Electronic supplementary information

The mechanism of *N*-vinylindole formation *via* tandem imine formation and cycloisomerisation of *o*-ethynylanilines

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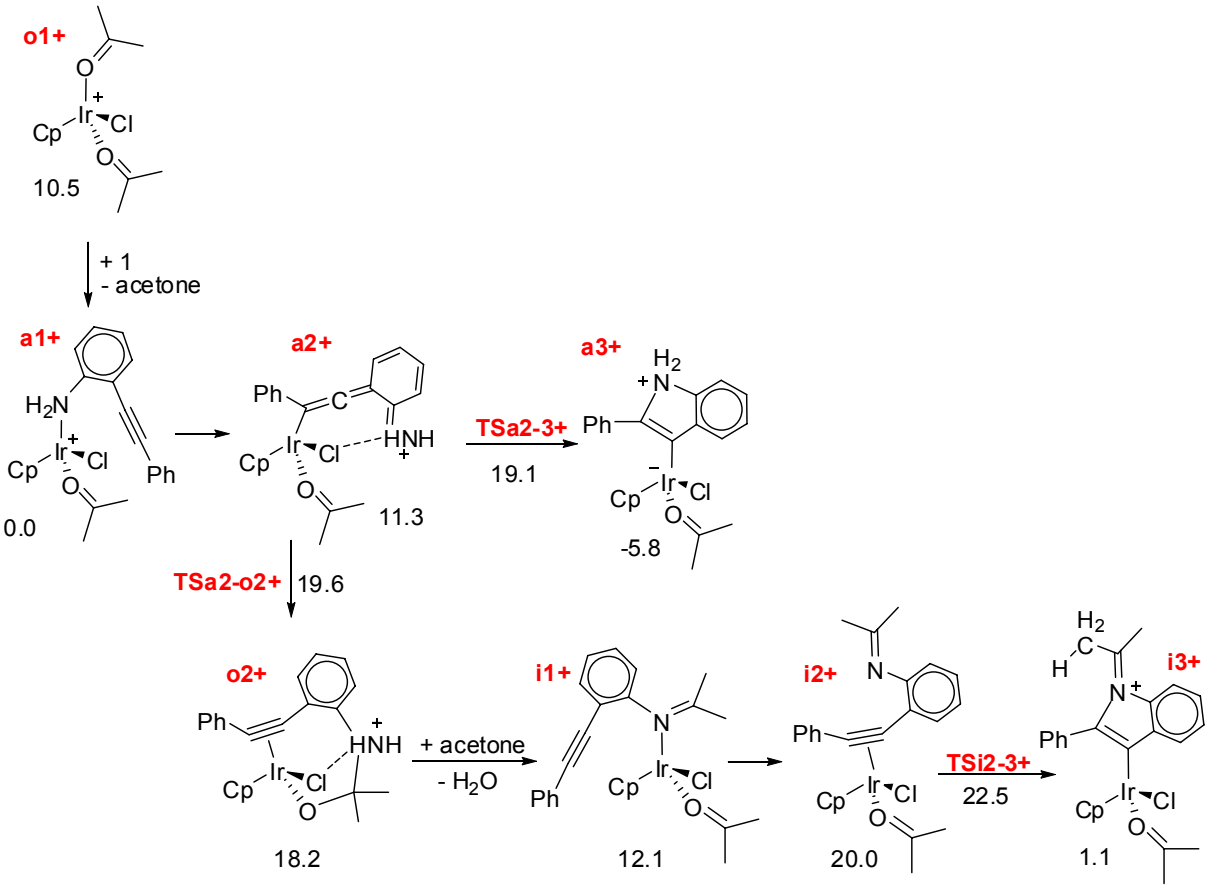
Results obtained with cationic Ir species:

Cationic Ir species with coordinated acetone have been considered as possible reactant to the imine formation. These species are less stable than the neutral equivalents with chloride as counterion (see Scheme 4); however they can be stabilized by the presence of $NaBF_4$. As it is showed in Scheme S1, the stability pattern of **o1+**, **a1+** and **a2+**, is the same of that found with the neutral equivalents (**o1**, **a1** and **a2**). Thus, **a1+** is the most stable complex but inactive for any reaction, **o1+** will be favored by the excess of acetone, and **a2+** is the less stable complex. This last complex can gives intramolecular nucleophilic addition to acetone to give imine, or to alkyne to give cyclization (see scheme S1). The energy barrier for both processes is very similar (**TSa2-3+** =19.1 kcal mol^{-1} and **TSa2-o2+** = 19.6 kcal mol^{-1}). However, **a2+** is unstable, and the formation of imine will be much easier if we consider and

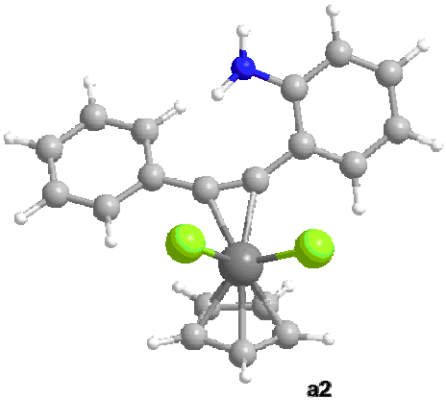
intermolecular attack of an external amine to the coordinated acetone present in the much stable complexes **o1**+ and **a1**+. The same that happens with the neutral species described in the paper.

Scheme S1 also shows that the energy profile obtained for the cyclization of amine and imine does not change significantly of that obtained with the neutrals species. The energies of **TSa2-3**+ and **TSi2-3**+ (19.1 kcal mol^{-1} and 22.5 kcal mol^{-1}, respectively) are slightly lower than those of **TSa2-3** and **TSi2-3** (21.4 kcal mol^{-1} and 25.5 kcal mol^{-1}, respectively). This could account for the enhanced rate observed when $NaBF_4$ was included with the catalyst.

