

Random polymer formation in copolymerization of L-lactide and ϵ -caprolactone initiated by aluminum pyridine-bis(phenolate): a quantum chemical study

Maxim V. Zabalov, Badma N. Mankaev, Mikhail P. Egorov and Sergey S. Karlov

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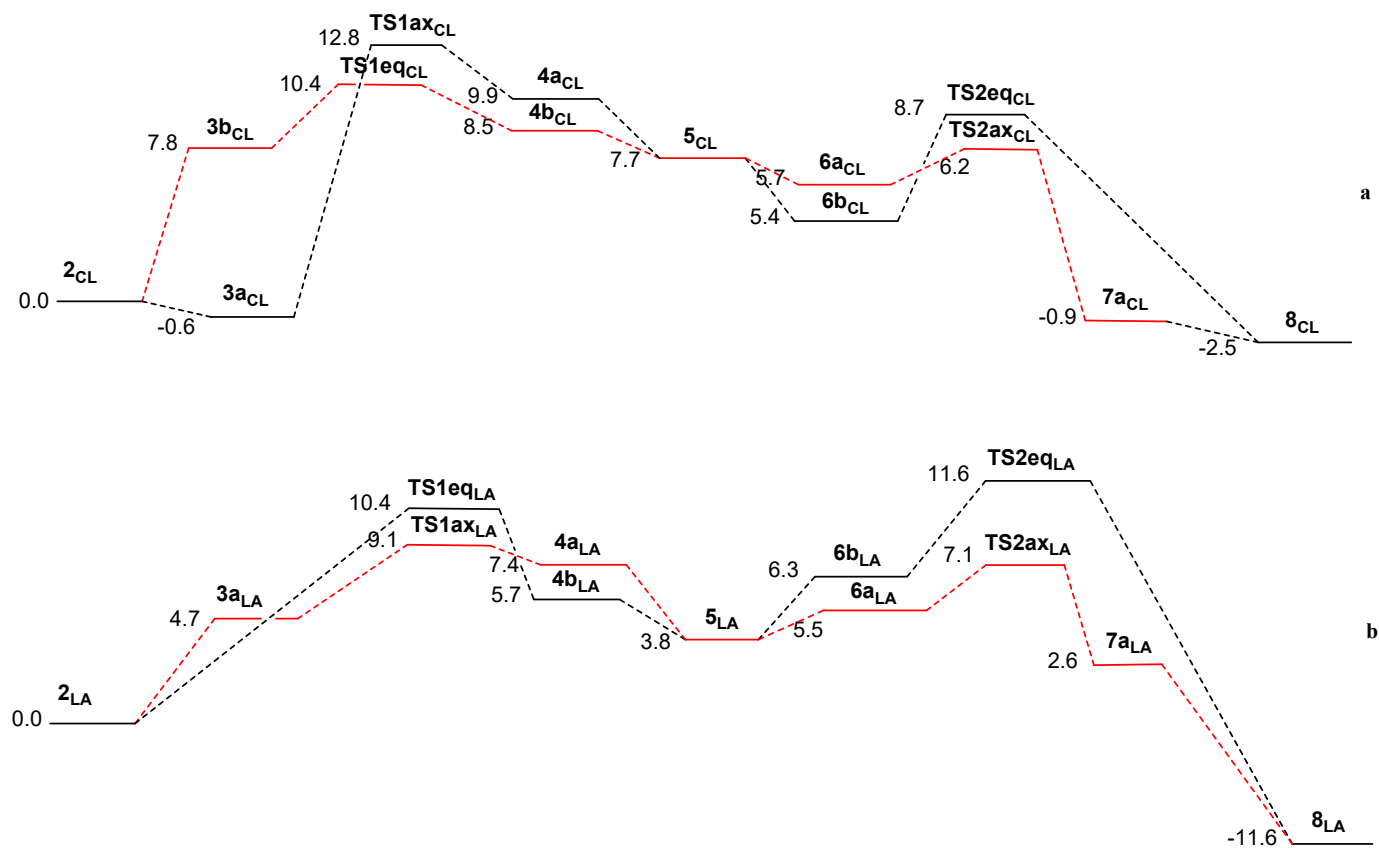
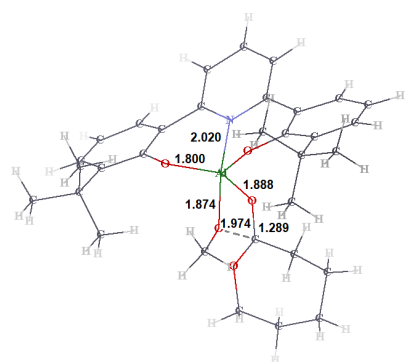
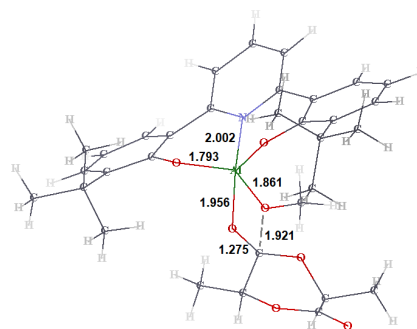


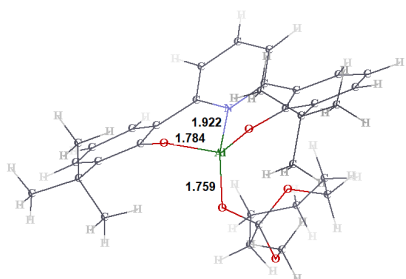
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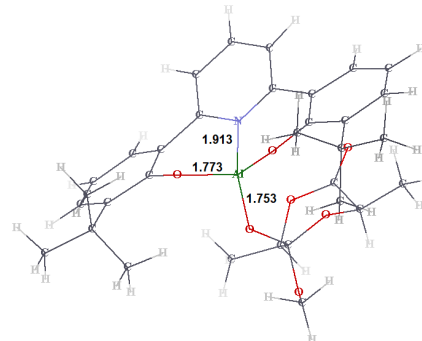
TS1eq_{CL}



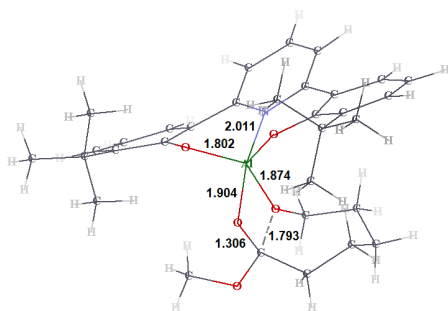
TS1ax_{LA}



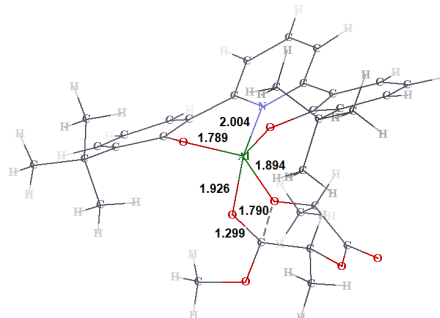
5_{CL}



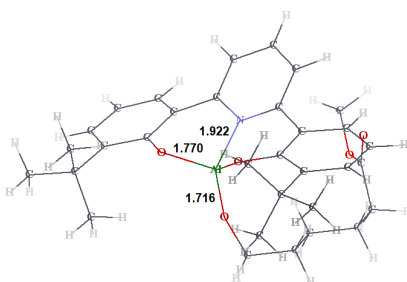
5_{LA}



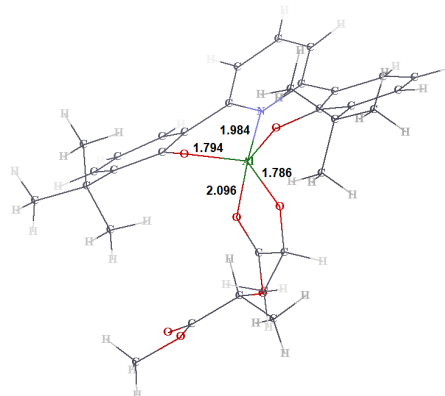
TS2ax_{CL}



TS2ax_{LA}

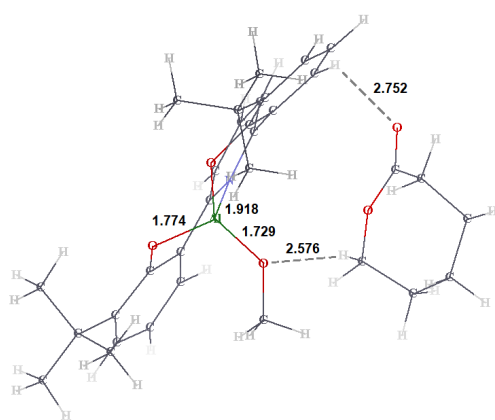


8_{CL}

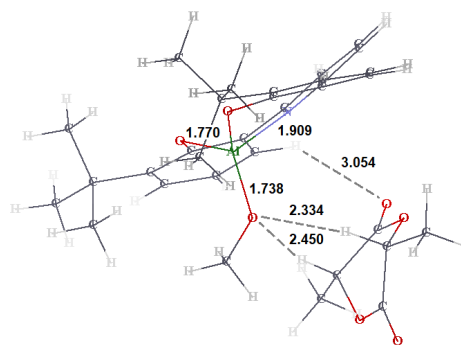


8_{LA}

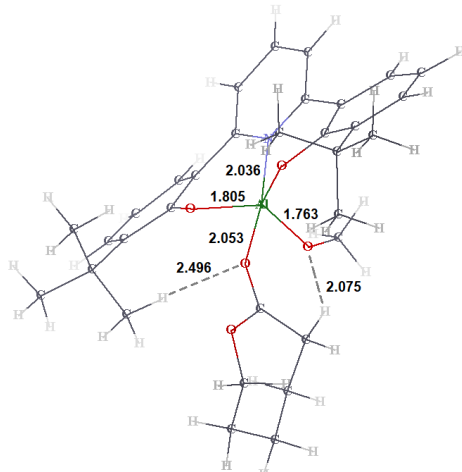
Fig. S2. The most characteristic structures of transition states and intermediates of the initiation stage.



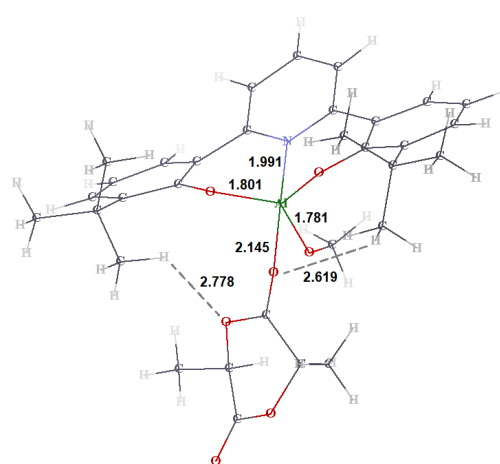
2_{CL} (-1.8)



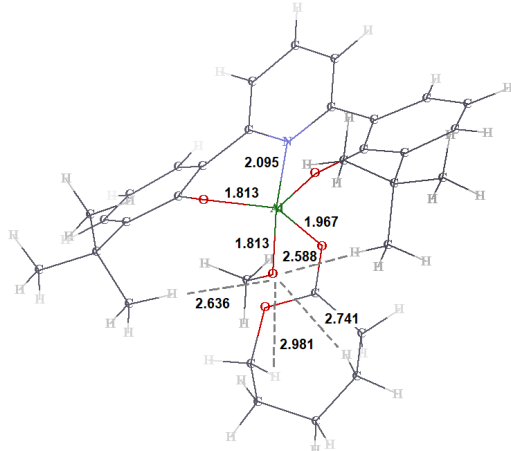
2_{LA} (-2.2)



3a_{CL} (-2.4)

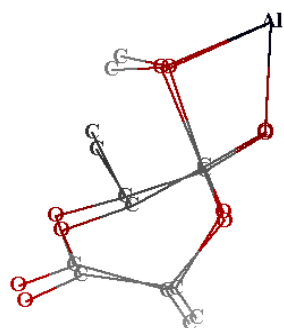


3a_{LA} (2.5)

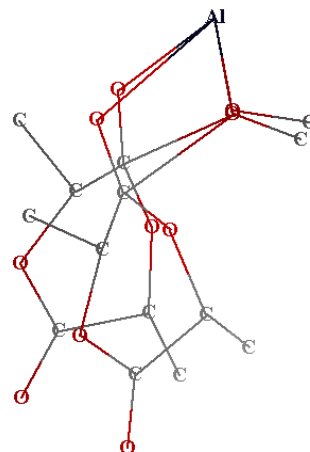


3b_{CL} (6.0)

Fig. S3. Structures and main geometric parameters (bonds of the aluminum atom with the ligand atoms and van der Waals interactions, in Å) of complexes of reagents of the initiation stage. The complex formation Gibbs free energies relative to the sum of the free energies of the starting reagents are given in parentheses (in kcal/mol).

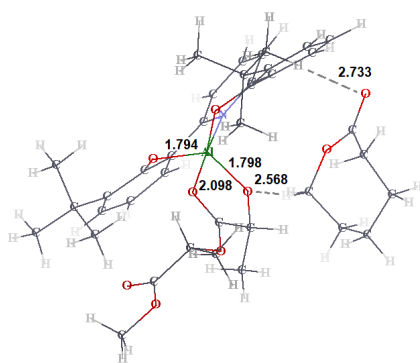


TS1ax_{Py} + TS1ax_{Amino}

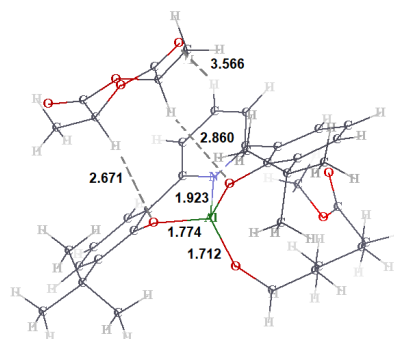


TS1eq_{Py} + TS1eq_{Amino}

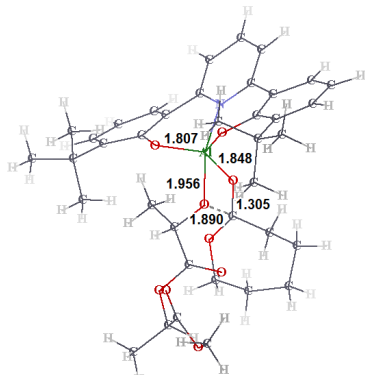
Fig. S4. Aligned in the plane of atoms O-Al-O structures of the main four-membered rings of **TS1** with axial and equatorial addition of LA for reactions with initiators with pyridine-bis(phenolate) (**TS1Py**) and amino-bis(phenolate) (**TS1Amino**) ligands. Ligands are not shown for clarity.



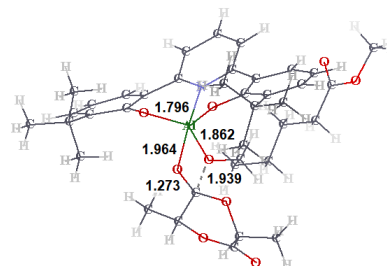
9_{LACL}



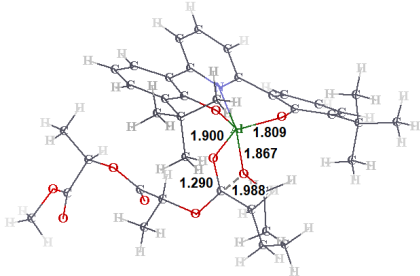
9_{CLLA}



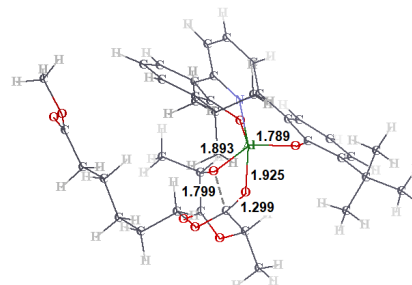
TS3eq_{LACL}



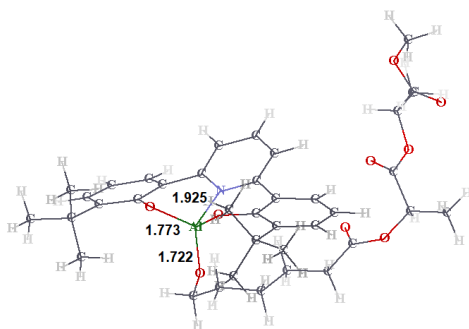
TS3ax_{CLLA}



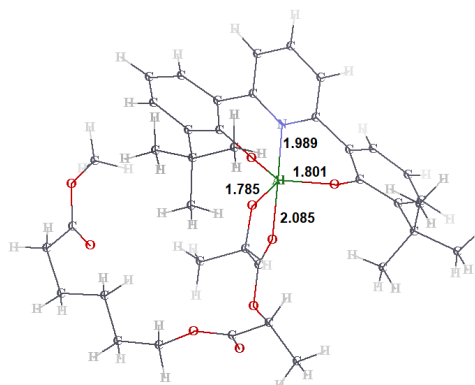
TS4eq_{LACL}



TS4ax_{CLLA}



15_{LACL}



15_{CLLA}

Fig. S5. The most characteristic structures of transition states and intermediates of the propagation stages.

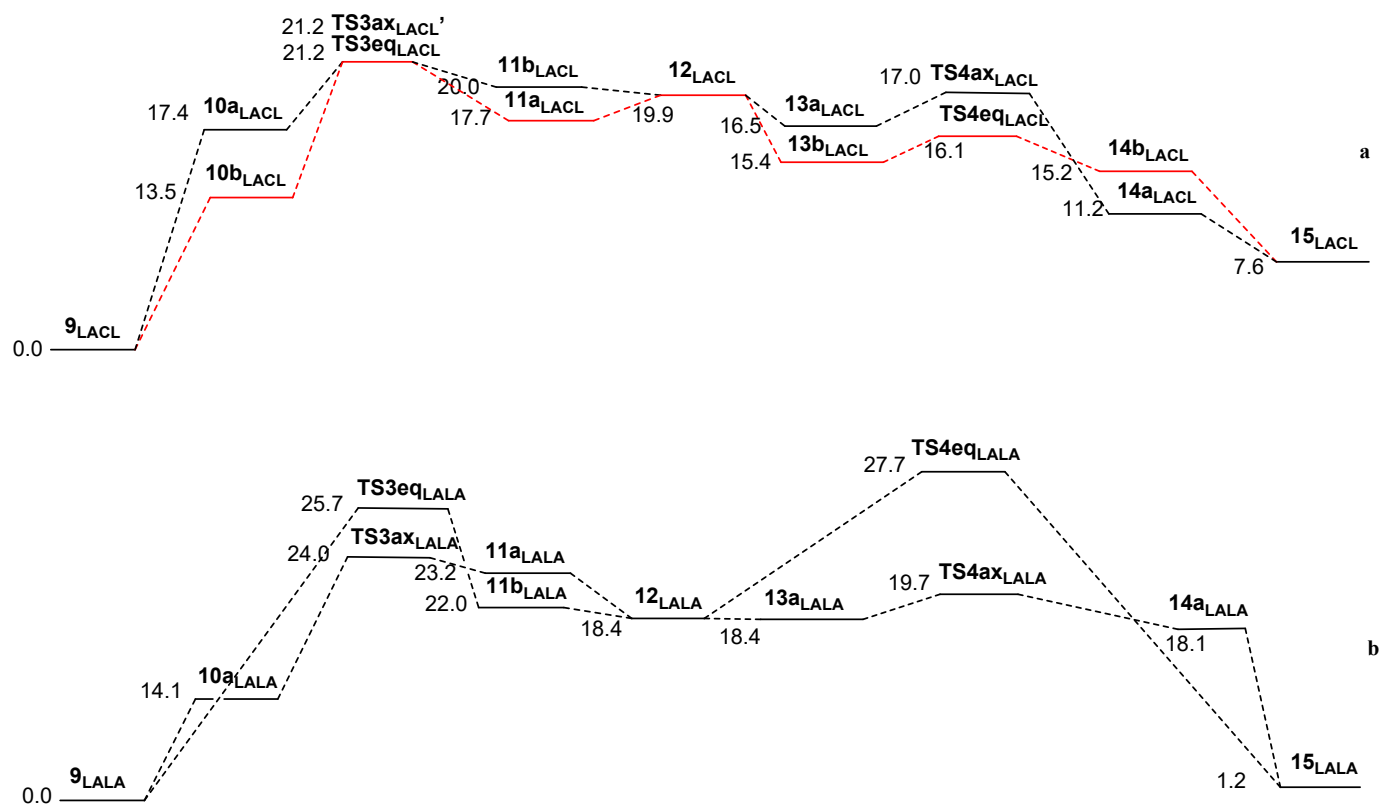


Fig. S6. Gibbs free energy profiles of propagation stages with CL (a) and LA (b) axial and equatorial addition to the product of LA addition on the initiation stage. The red line shows the most advantageous reaction path.

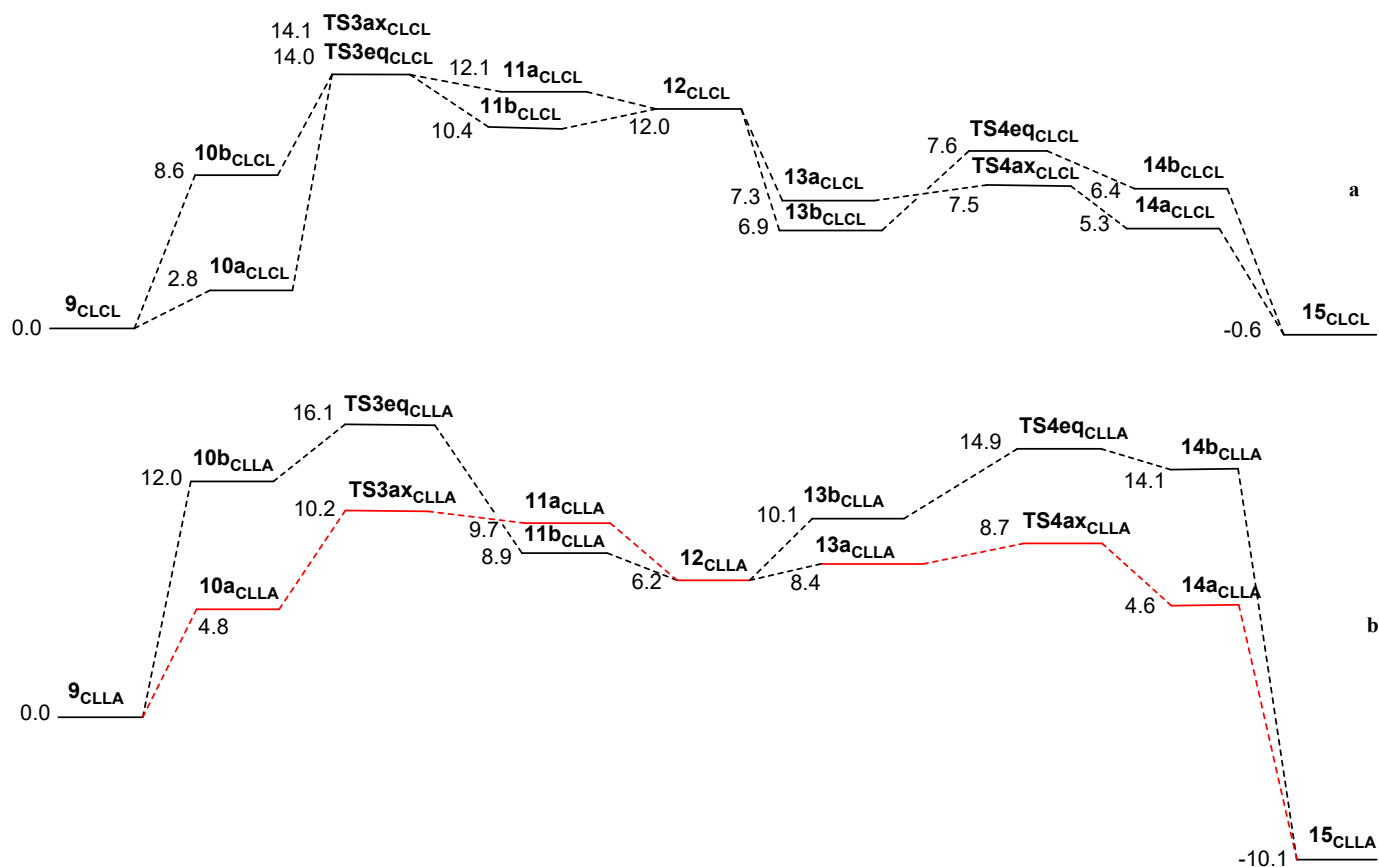


Fig. S7. Gibbs free energy profiles of propagation stages with CL (a) and LA (b) axial and equatorial addition to the product of CL addition on the initiation stage. The red line shows the most advantageous reaction path.

Methodological details

Calculations were carried out at the DFT level of theory using the non-empirically generalized gradient approximation and the PBE functional^{S1,S2} in the TZ2P basis implemented in PRIRODA program.^{S3,S4} The geometry optimization to find the energy minimum was performed for all stable complexes and intermediates (I); the saddle point search method was performed for the transition states (TS). The characters of the stationary points found (minima or saddle point on the PES) were determined by calculating the eigenvalues of the matrix of the second energy derivatives with respect to the nuclear coordinates. Correspondence between a particular TS and a transformation under study was verified by calculating the intrinsic reaction coordinate (IRC). For all structures the conformational analysis was performed to find structures close to the global minima. The reported Gibbs free energy values (kcal/mol) correspond to conformers with minimal energy, are calculated relative to vdW complexes of reagents (**RC_vdW**) of corresponding stage and are sums of the electronic energy, heat corrections (298 K), and dispersion corrections (PBE-D4).^{S5-S7} The activation Gibbs free energy values (kcal/mol) are calculated relative to the most stable structure (ground state), preceding the TS on each stage and which can be the complex of reagents or the intermediate. The stability of DFT determinants for **TS1eq_CL**, **TS1ax_CL**, **TS2eq_CL** and **TS2ax_CL** was verified (internal RKS/RKS, real/complex and RKS/UKS stability analysis)^{S8, S9} with using PySCF program package^{S10-S12} at the same level of theory (PBE/TZ2P).

References

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Initiation stage for CL

2_{CL}

Atomic N.	X	Y	Z
6	-3.73950947	-2.25577650	-2.16913420
6	-4.36017671	-1.85198825	-0.98031366
6	-3.81453841	-0.87882007	-0.13922103
6	-2.57393492	-0.28593934	-0.52719536
6	-1.97131474	-0.63497205	-1.78104408
6	-2.56391957	-1.64619836	-2.56903983
6	-0.78854438	0.06248803	-2.32877467
7	0.11838692	0.65652429	-1.48979460
6	1.19657837	1.36173676	-1.95490743
6	1.40656082	1.45168007	-3.33784078
6	0.51981109	0.82778366	-4.20978878
6	-0.58376679	0.14522440	-3.71475930
6	2.10319000	2.05276470	-1.01046474
6	1.65982782	2.59203373	0.24230705
6	2.51810932	3.45651478	0.99028535
6	3.82166175	3.64137578	0.52142069
6	4.29770485	3.03168689	-0.64613429
6	3.43915019	2.26301248	-1.41209830
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8	0.42913345	2.31665694	0.71538992
1	2.23307212	2.04502449	-3.71929029
1	0.67292731	0.90159184	-5.28662490
1	-1.30548215	-0.29929761	-4.39327118
1	-2.06396952	-1.98009708	-3.47764830
6	-4.51937902	-0.47746707	1.17319628
1	3.80182795	1.79130958	-2.32524392
1	4.50461368	4.27131076	1.08800342
6	2.02664161	4.16320567	2.27116586
1	-5.29448353	-2.33348447	-0.69793034
6	0.78684990	5.03215402	1.95021080
6	3.10234513	5.10062541	2.85275126
6	1.67901279	3.13084959	3.36944141
1	1.03782061	5.80352743	1.20761396
1	0.44661921	5.54224706	2.86399917
1	-0.04091393	4.42988041	1.56128838
1	2.55635103	2.51541365	3.61693265
1	0.86412951	2.46852789	3.05968411
1	1.36642374	3.65613164	4.28454686
1	2.69312913	5.60358468	3.74017953
1	3.40070471	5.88148598	2.13843826
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6	-3.64111352	-0.85605087	2.38974335
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6	-4.81891087	1.04074672	1.18009633
1	-5.74742979	-2.29571410	1.40957086
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1	-6.33775978	-0.86818370	2.27678499
1	-3.45839069	-1.94028266	2.41158464
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1	-5.33420011	1.31070646	2.11430876
1	-5.47966811	1.30714018	0.34214098
1	-3.90363151	1.63655393	1.10416796
1	5.33437681	3.17121262	-0.95204611
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8	0.45102345	-0.59594026	1.29956217
6	1.52732956	-0.63097472	2.21821805
1	1.17081399	-0.47471470	3.25065305
1	2.01262220	-1.62145247	2.18000062
1	2.29960722	0.12940562	2.00644328
13	-0.23961571	0.70523739	0.39375129
6	0.11282886	-4.21582464	-1.68335377
6	1.02440802	-5.37063627	-1.21589624
6	2.06560912	-4.96160646	-0.16900018
6	0.74362599	-3.31850113	-2.73476173
6	3.02483001	-3.85664556	-0.62409133
6	2.34082052	-2.55326409	-1.02638784
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1	1.51844729	-5.82242947	-2.09144426
1	1.53764900	-4.61768924	0.73702184
1	3.71817786	-3.62254377	0.20029404
1	-0.79426393	-4.61511833	-2.15110963
1	0.38221567	-6.15407676	-0.78623704
1	2.64691246	-5.84823836	0.12901170
1	3.64776681	-4.19893004	-1.46681771
1	3.06978077	-1.73319218	-1.04513776
1	1.53857483	-2.27240144	-0.32524039
8	0.34183395	-3.25271173	-3.88221119
8	1.82424482	-2.55660277	-2.38993880

Electronic energy = -1915.423419 a.u.

DFT-D4 dispersion correction = -0.119673 a.u.

Thermal free energy = 0.564027 a.u.

Gibbs free energy = -1914.979065 a.u.

Number of imaginary frequencies = 0.

3a_{CL}

Atomic N.	X	Y	Z
6	4.27141144	3.31193739	1.98963769
6	4.69875913	2.44516872	0.97529028
6	3.80848349	1.74404767	0.15907132
6	2.40463754	1.91370066	0.39877885
6	1.96707952	2.90041050	1.33618811
6	2.91843584	3.55245484	2.14880998
6	0.56046100	3.33994175	1.40951755
7	-0.46249420	2.49432786	1.07402975
6	-1.76260172	2.91826317	1.13987405
6	-2.05795361	4.23829412	1.52516584
6	-1.02847389	5.10932459	1.85365595
6	0.28498869	4.66475959	1.79401038
6	-2.87456198	2.02344231	0.76666391
6	-2.72047125	1.00163593	-0.22103088
6	-3.88596694	0.37438742	-0.77279997
6	-5.12192484	0.67553115	-0.19624379

6	-5.26011267	1.57519129	0.86915286
6	-4.14800577	2.26021123	1.32545635
8	1.52238607	1.17361244	-0.27355987
8	-1.50906625	0.65044662	-0.65290923
1	-3.08900598	4.58031508	1.51096795
1	-1.24747041	6.14327585	2.12329126
1	1.10800374	5.34549998	1.99233159
1	2.57927113	4.23389246	2.92894388
6	4.32836633	0.80757513	-0.95042157
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1	-6.01727424	0.18440388	-0.57319225
6	-3.78603673	-0.60949318	-1.95606405
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6	3.72078878	1.20977720	-2.31520182
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1	4.40529397	-0.96508910	0.33476462
1	4.34922860	-1.32468819	-1.41101615
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1	4.00583781	2.23980960	-2.57512817
1	2.62797638	1.14114087	-2.30475684
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8	0.80045665	-3.08275167	-1.45151155
6	0.64449452	-2.33489865	-0.34728341
6	0.79145268	-2.94356482	1.02086185
1	1.78195316	-3.42253199	1.09733026
1	0.74536131	-2.09470496	1.71742443
6	-0.31902458	-3.96513763	1.35553814
1	-1.29420135	-3.54597440	1.06273996
1	-0.34869076	-4.06801530	2.45001487
6	-0.11639756	-5.34935041	0.73182894
1	0.80796944	-5.79184256	1.14217675
1	-0.93870984	-6.01157963	1.04367781
6	-0.02181471	-5.35110464	-0.79775804
1	-0.96588260	-5.01126994	-1.25342830
1	0.13815657	-6.38336200	-1.14904299

6	1.11485952	-4.50563312	-1.36016077
1	2.04594746	-4.63471133	-0.78670211
1	1.31627478	-4.76901875	-2.40491264
13	-0.05084487	0.61396769	0.40983290
8	-0.10217380	-0.21650195	1.96360038
6	-0.39774123	0.28319229	3.25175102
1	-0.24692161	-0.51773395	3.99608276
1	0.25627703	1.12579852	3.54163982
1	-1.44658968	0.62087306	3.33885132

Electronic energy = -1915.427937 a.u.

DFT-D4 dispersion correction = -0.121852 a.u.

Thermal free energy = 0.569818 a.u.

Gibbs free energy = -1914.979971 a.u.

Number of imaginary frequencies = 0.

3b_{CL}

Atomic N.	X	Y	Z
6	4.24926928	3.12131590	-2.15764883
6	3.89141749	2.15214786	-3.10389141
6	2.69591141	1.43344272	-3.03321416
6	1.80821666	1.71620609	-1.94248785
6	2.12799589	2.76475969	-1.02952570
6	3.36788209	3.42879301	-1.13635875
6	1.16160455	3.23617422	-0.02187756
7	0.23049274	2.39077258	0.52418896
6	-0.62053345	2.85720703	1.49153043
6	-0.58720618	4.20613082	1.88880965
6	0.32555192	5.07679005	1.31142818
6	1.20376962	4.59198028	0.35400976
6	-1.62423054	1.97779159	2.11779132
6	-2.24648691	0.92376810	1.38449002
6	-3.40781304	0.27981696	1.92859657
6	-3.80059823	0.62996793	3.22289754
6	-3.11744599	1.58233516	3.99093958
6	-2.05035528	2.26354936	3.43082499
8	0.68538768	1.01506925	-1.78901332
8	-1.76282321	0.56170954	0.19749401
1	-1.31986055	4.56513011	2.60636198
1	0.33175133	6.13296510	1.58374368
1	1.89753018	5.25956095	-0.14918601
1	3.64526958	4.17149777	-0.38833705
6	2.37983780	0.33101668	-4.06178100
1	-1.51776114	3.01411761	4.01543796
1	-4.66381015	0.13595484	3.66589413
6	-4.17511021	-0.79764212	1.13866754
1	4.58962178	1.94033486	-3.91179369
6	-4.58292389	-0.26444957	-0.25494030
6	-5.47297040	-1.22592718	1.85045517
6	-3.28518585	-2.05499459	0.99956504
1	-5.24264999	0.60986611	-0.15221318
1	-5.13717379	-1.04257929	-0.80131418
1	-3.71179584	0.02813949	-0.84923054
1	-3.12236425	-2.50988960	1.98921305

1	-2.31090915	-1.81259056	0.56163095
1	-3.78180887	-2.80429996	0.36368329
1	-5.99286357	-1.96696958	1.22631972
1	-6.15823357	-0.37932044	2.00254159
1	-5.28104285	-1.69756466	2.82516249
6	2.42559348	-1.04452714	-3.35423038
6	3.41024830	0.29412032	-5.20707446
6	0.99604466	0.56646856	-4.71149120
1	4.42230683	0.05100816	-4.85244125
1	3.45252500	1.24678847	-5.75517209
1	3.11814297	-0.48827969	-5.92223269
1	3.44478342	-1.24838599	-2.99230522
1	2.15237515	-1.84223594	-4.06253812
1	1.74222184	-1.08655855	-2.49866519
1	0.79022116	-0.23025993	-5.44250778
1	0.98319715	1.52709290	-5.24771869
1	0.19370825	0.57515310	-3.96739237
1	-3.43438728	1.79241229	5.01253788
1	5.21333855	3.62525059	-2.22718813
8	0.00820244	-1.32846181	-0.59338917
6	-0.76474192	-1.86858352	-1.64548991
1	-0.73623294	-2.97281191	-1.60035728
8	1.37773511	0.00654203	1.10949860
1	-1.82800669	-1.56495916	-1.59596847
1	-0.38811357	-1.57056257	-2.64207632
13	-0.00256080	0.44618816	-0.22079544
6	2.62591368	-1.83551149	1.98801540
6	2.50214182	-3.16398055	1.19992314
6	1.67116238	-4.22743416	1.92510679
6	1.38237267	-1.00731403	1.83472663
6	0.23187695	-3.80427609	2.24538732
6	0.11399671	-2.59688091	3.16572428
1	2.82630284	-2.04185965	3.05147943
1	2.07206453	-2.94340636	0.21107467
1	2.18011026	-4.50419190	2.86521672
1	-0.32855298	-3.58679538	1.32319549
1	3.44732094	-1.23080102	1.58807565
1	3.51965070	-3.54808254	1.03832795
1	1.64604042	-5.13895723	1.30899711
1	-0.28611168	-4.63825878	2.74562205
1	-0.89422677	-2.51460808	3.58544912
1	0.83814164	-2.62500658	3.99501716
8	0.25764169	-1.32011774	2.45679469

Electronic energy = -1915.414729 a.u.

DFT-D4 dispersion correction = -0.124390 a.u.

Thermal free energy = 0.572497 a.u.

Gibbs free energy = -1914.966622 a.u.

Number of imaginary frequencies = 0.

TS1ax_{cl}

Atomic N.	X	Y	Z
6	5.10403299	1.65398777	0.95275885
6	5.10643721	0.93556035	-0.25149840

6	3.93867612	0.65000325	-0.96143842
6	2.69723630	1.10490346	-0.40971237
6	2.69888878	1.93451118	0.75609726
6	3.91352224	2.16405606	1.43813407
6	1.48589861	2.63941741	1.21115315
7	0.23855525	2.12674236	0.96137917
6	-0.88926971	2.79477835	1.36356509
6	-0.77436644	4.01631021	2.04985428
6	0.48228562	4.54498672	2.31459832
6	1.61561763	3.86551309	1.88794076
6	-2.23267579	2.27966237	1.03893936
6	-2.47871661	1.53764462	-0.15922154
6	-3.82554960	1.32184839	-0.59705853
6	-4.85540485	1.72122455	0.25760767
6	-4.61698008	2.33735347	1.49459732
6	-3.31805015	2.63591909	1.86669362
8	1.55100620	0.76917726	-0.99996269
8	-1.46177971	1.06788421	-0.88235337
1	-1.67381310	4.56450176	2.31643987
1	0.57738644	5.50719118	2.81936049
1	2.60329771	4.29533195	2.02916813
1	3.90796447	2.72570825	2.37235451
6	3.98277235	-0.14358395	-2.28254128
1	-3.12670040	3.12881517	2.82015800
1	-5.88794088	1.53728020	-0.03426336
6	-4.12672663	0.66672868	-1.96016788
1	6.06007957	0.57391840	-0.63190132
6	-3.45690966	1.48096645	-3.09311318
6	-5.63852787	0.63304877	-2.25489736
6	-3.61696553	-0.79328668	-1.98932087
1	-3.84636283	2.50949097	-3.11162424
1	-3.68266177	1.01688182	-4.06517029
1	-2.36921024	1.52006769	-2.97240496
1	-4.11914968	-1.39059174	-1.21290660
1	-2.53447294	-0.85126525	-1.83308589
1	-3.85189533	-1.24744070	-2.96431708
1	-5.79724026	0.19234450	-3.24937367
1	-6.08099890	1.63981998	-2.26373792
1	-6.19076490	0.01605411	-1.53093100
6	3.25195479	-1.49792123	-2.12381077
6	5.42959785	-0.44764689	-2.71619177
6	3.32955956	0.68164086	-3.41711450
1	5.95422649	-1.09096634	-1.99459863
1	6.02072287	0.46857440	-2.86082292
1	5.40734148	-0.98252195	-3.67628336
1	3.72678638	-2.10074115	-1.33530879
1	3.31623888	-2.06258440	-3.06693244
1	2.19568706	-1.36712229	-1.86795485
1	3.37265682	0.11329522	-4.35861349
1	3.87101102	1.62720072	-3.56858802
1	2.28115606	0.90937638	-3.19829893
1	-5.45131636	2.59126186	2.14837885
1	6.03561163	1.81455517	1.49540365
8	-0.12074662	-0.60981256	1.48112726

6	0.55082273	-0.56408471	2.73989081
1	0.96769899	0.43971959	2.89566064
6	-1.45822632	-2.74578786	0.81251866
6	-1.62645590	-3.34493113	2.21463823
6	-0.89143610	-4.66912556	2.44426346
6	-0.15644005	-2.03834677	0.45158079
6	0.63062245	-4.57527256	2.31427598
6	1.11466086	-4.08152056	0.95424056
1	-1.60474014	-3.52470088	0.04293611
1	-1.32581043	-2.60755849	2.97419119
1	-1.14828134	-5.05907059	3.44176173
1	1.05184162	-3.92235184	3.09601855
1	-2.23899102	-1.99735868	0.62835324
1	-2.70290971	-3.51343799	2.37276340
1	-1.26337850	-5.41275406	1.71781147
1	1.07115591	-5.57382011	2.47348237
1	2.18571186	-4.29119682	0.83615392
1	0.58291513	-4.59222841	0.13410830
8	-0.17043082	-1.36090243	-0.66640079
8	1.04536831	-2.64758468	0.75445014
1	1.37658906	-1.29107082	2.74700403
1	-0.15231375	-0.78651422	3.55630732
13	0.03101497	0.42984650	-0.11619880

Electronic energy = -1915.409280 a.u.

DFT-D4 dispersion correction = -0.124039 a.u.

Thermal free energy = 0.574576 a.u.

Gibbs free energy = -1914.958743 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 106.9i

TS1eq_{CL}

Atomic N.	X	Y	Z
6	4.07352811	3.36788218	-0.38681040
6	4.05020349	2.57158997	-1.53951292
6	2.93526578	1.81619107	-1.91067317
6	1.78828978	1.85002014	-1.05028733
6	1.75472563	2.77773172	0.03829136
6	2.92508042	3.48847912	0.37600760
6	0.49895773	3.10909543	0.74041903
7	-0.51724658	2.19745275	0.84128835
6	-1.69831235	2.53079918	1.44859324
6	-1.87807562	3.82569704	1.96926252
6	-0.85366034	4.75706403	1.88035691
6	0.33731646	4.40530833	1.25948730
6	-2.81400521	1.56953767	1.52561886
6	-2.99177659	0.53646994	0.55274451
6	-4.23293096	-0.17931809	0.50062518
6	-5.17131786	0.06927431	1.50406684
6	-4.94664899	0.98918413	2.53698097
6	-3.78712482	1.74307885	2.53270960
8	0.75619512	1.03503576	-1.27882599
8	-2.02073575	0.24671364	-0.31505394
1	-2.83937467	4.10266801	2.39221791

1	-0.99712761	5.76942378	2.26010981
1	1.12621294	5.13906926	1.12034975
1	2.92886497	4.12178565	1.26312074
6	2.94945581	0.96666801	-3.19724883
1	-3.60931998	2.46176902	3.33233193
1	-6.10844146	-0.48460120	1.50315373
6	-4.51428684	-1.21756719	-0.60330141
1	4.94577842	2.53395406	-2.15725431
6	-4.34456248	-0.57715866	-2.00146900
6	-5.95287958	-1.76389878	-0.52892595
6	-3.55321496	-2.41792092	-0.44527051
1	-5.05147286	0.25545970	-2.13174521
1	-4.55847680	-1.32574415	-2.77959940
1	-3.32903593	-0.19669612	-2.15201911
1	-3.72433567	-2.92333602	0.51679183
1	-2.50901415	-2.09376066	-0.48267676
1	-3.72854758	-3.14857286	-1.25034400
1	-6.10798284	-2.47095858	-1.35651221
1	-6.70308254	-0.96593237	-0.62857664
1	-6.14572331	-2.30809120	0.40691838
6	2.88512986	-0.53588557	-2.84346760
6	4.22954217	1.19278890	-4.02389175
6	1.75049048	1.34911654	-4.09742567
1	5.13532653	0.87453323	-3.48750206
1	4.35076223	2.24555199	-4.31730079
1	4.16804063	0.59605014	-4.94524845
1	3.76309468	-0.83106110	-2.24897228
1	2.88129158	-1.14029802	-3.76380808
1	1.98126491	-0.76308920	-2.27105206
1	1.76966843	0.74482372	-5.01717763
1	1.81010352	2.40797807	-4.38869125
1	0.79487014	1.18126385	-3.58955978
1	-5.68428485	1.11364023	3.32970006
1	4.98211094	3.90129663	-0.10761451
8	0.13850892	-1.45677698	-0.19866422
6	0.10261640	-2.42651562	-1.22062490
1	-0.52501352	-3.28782586	-0.93171273
6	2.42640750	-1.63213199	1.19788177
6	3.33842320	-1.82795585	2.42860372
6	3.29225073	-3.25062583	3.00071986
6	0.98850851	-1.34282396	1.57899545
6	1.91754630	-3.69224269	3.51711852
6	0.78624669	-3.57673889	2.50104827
1	2.48362807	-2.51951343	0.55018256
1	3.08162292	-1.08833529	3.20350183
1	3.61935819	-3.95339093	2.21469539
1	1.97076707	-4.74631332	3.83527962
1	2.75850108	-0.77437930	0.60213611
1	4.37081085	-1.60556552	2.12072225
1	4.02621150	-3.33981076	3.81662891
1	1.63223832	-3.11140483	4.40896784
1	-0.10416673	-4.11255690	2.85150733
1	1.06481079	-3.98304588	1.51689903
8	0.57552636	-0.12522965	1.67296389

8	0.31398417	-2.20736538	2.35289249
1	-0.31382605	-2.00024206	-2.14845861
1	1.11811542	-2.79641644	-1.45504626
13	-0.26164825	0.35665202	0.05043443

Electronic energy = -1915.412718 a.u.
DFT-D4 dispersion correction = -0.123129 a.u.
Thermal free energy = 0.573392 a.u.
Gibbs free energy = -1914.962455 a.u.
Number of imaginary frequencies = 1.
Imaginary frequency = 84.4i

4a_{CL}

Atomic N.	X	Y	Z
6	4.47986516	2.70889690	1.23973600
6	4.72286191	1.92388828	0.10262705
6	3.69835954	1.35495683	-0.65638674
6	2.35054283	1.57423621	-0.22263900
6	2.09370658	2.47422468	0.86329516
6	3.17654885	3.00011532	1.59947422
6	0.73369439	2.96811427	1.13980179
7	-0.35912542	2.19421269	0.84672571
6	-1.63726287	2.67103219	0.99248627
6	-1.83250080	3.97331222	1.48515481
6	-0.73721986	4.75531665	1.83266612
6	0.54920913	4.26328119	1.65297452
6	-2.80456541	1.85180472	0.60667011
6	-2.74046652	0.85344980	-0.42020322
6	-3.94919906	0.28560425	-0.93739836
6	-5.14956911	0.63469720	-0.31601650
6	-5.20846287	1.52178573	0.76801226
6	-4.05056741	2.13734173	1.20714983
8	1.34112516	0.96657968	-0.84651151
8	-1.56815231	0.45645522	-0.91813770
1	-2.83886597	4.37769222	1.54613614
1	-0.88738370	5.77078815	2.20129723
1	1.41542635	4.88962303	1.84787089
1	2.98057264	3.62091607	2.47407424
6	4.00542145	0.51148054	-1.90997143
1	-4.09572036	2.83137630	2.04629244
1	-6.07899369	0.19188269	-0.66931679
6	-3.92481059	-0.68769952	-2.13391482
1	5.75727352	1.74311279	-0.18454478
6	-3.25746904	-0.00791516	-3.35362017
6	-5.34636526	-1.09875026	-2.56305528
6	-3.16316634	-1.98391837	-1.76878444
1	-3.82025887	0.88901682	-3.65117702
1	-3.25379464	-0.70242031	-4.20730729
1	-2.22381516	0.28309405	-3.13956076
1	-3.65151973	-2.49228747	-0.92380502
1	-2.12014670	-1.78251769	-1.50271014
1	-3.17456393	-2.67332738	-2.62677917
1	-5.27602315	-1.76285390	-3.43609264
1	-5.95743334	-0.23217247	-2.85459547

1	-5.87734269	-1.65029954	-1.77346147
6	3.57580143	-0.95865420	-1.69357782
6	5.51026790	0.50674371	-2.24001296
6	3.27041117	1.10338130	-3.13669398
1	6.10997187	0.03906246	-1.44555331
1	5.89793241	1.52021603	-2.41925866
1	5.67099204	-0.07681675	-3.15760853
1	4.14585519	-1.40682989	-0.86592570
1	3.78784133	-1.54338016	-2.60189954
1	2.50821166	-1.04447568	-1.46585899
1	3.50498227	0.50554692	-4.03038500
1	3.60210645	2.13517741	-3.32465360
1	2.18454359	1.10531077	-2.99580713
1	-6.16221301	1.73068720	1.25237808
1	5.31421285	3.09508681	1.82501246
8	-0.70869717	-0.38769396	1.88031613
6	-0.94415903	-0.05779789	3.26049574
1	-0.01104738	-0.12880283	3.83213027
6	-0.98636880	-2.84570655	1.62528393
6	-0.40534587	-4.16252911	1.08933095
6	0.94656833	-4.59243026	1.68695923
6	-0.00296368	-1.68050332	1.50881283
6	2.12494932	-3.71503227	1.22913695
6	2.27156060	-2.39099501	1.99204523
1	-1.25092111	-2.96040856	2.68801878
1	-0.29559934	-4.08129723	-0.00375504
1	0.88728924	-4.60992904	2.78820599
1	2.01457626	-3.50963722	0.15434204
1	-1.89899997	-2.58510550	1.07058467
1	-1.14848642	-4.95414852	1.27268626
1	1.14155992	-5.62845955	1.36874899
1	3.07188009	-4.26525249	1.35130527
1	2.80214235	-1.64995270	1.37550859
1	2.84112511	-2.54271713	2.91961092
8	0.40161725	-1.36381391	0.26155112
8	1.02927895	-1.82908418	2.47074823
1	-1.70285437	-0.73272139	3.68050007
1	-1.32632538	0.96865797	3.28026528
13	-0.09153875	0.39017841	0.08055719

Electronic energy = -1915.413010 a.u.

DFT-D4 dispersion correction = -0.125055 a.u.

Thermal free energy = 0.574806 a.u.

Gibbs free energy = -1914.963259 a.u.

Number of imaginary frequencies = 0.

4b_{CL}

Atomic N.	X	Y	Z
6	4.22866248	2.96639136	-2.07347878
6	3.76504480	2.07782101	-3.05229652
6	2.53609216	1.42196486	-2.95173681
6	1.74144835	1.66728235	-1.78564057
6	2.14819555	2.67312561	-0.85094389
6	3.41593752	3.27489626	-0.99767246

6	1.24578703	3.18668304	0.19891178
7	0.24674727	2.40311233	0.71080299
6	-0.64051987	2.88584538	1.63447301
6	-0.51686385	4.21169234	2.08564990
6	0.50303614	5.01576386	1.59375976
6	1.38125964	4.51345539	0.64190019
6	-1.75918184	2.05351114	2.11982436
6	-2.35298748	1.02194896	1.32256262
6	-3.62023201	0.47547038	1.70611239
6	-4.14843622	0.85927177	2.94053197
6	-3.49954320	1.76281785	3.79212265
6	-2.33076273	2.36982291	3.37090372
8	0.61557095	0.96859449	-1.59522503
8	-1.75243920	0.58093835	0.20943269
1	-1.25283848	4.61467164	2.77536213
1	0.58831737	6.05216672	1.92271729
1	2.13822936	5.15321767	0.19741700
1	3.76888883	3.97167213	-0.23776734
6	2.06315978	0.45512881	-4.05635021
1	-1.82798061	3.08322928	4.02341419
1	-5.09304767	0.43000325	3.26926352
6	-4.37677943	-0.51597486	0.79914090
1	4.40174768	1.88269848	-3.91326388
6	-4.60290461	0.10960560	-0.59804397
6	-5.76437779	-0.87131282	1.36654381
6	-3.57926271	-1.83274116	0.66995630
1	-5.20646496	1.02555957	-0.51743419
1	-5.15109176	-0.59973468	-1.23665198
1	-3.65605360	0.35976013	-1.08815058
1	-3.45497355	-2.31009148	1.65267716
1	-2.58559208	-1.64996974	0.25258163
1	-4.11856377	-2.53427887	0.01452511
1	-6.27198600	-1.54850865	0.66485478
1	-6.40103570	0.01686269	1.48972890
1	-5.69937143	-1.39079152	2.33354033
6	1.98246616	-0.98716685	-3.50545871
6	3.02967505	0.43544308	-5.25591663
6	0.68038019	0.89658196	-4.59257005
1	4.02787264	0.06422695	-4.98195652
1	3.14076989	1.42927358	-5.71315315
1	2.62841228	-0.24018892	-6.02475283
1	2.97338281	-1.32796618	-3.16988655
1	1.63923841	-1.67140691	-4.29678725
1	1.28854029	-1.04735180	-2.66149154
1	0.35323565	0.20686224	-5.38550415
1	0.74041804	1.90502520	-5.02729109
1	-0.07736542	0.90345890	-3.80199202
1	-3.92203517	1.99459091	4.76968191
1	5.21603631	3.41809271	-2.16757715
8	0.20869487	-1.50563851	-0.29185767
6	-0.29937079	-2.70304673	-0.90416407
1	-0.82734422	-3.31625002	-0.16367663
8	1.09365872	-0.23952453	1.25661556
1	-0.99475904	-2.38010472	-1.68658713

1	0.52238179	-3.27359203	-1.36141446
13	0.02736212	0.56458868	0.04603285
6	2.38576723	-2.21210290	0.74424783
6	2.53919002	-3.71294865	1.03448965
6	2.63922572	-4.04904108	2.53123659
6	0.99813047	-1.57054322	0.96696011
6	1.33669194	-3.86706113	3.31905992
6	0.69424373	-2.49053089	3.17498404
1	3.08613045	-1.64539320	1.37622930
1	1.71781142	-4.28809806	0.57899956
1	3.42725172	-3.41845340	2.97880876
1	0.59716017	-4.61963778	2.99933570
1	2.66955081	-1.98338094	-0.29349294
1	3.46322474	-4.05448833	0.54133349
1	2.97823101	-5.09108523	2.64534969
1	1.52572407	-4.04809717	4.39091926
1	-0.16614482	-2.40088421	3.85355138
1	1.39524302	-1.67689904	3.42349037
8	0.15608342	-2.28884354	1.85014969

Electronic energy = -1915.417657 a.u.

DFT-D4 dispersion correction = -0.122904 a.u.

Thermal free energy = 0.575036 a.u.

Gibbs free energy = -1914.965525 a.u.

Number of imaginary frequencies = 0.

5_{CL}

Atomic N.	X	Y	Z
6	4.18901442	2.30376035	-1.63052674
6	3.89435627	1.39654006	-2.65749514
6	2.68336973	0.70469222	-2.72539990
6	1.73786567	0.91567063	-1.67159796
6	1.96277579	1.95987460	-0.71317146
6	3.21913971	2.60474941	-0.69225347
6	0.89926024	2.47919226	0.17030309
7	-0.16728051	1.69595325	0.52925110
6	-1.24195732	2.19158060	1.22372954
6	-1.21455498	3.52472540	1.66206292
6	-0.11611101	4.32314345	1.36376279
6	0.93088518	3.81593265	0.60262627
6	-2.42739859	1.34684223	1.46427262
6	-2.83099837	0.31490644	0.55098322
6	-4.10616695	-0.31376190	0.71011728
6	-4.87086201	0.04048826	1.82352517
6	-4.44289371	0.98270759	2.76924837
6	-3.24079429	1.63878044	2.58031819
8	0.64093107	0.15016485	-1.62225661
8	-2.03562760	-0.04470952	-0.46633758
1	-2.07587105	3.93747401	2.17994662
1	-0.09898030	5.36582614	1.68326584
1	1.74563473	4.46288830	0.29068418
1	3.43605077	3.33015317	0.09145635
6	2.36970560	-0.23077893	-3.91287388
1	-2.90028032	2.36810213	3.31533822

1	-5.83202326	-0.44499804	1.98186860
6	-4.60904640	-1.36684912	-0.29789293
1	4.64870764	1.22213671	-3.42223116
6	-4.65712451	-0.76298728	-1.72186480
6	-6.03392961	-1.84566598	0.04054617
6	-3.69003590	-2.61131832	-0.27548424
1	-5.34641948	0.09361900	-1.75521496
1	-5.02616011	-1.51998186	-2.43033721
1	-3.66898710	-0.42871151	-2.05440837
1	-3.67540472	-3.06387313	0.72643738
1	-2.66017549	-2.36445798	-0.55165758
1	-4.07048365	-3.36342529	-0.98341294
1	-6.35490623	-2.57012634	-0.72117746
1	-6.76008807	-1.01961432	0.03861596
1	-6.08329908	-2.35209332	1.01543230
6	2.21294260	-1.69767299	-3.45266057
6	3.49083374	-0.20219972	-4.96961841
6	1.07076183	0.24094037	-4.61043911
1	4.44374016	-0.58592123	-4.57686125
1	3.65891924	0.80861373	-5.36835497
1	3.20099310	-0.84609095	-5.81186115
1	3.13303160	-2.05331665	-2.96620020
1	2.02384723	-2.33974417	-4.32629087
1	1.37943611	-1.81330340	-2.75303881
1	0.85260640	-0.41402659	-5.46736295
1	1.18599190	1.26644118	-4.99056528
1	0.21310420	0.21499820	-3.92960723
1	-5.05624409	1.19522977	3.64469698
1	5.16611303	2.78464983	-1.58862212
8	1.69412312	-2.94608726	1.34356827
6	1.92388109	-3.20079818	-0.04769741
1	2.47960593	-4.14469194	-0.08904618
6	0.73906722	-1.79334895	3.14178612
6	0.64420992	-0.44836767	3.87259292
6	2.00834692	0.13413363	4.27883709
6	1.03683631	-1.72379746	1.62981053
6	2.88147429	0.63244174	3.11994452
6	3.08234179	-0.37353972	1.98912748
1	1.51019526	-2.41897594	3.61553436
1	0.08151375	0.27712479	3.26372880
1	2.56038026	-0.63972111	4.84033990
1	2.44305239	1.54635881	2.68729325
1	-0.20824580	-2.34338402	3.22258710
1	0.05031266	-0.59980650	4.78738112
1	1.85167750	0.96769080	4.98242869
1	3.87530764	0.91692585	3.50593004
1	3.81403182	0.01181883	1.26353341
1	3.45704023	-1.34165022	2.35994231
8	-0.10349427	-1.53409240	0.87771844
8	1.86647385	-0.58867314	1.24456007
1	0.97541867	-3.30838564	-0.59358878
1	2.52441877	-2.40117951	-0.50608715
13	-0.28388256	-0.10514347	-0.13163675

Electronic energy = -1915.416790 a.u.

