01160206	0.75829025
C	-2.55306981	-1.74652818	0.18170445
Mo	0.92820910	-0.44706018	0.03363794
S	-0.59295300	-0.88174769	-1.77065424
S	-0.08268144	-1.83905415	1.69749552
S	2.11754574	1.09141220	-1.49183638
S	2.68227854	0.13502640	1.66431738
C	-2.78447301	-0.33162172	0.61731215
N	-2.98261558	0.71985369	-0.26732666
C	-3.15050298	1.88040206	0.38493184
N	-3.10762160	1.57562708	1.68901243
C	-2.87480576	0.22116755	1.86313905
H	-3.20464578	2.25327085	2.43619953
C	-1.90003750	-3.36989906	-1.64997399
H	-2.79689354	-0.21852497	2.84275251

C	-1.73149224	-2.55167504	1.20921906
C	-2.07908429	-1.88978580	-1.27870415
C	2.06403959	-1.98438636	-0.60829352
N	5.48693285	2.35139696	0.06275032
C	-1.02187789	-4.13381179	-0.65928016
H	-1.50607437	-3.44250355	-2.66717628
H	-2.90153245	-3.82070688	-1.65973336
H	-2.58103771	-4.46435716	0.79034204
H	-0.95997037	-4.55324572	1.47695765
H	0.00446906	-3.75537180	-0.69275646
H	-0.97769208	-5.18881023	-0.94801662
H	-2.86164622	-1.47980890	-1.92444589
H	-2.28026325	-2.53504687	2.15464850
O	2.71311179	-2.85753866	-0.97376595
C	4.62694762	2.30028953	-1.00164179
H	4.84445118	2.79982402	-1.93243003
C	3.53904910	1.52949884	-0.60988671
C	3.78639099	1.10936972	0.75900932
C	5.01394408	1.64342341	1.13396799
H	5.56569760	1.57368487	2.05792066
H	6.36992160	2.84755310	0.05590230
H	-0.29477831	1.04023128	1.08645115
H	-3.53518252	-2.24398980	0.18473739
C	-3.26115774	3.23952100	-0.24809631
C	-1.87282503	3.60480928	-0.82494402
H	-1.93194347	4.58628698	-1.30419897
H	-1.11996102	3.64813015	-0.03258673
H	-1.54935330	2.87420775	-1.57229824
C	-3.68095698	4.27512768	0.80512790
H	-4.64973656	4.02449243	1.24782995
H	-2.93854922	4.36252375	1.60498706
H	-3.76783255	5.25283861	0.32489645
H	-2.91367541	0.65662988	-1.27591666
H	-0.19506727	1.42713835	0.44230450
C	-4.30374925	3.18581953	-1.38171286
H	-5.28621694	2.89632151	-0.99795543
H	-4.38597210	4.17678182	-1.83621394
H	-4.01323742	2.48024374	-2.16608693

Name-MoIII6tBu\\SCF E(UB3LYP-D3BJ/BS1)= -2790.7830047\\G=-
2790.415177\\H=-2790.306364\\ZeroPoint=0.441532

C	-0.89255312	4.04629029	-1.29547417
C	-1.98121438	1.80373895	-0.82262058
Mo	1.35645918	0.43869793	-0.02380035
S	-0.39576095	1.01671357	1.46581267
S	0.72584445	1.84095905	-1.86970014
S	2.21620698	-1.13081513	1.69720139
S	3.28669513	-0.28798718	-1.35847896
C	-2.16514498	0.37408940	-1.24764192

N	-2.69446810	-0.61102476	-0.42464360
C	-2.71096328	-1.75089373	-1.11835481
N	-2.23815359	-1.51666173	-2.36900901
C	-1.88244470	-0.18744660	-2.46975338
H	-2.12388391	-2.21284107	-3.09323295
C	-1.63021760	3.49500488	1.03945219
H	-1.46334151	0.21916645	-3.37458559
C	-0.98204528	2.57108528	-1.71219395
C	-1.76299888	2.00531015	0.68834032
C	2.45760361	1.94045147	0.74564711
N	5.70986173	-2.60410610	0.66372119
C	-0.58306335	4.21682484	0.19197751
H	-1.41784388	3.60142198	2.10706343
H	-2.61216370	3.95418257	0.86108587
H	-1.86652442	4.50553648	-1.51359838
H	-0.15101392	4.55846526	-1.91497881
H	0.41538889	3.82574332	0.41424336
H	-0.57060863	5.28131459	0.44818335
H	-2.63742909	1.61330589	1.20753982
H	-1.35073369	2.52365263	-2.74060624
O	3.08107846	2.79849942	1.18684645
C	4.70492398	-2.48234468	1.59259783
H	4.75920581	-2.97291294	2.55149448
C	3.73133708	-1.66460426	1.03847504
C	4.19604491	-1.28992638	-0.28358412
C	5.43519080	-1.89666743	-0.47142576
H	6.11476371	-1.87527243	-1.30881316
H	6.55277071	-3.14616237	0.80649044
H	0.02421030	-0.93559257	-1.08353751
H	-2.93651108	2.32222137	-1.00630209
C	-3.14811374	-3.10421298	-0.60783026
C	-2.31334624	-3.45731054	0.64111308
H	-2.60180547	-4.44731963	1.00853984
H	-1.24478630	-3.47546034	0.40250886
H	-2.47445015	-2.73482786	1.44436348
C	-2.92537946	-4.17734738	-1.68568237
H	-3.50943828	-3.97127340	-2.58897060
H	-1.86883633	-4.25611425	-1.96249838
H	-3.24325785	-5.14917016	-1.29867628
H	-3.21634286	-0.51905594	1.02306859
H	0.31613441	-1.42163305	-0.57707033
O	-5.40299279	0.23031951	3.08933087
O	-3.57772944	-0.48393092	2.01211114
C	-4.77176650	0.07512944	2.05335831
H	-5.16159747	0.39779352	1.07326120
C	-4.64539754	-3.05405549	-0.24149220
H	-4.83545596	-2.32398462	0.54789760
H	-5.25145425	-2.78742002	-1.11308469
H	-4.97028847	-4.03624849	0.11623499