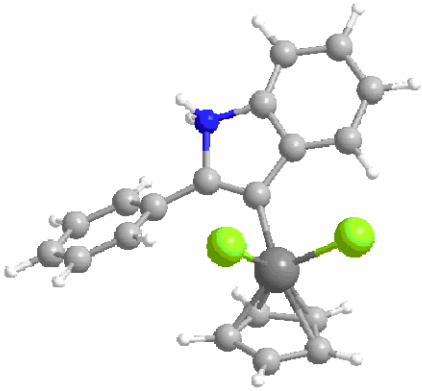


Scheme S1. Cyclization of amine (top) and imine (bottom) with cationic species. Energies are given relative to **a1**+, in kcalmol^{-1} and include the solvent (acetone) effect.

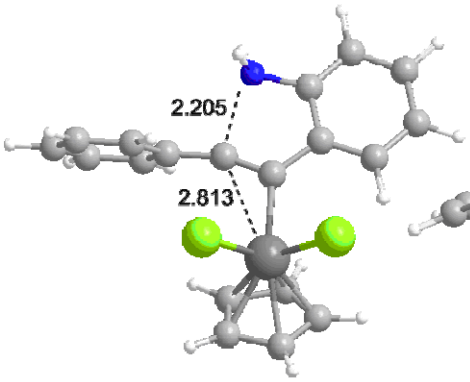
Geometries of some intermediates and transition states:



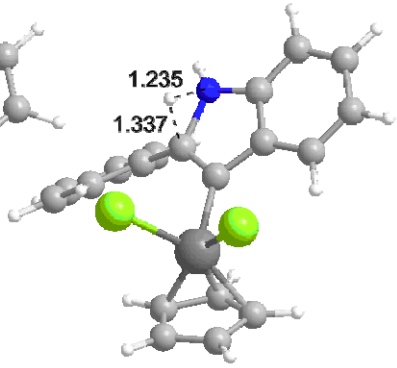
a2



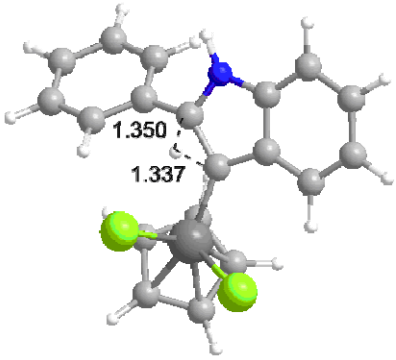
a3



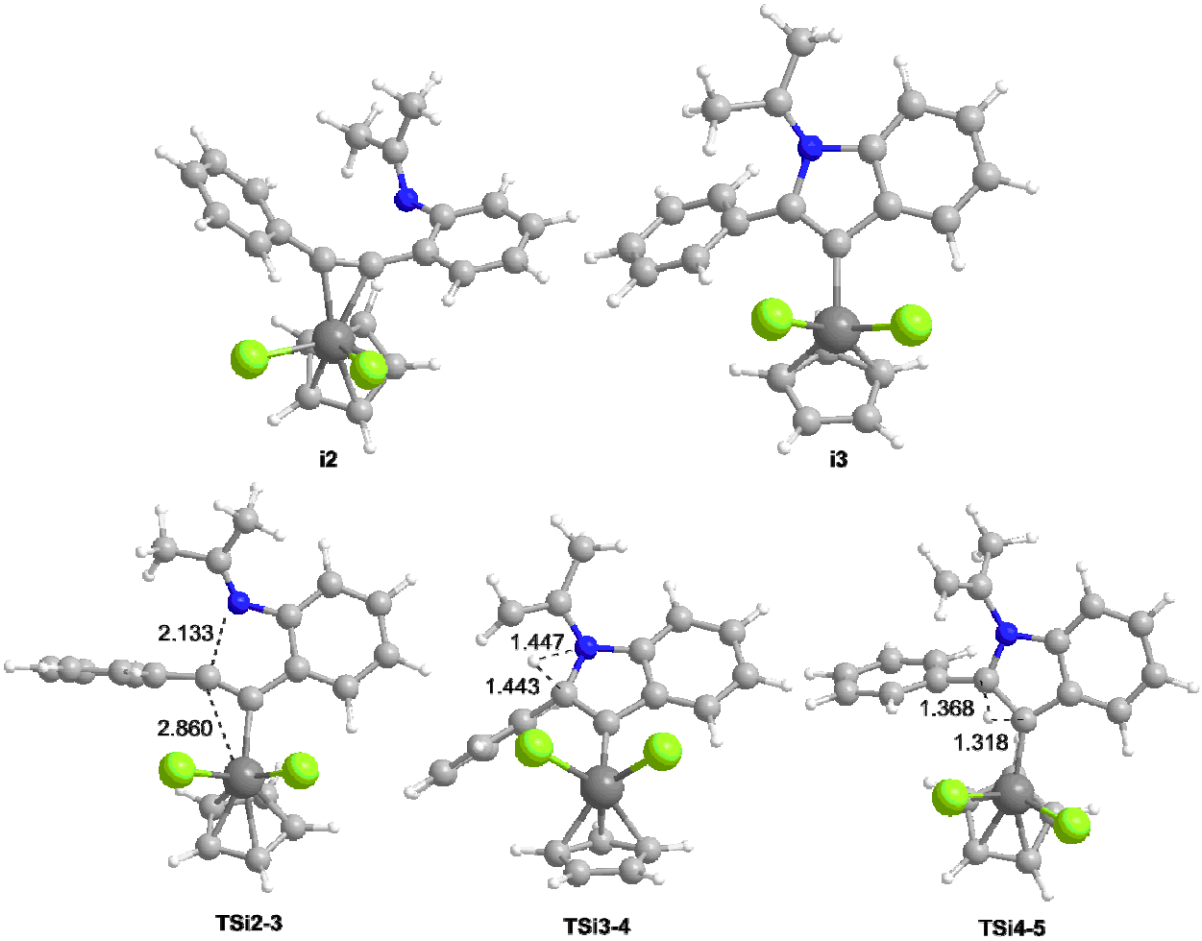
TSa2-3



TSa3-4



TSa4-5



Scheme S2. Geometries of some intermediates and transition states. Distances in Å.