DFT-D4 dispersion correction = -0.125640 a.u.
 Thermal free energy = 0.575570 a.u.
 Gibbs free energy = -1914.966859 a.u.
 Number of imaginary frequencies = 0.

6a_{cl}

Atomic N.	X	Y	Z
6	4.88903936	1.49861969	-0.58294235
6	4.27814810	1.63319495	-1.83827589
6	2.89928439	1.51638246	-2.01822441
6	2.09874993	1.22900399	-0.86419364
6	2.69835544	1.21733757	0.43680389
6	4.10418932	1.31485344	0.54057268
6	1.89458299	1.20436652	1.67546582
7	0.61799662	0.70141092	1.68637195
6	-0.15709125	0.75554307	2.81672728
6	0.37788772	1.27950354	4.00653085
6	1.67785641	1.76778813	4.02056338
6	2.43161431	1.75330352	2.85414915
6	-1.57490823	0.35046171	2.78286482
6	-2.35994343	0.49931898	1.59320826
6	-3.79014762	0.50467426	1.68594365
6	-4.35708385	0.14045211	2.90861452
6	-3.58577633	-0.17751431	4.03738753
6	-2.21081443	-0.03544408	3.98270570
8	0.80003781	0.98715228	-1.02120901
8	-1.77078922	0.66202446	0.41123355
1	-0.25306340	1.35886818	4.88745888
1	2.08865498	2.20503261	4.93140980
1	3.41828892	2.20666690	2.83403032
1	4.58058840	1.21409959	1.51541340
6	2.25854571	1.67831039	-3.41212786
1	-1.60861481	-0.24090149	4.86813405
1	-5.44105106	0.08867131	2.99562280
6	-4.66655123	0.91571960	0.48490087
1	4.91331473	1.81762647	-2.70277301
6	-4.25568452	2.33095017	0.01072064
6	-6.15810608	0.97565213	0.86559439
6	-4.52799119	-0.08601830	-0.68424500
1	-4.39118823	3.06464553	0.81880930
1	-4.89180551	2.63663415	-0.83355252
1	-3.21072335	2.35900575	-0.31668276
1	-4.86774920	-1.08666537	-0.37816036
1	-3.49435411	-0.15642547	-1.03947715
1	-5.16173988	0.23792428	-1.52387061
1	-6.73453126	1.31653074	-0.00604285
1	-6.34729467	1.68271193	1.68630645
1	-6.55416125	-0.00866380	1.15528458
6	1.60951575	0.35223936	-3.87573312
6	3.30204410	2.07437563	-4.47418686
6	1.19476937	2.80189532	-3.37494218
1	4.06765112	1.29767489	-4.61652446
1	3.80602389	3.02015449	-4.22712423

1	2.79276054	2.21259375	-5.43837744
1	2.36592370	-0.44391500	-3.94489589
1	1.17308085	0.48705643	-4.87724762
1	0.81596701	0.02422723	-3.19588924
1	0.75126016	2.92287073	-4.37476649
1	1.65438561	3.76023333	-3.09165889
1	0.39173740	2.57532738	-2.66589667
1	-4.07164165	-0.50540981	4.95618170
1	5.97417031	1.54994503	-0.49490007
8	-1.05642380	-3.49708140	-0.30332188
6	-2.28881273	-3.04774935	0.29269732
1	-2.83440979	-2.39075707	-0.39319427
6	0.88987429	-3.19192099	-1.57801741
6	2.33942432	-2.71278269	-1.42147739
6	3.07037194	-3.26578540	-0.18310793
6	-0.18848858	-2.49816635	-0.73047876
6	2.73335511	-2.58873283	1.15240823
6	1.25561362	-2.59234844	1.51739278
1	0.83847927	-4.27209179	-1.37766789
1	2.38966515	-1.61359038	-1.43815219
1	4.15556476	-3.16746167	-0.34320053
1	3.08764058	-1.54615350	1.13525713
1	0.55808347	-3.04317898	-2.61598999
1	2.88799568	-3.05063382	-2.31446341
1	2.86965105	-4.34886245	-0.10755314
1	3.28033654	-3.09320800	1.96689214
1	1.08970862	-2.14143682	2.50718731
1	0.83702531	-3.61155403	1.53565701
8	-0.72503863	-1.37033409	-1.20619959
8	0.46976500	-1.83344476	0.57608800
1	-2.10065162	-2.52184879	1.24111343
1	-2.86345706	-3.95905621	0.48993884
13	-0.17889166	-0.08389745	0.02310257

Electronic energy = -1915.417733 a.u.

DFT-D4 dispersion correction = -0.128217 a.u.

Thermal free energy = 0.575988 a.u.

Gibbs free energy = -1914.969962 a.u.

Number of imaginary frequencies = 0.

6b_{CL}

Atomic N.	X	Y	Z
6	3.11864264	3.60883472	2.71272651
6	3.90408854	2.64108247	2.07344526
6	3.37960542	1.74219277	1.14250680
6	1.97569753	1.81293554	0.86026717
6	1.20879274	2.90535113	1.38074894
6	1.79324356	3.75323497	2.34624469
6	-0.12431924	3.26028288	0.85413964
7	-0.92480597	2.32112144	0.26149366
6	-2.12516696	2.66129903	-0.30212395
6	-2.56285006	3.99640016	-0.25301840
6	-1.77477185	4.95864640	0.36393866
6	-0.54824946	4.60019919	0.90625242

6	-2.93645586	1.66308540	-1.02708754
6	-2.35016375	0.52407281	-1.66729678
6	-3.09734305	-0.18623252	-2.66314503
6	-4.44608430	0.14056523	-2.82071424
6	-5.07178377	1.14354841	-2.06819800
6	-4.31396387	1.91425458	-1.20515461
8	1.40596406	0.87102053	0.09999671
8	-1.10976550	0.12814877	-1.36451570
1	-3.48804593	4.27725675	-0.74757652
1	-2.09801591	6.00011854	0.38351765
1	0.11053344	5.35649076	1.32252070
1	1.18310390	4.51747681	2.82654345
6	4.28765460	0.69969513	0.45919656
1	-4.79004537	2.71365575	-0.63799756
1	-5.04513407	-0.41097891	-3.54289210
6	-2.44733479	-1.28207329	-3.53159020
1	4.95994084	2.58209227	2.33102634
6	-1.18909417	-0.72345007	-4.23803566
6	-3.40008922	-1.78379588	-4.63364658
6	-2.06913677	-2.49902367	-2.65932080
1	-1.45741039	0.11850542	-4.89271075
1	-0.73833431	-1.50732572	-4.86537442
1	-0.43884328	-0.37869044	-3.51872166
1	-2.96564962	-2.94385845	-2.20266192
1	-1.38119597	-2.20328154	-1.86118655
1	-1.58389627	-3.27106964	-3.27616993
1	-2.87226504	-2.52652412	-5.24871936
1	-3.72480498	-0.97107457	-5.29925248
1	-4.29359187	-2.27556484	-4.22268462
6	3.90630915	-0.72020791	0.93171574
6	5.77419370	0.91559275	0.80181804
6	4.15682304	0.80328862	-1.07907532
1	5.98118366	0.78037683	1.87318608
1	6.12525386	1.91365142	0.50234187
1	6.37599509	0.17451065	0.25652625
1	4.06456284	-0.82346176	2.01546814
1	4.53161256	-1.47056108	0.42357671
1	2.85529451	-0.93133292	0.71254361
1	4.81574099	0.06272897	-1.55729350
1	4.46579061	1.80076282	-1.42415181
1	3.12957001	0.62325175	-1.41275806
1	-6.13975003	1.32860620	-2.18203223
1	3.55514533	4.25295268	3.47580897
8	-1.80868227	-2.10316102	2.25514690
6	-2.97288006	-1.83263441	1.45091303
1	-2.74226062	-1.92191759	0.37915220
6	0.26631052	-1.44263749	3.20319986
6	0.58032786	-2.88887252	3.59325030
6	1.31937506	-3.70796591	2.52802262
6	-0.74005685	-1.23645142	2.07052183
6	0.54743179	-3.90141850	1.21359998
6	0.59111017	-2.72996092	0.23981012
1	1.18077725	-0.89871919	2.92437033
1	1.19517586	-2.86579247	4.50692940

1	1.54020139	-4.70075945	2.95129462
1	0.99483158	-4.74195845	0.65708175
1	-0.16758160	-0.91276708	4.06471966
1	-0.35668587	-3.40018302	3.86131739
1	2.29672948	-3.24349023	2.31076023
1	-0.49478143	-4.18467219	1.42263785
1	0.10706805	-3.02304655	-0.70352580
1	1.63882419	-2.47379776	0.01687832
8	-1.06534787	0.05671775	1.84496185
8	-0.06287027	-1.50900163	0.67603462
1	-3.70401005	-2.59762794	1.73390881
1	-3.36919555	-0.83129565	1.66062164
13	-0.33019173	0.43263039	0.22594824

Electronic energy = -1915.420891 a.u.

DFT-D4 dispersion correction = -0.125364 a.u.

Thermal free energy = 0.575751 a.u.

Gibbs free energy = -1914.970504 a.u.

Number of imaginary frequencies = 0.

TS2ax_{CL}

Atomic N.	X	Y	Z
6	4.89546394	1.55580699	-0.59695959
6	4.27481461	1.66365457	-1.85001922
6	2.89844012	1.51012003	-2.02126527
6	2.11169982	1.21054029	-0.86052722
6	2.71722078	1.23373556	0.43731853
6	4.12065220	1.36614621	0.53260565
6	1.91751564	1.22413445	1.67859352
7	0.64930290	0.70247930	1.69870830
6	-0.12231312	0.76056236	2.83037162
6	0.40672550	1.31084764	4.01123714
6	1.69920874	1.81838334	4.01549149
6	2.45007849	1.79798281	2.84756708
6	-1.53582203	0.33806458	2.80756283
6	-2.32609129	0.45491445	1.61777878
6	-3.75582910	0.48239335	1.72185302
6	-4.31819963	0.14678007	2.95497108
6	-3.54205084	-0.15767410	4.08382320
6	-2.16693830	-0.02067816	4.01821947
8	0.82184857	0.92302912	-1.00951922
8	-1.74569118	0.56970513	0.42599800
1	-0.22334546	1.39454508	4.89231396
1	2.10555053	2.27442718	4.91910839
1	3.43009877	2.26497555	2.81854868
1	4.60414457	1.28887784	1.50606024
6	2.24585581	1.64918077	-3.41205502
1	-1.56070197	-0.20770666	4.90493059
1	-5.40204430	0.10960782	3.05076265
6	-4.63631964	0.89878953	0.52545291
1	4.90059090	1.85677552	-2.71949410
6	-4.20170879	2.30218458	0.03743235
6	-6.12283325	0.98990875	0.91926736
6	-4.52797079	-0.11088582	-0.63914138

1	-4.31599188	3.04422212	0.84106940
1	-4.83779478	2.61467576	-0.80441231
1	-3.15878201	2.30629420	-0.29808605
1	-4.87393856	-1.10578036	-0.32116151
1	-3.49975538	-0.19208878	-1.00713670
1	-5.17048836	0.21505630	-1.47133720
1	-6.70066643	1.33620274	0.05066242
1	-6.29090261	1.70572984	1.73686409
1	-6.53480911	0.01523347	1.21933377
6	1.62358856	0.30734622	-3.86658454
6	3.27292299	2.06470060	-4.48263931
6	1.15640175	2.74785328	-3.37196398
1	4.05540228	1.30526316	-4.62655401
1	3.75661826	3.02277589	-4.24263668
1	2.75441909	2.18714738	-5.44408178
1	2.39616013	-0.47357345	-3.93166137
1	1.18343198	0.42693806	-4.86848974
1	0.83766949	-0.03067406	-3.18286157
1	0.70253247	2.85441685	-4.36883402
1	1.59563828	3.71774006	-3.09585762
1	0.36425549	2.50518250	-2.65587687
1	-4.02382374	-0.46573484	5.01159620
1	5.97950411	1.63387549	-0.51528656
8	-1.10953951	-3.51840758	-0.51746649
6	-2.40368867	-3.08020759	-0.04880412
1	-2.90620637	-2.48123193	-0.81501579
6	0.93218732	-3.19462276	-1.62668490
6	2.35386324	-2.68406558	-1.35174561
6	3.01947474	-3.24645638	-0.07905626
6	-0.23982327	-2.53725982	-0.89815462
6	2.66708446	-2.55067062	1.24327421
6	1.18505037	-2.55193377	1.59697402
1	0.88674712	-4.27614021	-1.43439436
1	2.37720704	-1.58453858	-1.34727943
1	4.11160374	-3.18100667	-0.20585880
1	3.02118278	-1.50816095	1.21129823
1	0.69293869	-3.05022240	-2.69237781
1	2.96814346	-2.99092817	-2.21261811
1	2.78787851	-4.32339907	-0.00220366
1	3.21221590	-3.04259181	2.06681371
1	1.01788533	-2.08220935	2.58028889
1	0.79094404	-3.58183908	1.65478921
8	-0.70086926	-1.37860918	-1.28632712
8	0.40153089	-1.85311472	0.62946254
1	-2.30152225	-2.49414468	0.87482005
1	-2.96082520	-4.00068617	0.15303464
13	-0.13640682	-0.15196300	0.05617142

Electronic energy = -1915.417329 a.u.

DFT-D4 dispersion correction = -0.128099 a.u.

Thermal free energy = 0.576217 a.u.

Gibbs free energy = -1914.969211 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 98.0i

TS2eq_{CL}

Atomic N.	X	Y	Z
6	3.60912253	3.34963146	-2.68236017
6	3.68543225	2.03595341	-3.16190616
6	2.74281272	1.05945629	-2.83463315
6	1.65889051	1.43312679	-1.97208242
6	1.50575164	2.80323492	-1.59060773
6	2.52103680	3.72760301	-1.91753785
6	0.27411272	3.31381262	-0.95921877
7	-0.54116061	2.49844844	-0.21834618
6	-1.69899113	2.98256423	0.32946499
6	-2.06209637	4.32783870	0.13986703
6	-1.24668197	5.16457182	-0.60832381
6	-0.08400065	4.65812257	-1.17041291
6	-2.62693377	2.10096435	1.06232743
6	-2.74386527	0.70907821	0.75422065
6	-3.90305244	-0.00973491	1.19935161
6	-4.76903444	0.63517969	2.08534354
6	-4.56061828	1.94864855	2.52590463
6	-3.51518498	2.68062225	1.99236892
8	0.79781742	0.50711446	-1.54515847
8	-1.79842351	0.08908740	0.04384143
1	-3.01109497	4.68484992	0.52913580
1	-1.53811661	6.20019352	-0.78774557
1	0.52921218	5.27893655	-1.81670563
1	2.45872562	4.74763393	-1.53983720
6	2.91143882	-0.38766381	-3.33825629
1	-3.36055863	3.71219851	2.30823601
1	-5.63398566	0.09559335	2.46695184
6	-4.18088107	-1.45665098	0.74650016
1	4.52956444	1.76742465	-3.79449322
6	-4.14524282	-1.55565499	-0.79686832
6	-5.56994494	-1.94816069	1.19721447
6	-3.12920889	-2.40126741	1.36737256
1	-4.91394806	-0.90655571	-1.24121846
1	-4.35828671	-2.59021168	-1.10614035
1	-3.17029139	-1.26369291	-1.20038456
1	-3.21346226	-2.40314684	2.46438344
1	-2.11749222	-2.08212512	1.09870632
1	-3.28314700	-3.43188227	1.01147454
1	-5.73208254	-2.96286347	0.80609172
1	-6.37742677	-1.30925229	0.81128122
1	-5.66156186	-2.00192336	2.29154185
6	3.28670120	-1.29041408	-2.14045369
6	4.03881825	-0.51215481	-4.38165276
6	1.61692871	-0.89464420	-4.01641386
1	5.02517299	-0.25972133	-3.96692979
1	3.85716087	0.12336543	-5.26059442
1	4.08816361	-1.55423060	-4.72905478
1	4.27329648	-1.00693421	-1.74477451
1	3.33578487	-2.34408923	-2.45707090
1	2.55437769	-1.19463095	-1.33245044
1	1.76989311	-1.92138998	-4.38240723

1	1.36528068	-0.26384101	-4.88174315
1	0.76677242	-0.88986821	-3.32758324
1	-5.23010714	2.39332670	3.26202718
1	4.39653896	4.06589730	-2.91670465
8	2.86285562	0.02426982	1.52626498
6	3.87768591	-0.83562671	2.06859614
1	4.81616517	-0.46509051	1.64376077
6	1.19308940	-0.63676098	3.28734865
6	1.38651635	-2.12901673	3.61235982
6	0.60303857	-3.15106158	2.77110348
6	1.57852178	-0.01460131	1.95146113
6	1.14663592	-3.39273337	1.35169408
6	0.59433083	-2.44319114	0.29026816
1	0.13138553	-0.38235074	3.40245961
1	2.45003365	-2.40706706	3.60817006
1	0.63164888	-4.10457974	3.32159698
1	2.24890765	-3.34418387	1.36589620
1	1.73255296	-0.03590795	4.04359049
1	1.06332035	-2.23732633	4.66053235
1	-0.45741351	-2.85745179	2.72033722
1	0.89895902	-4.41615537	1.02683675
1	1.16151370	-2.56419888	-0.64855792
1	-0.45323776	-2.71826362	0.07562148
8	0.91309692	1.03274394	1.56752303
8	0.60491053	-1.08675427	0.71582404
1	3.72591181	-1.87818926	1.75855123
1	3.92074460	-0.76681131	3.16401611
13	-0.05309841	0.55853478	0.04120849

Electronic energy = -1915.401368 a.u.
DFT-D4 dispersion correction = -0.125101 a.u.
Thermal free energy = 0.575214 a.u.
Gibbs free energy = -1914.951255 a.u.
Number of imaginary frequencies = 1.
Imaginary frequency = 76.4i

7a_{CL}

Atomic N.	X	Y	Z
6	3.98345199	3.91689426	0.17367895
6	4.20845952	3.07188041	-0.92035871
6	3.26590823	2.13757902	-1.35382147
6	2.02867374	2.04737201	-0.63464042
6	1.74456285	2.99275529	0.40068902
6	2.75759284	3.88536064	0.81273025
6	0.40382160	3.13388697	1.00180087
7	-0.47670121	2.08590231	1.02014818
6	-1.71683076	2.22463189	1.58038203
6	-2.11106583	3.45615510	2.13199556
6	-1.23621284	4.53377815	2.10304293
6	0.01904698	4.37995489	1.53129564
6	-2.68689579	1.11192651	1.56030735
6	-2.70677755	0.15122719	0.50112095
6	-3.87375975	-0.66025278	0.31251830
6	-4.85444140	-0.62817698	1.30702589

6	-4.75503619	0.18990682	2.44035777
6	-3.69785549	1.07691284	2.54313964
8	1.15120818	1.09515671	-0.95814174
8	-1.66442849	0.02457632	-0.32482769
1	-3.11849174	3.57019752	2.52243632
1	-1.54552660	5.50336230	2.49533175
1	0.69193131	5.22840397	1.44827137
1	2.58129919	4.53934946	1.66609025
6	3.57120455	1.21080571	-2.54797562
1	-3.63057486	1.74282350	3.40358671
1	-5.72875234	-1.26940889	1.21103755
6	-4.06011865	-1.52354109	-0.95231269
1	5.16626443	3.13798270	-1.43306876
6	-3.97283109	-0.62145409	-2.20670913
6	-5.43563388	-2.21635271	-0.97753333
6	-2.98450880	-2.62933647	-1.03565605
1	-4.76829354	0.13757401	-2.19251747
1	-4.10393909	-1.23074684	-3.11417014
1	-3.00452777	-0.11186602	-2.26692202
1	-3.00722923	-3.26767747	-0.13993405
1	-1.99030285	-2.18409056	-1.13300764
1	-3.17244893	-3.26833210	-1.91223152
1	-5.53430975	-2.77737350	-1.91784672
1	-6.26317543	-1.49390322	-0.93433995
1	-5.55634843	-2.93370912	-0.15262511
6	3.68546082	-0.25113709	-2.05759584
6	4.90410559	1.57164010	-3.23176760
6	2.46378066	1.32768808	-3.62200527
1	5.76681491	1.43796687	-2.56329337
1	4.90946624	2.60595854	-3.60506583
1	5.05265244	0.90677599	-4.09477916
1	4.49858420	-0.35102244	-1.32387065
1	3.91524019	-0.91214440	-2.90884245
1	2.75241452	-0.58271714	-1.59067624
1	2.70375993	0.67232620	-4.47360870
1	2.40142292	2.35873480	-3.99995557
1	1.48429174	1.04287313	-3.22440107
1	-5.51800174	0.14489037	3.21733107
1	4.76608554	4.59574417	0.51213834
8	0.79050722	-3.63020611	-1.32465508
6	1.00402252	-3.22203428	-2.70571303
1	1.89400561	-2.58699098	-2.77893886
6	0.30525883	-3.15233163	0.94499355
6	1.62162498	-3.17947059	1.77410606
6	1.39179580	-2.90245297	3.27616969
6	0.52491384	-2.64834679	-0.45260729
6	1.47430451	-1.42332155	3.69698136
6	0.48013972	-0.47333422	3.02141299
1	-0.41531218	-2.47758557	1.41665807
1	2.08706130	-4.16715322	1.64002183
1	2.15249683	-3.45503834	3.85042528
1	1.32762999	-1.35941390	4.78862795
1	-0.12712038	-4.16035883	0.89065065
1	2.32257801	-2.43080694	1.38150419

1	0.41903756	-3.32453997	3.58262145
1	2.49048452	-1.04785234	3.48984083
1	0.56800783	0.52572017	3.49425054
1	-0.55396539	-0.82549841	3.22220552
8	0.48866850	-1.46654610	-0.82490201
8	0.73921698	-0.40917999	1.64166935
1	1.14184966	-4.15698567	-3.25552280
1	0.12941634	-2.67244827	-3.07259535
13	0.04089233	0.30846467	0.21084040

Electronic energy = -1915.430077 a.u.

DFT-D4 dispersion correction = -0.123426 a.u.

Thermal free energy = 0.573050 a.u.

Gibbs free energy = -1914.980453 a.u.

Number of imaginary frequencies = 0.

8_{CL}

Atomic N.	X	Y	Z
6	1.82098499	3.89933690	1.74070038
6	0.95989377	3.59310942	2.80245525
6	0.37020072	2.33541519	2.95664197
6	0.66464289	1.34009526	1.97454344
6	1.63034923	1.61228318	0.94971995
6	2.16506499	2.91286456	0.83357470
6	2.16236292	0.56496385	0.05302064
7	1.38733192	-0.50936492	-0.29481195
6	1.86550391	-1.54560510	-1.05346729
6	3.18834348	-1.48760787	-1.52092349
6	3.98297004	-0.38881688	-1.21148841
6	3.48134709	0.63695818	-0.41891162
6	1.01190541	-2.71519807	-1.34591421
6	-0.04041917	-3.14960089	-0.47342633
6	-0.71151876	-4.38682439	-0.72494780
6	-0.36072393	-5.09500328	-1.87649018
6	0.61298401	-4.64066871	-2.77532688
6	1.29677607	-3.46980993	-2.50414186
8	0.04093873	0.14823419	2.03547454
8	-0.39122507	-2.42198662	0.59979546
1	3.59746853	-2.32423436	-2.08054228
1	5.01545980	-0.34957128	-1.56059895
1	4.11180684	1.47116182	-0.12494616
1	2.81404291	3.14690993	-0.00973027
6	-0.57696753	2.03988924	4.13817087
1	2.04344800	-3.10630564	-3.20968093
1	-0.87334078	-6.02812209	-2.10207606
6	-1.80433967	-4.91225197	0.22847491
1	0.72942245	4.37786319	3.52053629
6	-1.23177569	-5.08837211	1.65537405
6	-2.33806034	-6.28719825	-0.21771969
6	-3.00802302	-3.93997796	0.25000085
1	-0.40518499	-5.81407627	1.65248148
1	-2.01707214	-5.47502010	2.32244345
1	-0.86306785	-4.14255039	2.06526524
1	-3.44201626	-3.84023308	-0.75540950

1	-2.72208139	-2.94247537	0.59865234
1	-3.78817627	-4.33256172	0.91985000
1	-3.09441286	-6.62564855	0.50441807
1	-1.54549957	-7.04907596	-0.24801125
1	-2.82179504	-6.24693274	-1.20444768
6	-2.00595698	1.73881910	3.62747515
6	-0.68087075	3.23961534	5.09935169
6	-0.04308623	0.84115981	4.95816021
1	-1.11588680	4.12589275	4.61490790
1	0.29591280	3.51679304	5.52146912
1	-1.33813589	2.96785947	5.93734080
1	-2.39912751	2.58811011	3.04952828
1	-2.67793696	1.57192271	4.48291412
1	-2.02908735	0.84530958	2.99493908
1	-0.71961296	0.63986242	5.80253049
1	0.95117270	1.06789020	5.36999013
1	0.03034223	-0.06590005	4.34900064
1	0.82577075	-5.20606126	-3.68243685
1	2.21568714	4.90940568	1.63156446
8	1.62181211	2.53865905	-4.95386997
6	2.84854948	1.78419104	-5.09624084
1	2.86340837	0.94399114	-4.39017691
6	0.17209740	3.94089372	-3.69338950
6	-0.54991535	3.85392900	-2.34204380
6	-1.19685400	2.48889620	-2.08393064
6	1.45300970	3.12993572	-3.73577699
6	-1.90522327	2.41545644	-0.72838433
6	-2.55299275	1.05790290	-0.44000978
1	0.46786721	4.98491633	-3.89235814
1	0.16824887	4.08377072	-1.54019330
1	-0.43244395	1.69710730	-2.13111393
1	-1.19055937	2.65559527	0.07654603
1	-0.48030924	3.63155067	-4.52164111
1	-1.32256200	4.63903645	-2.31048265
1	-1.92145180	2.26652721	-2.88722785
1	-2.69912398	3.18228949	-0.68065014
1	-3.31468692	0.85017560	-1.21432493
1	-3.08567609	1.11293608	0.52739870
8	2.25946007	3.02823819	-2.82778812
8	-1.63951647	-0.02162939	-0.44312254
1	2.84611351	1.42032154	-6.12821391
1	3.71935215	2.42540112	-4.91035179
13	-0.35533624	-0.65476109	0.50203013

Electronic energy = -1915.432416 a.u.

DFT-D4 dispersion correction = -0.118009 a.u.

Thermal free energy = 0.567308 a.u.

Gibbs free energy = -1914.983116 a.u.

Number of imaginary frequencies = 0.

Initiation stage for LA

2_{LA}

Atomic N.	X	Y	Z
6	1.08857443	0.94968537	-4.99107916
6	-0.17806005	0.36564725	-5.11508554
6	-1.04629866	0.21036225	-4.03103012
6	-0.59817439	0.65949719	-2.75082377
6	0.65875351	1.34072167	-2.63095495
6	1.49223340	1.44632589	-3.76489830
6	1.09541564	2.01711586	-1.39024215
7	0.68129705	1.55515654	-0.16880354
6	0.99325817	2.18894913	1.00490389
6	1.81286314	3.32604741	0.96423993
6	2.27700210	3.79468949	-0.25942858
6	1.91040707	3.15742497	-1.44060710
6	0.44449131	1.69625541	2.28615410
6	-0.83293665	1.05202537	2.39173159
6	-1.39611408	0.79365413	3.67867684
6	-0.61800263	1.09504887	4.80001050
6	0.66833523	1.64079412	4.70355620
6	1.18650642	1.95193359	3.45908549
8	-1.38421554	0.46058601	-1.67374198
8	-1.52783845	0.70863835	1.28754312
1	2.04510154	3.85474846	1.88428415
1	2.90036621	4.68843080	-0.29643272
1	2.21212572	3.56152886	-2.40294304
1	2.47762533	1.90057991	-3.66288042
6	-2.43911144	-0.42757451	-4.21683587
1	2.19428354	2.35701446	3.37336270
1	-1.01374245	0.88394924	5.79150930
6	-2.81135485	0.19809367	3.83154804
1	-0.48498422	0.00709681	-6.09553181
6	-3.85028170	1.12414121	3.15495575
6	-3.21649875	0.06311927	5.31198616
6	-2.87776700	-1.21728883	3.21049324
1	-3.84896979	2.11625883	3.62928445
1	-4.85767204	0.69675785	3.27095343
1	-3.64778249	1.24885806	2.08596644
1	-2.14305685	-1.88519679	3.68359379
1	-2.68567356	-1.19392234	2.13280037
1	-3.87847659	-1.64523938	3.37186375
1	-4.23845312	-0.33760625	5.36551027
1	-3.21446693	1.03230369	5.83119435
1	-2.56293991	-0.62923476	5.86228454
6	-2.55140622	-1.74040837	-3.40640165
6	-2.71259398	-0.78041418	-5.69159746
6	-3.53833942	0.56680438	-3.77218681
1	-2.00935145	-1.53230376	-6.07810193
1	-2.67148090	0.10418961	-6.34328376
1	-3.72344647	-1.20372210	-5.77374892
1	-1.77198605	-2.45424536	-3.71060291
1	-3.52995899	-2.20776668	-3.59257022
1	-2.45904359	-1.55881336	-2.33067008

1	-4.52941153	0.11003956	-3.91372053
1	-3.49951349	1.48197745	-4.38067143
1	-3.43233447	0.84455467	-2.71820965
1	1.25571698	1.81817735	5.60433712
1	1.74767103	1.01486560	-5.85644242
8	0.19636261	-1.38355277	0.05779024
6	-0.34285409	-2.70000191	0.08461582
1	0.47836653	-3.42771560	0.18171528
1	-1.02329313	-2.84500458	0.94113474
1	-0.89325140	-2.93671250	-0.84171542
13	-0.60666765	0.14748802	-0.11567296
8	4.21966769	0.71131667	1.78735263
8	4.06436025	-0.41596323	-0.13717231
6	3.87013360	-0.29297195	1.20409465
6	3.18444139	-1.48992880	1.86121203
8	3.74090352	-2.74096919	1.33819035
6	3.83452233	-2.86070322	-0.01567497
6	3.47989130	-1.59377065	-0.79247791
8	4.16645911	-3.91001171	-0.52027399
6	3.98231097	-1.61973807	-2.22040129
6	3.34517621	-1.51743995	3.36674097
1	2.11468044	-1.44913345	1.58038134
1	2.37898424	-1.48175851	-0.76273126
1	3.69489817	-0.69623075	-2.73736044
1	3.53931558	-2.47372777	-2.74558912
1	5.07352432	-1.72882029	-2.24806975
1	2.89278826	-0.61894530	3.80232333
1	4.40604046	-1.54311879	3.64408145
1	2.84295019	-2.40289762	3.77520389

Electronic energy = -2064.604308 a.u.

DFT-D4 dispersion correction = -0.121909 a.u.

Thermal free energy = 0.548559 a.u.

Gibbs free energy = -2064.177659 a.u.

Number of imaginary frequencies = 0.

3a_{LA}

Atomic N.	X	Y	Z
6	1.19336841	4.42603669	-3.43355825
6	0.61781457	3.39766444	-4.19190767
6	0.03074230	2.27308953	-3.60936876
6	0.05203367	2.17143259	-2.17965027
6	0.49614805	3.28855852	-1.39920245
6	1.10670207	4.38053133	-2.05437611
6	0.24536382	3.39396690	0.05242919
7	0.06609058	2.27245463	0.81581685
6	-0.21228214	2.35668198	2.15325358
6	-0.29442789	3.61707454	2.77064834
6	-0.10659947	4.76636455	2.01370588
6	0.14714192	4.66271599	0.65192664
6	-0.50576605	1.14387549	2.94093173
6	-1.10900501	-0.00873089	2.34097927
6	-1.78127431	-0.96324934	3.17295819
6	-1.59273529	-0.86004264	4.55283195

6	-0.83130119	0.16250202	5.13875885
6	-0.33329448	1.17775516	4.34130479
8	-0.36952111	1.04520959	-1.59995641
8	-1.08473238	-0.18366464	1.02031432
1	-0.56342351	3.68404683	3.82112251
1	-0.19891374	5.74859221	2.47886439
1	0.22471673	5.55563809	0.03854975
1	1.53858532	5.18715448	-1.46267024
6	-0.61788474	1.17823630	-4.48075365
1	0.21403400	2.00467820	4.79444381
1	-2.04764138	-1.60163973	5.20726266
6	-2.71728128	-2.03346928	2.57249704
1	0.64844122	3.47909634	-5.27685874
6	-3.81636376	-1.32983853	1.73944222
6	-3.42427896	-2.84989916	3.67110857
6	-1.95282587	-3.03203268	1.67529345
1	-4.40710505	-0.65084151	2.37137822
1	-4.50101214	-2.08146212	1.31809986
1	-3.38576989	-0.75382450	0.91257095
1	-1.16998640	-3.55014096	2.24787239
1	-1.48924757	-2.52503079	0.82389655
1	-2.65137446	-3.79250842	1.29383588
1	-4.11653022	-3.55997094	3.19690898
1	-4.01355757	-2.21307589	4.34647034
1	-2.71563214	-3.43614940	4.27448946
6	0.14335588	-0.15884893	-4.33251996
6	-0.60512121	1.55281989	-5.97496315
6	-2.09721671	0.98813168	-4.06792970
1	0.41568874	1.64319665	-6.37422568
1	-1.13978824	2.49366903	-6.17001234
1	-1.11126165	0.76026688	-6.54425346
1	1.19641841	-0.03665116	-4.62899030
1	-0.30842697	-0.91832870	-4.98937198
1	0.10384641	-0.52152524	-3.30052950
1	-2.56079861	0.21234396	-4.69610687
1	-2.66085026	1.92125265	-4.21328675
1	-2.18717974	0.68446431	-3.01945050
1	-0.66871515	0.17465208	6.21640615
1	1.68827875	5.26112385	-3.92905776
8	1.97950465	0.24151331	0.26676794
6	2.90395892	1.15153378	0.83223496
1	2.97000165	2.09637170	0.26349903
8	0.45841916	-1.47596454	-0.88749715
1	3.90985452	0.69752063	0.82239871
1	2.66509830	1.40177785	1.88228718
13	0.23556259	0.47088762	-0.01474707
8	1.28655505	-2.47055957	0.92703835
6	1.30687108	-2.21121526	-0.37854334
6	2.41714021	-2.86795667	-1.18196130
8	2.78456448	-4.16664431	-0.62920081
6	2.94735036	-4.26412287	0.72233205
6	2.51620779	-3.02639903	1.50761866
8	3.39436264	-5.27002170	1.22012493
6	2.24580542	-3.30587845	2.96995192

6	2.07687255	-3.07316745	-2.64543799
1	3.28409570	-2.18672087	-1.08551701
1	3.29196809	-2.24800809	1.39706307
1	1.91923285	-2.38548487	3.46856196
1	3.16498167	-3.66982439	3.44344925
1	1.47330367	-4.07595019	3.08125582
1	1.85731455	-2.10685578	-3.11208150
1	1.20062457	-3.72413527	-2.75190970
1	2.93070521	-3.53504747	-3.15506024

Electronic energy = -2064.597211 a.u.

DFT-D4 dispersion correction = -0.124482 a.u.

Thermal free energy = 0.551566 a.u.

Gibbs free energy = -2064.170127 a.u.

Number of imaginary frequencies = 0.

TS1ax_{1A}

Atomic N.	X	Y	Z
6	3.59044075	3.75554991	0.87262636
6	3.22762966	3.80003023	-0.48115206
6	2.11105442	3.12945747	-0.98371226
6	1.33605886	2.34867525	-0.06585657
6	1.61559486	2.41678262	1.33685482
6	2.77601004	3.09327126	1.77295649
6	0.67328173	1.90378618	2.35050988
7	-0.18759726	0.87723362	2.05789781
6	-1.09727204	0.42966074	2.98055792
6	-1.13678157	1.01121366	4.26011705
6	-0.26239416	2.04240918	4.57730389
6	0.63452148	2.50292349	3.62212825
6	-2.08707619	-0.60671729	2.63053107
6	-2.57509470	-0.75445408	1.29308665
6	-3.78857970	-1.47868133	1.05725932
6	-4.33321238	-2.19073462	2.12782454
6	-3.76197004	-2.18444562	3.40895367
6	-2.67153168	-1.37183833	3.66272998
8	0.34638077	1.58424854	-0.52887571
8	-1.92847252	-0.20050120	0.26763725
1	-1.89185774	0.68862307	4.97141314
1	-0.30817869	2.51653385	5.55846500
1	1.27493870	3.35465097	3.83264756
1	3.04636073	3.07070279	2.82851648
6	1.72697723	3.22671461	-2.47436261
1	-2.24389529	-1.33730435	4.66480112
1	-5.23065948	-2.78574681	1.96775150
6	-4.47883081	-1.45521259	-0.32239163
1	3.85596442	4.36990499	-1.16328979
6	-4.76776457	0.01006357	-0.72947270
6	-5.82903433	-2.19662380	-0.29513556
6	-3.60254049	-2.13262844	-1.40097284
1	-5.42679691	0.49276337	0.00686166
1	-5.27841330	0.02952019	-1.70409667
1	-3.84558558	0.59547448	-0.81099683
1	-3.43683958	-3.19164371	-1.15113831

1	-2.63330317	-1.63342774	-1.50720572
1	-4.11899805	-2.09741569	-2.37244272
1	-6.29968023	-2.11581278	-1.28523755
1	-6.52354383	-1.76312566	0.43889198
1	-5.71216249	-3.26763988	-0.07402477
6	1.84266365	1.84740925	-3.16392040
6	2.64598441	4.20076895	-3.23620081
6	0.28089330	3.76205206	-2.60736656
1	3.69184947	3.86059856	-3.25166726
1	2.61563921	5.21574354	-2.81394291
1	2.30716896	4.26605034	-4.27986097
1	2.87116718	1.46437657	-3.08798552
1	1.59708714	1.94872773	-4.23238850
1	1.16533554	1.11199450	-2.71907806
1	0.01206012	3.84034085	-3.67169404
1	0.19748227	4.76502609	-2.16362524
1	-0.44069186	3.10042930	-2.11648655
1	-4.19194794	-2.79579878	4.20212889
1	4.49816942	4.25404930	1.21232259
8	2.30571818	-1.35460222	-1.57068026
6	0.98553485	-3.30571508	-0.98282748
8	2.16407919	-3.86948252	-0.33362317
6	3.38139343	-3.43476462	-0.75870484
6	3.33562255	-2.35632515	-1.84269655
8	4.39934635	-3.90258598	-0.30138525
6	4.65297222	-1.62715626	-2.00821733
6	-0.22984131	-3.79686260	-0.22716542
1	0.95550448	-3.68106484	-2.02498388
1	3.05875611	-2.85796523	-2.78941321
1	4.56535196	-0.87829268	-2.80454659
1	5.43831778	-2.34558201	-2.26981997
1	4.93769264	-1.12969208	-1.07329118
1	-1.13841081	-3.40384197	-0.69628942
1	-0.19246580	-3.45668602	0.81373197
1	-0.25889733	-4.89312267	-0.25256431
8	0.08518117	-1.06551921	-1.35506570
8	1.10136330	-1.23500168	0.73773581
6	2.19580531	-1.24772406	1.64780915
1	1.95820558	-0.63587856	2.53053260
1	2.39301586	-2.27665973	1.98041701
1	3.10281920	-0.83266854	1.17764914
13	-0.15235229	0.04612276	0.23729819
6	1.10527968	-1.78693783	-1.10209262

Electronic energy = -2064.592049 a.u.

DFT-D4 dispersion correction = -0.127131 a.u.

Thermal free energy = 0.556005 a.u.

Gibbs free energy = -2064.163175 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 109.8i

TS1eq_{LA}

Atomic N.	X	Y	Z
6	1.17124735	2.03454171	-4.88901082

6	0.16021887	1.07610459	-5.03654876
6	-0.55996871	0.56834551	-3.95317843
6	-0.22943405	1.05171285	-2.64494876
6	0.70307980	2.12613741	-2.50584212
6	1.42277230	2.56601107	-3.63726699
6	0.85934464	2.86965720	-1.24172833
7	0.60352132	2.28055366	-0.03113419
6	0.72509308	2.99539395	1.13110050
6	1.10544343	4.34792046	1.09175074
6	1.36360845	4.95850985	-0.12766030
6	1.23323826	4.22477166	-1.29776267
6	0.40797855	2.38808319	2.43760316
6	-0.57298654	1.35635415	2.56724506
6	-1.08514408	1.02989118	3.86611735
6	-0.47476143	1.62471879	4.97321068
6	0.58833147	2.52974932	4.85587574
6	1.00557413	2.92473998	3.59705334
8	-0.80550757	0.50990931	-1.56796510
8	-1.02093834	0.71205323	1.48640735
1	1.13885386	4.91977727	2.01467962
1	1.62902364	6.01555735	-0.16825990
1	1.36728388	4.70105787	-2.26459764
1	2.20489504	3.31516320	-3.51710748
6	-1.64584475	-0.50493133	-4.16453158
1	1.82055688	3.64150600	3.49713317
1	-0.82297763	1.36695828	5.97178206
6	-2.25206752	0.03891250	4.04731253
1	-0.05247153	0.70240313	-6.03649576
6	-3.46706618	0.48139448	3.19793643
6	-2.72574211	-0.03374700	5.51156977
6	-1.80244089	-1.38044175	3.63382087
1	-3.81296915	1.47753170	3.51049559
1	-4.29788391	-0.22510760	3.34531249
1	-3.22462178	0.51745773	2.13082348
1	-0.99147625	-1.73373750	4.28855794
1	-1.44745744	-1.39324547	2.59914894
1	-2.64287139	-2.08552109	3.72684976
1	-3.58167267	-0.72079723	5.57452289
1	-3.05717108	0.94526058	5.88682279
1	-1.94707136	-0.41972895	6.18518524
6	-1.17905685	-1.83955117	-3.54049020
6	-1.92067237	-0.76358572	-5.65824470
6	-2.98296175	-0.05551947	-3.52929705
1	-1.04192563	-1.16638619	-6.18223112
1	-2.25055292	0.14627146	-6.18031812
1	-2.72466513	-1.50804262	-5.74830872
1	-0.27552399	-2.20567132	-4.05092414
1	-1.96472711	-2.60338677	-3.64860716
1	-0.95094063	-1.71539967	-2.47774639
1	-3.75104019	-0.82481750	-3.70111297
1	-3.33321677	0.87884214	-3.99192491
1	-2.88588587	0.10690124	-2.45106470
1	1.06802202	2.92999324	5.74888872
1	1.74467800	2.36403595	-5.75528360

8	-0.02515040	-1.49133929	0.19755080
6	-1.06207634	-2.44931437	0.18028106
1	-0.96789937	-3.14316219	1.03593818
1	-2.05347390	-1.97034379	0.25531667
1	-1.04912876	-3.04461258	-0.74967049
13	-0.00953190	0.35501307	0.03521158
8	1.88972543	-0.06805393	0.09810039
8	2.44184797	-1.87734795	-1.06212406
6	2.09441591	-1.31346855	0.09450712
6	2.40109910	-2.13376650	1.35033032
8	3.71615878	-2.76766397	1.18458483
6	3.90074600	-3.48975732	0.04307113
6	2.79813913	-3.29936313	-1.00507925
8	4.87056861	-4.19594236	-0.10255763
6	3.21396851	-3.72574358	-2.39573095
6	2.44481700	-1.30827768	2.61726470
1	1.65058623	-2.93309673	1.43314769
1	1.89994762	-3.85272472	-0.67829018
1	2.38853736	-3.56191108	-3.09893547
1	3.47504114	-4.79026297	-2.38458674
1	4.09324994	-3.16013682	-2.72605836
1	1.45236866	-0.88682378	2.81622809
1	3.16455484	-0.48681893	2.52424240
1	2.73043898	-1.94964566	3.45964456

Electronic energy = -2064.588934 a.u.

DFT-D4 dispersion correction = -0.125296 a.u.

Thermal free energy = 0.553150 a.u.

Gibbs free energy = -2064.161079 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 49.3i

4a_{LA}

Atomic N.	X	Y	Z
6	3.59961678	3.72422281	0.94799325
6	3.26076314	3.79078043	-0.41096327
6	2.12757674	3.16717975	-0.93634561
6	1.30315138	2.42025955	-0.03538613
6	1.57633678	2.44570186	1.36997831
6	2.75362122	3.07664905	1.82939291
6	0.62125291	1.92679382	2.36847695
7	-0.25028048	0.91427257	2.05400291
6	-1.16887610	0.45679964	2.96428578
6	-1.20559786	1.01033109	4.25506778
6	-0.32257154	2.02740121	4.59515297
6	0.58237653	2.49870912	3.65243840
6	-2.15498046	-0.57195287	2.58639711
6	-2.65289447	-0.67273000	1.24796184
6	-3.80843221	-1.47358241	0.97714974
6	-4.31969153	-2.24388323	2.02419676
6	-3.76242892	-2.24004389	3.31116774
6	-2.70570255	-1.39286020	3.59322584
8	0.27059831	1.72344542	-0.51631194
8	-2.05913165	-0.00305606	0.25688116

1	-1.96511787	0.67749334	4.95713544
1	-0.36765898	2.48307233	5.58500577
1	1.22925194	3.34068597	3.88198954
1	3.01168013	3.02852814	2.88720773
6	1.78450178	3.26854324	-2.43638577
1	-2.27633939	-1.37592767	4.59514643
1	-5.17731055	-2.88784056	1.83780650
6	-4.45824439	-1.49311803	-0.42124109
1	3.92287048	4.33792337	-1.07946952
6	-4.84639154	-0.05548287	-0.84283513
6	-5.74807021	-2.33561608	-0.43833203
6	-3.49142303	-2.10694896	-1.46133412
1	-5.56676197	0.37444773	-0.13145625
1	-5.32418880	-0.07877758	-1.83381971
1	-3.97216438	0.60161293	-0.89544517
1	-3.26329810	-3.15237644	-1.20358418
1	-2.55067801	-1.55036732	-1.52819226
1	-3.96720503	-2.10476333	-2.45394001
1	-6.18998265	-2.28819054	-1.44362715
1	-6.49822475	-1.95816826	0.27174640
1	-5.55778633	-3.39541945	-0.21447243
6	1.86450329	1.87654083	-3.10648174
6	2.76465837	4.19391346	-3.18269126
6	0.36749706	3.86460528	-2.61501068
1	3.79515073	3.81010010	-3.16512987
1	2.76491318	5.21465978	-2.77327155
1	2.45790444	4.26016414	-4.23606886
1	2.87946708	1.46361027	-3.01116460
1	1.63624595	1.97165036	-4.17923151
1	1.16108015	1.16466384	-2.66332967
1	0.13411625	3.94539979	-3.68737303
1	0.31541429	4.87430940	-2.18174229
1	-0.39731471	3.24072027	-2.14100607
1	-4.16961667	-2.89128938	4.08436022
1	4.51850853	4.18853032	1.30556418
8	2.38228722	-1.33555245	-1.23183905
6	0.99540837	-3.23308244	-0.56085990
8	2.25792932	-3.89780504	-0.24518281
6	3.32740440	-3.56330895	-1.02908842
6	3.06162807	-2.38273953	-1.96634087
8	4.37545783	-4.15971929	-0.92414671
6	4.33681054	-1.79757784	-2.54039568
6	-0.03469458	-3.71892284	0.43984884
1	0.69058496	-3.52916302	-1.57864745
1	2.41027614	-2.73249315	-2.79068913
1	4.09269937	-0.96544367	-3.21173993
1	4.87759799	-2.56958278	-3.10032879
1	4.98950860	-1.43590844	-1.73641750
1	-1.00589611	-3.25890679	0.22223686
1	0.25769625	-3.46277921	1.46526654
1	-0.13629816	-4.80847580	0.36288442
8	0.07627783	-1.08151889	-1.09720250
8	1.20371543	-1.08845932	0.77100231
6	2.40125259	-1.13686098	1.57991977

1	2.18673126	-0.55398166	2.48193404
1	2.62270632	-2.17568394	1.85439245
1	3.24269449	-0.69280634	1.03559156
13	-0.27877912	0.18939190	0.20081014
6	1.16230869	-1.69994561	-0.61509693

Electronic energy = -2064.595419 a.u.
DFT-D4 dispersion correction = -0.126822 a.u.
Thermal free energy = 0.556319 a.u.
Gibbs free energy = -2064.165922 a.u.
Number of imaginary frequencies = 0.

4b_{LA}

Atomic N.	X	Y	Z
6	1.06267769	2.11655396	-5.06795579
6	0.05587205	1.14753253	-5.17412619
6	-0.61480172	0.63470700	-4.06148188
6	-0.21850216	1.10865539	-2.76973434
6	0.69275026	2.20917843	-2.66711739
6	1.35298237	2.66089759	-3.82997489
6	0.87174612	2.97137574	-1.41452007
7	0.65192667	2.38288428	-0.19821697
6	0.72865993	3.09033170	0.97122347
6	1.06233417	4.45536922	0.92799475
6	1.31587634	5.06551461	-0.29378623
6	1.21228095	4.33330067	-1.47014167
6	0.41235002	2.45394478	2.26595903
6	-0.49506531	1.35122736	2.38748449
6	-1.00950207	0.99854536	3.67619481
6	-0.46399118	1.63771137	4.79158881
6	0.53517959	2.61416957	4.68905129
6	0.94560133	3.03392122	3.43745291
8	-0.72646908	0.53088913	-1.67341474
8	-0.89255904	0.66037075	1.30819794
1	1.06891981	5.03651030	1.84552250
1	1.55439751	6.12904358	-0.33284196
1	1.33733524	4.81786717	-2.43419131
1	2.11852636	3.43181139	-3.74559852
6	-1.75028154	-0.39681899	-4.22502002
1	1.71111927	3.80451786	3.35195553
1	-0.81199757	1.35970637	5.78457444
6	-2.12508572	-0.05421842	3.83881085
1	-0.19852330	0.77543509	-6.16481596
6	-3.36063476	0.35413213	3.00123347
6	-2.58936776	-0.17766614	5.30265502
6	-1.62118079	-1.44570199	3.39631612
1	-3.75353467	1.32360882	3.34078287
1	-4.15714483	-0.39484308	3.12706404
1	-3.12061228	0.43036988	1.93532705
1	-0.75927758	-1.75953758	4.00280162
1	-1.31631327	-1.43548912	2.34658097
1	-2.42048994	-2.19154319	3.52633345
1	-3.40839675	-0.90900339	5.35456930
1	-2.97044082	0.77512998	5.69778740

1	-1.78862112	-0.53539223	5.96596846
6	-1.35768027	-1.75301827	-3.59651625
6	-2.07820781	-0.65702524	-5.70761335
6	-3.04068847	0.13989373	-3.55940435
1	-1.23267107	-1.10435182	-6.24999035
1	-2.38204736	0.26102427	-6.23093930
1	-2.91675456	-1.36527649	-5.76727270
1	-0.47760547	-2.17397979	-4.10466292
1	-2.18584229	-2.46931244	-3.70908419
1	-1.12881775	-1.64448494	-2.53181612
1	-3.85489019	-0.58882760	-3.69025128
1	-3.35361568	1.08282211	-4.03090531
1	-2.90146463	0.31610763	-2.48735929
1	0.97026222	3.04953511	5.58843438
1	1.59535781	2.45200852	-5.95755770
8	0.26549966	-1.64368671	-0.15652616
6	-0.42880716	-2.88216909	0.10862875
1	-0.27785523	-3.18878014	1.15032301
1	-1.48963636	-2.67899902	-0.07169124
1	-0.07759023	-3.66707851	-0.57445684
13	0.15673994	0.49296839	-0.12254407
8	1.84010688	-0.14621349	0.07750274
8	1.79143480	-1.93086636	1.56465772
6	1.68761296	-1.48648415	0.22247284
6	2.66613912	-2.25634260	-0.69115535
8	2.72731491	-3.67176781	-0.33726009
6	3.00047884	-3.94818124	0.97445228
6	2.96142296	-2.71818397	1.88604688
8	3.21237967	-5.08528488	1.33113691
6	2.88417289	-3.08490410	3.35520224
6	2.34909880	-2.16637129	-2.17015577
1	3.65486302	-1.80771961	-0.49873765
1	3.87313044	-2.11716579	1.70168625
1	2.85799799	-2.17189042	3.96241293
1	3.75963324	-3.68280709	3.63460655
1	1.98426708	-3.67928543	3.55563941
1	2.30865971	-1.11293198	-2.47347895
1	1.38522499	-2.63562390	-2.39767621
1	3.13463415	-2.67034471	-2.74664013

Electronic energy = -2064.600190 a.u.

DFT-D4 dispersion correction = -0.125542 a.u.

Thermal free energy = 0.557182 a.u.

Gibbs free energy = -2064.168550 a.u.

Number of imaginary frequencies = 0.

5_{LA}

Atomic N.	X	Y	Z
6	-4.89983047	0.08335799	-1.48794144
6	-4.76831245	-1.04378945	-0.66718658
6	-3.64042203	-1.26780987	0.12507641
6	-2.58994549	-0.29904343	0.07849867
6	-2.75613872	0.90590495	-0.68172629
6	-3.91048799	1.04881038	-1.48347444

6	-1.82482396	2.05155590	-0.60800961
7	-0.52328598	1.87901654	-0.21085578
6	0.33180241	2.93439385	-0.01540939
6	-0.10752258	4.23236349	-0.30712801
6	-1.40651547	4.43002798	-0.76271391
6	-2.27286076	3.35235681	-0.89267638
6	1.68001099	2.71059430	0.54805541
6	1.96271924	1.66049791	1.48368305
6	3.22249496	1.62634657	2.15679247
6	4.17679838	2.58148284	1.79648822
6	3.93952676	3.55812392	0.82053916
6	2.69791180	3.62919874	0.21521915
8	-1.46893748	-0.53473206	0.78041615
8	1.04100900	0.71497707	1.75035016
1	0.55100825	5.07658356	-0.12237073
1	-1.76158152	5.43928615	-0.97325806
1	-3.30994148	3.51662454	-1.16839309
1	-4.00155188	1.91035203	-2.14285461
6	-3.53511414	-2.52520614	1.01372206
1	2.50953347	4.37978302	-0.55209794
1	5.15392213	2.56036807	2.27517765
6	3.53058934	0.55966842	3.22750695
1	-5.57157368	-1.77776677	-0.66774251
6	2.49000405	0.63315660	4.37035734
6	4.91823301	0.77315691	3.86246191
6	3.52998463	-0.85188787	2.59372225
1	2.51891719	1.61961114	4.85593914
1	2.72619633	-0.12433302	5.13288890
1	1.47314554	0.45371120	4.00634040
1	4.28495566	-0.91879734	1.79721254
1	2.55537714	-1.10537803	2.16452748
1	3.77732478	-1.60101494	3.36118847
1	5.07610219	0.00824464	4.63575066
1	5.00462479	1.75645739	4.34724646
1	5.73253598	0.67183246	3.13042297
6	-2.35826550	-3.41759465	0.55402554
6	-4.81217588	-3.38448071	0.93905917
6	-3.34831241	-2.11654128	2.49470524
1	-4.99585315	-3.77181443	-0.07364811
1	-5.70362006	-2.83126501	1.26829251
1	-4.69656630	-4.25064648	1.60563427
1	-2.49486492	-3.72852241	-0.49200969
1	-2.31701518	-4.32468746	1.17595196
1	-1.39904239	-2.89725943	0.63731541
1	-3.28955264	-3.01881663	3.12192641
1	-4.20526925	-1.52080943	2.84143610
1	-2.43495353	-1.53155547	2.64405220
1	4.72898063	4.25618051	0.54286114
1	-5.77384472	0.19452651	-2.12931015
8	1.73723506	-2.34256401	-2.21480322
6	1.36623077	-3.39361658	-1.30822434
1	0.28275982	-3.58196383	-1.34135568
8	1.21847914	-0.72422294	-0.65071282
8	-0.29345229	-1.14839292	-2.27812534

1	1.90305793	-4.28347889	-1.65527158
1	1.67040711	-3.15335743	-0.28005170
13	0.09183806	0.15998526	0.35934261
8	0.97453726	0.97883733	-3.31987632
6	-0.24191376	0.63427621	-3.84572752
6	-0.58084333	-0.84843347	-3.66284656
6	1.11954969	-1.09524864	-1.96156672
6	1.84618479	-0.13458235	-2.95367607
8	-0.96228218	1.47936862	-4.33170111
6	3.13241308	0.44714901	-2.40649886
6	-2.03073698	-1.17426364	-3.95657478
1	0.07310380	-1.45544356	-4.31713627
1	2.05792320	-0.71495985	-3.86425791
1	3.60666746	1.08019986	-3.16730052
1	3.81898838	-0.36864626	-2.14735188
1	2.94274547	1.04207902	-1.50606834
1	-2.26500623	-0.90843041	-4.99490065
1	-2.70020619	-0.61052089	-3.29707845
1	-2.20320672	-2.24856976	-3.81427323

Electronic energy = -2064.600435 a.u.

DFT-D4 dispersion correction = -0.128195 a.u.

Thermal free energy = 0.557027 a.u.

Gibbs free energy = -2064.171602 a.u.

Number of imaginary frequencies = 0.