Name-MoIII21tBu\\SCF E(UB3LYP-D3BJ/BS1)= -2790.3131355\\G=-
2789.950810\\H=-2789.846479\\ZeroPoint=0.432030

C	-0.47384894	4.23947858	-0.74337753
C	-1.86517920	2.15688927	-0.39069879
Mo	1.19402400	0.04905188	-0.23421709
S	-0.13615147	0.89185859	1.56544395
S	0.69973678	1.90416437	-1.73422057
S	2.12533932	-1.72984974	1.24949814
S	2.98136296	-0.59405870	-1.81513674
C	-2.38078494	0.86903610	-0.96829003
N	-3.09247696	-0.08266493	-0.24465738
C	-3.45887510	-1.04452329	-1.09591485
N	-3.01562209	-0.72831833	-2.33907511
C	-2.33607925	0.47022978	-2.27986642
H	-3.15566689	-1.28490835	-3.17075888
C	-1.06608668	3.51569113	1.58464993
H	-1.87981943	0.90505822	-3.15253223
C	-0.83956015	2.85734969	-1.30619315
C	-1.44908760	2.11120679	1.09098130
C	2.83318281	1.34960722	0.62376601
N	5.87301475	-2.40445498	0.17334597
C	0.00237254	4.17026557	0.70820676
H	-0.74092708	3.45932998	2.62775747
H	-1.97489697	4.13378528	1.56453812
H	-1.37354749	4.86952907	-0.79410554
H	0.28043155	4.70665116	-1.38341187
H	0.93219481	3.59271597	0.76466258
H	0.22436090	5.17728961	1.07796435
H	-2.31108481	1.77138916	1.66884098
H	-1.31917604	3.00355167	-2.27858562
O	3.66989676	1.99957658	1.05076173
C	4.86465711	-2.50349175	1.10502553
H	5.02319451	-2.98865526	2.05589875
C	3.73981827	-1.89402363	0.57125671
C	4.10403405	-1.40824600	-0.73822819
C	5.43529256	-1.74114507	-0.94573345
H	6.08838513	-1.55650672	-1.78478540
H	6.81166020	-2.75518861	0.30262929
H	-3.29272751	-0.18067735	1.27150012
H	0.00431167	-1.04300125	-0.89166725
H	-2.72047187	2.85387119	-0.38282894
C	-4.23057900	-2.30353593	-0.76768456
C	-4.66439014	-3.01622893	-2.06031380
H	-5.25231164	-3.90135457	-1.80232350
H	-5.28593583	-2.37005268	-2.68854762

H	-3.80379145	-3.35389510	-2.64759611
C	-5.48356723	-1.93931215	0.05214025
H	-5.21811299	-1.45210131	0.99270808
H	-6.13794935	-1.26751523	-0.51248054
H	-6.04541239	-2.84914591	0.28628409
O	-3.45063398	-0.22173983	2.31642767
C	-2.53284247	-0.96118284	2.91133170
O	-2.48600973	-1.11277800	4.12607050
H	-1.81250680	-1.43917775	2.23332248
C	-3.33160281	-3.25518110	0.04909251
H	-2.41179637	-3.48845819	-0.49634442
H	-3.05918496	-2.81459861	1.00968174
H	-3.86450572	-4.19164859	0.24366840

Name-MoIII22tBu\\SCF E(UB3LYP-D3BJ/BS1)= -2600.5151446\\G=-
2600.182593\\H=-2600.087871\\ZeroPoint=0.396663

C	-1.13363400	3.41488100	-1.72121800
C	-2.14900800	1.99490900	0.11311900
Mo	0.99912500	-0.06360000	0.10846100
S	0.28020700	1.65628400	1.68578200
S	-0.27522600	0.75540200	-1.72138400
S	2.75148900	-0.59610600	1.75877200
S	2.14202400	-1.76123100	-1.35646700
C	-2.74866800	0.68304400	0.52148900
N	-3.54651500	-0.04484100	-0.35238700
C	-3.95121000	-1.11964700	0.31058300
N	-3.45884600	-1.09995500	1.58628900
C	-2.69183400	0.03923600	1.73281100
H	-3.59904200	-1.81480000	2.28699200
C	-0.78807900	4.03610100	0.69155600
H	-2.17255400	0.26160000	2.64971100
C	-1.59105100	2.00354300	-1.32292200
C	-1.21201200	2.63266200	1.15496000
C	2.60437700	1.32440500	-0.64023000
N	5.87426900	-2.15217600	-0.08741200
C	-0.16407100	4.02290700	-0.70551700
H	-0.10086500	4.47236500	1.42259400
H	-1.68638800	4.67022500	0.67563900
H	-2.03149200	4.04640600	-1.77958000
H	-0.69280200	3.39340000	-2.72251600
H	0.76535300	3.44319500	-0.68689200
H	0.09967900	5.04260400	-1.00721100
H	-1.78328800	2.73218800	2.08323000
H	-2.40333700	1.69371400	-1.98446900
O	3.44956300	1.98448600	-1.03592000
C	5.32705800	-1.54062900	1.01155100
H	5.91798800	-1.31358400	1.88566000
C	3.98554400	-1.31322900	0.73596100
C	3.72904900	-1.80753600	-0.59483400