Geometries and energies of all stationary points reported in the text:

Optimized geometries with basis set I and IEFPCM energies (acetone, E_{PCM}) with basis set II.

1

E_{PCM}: -594.743659

H	-1.564838	-0.627029	-1.125739
N	-1.939571	-1.079749	-0.304641
H	-1.685314	-2.049899	-0.207652
C	-3.233488	-0.740865	0.025943
C	-3.982737	-1.521101	0.920343
C	-3.821894	0.440498	-0.503275
C	-5.269218	-1.148428	1.286606
H	-3.538605	-2.424294	1.332084
C	-5.125092	0.797025	-0.113548
C	-5.850264	0.014589	0.773403
H	-5.824902	-1.773168	1.980812

H	-5.555220	1.702936	-0.529938
H	-6.855605	0.303712	1.062749
C	-3.090921	1.237630	-1.422345
C	-2.440736	1.900554	-2.213045
C	-1.717096	2.703805	-3.137117
C	-0.380863	2.404564	-3.463780
C	-2.328910	3.817953	-3.743459
C	0.317056	3.195760	-4.369036
H	0.100481	1.550050	-2.997858
C	-1.622311	4.603706	-4.646412
H	-3.359100	4.053878	-3.495542
C	-0.298640	4.297211	-4.964012
H	1.348063	2.952319	-4.610611
H	-2.107717	5.460434	-5.105741
H	0.250029	4.913468	-5.670534

2

E_{PCM}: -711.479709

N	1.648210	-0.043518	1.875219
C	2.556386	-0.347022	0.872079
C	3.906802	-0.005654	0.746751
C	1.904675	-1.181015	-0.072936
C	4.586034	-0.466181	-0.373556
H	4.418838	0.578783	1.504483
C	2.616713	-1.628637	-1.197681
C	3.945838	-1.262178	-1.342094
H	5.634902	-0.212499	-0.499395
H	2.132499	-2.261979	-1.936212
H	4.508419	-1.603176	-2.206691
C	0.578214	-1.386512	0.409605
C	0.442915	-0.696722	1.592821
C	-0.768015	-0.597817	2.417367
C	-1.561312	-1.742592	2.596330
C	-1.201395	0.608247	2.989947
C	-2.749543	-1.682871	3.318491
H	-1.226357	-2.685784	2.174376
C	-2.386243	0.664542	3.717484
H	-0.619566	1.512518	2.845563
C	-3.165976	-0.479368	3.885640
H	-3.346584	-2.581764	3.446317
H	-2.706796	1.609604	4.147612
H	-4.090678	-0.432418	4.453962
C	1.977553	0.701018	3.048844
C	1.964843	0.108294	4.244117
H	2.167392	0.675993	5.146443
H	1.730398	-0.945204	4.350005
H	-0.215062	-1.934806	-0.079370
C	2.281865	2.156114	2.827668
H	2.591068	2.635733	3.759019

H	3.073222	2.295815	2.085043
H	1.399639	2.679925	2.439997

3

E_{PCM}: -594.806189

H	-1.564838	-0.627029	-1.125739
N	-1.939571	-1.079749	-0.304641
H	-1.685314	-2.049899	-0.207652
C	-3.233488	-0.740865	0.025943
C	-3.982737	-1.521101	0.920343
C	-3.821894	0.440498	-0.503275
C	-5.269218	-1.148428	1.286606
H	-3.538605	-2.424294	1.332084
C	-5.125092	0.797025	-0.113548
C	-5.850264	0.014589	0.773403
H	-5.824902	-1.773168	1.980812
H	-5.555220	1.702936	-0.529938
H	-6.855605	0.303712	1.062749
C	-3.090921	1.237630	-1.422345
C	-2.440736	1.900554	-2.213045
C	-1.717096	2.703805	-3.137117
C	-0.380863	2.404564	-3.463780
C	-2.328910	3.817953	-3.743459
C	0.317056	3.195760	-4.369036
H	0.100481	1.550050	-2.997858
C	-1.622311	4.603706	-4.646412
H	-3.359100	4.053878	-3.495542
C	-0.298640	4.297211	-4.964012
H	1.348063	2.952319	-4.610611
H	-2.107717	5.460434	-5.105741
H	0.250029	4.913468	-5.670534

5

E_{PCM}: -711.432103

N	0.978029	1.164099	0.856734
C	2.164129	0.432632	0.767152
C	2.959323	0.281517	1.910979
C	2.530752	-0.253721	-0.420078
C	4.109012	-0.498764	1.885570
H	2.654005	0.792402	2.819275
C	3.691906	-1.050942	-0.417968
C	4.479246	-1.170673	0.718047
H	4.715391	-0.588606	2.782754
H	3.959737	-1.572068	-1.332143
H	5.371520	-1.789147	0.698178
C	1.740707	-0.155939	-1.597160
C	1.082544	-0.093846	-2.620204
C	0.308330	-0.023080	-3.811495
C	-1.010010	0.470167	-3.781506