6a_{LA}

Atomic N.	X	Y	Z
6	2.32432571	4.06948468	-2.24535300
6	2.04728945	3.16375728	-3.27894315
6	1.19923886	2.06681134	-3.11199062
6	0.62532756	1.86371979	-1.81597116
6	0.78906846	2.85997512	-0.79976440
6	1.67878076	3.93288354	-1.02987679
6	-0.02432616	2.86973469	0.43338708
7	-0.52573420	1.70566707	0.95813950
6	-1.32927828	1.71211963	2.06959154
6	-1.62337160	2.92997876	2.70674427
6	-1.10901132	4.11648073	2.20030602
6	-0.32102177	4.09437922	1.05609815
6	-1.93079357	0.46340704	2.57191197
6	-2.25323992	-0.61977114	1.69238980
6	-3.11263455	-1.67180709	2.14524153
6	-3.47231389	-1.67549047	3.49450519
6	-3.04984443	-0.68601862	4.39457587
6	-2.30962032	0.38575463	3.92963384
8	-0.07477757	0.75166813	-1.57688546
8	-1.78016667	-0.64040285	0.44447394
1	-2.29779788	2.93855058	3.55840840
1	-1.35708814	5.06673298	2.67442922
1	0.02711524	5.02098518	0.60870128
1	1.87891479	4.64609436	-0.23039054
6	0.88832723	1.11259283	-4.28396522
1	-1.99353851	1.16634887	4.62179062

1	-4.09462696	-2.48371702	3.87451320
6	-3.61993767	-2.76171870	1.17944770
1	2.52861878	3.32033899	-4.24244447
6	-4.36130371	-2.10434497	-0.00966624
6	-4.61736625	-3.71285551	1.86793155
6	-2.44520303	-3.62261549	0.65921473
1	-5.22407636	-1.52306607	0.34738426
1	-4.73813814	-2.88596308	-0.68629855
1	-3.70379297	-1.44006444	-0.58014508
1	-1.95011693	-4.14083324	1.49424480
1	-1.69990100	-3.02165500	0.12755839
1	-2.82721867	-4.39095417	-0.03010873
1	-4.97718640	-4.44467125	1.13101972
1	-5.49482655	-3.17871038	2.26050523
1	-4.15554761	-4.27752054	2.69094404
6	1.42627484	-0.30950117	-4.00038622
6	1.53694882	1.59394754	-5.59591258
6	-0.64037075	1.05857728	-4.51990905
1	2.63528947	1.60105019	-5.54041685
1	1.19543966	2.59931235	-5.88166950
1	1.25441103	0.90617018	-6.40528244
1	2.51757542	-0.28915942	-3.85948776
1	1.21406312	-0.96259858	-4.86044265
1	0.96080246	-0.75058956	-3.11242584
1	-0.86019753	0.38854491	-5.36460105
1	-1.02798289	2.05650000	-4.77165071
1	-1.17340603	0.68827867	-3.63773725
1	-3.31816521	-0.75599880	5.44852728
1	3.03143895	4.88282076	-2.40610225
8	2.28715910	-2.35575600	1.33157910
6	1.23233551	-2.84842328	2.18429898
1	0.76027995	-2.02752210	2.74480599
8	0.70110813	-1.64553977	-0.21944377
8	1.60675965	-0.06369144	1.00704332
1	1.72471668	-3.53320438	2.88233805
1	0.47456117	-3.37770422	1.59527840
13	-0.15349047	-0.01480449	0.03302664
8	4.22980507	-0.68361653	0.14578412
6	4.09111311	0.24410745	1.12247430
6	2.69406176	0.72290935	1.55867058
6	1.89088472	-1.45479617	0.36252627
6	3.06803823	-1.19701898	-0.58398363
8	5.07694750	0.71824698	1.64683764
6	3.52425857	-2.43772448	-1.32551459
6	2.59082318	0.78246912	3.08013648
1	2.59196933	1.73562987	1.13526142
1	2.74261596	-0.41828758	-1.28913205
1	4.33623866	-2.18179487	-2.01749032
1	2.68483859	-2.84763207	-1.90161838
1	3.87904159	-3.19620489	-0.61777056
1	3.39094953	1.41755965	3.47671289
1	2.69086809	-0.22068608	3.51351952
1	1.61878921	1.20084516	3.37086804

Electronic energy = -2064.595907 a.u.

DFT-D4 dispersion correction = -0.128702 a.u.
 Thermal free energy = 0.555737 a.u.
 Gibbs free energy = -2064.168872 a.u.
 Number of imaginary frequencies = 0.

6b_{LA}

Atomic N.	X	Y	Z
6	3.78399970	2.99302359	-2.57500119
6	3.42391372	1.87068081	-3.33284159
6	2.34931049	1.04616840	-2.99262936
6	1.62806510	1.35567021	-1.79503078
6	1.86693123	2.60380972	-1.13048121
6	2.98904513	3.37312811	-1.50990560
6	0.91054693	3.19053646	-0.17014564
7	0.04809685	2.39717237	0.53822390
6	-0.92658027	2.92117061	1.34525977
6	-1.02201023	4.31594103	1.48545277
6	-0.13126875	5.13952133	0.80783857
6	0.82660307	4.58690567	-0.03247976
6	-1.91459722	2.04520838	2.00925087
6	-2.28044906	0.75873135	1.49334121
6	-3.48245147	0.12781781	1.94887031
6	-4.14666616	0.70474108	3.03353268
6	-3.69681373	1.87647313	3.65628969
6	-2.61262891	2.55215549	3.12740239
8	0.72056752	0.48286910	-1.33149460
8	-1.52674150	0.13826466	0.57408642
1	-1.82335241	4.74554879	2.07912775
1	-0.21415643	6.22302490	0.90026235
1	1.47163588	5.22707154	-0.62698814
1	3.24287222	4.26625166	-0.93986328
6	1.94957442	-0.14203513	-3.89236497
1	-2.27704066	3.47767661	3.59384457
1	-5.04072042	0.22337937	3.42509191
6	-4.03669972	-1.14025644	1.26531117
1	4.01760188	1.63083841	-4.21280626
6	-4.23702745	-0.87389695	-0.24617121
6	-5.40707958	-1.54694655	1.84010689
6	-3.08085669	-2.33730620	1.46745198
1	-4.94940314	-0.05068443	-0.40143895
1	-4.65093607	-1.77246507	-0.72783751
1	-3.29539923	-0.61712412	-0.74318865
1	-2.97815856	-2.57806867	2.53586441
1	-2.08889531	-2.12201319	1.05742763
1	-3.48343973	-3.22730088	0.96039744
1	-5.77540972	-2.42566775	1.29212243
1	-6.15507700	-0.74888287	1.72850927
1	-5.34896939	-1.82508310	2.90234835
6	2.18036839	-1.48572378	-3.16792944
6	2.77220050	-0.17481550	-5.19463210
6	0.46093775	-0.00956914	-4.29525466
1	3.84303103	-0.34091401	-5.00825124
1	2.65835218	0.74955854	-5.77906965

1	2.41650339	-1.00732608	-5.81794530
1	3.24397830	-1.62030179	-2.92303869
1	1.87719659	-2.31906393	-3.81992118
1	1.59656424	-1.53738028	-2.24359160
1	0.18094662	-0.84528604	-4.95393649
1	0.29211206	0.92612471	-4.84784821
1	-0.19936481	-0.02218565	-3.42134110
1	-4.21345373	2.26291681	4.53448382
1	4.66478516	3.57584014	-2.84334214
8	1.28146381	-1.58801371	3.13224433
6	0.04717625	-1.08494740	3.67571066
1	-0.80715340	-1.32251027	3.02565875
8	1.41696669	0.23904330	1.68834423
8	0.81027626	-1.68597817	0.79364924
1	-0.07387769	-1.59597132	4.63683286
1	0.10315859	0.00023359	3.83242823
13	0.21120123	0.46848026	0.37370144
6	1.63804811	-1.08786165	1.87103185
6	3.08762373	-1.54755821	1.63591188
8	3.16176785	-3.00857715	1.51884811
6	2.10917714	-3.77521735	1.13980773
6	0.75004508	-3.13087019	0.83045149
8	2.24045652	-4.98044493	1.07632639
6	0.18573859	-3.64615697	-0.48646336
6	3.75541759	-0.91198330	0.43139532
1	3.65405761	-1.32992103	2.55193643
1	0.08880637	-3.43167740	1.66114278
1	-0.79586489	-3.19405397	-0.67602898
1	0.07583823	-4.73441515	-0.42294487
1	0.85542065	-3.40961339	-1.32198559
1	3.84327295	0.17113568	0.58214406
1	3.18046754	-1.09594405	-0.48423196
1	4.76042221	-1.33510044	0.30896093

Electronic energy = -2064.596855 a.u.

DFT-D4 dispersion correction = -0.128658 a.u.

Thermal free energy = 0.557821 a.u.

Gibbs free energy = -2064.167691 a.u.

Number of imaginary frequencies = 0.

TS2ax_{LA}

Atomic N.	X	Y	Z
6	2.28920364	4.09755325	-2.33839083
6	2.01080942	3.16643906	-3.34893966
6	1.19205606	2.05394983	-3.14295340
6	0.65450275	1.86101270	-1.82954025
6	0.80504757	2.88683796	-0.84239364
6	1.66692185	3.97338676	-1.10944855
6	-0.00896756	2.91150832	0.38921782
7	-0.49372315	1.75205672	0.93800122
6	-1.30324709	1.77671051	2.04467583
6	-1.62984526	3.00716591	2.64155531
6	-1.13004994	4.18867254	2.11007190
6	-0.32845357	4.14818478	0.97674829

6	-1.88781691	0.53529835	2.58674812
6	-2.17396212	-0.59095699	1.75118136
6	-3.05453110	-1.61821806	2.22129464
6	-3.44604683	-1.56982601	3.56082678
6	-3.03956628	-0.54818338	4.43125010
6	-2.29536486	0.50828487	3.93827081
8	0.00163276	0.73139262	-1.54707098
8	-1.64990246	-0.68128061	0.52729809
1	-2.31543779	3.02800822	3.48386145
1	-1.39967811	5.14676332	2.55582380
1	0.01177567	5.06750631	0.50888729
1	1.86268890	4.70860672	-0.32909402
6	0.87275231	1.07405818	-4.29085779
1	-1.99943149	1.31802261	4.60520840
1	-4.08190107	-2.35981846	3.95635438
6	-3.56200957	-2.73060894	1.28094423
1	2.46688294	3.31586862	-4.32585049
6	-4.27272129	-2.09514093	0.06163633
6	-4.58535671	-3.64490938	1.98105848
6	-2.39620829	-3.62499261	0.80093831
1	-5.13175821	-1.49044049	0.38706386
1	-4.64997816	-2.88834190	-0.60122091
1	-3.59387708	-1.45740366	-0.51463872
1	-1.90984714	-4.11413145	1.65845776
1	-1.64635670	-3.04948235	0.24809176
1	-2.78416038	-4.41600275	0.14108457
1	-4.94573879	-4.39258432	1.26046050
1	-5.45991993	-3.08558273	2.34357095
1	-4.14533663	-4.19153643	2.82790399
6	1.45308447	-0.32922363	-3.99994254
6	1.47149622	1.55035067	-5.62802935
6	-0.66017085	0.97842246	-4.48124743
1	2.57057118	1.58301485	-5.60487938
1	1.09906065	2.54357600	-5.91754007
1	1.18134511	0.84453821	-6.41905022
1	2.54652333	-0.27834573	-3.88649654
1	1.23627198	-1.00131619	-4.84428072
1	1.01989305	-0.76549715	-3.09342480
1	-0.88768923	0.28856361	-5.30779791
1	-1.07987618	1.96201980	-4.73784828
1	-1.15753961	0.61015815	-3.57752109
1	-3.32793021	-0.57800800	5.48179579
1	2.97572517	4.92210293	-2.52865624
8	2.29893017	-2.59502339	1.07032514
6	1.23375750	-3.30799365	1.74433017
1	0.61769509	-2.61045241	2.32719922
8	0.75274670	-1.69411993	-0.37670037
8	1.50385380	-0.16911867	1.14767528
1	1.74188542	-4.01185989	2.41028690
1	0.60993946	-3.83861470	1.01736212
13	-0.05382108	-0.00624025	0.08333153
8	4.16444540	-0.61743242	0.35697949
6	3.93203521	0.25088722	1.38159764
6	2.49423146	0.65707624	1.76307917

6	1.91233623	-1.63447368	0.20513333
6	3.11509395	-1.06946433	-0.54925013
8	4.87926626	0.70285952	1.98855233
6	3.75560904	-2.10347152	-1.46189237
6	2.33358932	0.65107805	3.28366923
1	2.38243437	1.68999767	1.38634360
1	2.75515056	-0.20967530	-1.13215804
1	4.57730818	-1.64206111	-2.02341557
1	3.01233792	-2.48445964	-2.17385507
1	4.15041828	-2.93820786	-0.87031966
1	3.09726739	1.28780901	3.74410820
1	2.44272161	-0.36943141	3.67365599
1	1.33692396	1.02419055	3.55079341

Electronic energy = -2064.595288 a.u.

DFT-D4 dispersion correction = -0.128456 a.u.

Thermal free energy = 0.557322 a.u.

Gibbs free energy = -2064.166421 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 76.1i

TS2eq_{LA}

Atomic N.	X	Y	Z
6	2.48505473	4.63582325	-1.32526207
6	1.92371166	4.09930277	-2.49185300
6	1.03842020	3.01964927	-2.46883225
6	0.71350139	2.45391059	-1.19487548
6	1.19245231	3.06366801	0.00732224
6	2.11039519	4.13205528	-0.09257516
6	0.71855223	2.66572523	1.34844398
7	0.19781043	1.41722786	1.58215368
6	-0.25898334	1.05437207	2.82018161
6	-0.17297611	1.95966911	3.89075279
6	0.34869364	3.22836113	3.67538595
6	0.77569318	3.59140921	2.40468621
6	-0.92333382	-0.24490681	3.02842855
6	-1.70436275	-0.84981996	1.99072969
6	-2.70895696	-1.80944228	2.34493470
6	-2.68552804	-2.31081724	3.64866328
6	-1.77588522	-1.86610329	4.61941338
6	-0.93829095	-0.80597508	4.32348442
8	-0.04751440	1.35711479	-1.14832187
8	-1.52394855	-0.49550730	0.71406317
1	-0.57811368	1.68188727	4.85983324
1	0.38435167	3.95153093	4.49096918
1	1.11905253	4.60338163	2.21160889
1	2.55659819	4.54526758	0.81107080
6	0.44741365	2.44510221	-3.77275729
1	-0.27160615	-0.40576521	5.08777761
1	-3.39876795	-3.08350515	3.92955351
6	-3.80821419	-2.23874617	1.35090458
1	2.20793629	4.53416586	-3.44829011
6	-4.55007172	-0.97745627	0.84571499
6	-4.85400295	-3.15175390	2.01879787

6	-3.22426915	-3.00809765	0.14764091
1	-5.02310896	-0.44394049	1.68282223
1	-5.34249449	-1.27110791	0.14100780
1	-3.86978650	-0.28903952	0.33128130
1	-2.67266893	-3.90033126	0.47894385
1	-2.55293822	-2.37267804	-0.43680558
1	-4.04001617	-3.34308076	-0.51074839
1	-5.64377308	-3.37903976	1.28897905
1	-5.33079624	-2.67111707	2.88507009
1	-4.42363310	-4.11015177	2.34396625
6	0.93947303	0.99526376	-3.99717903
6	0.87322217	3.26925015	-5.00296021
6	-1.09876084	2.47770691	-3.71623635
1	1.96133614	3.25102282	-5.16165018
1	0.54874396	4.31755543	-4.93114519
1	0.40475091	2.83822942	-5.89895296
1	2.03510594	0.97105354	-4.09918499
1	0.51031554	0.59900266	-4.93003082
1	0.65033841	0.33259630	-3.17467403
1	-1.51039803	2.08260083	-4.65717745
1	-1.45882571	3.51025820	-3.59815240
1	-1.48762655	1.87594962	-2.88838434
1	-1.76259744	-2.32476687	5.60781574
1	3.20763350	5.44922495	-1.39062071
8	3.89751649	-1.01277816	-0.50103486
6	4.25988293	0.23525551	-1.15820742
1	3.39898133	0.62149435	-1.71570098
8	2.36229348	0.13267186	0.70291656
8	0.75836790	-1.30541801	-0.72078502
1	5.07808161	-0.03069551	-1.83250928
1	4.58196211	0.97242302	-0.41425484
13	0.07079893	0.11255941	0.11120640
6	2.89112687	-0.93351555	0.36457300
6	2.56368518	-2.27691340	1.01742554
8	2.57481313	-3.36536860	0.07278560
6	1.53137529	-3.61910868	-0.79866761
6	0.33831015	-2.63797235	-0.88651991
8	1.59816206	-4.63761759	-1.44932663
6	-0.37383318	-2.83614254	-2.22659230
6	3.60543013	-2.61678934	2.08327603
1	1.57389641	-2.17166972	1.48118174
1	-0.35019079	-2.94310355	-0.07095945
1	-1.23695743	-2.16039920	-2.27903724
1	-0.71410584	-3.87137866	-2.34521842
1	0.31075180	-2.59699559	-3.05077171
1	3.66052556	-1.81465149	2.83166480
1	4.59204674	-2.75132060	1.62301779
1	3.31877255	-3.54875565	2.58580661

Electronic energy = -2064.587912 a.u.

DFT-D4 dispersion correction = -0.126055 a.u.

Thermal free energy = 0.554754 a.u.

Gibbs free energy = -2064.159213 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 99.4i

7a_{LA}

Atomic N.	X	Y	Z
6	2.74784159	3.17147260	-3.69927508
6	2.49411169	1.90889404	-4.24915593
6	1.62297913	0.99162174	-3.65650934
6	0.98526059	1.37086221	-2.43072847
6	1.13603146	2.70377819	-1.94158176
6	2.05717659	3.56885261	-2.56833671
6	0.28277229	3.24736794	-0.86692736
7	-0.24576292	2.43594932	0.10349058
6	-1.04865996	2.95945955	1.08398615
6	-1.36261094	4.33083619	1.07953579
6	-0.84297099	5.15931730	0.09593762
6	-0.01911368	4.62020599	-0.88210927
6	-1.63339461	2.10650059	2.13626080
6	-1.91943272	0.72344881	1.92691107
6	-2.74672972	0.01971722	2.86066509
6	-3.10905141	0.68392132	4.03422206
6	-2.71370659	1.99891602	4.31045173
6	-2.00454308	2.70787459	3.35884795
8	0.23344602	0.48435607	-1.76872143
8	-1.44084025	0.08221771	0.85476870
1	-2.05444814	4.72165572	1.81981624
1	-1.10709611	6.21721590	0.07155659
1	0.35242453	5.23891044	-1.69384847
1	2.24581006	4.55249191	-2.13893165
6	1.38640443	-0.39152481	-4.29640793
1	-1.69991256	3.73294556	3.56750155
1	-3.70382991	0.15875381	4.77891419
6	-3.21559817	-1.42627406	2.59875148
1	3.01456600	1.63235151	-5.16417387
6	-3.96675385	-1.50225259	1.24811749
6	-4.18648537	-1.92021643	3.68842227
6	-2.00668662	-2.38869639	2.58856483
1	-4.85578770	-0.85476868	1.26202927
1	-4.30659664	-2.53461791	1.07151012
1	-3.32675526	-1.19628995	0.41330870
1	-1.45769117	-2.34457794	3.53929724
1	-1.31359079	-2.13267686	1.78263121
1	-2.35591469	-3.42305934	2.44170655
1	-4.52278276	-2.93468781	3.43056008
1	-5.08021656	-1.28424564	3.76658634
1	-3.70827523	-1.97555420	4.67680971
6	1.97195403	-1.49481490	-3.38544508
6	2.07079452	-0.51829614	-5.67083170
6	-0.12584054	-0.63189318	-4.51719364
1	3.16541509	-0.44110915	-5.60239680
1	1.71211363	0.24075906	-6.38075097
1	1.83834400	-1.50572722	-6.09494677
1	3.05698918	-1.36193463	-3.26458283
1	1.79744024	-2.48637865	-3.83204254
1	1.50277053	-1.46060925	-2.39784109

1	-0.28049459	-1.61704189	-4.98410341
1	-0.54113768	0.12807903	-5.19495690
1	-0.68231648	-0.59647122	-3.57463721
1	-2.97142748	2.45915413	5.26409796
1	3.47442468	3.83641975	-4.16586108
8	0.67469011	-3.82731516	-0.42388622
6	-0.55501532	-4.03527073	-1.18008769
1	-0.54178293	-3.42043070	-2.08723122
8	0.11153261	-1.66338459	-0.27534646
8	1.67786190	0.40370483	0.79502130
1	-0.55717386	-5.10111389	-1.42183218
1	-1.41855043	-3.76488851	-0.56192039
13	0.10082248	0.45135773	0.02201167
8	1.69822180	-2.21364080	2.17889561
6	1.71908894	-0.98259650	2.81762434
6	2.27533195	0.23899009	2.05160612
6	0.89641522	-2.57838738	-0.01689782
6	2.17087172	-2.41223689	0.81743496
8	1.31419742	-0.95509214	3.95683524
6	3.10576407	-3.60872101	0.80807906
6	2.18518116	1.48921529	2.92541013
1	3.35452308	0.02094895	1.89057975
1	2.66046315	-1.50580791	0.43936535
1	3.99157298	-3.37677565	1.41299596
1	3.43226366	-3.83206899	-0.21643408
1	2.61695670	-4.49760178	1.22327188
1	2.76400017	1.36591990	3.84985578
1	1.14350675	1.69492688	3.20230235
1	2.58664159	2.33968098	2.35938446

Electronic energy = -2064.601483 a.u.

DFT-D4 dispersion correction = -0.127041 a.u.

Thermal free energy = 0.554962 a.u.

Gibbs free energy = -2064.173563 a.u.

Number of imaginary frequencies = 0.

8_{LA} (ax_chelate)

Atomic N.	X	Y	Z
6	-4.21802470	3.48473230	-2.07913847
6	-4.58754948	2.80351461	-0.91212095
6	-3.66047408	2.14862138	-0.09799986
6	-2.28610484	2.16761034	-0.50170071
6	-1.88755618	2.97238328	-1.61597675
6	-2.87860977	3.58580379	-2.41055647
6	-0.47067027	3.27111688	-1.90641194
7	0.51998830	2.39688163	-1.55002367
6	1.83767351	2.68599549	-1.77856522
6	2.18829130	3.90307310	-2.38906602
6	1.19557181	4.79914965	-2.76268689
6	-0.13636921	4.49240651	-2.51659053
6	2.90411718	1.76104097	-1.34574551
6	2.74782266	0.88894919	-0.22207030
6	3.89707731	0.24240820	0.33776841
6	5.10985631	0.36563583	-0.34383954

6	5.23888952	1.10861014	-1.52479980
6	4.15126253	1.81729783	-2.00306873
8	-1.38719759	1.44938295	0.18015387
8	1.54650546	0.68542151	0.32709798
1	3.23686463	4.15639367	-2.51681308
1	1.46293963	5.75601942	-3.21279095
1	-0.91968103	5.20959599	-2.74499049
1	-2.58498281	4.12133417	-3.31308674
6	-4.10960109	1.42841038	1.19020946
1	4.24993124	2.40570120	-2.91501187
1	5.99063396	-0.14459769	0.04185490
6	3.80264512	-0.56493363	1.64854640
1	-5.64252721	2.77472375	-0.64581888
6	3.26029904	0.33650371	2.78334233
6	5.17958235	-1.08856100	2.09945661
6	2.87955283	-1.79231637	1.46803070
1	3.93685596	1.18592696	2.95699719
1	3.19638515	-0.24087426	3.71828264
1	2.26413508	0.72548546	2.54699797
1	3.25552709	-2.44294423	0.66393186
1	1.85707495	-1.48746473	1.22479744
1	2.85763806	-2.37756474	2.40085294
1	5.06236342	-1.62211461	3.05352784
1	5.89866943	-0.27298876	2.26260519
1	5.61382803	-1.79587776	1.37764526
6	-3.85251543	-0.09329101	1.08348586
6	-5.61416169	1.62038411	1.46009536
6	-3.34722674	2.00401552	2.40740546
1	-6.23970330	1.17624786	0.67204379
1	-5.88324438	2.68158519	1.56115941
1	-5.87266189	1.12194064	2.40526265
1	-4.38241812	-0.51557238	0.21620188
1	-4.22593358	-0.59586777	1.98949616
1	-2.78260685	-0.30175731	0.98438720
1	-3.67043334	1.49066024	3.32593006
1	-3.56499650	3.07542336	2.52572421
1	-2.26450716	1.87740900	2.30083437
1	6.19250095	1.13790681	-2.05176791
1	-4.97978701	3.94035324	-2.71160649
8	0.62825945	-4.63187155	0.51328542
6	1.72161134	-5.47971584	0.95695246
1	1.35229316	-6.48963655	1.17163701
8	-0.40935879	-5.02502601	2.50243472
8	-0.16721913	-0.20432957	-2.15731573
1	2.43098648	-5.48928350	0.12489026
1	2.18178271	-5.05910903	1.85862889
13	0.03181778	0.70603090	-0.63356725
8	-1.27997956	-3.14532131	-0.45876851
6	-0.77810697	-1.93421507	-0.67441118
6	-0.56864720	-1.53595241	-2.12965477
6	-0.37055320	-4.49527341	1.40929200
6	-1.49495311	-3.57270742	0.92604751
8	-0.49870629	-1.12959448	0.22870811
6	-2.85033662	-4.26306498	0.99083911

6	0.45008972	-2.46972271	-2.80703884
1	-1.55054181	-1.66617505	-2.63213970
1	-1.47226079	-2.68396762	1.57233318
1	-3.64727147	-3.54725787	0.75579149
1	-3.00484653	-4.65226191	2.00399560
1	-2.89619881	-5.09777884	0.27937056
1	0.10634646	-3.51260370	-2.80114368
1	1.42055204	-2.40180663	-2.29747493
1	0.58030255	-2.13868546	-3.84456938

Electronic energy = -2064.627388 a.u.

DFT-D4 dispersion correction = -0.121247 a.u.

Thermal free energy = 0.552513 a.u.

Gibbs free energy = -2064.196122 a.u.

Number of imaginary frequencies = 0.

8_{LA} (eq_chelate)

Atomic N.	X	Y	Z
6	4.33730758	-1.86551194	-2.68120381
6	3.61693658	-1.24439910	-3.71280691
6	2.59073899	-0.32770064	-3.47573586
6	2.25936886	-0.03841700	-2.11159654
6	3.06297136	-0.58931791	-1.05932956
6	4.07519420	-1.52207914	-1.36710320
6	2.93919417	-0.09335043	0.32121386
7	1.73205020	0.35892991	0.78465199
6	1.61264931	0.93892329	2.02169246
6	2.74768044	1.04234606	2.84383008
6	3.96899027	0.53859270	2.41175095
6	4.07385907	-0.02480927	1.14669668
6	0.32257304	1.48994351	2.48947641
6	-0.68245080	1.98063133	1.59401662
6	-1.81639663	2.68596053	2.11053768
6	-1.95145468	2.77796362	3.49752137
6	-1.02218344	2.21529172	4.38273378
6	0.10683888	1.59233204	3.88035585
8	1.23349039	0.76072443	-1.82088624
8	-0.57869484	1.79468005	0.27562272
1	2.67235141	1.55630812	3.79786647
1	4.85150341	0.62834725	3.04638975
1	5.03502545	-0.35453424	0.76123751
1	4.63831515	-1.98933012	-0.55834986
6	1.82574732	0.33297389	-4.63922610
1	0.82212038	1.14265322	4.56827440
1	-2.81800905	3.28729100	3.91536454
6	-2.86748119	3.30332412	1.16527844
1	3.86489271	-1.50599767	-4.74011422
6	-2.19438296	4.32444706	0.21738154
6	-3.96359500	4.05590964	1.94348555
6	-3.56911959	2.19855383	0.33853544
1	-1.73844468	5.14215474	0.79444444
1	-2.94996179	4.76390685	-0.45143207
1	-1.41857348	3.85503270	-0.39637254
1	-4.05616943	1.46857903	1.00305070

1	-2.86177162	1.67224130	-0.31121464
1	-4.34907523	2.64798386	-0.29475954
1	-4.66846659	4.49986227	1.22634686
1	-3.55077665	4.87420749	2.55101894
1	-4.54041671	3.39008880	2.60214706
6	0.34798918	-0.12467416	-4.63656005
6	2.42521978	-0.04787960	-6.00642119
6	1.90460722	1.87387985	-4.51938551
1	2.34796133	-1.12596371	-6.20977589
1	3.48079989	0.24892152	-6.09342474
1	1.86744186	0.47455889	-6.79661496
1	0.28394787	-1.21411672	-4.77657963
1	-0.18811538	0.35609592	-5.46959059
1	-0.15919122	0.12740071	-3.69971098
1	1.36495964	2.33651364	-5.35969310
1	2.95042264	2.21250625	-4.56304209
1	1.46053175	2.22894903	-3.58365908
1	-1.18754581	2.27163786	5.45863027
1	5.10343655	-2.60374877	-2.91812012
8	-0.35846055	-4.11535699	1.91815760
6	0.82439762	-4.94138158	2.08636001
1	0.65649121	-5.68674552	2.87284029
8	-0.17691857	-3.49306209	4.10312852
8	-0.99625288	-0.62669586	-1.39013562
1	0.97865588	-5.42060697	1.11573477
1	1.68318114	-4.31476833	2.35476277
13	0.16587995	0.33022409	-0.42473436
8	-2.33720628	-2.42859476	1.39295199
6	-1.56129680	-1.63796886	0.65489282
6	-1.93765243	-1.46536333	-0.80827906
6	-0.72744507	-3.43167569	3.02202451
6	-1.97508901	-2.56863927	2.80563813
8	-0.57400209	-1.04110891	1.10599923
6	-3.18359112	-3.16874394	3.51194771
6	-2.02550454	-2.82086803	-1.52877377
1	-2.95031260	-1.00484278	-0.81149938
1	-1.73481792	-1.57305934	3.20230510
1	-4.04411283	-2.49515932	3.41886229
1	-2.94915452	-3.30084477	4.57502735
1	-3.44513304	-4.14309358	3.07931294
1	-2.79758543	-3.46282965	-1.08475686
1	-1.05561209	-3.33417567	-1.48807023
1	-2.27329817	-2.63345649	-2.58054007

Electronic energy = -2064.618125 a.u.

DFT-D4 dispersion correction = -0.121199 a.u.

Thermal free energy = 0.551830 a.u.

Gibbs free energy = -2064.187493 a.u.

Number of imaginary frequencies = 0.

8_{LA} (open tail)

Atomic N.	X	Y	Z
6	-1.87640343	-4.77508602	1.13566791
6	-1.23794016	-4.50690149	2.35292376

6	-0.82692511	-3.22349918	2.72112251
6	-1.07584167	-2.15630277	1.80352977
6	-1.79707651	-2.40712851	0.59001545
6	-2.16028252	-3.73317069	0.27165067
6	-2.24116370	-1.33213308	-0.32245195
7	-1.54468796	-0.15523451	-0.40087452
6	-1.94563668	0.88408114	-1.19627768
6	-3.09557727	0.73558709	-1.98587108
6	-3.81080441	-0.45486019	-1.93863933
6	-3.39765898	-1.48734770	-1.10278145
6	-1.20071550	2.15952826	-1.19011895
6	-0.52173992	2.65524993	-0.02932132
6	-0.00197849	3.98596737	-0.02102782
6	-0.09455200	4.72490196	-1.20374601
6	-0.67252830	4.21252942	-2.37224320
6	-1.23113686	2.94713212	-2.35972557
8	-0.64776067	-0.91842936	2.11055855
8	-0.38350276	1.88427764	1.06810883
1	-3.44165510	1.56893525	-2.59090708
1	-4.72005488	-0.56673169	-2.53035374
1	-3.98963779	-2.39383348	-1.01234763
1	-2.64432655	-3.94141933	-0.68225539
6	-0.10564039	-2.97626042	4.06224667
1	-1.65889328	2.52888357	-3.26999461
1	0.31675208	5.73209943	-1.23255401
6	0.65853683	4.58109079	1.23977910
1	-1.04083243	-5.33996033	3.02477187
6	-0.33491856	4.55713222	2.42572224
6	1.07623256	6.04872230	1.02594186
6	1.93855962	3.79016774	1.60154081
1	-1.22626928	5.15833044	2.19387908
1	0.14261599	4.99261012	3.31646670
1	-0.65497722	3.53823774	2.66708956
1	2.66223734	3.82514352	0.77377279
1	1.71805823	2.74178402	1.82906742
1	2.41535225	4.24054224	2.48528709
1	1.51335247	6.43328145	1.95820648
1	0.21914239	6.68963657	0.77330501
1	1.83632966	6.15576764	0.23856531
6	1.34204364	-2.49262543	3.80772002
6	-0.01524264	-4.26267037	4.90623112
6	-0.87962245	-1.93531382	4.90609412
1	0.57293529	-5.04810327	4.41007551
1	-1.00895911	-4.66768648	5.14702880
1	0.48564868	-4.02903557	5.85617241
1	1.90745370	-3.24742444	3.24225492
1	1.85330525	-2.33531708	4.76961620
1	1.36878606	-1.55412434	3.24474501
1	-0.36263193	-1.78153496	5.86531513
1	-1.89572587	-2.29507222	5.12529529
1	-0.95497708	-0.97066752	4.39426706
1	-0.67642769	4.80771793	-3.28517571
1	-2.14441237	-5.79825602	0.87267783
8	0.96684539	-1.29355838	-5.66463086

6	0.36826327	-0.48982924	-6.71114598
1	-0.72399801	-0.59409496	-6.69776400
8	-0.23671582	-0.10504760	-4.13830040
8	1.50794781	-0.25995688	0.31896286
1	0.78504028	-0.87609793	-7.64579537
1	0.63385821	0.56528763	-6.57308904
13	-0.09595138	0.15187350	0.82033240
6	0.56701792	-0.97466717	-4.40737431
6	1.22539933	-1.92797909	-3.40283409
8	1.32508584	-1.30138882	-2.10441297
6	2.23854053	-0.28924873	-2.03751255
6	2.36515311	0.31764329	-0.62973834
8	2.89065057	0.08894660	-2.99360905
6	3.82381509	0.19299847	-0.16666982
6	0.38905902	-3.19148299	-3.22617999
1	2.23414655	-2.16400146	-3.76785567
1	2.14696392	1.39362570	-0.78455696
1	3.94695509	0.74264511	0.77507834
1	4.50789391	0.60193761	-0.92024123
1	4.06762230	-0.86286416	0.01370614
1	0.32194127	-3.73134732	-4.17966923
1	-0.62363835	-2.94134160	-2.88514420
1	0.85987963	-3.84525923	-2.48160150

Electronic energy = -2064.613823 a.u.

DFT-D4 dispersion correction = -0.121155 a.u.

Thermal free energy = 0.550913 a.u.

Gibbs free energy = -2064.184065 a.u.

Number of imaginary frequencies = 0.

Propagation stage for CL-CL

9_{CLCL}

Atomic N.	X	Y	Z
6	3.99174358	0.73940223	-1.34357362
6	5.27203319	-0.08857373	-1.10086518
6	5.20165185	-1.00134672	0.12758183
6	3.89315068	1.98772336	-0.48359883
6	4.94248032	-0.27111488	1.44955657
6	3.64370987	0.52979270	1.48411345
1	3.10572724	0.10157565	-1.18898030
1	6.13745953	0.58985419	-1.02604176
1	4.39675528	-1.73985615	-0.02904366
1	4.89208453	-1.01182208	2.26423609
1	3.96695524	1.09852282	-2.37881922
1	5.44382369	-0.71095809	-1.99199263
1	6.13804731	-1.57564961	0.20670515
1	5.77617992	0.40701875	1.69561770
1	3.37076345	0.76406778	2.52053589
1	2.81056523	-0.03241343	1.03356479
8	3.95269012	3.11597139	-0.93482669
8	3.74308245	1.84602529	0.86942251
6	-1.21468976	0.81120064	4.55197079
6	-0.78875721	-0.52072644	4.62270790
6	-0.25940963	-1.20269683	3.52240758
6	-0.16803677	-0.49401270	2.28648183
6	-0.50449802	0.89760149	2.23322924
6	-1.05895745	1.51757067	3.37149890
6	-0.21618210	1.74455255	1.05498983
7	-0.23565002	1.20409689	-0.20227433
6	0.11108955	1.92641748	-1.31406395
6	0.47409591	3.27261363	-1.16375074
6	0.47211957	3.85057808	0.10114239
6	0.13041522	3.09287627	1.21525584
6	0.14067166	1.27790932	-2.64240997
6	0.43466332	-0.11274914	-2.82042270
6	0.61274960	-0.64414132	-4.13374948
6	0.41684518	0.21916210	-5.21542716
6	0.06289076	1.56400874	-5.05353499
6	-0.06182248	2.08744902	-3.77894466
8	0.25770952	-1.14170338	1.17999992
8	0.58151781	-0.92505550	-1.75373525
1	0.82345863	3.83525663	-2.02469616
1	0.79002629	4.88578134	0.22380159
1	0.18338691	3.51820967	2.21338106
1	-1.40739884	2.54728263	3.29776942
6	0.19448283	-2.67275379	3.64143712
1	-0.34577259	3.13128708	-3.64757843
1	0.52565842	-0.16560793	-6.22756425
6	0.98677157	-2.12412560	-4.35717108
1	-0.89533748	-1.04537432	5.57029232
6	2.32244735	-2.45356003	-3.64811887
6	1.17827554	-2.44562779	-5.85199294
6	-0.13905266	-3.04599500	-3.83119665

1	3.13409209	-1.82481999	-4.04353260
1	2.58968166	-3.50495116	-3.83322320
1	2.25438481	-2.29882192	-2.56616418
1	-1.08126223	-2.84510918	-4.36101745
1	-0.31479665	-2.90669540	-2.75963541
1	0.13186397	-4.09837171	-4.00625183
1	1.46184615	-3.50260986	-5.95467815
1	1.97781843	-1.84262013	-6.30651490
1	0.25598367	-2.29599533	-6.43154350
6	-0.67606059	-3.58503993	2.74542839
6	0.06587735	-3.19511692	5.08520913
6	1.68324589	-2.80337383	3.23941717
1	-0.97658234	-3.19975750	5.43487154
1	0.66820347	-2.60750361	5.79304437
1	0.42892516	-4.23189779	5.12251581
1	-1.73601833	-3.50993374	3.02893344
1	-0.36625174	-4.63365178	2.87050330
1	-0.57870130	-3.32317483	1.68660497
1	2.00391637	-3.85135760	3.33913026
1	2.31599789	-2.19315955	3.90087267
1	1.84893507	-2.48825683	2.20348930
1	-0.11183376	2.19205460	-5.92682943
1	-1.66627475	1.28696362	5.42236570
13	-0.49772071	-0.69278934	-0.36634413
8	-4.75803950	4.32113554	-0.11917041
6	-3.77231372	5.33284454	-0.43628632
1	-2.82487074	4.86336574	-0.73038794
6	-5.55094399	2.53783316	1.23997246
6	-5.02889889	1.17065858	1.70085421
6	-4.37977349	0.35631511	0.57646944
6	-4.44037730	3.52780273	0.94381844
6	-3.83796795	-0.99235199	1.05843271
6	-3.19399233	-1.83430118	-0.04674538
1	-6.15915531	2.99460292	2.03904770
1	-4.30519649	1.32383260	2.51593900
1	-3.55709489	0.93210934	0.12367098
1	-3.10547344	-0.82995607	1.86694785
1	-6.20115360	2.44774301	0.35871855
1	-5.87118488	0.60203925	2.12693053
1	-5.11672206	0.18735899	-0.22855345
1	-4.65862475	-1.58863225	1.49618406
1	-3.95174150	-2.05067121	-0.82241057
1	-2.88317778	-2.80681425	0.37795763
8	-3.40500048	3.64211135	1.57630208
8	-2.10218714	-1.20265813	-0.68587427
1	-4.19723511	5.89913322	-1.27057704
1	-3.59675834	5.98454473	0.42878229

Electronic energy = -2300.232439 a.u.

DFT-D4 dispersion correction = -0.145609 a.u.

Thermal free energy = 0.702903 a.u.

Gibbs free energy = -2299.675145 a.u.

Number of imaginary frequencies = 0.

10a_{CLCL}

Atomic N.	X	Y	Z
6	3.06777570	-1.27816506	-3.59465655
6	1.90715481	-0.82169580	-4.23383221
6	1.04028779	0.10510195	-3.65083240
6	1.35576425	0.57961479	-2.33469719
6	2.60405806	0.21978952	-1.73885287
6	3.42195054	-0.74133383	-2.36982122
6	3.11712410	0.90222297	-0.53646030
7	2.26275612	1.42662077	0.39693941
6	2.75514671	2.05715787	1.50832343
6	4.14345523	2.20225655	1.68342886
6	5.01805726	1.68917682	0.73587902
6	4.50819519	1.03856417	-0.37904571
6	1.85165966	2.63645504	2.51957313
6	0.56439022	3.15191633	2.17356028
6	-0.13499117	3.98305564	3.11019639
6	0.40342561	4.11613780	4.39194848
6	1.59797615	3.49415475	4.77856769
6	2.32514297	2.78382118	3.84030247
8	0.49912041	1.37141202	-1.69082472
8	0.02619231	2.89305761	0.98140171
1	4.51751373	2.76257917	2.53563905
1	6.09432334	1.82472742	0.84980035
1	5.17107772	0.67644586	-1.15987350
1	4.32931363	-1.08326412	-1.87177855
6	-0.22077895	0.58357487	-4.39827620
1	3.26303355	2.30924550	4.12886951
1	-0.12788215	4.71267118	5.13138622
6	-1.44599102	4.69955157	2.72876209
1	1.67091351	-1.22362387	-5.21742314
6	-1.22728006	5.57653067	1.47294129
6	-1.94419119	5.62806682	3.85257136
6	-2.55950453	3.66238377	2.45691381
1	-0.46283336	6.34302112	1.66735224
1	-2.16418077	6.09267407	1.21319409
1	-0.91050518	4.97655295	0.61341415
1	-2.74373935	3.04757769	3.35049430
1	-2.27387871	3.00823197	1.62850954
1	-3.49624474	4.17842669	2.19451037
1	-2.85572126	6.14022048	3.51246497
1	-1.20460989	6.40093735	4.10697545
1	-2.20009826	5.07653128	4.76900296
6	-1.49221799	0.10144601	-3.66226224
6	-0.28128276	0.03186317	-5.83537166
6	-0.22694314	2.12745654	-4.49925179
1	-0.35802401	-1.06496143	-5.85975554
1	0.59326846	0.33276491	-6.43019549
1	-1.17530351	0.43436831	-6.33285313
1	-1.50973918	-0.99694205	-3.59867868
1	-2.38770432	0.42789502	-4.21384410
1	-1.53449734	0.51731837	-2.65147562
1	-1.12364945	2.45893040	-5.04482574
1	0.65487420	2.48088177	-5.05366221

1	-0.22960101	2.59512527	-3.50923319
1	1.95555919	3.58377489	5.80425722
1	3.68940260	-2.03918819	-4.06619654
6	-3.12230293	-0.03498310	0.80913484
6	-3.59514429	-1.33547320	0.12108453
6	-5.07588635	-1.34261939	-0.27027055
6	-2.85654787	1.08601044	-0.15898691
6	-5.48726251	-0.21571615	-1.22384689
6	-5.23813534	1.18854597	-0.68614877
1	-3.87133860	0.29687320	1.54739135
1	-2.96022715	-1.53009737	-0.75718219
1	-5.32489924	-2.31223015	-0.72811363
1	-4.97499950	-0.31192002	-2.19479954
1	-2.16493153	-0.20775135	1.31839646
1	-3.40739888	-2.16269045	0.82105751
1	-5.68610870	-1.26855182	0.64664044
1	-6.56626976	-0.29516581	-1.43349117
1	-5.80305299	1.93119870	-1.26128162
1	-5.52612055	1.28076464	0.37264915
8	-1.73683595	1.55221924	-0.39192129
8	-3.86152033	1.64666000	-0.85077241
13	0.24943117	1.33490263	0.09570796
8	3.11451340	-8.23660787	0.88879176
6	3.00353299	-9.57190852	0.34170265
1	2.07334772	-10.04871966	0.67610069
6	2.28667374	-6.03247251	1.17786410
6	1.38330295	-4.94756915	0.59096643
6	1.52434153	-3.60707245	1.31995918
6	2.10477988	-7.38902906	0.52602692
6	0.64330720	-2.50591218	0.72186107
6	0.74903155	-1.17883727	1.47983704
1	2.08486123	-6.16354486	2.25523021
1	0.33769209	-5.28820211	0.63010341
1	1.27121981	-3.74443497	2.38641096
1	-0.41096507	-2.83109176	0.72126519
1	3.34956019	-5.75405773	1.11001616
1	1.61868315	-4.81557595	-0.47677388
1	2.57976885	-3.28394605	1.29520765
1	0.91945589	-2.33399647	-0.33140885
1	1.81072934	-0.86503865	1.50251560
1	0.45054371	-1.33860350	2.53461171
8	1.19199888	-7.71533274	-0.20890365
8	-0.08234546	-0.18735466	0.91384982
1	3.87503102	-10.11403633	0.72139392
1	3.01296700	-9.53974800	-0.75507470

Electronic energy = -2300.236532 a.u.

DFT-D4 dispersion correction = -0.141141 a.u.

Thermal free energy = 0.707055 a.u.

Gibbs free energy = -2299.670618 a.u.

Number of imaginary frequencies = 0.

10b_{CLCL}

Atomic N.	X	Y	Z
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6	3.70240492	3.86704322	-2.44838780
6	2.87875707	3.49764132	-3.52202185
6	1.61148320	2.94187977	-3.34123553
6	1.16027390	2.73224894	-1.99631764
6	1.93874197	3.22835200	-0.90393800
6	3.22496660	3.75243489	-1.15505403
6	1.38386557	3.31766680	0.45856922
7	0.40299260	2.45819703	0.88945603
6	-0.14172721	2.60197917	2.13756837
6	0.31227110	3.62164310	2.99637976
6	1.31503411	4.48464215	2.57853174
6	1.84461842	4.34387271	1.30379522
6	-1.26179040	1.75616184	2.58498092
6	-2.19195356	1.19518772	1.65157230
6	-3.48447582	0.78156919	2.12895396
6	-3.67256706	0.70383227	3.51006941
6	-2.67829447	1.05851534	4.43335367
6	-1.50168127	1.61875003	3.96923652
8	0.01446660	2.09775208	-1.76936757
8	-1.88162714	1.08304465	0.36641741
1	-0.17307273	3.76639603	3.95723589
1	1.65012361	5.29466223	3.22784239
1	2.57463648	5.05506732	0.92775429
1	3.85913137	4.04571612	-0.31823131
6	0.73764945	2.53870032	-4.54416720
1	-0.74446924	1.94987897	4.68051934
1	-4.62617189	0.34569095	3.89403038
6	-4.63295750	0.42728947	1.16315273
1	3.25894946	3.63441770	-4.53305695
6	-4.83685435	1.56974590	0.14001260
6	-5.97096405	0.24132438	1.90504206
6	-4.32093335	-0.89131948	0.42543492
1	-5.09676713	2.50710239	0.65359034
1	-5.66615537	1.31481083	-0.53696490
1	-3.93773887	1.73996621	-0.46132286
1	-4.21978783	-1.72162686	1.14037256
1	-3.39248646	-0.80849892	-0.14480666
1	-5.13814117	-1.13833872	-0.26999401
1	-6.76273834	0.05517184	1.16534133
1	-6.25330985	1.13625261	2.47843941
1	-5.95556726	-0.62010362	2.58845583
6	0.54268266	1.00498351	-4.56669396
6	1.38052145	2.94566956	-5.88351922
6	-0.63575025	3.24708419	-4.46264377
1	2.33811954	2.43407719	-6.05906718
1	1.54820504	4.03079372	-5.94904438
1	0.70367577	2.66415991	-6.70293731
1	1.51103007	0.49564030	-4.68334280
1	-0.09386933	0.72367066	-5.42031053
1	0.07547178	0.64621711	-3.64356279
1	-1.25256182	2.95885478	-5.32758464
1	-0.50851855	4.33951512	-4.48783060
1	-1.17320127	2.97862521	-3.54710151
1	-2.85032996	0.93140125	5.50221168

1	4.70531230	4.25107171	-2.63542693
8	1.59844573	0.21570184	0.18337187
8	0.63703945	-0.85263109	1.83832333
6	1.72026479	-0.60576232	1.10595161
6	3.03277483	-1.27711982	1.39505904
1	2.88694926	-2.37033139	1.33931529
1	3.70752667	-0.97984580	0.58423799
6	3.63316554	-0.89995398	2.76877153
1	3.56674143	0.19017206	2.91440589
1	4.70558516	-1.14144729	2.73380903
6	2.99859324	-1.63867200	3.95202077
1	3.16965758	-2.72059328	3.82547687
1	3.51834448	-1.34507359	4.87698306
6	1.49473892	-1.39531354	4.12296787
1	1.28490233	-0.33596389	4.34173370
1	1.13546788	-1.96609090	4.99444091
6	0.64480365	-1.82926975	2.93714101
1	0.95497384	-2.80372865	2.53218459
1	-0.41550978	-1.87375275	3.20901622
13	-0.22708563	0.95884783	-0.39116945
8	1.50337609	-6.59734555	0.21509282
6	1.46877749	-7.27452640	1.49531872
1	2.43041523	-7.16548903	2.01186758
6	1.70778853	-4.61676766	-1.08720599
6	0.36528637	-3.89040598	-1.32120425
6	0.40193861	-3.03034860	-2.58813145
6	1.74968313	-5.26254581	0.27532824
6	-0.90960335	-2.28996578	-2.88284427
6	-1.38873340	-1.39236803	-1.72824362
1	2.52544412	-3.88189622	-1.12693432
1	0.15063361	-3.24739167	-0.45524160
1	1.19955383	-2.27971886	-2.47644510
1	-1.71378441	-3.01080870	-3.11363056
1	1.87658988	-5.37041409	-1.86781760
1	-0.44509046	-4.63522038	-1.38298782
1	0.66750524	-3.65929020	-3.45462281
1	-0.76342929	-1.67644903	-3.78548178
1	-1.79514658	-2.04191039	-0.92526111
1	-2.24198789	-0.78699163	-2.09462623
8	1.94633628	-4.67013221	1.32932171
8	-0.34425410	-0.60068104	-1.23043188
1	1.27081353	-8.32448707	1.26054586
1	0.67158660	-6.86050148	2.12520596

Electronic energy = -2300.224483 a.u.

DFT-D4 dispersion correction = -0.145870 a.u.

Thermal free energy = 0.708936 a.u.

Gibbs free energy = -2299.661417 a.u.

Number of imaginary frequencies = 0.

TS3ax_{CLCL}

Atomic N.	X	Y	Z
6	1.19402146	2.83249974	-3.66389871
6	0.39020535	1.94590354	-4.39465714

6	-0.56791121	1.12675393	-3.79378986
6	-0.70382899	1.19941485	-2.36989236
6	0.02473111	2.18842220	-1.63610291
6	0.99725139	2.96833849	-2.30097795
6	-0.27714953	2.48793006	-0.22340728
7	-0.79675573	1.52671838	0.60616761
6	-1.10974312	1.82118440	1.90846336
6	-0.89083838	3.11619282	2.40833735
6	-0.35102448	4.09448147	1.58307672
6	-0.04948310	3.78730321	0.26381114
6	-1.72197676	0.80917001	2.79084134
6	-2.58715487	-0.20610689	2.27573466
6	-3.39783192	-0.97212958	3.17502356
6	-3.19124079	-0.79348958	4.54472017
6	-2.25130081	0.11248830	5.05635548
6	-1.54353178	0.92245626	4.18550396
8	-1.52532566	0.35604590	-1.74345338
8	-2.66107297	-0.42651564	0.96296245
1	-1.19412959	3.35344458	3.42438579
1	-0.19518305	5.10642433	1.95885754
1	0.33001614	4.55169773	-0.40774572
1	1.62205887	3.65708852	-1.73115993
6	-1.43748415	0.16829199	-4.63214016
1	-0.82195103	1.63948607	4.57783556
1	-3.76883125	-1.38823497	5.25028181
6	-4.45592165	-1.96312058	2.64965892
1	0.53774428	1.88684535	-5.47165298
6	-5.45745230	-1.22323704	1.73060429
6	-5.26877499	-2.59168720	3.79756093
6	-3.78292012	-3.11847353	1.87210882
1	-5.97781849	-0.42978492	2.28699446
1	-6.21588898	-1.93155253	1.36402309
1	-4.95578289	-0.77472311	0.86667955
1	-3.09522486	-3.67344666	2.52857184
1	-3.22369242	-2.75392342	1.00389993
1	-4.55133772	-3.82389402	1.51971459
1	-6.03095722	-3.25853801	3.36993408
1	-5.79114246	-1.83309996	4.39851809
1	-4.64251232	-3.19736266	4.46895695
6	-1.13111782	-1.30336833	-4.26686811
6	-1.17477655	0.33388224	-6.14125061
6	-2.93616915	0.47137821	-4.39323902
1	-0.14226143	0.07198639	-6.41540909
1	-1.37834513	1.35769689	-6.48774719
1	-1.84243846	-0.34211013	-6.69422150
1	-0.07108611	-1.53263271	-4.45270967
1	-1.73831856	-1.97248304	-4.89636421
1	-1.35115087	-1.51844239	-3.21639442
1	-3.55242658	-0.20962837	-4.99981165
1	-3.17494202	1.50196028	-4.69492912
1	-3.21060252	0.34178632	-3.34112120
1	-2.09232688	0.18590797	6.13221264
1	1.96145582	3.41856360	-4.16976452
6	0.07724181	-3.58598208	0.78972977

6	1.46924055	-3.96181107	1.31219506
6	2.25346112	-4.92846870	0.41838035
6	-0.03942205	-2.56372619	-0.33361787
6	2.60698342	-4.36181259	-0.95862448
6	1.40288901	-3.91352844	-1.77976000
1	-0.45488787	-4.48766804	0.43641528
1	2.05883694	-3.04930735	1.48955381
1	3.17825961	-5.23173523	0.93400592
1	3.29950237	-3.50917554	-0.86289167
1	-0.53776228	-3.18062496	1.60279262
1	1.33649743	-4.43050814	2.29947543
1	1.66024780	-5.84980154	0.28315425
1	3.13664412	-5.13033962	-1.54641914
1	1.69734788	-3.74667931	-2.82409811
1	0.60874128	-4.67841291	-1.77568960
8	-1.23754001	-2.14806199	-0.61436850
8	0.84340507	-2.63249612	-1.39096463
13	-1.22606170	-0.31703550	-0.11135626
8	5.98193216	4.89308214	0.38083431
6	5.97961283	6.21684885	-0.20788345
1	5.75491667	6.15918589	-1.28025532
6	4.91267252	2.84180689	0.89916497
6	3.57389379	2.10966301	0.97476268
6	3.69967532	0.69275749	1.55013669
6	4.79852343	4.22280312	0.28174803
6	2.35229087	-0.03905876	1.67515242
6	1.76254487	-0.42305022	0.31793928
1	5.63882160	2.27299762	0.29398581
1	3.13445711	2.08078885	-0.03178384
1	4.38820505	0.09787062	0.92396003
1	1.63501048	0.59975284	2.21366620
1	5.37624407	2.94681859	1.89286935
1	2.87630558	2.69385910	1.59505248
1	4.16611910	0.74767834	2.54748464
1	2.47493362	-0.94899935	2.28319621
1	2.40591192	-1.15961957	-0.19159929
1	1.70524395	0.45190316	-0.34661365
8	3.80565882	4.69254446	-0.24466771
8	0.45562553	-1.00661969	0.44389322
1	6.98819494	6.60769892	-0.04333516
1	5.23123503	6.85270452	0.28129187

Electronic energy = -2300.216028 a.u.

DFT-D4 dispersion correction = -0.147906 a.u.

Thermal free energy = 0.711260 a.u.

Gibbs free energy = -2299.652674 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 130.0i

TS3eq_{CLCL}

Atomic N.	X	Y	Z
6	2.89508700	3.04612660	-3.93122649
6	2.06369734	2.00791883	-4.37220764
6	1.00907850	1.51021469	-3.60335326

6	0.81400335	2.06858206	-2.29618955
6	1.53091061	3.25364232	-1.92896986
6	2.60360909	3.68368697	-2.73844934
6	1.09555578	4.12255192	-0.81641400
7	0.39014462	3.61732507	0.24121059
6	-0.09170546	4.43464804	1.22740328
6	0.15558165	5.81856298	1.16711557
6	0.88869762	6.34442663	0.11278974
6	1.35101569	5.50296545	-0.89063549
6	-0.92319494	3.89598846	2.31992626
6	-1.69754970	2.70176816	2.16440463
6	-2.74474239	2.41366601	3.10067225
6	-2.84309816	3.21964097	4.23595285
6	-1.97982192	4.29827166	4.47250700
6	-1.04976034	4.64492655	3.50974560
8	-0.04387922	1.49506474	-1.44802427
8	-1.47065973	1.86672246	1.14971519
1	-0.27385908	6.47423744	1.91883743
1	1.06419849	7.41913033	0.05014133
1	1.85922325	5.90949392	-1.76024616
1	3.22203183	4.51746178	-2.40665650
6	0.08377100	0.40643117	-4.15579653
1	-0.38848957	5.49348736	3.68266320
1	-3.60535073	2.99726963	4.98061705
6	-3.72406793	1.24539328	2.87206817
1	2.26107192	1.56927681	-5.34869480
6	-4.42325401	1.40303648	1.50061381
6	-4.82983065	1.20227575	3.94364882
6	-2.96965361	-0.10148024	2.92874956
1	-4.99845457	2.33984613	1.46688068
1	-5.12582302	0.57009470	1.34452212
1	-3.70101190	1.40880966	0.67714971
1	-2.50737524	-0.24459261	3.91668630
1	-2.18130231	-0.13766283	2.17113328
1	-3.67116070	-0.93268281	2.75567150
1	-5.51809597	0.37684381	3.71161127
1	-5.41954899	2.13016510	3.96618867
1	-4.42801571	1.02079260	4.95105028
6	0.24859978	-0.90081066	-3.35150027
6	0.39168239	0.08336614	-5.63033438
6	-1.38789797	0.88005435	-4.08795261
1	1.39824498	-0.33880061	-5.76430416
1	0.29625943	0.96852052	-6.27554750
1	-0.32793930	-0.66730309	-5.98706245
1	1.28607011	-1.26376736	-3.40235996
1	-0.40390202	-1.68412220	-3.76716185
1	-0.01883341	-0.74440008	-2.30294776
1	-2.04898238	0.09613747	-4.48780489
1	-1.53068471	1.78443074	-4.69709444
1	-1.69306660	1.10105896	-3.05925322
1	-2.05495453	4.86714411	5.39912796
1	3.74193597	3.36618948	-4.53809834
8	1.85031378	1.50603795	1.02593040
8	2.33991814	-0.10591238	2.45685625

6	2.09941483	0.23108089	1.16807640
6	2.84524226	-0.49349403	0.06194763
1	2.60541677	-1.56759822	0.06196846
1	2.46997690	-0.07772355	-0.88069105
6	4.37270355	-0.30024588	0.16358037
1	4.59150219	0.74323350	0.43961838
1	4.80114937	-0.45171875	-0.83814448
6	5.04808378	-1.27359354	1.13810360
1	4.86897945	-2.30386305	0.78416258
1	6.13848209	-1.12362301	1.10448492
6	4.57321310	-1.16321707	2.59202075
1	4.87192154	-0.19617645	3.02743173
1	5.06664181	-1.94426167	3.19364572
6	3.06692767	-1.31848311	2.78294587
1	2.66874218	-2.17265558	2.21305823
1	2.82793808	-1.47959089	3.84161687
13	0.12435442	1.63815093	0.34517646
8	-1.60321236	-7.69361448	-1.75966418
6	-1.06027162	-8.62738895	-2.72385192
1	-0.76378691	-8.10294342	-3.64085007
6	-1.38714957	-5.80556774	-0.34190920
6	-0.55691558	-4.56244993	-0.02300235
6	-1.19870067	-3.69888306	1.07070076
6	-0.73831695	-6.71128702	-1.37086070
6	-0.36462355	-2.47584605	1.48183644
6	-0.24313086	-1.42713797	0.37323064
1	-2.39222264	-5.53709078	-0.70284480
1	-0.41953412	-3.98040628	-0.94643426
1	-2.19680738	-3.36235046	0.74009502
1	0.64033556	-2.81078029	1.78858876
1	-1.55277228	-6.40884447	0.56711423
1	0.45152104	-4.87387323	0.29120237
1	-1.36995542	-4.32284737	1.96371698
1	-0.81852287	-1.99550641	2.36062455
1	-1.24838161	-1.19372535	-0.02163966
1	0.34451634	-1.82467794	-0.47253731
8	0.39556810	-6.60871410	-1.79986882
8	0.33071786	-0.20464569	0.82900184
1	-1.86849725	-9.33661366	-2.92645216
1	-0.18528226	-9.14317799	-2.30850387

Electronic energy = -2300.217382 a.u.