C	4.92517300	-2.31787300	-1.07282800
H	5.17165800	-2.77693000	-2.01794900
H	6.84366200	-2.42421600	-0.17078500
H	-0.13830800	-1.27202300	0.65320400
H	-2.98489000	2.71342300	0.05108000
C	-4.78485700	-2.25957600	-0.22562200
C	-5.92993000	-2.58337600	0.75474600
H	-6.54462700	-3.39574600	0.35369100
H	-5.55154200	-2.90634400	1.73008200
H	-6.57306900	-1.71104100	0.90931800
C	-3.88322700	-3.50340200	-0.38705000
H	-3.05730600	-3.29755100	-1.07572400
H	-3.45797500	-3.81130600	0.57355000
H	-4.46365700	-4.34217900	-0.78608500
C	-5.37541100	-1.87852500	-1.59016500
H	-6.02317900	-1.00033500	-1.51103000
H	-4.58919700	-1.65474300	-2.31571100
H	-5.97208500	-2.71117200	-1.97582400

Name-MoIII23tBu\\SCF E (UB3LYP-D3BJ/BS1)=-2789.1225121\\G=-

2788.776991\\H=-2788.676100\\ZeroPoint=0.412633

C	-1.28223610	3.83810635	-1.39734666
C	-2.11203177	2.15467552	0.31189725
Mo	1.34709001	0.66500999	-0.09260039
S	0.37600965	1.80460414	1.75329070
S	-0.28142540	1.22962456	-1.71307771
S	2.87356643	-0.39976752	1.52047046
S	2.35799705	-0.84940780	-1.75787066
C	-2.56739056	0.75380866	0.59700127
N	-3.32579797	0.04381598	-0.32333258
C	-3.58820873	-1.13291508	0.23114551
N	-3.06454686	-1.18675860	1.49179667
C	-2.39529542	-0.00326391	1.73035163
H	-3.01415312	-2.00697571	2.07936889
C	-0.85728628	4.22237330	1.05801053
H	-1.86260474	0.16779517	2.65050221
C	-1.63309320	2.36588281	-1.13663305
C	-1.18084090	2.75433113	1.37793420
C	2.59259892	2.17781431	-0.54962407
N	4.50753578	-3.62146382	-0.00294842
C	-0.31755502	4.41469425	-0.36005749
H	-0.15822534	4.61844700	1.80034048
H	-1.79316214	4.78786744	1.16508365
H	-2.22470299	4.40172227	-1.35987497
H	-0.88347846	3.95232976	-2.40971444
H	0.66118966	3.93557946	-0.45352924
H	-0.16309993	5.48156800	-0.55358765

H	-1.70758233	2.71312676	2.33544727
H	-2.45688477	2.07528705	-1.79092599
O	3.30196802	3.04553522	-0.81502155
C	4.26504829	-2.82355978	1.08271684
H	4.64843639	-3.06455735	2.06159297
C	3.48222354	-1.76174250	0.64353929
C	3.26006325	-1.95652617	-0.77920628
C	3.92035850	-3.12620161	-1.13711352
H	4.00373377	-3.63173072	-2.08611765
H	5.04230589	-4.48039953	0.03134480
H	0.12029211	-1.02335149	0.35448885
H	-3.00528910	2.79979333	0.36956249
C	-4.39554216	-2.25187631	-0.38721875
C	-5.89607021	-1.97470846	-0.15094953
H	-6.50282421	-2.77179387	-0.59418716
H	-6.12186781	-1.92783449	0.91934734
H	-6.19326525	-1.02432609	-0.60482793
C	-4.02011473	-3.60311445	0.24788240
H	-2.94991974	-3.80469149	0.14307735
H	-4.27922646	-3.63897791	1.31159173
H	-4.57271994	-4.40699566	-0.24787435
C	-0.25717748	-2.10843111	0.43739421
O	-0.71041526	-2.57884714	-0.62719330
O	-0.15197798	-2.60737881	1.57544798
C	-4.11447381	-2.30556841	-1.89839859
H	-4.38274026	-1.36401566	-2.38365809
H	-3.05448262	-2.49697332	-2.08867797
H	-4.70066412	-3.10846709	-2.35698690

Name-TS23\\SCF E(UB3LYP-D3BJ/BS1)=-2789.5786903\\G=-2789.22639\\H=-2789.121784\\ZeroPoint=0.423031

C	-1.40262902	3.91321978	-1.35796818
C	-2.12335672	2.18932067	0.35101036
Mo	1.31545739	0.66955991	-0.09160311
S	0.40941823	1.95896892	1.75189642
S	-0.31520104	1.33833937	-1.73395333
S	2.90039862	-0.34007038	1.49231561
S	2.35978435	-0.79453940	-1.78797211
C	-2.47740244	0.76773925	0.65760270
N	-3.19321726	-0.03448613	-0.22579951
C	-3.40721578	-1.25612626	0.28702080
N	-2.85562897	-1.23767601	1.50897739
C	-2.26998920	-0.00754777	1.76056263
H	-2.81516165	-2.03592254	2.13140023
C	-0.96479506	4.30592833	1.08340560
H	-1.73717870	0.18830299	2.67394286
C	-1.68484955	2.42221363	-1.11312913
C	-1.19876400	2.82294481	1.40980293