C	0.846468	-0.445135	-5.042059
C	-1.761660	0.539726	-4.948948
H	-1.432437	0.788323	-2.833421
C	0.086770	-0.372073	-6.204057
H	1.862110	-0.827571	-5.070515
C	-1.218000	0.120577	-6.163697
H	-2.778530	0.920786	-4.910715
H	0.515040	-0.701572	-7.146725
H	-1.808682	0.175812	-7.073726
C	0.822199	2.305948	0.305623
C	1.868653	3.057739	-0.476478
H	2.867430	2.643933	-0.326178
H	1.635175	3.003524	-1.546176
H	1.868501	4.116526	-0.196978
C	-0.516898	2.976577	0.438681
H	-0.926802	3.213067	-0.550409
H	-1.212275	2.330338	0.975950
H	-0.418731	3.928580	0.974244

acetone

E_{PCM}: -193.140797

C	4.196854	-0.179280	-2.906492
O	4.190906	-0.518158	-1.740496
C	5.485507	-0.048342	-3.692858
H	5.600438	0.973467	-4.072560
H	6.334782	-0.300324	-3.056514
H	5.470608	-0.710193	-4.566447
C	2.916015	0.135219	-3.652612
H	2.937267	1.162249	-4.034957
H	2.807530	-0.523400	-4.522050
H	2.060094	0.009017	-2.988406

a1

E_{PCM}: -922.863858

Ir	-0.164887	-0.879328	0.463937
C	-0.848326	0.218968	2.191508
C	0.279269	-0.584244	2.539705
C	1.404884	-0.179848	1.734962
C	0.952787	0.901487	0.893974
C	-0.426844	1.148001	1.161714
H	-1.048697	1.880594	0.665609
H	-1.841280	0.139110	2.612954
H	0.270237	-1.415237	3.232740
H	1.543406	1.390818	0.130767
H	2.398104	-0.604491	1.758914
Cl	-0.240975	-3.271608	0.682099
Cl	0.788072	-1.127082	-1.728517
H	-1.782842	-0.852847	-1.597679
N	-1.967208	-1.275347	-0.685751

H	-1.901974	-2.292668	-0.781142
C	-3.232593	-0.872068	-0.155270
C	-3.900730	-1.694846	0.749096
C	-3.782541	0.370932	-0.537326
C	-5.124865	-1.296084	1.278991
H	-3.448773	-2.640602	1.036167
C	-5.021652	0.752228	0.010013
C	-5.686317	-0.072170	0.908407
H	-5.641844	-1.945473	1.979178
H	-5.449485	1.703929	-0.288631
H	-6.643214	0.236711	1.318025
C	-3.083291	1.202477	-1.452294
C	-2.430630	1.876316	-2.230621
C	-1.662473	2.667801	-3.130096
C	-0.391900	2.226829	-3.547695
C	-2.159648	3.895497	-3.605257
C	0.357890	3.006067	-4.422052
H	-0.006849	1.279480	-3.179298
C	-1.399011	4.664176	-4.478518
H	-3.140254	4.232762	-3.283627
C	-0.140385	4.222886	-4.889230
H	1.336853	2.658979	-4.740395
H	-1.789769	5.610614	-4.841452
H	0.450267	4.826189	-5.572890

a2

E_{PCM}: -922.847109

Ir	-0.476665	-0.998949	-0.199715
C	-0.838456	-1.618000	1.900237
C	-1.745181	-2.292207	1.030756
C	-0.995979	-3.098728	0.103101
C	0.394251	-2.920144	0.421142
C	0.492871	-2.005901	1.513404
H	1.412559	-1.648746	1.957367
H	-1.100037	-0.932572	2.694554
H	-2.819360	-2.163395	1.018515
H	1.224578	-3.364548	-0.110756
H	-1.402537	-3.721377	-0.681092
Cl	-2.448864	-0.346727	-1.371476
Cl	0.528735	-1.057397	-2.361892
H	0.910611	2.824535	-1.261556
N	0.551356	3.659615	-0.816968
H	0.658229	4.483685	-1.389833
C	-0.682105	3.521923	-0.209721
C	-1.519871	4.633148	-0.021602
C	-1.109522	2.259905	0.285815
C	-2.743197	4.503834	0.619917
H	-1.197249	5.603630	-0.391364
C	-2.364342	2.150898	0.906486

C	-3.177073	3.259031	1.086160
H	-3.371368	5.381398	0.747127
H	-2.690670	1.169176	1.232142
H	-4.142021	3.157378	1.572373
C	-0.217532	1.144660	0.170158
C	0.937826	0.629349	0.065675
C	2.373251	0.650613	0.198550
C	3.195234	-0.397758	-0.246394
C	2.966554	1.775534	0.806981
C	4.573857	-0.328128	-0.074136
H	2.740146	-1.235634	-0.763688
C	4.346491	1.835879	0.967857
H	2.335765	2.594079	1.138644
C	5.154991	0.784220	0.535312
H	5.199165	-1.143023	-0.428504
H	4.791716	2.708404	1.438041
H	6.232131	0.834200	0.667268

a3

E_{PCM}: -922.864486

Ir	-0.571194	-1.072960	-0.141264
C	0.246869	-1.412589	1.809271
C	-1.136401	-1.811405	1.811011
C	-1.248475	-2.934846	0.904003
C	0.012777	-3.198102	0.338866
C	0.954283	-2.231592	0.871770
H	2.008925	-2.173115	0.643329
H	0.677896	-0.609862	2.393006
H	-1.926841	-1.409407	2.428864
H	0.225393	-3.925208	-0.432511
H	-2.176230	-3.417315	0.627062
Cl	-2.702961	-0.968584	-1.287365
Cl	0.394531	-1.045145	-2.363367
H	1.159146	3.462634	-0.775254
N	0.688771	3.080774	0.052320
H	1.111104	3.533572	0.867352
C	-0.757786	3.272954	-0.001951
C	-1.425537	4.481160	0.041126
C	-1.351476	2.012027	-0.070306
C	-2.820706	4.412529	0.030172
H	-0.905107	5.433992	0.088927
C	-2.749380	1.971830	-0.057398
C	-3.461548	3.171136	-0.011036
H	-3.403362	5.327992	0.060613
H	-3.251080	1.012916	-0.116787
H	-4.547355	3.136880	-0.010854
C	-0.315682	0.943235	-0.069624
C	0.885956	1.572770	0.072962
C	2.296599	1.199513	0.259824