DFT-D4 dispersion correction = -0.143565 a.u.

Thermal free energy = 0.708095 a.u.

Gibbs free energy = -2299.652852 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 92.6i

11a_{CLCL}

Atomic N.	X	Y	Z
6	1.21549384	2.67803732	-3.72710048
6	0.40247366	1.78332035	-4.43742275
6	-0.57303525	0.99806994	-3.81994865
6	-0.72059662	1.11615552	-2.40061681

6	0.02402130	2.11028845	-1.68853033
6	1.01342146	2.85418111	-2.36986593
6	-0.27429804	2.45511044	-0.28502618
7	-0.81243041	1.52659605	0.56997197
6	-1.12638620	1.85802632	1.86353659
6	-0.88075710	3.15963345	2.33180726
6	-0.31925893	4.10529289	1.48296635
6	-0.02287861	3.76103039	0.17130883
6	-1.75926156	0.87435785	2.76186040
6	-2.63750241	-0.13759061	2.25980630
6	-3.43636791	-0.90170053	3.17063767
6	-3.22724399	-0.70432356	4.53730777
6	-2.29037509	0.21194869	5.03640077
6	-1.57901909	1.00650708	4.15476381
8	-1.56962088	0.31149542	-1.75866139
8	-2.73015387	-0.35352417	0.94670266
1	-1.18015577	3.42819210	3.34128596
1	-0.14218296	5.12260325	1.83387386
1	0.37134536	4.50274586	-0.51692899
1	1.64385535	3.55055352	-1.81582322
6	-1.44671980	0.02355111	-4.63502398
1	-0.85311837	1.72482901	4.53679037
1	-3.79921703	-1.29441370	5.25126071
6	-4.47409215	-1.92135128	2.66105241
1	0.55682614	1.68975312	-5.51094755
6	-5.48830045	-1.22349479	1.72338192
6	-5.27904450	-2.54320215	3.81840289
6	-3.76831142	-3.07754965	1.91352665
1	-6.02554782	-0.42728724	2.25962807
1	-6.23173811	-1.95594715	1.37404891
1	-4.99545756	-0.78577932	0.84919683
1	-3.08054287	-3.60774749	2.58971724
1	-3.19681539	-2.72230744	1.04962191
1	-4.51908544	-3.80206232	1.56182591
1	-6.02529343	-3.23391241	3.40078852
1	-5.81978953	-1.78365759	4.40187194
1	-4.64389500	-3.12294167	4.50406641
6	-1.15515505	-1.43763333	-4.21899831
6	-1.16838479	0.13576690	-6.14629195
6	-2.94453533	0.34818751	-4.42123788
1	-0.13584162	-0.14411958	-6.40156273
1	-1.35989296	1.14894625	-6.52896314
1	-1.83677016	-0.55279377	-6.68255875
1	-0.09894131	-1.68323499	-4.40515677
1	-1.77386317	-2.12243078	-4.81950344
1	-1.36901074	-1.61256858	-3.15953839
1	-3.56101406	-0.34437512	-5.01421906
1	-3.16962838	1.37158389	-4.75601081
1	-3.23190758	0.25335112	-3.36906012
1	-2.13210264	0.30055614	6.11118754
1	1.99473640	3.23768397	-4.24458082
6	0.44390636	-3.37299429	0.98361290
6	1.84095629	-4.00315860	1.07757782
6	2.08756550	-5.11088632	0.04078628

6	0.19989049	-2.32483693	-0.11772237
6	2.18126442	-4.62754279	-1.41127376
6	1.00886144	-3.76659590	-1.87384590
1	-0.30592666	-4.16284585	0.82075452
1	2.62529578	-3.23312304	0.99798469
1	3.01476720	-5.64820786	0.29629198
1	3.10451504	-4.04231572	-1.55533672
1	0.16509791	-2.88812283	1.92960195
1	1.94677335	-4.44194254	2.08230725
1	1.27127043	-5.84933377	0.12413306
1	2.25411027	-5.49881868	-2.08408654
1	1.08134126	-3.57612136	-2.95398025
1	0.03769556	-4.25577060	-1.69261328
8	-1.10300083	-2.12997719	-0.37130290
8	1.02919348	-2.46052419	-1.25688305
13	-1.27849046	-0.30789786	-0.10836610
8	5.95248746	5.04421926	0.68309151
6	5.93542201	6.37141663	0.10202635
1	5.77745430	6.31329275	-0.98211163
6	4.93741000	2.94564288	1.11412555
6	3.61949336	2.17291524	1.11974396
6	3.76403267	0.74648380	1.66604798
6	4.80666330	4.32820904	0.50260500
6	2.43353589	-0.02526914	1.72206288
6	1.90119531	-0.35406287	0.33152811
1	5.70680808	2.40589109	0.53627232
1	3.22286070	2.15787409	0.09531552
1	4.49216482	0.18590230	1.05374875
1	1.68571659	0.57250526	2.26652179
1	5.35220798	3.05396207	2.12851215
1	2.88031559	2.72201005	1.72392571
1	4.18848061	0.78746544	2.68232319
1	2.56673498	-0.95885256	2.29001847
1	2.53586785	-1.08143834	-0.19015845
1	1.83846240	0.54140493	-0.29983318
8	3.83089567	4.76151437	-0.08361521
8	0.55750335	-0.91597409	0.39726751
1	6.91682182	6.79839685	0.32898391
1	5.13574629	6.97510142	0.54893817

Electronic energy = -2300.218713 a.u.

DFT-D4 dispersion correction = -0.147505 a.u.

Thermal free energy = 0.710411 a.u.

Gibbs free energy = -2299.655807 a.u.

Number of imaginary frequencies = 0.

11b_{CLCL}

Atomic N.	X	Y	Z
6	3.62744522	4.78877544	1.99622560
6	2.24348593	5.00323963	1.98691595
6	1.32075012	3.96599030	1.83292282
6	1.82946956	2.63599920	1.66902888
6	3.23354506	2.39789319	1.80915570
6	4.11216354	3.49535012	1.92725694

6	3.78991652	1.03857219	1.94876325
7	3.15749836	-0.04396819	1.39694667
6	3.64249277	-1.31194103	1.57325244
6	4.81285095	-1.51198995	2.32714105
6	5.47310972	-0.42458397	2.88190341
6	4.96089792	0.85332352	2.70359087
6	2.92598319	-2.48582101	1.03891110
6	1.50581932	-2.50562596	0.85958123
6	0.84258211	-3.76313281	0.67347342
6	1.63383448	-4.90096807	0.50114900
6	3.03304720	-4.85884857	0.52067775
6	3.66679406	-3.66537476	0.81189579
8	0.98888576	1.62846994	1.40596795
8	0.79237050	-1.37096965	0.88968194
1	5.16054726	-2.52310348	2.51729488
1	6.36623144	-0.57739788	3.48897099
1	5.42606640	1.70696723	3.18790460
1	5.18777657	3.32116127	1.93802202
6	-0.19209182	4.26139212	1.79891431
1	4.75522614	-3.62621927	0.84231788
1	1.15044963	-5.85971403	0.32323310
6	-0.69443935	-3.86987257	0.62587434
1	1.88089275	6.02491188	2.08367062
6	-1.31992817	-3.23165154	1.88867593
6	-1.17526603	-5.33340168	0.58337867
6	-1.21422291	-3.17660117	-0.65245616
1	-0.99666274	-3.77208972	2.79049373
1	-2.41739273	-3.29601645	1.83279085
1	-1.03567147	-2.18026495	1.99915683
1	-0.85362279	-3.70230389	-1.54840112
1	-0.86538935	-2.14187860	-0.70530713
1	-2.31536436	-3.18532610	-0.66931963
1	-2.27491331	-5.34478951	0.59524840
1	-0.82803953	-5.90751028	1.45459151
1	-0.85346609	-5.85479832	-0.32936090
6	-0.73423803	3.99772120	0.37522736
6	-0.50233209	5.73036718	2.14587092
6	-0.94070017	3.38731551	2.83293700
1	-0.08010361	6.43254805	1.41277516
1	-0.13269450	6.00471735	3.14455032
1	-1.59246194	5.87333202	2.14441276
1	-0.26638186	4.68393326	-0.34624401
1	-1.82195365	4.16840601	0.34682915
1	-0.52845496	2.97029567	0.05754942
1	-2.01678658	3.61715102	2.80096722
1	-0.58184135	3.60388589	3.84986472
1	-0.80352187	2.31876898	2.63863444
1	3.61238575	-5.76065779	0.32365248
1	4.31248999	5.63344765	2.06700230
8	2.21530461	0.43728253	-1.22557604
8	0.97091299	-0.54948890	-2.83318806
6	1.16642010	0.60943365	-2.06722808
6	1.20465076	1.94034755	-2.82301450
1	0.23656783	2.14256215	-3.30892348

1	1.33648801	2.70196557	-2.04366541
6	2.34551501	2.03102517	-3.85012937
1	3.24571085	1.56171083	-3.42356968
1	2.59051418	3.09330893	-4.00143528
6	2.00409770	1.41147316	-5.21075058
1	1.13800466	1.94933188	-5.63562536
1	2.84023881	1.57999110	-5.90784502
6	1.68014598	-0.08564934	-5.16787767
1	2.57045650	-0.66836900	-4.88226461
1	1.39158440	-0.42201352	-6.17791510
6	0.54968739	-0.46275675	-4.21089554
1	-0.31118342	0.21868134	-4.32503462
1	0.19564421	-1.47911584	-4.43261337
13	1.46529365	0.21899885	0.40037948
8	-5.81390953	-2.67938328	0.40282157
6	-5.91389227	-4.00169754	-0.17699990
1	-6.95447350	-4.22697830	-0.44197309
6	-6.07336283	-0.32136330	0.26934889
6	-4.61334705	0.01453266	0.62688786
6	-3.69210219	0.10578613	-0.59434366
6	-6.23140144	-1.66620171	-0.41409245
6	-2.24062943	0.41249329	-0.20884982
6	-1.33700264	0.47708395	-1.43308079
1	-6.49466228	0.43162867	-0.40929708
1	-4.22928381	-0.74429232	1.32511270
1	-3.72724295	-0.84317255	-1.15543664
1	-1.86390424	-0.36772531	0.46978089
1	-6.67905664	-0.33244711	1.18857324
1	-4.60246038	0.97408253	1.16809118
1	-4.07173777	0.88167381	-1.28126991
1	-2.18738914	1.36558914	0.33786985
1	-1.63925612	1.31390274	-2.08696842
1	-1.39873207	-0.45892957	-2.00975823
8	-6.66392374	-1.84872806	-1.53666449
8	0.03021089	0.68690276	-1.02519584
1	-5.55311584	-4.68590355	0.59723043
1	-5.29244614	-4.07268667	-1.07877803

Electronic energy = -2300.223448 a.u.

DFT-D4 dispersion correction = -0.146533 a.u.

Thermal free energy = 0.711436 a.u.

Gibbs free energy = -2299.658546 a.u.

Number of imaginary frequencies = 0.

12_{CLCL}

Atomic N.	X	Y	Z
6	-5.76682282	-2.70784288	0.44708140
6	-5.67896580	-2.25631952	1.77041863
6	-4.78381999	-1.26073518	2.16585771
6	-3.92981009	-0.69431615	1.16746976
6	-4.07203029	-1.08716913	-0.20498914
6	-4.98100266	-2.11963079	-0.52627544
6	-3.36517783	-0.41931621	-1.31780750
7	-2.18664376	0.24894055	-1.10559075

6	-1.56089579	0.96210951	-2.09535137
6	-2.08763066	0.94158507	-3.39498723
6	-3.25852418	0.23503519	-3.64702036
6	-3.91263969	-0.42380926	-2.61255916
6	-0.38175874	1.79109057	-1.77870781
6	-0.23568630	2.44492293	-0.50919423
6	0.79286755	3.42369451	-0.33259222
6	1.68657563	3.62470561	-1.38749642
6	1.60265335	2.92320688	-2.59855392
6	0.56511831	2.02953008	-2.79631362
8	-3.02017673	0.21490006	1.53992064
8	-1.07261068	2.16238637	0.49999767
1	-1.61228187	1.52895660	-4.17603402
1	-3.69218336	0.23913284	-4.64773692
1	-4.87188846	-0.90140918	-2.78923890
1	-5.03818974	-2.48444044	-1.55116046
6	-4.70445039	-0.80621768	3.63815709
1	0.49160710	1.48137458	-3.73593830
1	2.49466575	4.34392224	-1.26632591
6	0.92500305	4.21407593	0.98481240
1	-6.32270046	-2.71908347	2.51583783
6	-0.38952836	4.97386383	1.28381532
6	2.05027318	5.26397428	0.91061045
6	1.26542792	3.25821100	2.15270689
1	-0.61264586	5.69060699	0.47982251
1	-0.28221412	5.54109792	2.22077218
1	-1.23804125	4.28966717	1.38711407
1	2.21702414	2.74006986	1.96395131
1	0.48902315	2.50147903	2.30228370
1	1.37268345	3.83613547	3.08334796
1	2.08202484	5.81790354	1.85944133
1	1.88263099	5.99475793	0.10602284
1	3.03954763	4.80580374	0.76581782
6	-3.31598904	-1.14469673	4.23165348
6	-5.75683934	-1.51637345	4.51157139
6	-4.97505938	0.71360950	3.74559721
1	-5.60436946	-2.60492462	4.54643426
1	-6.78247457	-1.31819858	4.16780697
1	-5.67535403	-1.14080667	5.54128092
1	-3.12708123	-2.22699559	4.17984962
1	-3.28345411	-0.84479412	5.29009052
1	-2.50996952	-0.62703824	3.70190406
1	-4.92793549	1.02310605	4.80062259
1	-5.98008057	0.95389698	3.36877608
1	-4.24233203	1.29803050	3.17990308
1	2.34584999	3.08714716	-3.37888426
1	-6.44960675	-3.51726494	0.18926357
6	0.69021461	-2.30427749	2.35148989
6	1.00541486	-3.79895817	2.24342359
6	-0.12912389	-4.67934282	1.69511775
6	0.19676731	-1.61122382	1.07037759
6	-0.36687237	-4.48156576	0.19044880
6	-1.22059854	-3.26335288	-0.18092444
1	-0.09839786	-2.13380084	3.09958820

1	1.89594180	-3.94593001	1.60976505
1	0.13751815	-5.73345211	1.87030061
1	0.60805602	-4.41748451	-0.31382010
1	1.57707370	-1.75673355	2.70532923
1	1.28164107	-4.15335244	3.24937356
1	-1.05915097	-4.49416358	2.25811111
1	-0.88285211	-5.36179467	-0.22710587
1	-1.00702903	-2.95976827	-1.21781673
1	-2.28730192	-3.51585814	-0.10559531
8	-0.00245903	-0.27062969	1.31220680
8	-1.10575793	-2.11244560	0.69086955
13	-1.49069871	0.43128054	0.68105078
8	7.99862696	1.06588588	-4.26916552
6	8.56545038	1.36841755	-5.56644617
1	8.53090847	0.48475116	-6.21597937
6	6.17749291	0.42127957	-2.89390618
6	4.82267532	-0.28568567	-2.85912937
6	4.26870754	-0.42148042	-1.43722610
6	6.69041433	0.67283720	-4.29843649
6	2.91077976	-1.13047573	-1.39875901
6	2.32594925	-1.18169031	0.00637914
1	6.94403900	-0.14083044	-2.33864747
1	4.91829092	-1.28111298	-3.32123961
1	4.99255069	-0.96754616	-0.80725931
1	3.00844325	-2.15527993	-1.79265452
1	6.11297485	1.40327500	-2.39402068
1	4.10918091	0.27129643	-3.48449349
1	4.16677097	0.58317176	-0.99171011
1	2.19837400	-0.60269565	-2.05187812
1	2.20367542	-0.16313487	0.40754182
1	2.99630500	-1.74507184	0.68294331
8	6.04783582	0.56436606	-5.32579740
8	1.04118126	-1.82488332	-0.06474987
1	9.60024354	1.66402054	-5.36840311
1	8.01263366	2.18589237	-6.04640772

Electronic energy = -2300.221461 a.u.

DFT-D4 dispersion correction = -0.144480 a.u.

Thermal free energy = 0.709884 a.u.

Gibbs free energy = -2299.656057 a.u.

Number of imaginary frequencies = 0.

13a_{CLCL}

Atomic N.	X	Y	Z
6	0.22177411	3.08265802	-5.55255116
6	0.05725741	4.17686116	-4.69044425
6	0.19164934	4.06741848	-3.30596396
6	0.48930495	2.77295220	-2.76606929
6	0.79243309	1.68364441	-3.64554391
6	0.60688419	1.85945062	-5.03548918
6	1.38947500	0.42256813	-3.16077852
7	1.23204517	0.01546427	-1.85877960
6	1.87080488	-1.10315735	-1.38403587
6	2.63785983	-1.89263626	-2.25927250

6	2.77242191	-1.51787471	-3.58908363
6	2.17253168	-0.34892557	-4.03820056
6	1.84984417	-1.44271197	0.05204309
6	1.71619721	-0.42743536	1.05468303
6	2.12978729	-0.69985947	2.40015506
6	2.45323386	-2.01983529	2.71991705
6	2.41053803	-3.05950175	1.77768290
6	2.14327400	-2.76468680	0.45271054
8	0.48664903	2.60588602	-1.44686058
8	1.23911026	0.77366432	0.74406030
1	3.17492625	-2.75385061	-1.87238375
1	3.38938971	-2.11098507	-4.26514425
1	2.34533408	0.00019506	-5.05184355
1	0.73976915	1.01284016	-5.70847218
6	0.01612066	5.29306992	-2.38581593
1	2.14298501	-3.56555688	-0.28669303
1	2.73557994	-2.26363497	3.74291046
6	2.22636414	0.42807575	3.44860419
1	-0.20350092	5.14021087	-5.12495681
6	3.17608368	1.53507226	2.93046276
6	2.80511795	-0.08480100	4.78107596
6	0.83627719	1.03400608	3.75265934
1	4.18350866	1.13018847	2.75502850
1	3.25901446	2.33307993	3.68364545
1	2.80873504	1.97749113	1.99821789
1	0.15898847	0.26799878	4.15909432
1	0.37731068	1.47169913	2.85973471
1	0.93791750	1.82494053	4.51138964
1	2.89366468	0.75962475	5.47908372
1	3.80773347	-0.51919215	4.65717659
1	2.15604941	-0.83538458	5.25572563
6	-1.21271093	5.11814374	-1.46175108
6	-0.19968677	6.58517950	-3.19674020
6	1.29196873	5.49559853	-1.53329015
1	-1.12699269	6.55664562	-3.78748189
1	0.64024876	6.79326060	-3.87549860
1	-0.28083248	7.43209590	-2.50082346
1	-2.13195036	5.01447849	-2.05758484
1	-1.32455466	6.01008966	-0.82645412
1	-1.11513205	4.24230061	-0.81149301
1	1.16875870	6.37950047	-0.88944761
1	2.16540583	5.66785832	-2.17927044
1	1.49342109	4.62884011	-0.89513567
1	2.60889518	-4.08692375	2.08287401
1	0.05901548	3.20149756	-6.62366553
6	-3.50666414	1.57351874	-0.83089328
6	-3.27899087	1.85938138	-2.32081418
6	-3.51324454	0.65432712	-3.25132835
6	-2.38111601	0.88824568	-0.04125871
6	-2.37646841	-0.37414883	-3.31718594
6	-1.97632138	-0.97911583	-1.97858446
1	-4.42058907	0.97429322	-0.70848420
1	-2.27900219	2.28640059	-2.48752895
1	-3.68430425	1.02887413	-4.27277594

1	-1.48870808	0.09029409	-3.77331492
1	-3.67158775	2.51874287	-0.29219616
1	-3.99112355	2.64858931	-2.60821410
1	-4.44862356	0.15072961	-2.95028882
1	-2.67309632	-1.20378427	-3.98122538
1	-1.20128253	-1.74938754	-2.11152423
1	-2.83384975	-1.45108520	-1.47158681
8	-1.38157212	1.63990575	0.41059583
8	-1.44289725	0.00414760	-1.07167012
13	0.08592041	1.07994783	-0.60255754
8	-0.20991007	-7.14099887	4.77875023
6	0.24605284	-8.50646754	4.62357659
1	-0.38986743	-9.04426638	3.90934388
6	-0.62688040	-4.97549851	3.89805000
6	-1.22384491	-4.28281992	2.67080572
6	-1.46598095	-2.78862326	2.90521635
6	-0.19559437	-6.40359465	3.62895156
6	-2.06072662	-2.08784207	1.67833217
6	-2.20924826	-0.58507660	1.89425664
1	-1.31613495	-4.96291861	4.75440558
1	-2.16953658	-4.77754085	2.39467814
1	-2.13951742	-2.64928899	3.76883520
1	-3.05096779	-2.51437575	1.44914587
1	0.27788903	-4.43369610	4.22625149
1	-0.54226280	-4.41963270	1.81887084
1	-0.50952364	-2.31062745	3.17388966
1	-1.41878267	-2.27096941	0.80242913
1	-1.23889884	-0.07848661	1.96142753
1	-2.76422320	-0.38321545	2.82333609
8	0.14807789	-6.85370573	2.55155025
8	-2.99804093	0.01043821	0.83203127
1	0.17242892	-8.95127954	5.62062606
1	1.28271606	-8.52698552	4.26416001

Electronic energy = -2300.224207 a.u.

DFT-D4 dispersion correction = -0.150993 a.u.

Thermal free energy = 0.714283 a.u.

Gibbs free energy = -2299.660916 a.u.

Number of imaginary frequencies = 0.

13b_{CLCL}

Atomic N.	X	Y	Z
6	4.35747611	2.49471882	1.78678311
6	4.55796293	1.37225300	0.97163543
6	3.60340710	0.92667856	0.05492564
6	2.36053340	1.63861676	-0.01119571
6	2.22929657	2.88684354	0.67969951
6	3.21930570	3.26113155	1.61375257
6	1.17300227	3.86132882	0.34302355
7	-0.01609627	3.45334850	-0.19803904
6	-0.96403701	4.35485632	-0.60016474
6	-0.72227446	5.73120638	-0.44212240
6	0.46690067	6.16294517	0.12998606
6	1.42402040	5.23395560	0.51525516

6	-2.21043703	3.90972390	-1.25550932
6	-2.30017585	2.68294911	-1.99030284
6	-3.40081965	2.47883328	-2.88621889
6	-4.44162708	3.40936096	-2.86491034
6	-4.43346657	4.53025146	-2.02498995
6	-3.31643478	4.78691385	-1.25154681
8	1.34969507	1.14567485	-0.73390848
8	-1.36457596	1.73466449	-1.86894364
1	-1.44459741	6.45082716	-0.81575513
1	0.66640598	7.22993423	0.23642927
1	2.38813062	5.56048380	0.89407126
1	3.07262773	4.15482342	2.21992602
6	3.88712122	-0.28787880	-0.85232668
1	-3.29824601	5.66743161	-0.61025973
1	-5.30450354	3.25518801	-3.51015122
6	-3.45171777	1.26452082	-3.83552862
1	5.49191998	0.82237581	1.07218567
6	-2.17201873	1.21157298	-4.70374198
6	-4.65034906	1.33614725	-4.80084985
6	-3.59426736	-0.03820511	-3.01819894
1	-2.08665223	2.11991757	-5.31782170
1	-2.22194165	0.34836612	-5.38470150
1	-1.26904355	1.12067467	-4.09104839
1	-4.53663750	-0.03783751	-2.45047926
1	-2.76411298	-0.14590133	-2.31344337
1	-3.60303005	-0.90956375	-3.69119759
1	-4.61339628	0.47106596	-5.47830946
1	-4.62652348	2.24428909	-5.42032261
1	-5.61508071	1.29865677	-4.27459164
6	2.96452246	-1.46842411	-0.48026231
6	5.34054294	-0.78041779	-0.71571343
6	3.67573844	0.10491513	-2.33422742
1	5.56012223	-1.15753182	0.29331862
1	6.06823639	0.00625695	-0.96264246
1	5.49971373	-1.61325934	-1.41521129
1	3.16067939	-1.81242351	0.54530402
1	3.14785250	-2.31866494	-1.15449593
1	1.91309129	-1.17556593	-0.56169973
1	3.89467607	-0.75897823	-2.97985476
1	4.35756033	0.91978404	-2.61850045
1	2.64723806	0.42969238	-2.52530139
1	-5.29154133	5.20159876	-1.99764459
1	5.10576683	2.77431403	2.52822416
6	-3.08351319	-0.07973185	1.29443424
6	-3.60883875	-1.50217143	1.50022688
6	-3.25177206	-2.49896050	0.39071490
6	-1.56650605	0.11380770	1.33769461
6	-1.74684214	-2.75837394	0.22229806
6	-0.97496008	-1.71616263	-0.57797479
1	-3.43192565	0.33664695	0.33789797
1	-4.70590409	-1.44723665	1.58295903
1	-3.74687735	-3.45656777	0.61761521
1	-1.60429973	-3.69852567	-0.33630528
1	-3.47363024	0.57691771	2.08688339

1	-3.24312697	-1.88490866	2.46540131
1	-3.67318820	-2.15670931	-0.56999097
1	-1.27711380	-2.90590364	1.20628330
1	0.06466041	-2.05280110	-0.70454169
1	-1.42276713	-1.61341692	-1.57896205
8	-1.17584728	1.40510512	1.24013270
8	-0.91413591	-0.38329213	-0.00534250
13	-0.37473490	1.51653543	-0.38805718
8	2.29712341	-6.82191732	2.69391375
6	3.19690101	-7.61117589	1.87938684
1	2.99068073	-7.45124772	0.81357256
6	1.39445771	-4.73818049	3.37658328
6	1.50804325	-3.21759831	3.27454683
6	0.47571545	-2.49742046	4.14844033
6	2.38177241	-5.47381623	2.49129382
6	0.59494136	-0.96585239	4.12757601
6	0.31758317	-0.30106463	2.78525767
1	0.38273939	-5.07707654	3.09683991
1	1.39454981	-2.92472597	2.22086869
1	-0.54142296	-2.78435880	3.83568585
1	1.61314440	-0.67074442	4.43242131
1	1.54149796	-5.08394816	4.41237603
1	2.52497537	-2.90875426	3.56454378
1	0.58351985	-2.83952131	5.19146978
1	-0.09324628	-0.53713854	4.87284664
1	0.99296528	-0.67254448	1.99766985
1	0.44457968	0.78717893	2.86246855
8	3.14981398	-4.96311979	1.69774286
8	-1.05300100	-0.59502235	2.41520706
1	3.00427447	-8.65115629	2.15991010
1	4.23977254	-7.33948464	2.08562493

Electronic energy = -2300.227556 a.u.

DFT-D4 dispersion correction = -0.146374 a.u.

Thermal free energy = 0.709749 a.u.

Gibbs free energy = -2299.664181 a.u.

Number of imaginary frequencies = 0.

TS4ax_{CLCL}

Atomic N.	X	Y	Z
6	0.24640575	3.11443186	-5.55811405
6	0.06157172	4.19817686	-4.68706846
6	0.18143936	4.07612467	-3.30229425
6	0.48434058	2.77886844	-2.77176166
6	0.81047243	1.70234847	-3.65873027
6	0.63882411	1.89026201	-5.04879522
6	1.41663098	0.44324782	-3.17999816
7	1.25070846	0.02293305	-1.88389957
6	1.89287281	-1.09529388	-1.41440082
6	2.67533684	-1.87024820	-2.28892565
6	2.82178831	-1.48009956	-3.61315227
6	2.21664834	-0.31176311	-4.05673885
6	1.86029804	-1.44839406	0.01832497
6	1.71451640	-0.44177389	1.02793396

6	2.13109255	-0.72008175	2.37141609
6	2.45690179	-2.04132771	2.68380570
6	2.41852474	-3.07523394	1.73503375
6	2.15728045	-2.77188516	0.41059205
8	0.46487385	2.59827495	-1.45449877
8	1.22476208	0.75624019	0.72598249
1	3.21440315	-2.73159623	-1.90498948
1	3.45097232	-2.06099916	-4.28857136
1	2.39663315	0.04881160	-5.06511784
1	0.78865081	1.05192959	-5.72852039
6	-0.01246385	5.29168415	-2.37240124
1	2.16526794	-3.56671715	-0.33534074
1	2.73938441	-2.29051256	3.70549107
6	2.23334742	0.40380058	3.42382574
1	-0.20321292	5.16342163	-5.11493015
6	3.18163800	1.51094377	2.90322495
6	2.81910753	-0.11446658	4.75109720
6	0.84701264	1.01260698	3.73838234
1	4.18729258	1.10504675	2.72025037
1	3.27043867	2.30677867	3.65804124
1	2.80889845	1.95647359	1.97450805
1	0.16970508	0.24744464	4.14638758
1	0.38509277	1.45512903	2.84936500
1	0.95559734	1.80050135	4.49931955
1	2.91317844	0.72738791	5.45149803
1	3.82022285	-0.55004740	4.61969519
1	2.17167306	-0.86572021	5.22695208
6	-1.24728441	5.09911060	-1.46002221
6	-0.23170009	6.58960676	-3.17301011
6	1.25459468	5.49578190	-1.50720000
1	-1.15364933	6.55911016	-3.77199149
1	0.61223328	6.81066322	-3.84261584
1	-0.32552323	7.42935228	-2.47001719
1	-2.16059065	4.99112606	-2.06419182
1	-1.37263024	5.98553085	-0.81949341
1	-1.14590204	4.21973944	-0.81515908
1	1.11898482	6.37167978	-0.85492373
1	2.13178706	5.68197012	-2.14414620
1	1.45776713	4.62372875	-0.87674868
1	2.61912775	-4.10390806	2.03449321
1	0.09431001	3.24235082	-6.62974882
6	-3.51259565	1.57511950	-0.82313520
6	-3.27746773	1.83422589	-2.31719708
6	-3.50566673	0.61608559	-3.23355722
6	-2.39712286	0.91233510	-0.00671627
6	-2.34851480	-0.38760921	-3.32589221
6	-1.91888154	-0.99946404	-1.99898231
1	-4.42644167	0.97742498	-0.69456857
1	-2.27840686	2.26207399	-2.48572326
1	-3.70977998	0.98212594	-4.25204849
1	-1.47716951	0.10216425	-3.78766274
1	-3.68320584	2.53245616	-0.30657050
1	-3.99082541	2.61739159	-2.61796260
1	-4.42255735	0.09342822	-2.90892434

1	-2.63723707	-1.21410716	-3.99733663
1	-1.12450612	-1.74719274	-2.15275025
1	-2.76104450	-1.50947261	-1.50086665
8	-1.38393211	1.64155626	0.41460121
8	-1.41890728	-0.01724549	-1.08203375
13	0.07530372	1.05924273	-0.62692261
8	-0.21415091	-7.11202383	4.82785749
6	0.21010426	-8.48835182	4.67943573
1	-0.47160530	-9.02998066	4.01184273
6	-0.64241171	-4.95941305	3.92322731
6	-1.24673820	-4.26619244	2.70041370
6	-1.46867752	-2.76824737	2.93127537
6	-0.24887876	-6.39991045	3.66252875
6	-2.07583976	-2.06819201	1.71006942
6	-2.20617294	-0.56350905	1.91893327
1	-1.31631315	-4.92332792	4.79138613
1	-2.20159936	-4.75110769	2.43919563
1	-2.12695765	-2.61792517	3.80480862
1	-3.07312202	-2.48691869	1.49808919
1	0.27889225	-4.43444490	4.23206949
1	-0.57871825	-4.41490459	1.83973718
1	-0.50318950	-2.29905891	3.18233681
1	-1.44929445	-2.26032734	0.82517552
1	-1.23110008	-0.06531371	1.97107232
1	-2.75361586	-0.34701198	2.84894228
8	0.02915283	-6.87892675	2.57882404
8	-2.99827361	0.02741758	0.85367680
1	0.18200582	-8.91035271	5.68865442
1	1.22580922	-8.53506565	4.26659441

Electronic energy = -2300.224165 a.u.

DFT-D4 dispersion correction = -0.150822 a.u.

Thermal free energy = 0.711723 a.u.

Gibbs free energy = -2299.663263 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 63.2i

TS4eq_{CLCL}

Atomic N.	X	Y	Z
6	1.87946882	4.20128885	0.04853794
6	1.59876118	3.71005237	-1.23381026
6	0.61479242	2.74707880	-1.47205053
6	-0.09552431	2.22378314	-0.34119400
6	0.07233886	2.84278759	0.93754066
6	1.09821323	3.79478164	1.11577024
6	-0.88167183	2.61221220	2.03796238
7	-1.56534175	1.43057035	2.14635360
6	-2.49366017	1.24885745	3.13582571
6	-2.76046037	2.28914882	4.04561547
6	-2.06536957	3.48651423	3.95513388
6	-1.12605179	3.65576754	2.94774654
6	-3.27223217	-0.00040489	3.23887915
6	-3.54189572	-0.83070993	2.10486571
6	-4.58189651	-1.81620283	2.18858560

6	-5.16317756	-2.04817385	3.43672385
6	-4.78186490	-1.34845085	4.58859754
6	-3.86450254	-0.31963519	4.48001403
8	-0.91408654	1.17817381	-0.48265708
8	-2.85072382	-0.69012816	0.97154168
1	-3.54763030	2.16650280	4.78344960
1	-2.28476175	4.30215772	4.64521235
1	-0.61953471	4.60782749	2.81704996
1	1.29066520	4.19388112	2.11190262
6	0.32801211	2.25263509	-2.90422391
1	-3.57648113	0.23877152	5.37006489
1	-5.92964657	-2.81531079	3.53010672
6	-5.02924579	-2.62650783	0.95561200
1	2.19540689	4.08152952	-2.06470194
6	-5.39915922	-1.68057699	-0.21126122
6	-6.27404265	-3.48636745	1.24834695
6	-3.89400991	-3.58350133	0.53130803
1	-6.22825507	-1.01882168	0.07929216
1	-5.72975209	-2.27389712	-1.07722600
1	-4.55107400	-1.05946506	-0.51651798
1	-3.69246755	-4.31843499	1.32486058
1	-2.97265785	-3.02802816	0.33098134
1	-4.17800559	-4.13419976	-0.37887905
1	-6.57291189	-4.00435306	0.32577395
1	-7.12704232	-2.87611715	1.57882423
1	-6.08252917	-4.25773891	2.00803045
6	0.78824424	0.78627602	-3.05769501
6	1.07628507	3.08844721	-3.96040702
6	-1.18256483	2.36813217	-3.21732694
1	2.16840442	3.01428545	-3.85931826
1	0.79876916	4.15136862	-3.91377991
1	0.80868277	2.71816315	-4.96077494
1	1.87824306	0.70747738	-2.92697448
1	0.54060071	0.41346225	-4.06371881
1	0.30066450	0.14451092	-2.31679106
1	-1.37310461	2.03120389	-4.24765595
1	-1.51228094	3.41444030	-3.13908455
1	-1.78619190	1.76135889	-2.53432295
1	-5.21867731	-1.60140516	5.55454506
1	2.69351842	4.91120746	0.19347213
6	0.35144333	-3.03168162	2.04638436
6	0.85225988	-4.24825713	1.25920285
6	0.13095452	-4.55535455	-0.06396379
6	0.74427023	-1.66853844	1.52341109
6	0.32367610	-3.54727732	-1.21255863
6	-0.60556968	-2.33398805	-1.18736154
1	-0.74195218	-3.03744681	2.14731261
1	0.74053886	-5.12658649	1.91454300
1	0.49578562	-5.53758635	-0.40534227
1	0.13259040	-4.06110325	-2.16929892
1	0.76159552	-3.06485337	3.07189206
1	1.93204470	-4.14131343	1.07400227
1	-0.94784278	-4.68540721	0.12719194
1	1.37242650	-3.20940595	-1.24621729

1	-0.45134696	-1.74880231	-2.11149587
1	-1.65421850	-2.68223714	-1.19606680
8	0.19324965	-0.59779974	2.00195434
8	-0.38242743	-1.50158976	-0.05911645
13	-1.17501731	-0.04701115	0.82432899
8	6.17516117	1.52576818	-3.63485576
6	5.53319060	1.81024301	-4.90110769
1	4.44221617	1.74672077	-4.80062285
6	6.56632703	1.99863825	-1.34350052
6	5.99620335	0.69941279	-0.73813595
6	4.53529237	0.82613144	-0.29479240
6	5.87135911	2.39980677	-2.63007769
6	3.96112510	-0.49218205	0.23833010
6	2.51942869	-0.31808153	0.68415774
1	7.63680776	1.86105095	-1.55622822
1	6.62047857	0.41994011	0.12567638
1	4.45503393	1.60863079	0.47815412
1	4.56600131	-0.85806844	1.08376908
1	6.45430008	2.83418626	-0.64054551
1	6.09710746	-0.11305883	-1.47441415
1	3.91831406	1.17468343	-1.13863866
1	4.00629980	-1.26305329	-0.54750115
1	1.88795376	0.04973694	-0.13713804
1	2.43031210	0.37288867	1.53301102
8	5.12851978	3.35346947	-2.77550180
8	2.01032672	-1.62735719	1.08470891
1	5.90273394	1.04580301	-5.59125276
1	5.80246234	2.81470596	-5.25045130

Electronic energy = -2300.226500 a.u.

DFT-D4 dispersion correction = -0.148213 a.u.

Thermal free energy = 0.711653 a.u.

Gibbs free energy = -2299.663060 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 57.4i

14a_{CLCL}

Atomic N.	X	Y	Z
6	0.32120080	2.79479358	-5.61615346
6	0.05327960	3.89845338	-4.79365469
6	0.14069097	3.83498918	-3.40217583
6	0.48291476	2.57318744	-2.81257868
6	0.92929247	1.49838160	-3.64904497
6	0.78493441	1.62195973	-5.04868819
6	1.64673554	0.32531579	-3.10848999
7	1.50212075	-0.04256354	-1.79788477
6	2.22449325	-1.07572832	-1.26466388
6	3.10684621	-1.80428577	-2.08212463
6	3.24773568	-1.46077576	-3.42043271
6	2.53559072	-0.38608764	-3.93562451
6	2.16403645	-1.37623965	0.18040548
6	1.83537422	-0.36811349	1.14440205
6	2.24851483	-0.53780717	2.50814514
6	2.70965124	-1.79803714	2.89220177

6	2.82726300	-2.86377709	1.98697549
6	2.59869260	-2.63809315	0.64036655
8	0.39365411	2.42978312	-1.49157752
8	1.17889746	0.73427171	0.79346594
1	3.71714053	-2.59176646	-1.64946803
1	3.94803762	-2.00645710	-4.05400703
1	2.69614285	-0.06281234	-4.95984588
1	1.01852041	0.77269523	-5.69008795
6	-0.10346568	5.08439534	-2.53006855
1	2.74218414	-3.44928632	-0.07323076
1	2.98143429	-1.97165947	3.93227959
6	2.22985688	0.64295187	3.50359438
1	-0.24736843	4.83200744	-5.26590721
6	3.07353658	1.80442433	2.92422202
6	2.85305133	0.25313417	4.85773207
6	0.79512301	1.14342028	3.78448200
1	4.11500379	1.48696791	2.77091418
1	3.07726772	2.64850471	3.63039571
1	2.66934904	2.15627031	1.96834953
1	0.17763121	0.33635616	4.20623272
1	0.31739400	1.52187200	2.87455402
1	0.82816770	1.95911257	4.52294877
1	2.86658229	1.13761885	5.51027461
1	3.89002093	-0.09634944	4.75131706
1	2.27407837	-0.52664201	5.37408788
6	-1.34044786	4.90376959	-1.62030768
6	-0.34437770	6.33999193	-3.38951255
6	1.14703002	5.35530632	-1.65889182
1	-1.25767600	6.25967561	-3.99714052
1	0.50187105	6.55161137	-4.05889527
1	-0.46680859	7.20769481	-2.72578847
1	-2.24224555	4.72319103	-2.22460643
1	-1.50540522	5.82175888	-1.03527031
1	-1.20263771	4.06862936	-0.92561041
1	0.98281774	6.25247476	-1.04287274
1	2.02723089	5.53725839	-2.29256937
1	1.36259158	4.51310999	-0.99222448
1	3.13713358	-3.84853705	2.33710215
1	0.18723614	2.87092751	-6.69507739
6	-3.57879475	1.99959908	-0.40331598
6	-3.37116933	1.66915594	-1.89790718
6	-3.68823235	0.20941838	-2.31546819
6	-2.54707568	1.36717603	0.49849976
6	-2.52997855	-0.49739219	-3.04794600
6	-1.51985693	-1.14323835	-2.08840314
1	-4.58012835	1.69304358	-0.07404396
1	-2.33895742	1.92423359	-2.16881984
1	-4.57421697	0.21340786	-2.96778467
1	-2.01733472	0.22675747	-3.70227471
1	-3.48376432	3.08769269	-0.26598785
1	-4.01025949	2.36479033	-2.46250992
1	-3.96762922	-0.38621148	-1.43160815
1	-2.92272615	-1.29030413	-3.70610805
1	-0.63268338	-1.48108727	-2.65874954

1	-1.97953772	-2.05403231	-1.65605563
8	-1.34940674	1.70860328	0.52807922
8	-1.17907164	-0.28281381	-1.02682978
13	0.12188563	0.85815726	-0.66274318
8	0.01669934	-7.20807945	3.87713132
6	0.01752810	-8.63646693	3.64296313
1	-0.99402201	-9.04555551	3.75924462
6	-0.70964464	-5.01457334	3.34785796
6	-1.61608204	-4.15936008	2.46360032
6	-1.49962800	-2.66670878	2.78937961
6	-0.78029979	-6.49423078	3.02680840
6	-2.37914265	-1.79995021	1.87948294
6	-2.20468136	-0.32255264	2.19106485
1	-0.95499684	-4.88798064	4.41489026
1	-2.65961360	-4.49192245	2.57699089
1	-1.77411265	-2.49703589	3.84545774
1	-3.43795528	-2.08182838	1.99358240
1	0.34231011	-4.69920121	3.24994113
1	-1.35624143	-4.32931072	1.40794771
1	-0.44749486	-2.35346963	2.68666945
1	-2.10140408	-1.96318791	0.82756391
1	-1.17217737	0.00830567	2.04469987
1	-2.52563707	-0.07638363	3.21321510
8	-1.44071250	-7.00539871	2.14237829
8	-3.08283841	0.45985086	1.31181184
1	0.69300204	-9.05311984	4.39635451
1	0.37816306	-8.86004309	2.63096812

Electronic energy = -2300.231061 a.u.

DFT-D4 dispersion correction = -0.148699 a.u.

Thermal free energy = 0.713079 a.u.

Gibbs free energy = -2299.666680 a.u.

Number of imaginary frequencies = 0.

14b_{CLCL}

Atomic N.	X	Y	Z
6	2.44386641	5.86577978	-2.37157627
6	2.20711205	5.14911914	-3.55186709
6	1.40539984	4.00640398	-3.59164839
6	0.83060999	3.54798304	-2.35900000
6	0.92534903	4.37501332	-1.19553558
6	1.78309128	5.49587235	-1.21447648
6	0.05727000	4.17562143	-0.02000589
7	-0.45684673	2.94475541	0.28824056
6	-1.29709357	2.79179593	1.35899741
6	-1.65008781	3.90189775	2.14628559
6	-1.13741848	5.15546394	1.84351647
6	-0.28934863	5.29819786	0.75548360
6	-1.89609972	1.48229851	1.67952038
6	-2.16215388	0.51148153	0.66361592
6	-3.04179815	-0.58529856	0.95274097
6	-3.46488920	-0.74960995	2.27366932
6	-3.07999583	0.11783633	3.30507974
6	-2.32384295	1.23634819	3.00103703

8	0.20200312	2.37184406	-2.31071420
8	-1.61097501	0.63093583	-0.54347422
1	-2.36704560	3.77853037	2.95288396
1	-1.42967955	6.02651963	2.43121910
1	0.06785180	6.28079203	0.46175812
1	1.94337819	6.06284332	-0.29780520
6	1.18000736	3.25502423	-4.91876763
1	-2.03717232	1.92671040	3.79434715
1	-4.10706637	-1.59259481	2.52310019
6	-3.48266246	-1.57389427	-0.14447553
1	2.68474649	5.49286296	-4.46754578
6	-4.09997104	-0.81166978	-1.34087090
6	-4.55150771	-2.56110147	0.36220340
6	-2.26615848	-2.40440820	-0.61098170
1	-4.98381411	-0.24164605	-1.01884190
1	-4.42395972	-1.53018616	-2.10889204
1	-3.38413495	-0.11726243	-1.79225950
1	-1.88616236	-3.02741036	0.21301987
1	-1.45681921	-1.75393992	-0.95778621
1	-2.55706420	-3.07518239	-1.43401666
1	-4.85610085	-3.21276128	-0.46915536
1	-5.45096026	-2.04383037	0.72646762
1	-4.17446809	-3.21131048	1.16492904
6	1.91195454	1.89651657	-4.87284226
6	1.72997161	4.03756835	-6.12694189
6	-0.33149200	3.04116888	-5.16929211
1	2.82177192	4.16061683	-6.08596586
1	1.27032427	5.03251705	-6.21655799
1	1.49924615	3.47997426	-7.04594450
1	2.99819713	2.04640337	-4.78231065
1	1.72242339	1.32849140	-5.79676495
1	1.57120557	1.30052729	-4.02072366
1	-0.47676461	2.51884268	-6.12697247
1	-0.85139408	4.00845469	-5.23129847
1	-0.79558776	2.44830429	-4.37462775
1	-3.39220459	-0.07755512	4.33093665
1	3.12325403	6.71798617	-2.37367386
6	3.46522241	0.34767515	-0.83958277
6	4.04598683	-0.90300772	-1.51499521
6	3.33150713	-1.40802098	-2.78194761
6	2.25248322	0.15570908	0.03513656
6	1.94140162	-2.05191474	-2.61037012
6	0.76438536	-1.07541338	-2.58544843
1	3.21738214	1.12643644	-1.57214305
1	5.08360651	-0.66106415	-1.79453710
1	3.99937601	-2.15741355	-3.23690469
1	1.76517817	-2.73952602	-3.45438963
1	4.22663255	0.78208827	-0.16504945
1	4.11313276	-1.71750255	-0.77778981
1	3.26255009	-0.58589436	-3.51432382
1	1.92219006	-2.67008617	-1.69726804
1	-0.17757663	-1.65469635	-2.56995238
1	0.76213031	-0.49030040	-3.52412216
8	1.49575584	1.13245953	0.37380833

8	0.83036005	-0.21830429	-1.46473490
13	0.03348646	1.32870646	-0.84849524
8	-1.31888617	-5.89196656	6.86610399
6	-1.19516172	-7.10421923	7.64828950
1	-1.13818559	-7.98092338	6.99097441
6	-0.50197792	-4.37149332	5.24179152
6	0.60813353	-4.07019374	4.23577196
6	0.36455833	-2.76192758	3.47664682
6	-0.28074226	-5.66031174	6.01001608
6	1.47152241	-2.45799410	2.45942179
6	1.19933230	-1.16178061	1.71782915
1	-1.48261896	-4.43873770	4.74356925
1	0.69009920	-4.90633937	3.52441410
1	-0.60779728	-2.81018674	2.95800853
1	1.54906379	-3.28252350	1.73325294
1	-0.60266563	-3.55633120	5.97711122
1	1.57381564	-4.02568359	4.76217332
1	0.28601524	-1.92803630	4.19496477
1	2.44385534	-2.38868535	2.97271069
1	1.15269538	-0.29743507	2.39357587
1	0.26551894	-1.21058966	1.14022607
8	0.67710812	-6.40205466	5.90117635
8	2.29511252	-0.95298400	0.76804649
1	-2.09610018	-7.14182232	8.26808447
1	-0.29417977	-7.06735207	8.27351110

Electronic energy = -2300.227344 a.u.

DFT-D4 dispersion correction = -0.145043 a.u.

Thermal free energy = 0.707501 a.u.

Gibbs free energy = -2299.664886 a.u.

Number of imaginary frequencies = 0.

15_{CLCL}

Atomic N.	X	Y	Z
6	1.89835771	0.16598534	-4.47436740
6	0.85796893	-0.50525313	-5.12911981
6	-0.36872278	-0.76975486	-4.51632352
6	-0.54801726	-0.33231873	-3.16675232
6	0.48303634	0.41961973	-2.51293247
6	1.70569588	0.62980195	-3.18574149
6	0.30791494	1.04510831	-1.18447639
7	-0.58029383	0.51903478	-0.28188412
6	-0.81342428	1.09593707	0.93862781
6	-0.08818156	2.23900136	1.30448085
6	0.83661193	2.77862092	0.41756475
6	1.02841651	2.19656591	-0.83124191
6	-1.85019402	0.54776853	1.83960946
6	-3.04427535	-0.08031987	1.35448663
6	-4.12540771	-0.34164023	2.25184818
6	-3.91119594	-0.09787935	3.61141286
6	-2.70035988	0.40210898	4.10818454
6	-1.68816195	0.74185910	3.22748313
8	-1.70201906	-0.61480516	-2.53909844
8	-3.17220884	-0.40642184	0.05355509

1	-0.28590233	2.71569295	2.26050271
1	1.40088645	3.67539485	0.67442486
1	1.70663707	2.66067292	-1.54170245
1	2.51772667	1.14261290	-2.67129144
6	-1.48235783	-1.53060973	-5.26524141
1	-0.73805443	1.12117518	3.60354479
1	-4.70672382	-0.31819503	4.32090201
6	-5.48249675	-0.86976892	1.74090361
1	1.02674375	-0.84660411	-6.14865786
6	-6.06548518	0.11029698	0.69459344
6	-6.51356956	-0.98672914	2.87992734
6	-5.32948210	-2.27705428	1.11775284
1	-6.23200799	1.10020898	1.14388718
1	-7.03604654	-0.26511863	0.33635224
1	-5.39929894	0.22575716	-0.16700361
1	-4.93324115	-2.98869247	1.85701035
1	-4.66058482	-2.26615924	0.25096367
1	-6.31329801	-2.64520128	0.78916800
1	-7.46978451	-1.32958948	2.46002573
1	-6.69581320	-0.02114726	3.37335588
1	-6.20969789	-1.71723333	3.64380679
6	-1.76805205	-2.88232788	-4.56817836
6	-1.08002019	-1.84515419	-6.71917057
6	-2.77051910	-0.67520241	-5.32611193
1	-0.20194760	-2.50474915	-6.77560146
1	-0.87002692	-0.93341327	-7.29723067
1	-1.91287855	-2.36527613	-7.21316720
1	-0.86487207	-3.50954597	-4.55748709
1	-2.55175357	-3.42420876	-5.11932690
1	-2.10197636	-2.74729913	-3.53440944
1	-3.55207568	-1.22411639	-5.87305397
1	-2.58275476	0.26680534	-5.86210857
1	-3.14832958	-0.43729441	-4.32657986
1	-2.56140613	0.52907936	5.18182921
1	2.85272778	0.31857214	-4.97823084
6	1.93458567	-2.15564821	4.12802994
6	1.43081926	-3.25061661	3.16569431
6	0.24889147	-2.80727929	2.29814026
6	2.44747817	-0.92099453	3.41477020
6	-0.28538176	-3.92143212	1.39392400
6	-1.48528798	-3.49579837	0.54416394
1	1.12891039	-1.82778676	4.79765158
1	1.13664879	-4.12321204	3.77166946
1	-0.56606306	-2.44408918	2.94807283
1	-0.59522064	-4.78473410	2.00927621
1	2.75394226	-2.55886841	4.74311660
1	2.26407492	-3.57948627	2.52593444
1	0.54891043	-1.95433195	1.66857114
1	0.51260862	-4.27625210	0.72069211
1	-1.88446587	-4.38139604	0.01686909
1	-2.28655034	-3.12796639	1.21377912
8	1.96210446	0.19523981	3.48692870
8	-1.12850657	-2.51795397	-0.41805014
13	-1.71078301	-0.94314097	-0.80175907

8	5.42764095	5.98288810	-0.66834604
6	4.64526604	6.96747410	-1.38937599
1	4.22740801	6.52930953	-2.30420677
6	5.64692429	3.89337485	0.43036113
6	4.88484039	2.80602411	1.18820643
6	5.81518823	1.73815515	1.77747697
6	4.73526411	4.88115550	-0.27225194
6	5.09519923	0.69348315	2.64549899
6	4.08595051	-0.13436301	1.85586569
1	6.29038343	3.44461312	-0.34640881
1	4.15654672	2.34780415	0.50463527
1	6.35345248	1.22906196	0.95868007
1	4.57434493	1.19374509	3.47610162
1	6.32725350	4.45215561	1.09064626
1	4.29512058	3.26718418	1.99663662
1	6.58844022	2.22647747	2.39284734
1	5.83793350	0.01158071	3.08758386
1	4.56761674	-0.63695113	1.00542906
1	3.25205221	0.48045281	1.49521737
8	3.54445342	4.72620052	-0.48371236
8	3.54019704	-1.22378763	2.65306427
1	5.34612654	7.77236357	-1.62944956
1	3.82587783	7.33874863	-0.76168669

Electronic energy = -2300.242144 a.u.

DFT-D4 dispersion correction = -0.138426 a.u.

Thermal free energy = 0.704524 a.u.

Gibbs free energy = -2299.676046 a.u.

Number of imaginary frequencies = 0.

Propagation stage for CL-LA

9_{CLLA}

Atomic N.	X	Y	Z
8	2.58607118	3.33858712	2.14294075
8	3.56466997	2.48554301	0.32273582
6	3.14947564	2.40403132	1.61677292
6	3.44942913	1.06931096	2.30012692
8	4.80395448	0.62484164	1.96706070
6	5.16484639	0.64980832	0.65269586
6	4.12565420	1.27234547	-0.28147366
8	6.23007956	0.20027835	0.29713808
6	4.70338261	1.66033050	-1.62614911
6	3.35642541	1.14604759	3.80964429
1	2.73683932	0.32092391	1.90518922
1	3.30414239	0.54225975	-0.40460677
1	3.92036761	2.08084336	-2.26831807
1	5.12662625	0.77399602	-2.11157493
1	5.50509249	2.39831655	-1.49983530
1	2.34274917	1.44077356	4.10407712
1	4.05938278	1.89195206	4.20010474
1	3.58663994	0.16657295	4.24533081
6	-2.44888096	0.78047133	4.00230995
6	-1.84428254	-0.44226199	4.31690723
6	-0.91508591	-1.06408692	3.47622895
6	-0.58820291	-0.40561236	2.25272830
6	-1.13781867	0.88557061	1.96378698
6	-2.08983785	1.44312767	2.84128050
6	-0.69858920	1.70377936	0.81221164
7	-0.27876707	1.09607304	-0.34071299
6	0.20921738	1.80514681	-1.40618827
6	0.25562729	3.20471287	-1.32449752
6	-0.19254058	3.84506274	-0.17389032
6	-0.66634785	3.10159315	0.90028089
6	0.70547747	1.09550195	-2.60552770
6	1.26619222	-0.22197422	-2.55329164
6	1.83691976	-0.80755946	-3.72409704
6	1.79080117	-0.06524616	-4.90774085
6	1.20562904	1.20452619	-4.98071733
6	0.67234745	1.77720243	-3.83969035
8	0.25658376	-1.00182723	1.37906236
8	1.29087117	-0.90879583	-1.39113586
1	0.69545374	3.77631857	-2.13717493
1	-0.12718047	4.93018278	-0.09501775
1	-0.95677013	3.58904921	1.82618550
1	-2.57603593	2.37991217	2.57130945
6	-0.28885120	-2.42318316	3.85499140
1	0.19348107	2.75417720	-3.89913412
1	2.20627933	-0.49285360	-5.81800308
6	2.44675904	-2.22504840	-3.70134517
1	-2.12961566	-0.93275121	5.24548663
6	3.60207996	-2.31077523	-2.67618947
6	3.03157632	-2.61683691	-5.07227907
6	1.35097806	-3.26281622	-3.35868651

1	4.41088614	-1.61515522	-2.94378328
1	4.02353056	-3.32701349	-2.67967410
1	3.26333639	-2.08369366	-1.66016894
1	0.54842379	-3.23949664	-4.10975232
1	0.90263376	-3.07887759	-2.37686877
1	1.78699582	-4.27327741	-3.35757276
1	3.46418277	-3.62440699	-4.99833072
1	3.83401073	-1.93567911	-5.39107698
1	2.26442478	-2.64644377	-5.85933781
6	-0.69953546	-3.51209897	2.83605464
6	-0.75654221	-2.90040894	5.24346987
6	1.25248710	-2.30615566	3.90927427
1	-1.84158739	-3.07456703	5.28048069
1	-0.49018048	-2.18798349	6.03754145
1	-0.26299924	-3.85443046	5.47620531
1	-1.79384547	-3.61382346	2.79599947
1	-0.28091780	-4.48272555	3.14187887
1	-0.33247478	-3.28429279	1.82972703
1	1.68923417	-3.27696791	4.18755076
1	1.55597585	-1.57096846	4.66878648
1	1.66866729	-2.00756592	2.94101729
1	1.16394276	1.73268515	-5.93305381
1	-3.20113620	1.20430747	4.66732453
13	-0.13980575	-0.82234670	-0.34572595
8	-5.21644421	3.27531293	-1.75688794
6	-4.39426036	4.45310639	-1.93540589
1	-3.33396247	4.17409685	-1.98632938
6	-5.94095964	1.41652811	-0.46490010
6	-5.32046815	0.21953717	0.26573215
6	-4.26323356	-0.51916157	-0.56216850
6	-4.99374019	2.59400171	-0.59629660
6	-3.64454964	-1.70255955	0.18735860
6	-2.58296510	-2.45985734	-0.61489400
1	-6.81186355	1.79125418	0.09956515
1	-4.87568105	0.57084939	1.20923069
1	-3.46284984	0.17841392	-0.85539664
1	-3.20302222	-1.35186506	1.13534541
1	-6.31047138	1.13772109	-1.46173138
1	-6.12838095	-0.47921511	0.53651755
1	-4.71765010	-0.88022808	-1.50178032
1	-4.43485076	-2.42486247	0.45967849
1	-3.04316104	-2.85573152	-1.53895925
1	-2.24138878	-3.33168573	-0.02740371
8	-4.15917028	2.93102100	0.22527828
8	-1.47984491	-1.66278015	-0.99955475
1	-4.72283861	4.89465202	-2.88110436
1	-4.54124614	5.15529682	-1.10516793

Electronic energy = -2449.410936 a.u.