C	2.63063612	2.34553619	-0.60290125
N	4.11334445	-3.80042680	0.06276920
C	-0.43770297	4.51443350	-0.33648116
H	-0.28496175	4.73693948	1.82368801
H	-1.92774554	4.82554416	1.18799198
H	-2.36368382	4.44242210	-1.29311336
H	-1.03209813	4.04715120	-2.37827388
H	0.54933430	4.05285810	-0.43790854
H	-0.31155769	5.58442513	-0.53328289
H	-1.72104015	2.75901187	2.36897721
H	-2.52436805	2.14202625	-1.75680561
O	3.31807148	3.22112404	-0.87304779
C	3.97059495	-2.94284401	1.12290697
H	4.30898277	-3.20555504	2.11310155
C	3.33803592	-1.80055293	0.64843731
C	3.09807281	-2.00177861	-0.76595363
C	3.59665893	-3.25660609	-1.08785225
H	3.61466538	-3.79370548	-2.02329618
H	4.52652939	-4.72134469	0.12392664
H	-3.49321193	0.24292952	-1.15234791
H	0.29201622	-0.70089065	0.30062293
H	-3.05871572	2.76497157	0.43845062
C	-4.17513503	-2.37968294	-0.35579674
C	-5.67830483	-2.15135606	-0.07579603
H	-6.25537987	-2.95783971	-0.53768306
H	-5.88051816	-2.15055195	0.99915175
H	-6.01572480	-1.19931582	-0.49549644
C	-3.73389132	-3.72580422	0.24367638
H	-2.66642944	-3.90194823	0.08794456
H	-3.95130639	-3.78482614	1.31474296
H	-4.29050723	-4.52773514	-0.24810927
C	-0.14565868	-2.43962145	0.35366311
O	-0.51490800	-2.60737326	-0.75983528
O	0.09349713	-2.68437741	1.48793522
C	-3.91929814	-2.37204428	-1.87423865
H	-4.28718286	-1.45405573	-2.34391191
H	-2.85419592	-2.47825796	-2.09564159
H	-4.45498127	-3.21041962	-2.32720272

Name=TS5,6\\SCF E (UB3LYP-D3BJ/BS1)=-2790.7818624\\G=-2790.405793\\H=-2790.308957\\ZeroPoint=0.437997

C	-0.86973577	4.02007878	-1.30149393
C	-1.97231163	1.79393502	-0.79275558
Mo	1.37927513	0.41812162	-0.02686394
S	-0.36107565	1.00205919	1.47625099
S	0.71787356	1.79311813	-1.88320760
S	2.27265028	-1.11850799	1.70626571
S	3.29553374	-0.31769597	-1.37718844
C	-2.17513107	0.36506064	-1.20807349

N	-2.72657312	-0.60987867	-0.38656830
C	-2.76202210	-1.76331278	-1.06157579
N	-2.27584328	-1.54277032	-2.30323365
C	-1.89629144	-0.22045715	-2.41676509
H	-2.16695950	-2.24881979	-3.01944200
C	-1.57321307	3.49436871	1.04982330
H	-1.46250775	0.16719074	-3.32260188
C	-0.97935736	2.54269824	-1.70509612
C	-1.72726251	2.00333500	0.71392062
C	2.48364855	1.93420401	0.70768948
N	5.75902748	-2.58807639	0.64645138
C	-0.53421930	4.19990192	0.17915693
H	-1.34161092	3.60636821	2.11277992
H	-2.55375849	3.96145292	0.88486768
H	-1.84300134	4.48629280	-1.50743693
H	-0.13386421	4.51985432	-1.93753241
H	0.46464143	3.80312104	0.38846391
H	-0.50905538	5.26632768	0.42602695
H	-2.59705900	1.62431323	1.25031313
H	-1.36543564	2.49032232	-2.72685975
O	3.11000798	2.79956660	1.12976840
C	4.76701993	-2.45721409	1.58770231
H	4.83810827	-2.93180107	2.55350507
C	3.78061743	-1.65433351	1.03443768
C	4.22438427	-1.29831888	-0.30039319
C	5.46444710	-1.90093666	-0.49593769
H	6.13217359	-1.88909447	-1.34296454
H	6.60703990	-3.12314711	0.78579034
H	0.04120460	-0.98450020	-1.05294914
H	-2.92636590	2.31767899	-0.96581045
C	-3.23455784	-3.09703988	-0.53657217
C	-2.44216987	-3.43369339	0.74420756
H	-2.75497804	-4.41285199	1.11978935
H	-1.36735428	-3.46901180	0.53855963
H	-2.62070932	-2.69357977	1.52751478
C	-2.99485490	-4.19223873	-1.58791420
H	-3.55114494	-3.99640175	-2.51073235
H	-1.93200648	-4.28901288	-1.83262545
H	-3.33668176	-5.15155412	-1.19079980
H	-3.20128836	-0.47954705	0.81875220
H	0.32720577	-1.45792484	-0.53226544
O	-5.49386020	0.38015386	2.92967184
O	-3.64727507	-0.39630701	1.91815989
C	-4.81594265	0.17869294	1.92090321
H	-5.18229494	0.49296624	0.92440599
C	-4.74166452	-3.01350823	-0.21776018
H	-4.94166665	-2.26272337	0.54940296
H	-5.31619339	-2.75745382	-1.11333466
H	-5.09126218	-3.98270782	0.15116872