C	2.938616	0.271471	-0.575441
C	3.045615	1.807014	1.286081
C	4.283643	-0.034360	-0.379167
H	2.362370	-0.198444	-1.370382
C	4.392022	1.504970	1.470948
H	2.568925	2.494041	1.986447
C	5.017306	0.580857	0.635493
H	4.764063	-0.752727	-1.038206
H	4.946874	1.981393	2.274475
H	6.067727	0.341863	0.775875

a4

E_{PCM}: -922.882442

Ir	0.125595	-1.199457	0.131892
C	-0.931928	-1.013074	-1.752646
C	0.241561	-1.817734	-1.953829
C	0.047705	-3.039825	-1.195710
C	-1.174356	-2.960785	-0.512461
C	-1.784153	-1.679152	-0.818254
H	-2.737822	-1.320859	-0.458062
H	-1.123003	-0.042584	-2.190559
H	1.063536	-1.607237	-2.623349
H	-1.552244	-3.677478	0.203567
H	0.782645	-3.826592	-1.090744
Cl	2.321997	-1.759110	0.915558
Cl	-0.618114	-1.228613	2.425109
N	0.387990	2.947634	0.983786
C	1.547428	2.790923	0.318742
C	2.552022	3.735457	0.039549
C	1.670116	1.430817	-0.115273
C	3.652613	3.296915	-0.673134
H	2.466701	4.766258	0.368955
C	2.822429	1.025337	-0.831747
C	3.797106	1.957369	-1.111479
H	4.441417	4.008766	-0.903490
H	2.919676	-0.015386	-1.119493
H	4.690991	1.670479	-1.655762
C	0.539087	0.700984	0.314258
C	-0.353050	1.697298	1.034777
C	-1.762679	1.844927	0.481204
C	-2.845816	1.242737	1.126339
C	-1.985923	2.591998	-0.681395
C	-4.135357	1.387515	0.613349
H	-2.668710	0.645503	2.016229
C	-3.274387	2.732311	-1.193284
H	-1.148945	3.073117	-1.181737
C	-4.353840	2.130859	-0.545581
H	-4.971402	0.921287	1.127755
H	-3.435727	3.316847	-2.095040

H	-5.359682	2.246301	-0.939719
H	-0.410001	1.312549	2.068049
H	0.049049	3.813102	1.370480

a5

E_{PCM}: -922.907798

Ir	0.031281	-1.160124	-0.152663
C	0.584669	-0.625974	-2.166528
C	1.212318	-1.853398	-1.808696
C	0.174967	-2.813239	-1.490893
C	-1.088871	-2.155371	-1.683267
C	-0.851364	-0.806284	-2.097391
H	-1.608993	-0.068744	-2.322212
H	1.101198	0.289669	-2.422097
H	2.277093	-2.021614	-1.722466
H	-2.057786	-2.584802	-1.464450
H	0.324303	-3.830292	-1.156622
Cl	1.638069	-1.881753	1.481529
Cl	-1.655838	-1.556528	1.485589
N	-0.020132	2.515011	-0.683439
C	1.363233	2.406254	-0.594170
C	2.352971	3.085936	-1.301325
C	1.642982	1.448253	0.402563
C	3.672702	2.801060	-0.964638
H	2.109696	3.817295	-2.067152
C	2.978168	1.182856	0.724644
C	3.977298	1.866555	0.038455
H	4.477499	3.316016	-1.481085
H	3.214990	0.443143	1.480801
H	5.017857	1.672624	0.282506
C	0.360512	0.925321	0.876944
C	-0.634974	1.708909	0.223201
C	-2.075035	1.815036	0.443503
C	-2.624066	1.518630	1.700009
C	-2.928782	2.262267	-0.580751
C	-3.988715	1.674644	1.923375
H	-1.980153	1.176345	2.500794
C	-4.291574	2.411358	-0.354531
H	-2.534549	2.466356	-1.574183
C	-4.824943	2.120100	0.902145
H	-4.398463	1.441110	2.901346
H	-4.938915	2.748904	-1.158798
H	-5.889770	2.238126	1.081376
H	0.209001	0.513709	1.868139
H	-0.505361	3.202046	-1.238708

tsa2-3

E_{PCM}: -922.829749

Ir	-0.870737	0.095011	-0.438372

C	-0.881039	-2.066137	-0.447034
C	-2.168140	-1.588844	-0.058059
C	-2.720699	-0.827346	-1.158503
C	-1.752185	-0.835222	-2.205071
C	-0.607315	-1.592951	-1.784674
H	0.279519	-1.788027	-2.371388
H	-0.216725	-2.660355	0.166348
H	-2.643903	-1.747999	0.899963
H	-1.829073	-0.285704	-3.134061
H	-3.671740	-0.314280	-1.165692
Cl	-1.864064	1.455629	1.282735
Cl	-0.510896	2.145552	-1.623589
H	3.646729	1.456337	1.224258
N	3.478901	0.456206	1.295870
H	4.366896	-0.034498	1.304517
C	2.607073	0.109876	2.366514
C	3.032476	-0.169971	3.660718
C	1.244158	0.026167	2.015129
C	2.092148	-0.531975	4.626281
H	4.087029	-0.099687	3.915745
C	0.312869	-0.319195	2.996405
C	0.739749	-0.597966	4.293679
H	2.418087	-0.751176	5.639006
H	-0.738247	-0.338536	2.731954
H	0.008902	-0.867699	5.050671
C	0.963310	0.229676	0.589877
C	1.922761	0.377975	-0.264664
C	2.634496	0.552844	-1.488341
C	2.727231	1.819791	-2.096000
C	3.281788	-0.548765	-2.085658
C	3.437788	1.968715	-3.283328
H	2.213636	2.658306	-1.640894
C	3.992910	-0.388283	-3.266930
H	3.217305	-1.521648	-1.606750
C	4.069169	0.871646	-3.867821
H	3.494729	2.945148	-3.755296
H	4.487386	-1.240988	-3.723394
H	4.624170	0.995706	-4.793750

tsa3-4

E_{PCM}: -922.808520

Ir	0.099859	0.174251	1.627454
C	-0.784408	-1.783673	1.710286
C	0.304147	-1.723546	2.646745
C	-0.068214	-0.761114	3.666317
C	-1.321364	-0.218007	3.336669
C	-1.774573	-0.824204	2.098842
H	-2.714951	-0.636143	1.600912
H	-0.834789	-2.423145	0.838799