DFT-D4 dispersion correction = -0.147613 a.u.

Thermal free energy = 0.683893 a.u.

Gibbs free energy = -2448.874656 a.u.

Number of imaginary frequencies = 0.

10a_{CLLA}

Atomic N.	X	Y	Z
6	-0.45666089	5.89798455	2.56482393
6	0.60581832	5.47435810	1.75711273
6	0.58356863	4.26493378	1.05827020
6	-0.57458301	3.43272886	1.19799623
6	-1.71158869	3.92290757	1.90888539
6	-1.61057387	5.13671714	2.62018233
6	-3.02716527	3.25736735	1.84063378
7	-3.13299351	1.90605770	1.63656997
6	-4.36582622	1.31063738	1.56498143
6	-5.53243546	2.09069404	1.66484828
6	-5.43731968	3.46096267	1.85756930
6	-4.18367926	4.04975244	1.94507898
6	-4.50694681	-0.14097544	1.34273902
6	-3.53152324	-0.90165589	0.62994148
6	-3.84917556	-2.22608512	0.18637810
6	-5.05548125	-2.78187120	0.61720794
6	-5.95668210	-2.08887555	1.43541912
6	-5.69378658	-0.77406092	1.77215219
8	-0.59310481	2.21715122	0.64068867
8	-2.33108921	-0.38132176	0.35162013
1	-6.50194415	1.61812043	1.53768252
1	-6.33818505	4.07385379	1.90581773
1	-4.08498498	5.12730826	2.03961455
1	-2.44337285	5.46381915	3.24224294
6	1.78512661	3.83852483	0.19058788
1	-6.39522553	-0.22899879	2.40309693
1	-5.30308150	-3.80132051	0.32813478
6	-2.89539977	-3.02601756	-0.72462419
1	1.48740859	6.10933571	1.69206354
6	-2.60286792	-2.22314102	-2.01465945
6	-3.50831894	-4.37266426	-1.15429261
6	-1.57562996	-3.33553744	0.01702429
1	-3.53120763	-2.03674588	-2.57436336
1	-1.92901968	-2.80175496	-2.66560821
1	-2.13169161	-1.25977477	-1.79080968
1	-1.76381454	-3.89833668	0.94175031
1	-1.05274442	-2.41202382	0.27983616
1	-0.92093009	-3.94331524	-0.62760595
1	-2.80913987	-4.87959363	-1.83472642
1	-4.45892470	-4.24297159	-1.69174524
1	-3.67763376	-5.04336922	-0.29980745
6	2.46810573	2.60097268	0.81649693
6	2.84864388	4.94847736	0.08844523
6	1.32228570	3.51762513	-1.25033524
1	3.29722648	5.18921988	1.06292566
1	2.43896358	5.87262778	-0.34386451
1	3.66001765	4.60520985	-0.56941990
1	2.84630136	2.83440519	1.82246483
1	3.32165708	2.28546514	0.19591592
1	1.75747981	1.77285338	0.89280302
1	2.18999830	3.22395574	-1.86149724
1	0.87063196	4.40563122	-1.71601849

1	0.58740125	2.70579856	-1.26703924
1	-6.85996902	-2.58145241	1.79476861
1	-0.37681228	6.82378113	3.13430928
8	0.23885157	-0.26083478	0.67254808
8	-1.01571722	0.56098201	3.04199487
13	-1.45644351	0.81439693	1.35973103
8	0.29173959	-2.09725820	3.00222570
6	-0.90243335	-1.81109739	3.64642453
6	-1.17107467	-0.35588404	4.08943037
6	1.18788290	-0.84214283	1.20638809
6	1.30132532	-1.09001615	2.71501033
8	-1.65280760	-2.74014102	3.83803753
6	2.64631459	-1.61836507	3.18116921
6	-2.53541531	-0.25916168	4.77075103
1	-0.39796656	-0.13193911	4.85787129
1	1.04705340	-0.13645938	3.19516167
1	2.62648840	-1.73844014	4.27186975
1	3.44629001	-0.91171223	2.92296602
1	2.87223515	-2.58801977	2.72279442
1	-2.57928879	-0.90503488	5.65726421
1	-3.33441289	-0.56877590	4.08536429
1	-2.69966351	0.78256172	5.07516992
8	5.81039693	-2.52377462	-7.26299549
6	6.96513377	-3.03215117	-7.97452823
1	7.87140271	-2.49499768	-7.66801496
6	4.62932186	-2.08477111	-5.25646582
6	4.63428269	-2.21397145	-3.73383823
6	3.36864273	-1.63155195	-3.09615407
6	5.88014831	-2.64634795	-5.90610748
6	3.37071471	-1.75851427	-1.56723022
6	2.11064210	-1.16950132	-0.96210494
1	4.53534632	-1.03091745	-5.56578299
1	5.52446575	-1.70867816	-3.32901936
1	3.27050688	-0.56886349	-3.37711743
1	4.25037903	-1.24307887	-1.15064665
1	3.75984571	-2.59842702	-5.69771058
1	4.73803894	-3.27490085	-3.45931917
1	2.48052679	-2.14218620	-3.50621662
1	3.45203317	-2.81852339	-1.28008246
1	1.19994027	-1.67875670	-1.30690642
1	2.00546147	-0.09606705	-1.17141189
8	6.82645721	-3.14007850	-5.32284841
8	2.19489034	-1.34188285	0.49690523
1	6.75097194	-2.85955542	-9.03349208
1	7.09837163	-4.10253495	-7.77374719

Electronic energy = -2449.410008 a.u.

DFT-D4 dispersion correction = -0.144917 a.u.

Thermal free energy = 0.687896 a.u.

Gibbs free energy = -2448.867028 a.u.

Number of imaginary frequencies = 0.

10b_{CLLA}

Atomic N.	X	Y	Z
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6	1.85313734	3.34891840	-5.04528437
6	1.56785629	1.99198037	-5.24373913
6	0.87052316	1.22276987	-4.30917110
6	0.43730684	1.86665384	-3.10375908
6	0.63036126	3.27165944	-2.94841479
6	1.37466509	3.98300684	-3.91256625
6	-0.01179775	4.02667593	-1.85759831
7	-0.27728431	3.44557689	-0.64375630
6	-0.86163850	4.18440717	0.35302035
6	-1.23591295	5.52045979	0.12413991
6	-0.99556052	6.10804531	-1.10916853
6	-0.38154717	5.36139478	-2.10354281
6	-1.14934202	3.59996656	1.67558182
6	-1.47269102	2.21849189	1.82999436
6	-1.99440670	1.75017375	3.08151806
6	-2.05201368	2.65897912	4.14155014
6	-1.62871394	3.98908354	4.02396367
6	-1.19701673	4.45645803	2.79507819
8	-0.15782718	1.16226516	-2.13821748
8	-1.29823036	1.37468170	0.81023284
1	-1.76109578	6.06449823	0.90401898
1	-1.31436287	7.13253223	-1.30468192
1	-0.22784177	5.77938611	-3.09429489
1	1.59686339	5.03724751	-3.74803428
6	0.63400326	-0.28062608	-4.55031634
1	-0.86511929	5.48977536	2.69445617
1	-2.42149886	2.32027270	5.10774280
6	-2.42595682	0.28439535	3.28282394
1	1.92631669	1.51968937	-6.15663194
6	-3.44310251	-0.14628023	2.19980299
6	-3.10854247	0.06102666	4.64650838
6	-1.17170304	-0.62037983	3.24233828
1	-4.35314163	0.46850928	2.26398832
1	-3.73193589	-1.19521458	2.36338559
1	-3.03172777	-0.04747021	1.19039469
1	-0.51615293	-0.39813523	4.09821325
1	-0.59994634	-0.47070942	2.31954492
1	-1.46547664	-1.67890927	3.30724239
1	-3.42527436	-0.98918287	4.71520137
1	-4.00377318	0.68853648	4.76578204
1	-2.43214248	0.25366337	5.49169943
6	1.49516756	-1.08966004	-3.55139260
6	1.04710468	-0.71294128	-5.97060732
6	-0.86343460	-0.63472947	-4.39293426
1	2.12251383	-0.57736360	-6.15460806
1	0.48937972	-0.16708960	-6.74538313
1	0.82738196	-1.78311608	-6.09461210
1	2.56341749	-0.93443247	-3.76633097
1	1.28296095	-2.16569568	-3.65097765
1	1.30349724	-0.78597392	-2.51650280
1	-1.01048690	-1.70976042	-4.57759360
1	-1.46646011	-0.08205672	-5.12841325
1	-1.23671256	-0.39585544	-3.39237447
1	-1.64709102	4.64853594	4.89155512

1	2.44260398	3.89788194	-5.77949401
8	1.83703808	2.04847207	0.27981776
13	0.06419086	1.43551823	-0.37112466
8	-3.41294456	-7.02056723	1.56496528
6	-4.51275884	-7.34146337	2.44995315
1	-4.17621318	-7.34799797	3.49436411
6	-1.70520479	-5.55691911	0.81353833
6	-1.04214400	-4.19215699	0.99333074
6	0.11228743	-3.96651655	0.00865463
6	-2.84370330	-5.79894415	1.78580721
6	0.84729987	-2.63102763	0.20255688
6	0.01803302	-1.40140714	-0.17736150
1	-0.97660905	-6.37490571	0.93980983
1	-0.67031671	-4.10458349	2.02619212
1	0.83772261	-4.79091993	0.11331080
1	1.76237678	-2.62707054	-0.41408013
1	-2.10378853	-5.67504576	-0.20729065
1	-1.80498498	-3.40908256	0.87986766
1	-0.26769913	-4.02494228	-1.02639092
1	1.16625267	-2.53614821	1.25542820
1	-0.91241857	-1.38197698	0.41912640
1	-0.29083085	-1.49963702	-1.23704052
8	-3.21983370	-5.03239595	2.65271379
8	0.75895120	-0.20939540	0.02493463
1	-4.84892086	-8.33703502	2.14461981
1	-5.32088603	-6.60743862	2.33982672
8	3.54952055	0.83307172	-0.42085002
6	2.72066203	1.21105221	0.53730749
6	2.99842024	0.68609471	1.93834744
8	4.44191342	0.61104241	2.16788710
6	5.20410491	0.02532547	1.20186426
6	4.45758445	-0.28195028	-0.09775865
8	6.37408660	-0.21129973	1.38790393
6	5.37275327	-0.48509398	-1.28398395
6	2.40210633	1.54428580	3.03573720
1	2.57773133	-0.33254089	1.97247036
1	3.81414184	-1.16517335	0.06351881
1	4.77945222	-0.70392186	-2.17958148
1	6.04320160	-1.32758556	-1.07878818
1	5.98671620	0.40651249	-1.45855511
1	1.31098796	1.56883159	2.93631414
1	2.78556518	2.57020122	2.98275135
1	2.65805833	1.11271892	4.01050946

Electronic energy = -2449.396446 a.u.

DFT-D4 dispersion correction = -0.146672 a.u.

Thermal free energy = 0.687571 a.u.

Gibbs free energy = -2448.855546 a.u.

Number of imaginary frequencies = 0.

TS3ax_{CLLA}

Atomic N.	X	Y	Z
6	0.73145437	4.65587473	-0.34348786
6	0.12471903	4.50011349	-1.59764755

6	-0.63519508	3.37728500	-1.93149137
6	-0.76757324	2.34694481	-0.94538736
6	-0.27378657	2.56524396	0.38125595
6	0.51292247	3.70999765	0.64185745
6	-0.63301736	1.68709433	1.51361227
7	-0.97988117	0.37599814	1.30752921
6	-1.36036539	-0.42725456	2.35126281
6	-1.36529040	0.08341838	3.66042042
6	-0.99238706	1.40176344	3.88834214
6	-0.64088374	2.21228075	2.81778121
6	-1.84129024	-1.80283999	2.11579251
6	-2.51143551	-2.15991664	0.90299487
6	-3.30869699	-3.34941840	0.85701245
6	-3.22171283	-4.22589302	1.94077039
6	-2.42744637	-3.96005440	3.06596184
6	-1.77443218	-2.74393821	3.16509485
8	-1.36890566	1.20181870	-1.27622569
8	-2.42418981	-1.38082218	-0.17474627
1	-1.71390462	-0.54222429	4.47740030
1	-1.00919366	1.81044126	4.89923191
1	-0.40028697	3.25862551	2.97870278
1	0.97957921	3.83326912	1.61931527
6	-1.30350423	3.25125098	-3.31603956
1	-1.18598962	-2.51607132	4.05410242
1	-3.78141093	-5.15930557	1.91490567
6	-4.24581194	-3.63839698	-0.33419707
1	0.27154192	5.28172970	-2.34091139
6	-5.22360897	-2.45261288	-0.51880264
6	-5.09710884	-4.89990234	-0.09487903
6	-3.44711661	-3.86179590	-1.63893056
1	-5.83123207	-2.30841780	0.38646692
1	-5.90737009	-2.66337466	-1.35495079
1	-4.69044590	-1.52049077	-0.73495394
1	-2.79238677	-4.74136686	-1.54276288
1	-2.83839297	-2.98811126	-1.89606929
1	-4.14301348	-4.05628633	-2.46944952
1	-5.77665997	-5.03806210	-0.94784272
1	-5.71426344	-4.81584644	0.81127673
1	-4.48266792	-5.80859089	-0.01459682
6	-0.70422864	2.06690526	-4.10983658
6	-1.10110760	4.52201700	-4.16353178
6	-2.82889581	3.05327535	-3.14546514
1	-0.04126001	4.70432377	-4.39435244
1	-1.50989199	5.41719770	-3.67270184
1	-1.62855494	4.39874935	-5.12008333
1	0.37927312	2.20277405	-4.24441242
1	-1.16671765	2.02134705	-5.10804224
1	-0.87368596	1.11147869	-3.60399818
1	-3.30439377	2.97165799	-4.13470602
1	-3.27456379	3.91483784	-2.62689066
1	-3.05663538	2.14576268	-2.57638526
1	-2.34977388	-4.69585705	3.86622977
1	1.35849357	5.52463055	-0.14299288
8	-0.66300106	-1.34033942	-2.23224401

13	-0.97845262	-0.38219130	-0.54740715
8	4.96094656	3.20640111	5.07985592
6	4.66400290	4.44383574	5.77079678
1	4.51313400	5.25861692	5.05155087
6	4.40929031	1.50638664	3.52167678
6	3.26117706	0.82761574	2.77575588
6	3.71187067	-0.40070626	1.97411501
6	3.98622584	2.78180718	4.22540283
6	2.55744028	-1.13179362	1.26837242
6	1.93423843	-0.30293962	0.14633407
1	5.22001696	1.77730465	2.82356739
1	2.79170179	1.57029808	2.11629939
1	4.46781921	-0.09979000	1.22788787
1	1.77258241	-1.37984538	2.00175357
1	4.86949968	0.83525771	4.26296616
1	2.48589849	0.52856231	3.49930811
1	4.21815729	-1.11041915	2.64852595
1	2.91887617	-2.08414340	0.85214484
1	2.67787385	-0.12231607	-0.65125495
1	1.63934278	0.69053918	0.51393163
8	2.93567681	3.37643170	4.06146383
8	0.79400927	-0.94111449	-0.43808162
1	5.53678179	4.63957214	6.40094090
1	3.75967050	4.33420086	6.38235807
8	2.56836796	-2.96880460	-1.86202598
6	3.35433412	-2.10248733	-2.55560017
6	2.60420752	-1.21772051	-3.55298138
8	1.36146283	-0.70146292	-2.98091125
6	0.59020090	-1.56017613	-2.26397491
6	1.14413512	-2.98228908	-2.18130851
8	4.55155897	-2.07334900	-2.37833095
6	0.45979789	-3.88569880	-1.17900336
6	3.41888356	-0.03200780	-4.02625084
1	2.32757115	-1.85519326	-4.41406918
1	1.02735984	-3.40059733	-3.20080805
1	0.88067997	-4.89627695	-1.24974811
1	-0.61294031	-3.92975116	-1.39624977
1	0.60216087	-3.50150323	-0.16312921
1	4.33687258	-0.38736466	-4.50839758
1	3.69791698	0.60609972	-3.17908669
1	2.83523512	0.55609524	-4.74469328

Electronic energy = -2449.399355 a.u.

DFT-D4 dispersion correction = -0.150684 a.u.

Thermal free energy = 0.691660 a.u.

Gibbs free energy = -2448.858379 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 93.3i

TS3eq_{CLLA}

Atomic N.	X	Y	Z
6	2.00425577	3.05936480	-5.07363987
6	1.29230261	1.87283766	-5.29808998
6	0.48064840	1.28717673	-4.32474995

6	0.41246220	1.92431080	-3.04287195
6	0.99431098	3.22042608	-2.86923575
6	1.82943487	3.73907399	-3.88193178
6	0.63382167	4.08705235	-1.73143876
7	0.19868681	3.55416393	-0.54694957
6	-0.22159383	4.35784912	0.47831777
6	-0.19306806	5.75546169	0.32486093
6	0.27038282	6.31239176	-0.85937977
6	0.67381454	5.48307037	-1.89619207
6	-0.77696133	3.78512549	1.72131515
6	-1.39890099	2.49603319	1.75778794
6	-2.26765537	2.16477942	2.84976315
6	-2.28764653	3.02765846	3.94776440
6	-1.52624798	4.20280313	3.99738503
6	-0.80833811	4.59037256	2.88050985
8	-0.21169418	1.31828308	-2.03013325
8	-1.18941593	1.60394073	0.78555810
1	-0.58377200	6.39113235	1.11380279
1	0.27630880	7.39522028	-0.98955375
1	0.96740532	5.90148258	-2.85449338
1	2.36059117	4.67529821	-3.71202469
6	-0.31119907	-0.00144706	-4.62279797
1	-0.24185453	5.52079964	2.90212655
1	-2.90494108	2.77667785	4.80835295
6	-3.15596843	0.90355802	2.82314825
1	1.39452922	1.38655734	-6.26664162
6	-4.02499580	0.90196615	1.54278386
6	-4.11780548	0.85390055	4.02570581
6	-2.29017758	-0.37403980	2.87122297
1	-4.67868757	1.78595746	1.51895010
1	-4.66659594	0.00788759	1.53183496
1	-3.41024065	0.89988327	0.63614994
1	-1.68959653	-0.40522099	3.79252100
1	-1.61738575	-0.41860604	2.01010680
1	-2.93364716	-1.26709294	2.85911942
1	-4.76088190	-0.03245728	3.92954588
1	-4.77195978	1.73662519	4.06770849
1	-3.58533883	0.76848984	4.98396015
6	0.20848131	-1.16671240	-3.75235629
6	-0.18004125	-0.42967233	-6.09656143
6	-1.81563222	0.23239627	-4.34577465
1	0.85471749	-0.68610543	-6.36639833
1	-0.53649241	0.34924892	-6.78592396
1	-0.79410058	-1.32635856	-6.26277399
1	1.26844382	-1.36774111	-3.96828842
1	-0.36374840	-2.08215261	-3.96950841
1	0.10993696	-0.93038183	-2.68870568
1	-2.38089299	-0.68606776	-4.56592894
1	-2.20670700	1.03166997	-4.99199009
1	-1.99583161	0.50998652	-3.30151939
1	-1.52445817	4.81761742	4.89718390
1	2.67056417	3.45175576	-5.84162521
8	2.01648307	1.82942283	0.34313664
13	0.24185681	1.56754529	-0.30537185

8	-1.94742942	-7.64533472	1.81313765
6	-2.38947058	-8.31471825	3.01884866
1	-1.53166342	-8.56330681	3.65627885
6	-0.85759026	-5.85464621	0.70726204
6	-0.15799841	-4.50584412	0.87113398
6	0.27761930	-3.91238832	-0.47471985
6	-1.28416443	-6.47155905	2.02566051
6	1.06281984	-2.59670663	-0.36388668
6	0.23989955	-1.44180012	0.21613352
1	-0.20467369	-6.58010626	0.19417839
1	0.71856183	-4.63068581	1.52650273
1	0.90150481	-4.64904976	-1.00774920
1	1.42255712	-2.29614711	-1.35878825
1	-1.75221181	-5.76465988	0.07015979
1	-0.83358890	-3.81737208	1.39953864
1	-0.60898226	-3.74821067	-1.11133015
1	1.95586860	-2.76633501	0.26345968
1	0.03067882	-1.62343049	1.28620052
1	-0.74029219	-1.40476072	-0.29475638
8	-1.07536066	-6.00908470	3.13127947
8	0.86932838	-0.17757475	0.05281236
1	-2.89465523	-9.22293091	2.67661905
1	-3.07968402	-7.67423487	3.58208156
8	3.51751685	0.26722136	-0.13631810
6	2.52929401	0.70267618	0.66192210
6	2.59447932	0.18280663	2.10345507
8	3.99040413	0.26389757	2.55535102
6	4.91799498	-0.34140724	1.75991201
6	4.37823296	-0.78689808	0.39649892
8	6.06066179	-0.48379454	2.12813616
6	5.46977520	-1.04583573	-0.61985916
6	1.75577509	0.97314548	3.08144450
1	2.30585670	-0.87908125	2.11291122
1	3.76564479	-1.69504428	0.54327542
1	5.02629423	-1.36120915	-1.57202613
1	6.13207865	-1.83622181	-0.24827811
1	6.06911612	-0.14168575	-0.77967268
1	0.69354391	0.86260831	2.83333516
1	2.01683307	2.03706050	3.04660583
1	1.92046213	0.58945113	4.09547758

Electronic energy = -2449.393147 a.u.

DFT-D4 dispersion correction = -0.146140 a.u.

Thermal free energy = 0.690293 a.u.

Gibbs free energy = -2448.848994 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 78.2i

11a_{CLLA}

Atomic N.	X	Y	Z
6	-4.72886562	-0.12220215	0.96156710
6	-4.84873199	0.27724525	-0.37680125
6	-3.81505919	0.12230090	-1.30121517
6	-2.59098840	-0.46208155	-0.84078306

6	-2.49154568	-0.95988911	0.49837863
6	-3.57024288	-0.74511009	1.38651299
6	-1.33981025	-1.75628209	0.97025031
7	-0.11222189	-1.65968335	0.36126366
6	0.94511712	-2.43595266	0.76572955
6	0.79497743	-3.30839634	1.85547256
6	-0.43085262	-3.39719343	2.50283885
6	-1.50388741	-2.64302588	2.04903579
6	2.22470975	-2.41034627	0.03009917
6	2.26819849	-2.16418862	-1.37973917
6	3.45810580	-2.46203279	-2.11837387
6	4.59092855	-2.83742356	-1.39232862
6	4.59076595	-2.95396996	0.00527920
6	3.41106868	-2.76799107	0.70457762
8	-1.55929220	-0.54505664	-1.68179929
8	1.19669664	-1.67677808	-2.00955176
1	1.62411165	-3.94719625	2.14713526
1	-0.56239784	-4.07995892	3.34235239
1	-2.48051071	-2.75901771	2.50824118
1	-3.48019123	-1.04788792	2.42898035
6	-3.97829962	0.58566427	-2.76314330
1	3.40030408	-2.87817168	1.78921103
1	5.51992607	-3.03469491	-1.92440236
6	3.48909426	-2.36146140	-3.65704417
1	-5.78034353	0.74213767	-0.69385523
6	2.38332319	-3.25734234	-4.26501226
6	4.83425570	-2.84447622	-4.23203754
6	3.29077268	-0.89641261	-4.11303663
1	2.53846931	-4.30878353	-3.98177242
1	2.42110229	-3.19489217	-5.36301994
1	1.38564026	-2.94966626	-3.93501258
1	4.11328554	-0.26426029	-3.74526191
1	2.34262562	-0.47947890	-3.75694251
1	3.30025506	-0.84785986	-5.21266270
1	4.79237366	-2.78915405	-5.32902861
1	5.04928303	-3.88818908	-3.96032143
1	5.67717314	-2.21828461	-3.90503168
6	-2.99093461	1.73530185	-3.07745075
6	-5.39940929	1.11469913	-3.03664064
6	-3.74060631	-0.60045820	-3.72833562
1	-5.63519955	2.00579500	-2.43670177
1	-6.16928673	0.35244119	-2.84728765
1	-5.47313976	1.40317822	-4.09468317
1	-3.17467713	2.59162474	-2.41165638
1	-3.14000463	2.07389188	-4.11435461
1	-1.94728267	1.42628908	-2.96065784
1	-3.87075949	-0.26193976	-4.76735163
1	-4.46981287	-1.40253019	-3.54145122
1	-2.73218870	-1.01337516	-3.62299204
1	5.51087236	-3.20616055	0.53216660
1	-5.54635239	0.05522098	1.66033137
8	0.76004589	1.05194461	-2.09054351
13	0.15050939	-0.46075726	-1.20595610
8	-1.06460083	-0.21082447	7.81591082

6	-1.33354485	-1.40742207	8.58606052
1	-2.34110951	-1.78436792	8.37024021
6	-0.84637898	0.93430984	5.75274372
6	-0.79571265	0.79005909	4.23260403
6	-0.57515377	2.12846756	3.51625156
6	-1.12460208	-0.37658766	6.46390676
6	-0.55244672	2.01135635	1.98091364
6	0.75396734	1.40036011	1.48363578
1	-1.63037956	1.64831483	6.05576897
1	-1.73781264	0.34219339	3.88333654
1	-1.38352323	2.82171249	3.79861069
1	-0.68617737	3.00090837	1.52617812
1	0.09445792	1.34601963	6.15145350
1	-0.00438343	0.07094541	3.97353220
1	0.36000693	2.59731460	3.87002087
1	-1.39641297	1.39034343	1.64434135
1	0.99118900	0.47347322	2.02358842
1	1.59456193	2.09531999	1.61570477
8	-1.37599659	-1.44152939	5.92927885
8	0.72550583	0.99082273	0.08027107
1	-1.24985528	-1.10178494	9.63323975
1	-0.60027224	-2.18858433	8.34949875
8	2.62201047	3.60682297	-0.24517402
6	1.74017715	4.63382435	-0.44768694
6	0.57285202	4.26577663	-1.36643112
8	0.07307607	2.97040772	-0.95982236
6	1.00093687	1.90268493	-1.08216369
6	2.45299625	2.43857145	-1.10854793
8	1.89534116	5.69514751	0.11377736
6	3.51691103	1.43039620	-0.72132832
6	-0.56997812	5.25874758	-1.28618121
1	0.94254094	4.21158075	-2.40863538
1	2.61486292	2.75595570	-2.15175533
1	4.50946140	1.88139474	-0.84373927
1	3.45007706	0.55206007	-1.37364352
1	3.40561962	1.10643935	0.32022387
1	-0.21816728	6.25263071	-1.58725977
1	-0.95070773	5.32644892	-0.25978273
1	-1.38043356	4.94256926	-1.95412254

Electronic energy = -2449.399648 a.u.

DFT-D4 dispersion correction = -0.150441 a.u.

Thermal free energy = 0.690839 a.u.

Gibbs free energy = -2448.859250 a.u.

Number of imaginary frequencies = 0.

11b_{CLLA}

Atomic N.	X	Y	Z
6	2.51195970	4.22299696	-3.73677473
6	1.95995510	3.05913732	-4.28885935
6	1.01524547	2.28135494	-3.61568343
6	0.63757033	2.68840546	-2.29556233
6	1.06500586	3.96301880	-1.80143259
6	2.04182917	4.68461434	-2.52083652

6	0.41965731	4.61221213	-0.64332007
7	-0.18254944	3.86634935	0.33433958
6	-0.87024430	4.44976816	1.36394846
6	-0.94612967	5.85260806	1.43205754
6	-0.31451388	6.62725887	0.46813144
6	0.36217663	6.01447576	-0.57869200
6	-1.58431614	3.63182709	2.36506553
6	-2.07656157	2.31358274	2.08921628
6	-3.05737554	1.73436897	2.95910807
6	-3.35119621	2.40411299	4.14871065
6	-2.74414140	3.61496102	4.50371245
6	-1.89258540	4.23076278	3.60630232
8	-0.13189011	1.88466657	-1.54957835
8	-1.65469428	1.62429996	1.01848504
1	-1.54179776	6.32253923	2.20878592
1	-0.38719845	7.71471040	0.50897265
1	0.79566159	6.60799132	-1.37838532
1	2.44529929	5.60517072	-2.09973723
6	0.39768584	1.03429635	-4.27968548
1	-1.43283952	5.18266437	3.86920259
1	-4.06597566	1.96396792	4.84124722
6	-3.75823892	0.40254146	2.62098601
1	2.29582176	2.74779092	-5.27622724
6	-4.39651592	0.47030359	1.21318476
6	-4.89335987	0.07994884	3.61218554
6	-2.73805012	-0.75392644	2.69326083
1	-5.14791674	1.27228958	1.16897324
1	-4.90617730	-0.47991255	0.99327719
1	-3.64945461	0.65387195	0.43429219
1	-2.34137644	-0.85690895	3.71377133
1	-1.89793964	-0.57583939	2.01775622
1	-3.22107093	-1.70408084	2.41690505
1	-5.38494673	-0.85125247	3.29642634
1	-5.65893742	0.86899579	3.63449043
1	-4.52424082	-0.07774257	4.63567261
6	0.80517314	-0.24538431	-3.51730177
6	0.86295834	0.87046373	-5.73894910
6	-1.14415677	1.16640090	-4.30202955
1	1.94674810	0.70102329	-5.81497840
1	0.60159240	1.74187771	-6.35648507
1	0.36344020	-0.00635737	-6.17478831
1	1.89704068	-0.37774686	-3.53689044
1	0.34950335	-1.12644050	-3.99499575
1	0.47744224	-0.19987474	-2.47435320
1	-1.58438819	0.28189214	-4.78671045
1	-1.44715496	2.05241003	-4.87866970
1	-1.55833997	1.25016370	-3.29135917
1	-2.95847589	4.07461906	5.46830541
1	3.28602739	4.77024769	-4.27430852
13	-0.07605432	1.91237027	0.23781452
8	0.40687978	-8.61740570	-1.44281822
6	0.96527470	-9.71052296	-2.21063577
1	0.76304818	-9.57155113	-3.28021262
6	0.23735496	-6.30899347	-0.93037978

6	0.92148599	-4.94686028	-1.04431064
6	0.18360741	-3.85653954	-0.26013721
6	0.90509750	-7.38668870	-1.76290476
6	0.88430413	-2.49345411	-0.34847806
6	0.10656456	-1.43910558	0.42953433
1	-0.81308091	-6.24695266	-1.26308197
1	0.99237600	-4.66415513	-2.10522847
1	-0.84943007	-3.76850804	-0.64007209
1	0.96942944	-2.18971039	-1.40265471
1	0.19612855	-6.65415100	0.11418767
1	1.95763669	-5.02758336	-0.68117271
1	0.09936938	-4.15719655	0.79842583
1	1.90466682	-2.58369442	0.05162738
1	0.02753770	-1.70577369	1.49229705
1	-0.91044461	-1.33454336	0.02680354
8	1.75696261	-7.20905241	-2.61264942
8	0.66673752	-0.09249072	0.33750710
1	0.46877113	-10.61068422	-1.83574969
1	2.04996713	-9.77192577	-2.05735207
8	1.44194339	1.76794620	1.21236630
8	1.23539639	-0.08360203	2.59726228
6	1.63905924	0.43246120	1.34185346
6	3.11556476	0.08447136	1.04892043
8	3.45417669	-1.26455279	1.49365065
6	3.14331978	-1.56258413	2.79120828
6	2.30116993	-0.48990403	3.48753963
8	3.49535844	-2.61214383	3.28155044
6	1.66837276	-0.98751289	4.77204494
6	3.52245087	0.21169736	-0.40520430
1	3.69675517	0.79974046	1.65407987
1	2.94987485	0.38043025	3.70579952
1	1.07428597	-0.18477378	5.22552684
1	2.45073977	-1.30116928	5.47315388
1	1.02028955	-1.84971856	4.57254402
1	3.30202895	1.22699687	-0.75745205
1	2.98184507	-0.50509614	-1.03262444
1	4.60013482	0.03099073	-0.50275779

Electronic energy = -2449.405282 a.u.

DFT-D4 dispersion correction = -0.145573 a.u.

Thermal free energy = 0.690326 a.u.

Gibbs free energy = -2448.860529 a.u.

Number of imaginary frequencies = 0.

12_{CLLA}

Atomic N.	X	Y	Z
6	0.36989910	5.18688804	1.55027506
6	0.67746165	4.92132970	0.21019071
6	0.15533985	3.82252638	-0.47508789
6	-0.71100614	2.93916769	0.24238075
6	-1.11872033	3.26043091	1.57928681
6	-0.53042718	4.37623361	2.21546871
6	-2.18651987	2.53718268	2.30364039
7	-2.52360838	1.25094011	1.96608465

6	-3.58324920	0.59328971	2.53753232
6	-4.29984940	1.21748451	3.56713000
6	-3.94680707	2.50177300	3.96494380
6	-2.91352481	3.17366601	3.32310345
6	-3.99779422	-0.73256588	2.03383822
6	-3.85966864	-1.11198939	0.65713488
6	-4.48188534	-2.30731282	0.18291817
6	-5.12475254	-3.11957493	1.12144346
6	-5.18477966	-2.80122848	2.48436135
6	-4.63932229	-1.61127642	2.93130772
8	-1.14810429	1.83015245	-0.37609751
8	-3.16117745	-0.33958515	-0.19873378
1	-5.15670620	0.71454739	4.00673021
1	-4.51205735	3.00218560	4.75172576
1	-2.69620769	4.20679278	3.57641151
1	-0.76387838	4.58428275	3.25877025
6	0.50438983	3.57765347	-1.95868488
1	-4.67001739	-1.36152571	3.99143070
1	-5.58271329	-4.04973585	0.79052416
6	-4.42596341	-2.70375470	-1.30666386
1	1.36101502	5.59342396	-0.30456561
6	-5.03341951	-1.58122107	-2.18143654
6	-5.23433299	-3.98535788	-1.58649783
6	-2.96518620	-2.98166177	-1.73410471
1	-6.08698989	-1.41161266	-1.91511541
1	-4.99774253	-1.87918590	-3.24022370
1	-4.48892513	-0.63814507	-2.06772939
1	-2.53385090	-3.79628914	-1.13445097
1	-2.33063272	-2.09732351	-1.61757292
1	-2.94223043	-3.28886778	-2.79073402
1	-5.18868860	-4.20581813	-2.66230238
1	-6.29438195	-3.87321623	-1.31624711
1	-4.82923950	-4.85912544	-1.05578474
6	1.28356625	2.25241958	-2.12729867
6	1.39296518	4.70077829	-2.52784166
6	-0.78875181	3.54607691	-2.80851459
1	2.36679472	4.75988823	-2.02038354
1	0.90705146	5.68518498	-2.46632338
1	1.58836752	4.49491087	-3.58962921
1	2.21703423	2.27730570	-1.54600633
1	1.54744270	2.11109827	-3.18643199
1	0.69344541	1.39046715	-1.80052096
1	-0.53156042	3.38688188	-3.86655714
1	-1.32386863	4.50380560	-2.73234828
1	-1.46413462	2.74423090	-2.49256844
1	-5.65835673	-3.48818328	3.18534895
1	0.83241505	6.03101197	2.06132289
8	-0.55945231	-0.92990418	0.71130066
8	0.69225261	0.26522939	2.16688128
13	-1.69110012	0.38898257	0.47737164
8	-0.69358985	-1.30672091	3.85787194
6	-0.08410676	-0.19403044	4.36684091
6	1.12510705	0.26532061	3.54589651
6	0.42355882	-1.06572439	1.64960524

6	0.04902237	-2.02344755	2.82398582
8	-0.54362080	0.37017161	5.33684171
6	-0.79120385	-3.20824325	2.39580984
6	1.60893436	1.65000027	3.92433976
1	1.95053079	-0.46030354	3.67407328
1	0.99348546	-2.37472354	3.26607874
1	-0.98136450	-3.85949788	3.25831358
1	-0.24992709	-3.78147155	1.63254415
1	-1.74649174	-2.87679409	1.97393025
1	1.92504737	1.65533208	4.97478936
1	0.81060646	2.39010288	3.80236122
1	2.45955391	1.93184966	3.29126340
8	7.73309771	-1.38305478	-4.94404428
6	9.00412159	-1.92238233	-5.37920859
1	9.78368320	-1.71713812	-4.63470913
6	5.94308460	-1.26797144	-3.39407381
6	5.35335434	-1.81820979	-2.09606230
6	4.01779583	-1.15936961	-1.73569495
6	7.27269367	-1.89620629	-3.76460422
6	3.41598224	-1.71142281	-0.43847437
6	2.09375896	-1.04340088	-0.09021281
1	6.09495527	-0.17784665	-3.32991005
1	6.07593177	-1.67249887	-1.27857236
1	4.16086690	-0.06895764	-1.64058156
1	4.12357277	-1.56641180	0.39361534
1	5.25256942	-1.41728433	-4.24006991
1	5.22005444	-2.90690173	-2.19009975
1	3.30185820	-1.30339205	-2.56333857
1	3.25437479	-2.79711493	-0.53359517
1	1.35583482	-1.18961100	-0.89478344
1	2.23121071	0.03920478	0.06520328
8	7.87017539	-2.73882183	-3.12248511
8	1.60144133	-1.64488115	1.12646244
1	9.22602074	-1.41498111	-6.32297735
1	8.93016420	-3.00692728	-5.52873012

Electronic energy = -2449.408268 a.u.

DFT-D4 dispersion correction = -0.146418 a.u.

Thermal free energy = 0.689864 a.u.

Gibbs free energy = -2448.864823 a.u.

Number of imaginary frequencies = 0.

13a_{CLLA}

Atomic N.	X	Y	Z
6	3.54660390	5.54502039	0.54166041
6	3.08801023	5.63542513	-0.78014916
6	1.98700074	4.91389983	-1.24637991
6	1.33448074	4.03205630	-0.32612031
6	1.70749926	4.04136515	1.05681399
6	2.84556759	4.77787917	1.45421486
6	0.87813242	3.40438643	2.09985552
7	0.07967055	2.32779177	1.80792588
6	-0.73551979	1.76705500	2.75762701
6	-0.73727242	2.28332345	4.06489198

6	0.07853559	3.36150323	4.38294659
6	0.87776388	3.93465224	3.40180258
6	-1.65042768	0.66388121	2.41051157
6	-2.20496291	0.53519749	1.09661338
6	-3.32357028	-0.33203204	0.87894073
6	-3.72068824	-1.15103301	1.93792474
6	-3.09079393	-1.12849095	3.19112343
6	-2.08532478	-0.20931298	3.43080972
8	0.36961359	3.22139539	-0.76729289
8	-1.70404527	1.23920943	0.07971874
1	-1.41921972	1.86951667	4.80244040
1	0.06071878	3.78318342	5.38852241
1	1.46575336	4.82187056	3.61869764
1	3.19042672	4.71939333	2.48645731
6	1.49022300	5.06489213	-2.69916775
1	-1.60677746	-0.17346146	4.40960421
1	-4.54432408	-1.84710063	1.78926025
6	-4.06280073	-0.35921793	-0.47415253
1	3.62703691	6.28411052	-1.46807475
6	-4.56560109	1.06230097	-0.82355257
6	-5.29673619	-1.28064621	-0.43017913
6	-3.13633651	-0.88245131	-1.59617230
1	-5.25920919	1.42687630	-0.05176274
1	-5.10881186	1.03646116	-1.78013225
1	-3.73834864	1.77395377	-0.91497656
1	-2.82198145	-1.91523699	-1.38306242
1	-2.24211376	-0.26130246	-1.71321953
1	-3.68170997	-0.89026086	-2.55217737
1	-5.80840240	-1.23615061	-1.40191591
1	-6.01842057	-0.96982173	0.33912861
1	-5.02636341	-2.33146550	-0.25061672
6	1.64570300	3.73814786	-3.47876234
6	2.28561544	6.14087257	-3.46278662
6	0.00605016	5.50398516	-2.69928073
1	3.34814709	5.87761962	-3.56875660
1	2.21677047	7.12658071	-2.98036068
1	1.86985737	6.23842621	-4.47550287
1	2.70207393	3.43134186	-3.51244603
1	1.30625062	3.87783159	-4.51634337
1	1.05539046	2.93171113	-3.03059356
1	-0.34345396	5.62404822	-3.73572019
1	-0.11059313	6.47184467	-2.19021450
1	-0.63411207	4.76741027	-2.20216694
1	-3.40621963	-1.81843013	3.97359384
1	4.44016537	6.08794546	0.84851848
8	0.46694986	0.45764944	-1.44719970
8	1.64799918	0.52783460	0.40856950
13	0.04120566	1.61831304	-0.05389790
8	4.09048410	0.09879625	-0.95058565
6	4.11799734	0.11855402	0.40332951
6	2.85381470	0.46851334	1.21037299
6	1.62463706	-0.07520387	-1.04374267
6	2.89119346	0.49319812	-1.69341882
8	5.15329305	-0.12337187	0.98749744

6	3.08789469	0.03394437	-3.12464182
6	2.67133506	-0.49691375	2.37841232
1	3.02907799	1.48843430	1.59089632
1	2.80902209	1.58890742	-1.64356501
1	3.98572005	0.50248622	-3.54658917
1	2.21880106	0.33012172	-3.72579483
1	3.19825060	-1.05618081	-3.16364722
1	3.57551829	-0.49840683	2.99745417
1	2.49442877	-1.51624689	2.01233322
1	1.81432959	-0.18472004	2.98860522
8	-2.13553008	-8.92824756	0.93662606
6	-1.97071518	-10.35933909	1.08265318
1	-1.64311605	-10.80658599	0.13574099
6	-1.27458050	-6.77447029	0.44910628
6	-0.04814227	-5.96090111	0.03796104
6	-0.35866943	-4.46448874	-0.07228537
6	-0.99993386	-8.26042920	0.57606933
6	0.86086800	-3.63172618	-0.48466804
6	0.52519949	-2.15145207	-0.57116412
1	-2.09702977	-6.64592926	-0.27344680
1	0.33383088	-6.33721118	-0.92332959
1	-1.17064042	-4.31178285	-0.80405052
1	1.23607883	-3.97313718	-1.46238121
1	-1.67644586	-6.42463981	1.41417524
1	0.75899898	-6.12417010	0.76830615
1	-0.74406940	-4.09770156	0.89486301
1	1.67850692	-3.78015000	0.23875682
1	0.19546569	-1.76650997	0.40815179
1	-0.27048089	-1.95873030	-1.30352586
8	0.06957568	-8.80872968	0.38985855
8	1.72529726	-1.44767630	-0.98734110
1	-2.95714388	-10.73651792	1.36904419
1	-1.22819677	-10.58313342	1.85892700

Electronic energy = -2449.403863 a.u.

DFT-D4 dispersion correction = -0.147470 a.u.

Thermal free energy = 0.690019 a.u.

Gibbs free energy = -2448.861314 a.u.

Number of imaginary frequencies = 0.

13b_{CLLA}

Atomic N.	X	Y	Z
6	3.48264293	5.20281289	-2.58667971
6	3.18992097	4.42280751	-3.71341224
6	2.25330903	3.38719857	-3.68926577
6	1.60923702	3.10328620	-2.44215679
6	1.75881575	4.01719066	-1.34730637
6	2.74630195	5.02363661	-1.43065966
6	0.82815518	4.04525182	-0.20107536
7	0.12661153	2.92748266	0.16446642
6	-0.82785957	2.95790452	1.14619700
6	-1.06932971	4.16121504	1.83019774
6	-0.34053034	5.29825930	1.50348271
6	0.59735862	5.25303346	0.48036548

6	-1.65125355	1.76668636	1.44219208
6	-1.91117658	0.74509953	0.47080771
6	-2.99829151	-0.16514413	0.67379715
6	-3.63469735	-0.14843813	1.91670142
6	-3.26721921	0.73548618	2.93995125
6	-2.30901840	1.70055479	2.69010462
8	0.85503276	1.99975548	-2.32893274
8	-1.16643833	0.63484606	-0.63767202
1	-1.86049286	4.21139778	2.57226783
1	-0.53827076	6.23840143	2.01963472
1	1.11118759	6.15638896	0.16541679
1	2.94402596	5.65214721	-0.56300839
6	1.91957653	2.59450387	-4.97037755
1	-2.04155919	2.40759390	3.47458502
1	-4.43852370	-0.85604699	2.11080071
6	-3.46206640	-1.12835622	-0.43948048
1	3.72741998	4.62923018	-4.63689824
6	-3.80041366	-0.32582287	-1.71893560
6	-4.73502654	-1.89731755	-0.03690996
6	-2.37017143	-2.17686668	-0.74858512
1	-4.60630174	0.39535974	-1.51977788
1	-4.14987043	-1.01272145	-2.50428308
1	-2.93083985	0.22109831	-2.09868041
1	-2.16784000	-2.80156831	0.13406731
1	-1.43822371	-1.69351406	-1.05847696
1	-2.70704099	-2.84080267	-1.55908363
1	-5.04608915	-2.53396509	-0.87714367
1	-5.57046119	-1.22085060	0.19385991
1	-4.56993355	-2.55575396	0.82821540
6	2.37591579	1.12515024	-4.84333316
6	2.61897804	3.18772388	-6.20841537
6	0.39567157	2.65221814	-5.23538713
1	3.71442634	3.12022592	-6.14185600
1	2.34311403	4.23895896	-6.37513566
1	2.31045717	2.61870537	-7.09675110
1	3.46565519	1.06429878	-4.70891137
1	2.11852032	0.57250672	-5.75974473
1	1.88843038	0.63634366	-3.99403779
1	0.16077423	2.10419869	-6.16014547
1	0.06571598	3.69292092	-5.36752492
1	-0.17691019	2.20682411	-4.41465603
1	-3.75227910	0.67784747	3.91409892
1	4.26262026	5.96235070	-2.63354510
8	1.83887657	0.72126737	0.33280618
8	1.36063565	-0.76148276	-1.22850299
13	0.50199298	1.25226160	-0.75169318
6	2.21501121	-0.53167070	-0.03002430
6	3.67666905	-0.67122960	-0.49171508
8	3.88740797	-1.94502436	-1.19016049
6	2.88944252	-2.63092509	-1.80037434
6	1.44896240	-2.09940579	-1.77021519
8	3.13707657	-3.68632247	-2.34685726
6	0.82461539	-2.12681601	-3.15853679
6	4.16675783	0.46788946	-1.36508213

1	4.29847451	-0.76244763	0.40958784
1	0.89865990	-2.78337702	-1.10153568
1	-0.21038387	-1.76571739	-3.11152894
1	0.83044359	-3.15795774	-3.52882139
1	1.38999997	-1.50002506	-3.85837545
1	4.15621836	1.40540363	-0.79542814
1	3.53500631	0.58739159	-2.25351510
1	5.19491064	0.26081830	-1.68772552
8	-2.88052658	-4.83272339	7.22059341
6	-2.98912841	-5.86154521	8.23348830
1	-2.93726521	-6.85761467	7.77614926
6	-1.69572775	-3.74574303	5.47864953
6	-0.44260331	-3.74840775	4.60394146
6	-0.44382253	-2.60494257	3.58410611
6	-1.71606037	-4.86093481	6.50613520
6	0.80675202	-2.60263827	2.69751827
6	0.79641947	-1.45333252	1.70064012
1	-2.60831833	-3.83337101	4.86702471
1	-0.36424886	-4.71527251	4.08340033
1	-1.34531476	-2.67740964	2.95171618
1	0.88259023	-3.55695771	2.15232231
1	-1.79731447	-2.79095340	6.02066141
1	0.44889956	-3.67827942	5.24557242
1	-0.52038898	-1.63992184	4.11400622
1	1.70972847	-2.52175657	3.32312825
1	0.74775620	-0.48290409	2.21685949
1	-0.06974683	-1.53048883	1.02357219
8	-0.83540845	-5.67833269	6.69337493
8	2.02476515	-1.52531324	0.93795093
1	-3.96334098	-5.70160430	8.70543668
1	-2.18021896	-5.76391675	8.96848553

Electronic energy = -2449.404793 a.u.

DFT-D4 dispersion correction = -0.148417 a.u.

Thermal free energy = 0.694688 a.u.

Gibbs free energy = -2448.858522 a.u.

Number of imaginary frequencies = 0.

TS4ax_{CLLA}

Atomic N.	X	Y	Z
6	3.69287562	5.30310726	0.08961356
6	3.24124932	5.28211927	-1.23740971
6	2.18486452	4.47230673	-1.65973496
6	1.57633746	3.61461830	-0.68720239
6	1.92647123	3.74614000	0.69496447
6	3.02153254	4.56560183	1.04782045
6	1.10985684	3.15181327	1.77254367
7	0.35080722	2.03295302	1.54655445
6	-0.45084748	1.50953817	2.52805710
6	-0.48304027	2.11183357	3.79768848
6	0.29110518	3.23743653	4.04762983
6	1.07854462	3.77019882	3.03512239
6	-1.32937205	0.35668203	2.25435591
6	-1.87365961	0.12228494	0.95171839

6	-2.99276972	-0.75824034	0.79932344
6	-3.37455940	-1.51369214	1.91072726
6	-2.73258519	-1.40995932	3.15333223
6	-1.74544990	-0.45724216	3.32981181
8	0.67462760	2.71391106	-1.08393443
8	-1.36295629	0.73606735	-0.11777966
1	-1.15530586	1.72272289	4.55722904
1	0.25024065	3.72463989	5.02245951
1	1.63468885	4.68917465	3.19614697
1	3.35747480	4.59663153	2.08405542
6	1.68600428	4.50826883	-3.11925197
1	-1.26234365	-0.35320821	4.30139780
1	-4.19219971	-2.22597480	1.81114483
6	-3.75298452	-0.86193126	-0.53875130
1	3.74938273	5.91354370	-1.96387792
6	-4.24791145	0.54116380	-0.96507722
6	-4.99381208	-1.76725376	-0.41944325
6	-2.85071659	-1.45700002	-1.64390242
1	-4.92548943	0.95910043	-0.20629504
1	-4.80572891	0.46483490	-1.91056514
1	-3.41411757	1.23624361	-1.11087739
1	-2.53898096	-2.47764301	-1.37523663
1	-1.95643651	-0.84730554	-1.81065941
1	-3.41262197	-1.51772225	-2.58848524
1	-5.52303076	-1.77467108	-1.38283539
1	-5.69787741	-1.40486300	0.34349337
1	-4.73070097	-2.80859590	-0.18243274
6	1.91424751	3.14850950	-3.81914043
6	2.42351866	5.57892895	-3.94581747
6	0.18001622	4.86435747	-3.14412594
1	3.49876499	5.36699390	-4.03817749
1	2.30156565	6.58583498	-3.52127981
1	2.00419497	5.59516239	-4.96169472
1	2.98428845	2.89137530	-3.82359052
1	1.58178258	3.21149039	-4.86658049
1	1.35555041	2.34390950	-3.32916236
1	-0.17436428	4.90078306	-4.18528080
1	0.00949452	5.85365534	-2.69507909
1	-0.41895708	4.12518692	-2.60132551
1	-3.01624084	-2.06837034	3.97372580
1	4.55467367	5.91072226	0.36451188
8	0.72775018	-0.01664973	-1.73781085
8	1.81631446	0.05031651	0.27221307
13	0.37352058	1.15737665	-0.25450873
8	4.28305531	-0.40080956	-1.00390196
6	4.26265383	-0.31321442	0.35660049
6	2.97812128	0.10419964	1.10193276
6	1.84921908	-0.58516473	-1.41005588
6	3.17381167	0.04430327	-1.83849621
8	5.27825880	-0.56106764	0.97060543
6	3.54343677	-0.31480667	-3.26926470
6	2.79258990	-0.75815642	2.35067368
1	3.15559292	1.15290654	1.40376413
1	3.06175065	1.13259780	-1.73104763

1	4.47108746	0.19852439	-3.55097866
1	2.74399471	0.00153996	-3.95143414
1	3.69115305	-1.39747548	-3.36272407
1	3.69175744	-0.71290153	2.97519231
1	2.61177135	-1.80357432	2.06796169
1	1.93057036	-0.39716509	2.92529202
8	-3.98313665	-5.74827814	2.37162852
6	-4.63977814	-5.70488882	3.66138530
1	-4.18715954	-6.43132639	4.34787560
6	-2.02812886	-5.63555050	1.02885735
6	-0.80856121	-4.73393965	0.81737417
6	-0.13179743	-4.99312687	-0.53490579
6	-2.64037967	-5.49528599	2.40894246
6	1.09460485	-4.10767555	-0.80922556
6	0.72155786	-2.65082407	-1.03493452
1	-1.73638213	-6.69551659	0.92288059
1	-0.09119058	-4.90150309	1.63471413
1	0.18446405	-6.04802608	-0.57853079
1	1.62095189	-4.47502184	-1.70352507
1	-2.80303597	-5.45293379	0.27088642
1	-1.12837791	-3.68405724	0.89760965
1	-0.86471289	-4.86278248	-1.35014999
1	1.80399084	-4.17726088	0.03064127
1	0.26826960	-2.19605088	-0.14335699
1	0.02753206	-2.53530741	-1.87863076
8	-2.03943110	-5.22271347	3.43062973
8	1.95002484	-1.92639959	-1.34427655
1	-5.68586111	-5.95662975	3.46249437
1	-4.55897284	-4.70185232	4.09918118

Electronic energy = -2449.402924 a.u.

DFT-D4 dispersion correction = -0.151116 a.u.

Thermal free energy = 0.693305 a.u.

Gibbs free energy = -2448.860735 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 80.1i

TS4eq_{CLLA}

Atomic N.	X	Y	Z
6	4.12642002	4.76688528	-2.32756758
6	3.59826851	4.35845518	-3.56220818
6	2.47192097	3.54080939	-3.66979122
6	1.90925169	3.04046750	-2.44963598
6	2.27631903	3.66136956	-1.21437716
6	3.43226790	4.47179317	-1.16920888
6	1.36119747	3.64431214	-0.06267210
7	0.46326444	2.62621903	0.11736299
6	-0.46694988	2.67961550	1.12412107
6	-0.51728684	3.80032682	1.96998310
6	0.40631655	4.82752037	1.81811738
6	1.34800482	4.75491905	0.80387497
6	-1.44166172	1.58595288	1.32573247
6	-1.83753407	0.71267074	0.26449779
6	-2.95323253	-0.17108557	0.44065768

6	-3.54106498	-0.23115788	1.70589864
6	-3.08224225	0.53716993	2.78513360
6	-2.05539608	1.44493985	2.58899426
8	1.02468753	2.04223251	-2.47067928
8	-1.18330801	0.71269172	-0.89283490
1	-1.30312788	3.87596178	2.71570373
1	0.36396596	5.70350170	2.46659994
1	2.03091455	5.57994270	0.62268245
1	3.78522754	4.85132647	-0.21000949
6	1.81885219	3.26378751	-5.03969622
1	-1.70098436	2.04075861	3.42958498
1	-4.37563229	-0.91002321	1.87331676
6	-3.47157240	-1.03903151	-0.72366387
1	4.09533882	4.69415522	-4.47046995
6	-3.86483693	-0.13985850	-1.92022407
6	-4.72600508	-1.83931339	-0.32447156
6	-2.39156342	-2.05806541	-1.16044128
1	-4.66268301	0.55988085	-1.63105917
1	-4.24539614	-0.76485711	-2.74221849
1	-3.01038814	0.43624613	-2.28989816
1	-2.14748621	-2.73888183	-0.32968646
1	-1.47088289	-1.56448221	-1.49144769
1	-2.77738714	-2.67175722	-1.98910975
1	-5.07139683	-2.41597414	-1.19413912
1	-5.55266380	-1.18506813	-0.01122177
1	-4.52361107	-2.55668926	0.48462689
6	1.81973743	1.76580083	-5.40185070
6	2.53875113	4.01670170	-6.17424154
6	0.35826278	3.77627420	-4.99164820
1	3.57182765	3.66570044	-6.31183720
1	2.55743456	5.10336685	-6.00693178
1	2.00196338	3.83524132	-7.11623526
1	2.83488321	1.34851563	-5.38403845
1	1.40302920	1.63058245	-6.41199732
1	1.20543599	1.20254564	-4.69415617
1	-0.12972493	3.59973907	-5.96224594
1	0.32876667	4.85665035	-4.78810501
1	-0.22165094	3.25783086	-4.21827841
1	-3.54072928	0.42832789	3.76820183
1	5.04414988	5.35348320	-2.29153681
8	1.61110508	0.37458697	0.60477871
8	0.95812738	-0.68107051	-1.66844046
13	0.57778388	0.99091363	-1.07408857
6	2.19526005	-0.72271216	0.60161895
6	3.52847075	-0.99524677	-0.09012876
8	3.75299835	-0.16538751	-1.23554313
6	3.23183560	-0.54157805	-2.48438692
6	1.91986239	-1.34164572	-2.44740033
8	3.81324244	-0.15315209	-3.46605325
6	1.43036377	-1.69131947	-3.85042620
6	4.66021872	-0.69023097	0.89895827
1	3.55492926	-2.05944729	-0.36702895
1	2.16320610	-2.30915737	-1.95203567
1	0.51358223	-2.28811026	-3.76013422

1	2.18689752	-2.27674127	-4.39083576
1	1.21229362	-0.78769398	-4.42836094
1	4.56755829	-1.31184995	1.79858971
1	4.63648796	0.36972797	1.18200433
1	5.62011528	-0.90306401	0.41391405
8	-3.79663730	-5.26783180	6.88559389
6	-4.07762480	-6.41110039	7.72944021
1	-4.09524441	-7.33215380	7.13355494
6	-2.39547634	-4.08103609	5.38770151
6	-1.10100555	-4.11331320	4.57613564
6	-0.90316325	-2.84065127	3.74649143
6	-2.59862971	-5.32296371	6.23503971
6	0.38716039	-2.88142872	2.91742444
6	0.57164812	-1.60614896	2.11787128
1	-3.27445030	-3.96791983	4.73313808
1	-1.10921860	-4.99350452	3.91491747
1	-1.76537311	-2.69559765	3.07470417
1	0.35954121	-3.73965001	2.22788119
1	-2.41781306	-3.20952797	6.06267786
1	-0.24871115	-4.25559378	5.25789690
1	-0.88533270	-1.96295154	4.41475344
1	1.25439203	-3.02687407	3.58096743
1	0.67616928	-0.71775836	2.75419903
1	-0.24609126	-1.43581402	1.40526950
8	-1.81806898	-6.24985743	6.34070969
8	1.81535304	-1.75457442	1.33389926
1	-5.06070375	-6.21280384	8.16681957
1	-3.31511879	-6.50619268	8.51265812

Electronic energy = -2449.390669 a.u.