Name-TS2,21SCF E (UB3LYP-D3BJ/BS1)=-2790.3123905\\G=-2789.95243\\H=-2789.849455\\ZeroPoint=0.428440

C	-0.45644368	4.17163226	-0.94507309
C	-1.84149749	2.09769610	-0.53425629
Mo	1.23594389	0.02866873	-0.20814039
S	-0.17034232	0.90520157	1.51248356
S	0.75642955	1.80884101	-1.80884234
S	2.15646619	-1.68934707	1.35907321
S	3.07591794	-0.62795033	-1.71353982
C	-2.32653736	0.77723507	-1.05922982
N	-3.07587180	-0.13025180	-0.31668683
C	-3.38699874	-1.16306380	-1.10706769
N	-2.87211953	-0.93016616	-2.33577699
C	-2.20351077	0.27638220	-2.32805631
H	-2.95332466	-1.55381310	-3.12735909
C	-1.08040204	3.54042681	1.40004472
H	-1.69186320	0.64545486	-3.19981789
C	-0.80044082	2.76463577	-1.45765918
C	-1.45834532	2.11772880	0.95801908
C	2.82390702	1.38808073	0.65533351
N	5.93159673	-2.36826411	0.38320281
C	-0.00093203	4.16325643	0.51468251
H	-0.77132012	3.52492849	2.44938360
H	-1.98946560	4.15574620	1.34246412
H	-1.36051308	4.79119392	-1.03348688
H	0.30336480	4.61921794	-1.59242098
H	0.93068170	3.59365395	0.60805871
H	0.21078449	5.18541348	0.84697730
H	-2.33657372	1.81037408	1.52837178
H	-1.26082322	2.86579653	-2.44512537
O	3.63895135	2.06000444	1.09038173
C	4.90300162	-2.44972374	1.29500483
H	5.04341750	-2.90996642	2.26096803
C	3.78694669	-1.86091775	0.72157706
C	4.17770169	-1.40705156	-0.59143705
C	5.51534432	-1.73669492	-0.76146058
H	6.18547195	-1.56963805	-1.59071316
H	6.86895633	-2.71049498	0.54160704
H	-3.42666528	-0.04522576	0.96822482
H	0.08138780	-1.10559118	-0.85183626
H	-2.70428548	2.78338239	-0.57788305
C	-4.16493278	-2.40033140	-0.72409486
C	-4.44144731	-3.25829053	-1.97017455
H	-5.02537354	-4.13524452	-1.67822444
H	-5.01592757	-2.70636377	-2.72111610
H	-3.51475796	-3.61708725	-2.43040358
C	-5.50551194	-1.98705222	-0.08476789
H	-5.34995336	-1.39302186	0.81825439
H	-6.10753012	-1.40089942	-0.78631076
H	-6.07102070	-2.88360236	0.18783466
O	-3.78527391	0.05810651	2.07164053

C	-3.00420084	-0.55975834	2.91676245
O	-3.17601370	-0.56464590	4.13664118
H	-2.15121597	-1.09168489	2.46292884
C	-3.33620128	-3.22673183	0.28138944
H	-2.36520187	-3.49872600	-0.14412397
H	-3.16310017	-2.67092366	1.20465594
H	-3.87387508	-4.14658257	0.53249665

Name-TS22,23\\SCF E (UB3LYP-D3BJ/BS1)=-2789.0996122\\G=-

2788.758591\\H=-2788.657077\\ZeroPoint=0.408729

C	-1.43988787	3.87324323	-1.37543396
C	-2.14103595	2.13009488	0.32421576
Mo	1.31416269	0.64718827	-0.07583122
S	0.39515992	1.95688686	1.74489133
S	-0.25679082	1.35479797	-1.73597157
S	2.86112129	-0.37230303	1.54018062
S	2.43620077	-0.78453509	-1.76723142
C	-2.53173958	0.70889748	0.60671501
N	-3.31309775	-0.01318146	-0.28613132
C	-3.50177099	-1.20992565	0.25576482
N	-2.89780361	-1.27162983	1.48073863
C	-2.27002070	-0.06267584	1.71205189
H	-2.82793212	-2.08791406	2.07182250
C	-1.02907196	4.26663479	1.07583540
H	-1.67889028	0.10990321	2.59537628
C	-1.68306068	2.37643593	-1.12853599
C	-1.23740049	2.77621201	1.39042587
C	2.63142467	2.34362738	-0.54756551
N	4.38650615	-3.68726693	0.06106366
C	-0.50026207	4.49620113	-0.34140644
H	-0.36059908	4.71022877	1.81973365
H	-2.00259385	4.76710799	1.17908085
H	-2.41519237	4.37754101	-1.31914302
H	-1.06146607	4.02411433	-2.39110094
H	0.49884499	4.05895161	-0.43747140
H	-0.39852170	5.57045506	-0.53141525
H	-1.76055795	2.69344921	2.34806363
H	-2.49664277	2.04165332	-1.77531034
O	3.30638592	3.23367217	-0.80298326
C	4.14853071	-2.86953650	1.13557327
H	4.48524459	-3.12656534	2.12796170
C	3.43468295	-1.77167723	0.67065668
C	3.24510933	-1.95557717	-0.75116540
C	3.85187801	-3.15692155	-1.08941947
H	3.93796213	-3.66555058	-2.03705564
H	4.86957277	-4.57388328	0.11211398
H	0.28110132	-0.72006166	0.26526435
H	-3.06816816	2.72552011	0.38873477