H	1.194367	-2.336933	2.644008
H	-1.818973	0.588990	3.856946
H	0.567454	-0.439437	4.479995
Cl	2.200933	1.209754	2.203631
Cl	-0.691502	2.422264	1.221957
N	0.550542	0.205807	-2.668735
C	1.850535	-0.131715	-2.314082
C	2.954940	-0.300727	-3.151208
C	1.915905	-0.202608	-0.904488
C	4.154144	-0.628400	-2.538560
H	2.872557	-0.210680	-4.230196
C	3.156490	-0.523717	-0.317780
C	4.249402	-0.744332	-1.137721
H	5.034329	-0.802093	-3.150904
H	3.232695	-0.567721	0.761897
H	5.207071	-0.999210	-0.693604
C	0.615441	0.060595	-0.311199
C	-0.282555	0.225045	-1.376936
C	-1.732046	0.002173	-1.579570
C	-2.698953	0.812739	-0.971122
C	-2.146820	-1.056047	-2.405424
C	-4.052386	0.557996	-1.183421
H	-2.367407	1.623151	-0.326231
C	-3.501372	-1.299736	-2.618947
H	-1.408148	-1.711467	-2.863398
C	-4.458894	-0.491234	-2.007827
H	-4.793601	1.194273	-0.707444
H	-3.806925	-2.124923	-3.256185
H	-5.516003	-0.678151	-2.174827
H	0.168942	1.242683	-2.117407
H	0.113860	-0.003749	-3.559094

tsa4-5

E_{PCM}: -922.856292

Ir	0.078668	0.115477	1.654167
C	-0.986202	-1.747566	1.625455
C	0.106260	-1.840529	2.559298
C	-0.169875	-0.896751	3.622584
C	-1.369858	-0.219307	3.332891
C	-1.880072	-0.723844	2.072436
H	-2.792668	-0.415761	1.582774
H	-1.099336	-2.329713	0.720511
H	0.935297	-2.532818	2.520437
H	-1.792268	0.596637	3.903017
H	0.498453	-0.673768	4.443387
Cl	2.174702	1.040107	2.398556
Cl	-0.531860	2.407623	1.133752
N	0.517167	-0.117263	-2.602335
C	1.858087	-0.220445	-2.310501

C	2.939647	-0.377959	-3.180259
C	2.003413	-0.139409	-0.907825
C	4.193839	-0.502819	-2.601260
H	2.803745	-0.416244	-4.256953
C	3.284787	-0.281763	-0.352715
C	4.362799	-0.467139	-1.205240
H	5.061946	-0.637126	-3.240680
H	3.407069	-0.221426	0.722162
H	5.359754	-0.575418	-0.788763
C	0.679369	0.021654	-0.296859
C	-0.214676	0.050978	-1.445301
C	-1.690783	-0.081045	-1.559928
C	-2.601677	0.830178	-1.013071
C	-2.172517	-1.179120	-2.291556
C	-3.969688	0.636286	-1.194149
H	-2.231738	1.675268	-0.439540
C	-3.541737	-1.367180	-2.463664
H	-1.470877	-1.894712	-2.712180
C	-4.445091	-0.457896	-1.916422
H	-4.666746	1.353909	-0.770370
H	-3.899585	-2.225154	-3.025684
H	-5.513249	-0.599936	-2.054268
H	0.166171	1.159305	-0.776048
H	0.129950	0.041241	-3.520049

a4ass

E_{PCM}: -1115.995779

Ir	-1.465721	-0.396772	-0.034580
C	-2.216624	0.494985	-1.816044
C	-2.700704	-0.857368	-1.725097
C	-3.587180	-0.916439	-0.575355
C	-3.603962	0.341087	0.047802
C	-2.721907	1.227274	-0.693216
H	-2.534363	2.269652	-0.477917
H	-1.548174	0.881587	-2.573801
H	-2.520476	-1.654932	-2.432178
H	-4.104613	0.585330	0.974807
H	-4.066747	-1.812857	-0.205367
Cl	-1.040272	-2.586123	0.935836
Cl	-0.854637	0.400696	2.209361
N	2.677469	0.474560	-0.814581
C	2.656076	-0.865415	-1.254469
C	3.712560	-1.649489	-1.704603
C	1.336268	-1.334173	-1.107649
C	3.416761	-2.961001	-2.071443
H	4.720508	-1.251878	-1.794150
C	1.070106	-2.660356	-1.481972
C	2.106994	-3.452282	-1.965582
H	4.206395	-3.602507	-2.452212

H	0.067967	-3.057105	-1.375421
H	1.899075	-4.476105	-2.264430
C	0.484579	-0.237952	-0.621676
C	1.292319	0.878789	-0.636237
H	2.931734	0.422070	0.704631
H	3.301190	1.120438	-1.288169
C	2.503634	-0.320297	2.534395
O	2.939256	0.583026	1.761989
C	2.161849	-1.674129	2.082415
H	1.074619	-1.694440	1.843762
H	2.694102	-1.964812	1.175317
H	2.309649	-2.401231	2.883206
C	2.300400	0.073162	3.947089
H	1.208695	0.122770	4.078778
H	2.680364	-0.689319	4.631385
H	2.732129	1.051843	4.155600
C	1.060109	2.334477	-0.597349
C	0.209352	2.966276	0.323362
C	0.022230	4.346468	0.284523
C	0.676668	5.132221	-0.663708
C	1.523835	4.520107	-1.585516
C	1.709991	3.140997	-1.552981
H	-0.281174	2.362872	1.080493
H	-0.634647	4.811961	1.015309
H	0.528834	6.208460	-0.684708
H	2.032744	5.113619	-2.340478
H	2.336646	2.683715	-2.316825