DFT-D4 dispersion correction = -0.147494 a.u.

Thermal free energy = 0.693122 a.u.

Gibbs free energy = -2448.845041 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 42.1i

14a_{CLLA}

Atomic N.	X	Y	Z
6	-0.25932521	6.04284671	0.62419292
6	0.74413810	5.34394877	-0.05793226
6	0.59229761	4.01628697	-0.46538273
6	-0.63987243	3.35640499	-0.14968120
6	-1.71245133	4.10569642	0.42148916
6	-1.48210263	5.43263609	0.84025010
6	-3.08843408	3.57667570	0.49224329
7	-3.33065758	2.23209738	0.60387629
6	-4.61773920	1.76241602	0.65530970
6	-5.69911055	2.65705183	0.55532095
6	-5.46549196	4.01829337	0.42873493
6	-4.15833295	4.48336747	0.39640835
6	-4.90633310	0.32074159	0.77536300
6	-4.01803417	-0.67963888	0.27724287
6	-4.46978283	-2.03348678	0.15446372
6	-5.72292432	-2.34904900	0.68331358

6	-6.54418724	-1.39631841	1.29951820
6	-6.14766625	-0.07218272	1.32200453
8	-0.78684064	2.05385404	-0.41573717
8	-2.77371391	-0.36265515	-0.09695120
1	-6.71226293	2.26707595	0.52640223
1	-6.29992693	4.71238610	0.32165790
1	-3.95082771	5.53834719	0.24212580
1	-2.27033117	5.97303294	1.36390193
6	1.73219753	3.28852537	-1.20645869
1	-6.78585263	0.67296002	1.79592865
1	-6.07365474	-3.37818568	0.63865774
6	-3.60587926	-3.11799529	-0.52136973
1	1.68296482	5.85695119	-0.25811603
6	-3.23521133	-2.67994074	-1.95833085
6	-4.35431051	-4.46017860	-0.63277032
6	-2.32370228	-3.37292852	0.30280561
1	-4.14078032	-2.54013203	-2.56679807
1	-2.62634742	-3.46208999	-2.43784627
1	-2.66683886	-1.74344306	-1.95979801
1	-2.56747359	-3.68031799	1.32913828
1	-1.70907009	-2.47011502	0.35389459
1	-1.73461738	-4.17739137	-0.16546314
1	-3.71271253	-5.18135424	-1.15907582
1	-5.28855465	-4.36780968	-1.20547988
1	-4.58809851	-4.88849976	0.35239845
6	2.30059886	2.16202415	-0.31345199
6	2.89763384	4.23586603	-1.54971735
6	1.21661932	2.69919342	-2.54070432
1	3.38351670	4.64446697	-0.65206500
1	2.57360222	5.07464107	-2.18232645
1	3.66046609	3.67428966	-2.10804901
1	2.71279087	2.57672139	0.61808643
1	3.11110864	1.63417868	-0.84047325
1	1.51420432	1.44492879	-0.06067321
1	2.04046786	2.18949654	-3.06418480
1	0.84774391	3.50016217	-3.19776583
1	0.40458027	1.98251619	-2.37841857
1	-7.49010483	-1.69768691	1.74909199
1	-0.08011639	7.06074627	0.96995082
8	-0.20137482	-0.42140894	0.19320406
8	-1.32688768	1.05188787	2.29958059
13	-1.77202328	0.94724405	0.60274220
8	-0.25872271	-1.64511931	2.90070435
6	-1.41215256	-1.11124176	3.45565647
6	-1.55381036	0.42603490	3.53208124
6	0.70028379	-0.94598448	0.85313805
6	0.82480168	-0.82787008	2.37661500
8	-2.23006782	-1.89953803	3.87075018
6	2.13047888	-1.34137902	2.95722807
6	-2.90090497	0.79637168	4.15105027
1	-0.75917834	0.75989095	4.23603732
1	0.66065368	0.23172299	2.61024243
1	2.12382955	-1.19129759	4.04436318
1	2.98067217	-0.78900601	2.53483030

1	2.26473229	-2.40904145	2.74857214
1	-2.99613930	0.38336712	5.16353308
1	-3.72718569	0.40373490	3.54502446
1	-2.97308109	1.89058250	4.19963618
8	8.93590896	-2.20624415	-2.10741215
6	10.12708828	-2.89891069	-2.55388067
1	10.24185991	-3.84907609	-2.01738912
6	6.58848542	-2.08235764	-1.81073281
6	5.25464728	-2.81203074	-1.96426850
6	4.07152054	-1.97526140	-1.46779614
6	7.77285343	-2.89226952	-2.30375788
6	2.73150054	-2.70452348	-1.61715258
6	1.53006677	-1.89483277	-1.16832253
1	6.77723772	-1.81332817	-0.75887318
1	5.29691026	-3.76456090	-1.41387732
1	4.22618387	-1.70742292	-0.40996939
1	2.75243697	-3.65810682	-1.06566402
1	6.58414831	-1.12734101	-2.36148304
1	5.10822250	-3.08139961	-3.02159823
1	4.02971859	-1.02410275	-2.02654949
1	2.56433480	-2.96209932	-2.67630120
1	0.57988229	-2.40939657	-1.36370792
1	1.49160616	-0.90197426	-1.63742762
8	7.72091081	-3.99770595	-2.80841966
8	1.63621819	-1.70234946	0.28915102
1	10.95672011	-2.22256166	-2.32730443
1	10.07235835	-3.10052205	-3.63100360

Electronic energy = -2449.410065 a.u.

DFT-D4 dispersion correction = -0.145634 a.u.

Thermal free energy = 0.688297 a.u.

Gibbs free energy = -2448.867402 a.u.

Number of imaginary frequencies = 0.

14b_{CLLA}

Atomic N.	X	Y	Z
6	3.20843703	4.31030682	-2.14773074
6	2.48355936	4.17373923	-3.34232108
6	1.22395008	3.57549540	-3.39996696
6	0.68770085	3.04891649	-2.18051608
6	1.35929511	3.30855373	-0.94288028
6	2.63547823	3.91063856	-0.95443052
6	0.66189814	3.10785272	0.33502888
7	-0.29507091	2.13445684	0.46274268
6	-1.03984054	2.02348355	1.60961581
6	-0.81550748	2.91348493	2.67299990
6	0.18644682	3.87334932	2.57779812
6	0.92781657	3.97606904	1.41027011
6	-2.09438325	0.99350106	1.74000783
6	-2.78744764	0.45481275	0.60876745
6	-3.92421623	-0.39658082	0.80446857
6	-4.25212945	-0.75680401	2.11332231
6	-3.52119568	-0.30775699	3.22214069
6	-2.46635846	0.56996695	3.03385408

8	-0.44720619	2.35340538	-2.18905770
8	-2.39543584	0.73922698	-0.62968884
1	-1.45497795	2.87281692	3.55022051
1	0.35667178	4.57025598	3.39943637
1	1.66500835	4.76481375	1.28611182
1	3.18062916	4.03666007	-0.01824273
6	0.43671980	3.48415280	-4.72183119
1	-1.89633704	0.91469964	3.89648654
1	-5.09727960	-1.42066005	2.28714527
6	-4.74552256	-0.91099778	-0.39521443
1	2.93767128	4.53874389	-4.26192828
6	-5.29767557	0.28365834	-1.20950919
6	-5.95459260	-1.75081784	0.05897907
6	-3.87384651	-1.81122185	-1.30424192
1	-5.95381451	0.90602706	-0.58348203
1	-5.89344387	-0.09009091	-2.05593881
1	-4.49124482	0.91056863	-1.60344390
1	-3.51141464	-2.68792681	-0.74480673
1	-3.01272236	-1.27003483	-1.71163563
1	-4.47956686	-2.18183917	-2.14534515
1	-6.51976049	-2.06949582	-0.82822019
1	-6.64004334	-1.17683905	0.69938764
1	-5.65251098	-2.66019194	0.59938345
6	0.22811579	2.01084586	-5.14222435
6	1.17479506	4.19341029	-5.87281881
6	-0.93418622	4.18262043	-4.55161409
1	2.13933389	3.71729981	-6.10154659
1	1.35160581	5.25802116	-5.65961623
1	0.55691341	4.13516957	-6.78019873
1	1.19351074	1.50410369	-5.27948472
1	-0.31629189	1.97800321	-6.09899003
1	-0.34610768	1.45324829	-4.39489582
1	-1.49627558	4.12775105	-5.49636318
1	-0.80100740	5.24503866	-4.29869768
1	-1.53203546	3.70677345	-3.76640668
1	-3.79072282	-0.63819534	4.22549776
1	4.20850076	4.74335658	-2.16359109
8	0.19139471	-0.43640866	0.19558114
8	-0.46620156	-0.32743656	-2.36318833
13	-0.68142749	0.92527544	-1.10458257
6	1.00832072	-1.35810925	0.27622984
6	2.38291301	-1.37174157	-0.38839518
8	2.46863246	-0.47656503	-1.50505926
6	1.82529948	-0.79214425	-2.71416807
6	0.40404928	-1.38758286	-2.61252028
8	2.35466359	-0.43010504	-3.73460086
6	0.02494757	-2.11443541	-3.89955862
6	3.45092267	-0.92270548	0.61361209
1	2.58941846	-2.40518604	-0.70903305
1	0.38049293	-2.13622990	-1.78537809
1	-1.00874556	-2.47344674	-3.81429967
1	0.68907281	-2.97224910	-4.07864547
1	0.09888027	-1.42737345	-4.75034029
1	3.49099357	-1.59333935	1.48151595

1	3.24638596	0.10185267	0.95026795
1	4.42597237	-0.93529827	0.11243892
8	4.68522762	-3.59021277	6.07173968
6	6.09043676	-3.23520850	6.05444283
1	6.59706469	-3.72098997	5.21143515
6	2.52642998	-3.59819029	5.08822663
6	1.78140778	-3.51104566	3.75648093
6	0.27296531	-3.73577994	3.90415409
6	3.99165653	-3.22466561	4.95859548
6	-0.50463579	-3.78007103	2.57917848
6	-0.48234802	-2.50440127	1.75351124
1	2.45578775	-4.60118675	5.53537344
1	2.20292259	-4.24752874	3.05414580
1	0.09318255	-4.68446014	4.43657411
1	-1.56409519	-3.98746158	2.79844739
1	2.08274673	-2.90958317	5.82805962
1	1.97787358	-2.52572595	3.31376074
1	-0.15403001	-2.94258796	4.54186080
1	-0.15174133	-4.61512281	1.95254652
1	-0.58133986	-1.59926901	2.36791359
1	-1.27530150	-2.49247946	0.99453026
8	4.49844156	-2.66000301	4.00562483
8	0.80761138	-2.43411267	1.03253067
1	6.49018846	-3.59439260	7.00731306
1	6.20967760	-2.14813792	5.96689399

Electronic energy = -2449.393847 a.u.

DFT-D4 dispersion correction = -0.147944 a.u.

Thermal free energy = 0.689677 a.u.

Gibbs free energy = -2448.852114 a.u.

Number of imaginary frequencies = 0.

15_{CLLA} (ax_chelate)

Atomic N.	X	Y	Z
6	6.29592142	1.40308387	1.71307262
6	6.29351699	0.19038536	1.01115713
6	5.24956881	-0.18625310	0.16275817
6	4.13470881	0.70487392	0.04081952
6	4.19882600	2.00163460	0.64237362
6	5.27013055	2.30847943	1.50669241
6	3.24562488	3.07342186	0.29272336
7	1.96589255	2.78032028	-0.09507414
6	1.10092246	3.76717036	-0.48407287
6	1.53037351	5.10650787	-0.48919209
6	2.81969210	5.42226723	-0.08226318
6	3.68542186	4.40816167	0.30483241
6	-0.26469102	3.44418896	-0.94518011
6	-0.59777034	2.18164302	-1.53158237
6	-1.85255723	2.01991232	-2.20564488
6	-2.76774850	3.07231925	-2.14132025
6	-2.49360695	4.26837474	-1.46463128
6	-1.24871468	4.45471313	-0.89093350
8	3.05459765	0.32751076	-0.65148087
8	0.25156703	1.15394313	-1.48087490

1	0.86624587	5.88220794	-0.85900860
1	3.16295940	6.45731430	-0.10498163
1	4.71737354	4.62918148	0.56269381
1	5.27301531	3.25991812	2.03843482
6	5.30133168	-1.51792383	-0.61363095
1	-1.03310644	5.38557213	-0.36711048
1	-3.73969647	2.96223836	-2.61852865
6	-2.18707827	0.72561387	-2.97533270
1	7.13513831	-0.48573071	1.15036372
6	-1.12452589	0.47483712	-4.07202170
6	-3.55546442	0.81554217	-3.67768762
6	-2.24398689	-0.48281309	-2.01155178
1	-1.11230092	1.30481839	-4.79353681
1	-1.36882944	-0.44695209	-4.62156669
1	-0.12196860	0.36836478	-3.64438466
1	-2.99128146	-0.31308940	-1.22225205
1	-1.27185659	-0.66278522	-1.54233179
1	-2.53534924	-1.38685570	-2.56880024
1	-3.72949014	-0.11463219	-4.23707098
1	-3.59786712	1.64678044	-4.39619921
1	-4.38349351	0.93052898	-2.96285707
6	4.16686323	-2.46362284	-0.15457670
6	6.63362231	-2.25915578	-0.39300515
6	5.17126633	-1.24502264	-2.13112654
1	6.77705829	-2.55657764	0.65610082
1	7.49810633	-1.65566545	-0.70477654
1	6.63499873	-3.17686704	-0.99830507
1	4.23442793	-2.65081937	0.92802904
1	4.25760896	-3.43033914	-0.67418732
1	3.18572007	-2.03548202	-0.38311269
1	5.20746474	-2.19553561	-2.68507080
1	6.00397516	-0.61835270	-2.48208369
1	4.22890441	-0.73975399	-2.36898892
1	-3.25282877	5.04831416	-1.40294268
1	7.10741645	1.63462913	2.40281336
8	-1.31924105	-5.04405891	-0.84049669
8	0.96289021	0.81356013	1.58025404
13	1.41366305	0.86997797	-0.14634863
8	0.22810194	-2.68693549	1.42719018
6	0.54404592	-1.45048820	1.05912608
6	0.62149934	-0.40487706	2.16521170
6	-1.16010302	-4.20783420	0.02889555
6	0.24886854	-3.74153323	0.40825604
8	0.80454236	-1.12335956	-0.11109774
6	1.07004178	-4.89988991	0.96378149
6	-0.68068124	-0.32954580	2.97341659
1	1.43058474	-0.75701777	2.84296389
1	0.70411741	-3.33605149	-0.50475856
1	2.10737751	-4.58169070	1.12361910
1	1.05658869	-5.72586043	0.24277858
1	0.65172918	-5.25062249	1.91627933
1	-0.91530823	-1.29175146	3.44692265
1	-1.51966662	-0.03175014	2.33273347
1	-0.56243689	0.43145135	3.75390880

8	-4.74773194	2.16219357	1.61925684
6	-3.68874944	3.05232436	2.05814367
1	-2.70824069	2.59323658	1.88293756
6	-5.97731308	0.13824375	1.79497555
6	-5.76235479	-1.36034918	2.02816214
6	-4.67604126	-1.96184939	1.12945156
6	-4.81943540	0.98478476	2.29516054
6	-4.48421316	-3.46325991	1.36466898
6	-3.48966039	-4.12555090	0.42842410
1	-6.87221399	0.48227952	2.34014573
1	-5.49775139	-1.51952687	3.08455800
1	-3.72291636	-1.44072632	1.30473955
1	-4.18069373	-3.64999042	2.40730503
1	-6.15675632	0.36439839	0.73394995
1	-6.71602474	-1.88378594	1.85190272
1	-4.94156119	-1.79300925	0.07139316
1	-5.44600433	-3.98538344	1.22194185
1	-3.69494619	-3.89099987	-0.62617991
1	-3.48525389	-5.21836121	0.54019130
8	-4.06159279	0.67591770	3.19767704
8	-2.14371457	-3.63574234	0.74970942
1	-3.80046532	3.95372402	1.44940234
1	-3.79902744	3.27916622	3.12586235

Electronic energy = -2449.436799 a.u.

DFT-D4 dispersion correction = -0.143546 a.u.

Thermal free energy = 0.689629 a.u.

Gibbs free energy = -2448.890716 a.u.

Number of imaginary frequencies = 0.

15_{CLLA} (eq_chelate)

Atomic N.	X	Y	Z
6	4.47837581	4.52914558	-3.08110748
6	4.03666236	3.87064077	-4.23609571
6	2.78441421	3.25871019	-4.31651705
6	1.94309664	3.29756835	-3.15766491
6	2.32927216	4.08988080	-2.02529387
6	3.62309309	4.65410152	-2.00161240
6	1.40444582	4.42715987	-0.92137872
7	0.32312266	3.63659497	-0.63053557
6	-0.60809321	4.00112949	0.30557258
6	-0.40960859	5.16582804	1.06415681
6	0.70358893	5.95986204	0.81863072
6	1.59470238	5.61290170	-0.19033344
6	-1.84412517	3.21599280	0.45891853
6	-2.43388031	2.54682020	-0.66639086
6	-3.77155689	2.04207934	-0.56117971
6	-4.39742551	2.11480257	0.68451614
6	-3.78118197	2.67346028	1.81456993
6	-2.52402720	3.23743581	1.69430659
8	0.80135152	2.60383677	-3.16648022
8	-1.75429755	2.42442723	-1.80553943
1	-1.16156169	5.46778768	1.78837629
1	0.85071811	6.88330601	1.38026242

1	2.41251637	6.27877224	-0.45013528
1	3.96501176	5.17008357	-1.10516725
6	2.32453894	2.56306852	-5.61511934
1	-2.04040200	3.68167697	2.56486604
1	-5.40092134	1.70752763	0.79704385
6	-4.48337351	1.41739817	-1.77721906
1	4.70785573	3.82466810	-5.09172490
6	-4.52065833	2.42795932	-2.94856724
6	-5.94224818	1.04089392	-1.45528131
6	-3.75708663	0.12362398	-2.21526640
1	-5.07395230	3.33386742	-2.65965627
1	-5.03804145	1.97666341	-3.80900752
1	-3.51246648	2.71881790	-3.26139600
1	-3.77609937	-0.61970351	-1.40443777
1	-2.71112544	0.31156363	-2.47750612
1	-4.26992107	-0.31060097	-3.08775251
1	-6.41240832	0.63306582	-2.36155544
1	-6.53402044	1.91175487	-1.13707022
1	-6.01087989	0.26894251	-0.67488226
6	2.11942503	1.04708846	-5.38823501
6	3.36142482	2.71823345	-6.74418116
6	1.00544552	3.20157876	-6.11228608
1	4.31781067	2.23211907	-6.50174397
1	3.55789248	3.77345625	-6.98268891
1	2.97096542	2.24037102	-7.65391347
1	3.04670494	0.58097304	-5.02217933
1	1.84977457	0.56221372	-6.33901125
1	1.31806443	0.85915291	-4.66641243
1	0.68027498	2.70797301	-7.04083391
1	1.15319230	4.26914124	-6.33124899
1	0.20635653	3.10465522	-5.36960666
1	-4.29607005	2.66943886	2.77532228
1	5.48283204	4.95042634	-3.04086002
8	1.28547774	-0.64832792	2.35647286
8	-0.26285034	0.25445968	-1.49430805
13	0.01026701	2.01195889	-1.68026311
6	1.85580679	-1.63060901	1.93240587
6	2.83698237	-1.64278438	0.74609553
8	2.91229727	-0.31399076	0.17489693
6	1.87326152	0.20169500	-0.50066546
6	0.72887886	-0.62628813	-1.09017837
8	1.87947719	1.41550543	-0.71643531
6	1.24421043	-1.47220493	-2.27669507
6	4.25485416	-2.00741868	1.17336349
1	2.47044298	-2.36583242	0.00411281
1	0.33382645	-1.30395411	-0.30755264
1	0.37778013	-1.97101913	-2.72791194
1	1.97524366	-2.23933699	-1.98355016
1	1.70011416	-0.82007736	-3.03245090
1	4.26252833	-3.00714111	1.62271565
1	4.63163489	-1.28045905	1.90395971
1	4.91759063	-2.00375361	0.29926907
8	-2.14812708	-8.03355924	8.18123290
6	-2.26039367	-9.38728275	8.68446178

1	-2.57140750	-10.06933457	7.88334541
6	-1.19060210	-6.42604548	6.72779150
6	-0.23766914	-6.19234727	5.55631122
6	-0.18459710	-4.72094060	5.13219813
6	-1.23964697	-7.87474480	7.17618234
6	0.76385354	-4.48408179	3.94998599
6	0.80786924	-3.01897388	3.55550207
1	-2.21712560	-6.11371461	6.47725418
1	-0.54910367	-6.81604570	4.70435483
1	-1.19849822	-4.37781260	4.86399511
1	0.43899779	-5.08390866	3.08525393
1	-0.90314809	-5.81659993	7.60045218
1	0.76939147	-6.53982102	5.83259943
1	0.13370760	-4.10277956	5.98927474
1	1.77903667	-4.82177085	4.21207149
1	1.17639511	-2.38102153	4.37155708
1	-0.17794781	-2.64171182	3.24802162
8	-0.57174274	-8.78453878	6.72261034
8	1.72359295	-2.88643889	2.41923184
1	-3.01914384	-9.34096430	9.47134997
1	-1.29901237	-9.72631966	9.09021425

Electronic energy = -2449.413737 a.u.

DFT-D4 dispersion correction = -0.137548 a.u.

Thermal free energy = 0.690146 a.u.

Gibbs free energy = -2448.861139 a.u.

Number of imaginary frequencies = 0.

15_{CLLA} (open tail)

Atomic N.	X	Y	Z
6	3.77352951	4.57189391	-2.14193633
6	3.36377298	4.20528316	-3.43041356
6	2.22321659	3.43408115	-3.66846520
6	1.47241682	2.99441208	-2.53446840
6	1.81158773	3.47154334	-1.22565539
6	2.99053909	4.22786342	-1.05563871
6	0.92747091	3.29751552	-0.05655277
7	0.07933301	2.22531474	0.02509613
6	-0.83838144	2.08733811	1.03298122
6	-0.87912278	3.05374642	2.04899704
6	0.00562228	4.12694602	2.01567009
6	0.90003252	4.26346859	0.96170551
6	-1.80158964	0.96393267	1.02738776
6	-2.27061133	0.33574915	-0.17463650
6	-3.38294176	-0.56209293	-0.12207915
6	-3.88929144	-0.89680112	1.13608222
6	-3.36474314	-0.37384972	2.32471354
6	-2.34750621	0.56094221	2.26559868
8	0.43421363	2.15543414	-2.71643573
8	-1.70045299	0.60086222	-1.36441767
1	-1.63406351	2.98682606	2.82708575
1	-0.03549466	4.88829309	2.79536909
1	1.53943429	5.13859686	0.88892871
1	3.30282271	4.50916946	-0.05058509

6	1.79530454	3.07607766	-5.10706779
1	-1.94200808	0.97559180	3.18816051
1	-4.71473012	-1.60241087	1.20440640
6	-4.00978776	-1.14464026	-1.40621610
1	3.97272710	4.52423677	-4.27395778
6	-4.48722750	0.00450514	-2.32655737
6	-5.23971963	-2.01900023	-1.09479878
6	-2.99324028	-2.03694521	-2.15504456
1	-5.25218581	0.61165687	-1.82100961
1	-4.93912144	-0.41622790	-3.23730369
1	-3.66098913	0.66003186	-2.62159258
1	-2.64731194	-2.86055114	-1.51384899
1	-2.12307143	-1.46123610	-2.48510534
1	-3.46938752	-2.47819270	-3.04340932
1	-5.66645182	-2.37983066	-2.04104787
1	-6.02602081	-1.45627667	-0.57122683
1	-4.98250466	-2.90308879	-0.49359212
6	1.86230847	1.54870990	-5.33581751
6	2.71177451	3.73556235	-6.15545226
6	0.35810901	3.58722805	-5.36859461
1	3.74958827	3.37871328	-6.08568112
1	2.71305449	4.83203706	-6.07321994
1	2.34420010	3.47966506	-7.15907835
1	2.87985266	1.17152281	-5.15646872
1	1.59455174	1.31763843	-6.37782075
1	1.17106735	1.01452064	-4.67709423
1	0.05880045	3.33857481	-6.39789243
1	0.31108770	4.68048177	-5.25903123
1	-0.36450755	3.13628865	-4.68004244
1	-3.76478856	-0.69432357	3.28657639
1	4.69757742	5.13211825	-2.00090642
8	2.89122431	0.79947915	1.12616210
8	1.12259491	-0.33803722	-1.24338565
13	0.02491348	0.99941611	-1.43792788
6	2.92529681	-0.35851925	0.75070726
6	3.82340860	-0.85448321	-0.38727070
8	3.46222436	-2.15920264	-0.91143081
6	2.23202933	-2.58958307	-1.33082100
6	1.05067795	-1.66671558	-1.71458491
8	2.09645326	-3.78459293	-1.50034868
6	0.92167989	-1.72865517	-3.24696902
6	4.12318689	0.17855697	-1.46351105
1	4.77564969	-1.08659151	0.12384951
1	0.18057749	-2.18116702	-1.26996540
1	0.01265678	-1.19642972	-3.56471218
1	0.85083462	-2.76968385	-3.58421009
1	1.78813429	-1.25212748	-3.72509665
1	4.48878346	1.09851832	-0.99017532
1	3.22755307	0.41631468	-2.04455130
1	4.90388546	-0.21028111	-2.12970245
8	-2.43630490	-4.15464002	8.01813636
6	-2.82319000	-5.29607386	8.82113204
1	-3.17343900	-6.11475292	8.18017357
6	-1.06578726	-3.13943630	6.37119810

6	-0.16465256	-3.39635974	5.16338341
6	0.23260058	-2.10028711	4.44906129
6	-1.42549932	-4.40093336	7.13272247
6	1.10954541	-2.35024939	3.21649875
6	1.51371006	-1.05077482	2.53986585
1	-1.99818575	-2.63238957	6.07881516
1	-0.68200314	-4.06526285	4.45809226
1	-0.67725576	-1.55476462	4.14504638
1	0.56814516	-2.98092221	2.49436165
1	-0.57113959	-2.46048691	7.08714772
1	0.73490346	-3.93868522	5.49027715
1	0.76778778	-1.44304201	5.15678496
1	2.01607366	-2.90457404	3.50611547
1	2.11360071	-0.40771385	3.20001381
1	0.63551176	-0.47826719	2.20673094
8	-0.89658113	-5.48827088	7.00465334
8	2.30798071	-1.39177454	1.36861507
1	-3.62997443	-4.93583051	9.46660714
1	-1.97435409	-5.64962917	9.41991556

Electronic energy = -2449.400330 a.u.

DFT-D4 dispersion correction = -0.145117 a.u.

Thermal free energy = 0.687481 a.u.

Gibbs free energy = -2448.857966 a.u.

Number of imaginary frequencies = 0.

Propagation stage for LA-CL

9_{LACL}

Atomic N.	X	Y	Z
6	-2.04374426	3.11049400	2.94271337
6	-3.49995452	2.90090358	3.41133019
6	-4.39881081	2.21908857	2.37442344
6	-1.86011133	4.33605707	2.06425830
6	-4.51009024	2.96190161	1.03824177
6	-3.17768218	3.19657377	0.33053567
1	-1.68445774	2.21214034	2.41325439
1	-3.93042670	3.86989787	3.71232052
1	-4.00411596	1.20623132	2.18326947
1	-5.14797310	2.37718734	0.35497029
1	-1.38818932	3.27065140	3.80620867
1	-3.47770575	2.27958530	4.31945876
1	-5.40555011	2.08282332	2.80014105
1	-5.00996773	3.93533179	1.17240023
1	-3.35083939	3.45373281	-0.72206753
1	-2.53180198	2.30474533	0.36183997
8	-1.22921496	5.31775652	2.41122146
8	-2.44884769	4.35490025	0.83147618
6	2.42398807	2.89502772	3.91333564
6	3.06650234	1.65074153	3.93785639
6	3.02232574	0.76006623	2.86208106
6	2.26893868	1.14681052	1.70787688
6	1.72407352	2.46692351	1.62719978
6	1.77926598	3.30715441	2.76003622
6	1.19337466	3.02526198	0.36638426
7	0.65248209	2.21043518	-0.59320620
6	0.19506441	2.72149713	-1.77810953
6	0.27786941	4.10198244	-2.02127538
6	0.81113540	4.94331213	-1.05334934
6	1.27975934	4.40856648	0.13806990
6	-0.34141159	1.83364805	-2.83065306
6	0.11812027	0.48980283	-2.99806844
6	-0.19164330	-0.21939668	-4.20295254
6	-1.08008573	0.37912226	-5.10005679
6	-1.64412861	1.64124779	-4.87345165
6	-1.25492484	2.36906128	-3.76216764
8	2.10079295	0.27334725	0.70625077
8	0.85420492	-0.10446491	-2.05197753
1	-0.03562202	4.49590308	-2.98406152
1	0.88719497	6.01492662	-1.23849941
1	1.73911264	5.04794154	0.88572930
1	1.27513935	4.27331761	2.73767620
6	3.76166921	-0.59260112	2.92502465
1	-1.67372815	3.36084608	-3.59134466
1	-1.35949440	-0.15408662	-6.00695309
6	0.43709225	-1.59444814	-4.50799473
1	3.60603695	1.36788667	4.83994432
6	1.98016965	-1.47875708	-4.49414736
6	0.02893847	-2.11533029	-5.89917107
6	-0.01696910	-2.64698185	-3.47051419

1	2.32045096	-0.77184426	-5.26466732
1	2.42876146	-2.45953848	-4.71414196
1	2.34912028	-1.13906519	-3.52037858
1	-1.11371114	-2.73964731	-3.46786296
1	0.31765334	-2.37972151	-2.46346460
1	0.40877554	-3.62884496	-3.73088383
1	0.53308706	-3.07505124	-6.08203268
1	0.32758667	-1.42654182	-6.70233037
1	-1.05400864	-2.29166939	-5.97710128
6	2.75608245	-1.76697765	2.87379137
6	4.57391117	-0.74260661	4.22552444
6	4.75791292	-0.70457890	1.74645484
1	3.93398746	-0.74389268	5.11999464
1	5.32478380	0.05266811	4.33659817
1	5.10927214	-1.70256381	4.20232587
1	2.03398284	-1.69421168	3.70123157
1	3.29588056	-2.72162934	2.97523914
1	2.21182180	-1.77221537	1.92413206
1	5.28596936	-1.66923062	1.79528679
1	5.51090712	0.09482677	1.80272950
1	4.24766679	-0.63577446	0.77973315
1	-2.36796073	2.05185213	-5.57736455
1	2.44261840	3.53854242	4.79288013
8	-1.45295803	-4.87437828	-0.86303652
6	-1.87408678	-5.72944410	-1.96003642
1	-2.10954577	-6.73316880	-1.58659463
8	0.25927087	-6.32333476	-0.46628797
8	-1.01292090	0.23500937	0.43537837
1	-2.76289962	-5.24554370	-2.37408966
1	-1.07894514	-5.79611448	-2.71166159
13	0.62407742	0.25032556	-0.30865703
8	-0.86745464	-3.27142535	1.10454226
6	-0.55273685	-2.07427272	0.62334316
6	-1.58723885	-0.97511883	0.82414962
6	-0.35421594	-5.30616727	-0.21032802
6	0.08688550	-4.36908906	0.91913499
8	0.51329455	-1.81441476	0.04567338
6	0.20708907	-5.10816689	2.24462690
6	-2.86445047	-1.30454936	0.02909429
1	-1.83678068	-0.96728172	1.90550123
1	1.05301286	-3.94197618	0.61570515
1	0.63914018	-4.44670551	3.00523925
1	0.86292644	-5.97635706	2.11042393
1	-0.77612954	-5.45615956	2.58696522
1	-3.30599561	-2.25549793	0.35551945
1	-2.63670685	-1.35749601	-1.04385541
1	-3.59294255	-0.49972253	0.18804910

Electronic energy = -2449.428035 a.u.

DFT-D4 dispersion correction = -0.148531 a.u.

Thermal free energy = 0.690376 a.u.

Gibbs free energy = -2448.886190 a.u.

Number of imaginary frequencies = 0.

10a_{LACL}

Atomic N.	X	Y	Z
6	3.54969256	2.33748592	-1.94177590
6	3.22489676	1.47217987	-2.99640713
6	1.96592570	0.88352859	-3.12534443
6	0.99574347	1.15574519	-2.10540110
6	1.26156226	2.17567700	-1.13380049
6	2.56612194	2.71034039	-1.04466698
6	0.19203614	2.78190356	-0.31691038
7	-0.96037824	2.09360574	-0.04457468
6	-1.99566660	2.67380759	0.63908271
6	-1.86573376	3.99369602	1.10637141
6	-0.69410007	4.69849838	0.86244862
6	0.33174183	4.10567297	0.13775033
6	-3.27379103	1.96000699	0.82498058
6	-3.72370714	0.96292853	-0.10079419
6	-5.11475626	0.61854436	-0.14340256
6	-5.93050695	1.09330688	0.88513803
6	-5.44822976	1.91951612	1.91085574
6	-4.14442094	2.37754446	1.85524915
8	-0.14980284	0.47338380	-2.09547019
8	-2.87739342	0.37572459	-0.94630487
1	-2.70358811	4.47298794	1.60440597
1	-0.59713917	5.73059727	1.20159184
1	1.21924071	4.67409935	-0.12461286
1	2.80706955	3.40690590	-0.24196309
6	1.62871528	-0.01448249	-4.33361867
1	-3.77690148	3.05412238	2.62664393
1	-6.98088349	0.80797487	0.90475914
6	-5.69636463	-0.22015070	-1.30053692
1	3.99514858	1.24528438	-3.73127764
6	-5.37534972	0.47175749	-2.64760745
6	-7.22900150	-0.34083495	-1.20204622
6	-5.11951735	-1.65360394	-1.30334829
1	-5.81707670	1.47834378	-2.67954097
1	-5.80459682	-0.11230729	-3.47575208
1	-4.29522096	0.55791365	-2.80899427
1	-5.37653499	-2.17111416	-0.36661405
1	-4.03082720	-1.64346044	-1.42243529
1	-5.55758217	-2.22779143	-2.13429281
1	-7.59832486	-0.90403330	-2.07088412
1	-7.72181621	0.64200175	-1.20953264
1	-7.54755191	-0.88315448	-0.29977594
6	1.35139998	-1.46764290	-3.88734775
6	2.78446771	-0.05725060	-5.35147898
6	0.38970131	0.55155284	-5.06864467
1	3.69204035	-0.51565326	-4.93204799
1	3.04177937	0.94298675	-5.72881038
1	2.47694066	-0.66735560	-6.21269703
1	2.22506418	-1.88241473	-3.36294531
1	1.15574449	-2.09424390	-4.77147488
1	0.48641722	-1.52219456	-3.22006014
1	0.15100099	-0.08353949	-5.93527629
1	0.59054578	1.56717864	-5.43974978

1	-0.48703051	0.58478306	-4.41268800
1	-6.10646255	2.22219910	2.72501385
1	4.56194101	2.72990339	-1.84714799
8	-1.36123507	-1.88458493	-1.15863938
13	-1.12120106	0.20011332	-0.61351009
8	-0.33317132	-3.86969833	1.60287128
6	0.95206389	-4.14743874	1.26086247
6	1.24520252	-4.09562965	-0.23987990
8	0.56191978	-2.95917178	-0.87042400
6	-0.71114313	-2.72752477	-0.53966674
6	-1.29662367	-3.64536806	0.52995515
8	1.77219782	-4.43200607	2.10256937
6	-2.56640373	-3.12012508	1.16333200
6	2.72043501	-3.96859697	-0.55484793
1	0.82930367	-5.01422291	-0.69297844
1	-1.48783116	-4.61986896	0.03813583
1	-2.91168720	-3.82812819	1.92638084
1	-3.34323688	-3.00847900	0.39930442
1	-2.37462486	-2.14131145	1.61756991
1	3.25906336	-4.81623657	-0.11620758
1	3.12346778	-3.04288021	-0.12726375
1	2.87282311	-3.96360399	-1.64069121
8	6.44565311	0.89612712	5.87379549
6	7.88756689	0.83899736	5.98374986
1	8.24888579	-0.17573711	5.77438067
6	4.44540254	0.68084852	4.61834322
6	3.81123621	0.13540230	3.33908376
6	2.29039433	0.32171335	3.31259759
6	5.95702379	0.56605750	4.64031802
6	1.64538126	-0.23731135	2.04005023
6	0.12660569	-0.05095478	2.01555947
1	4.04921259	0.17380321	5.51210638
1	4.05493761	-0.93374879	3.23945289
1	1.84469251	-0.16865918	4.19569940
1	1.87749387	-1.31148328	1.95677153
1	4.19786769	1.74778165	4.75289048
1	4.26494573	0.63210710	2.46830640
1	2.05204613	1.39618866	3.40453305
1	2.07979888	0.25139390	1.15262052
1	-0.10565973	1.02397919	2.13842481
1	-0.31784931	-0.56536653	2.88835160
8	6.66572581	0.24039825	3.70697850
8	-0.46172782	-0.58064291	0.83924903
1	8.11099664	1.12479213	7.01620366
1	8.35537041	1.53661474	5.27742527

Electronic energy = -2449.402626 a.u.

DFT-D4 dispersion correction = -0.145083 a.u.

Thermal free energy = 0.689226 a.u.

Gibbs free energy = -2448.858483 a.u.

Number of imaginary frequencies = 0.

10b_{LACL}

Atomic N.	X	Y	Z
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6	3.69409929	3.85671782	-1.92617015
6	3.14779631	3.20751490	-3.04266339
6	1.92314802	2.53920245	-2.99503385
6	1.22605835	2.51248095	-1.74153486
6	1.70894368	3.28552846	-0.63872764
6	2.97002635	3.91188454	-0.74777188
6	0.89361141	3.53195825	0.57053264
7	-0.10170781	2.66804717	0.94833021
6	-0.85391114	2.91569964	2.06489343
6	-0.60125201	4.05742784	2.84877316
6	0.39453281	4.94541957	2.47192114
6	1.13227180	4.69637600	1.32164473
6	-1.99841741	2.05894400	2.41795140
6	-2.74252072	1.38159603	1.40128165
6	-4.09933439	0.99683385	1.66833369
6	-4.52418374	1.03200042	2.99783333
6	-3.70750722	1.48977683	4.04391871
6	-2.47668357	2.04659180	3.74574350
8	0.12976323	1.77119901	-1.62594302
8	-2.19790311	1.14333178	0.21276433
1	-1.23573131	4.26748975	3.70523067
1	0.57018843	5.85294461	3.05093045
1	1.86724997	5.41711938	0.97552436
1	3.39282782	4.42349127	0.11649161
6	1.33657993	1.85054577	-4.24467564
1	-1.86025798	2.46361323	4.54252415
1	-5.52779034	0.68816900	3.24254551
6	-5.07027927	0.62045832	0.52948296
1	3.71363390	3.21666037	-3.97278901
6	-5.13908739	1.79854721	-0.47266370
6	-6.49695167	0.37802008	1.05762886
6	-4.63125786	-0.65671134	-0.21882235
1	-5.50894797	2.70842620	0.02189085
1	-5.83222788	1.55133944	-1.29114634
1	-4.15520444	2.01059924	-0.90751565
1	-4.52395365	-1.50379687	0.47463799
1	-3.68038397	-0.50001852	-0.73718656
1	-5.39294096	-0.92690812	-0.96626522
1	-7.16132310	0.17301297	0.20617619
1	-6.89705621	1.25430619	1.58764056
1	-6.54839512	-0.49014816	1.73108905
6	1.23321715	0.32042291	-4.03867191
6	2.21320864	2.08899279	-5.48893819
6	-0.06421550	2.43315073	-4.55150613
1	3.21617929	1.64982709	-5.38236484
1	2.32414581	3.15873937	-5.71871784
1	1.73686605	1.61123598	-6.35674919
1	2.22876766	-0.11308848	-3.85601801
1	0.83227151	-0.14733220	-4.95107300
1	0.57479828	0.06106516	-3.20200817
1	-0.47499306	1.95275756	-5.45246040
1	0.00078732	3.51400815	-4.74474576
1	-0.75979536	2.26551298	-3.72247390
1	-4.06157561	1.44586416	5.07377379

1	4.67582649	4.32591976	-1.99256214
8	1.13130750	0.41845216	1.04894796
8	2.74995546	-0.65796959	2.01772843
6	2.15874925	-0.26443187	0.88965805
6	2.76387242	-0.57884018	-0.44919394
1	2.80419553	-1.67426883	-0.54959123
1	2.05321886	-0.23063973	-1.20435298
6	4.16199713	0.04162044	-0.66385369
1	4.16879373	1.08519374	-0.31283825
1	4.33322805	0.08900823	-1.74876680
6	5.30017884	-0.75223402	-0.01525774
1	5.32955481	-1.76087295	-0.46233756
1	6.26175125	-0.27627832	-0.26194707
6	5.18492906	-0.89246326	1.50612359
1	5.27177945	0.08963529	1.99881227
1	6.02346395	-1.50205257	1.88058533
6	3.90141847	-1.55949074	1.98412903
1	3.63416327	-2.44287928	1.38639228
1	3.99040857	-1.86531396	3.03304815
13	-0.41734590	0.95578267	-0.12346699
8	1.14022886	-6.14502530	2.16504641
6	1.83959573	-7.24575543	1.53285630
1	1.13887899	-8.05282124	1.28497945
8	-0.11937695	-5.94632970	0.27570455
8	-0.43709787	-0.72292686	-0.74720832
1	2.57553533	-7.58228060	2.26911095
1	2.33258573	-6.90380801	0.61453295
6	0.16188524	-5.58799289	1.39912304
6	-0.56099039	-4.50046690	2.20247278
8	-1.19708453	-3.55940919	1.31323463
6	-0.34759573	-2.75627258	0.59770318
6	-1.15102251	-1.84656010	-0.34827034
8	0.86376493	-2.80920691	0.72484569
6	-1.55626574	-2.68976205	-1.57369166
6	-1.66152249	-5.11015932	3.06618720
1	0.18178005	-3.97396573	2.81739470
1	-2.06941822	-1.58306449	0.20780226
1	-2.18652769	-2.07091101	-2.22556217
1	-2.10860568	-3.59302319	-1.28362636
1	-0.65788324	-2.98253976	-2.13364499
1	-1.22806917	-5.82411169	3.77829749
1	-2.39692765	-5.63042768	2.43917805
1	-2.17249639	-4.31790387	3.62742522

Electronic energy = -2449.408335 a.u.

DFT-D4 dispersion correction = -0.149008 a.u.

Thermal free energy = 0.692634 a.u.

Gibbs free energy = -2448.864709 a.u.

Number of imaginary frequencies = 0.

TS3ax_{LACL}

Atomic N.	X	Y	Z
6	3.53984189	2.39801288	-1.63548803
6	3.30227971	1.56286764	-2.73667002

6	2.05612087	0.98778778	-2.99055481
6	0.99712002	1.25792217	-2.06398368
6	1.19847286	2.20491409	-1.00860083
6	2.49234867	2.73173809	-0.79724091
6	0.08442966	2.72466087	-0.19226262
7	-1.05407226	1.98449671	0.00419793
6	-2.11007762	2.48580980	0.72154105
6	-2.01800728	3.76233768	1.30259907
6	-0.86636460	4.51846218	1.12657249
6	0.17939173	4.01242542	0.36569679
6	-3.37481856	1.73539698	0.83232939
6	-3.81588721	0.86774063	-0.21737874
6	-5.18997240	0.46579185	-0.27447280
6	-5.99715567	0.77403760	0.82264739
6	-5.52388144	1.48690152	1.93465459
6	-4.23603821	1.99270499	1.92034292
8	-0.17218243	0.63443524	-2.20826411
8	-2.96560431	0.45533961	-1.15566659
1	-2.87425089	4.17191696	1.83129263
1	-0.80114359	5.52277613	1.54689932
1	1.05388987	4.62232351	0.15811472
1	2.67516708	3.38283467	0.05738771
6	1.83210182	0.08235181	-4.21873474
1	-3.87382460	2.57845521	2.76556087
1	-7.03412485	0.44254503	0.82780963
6	-5.75811672	-0.26430371	-1.50918937
1	4.13375568	1.34419882	-3.40411210
6	-5.50636911	0.59117603	-2.77451158
6	-7.27991009	-0.47445428	-1.39446723
6	-5.11182356	-1.65799129	-1.68568325
1	-5.99706650	1.57112396	-2.68244648
1	-5.92907715	0.08295240	-3.65426922
1	-4.43662405	0.74990392	-2.94822025
1	-5.34012747	-2.30071592	-0.82173902
1	-4.02476597	-1.59103143	-1.80383706
1	-5.52740049	-2.14656520	-2.58025718
1	-7.64292002	-0.95756155	-2.31268358
1	-7.82096004	0.47636530	-1.28336620
1	-7.54841423	-1.12847137	-0.55194181
6	1.49716616	-1.36210632	-3.77782536
6	3.08689809	0.01204519	-5.11000013
6	0.68423647	0.64935684	-5.08830070
1	3.94186425	-0.44503766	-4.59067678
1	3.39090037	1.00314474	-5.47717810
1	2.86458659	-0.61196750	-5.98716164
1	2.31330585	-1.77811003	-3.16865134
1	1.37950540	-1.99941480	-4.66787195
1	0.57288140	-1.40814948	-3.19369912
1	0.53409374	0.00445054	-5.96736097
1	0.93416250	1.65803039	-5.44894695
1	-0.25732312	0.69941401	-4.53145695
1	-6.17694235	1.66215372	2.78938103
1	4.54146910	2.78437161	-1.44818985
8	-1.31797934	-1.71273446	-1.16993022

13	-1.21888387	0.17371339	-0.83618665
8	-0.61698812	-3.45867705	1.96329248
6	0.63782918	-3.91969705	1.69446838
6	0.98393446	-3.96165085	0.20621197
8	0.56248081	-2.74064660	-0.46985444
6	-0.68735671	-2.25331140	-0.18254843
6	-1.45812285	-3.12044477	0.81855214
8	1.37340927	-4.26431799	2.59189105
6	-2.73879671	-2.51724958	1.35409689
6	2.46247888	-4.15456486	-0.06134980
1	0.41313890	-4.80173349	-0.23488326
1	-1.69023168	-4.05478811	0.27229005
1	-3.25152898	-3.24947166	1.98998940
1	-3.39565754	-2.25169706	0.51859778
1	-2.53070211	-1.61573720	1.94132543
1	2.79647470	-5.09832859	0.38542259
1	3.04720068	-3.33784771	0.37819305
1	2.64078808	-4.18304586	-1.14313424
8	6.66009092	0.87910634	5.42801380
6	8.10633278	0.93719560	5.45791578
1	8.53530216	-0.02957901	5.16593981
6	4.61420774	0.56461209	4.27272224
6	3.95557618	0.08334750	2.98038268
6	2.42556334	0.12122232	3.05538964
6	6.12913132	0.58327180	4.20458984
6	1.75943995	-0.37285954	1.76591814
6	0.23782898	-0.32709172	1.87136626
1	4.31765556	-0.05847507	5.13118267
1	4.29042721	-0.94245845	2.76219678
1	2.08368945	-0.49401629	3.90564919
1	2.09151030	-1.40113485	1.55991232
1	4.28472424	1.58692873	4.52457523
1	4.30565310	0.70117140	2.13992548
1	2.09427738	1.15315390	3.26778769
1	2.08349037	0.24229899	0.91259325
1	-0.09042569	0.69351310	2.12802505
1	-0.11699071	-0.99351716	2.67263913
8	6.80396795	0.37720224	3.21392751
8	-0.44284520	-0.68306136	0.65243429
1	8.36492729	1.17944515	6.49319792
1	8.47423553	1.71216094	4.77360535

Electronic energy = -2449.397487 a.u.

DFT-D4 dispersion correction = -0.148614 a.u.

Thermal free energy = 0.693643 a.u.

Gibbs free energy = -2448.852458 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 130.9i

TS3eq_{LACL}

Atomic N.	X	Y	Z
6	3.29294062	3.83348536	-3.25847483
6	2.82517672	2.68443727	-3.91014814
6	1.75447619	1.92817843	-3.42927194

6	1.12722266	2.35675192	-2.21260238
6	1.51318324	3.59965777	-1.62001801
6	2.62939024	4.29309464	-2.13568401
6	0.72030348	4.23347712	-0.55094111
7	-0.06437530	3.48638105	0.28770679
6	-0.81844550	4.08530092	1.25880432
6	-0.80129552	5.48466396	1.40125740
6	-0.01223566	6.25484991	0.55866390
6	0.74372196	5.63438749	-0.42550761
6	-1.72079897	3.30110002	2.12325478
6	-2.34462881	2.09164405	1.67919993
6	-3.52991128	1.64017165	2.35116029
6	-3.86499691	2.25388908	3.56089449
6	-3.12331080	3.30785728	4.10776520
6	-2.08712816	3.84992671	3.37026691
8	0.17985645	1.60271907	-1.65125215
8	-1.85075080	1.40808570	0.63756210
1	-1.45233071	5.95593977	2.13172698
1	-0.01670462	7.34222126	0.64406359
1	1.31598222	6.22538376	-1.13446975
1	2.98775959	5.18777227	-1.62734926
6	1.30024672	0.65176374	-4.16385794
1	-1.52971506	4.70032406	3.76225853
1	-4.73113155	1.89404464	4.11293507
6	-4.42200899	0.51742136	1.78248131
1	3.33626318	2.36234450	-4.81563807
6	-4.79218674	0.82686949	0.31288478
6	-5.74783373	0.38422292	2.55762410
6	-3.69415116	-0.83877891	1.87959468
1	-5.36480761	1.76384068	0.25110903
1	-5.42194796	0.01944042	-0.09007388
1	-3.90422201	0.92563158	-0.32013026
1	-3.47442126	-1.08629787	2.92837906
1	-2.75203538	-0.80902982	1.32738149
1	-4.32076025	-1.64107597	1.46052384
1	-6.36929941	-0.37931776	2.06794310
1	-6.31784916	1.32436872	2.56429434
1	-5.59541273	0.06137745	3.59747958
6	1.63592231	-0.58525294	-3.29968143
6	2.01653790	0.47931004	-5.51734495
6	-0.21676148	0.70858967	-4.46322346
1	3.10170460	0.34467959	-5.40182972
1	1.83986080	1.33094013	-6.19069052
1	1.62704337	-0.42231411	-6.01138544
1	2.72447872	-0.68217832	-3.17399192
1	1.27107286	-1.50104284	-3.79006124
1	1.18576813	-0.51842803	-2.30446744
1	-0.52255839	-0.20693751	-4.99196100
1	-0.44948301	1.56585073	-5.11229515
1	-0.80927986	0.79737043	-3.54719758
1	-3.38383913	3.71560192	5.08429623
1	4.16576672	4.36296368	-3.64044595
8	1.15449107	1.37174881	1.45060623
8	0.97328192	-0.47032291	2.68301177

6	1.48828709	0.11645850	1.57606530
6	2.85470986	-0.30044407	1.06896400
1	2.86375332	-1.35792542	0.77795583
1	3.01783800	0.28127038	0.15417106
6	3.96104360	-0.00035021	2.10301304
1	3.77579808	0.97822839	2.57390761
1	4.91321898	0.09347038	1.56000054
6	4.11250830	-1.09479916	3.16754484
1	4.37802267	-2.03903317	2.66167140
1	4.95997286	-0.84902430	3.82658672
6	2.86538577	-1.33300471	4.02797365
1	2.65221834	-0.45623526	4.66045046
1	3.05456853	-2.17529202	4.71385050
6	1.60240805	-1.66153598	3.23734021
1	1.80115259	-2.39524364	2.44143081
1	0.82718170	-2.06852770	3.89845085
13	-0.12171826	1.48373127	0.11836382
8	1.43691492	-6.42430782	-1.47466612
6	1.63911974	-6.81659031	-2.85667491
1	0.71840245	-7.24615812	-3.27039409
8	-0.21389291	-5.01595879	-2.17383242
8	0.36566284	-0.41017577	0.15027311
1	2.44012666	-7.56092834	-2.83072162
1	1.93362975	-5.94604445	-3.45501304
6	0.46096420	-5.49891472	-1.29001212
6	0.30706096	-5.21058178	0.21005014
8	-0.33357951	-3.93030238	0.40206096
6	0.41154310	-2.84266257	0.02497324
6	-0.43496171	-1.57161570	0.16682187
8	1.56170213	-2.92389274	-0.35732758
6	-1.45880508	-1.55046177	-0.98201579
6	-0.57915854	-6.25715256	0.87770635
1	1.30961061	-5.18872309	0.65939093
1	-0.97050035	-1.65889406	1.13025975
1	-2.08735991	-0.65629041	-0.89344913
1	-2.09733915	-2.44095945	-0.93696404
1	-0.94319618	-1.53215873	-1.94923186
1	-0.12656292	-7.25132561	0.77282488
1	-1.57535601	-6.26669741	0.41711551
1	-0.68620849	-6.03005123	1.94595003

Electronic energy = -2449.397933 a.u.

DFT-D4 dispersion correction = -0.150225 a.u.

Thermal free energy = 0.695808 a.u.

Gibbs free energy = -2448.852350 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 90.3i

11a_{LACL}

Atomic N.	X	Y	Z
6	3.60884686	2.40236723	-1.63723951
6	3.38227656	1.54897013	-2.72640944
6	2.13813197	0.97112902	-2.98344841
6	1.06787607	1.26724739	-2.07941473

6	1.26276004	2.21461521	-1.02411564
6	2.55623266	2.74236862	-0.80865318
6	0.15070180	2.71921615	-0.19610699
7	-0.98959949	1.97723566	-0.00821132
6	-2.04152364	2.46650084	0.72530598
6	-1.94250611	3.72574632	1.33874339
6	-0.78996096	4.48358455	1.17226683
6	0.24849621	3.99389965	0.39161343
6	-3.30825294	1.71686424	0.82011457
6	-3.77244995	0.90869030	-0.26655882
6	-5.13407003	0.46666405	-0.29282152
6	-5.91374233	0.71431063	0.83958812
6	-5.42346493	1.39339268	1.96475758
6	-4.14146237	1.91410472	1.94111157
8	-0.10920073	0.66183967	-2.24579194
8	-2.94556410	0.58787202	-1.26405836
1	-2.79550813	4.12332651	1.88187889
1	-0.71937570	5.47793947	1.61470361
1	1.12130945	4.60864509	0.19223582
1	2.73718466	3.39701784	0.04335865
6	1.93100377	0.02707716	-4.18518374
1	-3.76170191	2.46396629	2.80278848
1	-6.94158123	0.35649732	0.86318809
6	-5.71433105	-0.26093785	-1.52265869
1	4.22096807	1.31650910	-3.37989873
6	-5.53550477	0.61807906	-2.78384750
6	-7.22286306	-0.53064770	-1.36489006
6	-5.01928871	-1.62745547	-1.72981959
1	-6.06208961	1.57639561	-2.66507669
1	-5.96559367	0.10281162	-3.65583142
1	-4.47935328	0.82201685	-2.98887307
1	-5.20299863	-2.28725764	-0.86828322
1	-3.93760004	-1.52260105	-1.86621978
1	-5.43539106	-2.12124528	-2.62119500
1	-7.59484903	-1.01457147	-2.27899875
1	-7.79645347	0.39698083	-1.22382968
1	-7.44067767	-1.20667633	-0.52519918
6	1.58540799	-1.39997099	-3.69604853
6	3.20211478	-0.07978748	-5.04947273
6	0.80296305	0.56578873	-5.09738671
1	4.04607964	-0.51774826	-4.49691113
1	3.51510651	0.89590809	-5.44900027
1	2.99479512	-0.73672260	-5.90593737
1	2.39643855	-1.79663262	-3.06745645
1	1.47145798	-2.06765234	-4.56395322
1	0.65709543	-1.42402109	-3.11633882
1	0.67098760	-0.10818091	-5.95726964
1	1.06304000	1.56124313	-5.48648257
1	-0.15071577	0.63684933	-4.56437509
1	-6.05657282	1.52390096	2.84219371
1	4.60848103	2.79149123	-1.44568707
8	-1.30595778	-1.62540770	-1.06188310
13	-1.22034068	0.22213225	-0.93016969
8	-0.83140678	-3.71029450	1.90802766

6	0.27797916	-4.37555516	1.46101259
6	0.67288218	-4.01369035	0.02763616
8	0.59822733	-2.57472753	-0.10599181
6	-0.69972433	-2.02458698	0.06583042
6	-1.59365919	-2.97936932	0.89619228
8	0.87856244	-5.12814789	2.19490286
6	-2.75835495	-2.31442245	1.60304881
6	2.08460132	-4.44641398	-0.31610786
1	-0.04140307	-4.48945651	-0.67166472
1	-1.97830353	-3.70805935	0.16403346
1	-3.37370956	-3.07939841	2.09265193
1	-3.37962462	-1.78096550	0.87442587
1	-2.41384892	-1.60336940	2.36328970
1	2.17537185	-5.53360931	-0.20729317
1	2.80712949	-3.97252758	0.35959096
1	2.31577117	-4.16386473	-1.35032102
8	6.72157222	0.84728669	5.36000131
6	8.10422118	1.27733474	5.33511955
1	8.68079042	0.67304670	4.62373847
6	4.62566560	0.51825729	4.30220354
6	3.92768719	0.30448554	2.95903392
6	2.43798007	-0.01693800	3.12022545
6	6.07283775	0.95155206	4.16346163
6	1.74061862	-0.25414822	1.77443145
6	0.25417951	-0.51633333	1.97144098
1	4.58992847	-0.38674562	4.92742295
1	4.42649447	-0.51196921	2.41399654
1	2.31852948	-0.90805275	3.76036837
1	2.19721344	-1.10853681	1.25617902
1	4.11131752	1.30183052	4.88537318
1	4.05325716	1.20319031	2.33740650
1	1.94304384	0.81392216	3.65383126
1	1.87595497	0.62255095	1.12385724
1	-0.23412664	0.33514807	2.46838093
1	0.08154913	-1.41111534	2.58447771
8	6.60288657	1.35626587	3.14607479
8	-0.48512388	-0.69031197	0.72046923
1	8.47098794	1.13070054	6.35550459
1	8.17283481	2.33336002	5.04489595

Electronic energy = -2449.400077 a.u.