C	-4.32426071	-2.33629201	-0.32945663
C	-5.81191266	-2.08910097	0.00464486
H	-6.43197208	-2.89098697	-0.41063440
H	-5.97012015	-2.06025172	1.08764293
H	-6.15299603	-1.13817922	-0.41575446
C	-3.89208285	-3.69076700	0.26015102
H	-2.83111284	-3.88624638	0.07758224
H	-4.07491992	-3.74376039	1.33877436
H	-4.47103141	-4.49368899	-0.20619199
C	-0.24685421	-2.44917871	0.23017746
O	-0.64529633	-2.53021632	-0.88190502
O	0.02150743	-2.76604942	1.33906828
C	-4.14109007	-2.36535653	-1.85631783
H	-4.43931817	-1.41609185	-2.30766669
H	-3.09675134	-2.55529165	-2.12133260
H	-4.75688950	-3.16063723	-2.28866833

5. Optimized geometrical parameters of MIII(tBu)(CO) in different oxidation states along with their thermochemical and single point data.

Name-MoIII(tBu)(CO), Oxid 2\\SCF E(UB3LYP-D3BJ/BS1)= -2600.0692072\\G=-2599.738597\\H= -2599.649619\\ZeroPoint= 0.390281

C	4.48632443	-0.92024773	-1.22169871
C	3.10144634	0.79777787	-0.01471720
Mo	0.01422486	-0.87995126	0.01915425
S	1.67742689	-0.89661678	1.87494257
S	1.75819028	-1.08046703	-1.75841028
S	-1.89765994	-0.38824804	1.69340999
S	-1.84972877	-1.18682038	-1.69374347
C	2.01815435	1.83344809	-0.04699737
N	0.63704432	1.62447220	-0.11628935
C	0.07120610	2.83992460	-0.13504907
N	1.04101335	3.79746746	-0.07637826
C	2.26819433	3.18107066	-0.02035691
H	0.87971434	4.79380796	-0.08538042
C	4.44128576	-0.90067947	1.28921625
H	3.19182982	3.73684775	0.02099777
C	3.22490994	-0.04241238	-1.30766402
C	3.20013290	0.00740466	1.31517990
C	-0.24090977	-2.76775061	0.09633324
N	-5.40694226	-1.33614664	0.06737539
C	4.49619644	-1.78348201	0.04192525
H	4.46987565	-1.50600452	2.20135716
H	5.33559043	-0.25806840	1.30451727
H	5.37191083	-0.26526191	-1.21165442

H	4.55953064	-1.54238923	-2.12010148
H	3.62369226	-2.44539223	0.02818534
H	5.39266532	-2.41476420	0.06475792
H	4.02708536	1.39574619	-0.01268523
H	3.35685089	0.76341295	2.09281274
H	3.36491536	0.67837612	-2.12214987
O	-0.39846699	-3.95212358	0.14831969
C	-4.63545201	-0.97305583	1.15499507
H	-5.08106024	-0.82286588	2.12763734
C	-3.31475191	-0.86803926	0.74088250
C	-3.29603069	-1.18813808	-0.66742460
C	-4.60147166	-1.47628607	-1.04159521
H	-5.01239542	-1.75996385	-1.99961357
H	-6.40094420	-1.50648244	0.08958905
C	-1.39142462	3.24496391	-0.14066363
C	-1.90087942	3.28783306	1.31670288
H	-1.86305893	2.28728651	1.75697817
H	-1.30131460	3.97626153	1.92225668
H	-2.94012106	3.63635555	1.33534421
C	-1.55124309	4.64673132	-0.76491438
H	-1.08470811	5.43327729	-0.16170845
H	-1.13265576	4.68840045	-1.77575332
H	-2.61673113	4.88661017	-0.82968414
C	-2.22975874	2.25161823	-0.94993814
H	-1.90512270	2.22341328	-1.99501381
H	-2.14892517	1.24750576	-0.54249538
H	-3.28136685	2.55863136	-0.92665989

Name-MoIII(tBu)(CO), Oxid 3\\SCF E(UB3LYP-D3BJ/BS1)=-2599.9748467\\G=-2599.642013\\H= -2599.553948\\ZeroPoint= 0.391801

C	4.41456737	-0.95966999	-1.19494556
C	3.05050275	0.88767811	-0.12207507
Mo	0.05287600	-0.70212277	0.03060851
S	1.67266223	-0.68369699	1.89593360
S	1.68043323	-1.02169543	-1.80081997
S	-1.84099768	-0.74584642	1.69723478
S	-1.71667382	-1.18049841	-1.72952098
C	1.92217480	1.87132463	-0.20817194
N	0.55055454	1.58960798	-0.12123227
C	-0.09105711	2.76984870	-0.17125154
N	0.82298125	3.76561050	-0.31024445
C	2.08576875	3.22309448	-0.33185184
H	0.60324731	4.74894157	-0.37704769
C	4.40649609	-0.71484508	1.29780545
H	2.97298802	3.82813920	-0.42922167
C	3.18844954	-0.04636160	-1.34804014
C	3.17608351	0.20479686	1.26482171
C	0.10126289	-2.71069945	0.22131119
N	-5.31120377	-1.46681035	-0.07893060