Tsa3-4ass

E_{PCM}: -1115.996124

Ir	-1.496789	-0.182814	-0.011363
C	-2.131900	0.728838	-1.826800
C	-2.814565	-0.527245	-1.665892
C	-3.683829	-0.396121	-0.507969
C	-3.496417	0.876695	0.052829
C	-2.500856	1.583268	-0.736199
H	-2.157107	2.595102	-0.575005
H	-1.424688	0.972645	-2.608318
H	-2.765228	-1.376020	-2.334057
H	-3.938644	1.236724	0.971854
H	-4.289954	-1.189709	-0.092046
Cl	-1.371740	-2.392859	0.997547
Cl	-0.774016	0.557374	2.218262
N	2.725847	0.091946	-0.820587
C	2.508512	-1.237043	-1.245244
C	3.438490	-2.168416	-1.692516
C	1.137891	-1.511531	-1.081824
C	2.955825	-3.429576	-2.038321
H	4.491760	-1.919382	-1.795950

C	0.682107	-2.791183	-1.433261
C	1.591286	-3.728897	-1.913544
H	3.642771	-4.181207	-2.416757
H	-0.365332	-3.038583	-1.310770
H	1.237316	-4.716955	-2.194902
C	0.454427	-0.299858	-0.604955
C	1.411041	0.692201	-0.639586
H	3.003685	0.033733	0.670281
H	3.426316	0.635091	-1.315838
C	2.492303	-0.591750	2.531247
O	3.055706	0.211010	1.732959
C	1.938521	-1.886964	2.117772
H	0.854946	-1.746584	1.906644
H	2.397428	-2.270726	1.205308
H	1.997545	-2.613461	2.930560
C	2.362389	-0.132826	3.933272
H	1.299864	0.131593	4.049750
H	2.581073	-0.935944	4.640619
H	2.973604	0.749391	4.123278
C	1.388622	2.165727	-0.615269
C	0.601448	2.919277	0.270601
C	0.609052	4.311339	0.219110
C	1.400569	4.990634	-0.706552
C	2.187633	4.258035	-1.593003
C	2.178379	2.866736	-1.548646
H	0.006923	2.397890	1.013832
H	-0.002449	4.869521	0.923917
H	1.404731	6.076689	-0.737266
H	2.801655	4.767874	-2.330689
H	2.762203	2.322514	-2.289280

Tsa4-5ass

E_{PCM}: -1115.994726

Ir	0.231175	-1.214936	-0.514906
C	0.858637	-1.419281	-2.566267
C	0.773752	-2.762737	-2.022862
C	-0.551079	-2.990173	-1.602078
C	-1.332077	-1.795110	-1.862988
C	-0.456346	-0.851526	-2.499955
H	-0.731299	0.141823	-2.829081
H	1.734360	-0.955702	-2.998341
H	1.607924	-3.437578	-1.885884
H	-2.387247	-1.665491	-1.667963
H	-0.906339	-3.865021	-1.074603
Cl	2.387185	-1.328251	0.646586
Cl	-0.684809	-2.064294	1.575688
N	-0.798720	2.957130	-0.362710
C	0.527152	3.086900	-0.695945
C	1.246691	4.220768	-1.079403

C	1.096765	1.792757	-0.606589
C	2.581049	4.041697	-1.418955
H	0.778883	5.200794	-1.124753
C	2.445862	1.646039	-0.977848
C	3.169011	2.764320	-1.376914
H	3.173908	4.897066	-1.730787
H	2.908149	0.665292	-0.930878
H	4.210730	2.650343	-1.665125
C	0.072353	0.849702	-0.135757
C	-1.093540	1.646549	-0.044669
C	-2.506105	1.350406	0.240992
C	-2.902058	0.408013	1.201082
C	-3.505562	2.058010	-0.455280
C	-4.253306	0.188934	1.456016
H	-2.151745	-0.169619	1.730050
C	-4.854239	1.837400	-0.192921
H	-3.224604	2.760463	-1.236519
C	-5.234768	0.902706	0.769164
H	-4.536344	-0.548748	2.201990
H	-5.607509	2.389458	-0.748680
H	-6.287078	0.728687	0.976640
H	0.359863	0.847764	1.450789
C	1.609284	0.485479	3.009518
O	0.463906	0.619092	2.512755
C	1.701910	-0.387138	4.205506
H	2.536665	-0.120711	4.856007
H	0.753509	-0.411598	4.744264
H	1.872605	-1.395869	3.801833
C	2.801039	1.232627	2.536296
H	2.933954	2.064402	3.245860
H	3.692839	0.606163	2.590692
H	2.679346	1.629511	1.529704
H	-1.438227	3.721197	-0.210028

a1+

E_{PCM}: -1100.774793

Ir	-0.694281	-0.018930	-1.386752
C	0.151929	1.828511	-1.995533
C	-1.084397	1.631966	-2.702685
C	-2.145786	1.548874	-1.752824
C	-1.566148	1.731746	-0.437117
C	-0.166011	1.922330	-0.586589
H	0.541947	2.053897	0.221226
H	1.132319	1.930774	-2.440288
H	-1.178200	1.478495	-3.770381
H	-2.100717	1.708562	0.503617
H	-3.192772	1.402547	-1.978814
Cl	-0.563415	-1.616711	-3.144836
H	0.697135	-1.436528	0.350713