DFT-D4 dispersion correction = -0.148173 a.u.

Thermal free energy = 0.690246 a.u.

Gibbs free energy = -2448.858004 a.u.

Number of imaginary frequencies = 0.

11b_{LACL}

Atomic N.	X	Y	Z
6	3.87418776	4.54890577	0.91573977
6	3.84126470	3.99159150	-0.36902587
6	2.77046121	3.22327000	-0.83082215
6	1.67611121	2.99456682	0.06635942
6	1.63921233	3.68360415	1.32036624
6	2.77274671	4.41283396	1.73996049

6	0.41591251	3.75934318	2.14015227
7	-0.54369093	2.78435555	2.07033502
6	-1.70957915	2.88456832	2.77944631
6	-1.92960082	4.00150130	3.60482814
6	-0.96043447	4.99072221	3.70124353
6	0.20981302	4.88056978	2.96326423
6	-2.77737207	1.87506757	2.64293166
6	-2.98063016	1.12066209	1.44230844
6	-4.24310120	0.47131626	1.23680971
6	-5.13933000	0.43008082	2.30749755
6	-4.86332038	1.01454442	3.54886751
6	-3.70597189	1.75491225	3.69888999
8	0.69277881	2.15682821	-0.28433179
8	-2.02128856	1.04163262	0.50587784
1	-2.88078186	4.11056074	4.11724158
1	-1.13639156	5.87096104	4.32076070
1	0.94432143	5.68038621	2.97311225
1	2.78822128	4.85250843	2.73675479
6	2.79691545	2.61365735	-2.24630838
1	-3.49295092	2.23637672	4.65275519
1	-6.08571514	-0.09278605	2.18394827
6	-4.61241620	-0.19403170	-0.10421189
1	4.69826554	4.15032728	-1.02085164
6	-4.41507902	0.80052547	-1.27239964
6	-6.08764472	-0.63881353	-0.14727201
6	-3.74560653	-1.45546658	-0.30314702
1	-5.08368158	1.66577740	-1.15384152
1	-4.66648435	0.30957269	-2.22467756
1	-3.38631793	1.17021193	-1.32910701
1	-3.97359647	-2.20317305	0.47019593
1	-2.68334842	-1.20949039	-0.23216338
1	-3.94246346	-1.90743879	-1.28763276
1	-6.30304898	-1.05430268	-1.14225070
1	-6.77686064	0.20165220	0.01895811
1	-6.31089578	-1.42444844	0.58844432
6	2.93969445	1.07924817	-2.14113966
6	3.98630178	3.13417493	-3.07661115
6	1.51123963	2.98788403	-3.02164662
1	4.95541068	2.83952915	-2.64930215
1	3.96928486	4.22869222	-3.18350683
1	3.93069390	2.70013820	-4.08526060
1	3.90165698	0.80977210	-1.68191426
1	2.90887965	0.62511287	-3.14398041
1	2.14439402	0.63932507	-1.53280482
1	1.55204348	2.55444980	-4.03271344
1	1.42883513	4.07966539	-3.12819281
1	0.61035106	2.62115692	-2.51936347
1	-5.56424089	0.90550495	4.37619728
1	4.75476470	5.09462752	1.25426827
8	0.40226761	0.15552216	2.18125976
8	-0.27494032	-1.98123492	1.91037223
6	0.68977627	-1.02322530	1.59234624
6	2.15667510	-1.42374070	1.73820328
1	2.41210196	-2.26298883	1.07833913

1	2.72260566	-0.55877924	1.37018001
6	2.54417086	-1.73821233	3.19379688
1	2.04929995	-1.01832253	3.86387893
1	3.62668163	-1.57350065	3.30370467
6	2.22726707	-3.17878062	3.61478380
1	2.80120159	-3.86775542	2.97031882
1	2.58818149	-3.34761007	4.64176182
6	0.74379979	-3.55694698	3.53783335
1	0.15564967	-2.98186098	4.27078315
1	0.62795090	-4.62091299	3.80458198
6	0.10581950	-3.35252182	2.16449365
1	0.75689340	-3.74080724	1.36246879
1	-0.84877245	-3.89325696	2.10794143
13	-0.27492019	1.21747235	0.89565549
8	1.25583282	-3.08400224	-4.33774256
6	1.79457266	-2.61803036	-5.60203235
1	2.82890348	-2.27960171	-5.46698616
8	2.85810989	-4.70341065	-4.31964708
8	0.44467353	-0.59432237	0.07701723
1	1.14837539	-1.78772140	-5.90081710
1	1.76975903	-3.42345261	-6.34593078
6	1.91870571	-4.13313029	-3.80108848
6	1.32907054	-4.59507131	-2.46369417
8	0.43274402	-3.62845707	-1.85797612
6	1.03131959	-2.49557792	-1.37316433
6	-0.05647173	-1.53122895	-0.88085203
8	2.22871903	-2.30604623	-1.38102290
6	-0.59652004	-0.76229717	-2.09140515
6	0.53749539	-5.88600908	-2.64557587
1	2.18980470	-4.74915357	-1.79802622
1	-0.85839500	-2.12984147	-0.42381879
1	-1.38545221	-0.07361369	-1.76687712
1	-1.01796293	-1.46628975	-2.81959891
1	0.20609395	-0.18904700	-2.57029191
1	1.17947901	-6.64510145	-3.10886125
1	-0.33788319	-5.71804601	-3.28640938
1	0.19539864	-6.25580908	-1.67093724

Electronic energy = -2449.398511 a.u.

DFT-D4 dispersion correction = -0.150564 a.u.

Thermal free energy = 0.694693 a.u.

Gibbs free energy = -2448.854383 a.u.

Number of imaginary frequencies = 0.

12_{LACL}

Atomic N.	X	Y	Z
6	4.01679755	2.14676186	-2.60851092
6	3.16189536	2.44410787	-3.67831275
6	1.77827643	2.57184572	-3.52917855
6	1.23313670	2.37694693	-2.22283210
6	2.10839433	2.15086469	-1.10879019
6	3.49470339	2.01701387	-1.33441604
6	1.62672235	2.14788803	0.28696685
7	0.35950915	1.71038881	0.57953526

6	-0.17254480	1.79023883	1.84121314
6	0.63055710	2.29083114	2.87957558
6	1.93741410	2.68655941	2.61859949
6	2.43987581	2.62905679	1.32319057
6	-1.56912515	1.38396290	2.10215507
6	-2.59522905	1.40503711	1.10153239
6	-3.95925806	1.18543123	1.46875871
6	-4.22986869	0.85596561	2.79849942
6	-3.22388702	0.74349157	3.76664839
6	-1.91351035	1.01829572	3.42220975
8	-0.10023304	2.43011389	-2.04107109
8	-2.30585323	1.65283390	-0.18594517
1	0.21245299	2.40789232	3.87499041
1	2.55553672	3.08241572	3.42497367
1	3.43324133	3.00573957	1.09507307
1	4.15275184	1.77904805	-0.49864596
6	0.87411910	2.88693145	-4.73826142
1	-1.13119379	0.92005404	4.17398005
1	-5.25730654	0.66010029	3.09856115
6	-5.09704643	1.29260827	0.43199883
1	3.59941849	2.56042112	-4.66788537
6	-5.11307480	2.70645526	-0.19705317
6	-6.47841694	1.06661341	1.07640694
6	-4.92809553	0.22049841	-0.67066083
1	-5.28139664	3.47038776	0.57600972
1	-5.93487442	2.77725975	-0.92533102
1	-4.17418137	2.93378416	-0.71235553
1	-4.92778892	-0.78845032	-0.23265419
1	-3.99702769	0.35889125	-1.22957017
1	-5.76779985	0.28226980	-1.37908441
1	-7.25267885	1.17943869	0.30467795
1	-6.69165232	1.79998870	1.86749718
1	-6.58126558	0.05654741	1.49898875
6	-0.07713890	1.70005054	-5.02254054
6	1.69841435	3.12595953	-6.01806946
6	0.05908146	4.17539291	-4.47323467
1	2.26208652	2.23269766	-6.32349913
1	2.40155451	3.96454338	-5.90813672
1	1.01214367	3.37511239	-6.83946585
1	0.49189129	0.78604598	-5.24511275
1	-0.69973036	1.93003868	-5.90019996
1	-0.74049816	1.49327027	-4.17680999
1	-0.57200681	4.39642105	-5.34712683
1	0.73036332	5.03280432	-4.31736948
1	-0.58774686	4.07474556	-3.59561565
1	-3.47493915	0.44417684	4.78408952
1	5.08512974	2.01981161	-2.78251349
8	-0.60864649	-0.30465359	-1.72871589
13	-0.75365915	1.23365130	-0.90665903
8	4.70976913	-3.79799900	6.30476528
6	5.76908501	-3.35374777	7.18649257
1	6.57508875	-2.88235496	6.61035543
6	3.00312804	-3.36320814	4.71782057
6	2.46403561	-2.35692482	3.70167004

6	1.27636955	-2.90096852	2.90069090
6	4.11871467	-2.80383882	5.58002043
6	0.75165318	-1.88917511	1.87544678
6	-0.47638113	-2.40936516	1.13479726
1	3.36932892	-4.27828985	4.22730420
1	3.27278902	-2.06567266	3.01329064
1	1.57222373	-3.83016980	2.38378172
1	1.53687130	-1.65639438	1.14071543
1	2.20182935	-3.69522977	5.40010633
1	2.16845662	-1.43685730	4.22785603
1	0.46492364	-3.17945593	3.59626447
1	0.48933148	-0.95121574	2.38820287
1	-1.30096124	-2.59155680	1.84170041
1	-0.24160868	-3.35370625	0.62805636
8	4.45268201	-1.63565555	5.64785776
8	-0.99474447	-1.44088698	0.18583985
1	6.12766067	-4.25851802	7.68648520
1	5.38296863	-2.63229379	7.91757340
8	0.58269590	-2.24419472	-1.30344920
6	-0.66803821	-1.56586179	-1.19456747
6	-1.72989449	-2.39355281	-1.95860260
8	-1.31981774	-2.56796177	-3.35552477
6	-0.01043858	-2.55212010	-3.71677130
6	1.06335467	-2.25774186	-2.66187831
8	0.28871642	-2.72652706	-4.88101196
6	2.20444366	-3.26421987	-2.73718409
6	-2.05994201	-3.76279301	-1.38472551
1	-2.63952128	-1.78014803	-2.02316708
1	1.43667901	-1.24974442	-2.91429891
1	2.99835520	-2.97198127	-2.03816532
1	2.60757054	-3.28543568	-3.75566638
1	1.85333417	-4.27086420	-2.47307849
1	-2.53302124	-3.66462493	-0.39922411
1	-1.16018997	-4.38586182	-1.29443109
1	-2.76529247	-4.26948093	-2.05585087

Electronic energy = -2449.399303 a.u.

DFT-D4 dispersion correction = -0.145114 a.u.

Thermal free energy = 0.689967 a.u.

Gibbs free energy = -2448.854449 a.u.

Number of imaginary frequencies = 0.

13a_{LACL}

Atomic N.	X	Y	Z
6	5.96969110	1.82057003	0.75011859
6	6.11279746	1.16354045	-0.48011504
6	5.02009833	0.79720319	-1.26836920
6	3.71108682	1.08830082	-0.76484067
6	3.56218211	1.89165967	0.41179305
6	4.71054575	2.20455037	1.17367339
6	2.27177339	2.50088504	0.79627246
7	1.07959725	1.93420389	0.42107029
6	-0.11862487	2.53574266	0.71552818
6	-0.13357306	3.72845436	1.45915991

6	1.06255578	4.30278103	1.86758056
6	2.26794172	3.70448053	1.52208668
6	-1.38756945	1.98383779	0.20812350
6	-1.44418693	1.26251314	-1.02773456
6	-2.70706113	1.04633775	-1.66704415
6	-3.85701645	1.40575769	-0.96008112
6	-3.81387406	1.98136146	0.31895280
6	-2.58929422	2.29311785	0.88161844
8	2.64431067	0.61647360	-1.41311143
8	-0.32469003	0.81544156	-1.59939891
1	-1.08035167	4.22236665	1.65836653
1	1.05762916	5.24306630	2.41989026
1	3.21016226	4.18536337	1.76813965
1	4.59986820	2.73156292	2.12099290
6	5.21767571	0.11023774	-2.63584450
1	-2.55304503	2.75562773	1.86794392
1	-4.83235562	1.22055154	-1.40736900
6	-2.79246716	0.44074987	-3.08293407
1	7.11772090	0.91914942	-0.81907176
6	-1.97121950	1.30429237	-4.07053713
6	-4.24277503	0.40937403	-3.60174014
6	-2.26721853	-1.01394810	-3.09396518
1	-2.36393276	2.33102319	-4.10497120
1	-2.04684666	0.87992074	-5.08302722
1	-0.91322728	1.34337878	-3.79032607
1	-2.87716485	-1.64938817	-2.43416398
1	-1.22230625	-1.07501785	-2.77184687
1	-2.34072395	-1.42500275	-4.11237468
1	-4.24586384	0.00684200	-4.62451529
1	-4.69098932	1.41282814	-3.63900372
1	-4.88971682	-0.23920966	-2.99300857
6	4.64082620	-1.32449524	-2.62609972
6	6.70925869	0.00323371	-3.00709430
6	4.52830324	0.94505897	-3.74201362
1	7.27103441	-0.62905731	-2.30427902
1	7.19278379	0.98958795	-3.05469207
1	6.79579647	-0.45575831	-4.00190936
1	5.13456414	-1.93549440	-1.85538847
1	4.82475437	-1.80316401	-3.59992729
1	3.56097976	-1.32440617	-2.44322159
1	4.68086285	0.46168138	-4.71867306
1	4.96410159	1.95343775	-3.79354163
1	3.45103605	1.03766233	-3.56744664
1	-4.73500833	2.18704528	0.86394601
1	6.84704249	2.04153819	1.35744776
8	0.86389081	-1.56942566	-0.97034447
8	1.21925494	-0.78682749	1.07476280
13	1.07901193	0.24909110	-0.63697889
8	2.85240017	-3.02558758	1.74664541
6	2.56245273	-2.11988800	2.71349809
6	1.98811362	-0.74775873	2.31003038
6	1.16015656	-2.12803764	0.20272602
6	2.57415648	-2.70635319	0.34840529
8	2.82010793	-2.37326023	3.87080756

6	2.77703060	-3.98182789	-0.44580026
6	1.14986934	-0.15378806	3.43364197
1	2.87290818	-0.11110500	2.12654196
1	3.27896061	-1.92728612	0.02041660
1	3.81257813	-4.32796551	-0.33817420
1	2.57687263	-3.78918438	-1.50732939
1	2.09730934	-4.76346135	-0.08629690
1	1.75772054	-0.07771950	4.34217578
1	0.28443514	-0.79237745	3.64851030
1	0.79440490	0.84546164	3.15382621
8	-7.51076900	-0.77651100	3.60060124
6	-8.26895108	0.11005457	4.45908956
1	-7.67391970	0.39605959	5.33526385
6	-5.64158271	-1.21346320	2.19328117
6	-4.12906224	-1.26751410	2.44643870
6	-3.38478836	-2.05816953	1.36591161
6	-6.35190730	-0.24347123	3.11598421
6	-1.86887342	-2.08736840	1.59658237
6	-1.14740191	-2.82551629	0.47387999
1	-6.10384353	-2.20646693	2.27256728
1	-3.93852030	-1.71697020	3.43496086
1	-3.77289334	-3.09072765	1.32354924
1	-1.64390654	-2.58143931	2.55572651
1	-5.82269678	-0.85233497	1.16613360
1	-3.74138445	-0.23941592	2.48574208
1	-3.59633412	-1.60312506	0.38352103
1	-1.49058494	-1.05628177	1.66468246
1	-1.25657496	-2.30837551	-0.48792917
1	-1.54224999	-3.84647748	0.37083695
8	-5.96705739	0.87931699	3.38976682
8	0.26710439	-3.01617319	0.75155301
1	-9.15184809	-0.46257632	4.75872170
1	-8.55946673	1.01639671	3.91304704

Electronic energy = -2449.402824 a.u.

DFT-D4 dispersion correction = -0.152221 a.u.

Thermal free energy = 0.695205 a.u.

Gibbs free energy = -2448.859840 a.u.

Number of imaginary frequencies = 0.

13b_{LACL}

Atomic N.	X	Y	Z
6	0.17713981	2.07403891	-5.44074225
6	-0.74542383	1.03495066	-5.61959055
6	-1.42367327	0.43649269	-4.55516685
6	-1.12193880	0.89403702	-3.23058506
6	-0.32882457	2.07486534	-3.06423710
6	0.35293936	2.60929919	-4.17794466
6	-0.33055345	2.84665196	-1.80677255
7	-0.55517492	2.23890811	-0.59965124
6	-0.67815668	2.97251579	0.55208602
6	-0.55104030	4.37239837	0.49725957
6	-0.28399792	4.99987650	-0.71181887
6	-0.18162476	4.24305243	-1.87045500

6	-0.99254661	2.32698569	1.84229561
6	-1.65974014	1.06366661	1.93156466
6	-2.18201956	0.62368647	3.19246437
6	-1.90255259	1.39598071	4.32101368
6	-1.14263616	2.57061608	4.25978253
6	-0.70827151	3.03299097	3.03190238
8	-1.60073384	0.23599596	-2.16712132
8	-1.81318288	0.28809673	0.85440185
1	-0.71264137	4.96280929	1.39387587
1	-0.20149941	6.08643469	-0.75788282
1	-0.05368822	4.72440183	-2.83560156
1	1.04086563	3.44199773	-4.03300956
6	-2.45421731	-0.68194491	-4.81055253
1	-0.11702370	3.94656521	2.98733888
1	-2.26623151	1.06767022	5.29275910
6	-2.98894005	-0.68435057	3.31772763
1	-0.92486630	0.67459668	-6.63083941
6	-4.19235760	-0.68093858	2.34543971
6	-3.55952626	-0.87711987	4.73615182
6	-2.06168517	-1.88675643	3.02652893
1	-4.86795907	0.15635112	2.57394345
1	-4.76342409	-1.61450842	2.46217103
1	-3.87426959	-0.59348732	1.30181877
1	-1.26359968	-1.94779172	3.78109875
1	-1.59672651	-1.79501770	2.03949854
1	-2.63529553	-2.82584955	3.06375627
1	-4.15056222	-1.80385218	4.75935818
1	-4.22510378	-0.05175254	5.02767150
1	-2.77064517	-0.97410376	5.49571593
6	-1.92490645	-2.02507018	-4.26503064
6	-2.73829027	-0.87279963	-6.31273506
6	-3.79991841	-0.32764780	-4.13420442
1	-1.85174728	-1.21273582	-6.86719876
1	-3.11031575	0.04936433	-6.78194927
1	-3.51351641	-1.64306951	-6.43255333
1	-1.00042078	-2.31848725	-4.78396425
1	-2.67052075	-2.81992155	-4.42115433
1	-1.71337644	-1.94839457	-3.19439420
1	-4.53321100	-1.12493467	-4.32848828
1	-4.20331527	0.60838321	-4.54721189
1	-3.69113279	-0.21067906	-3.05076333
1	-0.90186413	3.11561329	5.17232047
1	0.72737559	2.47187868	-6.29312948
6	1.64905921	-1.99739690	-1.91583113
6	1.91178482	-3.50533713	-1.94888610
6	0.66320780	-4.39188921	-1.86711612
6	1.11823052	-1.42253561	-0.60263767
6	-0.17171373	-4.22278027	-0.58838230
6	-1.07576527	-2.99692004	-0.55079827
1	0.95398123	-1.69371631	-2.71267919
1	2.44220814	-3.73376908	-2.88667858
1	0.98339585	-5.44363063	-1.93757629
1	-0.85908723	-5.08051892	-0.49810218
1	2.59208569	-1.45753875	-2.08823634

1	2.60073889	-3.76379831	-1.13116701
1	0.01804891	-4.20932963	-2.74392000
1	0.47624128	-4.24655198	0.30019675
1	-1.74610512	-3.05802438	0.31846489
1	-1.69913046	-2.96892137	-1.45798978
8	1.04516507	-0.07087501	-0.56654839
8	-0.40727982	-1.71017587	-0.43915155
13	-0.74557589	0.26525947	-0.58361381
8	6.18663945	1.93196433	2.92564093
6	7.35074804	1.49285233	3.66987994
1	7.17493784	1.59156050	4.74834855
8	4.97323691	0.31825107	3.98234154
8	1.81174697	-2.01543167	0.45905814
1	8.16448327	2.14800950	3.34560973
1	7.57535378	0.44552947	3.43435119
6	5.05175672	1.23447886	3.19124270
6	3.88861723	1.81984388	2.37919399
8	2.81045735	0.86240016	2.31604519
6	3.05762351	-0.22329927	1.52105098
6	1.92374114	-1.24500388	1.66369522
8	4.06115139	-0.36811176	0.85726832
6	2.25867531	-2.21591308	2.79479715
6	3.33675744	3.08064131	3.03625175
1	4.24986957	2.02516504	1.36221769
1	0.98915889	-0.71049478	1.88169058
1	1.43013408	-2.92255744	2.93220586
1	2.42069926	-1.66607009	3.73048433
1	3.17154475	-2.77530565	2.55347447
1	4.12701610	3.83821622	3.11302889
1	2.95414244	2.85736342	4.04050948
1	2.51858834	3.48440261	2.42706951

Electronic energy = -2449.406338 a.u.

DFT-D4 dispersion correction = -0.151425 a.u.

Thermal free energy = 0.696097 a.u.

Gibbs free energy = -2448.861665 a.u.

Number of imaginary frequencies = 0.

TS4ax_{LACL}

Atomic N.	X	Y	Z
6	5.90013456	2.60777116	1.69249427
6	6.12287760	2.12259889	0.39602640
6	5.08256960	1.84937918	-0.49470153
6	3.74267650	2.05023694	-0.03031376
6	3.51559687	2.69033432	1.23005629
6	4.61215878	2.91616845	2.09111285
6	2.19535971	3.23647261	1.60260582
7	1.04035711	2.69767046	1.09638512
6	-0.18346088	3.24254417	1.38973033
6	-0.26303002	4.35975933	2.23956776
6	0.89586908	4.90470505	2.77662969
6	2.12913442	4.35488081	2.45212841
6	-1.41748130	2.71132255	0.77981311
6	-1.41282201	2.08729482	-0.50833744

6	-2.64514971	1.91207910	-1.21722460
6	-3.82956600	2.18874335	-0.53131729
6	-3.84641171	2.65546536	0.79114562
6	-2.65136552	2.94258928	1.42576897
8	2.71872139	1.65401220	-0.78932875
8	-0.26876798	1.69066608	-1.06780624
1	-1.22791898	4.82231617	2.42662406
1	0.84090483	5.78575039	3.41699505
1	3.04768729	4.81283617	2.80758786
1	4.43780088	3.31449866	3.09050107
6	5.36736202	1.35619223	-1.92839241
1	-2.66055512	3.33008409	2.44452214
1	-4.78256655	2.02703190	-1.03193641
6	-2.66326308	1.44417405	-2.68676758
1	7.14968252	1.93993914	0.08457586
6	-1.81541121	2.40906620	-3.55030084
6	-4.09031010	1.44654691	-3.26728129
6	-2.11523628	0.00438873	-2.81515121
1	-2.22173285	3.42986250	-3.50110269
1	-1.84288979	2.08509398	-4.60155916
1	-0.77044791	2.43202615	-3.22318530
1	-2.74010539	-0.69591969	-2.24065471
1	-1.08234179	-0.07022427	-2.45916867
1	-2.14372802	-0.30972576	-3.86975241
1	-4.04485941	1.14717257	-4.32389784
1	-4.55284071	2.44323325	-3.22473288
1	-4.75078440	0.73330492	-2.75278497
6	4.82252693	-0.07516295	-2.14098001
6	6.87807703	1.32150614	-2.22818351
6	4.71788454	2.32199216	-2.94857097
1	7.41383171	0.60463607	-1.58895051
1	7.34571457	2.30985808	-2.11193085
1	7.02654886	1.00569975	-3.27043939
1	5.29580832	-0.77639610	-1.43719101
1	5.06149912	-0.41399825	-3.16063428
1	3.73584437	-0.11788006	-2.01056027
1	4.93104315	1.97708213	-3.97153616
1	5.13331985	3.33454490	-2.84079742
1	3.63123846	2.37363052	-2.82112598
1	-4.79534864	2.81104040	1.30403757
1	6.73883438	2.75709128	2.37196064
8	1.14759719	-0.66696411	-0.83152044
8	1.05117595	-0.06611946	1.35710466
13	1.14334488	1.11602592	-0.13075799
8	2.77916956	-2.16741443	2.07571387
6	2.26567578	-1.38758349	3.06666994
6	1.43594718	-0.13148092	2.73386645
6	1.31064653	-1.40064359	0.23449598
6	2.72498608	-1.78852725	0.66747457
8	2.47705984	-1.69292009	4.22096682
6	3.26169205	-2.97536635	-0.11597785
6	0.20757298	-0.05574969	3.64083791
1	2.10754037	0.71793884	2.95330000
1	3.36198473	-0.90534651	0.51577735

1	4.29445267	-3.18395591	0.18951856
1	3.25040340	-2.74838829	-1.18967533
1	2.64628172	-3.86332273	0.07204853
1	0.51478106	-0.09846352	4.69175386
1	-0.46936050	-0.89579409	3.43682885
1	-0.33086249	0.88208652	3.45514202
8	-7.70230007	-5.26700068	0.39449435
6	-8.61153126	-6.29087114	0.86553234
1	-8.29456806	-7.27904415	0.50912142
6	-5.53953457	-4.30637932	0.26177782
6	-4.08587265	-4.39352703	0.72489536
6	-3.22386932	-3.26235008	0.15465409
6	-6.41097784	-5.41975260	0.81116116
6	-1.76434445	-3.34365106	0.61791587
6	-0.92915112	-2.20913434	0.04888105
1	-5.60833406	-4.34010553	-0.83805192
1	-3.66819263	-5.36836052	0.43058345
1	-3.26192498	-3.29138470	-0.94796687
1	-1.32588696	-4.30553436	0.30833378
1	-5.99432373	-3.34605217	0.55420387
1	-4.05259180	-4.37106800	1.82492459
1	-3.65037155	-2.28876591	0.45188895
1	-1.71833467	-3.31175399	1.71799111
1	-1.29988706	-1.22856867	0.38418955
1	-0.91484731	-2.21917391	-1.04916871
8	-6.03924990	-6.33317518	1.52288675
8	0.43544063	-2.38435984	0.53175527
1	-9.58808422	-6.02373695	0.45051441
1	-8.64402103	-6.30024719	1.96224368

Electronic energy = -2449.403384 a.u.

DFT-D4 dispersion correction = -0.147068 a.u.

Thermal free energy = 0.691396 a.u.

Gibbs free energy = -2448.859056 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 76.4i

TS4eq_{LACL}

Atomic N.	X	Y	Z
6	1.15173005	3.03800451	-4.93945966
6	0.50107309	1.91777305	-5.47064176
6	-0.22708968	1.02855590	-4.67844384
6	-0.29018748	1.27990837	-3.26680515
6	0.23311669	2.50778447	-2.74650319
6	0.99792509	3.33532727	-3.59818267
6	-0.06753572	2.99807914	-1.38507113
7	-0.47637143	2.14368968	-0.39887370
6	-0.77863399	2.60157265	0.85434743
6	-0.65185097	3.96743867	1.15572257
6	-0.24883065	4.85139959	0.16450345
6	0.02435893	4.37575281	-1.11085002
6	-1.31975758	1.69124129	1.88115513
6	-2.13453437	0.57038072	1.52063918
6	-2.98217328	-0.02520433	2.51108615

6	-2.79681302	0.36735073	3.83918430
6	-1.85490173	1.33405262	4.21981653
6	-1.15071786	2.01659975	3.24311933
8	-0.84325388	0.36436705	-2.46686584
8	-2.11674054	0.10063604	0.26936101
1	-0.92742792	4.32534203	2.14378320
1	-0.18332864	5.91951681	0.37525066
1	0.27091580	5.06947727	-1.90865762
1	1.49675857	4.21174957	-3.18720094
6	-0.91194231	-0.20000478	-5.31126623
1	-0.43181814	2.78623767	3.52343271
1	-3.39347394	-0.10427790	4.61826227
6	-4.06429830	-1.05474319	2.12938105
1	0.58799522	1.72895338	-6.53896178
6	-4.98957774	-0.45627215	1.04302010
6	-4.95172646	-1.42808795	3.33176355
6	-3.41837781	-2.35588674	1.60642541
1	-5.48896155	0.44903096	1.41780243
1	-5.76898901	-1.18609646	0.77607416
1	-4.43151150	-0.19697098	0.13664776
1	-2.80074863	-2.82377300	2.38736464
1	-2.78919992	-2.15188205	0.73463745
1	-4.20018597	-3.07495659	1.31705449
1	-5.73355203	-2.12383201	2.99492033
1	-5.45184072	-0.54927469	3.76373309
1	-4.38539054	-1.93263432	4.12801315
6	-0.19845968	-1.48864288	-4.84617960
6	-0.84714071	-0.16859965	-6.85063627
6	-2.40930867	-0.24587632	-4.92465929
1	0.18396496	-0.22198367	-7.22860132
1	-1.32363194	0.73197460	-7.26425615
1	-1.38565179	-1.04137549	-7.24685622
1	0.84554047	-1.49866835	-5.19313097
1	-0.70346840	-2.37479314	-5.26088858
1	-0.20221587	-1.56364029	-3.75436973
1	-2.88629882	-1.11827200	-5.39652432
1	-2.92632643	0.65567503	-5.28452019
1	-2.54858688	-0.31540713	-3.84115712
1	-1.69857513	1.55994267	5.27438472
1	1.75890172	3.67629029	-5.58118193
6	2.45058217	-1.56317397	-1.21201118
6	2.72814848	-3.06193713	-1.36830142
6	1.58377475	-3.91025977	-1.94500426
6	1.56324804	-1.13762198	-0.06127667
6	0.32411796	-4.05178353	-1.07212172
6	-0.67744207	-2.90085474	-1.15921561
1	2.02259029	-1.13446413	-2.12815234
1	3.59529564	-3.16341787	-2.03997244
1	1.98989992	-4.91819398	-2.12795482
1	-0.22422533	-4.95456142	-1.38867989
1	3.40122252	-1.03110079	-1.02932721
1	3.04256713	-3.47675710	-0.39851373
1	1.29701170	-3.51699381	-2.93513518
1	0.60961748	-4.21795046	-0.02073387

1	-1.58498853	-3.17987123	-0.59590085
1	-0.97634608	-2.75904542	-2.21322014
8	1.15360575	0.08844641	0.02183928
8	-0.17211645	-1.67646918	-0.63411556
13	-0.58772174	0.16599835	-0.70265203
8	4.35882167	2.06478639	5.15159803
6	3.88119605	3.18381934	5.93993665
1	3.82933715	4.09079917	5.32483657
8	2.58087390	2.35655892	3.75443778
8	1.84010267	-1.83132898	1.06594176
1	4.61068014	3.30046915	6.74653220
1	2.88601156	2.96141755	6.34363218
6	3.58895814	1.76341508	4.07438045
6	4.23781893	0.60826000	3.29860072
8	3.24515414	-0.08080094	2.50304982
6	2.30719835	-0.75481986	3.21882633
6	1.24321200	-1.39027048	2.31719334
8	2.28609224	-0.81199334	4.43274915
6	0.56654436	-2.57690911	2.98127874
6	5.29367886	1.12965642	2.32976633
1	4.66886191	-0.09353341	4.02559354
1	0.51891733	-0.58933973	2.10310872
1	-0.23834766	-2.94663206	2.33574821
1	0.14114414	-2.26592486	3.94230260
1	1.28491540	-3.38632203	3.16507239
1	6.08139151	1.65564932	2.88395878
1	4.84077267	1.81884795	1.60575819
1	5.74694996	0.29125878	1.78600611

Electronic energy = -2449.401309 a.u.

DFT-D4 dispersion correction = -0.151614 a.u.

Thermal free energy = 0.693741 a.u.

Gibbs free energy = -2448.859183 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 78.0i

14a_{LACL}

Atomic N.	X	Y	Z
6	-0.33886536	6.22021867	1.13343484
6	0.37704064	6.12954796	-0.06902940
6	0.38751049	4.97317026	-0.85106715
6	-0.33294796	3.83352190	-0.36209789
6	-1.21161666	3.98116291	0.75970599
6	-1.15110904	5.16948822	1.52016549
6	-2.26396711	2.99139655	1.06579609
7	-2.14494927	1.69070610	0.65708151
6	-3.14914091	0.78464389	0.86652919
6	-4.32095155	1.18407569	1.53327400
6	-4.44965172	2.49478219	1.97476018
6	-3.43151026	3.40699125	1.73223375
6	-3.05272117	-0.58986963	0.33416585
6	-2.28355436	-0.89585241	-0.83583269
6	-2.54464960	-2.10951519	-1.55357205
6	-3.37942428	-3.05180002	-0.95019927

6	-3.99085258	-2.83239074	0.29321180
6	-3.85554437	-1.59948708	0.90697313
8	-0.18643066	2.65984857	-0.97400196
8	-1.35219804	-0.05629723	-1.28395817
1	-5.14050945	0.48065948	1.64953063
1	-5.36510415	2.81689280	2.47262204
1	-3.55209851	4.45055932	2.00791794
1	-1.73537394	5.25096441	2.43649185
6	1.12423270	4.93373226	-2.20686187
1	-4.36095441	-1.40980056	1.85388688
1	-3.55918603	-4.00102719	-1.45221456
6	-1.94678830	-2.35415648	-2.95463170
1	0.95343268	6.99483381	-0.39159602
6	-2.37313463	-1.20569981	-3.90065976
6	-2.45865334	-3.67059336	-3.56967113
6	-0.40427874	-2.43933798	-2.90370754
1	-3.46841906	-1.16544793	-3.99069953
1	-1.95732438	-1.37808897	-4.90502200
1	-2.01487466	-0.23507184	-3.54011766
1	-0.08480397	-3.25048383	-2.23249273
1	0.03250182	-1.49488016	-2.56132632
1	-0.01247918	-2.65916033	-3.90875085
1	-2.04314446	-3.77610094	-4.58186439
1	-3.55453828	-3.68770016	-3.65770210
1	-2.14140205	-4.55055808	-2.99088713
6	2.29029976	3.91897269	-2.19341061
6	1.71682258	6.30839337	-2.57123898
6	0.12065038	4.55397424	-3.32261900
1	2.49403901	6.62824659	-1.86169640
1	0.94626755	7.09120969	-2.61997707
1	2.18551609	6.24224701	-3.56336374
1	3.01713795	4.17265541	-1.40714123
1	2.81686888	3.95018347	-3.15967570
1	1.92909242	2.89854305	-2.02953237
1	0.63652746	4.53407913	-4.29460851
1	-0.68807261	5.29658568	-3.38457781
1	-0.32167484	3.56721193	-3.14636810
1	-4.59244638	-3.61615852	0.75378926
1	-0.27577410	7.12265500	1.74125689
6	2.90849532	1.49457498	0.54959372
6	3.41778112	1.37222870	1.99839374
6	2.41599236	1.69274006	3.12678036
6	2.23386361	0.29496053	-0.06578171
6	1.36844627	0.61887115	3.48730469
6	0.06402164	0.70474538	2.69527477
1	2.23390390	2.35013248	0.42878174
1	4.25482417	2.08158120	2.09426321
1	3.02280232	1.88616300	4.02588975
1	1.10638593	0.72097997	4.55425843
1	3.77125291	1.68757125	-0.11540692
1	3.84611494	0.37173833	2.15569163
1	1.90371618	2.64462855	2.90151274
1	1.80204610	-0.38674820	3.36475658
1	-0.63956403	-0.06336844	3.07078285

1	-0.40059456	1.69288191	2.88329486
8	1.32724776	0.34989609	-0.92862987
8	0.31371993	0.50624782	1.31895366
13	-0.44763931	1.05755880	-0.19564332
8	1.54152622	-6.35996451	3.13176739
6	2.54424306	-7.35580852	3.45961493
1	2.55328562	-8.15102863	2.70400608
8	2.63909975	-5.97595198	1.17166751
8	2.85657335	-0.84545834	0.24211897
1	2.25045812	-7.74913338	4.43693647
1	3.53579432	-6.88984680	3.50757666
6	1.72652027	-5.74486499	1.93702635
6	0.57987985	-4.75624099	1.68823955
8	0.96256248	-3.82754920	0.64649150
6	1.90952434	-2.91413163	1.00116704
6	2.28754403	-2.09621776	-0.23555463
8	2.38318245	-2.80146187	2.11049013
6	3.32778238	-2.82361744	-1.08087774
6	-0.68027958	-5.46891848	1.20972100
1	0.39566944	-4.19799959	2.61620727
1	1.38486056	-1.87788517	-0.81577683
1	3.55655930	-2.23279917	-1.97696813
1	2.93481513	-3.79967097	-1.39133802
1	4.24871972	-2.98416041	-0.50630166
1	-1.02301588	-6.17245152	1.97874058
1	-0.48213199	-6.02159921	0.28205946
1	-1.47280950	-4.73329806	1.02226131

Electronic energy = -2449.411314 a.u.

DFT-D4 dispersion correction = -0.150689 a.u.

Thermal free energy = 0.693633 a.u.

Gibbs free energy = -2448.868371 a.u.

Number of imaginary frequencies = 0.

14b_{LACL}

Atomic N.	X	Y	Z
6	0.22694750	1.85398171	-5.53776420
6	-0.75064224	0.86553159	-5.71512519
6	-1.47665431	0.32094831	-4.65297772
6	-1.15944455	0.77383934	-3.32910092
6	-0.31816617	1.92014259	-3.17244560
6	0.40820268	2.40300762	-4.28099713
6	-0.33066349	2.71653165	-1.93189392
7	-0.59091832	2.14242078	-0.71602030
6	-0.69605264	2.91899621	0.40899087
6	-0.55769396	4.31610749	0.31288933
6	-0.27169512	4.90609413	-0.90976057
6	-0.15731656	4.10828369	-2.03833624
6	-0.98862023	2.32474684	1.72754387
6	-1.67496268	1.07826955	1.86670896
6	-2.14374265	0.66611271	3.15929359
6	-1.81266151	1.46014897	4.25842473
6	-1.04818203	2.62830693	4.14132592
6	-0.65300244	3.05667078	2.88725697

8	-1.66242948	0.15326751	-2.25903921
8	-1.89081979	0.29961278	0.80833902
1	-0.72193976	4.93208983	1.19176898
1	-0.17997086	5.98994569	-0.98976650
1	-0.00543548	4.55256614	-3.01782861
1	1.13127625	3.20600861	-4.13717436
6	-2.57412038	-0.73097860	-4.91012837
1	-0.05608847	3.96366406	2.79576856
1	-2.13894741	1.15559702	5.25114588
6	-2.94255913	-0.63897005	3.34463052
1	-0.93864002	0.50328293	-6.72426568
6	-4.18991317	-0.65452104	2.42969788
6	-3.44457189	-0.80891991	4.79147818
6	-2.02630249	-1.84414235	3.02819948
1	-4.85529552	0.18683342	2.67326285
1	-4.75325190	-1.58622363	2.59038428
1	-3.91907616	-0.58771591	1.37148003
1	-1.19303801	-1.88898161	3.74576643
1	-1.61220731	-1.77332892	2.01660231
1	-2.59424167	-2.78360848	3.11184663
1	-4.03025351	-1.73691593	4.85782863
1	-4.09877420	0.01929337	5.10055323
1	-2.62015708	-0.89048906	5.51446859
6	-2.12591293	-2.10692178	-4.37567011
6	-2.87679749	-0.89224749	-6.41233343
6	-3.89224192	-0.30000499	-4.22438628
1	-2.01819631	-1.28851348	-6.97338317
1	-3.18650283	0.05645145	-6.87398641
1	-3.70311875	-1.60728693	-6.53314530
1	-1.22204934	-2.45073174	-4.90039993
1	-2.91776352	-2.85485541	-4.53589694
1	-1.90847304	-2.05436644	-3.30463448
1	-4.67418606	-1.04849092	-4.42274365
1	-4.23846641	0.66345443	-4.62628964
1	-3.77182612	-0.20150029	-3.14037051
1	-0.77222224	3.19370743	5.03149468
1	0.81055096	2.20732893	-6.38764425
6	1.75826108	-1.83250602	-1.97843842
6	1.83389964	-3.36585098	-1.99758562
6	0.49923242	-4.13324006	-2.01873333
6	1.46997916	-1.17634839	-0.65365221
6	-0.36372069	-4.10450809	-0.74193581
6	-1.28281798	-2.89071565	-0.59503714
1	1.02717473	-1.45221981	-2.70316899
1	2.38954675	-3.64447399	-2.90687300
1	0.74912599	-5.18450470	-2.23593340
1	-1.01356470	-4.99558661	-0.73619190
1	2.74063387	-1.41766594	-2.27157531
1	2.44752629	-3.71042903	-1.15164411
1	-0.10648830	-3.78768052	-2.87303480
1	0.27999545	-4.18522898	0.14994944
1	-1.92286601	-3.03439615	0.29547482
1	-1.95868240	-2.84179523	-1.46909043
8	1.07584906	0.03791250	-0.55605868

8	-0.54378617	-1.69251577	-0.46850256
13	-0.84080002	0.12322954	-0.64590079
8	6.23027512	2.01770750	3.17976316
6	7.53512040	1.52957732	3.58423924
1	7.54517620	1.31282618	4.65957726
8	5.32937645	0.05315521	3.90415258
8	2.08627212	-1.77760599	0.36814127
1	8.23227848	2.33671648	3.34193373
1	7.78418320	0.61789127	3.02805610
6	5.21028667	1.15239137	3.40508127
6	3.88480541	1.80553974	2.99089000
8	2.88450934	0.78276271	2.77201477
6	3.10670640	-0.01739093	1.69298976
6	2.04682758	-1.12316799	1.66125939
8	4.02165414	0.11300515	0.90965830
6	2.33417366	-2.19216898	2.71003383
6	3.35668808	2.71553859	4.09421227
1	4.04537120	2.35701085	2.05461691
1	1.05592916	-0.67665042	1.81481813
1	1.55657262	-2.96492849	2.66840736
1	2.33482505	-1.73855642	3.70799329
1	3.31382413	-2.65379355	2.53348523
1	4.07013714	3.52858356	4.27885865
1	3.21069103	2.14919117	5.02301571
1	2.39505043	3.14736003	3.79109223

Electronic energy = -2449.404133 a.u.

DFT-D4 dispersion correction = -0.150902 a.u.

Thermal free energy = 0.693092 a.u.

Gibbs free energy = -2448.861943 a.u.

Number of imaginary frequencies = 0.

15_{LACL}

Atomic N.	X	Y	Z
6	2.08891726	-1.37419724	-2.80382323
6	1.63311827	-0.60569412	-3.88257384
6	0.78981298	0.49618858	-3.72002506
6	0.38288009	0.83115888	-2.39164996
6	0.90340924	0.09451227	-1.27521861
6	1.73931086	-1.01924300	-1.51341975
6	0.67125124	0.49291930	0.12899165
7	-0.45831588	1.18944132	0.47530481
6	-0.68079340	1.64242029	1.74947822
6	0.26574817	1.36117756	2.74582529
6	1.39731658	0.61633050	2.42878389
6	1.61202765	0.18457751	1.12542379
6	-1.89277458	2.43077183	2.06157756
6	-2.55236554	3.26374507	1.09800768
6	-3.60253787	4.14130449	1.51228213
6	-4.00810719	4.08551359	2.84789324
6	-3.42560029	3.21497703	3.77792406
6	-2.37244654	2.40725398	3.38885212
8	-0.46871418	1.85709500	-2.20759654
8	-2.18059659	3.25085568	-0.19381638

1	0.12653694	1.75685930	3.74804592
1	2.13695025	0.39627695	3.19934011
1	2.51428938	-0.36394632	0.87086666
1	2.09179783	-1.62410009	-0.67752105
6	0.29650003	1.30493784	-4.93768358
1	-1.92579281	1.71977460	4.10664272
1	-4.82108927	4.72690487	3.18261766
6	-4.28150272	5.10313034	0.51533312
1	1.93871713	-0.89548308	-4.88615608
6	-3.23191929	6.04930925	-0.11534430
6	-5.33460045	5.99067211	1.20645940
6	-5.01265526	4.30313730	-0.58919138
1	-2.74243307	6.65462112	0.66169208
1	-3.72944164	6.73767328	-0.81511188
1	-2.46185780	5.49566889	-0.66219640
1	-5.78196573	3.65134668	-0.14968336
1	-4.32281590	3.68193388	-1.16973424
1	-5.51374245	4.99852371	-1.27951169
1	-5.76863670	6.67216587	0.46135047
1	-4.89625263	6.60831642	2.00379610
1	-6.16027546	5.40329981	1.63375103
6	-1.23880649	1.17507029	-5.07989120
6	0.91951632	0.79424536	-6.25142765
6	0.69811326	2.79238176	-4.79314756
1	0.63498324	-0.24487141	-6.47156191
1	2.01719046	0.86180729	-6.24304962
1	0.55617672	1.41630208	-7.08160400
1	-1.52592051	0.12315892	-5.22203922
1	-1.57751405	1.74166846	-5.96067953
1	-1.76667583	1.55602646	-4.19990015
1	0.35189521	3.35476899	-5.67353058
1	1.79212761	2.89292288	-4.73820734
1	0.26136538	3.24616647	-3.89773035
1	-3.80198193	3.17546439	4.79995203
1	2.71681809	-2.24742866	-2.98051071
6	-0.74414653	-3.84237027	0.05090046
6	-1.72685111	-2.87969208	0.72287041
6	-2.60061574	-2.14321423	-0.29725450
6	0.34481236	-4.33084965	0.97835493
6	-3.48419333	-1.05703843	0.32935080
6	-3.98171163	-0.02623268	-0.69173807
1	-0.25635988	-3.36568356	-0.81330884
1	-2.34578919	-3.42277145	1.45349038
1	-3.23044682	-2.86088681	-0.85063982
1	-4.35573673	-1.50506473	0.83617151
1	-1.26280236	-4.72749710	-0.35482070
1	-1.15438211	-2.14175129	1.30620956
1	-1.94762695	-1.66688180	-1.04585505
1	-2.91357493	-0.52560413	1.11098075
1	-4.62553406	0.71295106	-0.17936639
1	-4.60859060	-0.53026748	-1.44984925
8	0.35121369	-4.25728607	2.19233584
8	-2.91859555	0.61549842	-1.37356198
13	-1.67351270	1.71588862	-0.92185909

8	6.36473179	-1.99456084	2.89645910
6	7.53601170	-1.57378983	2.14930367
1	8.35834122	-2.28422809	2.29839993
8	6.35771608	-3.93137145	1.69372487
8	1.37918770	-4.88379622	0.26041687
1	7.79382610	-0.58880961	2.54856658
1	7.29849863	-1.51308870	1.08053005
6	5.88488007	-3.21571779	2.55123162
6	4.69498062	-3.57240510	3.45213199
8	3.87884951	-4.57832432	2.80749512
6	3.20465994	-4.15722704	1.70325267
6	2.48957586	-5.34751463	1.05598128
8	3.22153258	-3.01853299	1.28032744
6	3.43827295	-6.09138966	0.12068845
6	5.16611290	-4.16310787	4.77639532
1	4.09157658	-2.66824532	3.60909224
1	2.12164044	-6.00142479	1.85868824
1	2.91882968	-6.94733000	-0.32817715
1	4.30885839	-6.45465422	0.68051791
1	3.78766775	-5.42650890	-0.67911166
1	5.77771235	-3.42844677	5.31522751
1	5.76328421	-5.06762743	4.60355568
1	4.29905891	-4.42296028	5.39623690

Electronic energy = -2449.420790 a.u.

DFT-D4 dispersion correction = -0.141638 a.u.

Thermal free energy = 0.688400 a.u.

Gibbs free energy = -2448.874028 a.u.

Number of imaginary frequencies = 0.

Propagation stage for LA-LA

9_{LALA}

Atomic N.	X	Y	Z
8	-3.11339566	4.38298002	-2.07779234
8	-3.37538984	3.81404023	0.06873399
6	-3.32690377	3.51572825	-1.25828323
6	-3.54653176	2.04082151	-1.58757740
8	-4.63893092	1.49780113	-0.77237637
6	-4.58590068	1.73079481	0.56894214
6	-3.48170682	2.69088977	1.00592923
8	-5.36317251	1.18386476	1.31963383
6	-3.71749399	3.26960049	2.38520114
6	-3.90446766	1.79964850	-3.03880289
1	-2.62469187	1.49468207	-1.31305029
1	-2.53458422	2.12113420	0.97298981
1	-2.90177758	3.95451780	2.64545936
1	-3.75104236	2.45828684	3.12116977
1	-4.67022822	3.81178315	2.42263572
1	-3.08835384	2.14806532	-3.68177942
1	-4.81835405	2.34244604	-3.30932581
1	-4.05700845	0.72664284	-3.20862039
6	0.39677246	2.58244992	4.99487817
6	1.13500680	1.40182183	5.14767757
6	1.58603940	0.65058574	4.05992978
6	1.24634284	1.10876090	2.74585080
6	0.61056949	2.37955457	2.58138167
6	0.16129440	3.07537313	3.72393786
6	0.50957837	3.04467491	1.26617121
7	0.45765259	2.31548075	0.10612610
6	0.41750631	2.93650060	-1.11582031
6	0.41188731	4.33978720	-1.18692920
6	0.44948450	5.09157863	-0.02131942
6	0.51250199	4.44852267	1.20781929
6	0.42610869	2.15378560	-2.36820246
6	1.05943936	0.87425632	-2.46058149
6	1.31260146	0.29949804	-3.74738450
6	0.78259526	0.94926521	-4.86449205
6	0.04457728	2.13659512	-4.76748994
6	-0.10935609	2.74415853	-3.53379684
8	1.54969087	0.35471192	1.68423588
8	1.43967140	0.21728302	-1.35976339
1	0.41883929	4.82727784	-2.15712773
1	0.46377550	6.18050555	-0.07251734
1	0.61256552	5.02224148	2.12479432
1	-0.39567289	4.00417910	3.60273512
6	2.42151748	-0.62812395	4.27561853
1	-0.67819751	3.67047090	-3.45377817
1	0.93220070	0.51571171	-5.85165184
6	2.14236650	-0.99157391	-3.89985830
1	1.34951410	1.05666423	6.15730499
6	3.54191897	-0.79475625	-3.26966695
6	2.35497481	-1.36423290	-5.37945853
6	1.42609659	-2.18311758	-3.22282003

1	4.08245788	0.01731714	-3.77717299
1	4.13323020	-1.71604074	-3.38334111
1	3.47366240	-0.55621607	-2.20290945
1	0.42934421	-2.33637379	-3.66370027
1	1.31441922	-2.01944896	-2.14653301
1	2.01383068	-3.10158205	-3.37720478
1	2.98036640	-2.26672775	-5.43288847
1	2.87275671	-0.56954787	-5.93539204
1	1.40860813	-1.58832422	-5.89324779
6	1.65744605	-1.87183197	3.76406656
6	2.73466791	-0.86422564	5.76542419
6	3.77450104	-0.50348231	3.53523693
1	1.82621899	-1.03471596	6.36134718
1	3.28957042	-0.02500232	6.20858213
1	3.36247930	-1.76171810	5.85905227
1	0.68633357	-1.96689757	4.27302356
1	2.24388091	-2.77942461	3.97632302
1	1.49104676	-1.80799211	2.68420823
1	4.36996955	-1.41564512	3.69269926
1	4.35098036	0.34662563	3.92782364
1	3.63362951	-0.36218568	2.45824183
1	-0.39142565	2.58466751	-5.66037640
1	0.02537468	3.11329232	5.87120051
8	-0.57345086	-4.79524524	-1.37771408
6	-0.49425993	-5.52533782	-2.63219010
1	-0.68467756	-6.59127435	-2.45960830
8	1.12861063	-6.08445082	-0.58299260
8	-1.23292728	0.10103641	0.27911251
1	-1.26827350	-5.08598570	-3.26729685
1	0.49837742	-5.39838326	-3.07939366
13	0.55297110	0.33009202	0.19188451
8	-0.87118085	-3.41738923	0.81726616
6	-0.57724938	-2.15700978	0.52863735
6	-1.74878401	-1.18697351	0.47852814
6	0.31566147	-5.19218635	-0.44461072
6	0.22059730	-4.39579692	0.86151559
8	0.57423019	-1.74310830	0.31811253
6	-0.03199059	-5.30943127	2.05280738
6	-2.74266869	-1.61277690	-0.61546632
1	-2.25833904	-1.25805040	1.46129934
1	1.17021930	-3.85405737	0.97095533
1	0.02145830	-4.73436916	2.98503750
1	0.73539320	-6.09221757	2.07012901
1	-1.01985470	-5.78214380	1.97833342
1	-3.09819492	-2.63718021	-0.44506994
1	-2.26147388	-1.55723624	-1.60149734
1	-3.60747253	-0.93866254	-0.60113148

Electronic energy = -2598.609838 a.u.

DFT-D4 dispersion correction = -0.151931 a.u.

Thermal free energy = 0.672367 a.u.

Gibbs free energy = -2598.089402 a.u.

Number of imaginary frequencies = 0.

10a_{LALA}

Atomic N.	X	Y	Z
6	2.03524272	2.89151930	-3.33276879
6	1.69134104	1.73500327	-4.04825215
6	0.70018858	0.85074094	-3.61971773
6	0.05718256	1.12937031	-2.36901349
6	0.26404499	2.40143105	-1.74224336
6	1.29932331	3.23816514	-2.21464564
6	-0.65680692	2.92721745	-0.71678607
7	-1.37855997	2.07733058	0.07800371
6	-2.28576578	2.55098384	0.98779819
6	-2.47212197	3.93826054	1.12556197
6	-1.73526941	4.81521262	0.33985982
6	-0.83471942	4.31690330	-0.59239350
6	-3.12229203	1.62505248	1.77484518
6	-3.46700610	0.32118790	1.29195036
6	-4.59073814	-0.36462190	1.85963469
6	-5.15496626	0.16732895	3.02072396
6	-4.69429867	1.35395367	3.60898097
6	-3.71547667	2.09156532	2.96825744
8	-0.74872584	0.21601255	-1.82540961
8	-2.78145990	-0.25096022	0.30230944
1	-3.23067583	4.31369728	1.80629898
1	-1.89302991	5.89092748	0.42676388
1	-0.30472211	4.98864507	-1.26145445
1	1.53054965	4.15768511	-1.67694534
6	0.29863868	-0.36817963	-4.47534609
1	-3.38220980	3.03529048	3.39963139
1	-5.97861772	-0.35885024	3.50009955
6	-5.17564241	-1.63006559	1.19890763
1	2.23256140	1.51962345	-4.96775788
6	-5.55701353	-1.31395122	-0.26768472
6	-6.45542593	-2.10661095	1.91180286
6	-4.16592289	-2.79916459	1.23211540
1	-6.30952645	-0.51298796	-0.30675578
1	-5.99081590	-2.20874140	-0.73926938
1	-4.68442753	-1.00357788	-0.85283263
1	-3.91409660	-3.05742606	2.27192010
1	-3.24786936	-2.54509372	0.69171939
1	-4.61360498	-3.68962627	0.76440003
1	-6.85714796	-2.97871171	1.37651767
1	-7.23657662	-1.33290735	1.91899881
1	-6.26396063	-2.41777018	2.94917030
6	0.63349420	-1.69222197	-3.75415033
6	1.03413318	-0.38018361	-5.82902700
6	-1.21844386	-0.30697320	-4.77629159
1	2.12154058	-0.49499910	-5.71072387
1	0.84114923	0.53068644	-6.41406808
1	0.67648112	-1.23552406	-6.41971842
1	1.70826077	-1.74719899	-3.52822792
1	0.37575484	-2.54173712	-4.40579987
1	0.07822156	-1.78707282	-2.81680600
1	-1.50783972	-1.16977726	-5.39526891
1	-1.46638911	0.60741110	-5.33490695

1	-1.81236380	-0.32786561	-3.85588981
1	-5.12746747	1.70488390	4.54543632
1	2.85371866	3.52428439	-3.67589168
8	-0.76219581	-1.99956786	-0.09833128
13	-1.06224103	0.11457337	-0.06136569
8	1.76289659	-3.00467305	2.15397269
6	2.83125283	-3.14185465	1.32165668
6	2.47898027	-3.43027585	-0.13864357
8	1.30330269	-2.65711044	-0.56731149
6	0.27163996	-2.56500831	0.26294300
6	0.43701960	-3.27030825	1.60628921
8	3.96028226	-3.08144924	1.74912275
6	-0.58182798	-2.86867770	2.64980928
6	3.60641316	-3.11856553	-1.09918662
1	2.19580956	-4.49763228	-0.20102750
1	0.36690755	-4.35711767	1.40175495
1	-0.37235312	-3.40217909	3.58499165
1	-1.58774950	-3.13274501	2.30542937
1	-0.53787684	-1.78649641	2.81581240
1	4.49324467	-3.69396214	-0.80954435
1	3.84757849	-2.05066280	-1.05647095
1	3.31500066	-3.39399351	-2.11986661
8	5.16450316	0.63157876	2.28058220
6	6.03722240	-0.36621290	2.87448931
1	5.89402685	-1.32953975	2.37086018
8	6.42239731	0.53963546	0.38162956
8	0.22561121	0.01315325	1.16451933
1	5.72491361	-0.43142043	3.92076313
1	7.08459245	-0.05208064	2.79296140
6	5.46437168	0.95632121	1.00418896
6	4.49886910	1.99144981	0.41538000
8	3.19823559	2.00721384	1.06006237
6	2.46463173	0.86627491	0.89991653
6	1.12361099	0.97216886	1.64443900
8	2.85316653	-0.09318611	0.26224854
6	1.36726080	0.78281110	3.15146860
6	5.07469682	3.39764712	0.53995739
1	4.36699418	1.71054753	-0.63844460
1	0.76429984	2.00660467	1.48804743
1	0.41008295	0.89007293	3.67916854
1	2.07206870	1.53199750	3.53496875
1	1.76944400	-0.21934033	3.35036367
1	6.06121306	3.43296597	0.06089432
1	5.17824474	3.68386566	1.59473511
1	4.41362848	4.11760469	0.04110535

Electronic energy = -2598.587772 a.u.