C	4.41375168	-1.71027113	0.13714598
H	4.44971369	-1.23098531	2.26197636
H	5.30581437	-0.08465312	1.23049707
H	5.31633372	-0.33157648	-1.24729495
H	4.45917714	-1.65355545	-2.04025993
H	3.52419502	-2.34816336	0.19749412
H	5.29176681	-2.36250944	0.20374545
H	3.95447450	1.51213303	-0.17616100
H	3.32914053	1.01568274	1.98396673
H	3.35124450	0.61001136	-2.20895268
O	0.17752619	-3.86066900	0.33567101
C	-4.56781814	-1.21584838	1.05295455
H	-5.03130692	-1.14871459	2.02580578
C	-3.24049106	-1.08808876	0.67185861
C	-3.18867076	-1.27593265	-0.75458992
C	-4.48719773	-1.50931821	-1.18186997
H	-4.88102953	-1.69505688	-2.16991869
H	-6.30937791	-1.61576069	-0.09544747
C	-1.55920886	3.09245303	0.02914473
C	-1.88203634	2.94712889	1.53235735
H	-1.73326615	1.91598603	1.86094706
H	-1.24911724	3.60981606	2.13210335
H	-2.92820598	3.21887564	1.71139573
C	-1.85036239	4.54377827	-0.40000254
H	-1.33691372	5.27634866	0.23215032
H	-1.57302051	4.72202646	-1.44411082
H	-2.92310424	4.73107976	-0.30081724
C	-2.45106953	2.15305322	-0.78954621
H	-2.24892463	2.25336781	-1.86063390
H	-2.29270532	1.11543384	-0.51189302
H	-3.50210527	2.40385503	-0.61196492

Name-MoIII1(tBu)(CO), Oxid 3\\SCF E(UB3LYP-D3BJ/BS1)= -

2601.1263856\\G= -2600.784503\\H= -2600.689379\\ZeroPoint= 0.406130

C	1.64260939	-3.65130699	-1.26084871
C	2.65188535	-1.71268481	-0.00012280
Mo	-1.00986888	-0.48659038	-0.00012726
S	0.43902387	-1.17408451	1.83213074
S	0.43906162	-1.17395407	-1.83239444
S	-2.51803423	0.56228742	1.71826140
S	-2.51830257	0.56197623	-1.71850149
C	3.22347371	-0.32425631	-0.00002742
N	2.50342096	0.85893786	0.00021041
C	3.38542232	1.84987177	0.00030242
N	4.65559743	1.34881837	0.00009569
C	4.56805215	-0.02915771	-0.00010156
H	5.50950713	1.88913131	0.00012454
C	1.64255162	-3.65141312	1.26040064

H	5.44456882	-0.65865244	-0.00026387
C	1.93258964	-2.14044750	-1.30085135
C	1.93254881	-2.14056093	1.30054527
C	-2.11039512	-2.12573714	0.00000251
N	-5.65903738	2.25736576	-0.00002584
C	0.88933727	-4.07923362	-0.00025958
H	1.09422460	-3.94548813	2.16062695
H	2.61015520	-4.17376219	1.28862312
H	2.61021943	-4.17364428	-1.28906835
H	1.09432769	-3.94531224	-2.16112534
H	-0.10913298	-3.63589001	-0.00026769
H	0.75382764	-5.16687675	-0.00030681
H	2.63635485	-1.95013921	2.11666774
H	2.63641773	-1.94994187	-2.11693498
O	-2.78907253	-3.07007766	0.00009114
C	-4.96646942	1.87986776	1.12825829
H	-5.34814114	2.08496622	2.11707541
C	-3.80062157	1.24993706	0.71911802
C	-3.80073970	1.24979730	-0.71928254
C	-4.96665076	1.87965680	-1.12835150
H	-5.34848156	2.08457391	-2.11714477
H	-6.54861899	2.73494282	0.00000116
H	0.50775027	1.19064687	-0.00017377
H	-0.20407946	1.48885642	-0.00027851
H	3.54311620	-2.35988199	-0.00014491
C	3.04041884	3.32185137	0.00055174
C	2.20904803	3.64063832	-1.25887512
H	2.77770526	3.41861945	-2.16790153
H	1.28749444	3.05299469	-1.28015754
H	1.94108344	4.70247442	-1.27272649
C	4.31376595	4.18163260	0.00092740
H	4.04121775	5.24095938	0.00111435
H	4.92584875	3.99464875	0.88975227
H	4.92611820	3.99504271	-0.88779547
C	2.20865892	3.64012922	1.25984786
H	1.28710829	3.05246558	1.28063024
H	2.77704609	3.41776795	2.16895952
H	1.94067723	4.70195640	1.27402781

Name-TS12, Oxid 2\\SCF E(UB3LYP-D3BJ/BS1)=-2601.2140395\\G=-
2600.871211\\H= -2600.780590\\ZeroPoint= 0.403601

C	-1.44725760	-3.69343211	1.33104819
C	-2.63999581	-1.85595260	0.07456098
Mo	0.93400275	-0.30986925	-0.01482470
S	-0.57343578	-1.22310957	-1.89300948
S	-0.45847862	-1.10915227	1.86744141
S	2.51951692	0.72006710	-1.76048674
S	2.28606191	1.15537587	1.65052950

C	-3.23364407	-0.48167395	0.06488169
N	-2.54619110	0.72022394	-0.03994631
C	-3.42037500	1.72842857	-0.01525934
N	-4.66146827	1.20535507	0.10025037
C	-4.56632777	-0.17313308	0.15161231
H	-5.51792681	1.74143058	0.14246258
C	-1.56304830	-3.75828020	-1.17034959
H	-5.43703217	-0.80281020	0.24086589
C	-1.86051570	-2.21171650	1.36956056
C	-1.95706408	-2.27241994	-1.25595893
C	2.24651758	-1.72630897	-0.00627365
N	5.92798854	1.59510292	0.09602113
C	-0.69479198	-4.06102534	0.05167973
H	-1.05412497	-4.04683453	-2.09516067
H	-2.48303628	-4.36174674	-1.10572636
H	-2.36099932	-4.30560926	1.38831892
H	-0.85210778	-3.92489487	2.22017490
H	0.23173800	-3.48156872	-0.00860699
H	-0.42255376	-5.12352084	0.06926894
H	-2.73423720	-2.17934508	-2.02335287
H	-2.57791919	-2.08722674	2.18820089
O	3.09396467	-2.57147923	-0.01992769
C	5.21836655	1.30316616	-1.05103984
H	5.70625914	1.26271810	-2.01410403
C	3.89229912	1.10145659	-0.69946224
C	3.80002683	1.26619255	0.73226230
C	5.07691643	1.56238307	1.18475435
H	5.44249207	1.75663387	2.18273409
H	6.92395965	1.74808680	0.14066004
H	-1.32228128	0.90685327	-0.09974887
H	-0.30431783	1.23462886	-0.14097093
H	-3.52099822	-2.51506326	0.12729858
C	-3.08438386	3.19698167	-0.09518072
C	-2.20812125	3.57436385	1.11814928
H	-2.73620948	3.37764634	2.05650286
H	-1.27379209	3.00641294	1.12025518
H	-1.96397420	4.64065418	1.07666661
C	-4.37024041	4.03824471	-0.08150334
H	-4.10770052	5.09776908	-0.14288399
H	-5.01483570	3.80220296	-0.93464839
H	-4.94123161	3.88838255	0.84092871
C	-2.30951843	3.46350776	-1.40253915
H	-1.37556135	2.89565496	-1.42955153
H	-2.90957293	3.18679124	-2.27511635
H	-2.06785759	4.52873170	-1.47393498

Name-TS12, Oxid 3\\SCF E(UB3LYP-D3BJ/BS1)=-2601.1207443\\G=-
2600.777303\\H= -2600.685425\\ZeroPoint= 0.405434

C	-1.84936479	-3.61763179	1.25455372
C	-2.75462775	-1.62231673	0.00120622
Mo	0.88908558	-0.46038087	-0.00011727
S	-0.54616008	-1.19135196	-1.85721253
S	-0.54239315	-1.19777331	1.85699775
S	2.45315088	0.52206835	-1.72356876
S	2.46261198	0.50198029	1.72657036
C	-3.20122321	-0.19105762	0.00237367
N	-2.38331835	0.93015970	0.00364795
C	-3.15116173	2.01849706	0.00246977
N	-4.44881565	1.63035938	0.00074039
C	-4.50054864	0.24919375	0.00066573
H	-5.24500514	2.25377284	-0.00041415
C	-1.84983115	-3.61454253	-1.25790208
H	-5.43522826	-0.28862553	-0.00068339
C	-2.06894481	-2.09616375	1.30630202
C	-2.07055638	-2.09309695	-1.30591229
C	2.00196950	-2.15826617	-0.00854223
N	5.76039133	1.86881692	0.00034585
C	-1.10194375	-4.06425911	-0.00235655
H	-1.32590484	-3.93523828	-2.16334768
H	-2.83878960	-4.09649092	-1.27062197
H	-2.83859176	-4.09905411	1.26632466
H	-1.32533431	-3.94089404	2.15902764
H	-0.09386260	-3.64085267	-0.00191665
H	-0.99243097	-5.15479432	-0.00376005
H	-2.77900276	-1.87838070	-2.11204423
H	-2.77587358	-1.88250702	2.11404752
O	2.66797669	-3.10758572	-0.01368529
C	5.02774491	1.57036122	-1.12733267
H	5.42628490	1.73869227	-2.11659414
C	3.80348225	1.06359895	-0.71834370
C	3.80753710	1.05494590	0.72033113
C	5.03406342	1.55689553	1.12847084
H	5.43803846	1.71367537	2.11742544
H	6.69553262	2.24863713	-0.00001221
H	-1.01886081	0.99508385	0.00498804
H	-0.07816713	1.18443717	0.00638280
H	-3.69816584	-2.18887685	0.00120080
C	-2.65276029	3.44262395	0.00205464
C	-1.79445233	3.66942515	1.26423355
H	-2.38188454	3.49733623	2.17167216
H	-0.93055835	2.99924660	1.27986201
H	-1.42937664	4.70129093	1.28039064
C	-3.83417940	4.42493563	0.00029110
H	-3.45240790	5.44947519	0.00000567
H	-4.46027330	4.30033265	-0.88950226
H	-4.46201822	4.30143610	0.88900401
C	-1.79233000	3.66753782	-1.25906993
H	-0.92827454	2.99751381	-1.27215599
H	-2.37819168	3.49380183	-2.16721364
H	-1.42745423	4.69945713	-1.27634340