DFT-D4 dispersion correction = -0.154182 a.u.

Thermal free energy = 0.675091 a.u.

Gibbs free energy = -2598.066863 a.u.

Number of imaginary frequencies = 0.

TS3ax_{LALA}

Atomic N.	X	Y	Z
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6	-0.45329714	4.49892092	-3.51060724
6	-0.60006601	3.44980168	-4.42862177
6	-0.93724161	2.15403414	-4.03644037
6	-1.12644029	1.90789795	-2.63689685
6	-1.09827507	2.99544311	-1.70734990
6	-0.71532011	4.27465010	-2.17203736
6	-1.51435494	2.85277057	-0.29657826
7	-1.51460969	1.62941957	0.32915968
6	-1.94672167	1.50022256	1.62682772
6	-2.30206108	2.64201593	2.36468625
6	-2.28789401	3.88733983	1.75333190
6	-1.93027031	3.99144840	0.41529706
6	-2.16345525	0.17378269	2.23018503
6	-2.58074856	-0.92821372	1.41961992
6	-3.24203491	-2.04415798	2.02612829
6	-3.22883129	-2.11371875	3.42083597
6	-2.64563894	-1.12027371	4.22299862
6	-2.15673733	0.03191434	3.63338661
8	-1.33323181	0.65808588	-2.22828865
8	-2.38097787	-0.90470827	0.10262068
1	-2.65993190	2.52723193	3.38405466
1	-2.60177565	4.77348661	2.30613637
1	-1.99918354	4.94787884	-0.09351738
1	-0.58958918	5.09126902	-1.46266794
6	-1.08751309	1.02278852	-5.07427263
1	-1.73890281	0.82661396	4.25132942
1	-3.67759132	-2.97478533	3.91351342
6	-3.96650338	-3.10538840	1.17138445
1	-0.42239383	3.65816689	-5.48201227
6	-5.01129103	-2.40399599	0.26975277
6	-4.72412443	-4.11929369	2.04926085
6	-2.97914600	-3.90457916	0.28992921
1	-5.75063896	-1.86582935	0.88063353
1	-5.54892159	-3.15537214	-0.32823074
1	-4.53778028	-1.69205475	-0.41537747
1	-2.27270150	-4.47057343	0.91579133
1	-2.41590047	-3.24909186	-0.38356939
1	-3.53610301	-4.63208532	-0.32032275
1	-5.26156855	-4.82355595	1.39832342
1	-5.46709538	-3.63071561	2.69600916
1	-4.04619026	-4.70986938	2.68274331
6	-0.01557970	-0.06988779	-4.84767723
6	-0.91467977	1.54450548	-6.51364899
6	-2.50235438	0.40280616	-4.97970438
1	0.09284672	1.94754815	-6.69304752
1	-1.65085435	2.32227612	-6.76380825
1	-1.06385267	0.71047586	-7.21396017
1	0.99479771	0.35991690	-4.92026091
1	-0.11064231	-0.84412754	-5.62475061
1	-0.12260339	-0.54693896	-3.86860251
1	-2.60612941	-0.39736199	-5.72819614
1	-3.27104640	1.16142440	-5.18814230
1	-2.69091439	-0.02414997	-3.98921180
1	-2.60797071	-1.24586713	5.30489540

1	-0.13954309	5.48519468	-3.85230279
8	-0.23057111	-1.68247724	-1.31512523
13	-0.97843879	-0.03820815	-0.62770498
8	2.82526588	-2.46415281	0.52533376
6	3.75756097	-2.23378181	-0.43775070
6	3.19474339	-2.12779856	-1.85591829
8	1.93675137	-1.38324571	-1.88079274
6	0.99246526	-1.69901371	-0.94388604
6	1.45929134	-2.73596597	0.07925115
8	4.93055391	-2.13153219	-0.15394793
6	0.59404230	-2.88045597	1.31151831
6	4.14567041	-1.45070612	-2.82164288
1	2.97601581	-3.15616918	-2.20096707
1	1.47109938	-3.69177890	-0.48064932
1	0.96405691	-3.71645045	1.91814995
1	-0.43563521	-3.09508014	1.00786757
1	0.61194390	-1.96272194	1.90996909
1	5.08169937	-2.01864910	-2.87269735
1	4.37817097	-0.43317169	-2.48452425
1	3.69195151	-1.40707040	-3.81904244
8	4.34657145	1.07710850	5.34791374
6	4.16462183	2.14217496	6.31455421
1	4.83521032	2.98085117	6.08978510
8	3.74001431	2.53745580	3.70689845
8	0.80657572	-0.09829732	0.03169831
1	4.40836906	1.69693255	7.28346586
1	3.12624478	2.49486256	6.29705858
6	4.09483528	1.43282342	4.06161022
6	4.37379217	0.24077992	3.13851142
8	3.77436590	0.48064485	1.84547484
6	2.41868329	0.35627359	1.79066432
6	1.93420637	0.69605911	0.37425032
8	1.71378982	0.05218620	2.73064160
6	1.71085036	2.20840812	0.29613140
6	5.86846256	0.04409425	2.90586662
1	3.91878176	-0.65461916	3.58381724
1	2.74316716	0.44501430	-0.33226839
1	1.37468481	2.48919392	-0.70955944
1	2.66156602	2.71678376	0.50441855
1	0.97730309	2.54092360	1.03898776
1	6.36763477	-0.17475222	3.85801864
1	6.31302691	0.94743842	2.46803403
1	6.02218533	-0.79664522	2.21785641

Electronic energy = -2598.572641 a.u.

DFT-D4 dispersion correction = -0.155734 a.u.

Thermal free energy = 0.677178 a.u.

Gibbs free energy = -2598.051196 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 122.2i

TS3eq_{LALA}

Atomic N.	X	Y	Z
6	3.90293415	4.46058262	0.50369573

6	3.98728836	4.09119121	-0.84885286
6	3.05728008	3.24705250	-1.45672841
6	2.02541345	2.68811393	-0.62615836
6	1.79413784	3.26387987	0.67360991
6	2.78895800	4.09273888	1.23627370
6	0.47067470	3.18251888	1.31534499
7	-0.41638228	2.19798072	0.95863842
6	-1.75238230	2.28994924	1.24684965
6	-2.19104015	3.30821913	2.11068838
6	-1.27552415	4.22373510	2.61888803
6	0.04620445	4.19514372	2.19393406
6	-2.72545371	1.41186695	0.56470895
6	-2.40807494	0.72044958	-0.65791635
6	-3.48061226	0.28060591	-1.50909690
6	-4.77713351	0.30939730	-0.99380372
6	-5.06605301	0.79401190	0.29051044
6	-4.05506691	1.37123835	1.03808712
8	1.29061155	1.68363451	-1.07704682
8	-1.15626189	0.48633925	-1.02618272
1	-3.24760001	3.41665923	2.33574046
1	-1.61328584	5.01116874	3.29398812
1	0.73240221	4.98815970	2.47744401
1	2.68274082	4.43624817	2.26534004
6	3.09313952	2.97635122	-2.97702883
1	-4.29071405	1.78927277	2.01597111
1	-5.60031512	-0.06367747	-1.60044211
6	-3.21845169	-0.16135035	-2.96541086
1	4.81547494	4.48179694	-1.43805280
6	-2.51578318	0.99047373	-3.72458149
6	-4.53159858	-0.47023087	-3.71015031
6	-2.34063235	-1.43169177	-3.04453915
1	-3.15310372	1.88609835	-3.74388975
1	-2.32372024	0.68874884	-4.76550151
1	-1.55912169	1.25111170	-3.25758676
1	-2.76672133	-2.24605986	-2.43895106
1	-1.32058756	-1.22165896	-2.70559513
1	-2.28688523	-1.78160017	-4.08661905
1	-4.29783923	-0.72075054	-4.75454457
1	-5.21276252	0.39238969	-3.72120775
1	-5.06498164	-1.32936646	-3.27703789
6	3.38235602	1.49659302	-3.31067485
6	4.17359106	3.82291991	-3.67661213
6	1.72592718	3.37637422	-3.58515699
1	5.18887703	3.55467887	-3.34933307
1	4.02750451	4.89972526	-3.50951957
1	4.12050397	3.64372618	-4.75995763
1	4.36251296	1.19009946	-2.91711671
1	3.40433996	1.36436745	-4.40342548
1	2.61196598	0.83834821	-2.89679575
1	1.74019632	3.20990472	-4.67305544
1	1.51830972	4.44159843	-3.40804916
1	0.91022214	2.78398699	-3.15501907
1	-6.08370488	0.74860989	0.67823767
1	4.68315604	5.07493622	0.95283072

8	1.71623903	0.36266973	1.35849338
8	1.62698901	-1.74226804	2.20988182
6	2.06874982	-0.86769044	1.22510455
6	3.50337582	-1.17041187	0.77686427
8	3.74176007	-2.60499950	0.64511528
6	3.38936310	-3.38156658	1.70314597
6	2.62120502	-2.63435143	2.79364331
8	3.67157181	-4.55920584	1.73677236
6	1.90738474	-3.55855777	3.75893853
6	3.94054523	-0.52104668	-0.51436981
1	4.13150780	-0.79533140	1.60735460
1	3.34852474	-2.01013421	3.34675688
1	1.39231769	-2.96635912	4.52557655
1	2.64005543	-4.21545616	4.24243747
1	1.17747062	-4.18445838	3.23133738
1	3.80936524	0.56431648	-0.44619917
1	3.34584036	-0.89907353	-1.35199027
1	5.00078971	-0.74159699	-0.69000368
13	0.31547364	0.62815216	0.06197154
8	-1.63825193	-4.69280842	3.37232551
6	-1.57824021	-5.72710691	4.39083326
1	-1.18025737	-5.31531657	5.32615896
8	-3.07263149	-3.54728566	4.71903903
8	1.03838332	-1.20488890	-0.23427735
1	-0.90990107	-6.49077321	3.98325528
1	-2.57867015	-6.13694459	4.57363059
6	-2.44019261	-3.65131924	3.68581998
6	-2.51914851	-2.58099176	2.59797088
8	-1.56987482	-2.88370536	1.52394242
6	-0.85162596	-1.86959733	1.03902909
6	0.04115770	-2.22384893	-0.14738304
8	-0.91319111	-0.70768589	1.44517691
6	0.56191305	-3.65427927	-0.20690532
6	-3.92776577	-2.49271213	2.01923674
1	-2.22851461	-1.62587179	3.05607814
1	-0.61186491	-2.06538391	-1.02635192
1	1.24836207	-3.74981098	-1.05686507
1	-0.27846449	-4.34323920	-0.35903356
1	1.08355874	-3.96010436	0.70462242
1	-4.64209017	-2.33855551	2.83728043
1	-4.18648226	-3.42032748	1.49170399
1	-3.99966535	-1.64668404	1.32474116

Electronic energy = -2598.563030 a.u.

DFT-D4 dispersion correction = -0.159905 a.u.

Thermal free energy = 0.682799 a.u.

Gibbs free energy = -2598.040135 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 132.7i

11a_{LALA}

Atomic N.	X	Y	Z
6	0.50431575	4.58731136	-2.01111777
6	0.04782829	3.81430726	-3.08910168

6	-0.52194779	2.55337657	-2.91489917
6	-0.64721959	2.05612777	-1.57576487
6	-0.29378871	2.88606637	-0.46297896
6	0.32902791	4.12943222	-0.71856686
6	-0.65298178	2.54609071	0.92776641
7	-0.99690240	1.26367080	1.28740938
6	-1.47408168	0.97831681	2.54644937
6	-1.51812873	1.98805169	3.52017553
6	-1.11228389	3.27596723	3.19376349
6	-0.70965487	3.56400628	1.89820275
6	-2.03069945	-0.35077629	2.86874436
6	-2.67647379	-1.14829798	1.86889808
6	-3.58417192	-2.18369716	2.26342555
6	-3.61816358	-2.52579959	3.61665464
6	-2.84233303	-1.86751105	4.58337834
6	-2.08927101	-0.76608878	4.21692882
8	-1.09995738	0.81920322	-1.39719124
8	-2.45392331	-0.91946284	0.57510717
1	-1.93088492	1.76918271	4.50088047
1	-1.15977839	4.07036498	3.93927554
1	-0.47942633	4.58697131	1.61968790
1	0.71120100	4.72335644	0.10939219
6	-0.98358132	1.71235799	-4.12271991
1	-1.52266753	-0.22155216	4.97273231
1	-4.26096195	-3.34212265	3.94156310
6	-4.50467725	-2.87410057	1.23463190
1	0.17306195	4.20809801	-4.09601629
6	-5.34489764	-1.80061826	0.50102650
6	-5.49129371	-3.84022118	1.91745984
6	-3.69590076	-3.69466058	0.20316103
1	-5.96046249	-1.23543413	1.21592950
1	-6.02198476	-2.28830987	-0.21623055
1	-4.71017600	-1.09648528	-0.04797976
1	-3.14712984	-4.50918578	0.69872427
1	-2.98405191	-3.06974149	-0.34731470
1	-4.38485687	-4.15300543	-0.52253386
1	-6.15589091	-4.26891764	1.15410470
1	-6.12291955	-3.32961447	2.65867996
1	-4.97967877	-4.67791851	2.41349614
6	-0.14300151	0.41700807	-4.23134856
6	-0.81414649	2.48009782	-5.44790722
6	-2.48549286	1.36373294	-3.98875147
1	0.23811369	2.72031647	-5.65910383
1	-1.39488684	3.41391092	-5.46268534
1	-1.17857582	1.85104397	-6.27226653
1	0.91936696	0.66058730	-4.38269628
1	-0.47974948	-0.16805567	-5.10080779
1	-0.23387785	-0.20828016	-3.33708743
1	-2.80721964	0.77781579	-4.86292123
1	-3.09246542	2.28039918	-3.95523758
1	-2.68810573	0.77767802	-3.08658430
1	-2.86092139	-2.20384230	5.61978914
1	0.99762356	5.54201886	-2.19344070
8	-0.12330817	-1.71357803	-0.81918922

13	-0.88741194	-0.24653580	0.00987832
8	2.24723811	-3.88062205	0.92492858
6	3.29983425	-3.70799675	0.06957934
6	2.98028991	-2.81036492	-1.12768357
8	2.19871597	-1.67320603	-0.68116259
6	0.95815715	-1.98368921	-0.08102185
6	0.94491052	-3.44210506	0.43396684
8	4.37251965	-4.21665742	0.30069771
6	-0.07547795	-3.74723020	1.50988593
6	4.23299599	-2.28283686	-1.80014802
1	2.38413738	-3.39444099	-1.85489193
1	0.70668407	-4.03308116	-0.46660974
1	-0.07660077	-4.82497445	1.71493113
1	-1.07175305	-3.45553210	1.16273799
1	0.14848747	-3.21227222	2.43851624
1	4.84002871	-3.12417764	-2.15434538
1	4.83494244	-1.70472582	-1.08826687
1	3.95892833	-1.65172437	-2.65457696
8	5.32786115	3.38885892	-0.36046538
6	5.84970665	4.59779569	0.24630701
1	5.11954729	5.41221537	0.16233452
8	3.62108435	3.43291545	1.14735894
8	0.75846850	-0.92100953	1.01729950
1	6.75964562	4.83163307	-0.31373348
1	6.07654480	4.42272364	1.30496486
6	4.18716509	2.91714086	0.20621157
6	3.73972404	1.65076725	-0.53525256
8	2.64763710	1.04825300	0.19825062
6	3.01352913	0.16534069	1.16219076
6	1.77975320	-0.37368334	1.90843389
8	4.15896365	-0.10079434	1.46533348
6	2.15880656	-1.30270405	3.04736718
6	3.26118018	1.93897983	-1.95317638
1	4.59010038	0.95462908	-0.53806770
1	1.28011886	0.51751339	2.31799785
1	1.26108451	-1.58299590	3.61249724
1	2.84267429	-0.77074476	3.72085517
1	2.66988833	-2.20589968	2.69780394
1	4.08807248	2.35713654	-2.54058815
1	2.42704363	2.65046939	-1.95435636
1	2.92918989	1.00404125	-2.42097694

Electronic energy = -2598.571100 a.u.

DFT-D4 dispersion correction = -0.159578 a.u.

Thermal free energy = 0.678304 a.u.

Gibbs free energy = -2598.052373 a.u.

Number of imaginary frequencies = 0.

11b_{LALA}

Atomic N.	X	Y	Z
6	3.58978955	4.43234815	-0.29717404
6	3.48451043	3.63972168	-1.44761860
6	2.38474985	2.81663426	-1.69900339
6	1.34473667	2.77716442	-0.71448253

6	1.36902249	3.70740746	0.37492710
6	2.52898883	4.48470809	0.58717589
6	0.18416565	3.98055932	1.21027497
7	-0.80010669	3.04102966	1.36734821
6	-1.94431788	3.30732374	2.06931263
6	-2.11024745	4.56923295	2.66586664
6	-1.11288059	5.52759375	2.54042567
6	0.03034368	5.24517568	1.80466885
6	-3.03617085	2.31699387	2.15108244
6	-3.28300141	1.34308067	1.12815713
6	-4.56674354	0.70852320	1.06735406
6	-5.44032987	0.90173327	2.14030203
6	-5.12316426	1.70794089	3.23985632
6	-3.94732979	2.43363977	3.22311449
8	0.35067801	1.88587723	-0.83896885
8	-2.34309647	1.04353332	0.21361149
1	-3.04080289	4.80624885	3.17288212
1	-1.24717617	6.51569094	2.98216076
1	0.78066632	6.01226545	1.63801197
1	2.59639829	5.11582245	1.47268511
6	2.31517393	1.97049645	-2.98618389
1	-3.70586436	3.08953152	4.05884780
1	-6.40285699	0.39422862	2.13488608
6	-4.98951277	-0.17344674	-0.12541504
1	4.30552235	3.65684895	-2.16171261
6	-4.79510289	0.59482978	-1.45416513
6	-6.47711187	-0.57000508	-0.05297808
6	-4.16475063	-1.47711700	-0.12947054
1	-5.42195342	1.49839890	-1.47051964
1	-5.10102922	-0.04187558	-2.29779238
1	-3.75361210	0.89715005	-1.60487984
1	-4.35303381	-2.05961803	0.78373212
1	-3.09610192	-1.25603340	-0.17952327
1	-4.43780347	-2.09959645	-0.99521312
1	-6.73337746	-1.14642952	-0.95328676
1	-7.13784475	0.30830657	-0.02071959
1	-6.69969369	-1.20712299	0.81479247
6	2.44329564	0.47188286	-2.63717302
6	3.45650324	2.31623908	-3.96238811
6	0.98689258	2.24094182	-3.73292811
1	4.44631976	2.07476873	-3.54958372
1	3.44632955	3.37685388	-4.25340917
1	3.33195504	1.71910469	-4.87691009
1	3.42574111	0.25101015	-2.19771378
1	2.34280561	-0.13764691	-3.54837720
1	1.67540462	0.16071950	-1.92298046
1	0.95989358	1.64834435	-4.65982517
1	0.90779696	3.30240524	-4.01066683
1	0.11520435	1.97608956	-3.12571257
1	-5.80935838	1.78214450	4.08316258
1	4.49183384	5.01590397	-0.11425079
8	0.09641762	0.45229897	1.97348279
13	-0.60148854	1.28277019	0.54170543
8	-0.59171291	-1.75543449	2.15698793

6	0.34262730	-0.83769304	1.63202064
6	1.78214443	-1.21100910	2.04176966
8	2.00023184	-2.65482445	1.99252481
6	1.12206246	-3.40966754	2.71978008
6	-0.11535848	-2.64199191	3.19849897
8	1.34066901	-4.58223989	2.92353462
6	-1.25860284	-3.56884656	3.56650925
6	2.87263552	-0.53845141	1.23498209
1	1.85766755	-0.89511080	3.09595580
1	0.17639347	-2.03981522	4.08096950
1	-2.11611210	-2.97821346	3.91140123
1	-0.93988603	-4.24866721	4.36514144
1	-1.55464623	-4.17068899	2.69857754
1	2.74175739	0.54974629	1.28549161
1	2.85281122	-0.85877045	0.18890816
1	3.85146483	-0.78951869	1.66255811
8	4.79512308	-4.57022158	-0.75983869
6	6.20132774	-4.24731683	-0.62085008
1	6.59071746	-3.82321142	-1.55471429
8	4.39504085	-2.37879261	-1.23354928
8	0.12629144	-0.80340829	0.14266783
1	6.69255204	-5.19630411	-0.38780714
1	6.34444430	-3.52498339	0.19198875
6	4.00063886	-3.51580854	-1.08049366
6	2.56931931	-4.01711797	-1.26710723
8	1.69124999	-2.86881296	-1.10393535
6	0.44175605	-3.17045133	-0.67082244
6	-0.46630782	-1.94044986	-0.53975682
8	0.02685659	-4.29708425	-0.47143037
6	-0.89318160	-1.47719717	-1.93088661
6	2.38938880	-4.63779027	-2.65327381
1	2.33416192	-4.75129494	-0.48557604
1	-1.33025042	-2.28731956	0.03715098
1	-1.59623758	-0.63902245	-1.84721224
1	-1.40135957	-2.30368235	-2.44571942
1	-0.02722715	-1.16389898	-2.52469632
1	3.08376146	-5.47896384	-2.77642779
1	2.58748368	-3.89318892	-3.43536511
1	1.36502874	-5.01510713	-2.75675717

Electronic energy = -2598.577338 a.u.

DFT-D4 dispersion correction = -0.155321 a.u.

Thermal free energy = 0.678377 a.u.

Gibbs free energy = -2598.054282 a.u.

Number of imaginary frequencies = 0.

12_{LALA}

Atomic N.	X	Y	Z
6	4.12206782	2.26143678	-2.73041861
6	3.74883030	1.26159523	-3.63901661
6	2.50143548	0.63367518	-3.59991847
6	1.60383441	1.01577740	-2.55565929
6	1.91214722	2.14743702	-1.72923379
6	3.19899517	2.72215300	-1.80981569

6	0.89824544	2.82749446	-0.89719029
7	-0.16288313	2.13173310	-0.38207545
6	-1.19597713	2.73978550	0.28056248
6	-1.14116724	4.13006087	0.47718831
6	-0.05027628	4.85258830	0.00771456
6	0.96813393	4.21344571	-0.68953441
6	-2.37300281	1.96466076	0.72692589
6	-2.78770276	0.73297943	0.11953034
6	-4.07055039	0.18095612	0.42659592
6	-4.82621838	0.80592924	1.42121982
6	-4.37615739	1.94000595	2.10748162
6	-3.17306188	2.51744770	1.75039682
8	0.45904531	0.32590670	-2.38684598
8	-2.00294273	0.08399221	-0.76091828
1	-1.97480241	4.64134643	0.94936921
1	-0.01755748	5.93428684	0.14510091
1	1.78286015	4.78267451	-1.12808889
1	3.47144929	3.51748341	-1.11645045
6	2.10280139	-0.41291970	-4.66092287
1	-2.81695518	3.39108774	2.29382240
1	-5.79406515	0.38934999	1.69287439
6	-4.60685082	-1.06722126	-0.30572040
1	4.47009384	0.95696011	-4.39482378
6	-4.64415586	-0.81503193	-1.83226290
6	-6.04442312	-1.41075903	0.13023115
6	-3.72619211	-2.29867644	0.00894718
1	-5.30411446	0.03299295	-2.06671265
1	-5.04366666	-1.70395865	-2.34328491
1	-3.64834694	-0.60321769	-2.23488251
1	-3.73446413	-2.51199222	1.08859121
1	-2.68954557	-2.15033516	-0.30940090
1	-4.12607611	-3.18268369	-0.51144309
1	-6.38885555	-2.28416550	-0.44132911
1	-6.74554077	-0.58740425	-0.06900948
1	-6.10635600	-1.67182377	1.19666882
6	1.87814089	-1.80190211	-4.02438527
6	3.19484125	-0.57478502	-5.73599500
6	0.81427905	0.05311591	-5.38142872
1	4.13264522	-0.96829842	-5.31793346
1	3.41051839	0.37007955	-6.25602352
1	2.84551475	-1.29535901	-6.48865559
1	2.78195764	-2.15445965	-3.51010680
1	1.63233449	-2.53266734	-4.80911562
1	1.05534394	-1.78486898	-3.30264264
1	0.53449600	-0.68496025	-6.14810411
1	0.97604660	1.01780993	-5.88462556
1	-0.02401160	0.15854050	-4.68384753
1	-4.97210133	2.36272416	2.91588987
1	5.12519016	2.68598009	-2.76653863
8	0.69215001	-0.51121477	0.49939690
8	0.01680611	-2.55762113	-0.13010257
13	-0.24902558	0.26498178	-0.76737927
6	0.89731969	-1.82905971	0.74677569
6	2.37078833	-2.32184947	0.57091070

8	2.60393274	-2.91329364	-0.74340769
6	1.74511305	-3.90074333	-1.12890339
6	0.42878680	-3.92615421	-0.34521557
8	2.02567701	-4.63730070	-2.04938020
6	-0.67100686	-4.66045963	-1.08843852
6	3.39210553	-1.21880187	0.75187978
1	2.52724939	-3.11319636	1.31916156
1	0.60876135	-4.40877259	0.63465688
1	-1.57891017	-4.69942733	-0.47414640
1	-0.34283813	-5.68096821	-1.31757816
1	-0.89803344	-4.15274983	-2.03429822
1	3.25554675	-0.74645987	1.73231819
1	3.26678108	-0.44912611	-0.01864248
1	4.40502335	-1.63618941	0.68843267
8	1.40928730	3.25162884	4.75229608
6	1.44355428	4.56265677	4.13814204
1	2.38957545	4.71181019	3.60290033
8	1.76436077	2.33268762	2.69486877
8	0.62876378	-2.17336073	2.11652311
1	1.34686100	5.27196289	4.96540739
1	0.60816600	4.67093711	3.43507538
6	1.58873936	2.21623366	3.88877344
6	1.61622500	0.90201691	4.67885748
8	1.23612864	-0.21091962	3.83690917
6	-0.07773269	-0.22744758	3.47731534
6	-0.47650397	-1.50556406	2.72758810
8	-0.87512070	0.63597931	3.79142813
6	-1.12328544	-2.47776001	3.71866058
6	3.02476743	0.61072732	5.18745935
1	0.90032540	0.98763198	5.50781374
1	-1.21891576	-1.20007694	1.97714607
1	-1.51438731	-3.34587369	3.17332213
1	-1.94973591	-1.98611825	4.24731683
1	-0.38363880	-2.82803428	4.45105915
1	3.35188677	1.41304533	5.86117408
1	3.72913697	0.53731219	4.34898101
1	3.03208867	-0.33707131	5.74019274

Electronic energy = -2598.582264 a.u.

DFT-D4 dispersion correction = -0.154053 a.u.

Thermal free energy = 0.676309 a.u.

Gibbs free energy = -2598.060009 a.u.

Number of imaginary frequencies = 0.

13a_{LALA}

Atomic N.	X	Y	Z
6	3.43993112	4.59624235	-2.28070074
6	2.80805823	4.12985974	-3.44200949
6	1.65771528	3.33884155	-3.40762028
6	1.13882252	2.97955436	-2.12230128
6	1.69021547	3.57073090	-0.94044869
6	2.86911148	4.34214355	-1.04703123
6	1.00785511	3.49918606	0.36747168
7	0.17194816	2.45510959	0.67508075

6	-0.51247585	2.42040905	1.86415531
6	-0.32907874	3.45049254	2.80246625
6	0.52973794	4.50308261	2.51604985
6	1.18779842	4.54085784	1.29360583
6	-1.48624043	1.35044087	2.14942389
6	-2.21832203	0.70603268	1.10181301
6	-3.38305490	-0.06519648	1.41690448
6	-3.66129841	-0.28999984	2.76662391
6	-2.86325002	0.22212770	3.80056760
6	-1.80218601	1.05465141	3.49284837
8	0.13241851	2.10562941	-2.04298329
8	-1.83727087	0.84065176	-0.16978409
1	-0.90601477	3.44408594	3.72276123
1	0.65491642	5.31753973	3.23025791
1	1.80409399	5.39435995	1.02650650
1	3.34934211	4.71798644	-0.14391134
6	0.97086040	2.87456305	-4.70877845
1	-1.19111777	1.47124808	4.29335587
1	-4.52373544	-0.89769383	3.03520887
6	-4.29756724	-0.62481826	0.30803323
1	3.24732811	4.38552996	-4.40432214
6	-4.80407917	0.53242592	-0.58600972
6	-5.53759498	-1.32552834	0.89535165
6	-3.54472525	-1.66621777	-0.55288306
1	-5.38047217	1.25611861	0.00863897
1	-5.46808527	0.13248563	-1.36699249
1	-3.97665576	1.05968404	-1.07260723
1	-3.21313922	-2.51167435	0.06851931
1	-2.67285450	-1.22969580	-1.05216932
1	-4.22033893	-2.06449720	-1.32513425
1	-6.17640673	-1.67344931	0.07221842
1	-6.14041209	-0.64733172	1.51656167
1	-5.27176549	-2.20703237	1.49699318
6	1.02740336	1.33571482	-4.84611147
6	1.65399928	3.47176067	-5.95396389
6	-0.50173703	3.34993910	-4.71884236
1	2.69337050	3.12987208	-6.06400905
1	1.64721238	4.57121600	-5.94214225
1	1.10592175	3.14749518	-6.84975415
1	2.07115152	0.98764269	-4.86738943
1	0.55532077	1.03097879	-5.79259043
1	0.50260654	0.83635871	-4.02460103
1	-0.98856906	3.02538719	-5.65077243
1	-0.55363806	4.44753501	-4.67595284
1	-1.06534815	2.93934549	-3.87418989
1	-3.09210692	-0.01831785	4.83886910
1	4.36479190	5.16784553	-2.35339529
8	0.06501040	-0.66533092	-1.46042722
8	1.50381142	0.06000735	0.04907944
13	-0.12152329	1.00636051	-0.65876630
8	3.69841192	-1.16169114	-1.30455465
6	3.93509640	-0.54050998	-0.11938912
6	2.86918015	0.41869009	0.44185784
6	1.26110528	-1.06170900	-1.01411214

6	2.43504871	-0.92688532	-1.99417203
8	5.00346640	-0.68549516	0.43160019
6	2.36599987	-1.91088752	-3.14535474
6	2.96485820	0.53367957	1.95462312
1	3.08936782	1.39375595	-0.03009337
1	2.42524008	0.10883317	-2.36839992
1	3.20173724	-1.73709416	-3.83460130
1	1.42362852	-1.77458028	-3.69056703
1	2.42100749	-2.93870479	-2.76771746
1	3.98316706	0.83354443	2.22722419
1	2.73929896	-0.43094764	2.42261857
1	2.26047868	1.28972415	2.32270599
8	0.80060332	-5.33236635	3.45768217
6	1.78273337	-6.29674215	3.91629821
1	2.72418165	-5.78827944	4.15632905
8	0.91822092	-4.33298307	5.50173859
8	1.34346369	-2.31643762	-0.42702877
1	1.91639824	-6.99021293	3.08108640
1	1.41506352	-6.82050876	4.80707577
6	0.48581159	-4.38196890	4.36703111
6	-0.55606575	-3.38357176	3.85225996
8	-0.65512068	-3.33676720	2.40450361
6	0.43893147	-2.83242735	1.76284530
6	0.18084494	-2.81753439	0.25226295
8	1.44232791	-2.45423991	2.32903449
6	-0.12734885	-4.21136473	-0.29608751
6	-1.94075953	-3.74245996	4.38053955
1	-0.23537905	-2.39836386	4.21751503
1	-0.67162532	-2.14915757	0.06144656
1	-0.35039674	-4.13550158	-1.36755351
1	-0.99317534	-4.64309500	0.21888930
1	0.73558190	-4.87625519	-0.15932320
1	-1.91228965	-3.78555049	5.47639001
1	-2.26362472	-4.71765379	3.99297965
1	-2.66515817	-2.97902680	4.07164594

Electronic energy = -2598.580529 a.u.

DFT-D4 dispersion correction = -0.155977 a.u.

Thermal free energy = 0.676413 a.u.

Gibbs free energy = -2598.060093 a.u.

Number of imaginary frequencies = 0.

TS4ax_{LALA}

Atomic N.	X	Y	Z
6	2.07506204	5.92057133	0.05875712
6	1.89156723	5.69053984	-1.31213152
6	1.12081861	4.63371849	-1.80092669
6	0.53421825	3.74349141	-0.84428984
6	0.57922161	4.06821823	0.54923725
6	1.39921379	5.13651228	0.97582316
6	-0.30037341	3.40898228	1.53543937
7	-0.77363569	2.13903570	1.32435811
6	-1.65439987	1.55764019	2.20069695
6	-2.05727744	2.25827837	3.35109687

6	-1.56490362	3.53365421	3.59333181
6	-0.69761252	4.12005043	2.68156195
6	-2.24471617	0.23337708	1.92427099
6	-2.43267655	-0.24332362	0.58790517
6	-3.34002399	-1.32398605	0.33932093
6	-3.85627198	-2.00028563	1.44627523
6	-3.54078412	-1.64192450	2.76544118
6	-2.76833415	-0.51811218	2.99858212
8	-0.06336491	2.62819004	-1.26842034
8	-1.79257917	0.32453489	-0.43398765
1	-2.79517293	1.81810093	4.01545048
1	-1.89186311	4.08894253	4.47312117
1	-0.36400747	5.14434433	2.81964040
1	1.52102959	5.32846928	2.04159141
6	0.90096617	4.43945837	-3.31549382
1	-2.54559588	-0.21973509	4.02285194
1	-4.52007914	-2.84844637	1.28758621
6	-3.74618626	-1.71528232	-1.09664392
1	2.38530993	6.35749865	-2.01645207
6	-4.36012554	-0.48802060	-1.81244636
6	-4.81055641	-2.82914329	-1.10206318
6	-2.53200340	-2.23650408	-1.89993274
1	-5.25571537	-0.13742304	-1.27912569
1	-4.66230679	-0.76729357	-2.83303857
1	-3.64539242	0.33947781	-1.87853432
1	-2.09300613	-3.11696792	-1.40730512
1	-1.76136291	-1.46579921	-2.01069689
1	-2.85887218	-2.54348755	-2.90511966
1	-5.09780645	-3.04173088	-2.14144397
1	-5.72120380	-2.53452325	-0.56077069
1	-4.43369055	-3.76682782	-0.66788948
6	1.53356993	3.11629820	-3.80454731
6	1.53472948	5.58112764	-4.13292551
6	-0.61596525	4.44008780	-3.62260985
1	2.62894702	5.61243153	-4.02677393
1	1.12894011	6.56423426	-3.85396290
1	1.31323969	5.42163277	-5.19762850
1	2.61597919	3.10950065	-3.60650206
1	1.39233470	3.01855135	-4.89182234
1	1.07594025	2.24780893	-3.31890297
1	-0.77446169	4.31222296	-4.70399952
1	-1.06992280	5.39687967	-3.32618618
1	-1.13442111	3.62914538	-3.09966731
1	-3.92519879	-2.22965026	3.59916782
1	2.72935510	6.72417116	0.39571503
8	0.65287113	-0.05159776	-1.59056127
8	1.29134154	0.39613891	0.58699024
13	-0.19513261	1.12494671	-0.30363718
8	3.99278378	0.40637541	-0.20975748
6	3.69705224	0.62284869	1.10753322
6	2.24056101	0.87409192	1.54682291
6	1.78758287	-0.33387321	-1.03989220
6	3.00621653	0.56003737	-1.26473451
8	4.60620356	0.64336246	1.90734303

6	3.71850944	0.22647288	-2.56788778
6	1.98954248	0.25559792	2.92071533
1	2.15894938	1.97549653	1.61984396
1	2.64455914	1.59834361	-1.27888691
1	4.54922199	0.92614204	-2.72200060
1	3.02171493	0.31495979	-3.41116405
1	4.11513186	-0.79520780	-2.52972388
1	2.71884084	0.64316320	3.64108372
1	2.08840299	-0.83552670	2.86715269
1	0.97696424	0.50913376	3.25940204
8	1.33914089	-6.06400299	3.48298407
6	2.32146883	-7.11840773	3.65251565
1	1.98426545	-8.03735352	3.15730476
8	1.60823905	-6.24807835	1.22705281
8	2.16969872	-1.60945797	-0.83829623
1	2.40331960	-7.26429701	4.73332310
1	3.28276110	-6.80776691	3.22610998
6	1.08737171	-5.73086023	2.19284844
6	0.00278785	-4.64584446	2.14658380
8	0.05893370	-3.95900178	0.87354988
6	1.16739392	-3.18553400	0.68475115
6	1.14037561	-2.62330723	-0.73821026
8	2.02663732	-3.00243068	1.51867807
6	1.42868888	-3.70773506	-1.77382386
6	-1.38944936	-5.25522614	2.26510572
1	0.19600634	-3.92554879	2.95279956
1	0.16131562	-2.16406155	-0.92285562
1	1.36682379	-3.27723575	-2.78122711
1	0.69225174	-4.51505375	-1.68516457
1	2.43026471	-4.12903404	-1.62072623
1	-1.48428369	-5.77866030	3.22488117
1	-1.56788206	-5.96867371	1.45004404
1	-2.14601922	-4.46204472	2.21814871

Electronic energy = -2598.580290 a.u.

DFT-D4 dispersion correction = -0.155000 a.u.

Thermal free energy = 0.677261 a.u.

Gibbs free energy = -2598.058029 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 67.2i

TS4eq_{LALA}

Atomic N.	X	Y	Z
6	4.01114225	2.80837893	-3.55683875
6	3.39136887	2.10868669	-4.60396242
6	2.17005706	1.44907606	-4.45454073
6	1.59740543	1.42680538	-3.14051986
6	2.08043456	2.35169172	-2.16198277
6	3.32797122	2.98119116	-2.36773109
6	1.20672262	2.81765199	-1.07434177
7	0.19414894	2.03308511	-0.58997267
6	-0.69865608	2.52400541	0.32860294
6	-0.58876300	3.85487676	0.76483476
6	0.45477572	4.65206861	0.30977729

6	1.35627210	4.13857174	-0.60878599
6	-1.79646814	1.68409908	0.85586590
6	-2.31651425	0.56355131	0.13419369
6	-3.52434945	-0.07474495	0.57065523
6	-4.08927298	0.35563931	1.77275348
6	-3.52373004	1.38064778	2.54363704
6	-2.40070581	2.04369855	2.08012557
8	0.60042024	0.58923924	-2.84807491
8	-1.69359112	0.10478294	-0.94723952
1	-1.34218097	4.26740170	1.42921793
1	0.53901505	5.68748569	0.64203256
1	2.13418746	4.76743555	-1.03208864
1	3.75866890	3.59242082	-1.57428944
6	1.43570364	0.85118169	-5.67247581
1	-1.96360314	2.84086037	2.68075967
1	-4.99317265	-0.12750393	2.13958764
6	-4.16970778	-1.20480561	-0.25632778
1	3.89176464	2.07987428	-5.57011414
6	-4.48010206	-0.70193249	-1.68679869
6	-5.50167608	-1.67354941	0.35967919
6	-3.23114944	-2.43375039	-0.31949922
1	-5.18071890	0.14531472	-1.65370274
1	-4.95344114	-1.50858653	-2.26674199
1	-3.57188892	-0.38565049	-2.20995045
1	-3.06157660	-2.83669925	0.69119847
1	-2.26209354	-2.18832850	-0.76828516
1	-3.70347071	-3.22808647	-0.91789120
1	-5.93353081	-2.45590663	-0.28037277
1	-6.23644018	-0.85806733	0.42746377
1	-5.36845255	-2.10674334	1.36197865
6	1.23994589	-0.67288095	-5.55589771
6	2.19697189	1.12321341	-6.98353148
6	0.05100919	1.53553414	-5.78529644
1	3.17338729	0.61779892	-7.00665569
1	2.35458064	2.19730997	-7.15854168
1	1.60534894	0.73352069	-7.82409954
1	2.19596577	-1.19103372	-5.40604544
1	0.77377856	-1.05630445	-6.47674131
1	0.58638418	-0.90876406	-4.71173286
1	-0.49234882	1.13427961	-6.65427351
1	0.16060382	2.62088943	-5.92479563
1	-0.55688137	1.35682380	-4.88985729
1	-3.97492504	1.65887094	3.49632883
1	4.99511766	3.25351906	-3.70244622
8	1.04788935	-0.06558920	0.64502740
8	0.26571128	-1.70201278	-1.19581521
13	0.08080203	0.10618060	-1.18870091
6	1.53047287	-1.17271936	0.93268692
6	2.81976914	-1.74434149	0.35206690
8	3.07262492	-1.33872700	-1.00011182
6	2.49428678	-2.06050706	-2.05567551
6	1.11501300	-2.66740513	-1.75809038
8	3.08564425	-2.08636808	-3.10562968
6	0.52106977	-3.36875701	-2.97661352

6	3.98843694	-1.21860385	1.19465256
1	2.76940751	-2.84047341	0.42642674
1	1.28905833	-3.46016574	-0.99520767
1	-0.43612140	-3.82119322	-2.68689847
1	1.19542396	-4.15718555	-3.33774447
1	0.34705985	-2.66019344	-3.79252386
1	3.85378289	-1.47745657	2.25187635
1	4.05230570	-0.12762003	1.10090721
1	4.91840076	-1.66353154	0.82140708
8	0.64923632	-1.27626073	6.77433920
6	1.37741506	-1.97257543	7.81989098
1	2.45133424	-1.77070296	7.72840691
8	1.40279901	0.68907982	7.64673424
8	1.08124506	-1.94287467	1.91883278
1	1.16382360	-3.03340888	7.66124487
1	1.02948260	-1.64534724	8.80698490
6	0.77594352	0.06976208	6.81079054
6	-0.01478882	0.77908456	5.70644569
8	-0.43304816	-0.10948724	4.63230801
6	0.55800283	-0.53971094	3.81450701
6	-0.03036910	-1.45020390	2.72751379
8	1.72988999	-0.24580680	3.92268085
6	-0.75052214	-2.66943359	3.28460050
6	-1.27833998	1.41381800	6.27583027
1	0.66116613	1.53905499	5.29138470
1	-0.69451374	-0.84752280	2.09182358
1	-1.11682463	-3.28859425	2.45683599
1	-1.60538375	-2.34330344	3.88750577
1	-0.07996523	-3.26843572	3.91398335
1	-1.00617838	2.09179044	7.09385586
1	-1.96072984	0.64488500	6.66066265
1	-1.79445374	1.98471940	5.49454975

Electronic energy = -2598.566747 a.u.

DFT-D4 dispersion correction = -0.153844 a.u.

Thermal free energy = 0.675320 a.u.

Gibbs free energy = -2598.045271 a.u.

Number of imaginary frequencies = 1.

Imaginary frequency = 37.9i

14a_{LALA}

Atomic N.	X	Y	Z
6	1.97465730	6.02443641	-0.03610782
6	1.81695811	5.72819485	-1.39724899
6	1.09699059	4.61916314	-1.84596027
6	0.54064779	3.74479472	-0.85669739
6	0.54115138	4.14022651	0.51951293
6	1.31415102	5.25765088	0.90621384
6	-0.33947354	3.50472727	1.52095363
7	-0.79400259	2.22343110	1.34974951
6	-1.67977134	1.66044173	2.23149504
6	-2.10921571	2.39451294	3.35084567
6	-1.63637866	3.68419869	3.55445678
6	-0.76368048	4.25067160	2.63549965

6	-2.25206625	0.32112063	1.98719702
6	-2.40295547	-0.20690851	0.66503684
6	-3.31703234	-1.28557410	0.43222706
6	-3.85874574	-1.92447671	1.54918978
6	-3.56664691	-1.52648424	2.86223928
6	-2.79983638	-0.39452629	3.07386024
8	0.01455295	2.57897643	-1.23972510
8	-1.72582028	0.31069327	-0.36043472
1	-2.85144146	1.96901214	4.01988387
1	-1.98297582	4.26538885	4.40970197
1	-0.44692596	5.28370377	2.74387400
1	1.41118511	5.50420322	1.96307899
6	0.89323521	4.35774663	-3.35293410
1	-2.60111257	-0.06105209	4.09218342
1	-4.52570173	-2.77264147	1.40420915
6	-3.71111876	-1.70819758	-0.99844984
1	2.28949324	6.38482802	-2.12539313
6	-4.30437406	-0.49061684	-1.74755235
6	-4.78727306	-2.81068200	-0.98874127
6	-2.49645353	-2.25912742	-1.78006724
1	-5.20093443	-0.11804045	-1.23116860
1	-4.59948085	-0.78867944	-2.76496796
1	-3.57904679	0.32692775	-1.82437149
1	-2.06357250	-3.12637073	-1.25942473
1	-1.72428863	-1.49253796	-1.90739585
1	-2.81988211	-2.59303449	-2.77779584
1	-5.06603911	-3.04502812	-2.02578453
1	-5.70018794	-2.49392787	-0.46414685
1	-4.42482601	-3.74142365	-0.52807395
6	1.58223527	3.04598313	-3.79248142
6	1.48049613	5.49429967	-4.21131953
6	-0.62123612	4.28142666	-3.66281835
1	2.57219743	5.57530081	-4.10540915
1	1.03339035	6.46899917	-3.96866594
1	1.26823955	5.28690245	-5.26966249
1	2.66102951	3.08667010	-3.58001292
1	1.45941976	2.90884427	-4.87781719
1	1.14901506	2.17781607	-3.28456495
1	-0.77078210	4.10504166	-4.73869257
1	-1.11691086	5.22835259	-3.40416009
1	-1.10590782	3.46944213	-3.10964991
1	-3.96768585	-2.08732186	3.70652465
1	2.59284199	6.86703175	0.27261426
8	0.67137812	-0.11481745	-1.57838243
8	1.24836585	0.40956536	0.72335263
13	-0.14239613	1.13281916	-0.19287745
8	3.92683026	0.34156230	-0.09687721
6	3.63528705	0.63838234	1.21663145
6	2.17932481	0.89138621	1.66715262
6	1.82335091	-0.42556018	-1.16603841
6	3.00886457	0.53694086	-1.19794615
8	4.56080907	0.68987955	1.99540862
6	3.83243571	0.32623468	-2.46712730
6	1.95727779	0.25685143	3.04366041

1	2.10846744	1.99356729	1.76846789
1	2.59676781	1.55455762	-1.17485428
1	4.63245464	1.07539166	-2.50950020
1	3.19983722	0.43500873	-3.35762068
1	4.28228452	-0.67403713	-2.45983051
1	2.70295229	0.62193730	3.75891459
1	2.04038083	-0.83506229	2.96784089
1	0.95191491	0.51289380	3.40213777
8	1.31525076	-6.16217425	3.35360617
6	2.24117858	-7.26953396	3.50307919
1	1.84777518	-8.16521345	3.00677607
8	1.54311460	-6.34261361	1.09289354
8	2.21700341	-1.68034387	-0.97070001
1	2.32920964	-7.42704272	4.58172489
1	3.21215134	-7.00835571	3.06563198
6	1.06425705	-5.80603647	2.07005881
6	0.04258253	-4.66096190	2.04729121
8	0.10210890	-3.98765649	0.76626871
6	1.23805932	-3.26485015	0.54920339
6	1.20434358	-2.72174016	-0.88254144
8	2.12336832	-3.10688456	1.35899540
6	1.53562222	-3.80572155	-1.90272855
6	-1.37960700	-5.18370369	2.21278998
1	0.30235617	-3.94642883	2.83986642
1	0.22043741	-2.27993347	-1.07790880
1	1.47382061	-3.39145661	-2.91707625
1	0.81776729	-4.62967404	-1.81171157
1	2.54482334	-4.20123120	-1.73272274
1	-1.47585527	-5.69483601	3.17896190
1	-1.62680044	-5.88962916	1.40914718
1	-2.08765918	-4.34598857	2.18373125

Electronic energy = -2598.580657 a.u.

DFT-D4 dispersion correction = -0.154265 a.u.

Thermal free energy = 0.674399 a.u.

Gibbs free energy = -2598.060523 a.u.

Number of imaginary frequencies = 0.

15_{LALA} (eq_chelate)

Atomic N.	X	Y	Z
6	-0.34929964	3.66451240	-0.00800513
6	0.69817650	3.27240634	0.83672047
6	1.48008740	2.14449930	0.58473891
6	1.18744624	1.37097538	-0.58609921
6	0.18882574	1.82595086	-1.51227093
6	-0.58945584	2.95322943	-1.16986597
6	-0.00654474	1.23057461	-2.85302830
7	0.39061114	-0.05290591	-3.12817907
6	0.33094928	-0.57224357	-4.39551115
6	-0.25753874	0.17787533	-5.42627048
6	-0.71099186	1.46356952	-5.16076231
6	-0.55713964	2.00517845	-3.88933754
6	0.95484567	-1.87256753	-4.68678474
6	2.14161086	-2.28647208	-3.99092817

6	2.89544487	-3.39859605	-4.49005461
6	2.36559415	-4.11032104	-5.56770468
6	1.15207219	-3.76909232	-6.18488455
6	0.46597847	-2.64598131	-5.76031637
8	1.87040043	0.24520876	-0.79561639
8	2.55054998	-1.61979091	-2.91200185
1	-0.28469816	-0.22750929	-6.43432617
1	-1.13549447	2.06987166	-5.96199560
1	-0.81663138	3.04362488	-3.70625758
1	-1.40813434	3.25671482	-1.82119334
6	2.61651254	1.73850143	1.54595315
1	-0.47203609	-2.36522937	-6.24088669
1	2.90275145	-4.98042345	-5.94151354
6	4.23082542	-3.80988312	-3.83990645
1	0.88867772	3.86343646	1.73062742
6	5.21584988	-2.61638403	-3.84889984
6	4.90716171	-4.96410561	-4.60404539
6	3.99278808	-4.29157019	-2.38920879
1	5.42556286	-2.29566598	-4.88014555
1	6.16871119	-2.92184973	-3.39045095
1	4.81908512	-1.76210320	-3.29058313
1	3.33438516	-5.17259359	-2.38006330
1	3.52803087	-3.51638699	-1.77196276
1	4.95314026	-4.57916451	-1.93378162
1	5.86767960	-5.19477654	-4.12165833
1	5.11633301	-4.70122957	-5.65145302
1	4.30425358	-5.88377094	-4.58871698
6	2.32881904	0.35422689	2.17469001
6	2.76719475	2.74151111	2.70597315
6	3.96527791	1.70780849	0.78800786
1	1.86772645	2.78456974	3.33774400
1	2.99360418	3.75725532	2.35022521
1	3.60274935	2.42212582	3.34461403
1	1.36028552	0.35507572	2.69548607
1	3.11268258	0.11257631	2.90859795
1	2.31577253	-0.43340111	1.41476274
1	4.77191544	1.42110479	1.47966850
1	4.20443153	2.70270085	0.38450938
1	3.94724464	0.99054480	-0.03921557
1	0.76189595	-4.38190269	-6.99742460
1	-0.95935452	4.53282785	0.24317098
8	-1.71577680	-0.21261930	2.29733157
8	1.08180928	-2.73309731	-0.99589401
13	1.25188041	-1.13146114	-1.74113655
6	-2.61513233	-0.09791908	1.49400699
6	-3.11769056	-1.19904077	0.55206019
8	-2.13072252	-2.26804948	0.50005537
6	-1.00124907	-2.01212454	-0.16517963
6	0.04148971	-3.11715937	-0.15656579
8	-0.79173058	-0.96398097	-0.78444934
6	0.51189172	-3.42472696	1.27541995
6	-4.41312504	-1.81676841	1.06368530
1	-3.23866582	-0.77460229	-0.45375428
1	-0.45923024	-4.02343941	-0.55770123

1	1.28777301	-4.19819593	1.22187984
1	-0.31771499	-3.78776383	1.89602816
1	0.94079906	-2.52794051	1.74064779
1	-5.19222260	-1.04739857	1.11778033
1	-4.26881695	-2.23914385	2.06579351
1	-4.74113083	-2.61134028	0.38188338
8	-4.95401955	3.69022155	5.45284748
6	-6.22980452	4.26804781	5.83338737
1	-6.97998667	3.47755480	5.95540714
8	-4.95482159	2.55765200	7.42908716
8	-3.36777282	1.01873052	1.31397533
1	-6.49846888	4.93831825	5.01180124
1	-6.13051891	4.82163048	6.77487087
6	-4.44203424	2.82714295	6.36123371
6	-3.09296703	2.23714638	5.93887901
8	-2.77442765	2.46742749	4.54002810
6	-3.46557403	1.70647359	3.64977694
6	-3.06937981	2.10844541	2.22449541
8	-4.29565859	0.87205523	3.94189906
6	-3.87616515	3.31315804	1.75695443
6	-1.95969915	2.84131408	6.76089573
1	-3.17052674	1.15438187	6.10815716
1	-1.99035108	2.31092691	2.19611859
1	-3.57797527	3.58481431	0.73685354
1	-3.68609142	4.16531706	2.42129898
1	-4.94995260	3.08613467	1.76881695
1	-2.16653085	2.69403458	7.82780409
1	-1.86272824	3.91637468	6.56053877
1	-1.01360166	2.34693241	6.50880194

Electronic energy = -2598.605122 a.u.

DFT-D4 dispersion correction = -0.146395 a.u.

Thermal free energy = 0.673523 a.u.

Gibbs free energy = -2598.077994 a.u.

Number of imaginary frequencies = 0.

15_{LALA} (ax_chelate)

Atomic N.	X	Y	Z
8	-0.23532514	-8.30716705	-4.41763544
6	-0.85919815	-9.57372761	-4.08183527
1	-0.12312201	-10.25523853	-3.63806438
8	0.29359356	-8.04093170	-2.21647286
1	-1.23580790	-9.96892643	-5.02946377
1	-1.67905641	-9.41247177	-3.37169719
6	0.30502751	-7.64716101	-3.36369181
6	0.97026670	-6.35531330	-3.85836983
8	1.19908369	-5.47095633	-2.73538899
6	0.08056163	-4.90501118	-2.20598674
6	0.46127120	-4.10786772	-0.95388401
8	-1.04181302	-5.04157782	-2.64375854
6	0.61294425	-5.02408743	0.25445393
6	2.32902265	-6.63511753	-4.49083376
1	0.29025698	-5.86564493	-4.56867313
1	1.38707221	-3.55399156	-1.16020727

1	0.88822198	-4.43110323	1.13568997
1	1.39826441	-5.76468277	0.06120998
1	-0.32593298	-5.55452633	0.45640910
1	2.20540285	-7.29243565	-5.36039305
1	2.99933934	-7.11899614	-3.76874518
1	2.78482723	-5.69397306	-4.82243299
6	-4.00904989	5.68151093	2.39861703
6	-4.36478090	4.36792803	2.73067069
6	-3.46444154	3.30283356	2.65352654
6	-2.13637328	3.58172798	2.19385958
6	-1.73238170	4.93841171	1.98114634
6	-2.69984341	5.96260357	2.05067945
6	-0.31883341	5.32137394	1.78828025
7	0.57787973	4.44592428	1.23965108
6	1.89641786	4.77870941	1.09191656
6	2.34701276	6.04356432	1.50939620
6	1.44993627	6.94632721	2.06468463
6	0.11654322	6.58782625	2.21556163
6	2.86716247	3.80728531	0.55040944
6	2.69684434	2.39487457	0.70527893
6	3.80038214	1.51724339	0.45358065
6	4.95488453	2.06894135	-0.10634998
6	5.07442951	3.43481588	-0.39586058
6	4.05022335	4.29539919	-0.04332789
8	-1.28345358	2.57238173	1.98867738
8	1.52821076	1.88440692	1.10474396
1	3.40405846	6.28513193	1.44289601
1	1.79832327	7.91860390	2.41547203
1	-0.58343810	7.25868797	2.70550132
1	-2.41684604	6.98408461	1.79759800
6	-3.89450407	1.87465620	3.04748130
1	4.14445162	5.36092091	-0.25189620
1	5.79383898	1.41737974	-0.34406820
6	3.72408152	0.01621496	0.79958802
1	-5.38942719	4.17625332	3.04389906
6	3.41569042	-0.15208088	2.30683947
6	5.05769253	-0.70299751	0.52107954
6	2.63464785	-0.69261009	-0.03728343
1	4.20947075	0.30288044	2.91705585
1	3.36776876	-1.22265959	2.55924749
1	2.45944476	0.31048086	2.57477474
1	2.83119822	-0.58686382	-1.11404526
1	1.64108491	-0.28818271	0.17898791
1	2.63565326	-1.76798129	0.20320979
1	4.96303368	-1.75677025	0.82022280
1	5.88945866	-0.26950920	1.09484041
1	5.32424212	-0.68636268	-0.54580784
6	-3.83783531	0.92984319	1.82390344
6	-5.33699322	1.83795798	3.58718729
6	-2.97100997	1.33729172	4.16663218
1	-6.07396460	2.14097691	2.82916546
1	-5.46349335	2.47893548	4.47146940
1	-5.57832813	0.80833966	3.88773346
1	-4.47856712	1.30692053	1.01252699

1	-4.20310545	-0.06890780	2.11005473
1	-2.81227255	0.83447295	1.45379674
1	-3.27928686	0.31823653	4.44649744
1	-3.04503155	1.96987414	5.06316090
1	-1.92434001	1.30839682	3.84504437
1	5.97410774	3.81511307	-0.87947780
1	-4.75615740	6.47461891	2.42577291
8	-0.59759963	-3.16545391	-0.64738172
8	0.03174824	-1.89978635	-2.44234467
8	-0.49922448	3.18143773	-0.95151681
13	-0.04361820	2.64362192	0.68893027
8	-1.87152147	-0.00847273	-1.79477978
6	-1.21217823	0.94244218	-1.14189625
6	-1.09416783	2.28993750	-1.83938193
6	-0.71548641	-2.12672687	-1.51629603
6	-1.96990085	-1.32101786	-1.16148496
8	-0.72166932	0.78822559	-0.01141011
6	-3.22344017	-1.99016368	-1.71065485
6	-0.30305260	2.15070200	-3.15207577
1	-2.12981987	2.60603356	-2.08639836
1	-2.01993775	-1.19278502	-0.07283076
1	-4.10912657	-1.40506220	-1.43332052
1	-3.31483912	-2.99911880	-1.29088426
1	-3.16894984	-2.07030582	-2.80338001
1	-0.80095100	1.46539855	-3.85042691
1	0.71056229	1.78268445	-2.94565868
1	-0.22614388	3.14388227	-3.61123919

Electronic energy = -2598.615259 a.u.

DFT-D4 dispersion correction = -0.143913 a.u.

Thermal free energy = 0.671622 a.u.

Gibbs free energy = -2598.087550 a.u.

Number of imaginary frequencies = 0.