N	0.946566	-1.183842	-0.608347
H	0.926124	-2.029911	-1.183486
C	2.264590	-0.597075	-0.627149
C	3.035876	-0.663642	-1.783416
C	2.743084	0.043946	0.533743
C	4.304313	-0.088265	-1.798674
H	2.642969	-1.163756	-2.664656
C	4.027818	0.618549	0.493514
C	4.797830	0.552801	-0.660388
H	4.908543	-0.147589	-2.698433
H	4.407871	1.106019	1.385201
H	5.788399	0.996300	-0.671581
C	1.941576	0.099291	1.706089
C	1.243359	0.147559	2.705415
C	0.466594	0.234821	3.894702
C	-0.802094	-0.369609	3.972618
C	0.965819	0.932887	5.010475
C	-1.551530	-0.273298	5.139062
H	-1.183591	-0.918642	3.116572
C	0.207554	1.023114	6.171696
H	1.945720	1.396077	4.954431
C	-1.050268	0.422926	6.239701
H	-2.528005	-0.745559	5.194486
H	0.600244	1.562058	7.028578
H	-1.637649	0.494713	7.150130
C	-2.716334	-2.241282	-0.499952
O	-1.665412	-1.607727	-0.298081
C	-3.016601	-3.404826	0.388087
H	-2.870970	-4.323893	-0.194419
H	-2.355889	-3.425892	1.254844
H	-4.065139	-3.397086	0.701356
C	-3.697748	-1.893023	-1.566153
H	-4.117485	-2.799469	-2.011027
H	-4.533925	-1.359345	-1.094005
H	-3.249042	-1.271623	-2.339878

a2+

E_{PCM}: -1100.756817

Ir	-1.555866	0.314287	-0.445848
C	-2.353291	-1.704976	-0.183291
C	-3.420773	-0.877017	-0.707553
C	-3.009154	-0.352175	-1.953449
C	-1.668425	-0.831554	-2.225930
C	-1.296538	-1.701301	-1.143518
H	-0.349730	-2.217710	-1.052050
H	-2.381671	-2.285042	0.728424
H	-4.355676	-0.654302	-0.209667
H	-1.082847	-0.628488	-3.111262
H	-3.561584	0.351514	-2.562197

Cl	-1.390391	2.517256	-1.371290
H	0.079255	3.407851	0.166835
N	0.523497	3.941925	0.916541
H	0.507503	4.946856	0.836372
C	0.987085	3.367492	2.025706
C	1.439187	4.148689	3.122532
C	1.031109	1.920844	2.160731
C	1.852286	3.547021	4.286105
H	1.442593	5.231247	3.032867
C	1.448246	1.346476	3.409740
C	1.851941	2.135599	4.449705
H	2.186760	4.173328	5.108657
H	1.469917	0.263666	3.484361
H	2.190282	1.698345	5.382674
C	0.780748	1.132593	1.073225
C	0.515263	0.534526	-0.028286
C	1.517709	0.024574	-1.001011
C	2.493295	-0.891470	-0.583611
C	1.509495	0.468031	-2.330816
C	3.440879	-1.365374	-1.489324
H	2.505014	-1.231979	0.448029
C	2.469605	0.000176	-3.224799
H	0.766133	1.195235	-2.644242
C	3.432255	-0.921110	-2.810228
H	4.190698	-2.077775	-1.157760
H	2.467204	0.360540	-4.249571
H	4.174697	-1.287105	-3.512962
C	-2.340470	1.181465	2.487300
O	-2.109461	1.463760	1.304087
C	-2.856173	2.259218	3.386882
H	-2.090062	2.496435	4.135021
H	-3.101658	3.155100	2.816856
H	-3.733618	1.907083	3.940132
C	-2.140146	-0.187473	3.053725
H	-1.820365	-0.138275	4.097607
H	-3.104073	-0.712975	3.042167
H	-1.425532	-0.753749	2.454342

a3+

E_{PCM}: -1100.783970

Ir	0.626046	-0.795273	-0.176121
C	0.056338	-0.933558	-2.238733
C	1.457957	-1.181043	-2.154337
C	1.646913	-2.412966	-1.407227
C	0.385009	-2.867967	-0.990019
C	-0.624783	-1.935226	-1.456194
H	-1.693422	-2.039985	-1.334239
H	-0.410951	-0.107816	-2.758048
H	2.236290	-0.596867	-2.626875

H	0.194424	-3.719064	-0.349168
H	2.598640	-2.879826	-1.192741
Cl	-0.017499	-1.395120	2.049369
H	-2.407003	2.808920	1.257560
N	-1.976167	2.648010	0.339723
H	-2.660415	2.953783	-0.360321
C	-0.687970	3.325482	0.201286
C	-0.467455	4.688253	0.191280
C	0.289723	2.342848	0.030549
C	0.850388	5.098711	-0.026953
H	-1.266637	5.410196	0.332903
C	1.594328	2.782286	-0.211771
C	1.857363	4.152993	-0.235649
H	1.085196	6.157841	-0.046685
H	2.387434	2.064847	-0.374874
H	2.870737	4.494776	-0.424607
C	-0.327203	0.993281	0.066358
C	-1.667086	1.165473	0.191812
C	-2.887042	0.338050	0.142149
C	-3.200086	-0.605136	1.131085
C	-3.796550	0.545613	-0.912084
C	-4.388891	-1.329265	1.053991
H	-2.499445	-0.774941	1.940889
C	-4.985951	-0.174227	-0.979493
H	-3.558811	1.250760	-1.708491
C	-5.283804	-1.115123	0.006510
H	-4.618314	-2.059663	1.824375
H	-5.673572	-0.007626	-1.803374
H	-6.210741	-1.678732	-0.042985
C	3.122235	-0.356432	1.669044
O	2.281856	0.120324	0.892342
C	4.047526	0.591357	2.369929
H	5.079285	0.406860	2.048777
H	3.776145	1.626708	2.165474
H	4.018324	0.404511	3.448928
C	3.279447	-1.813035	1.950364
H	4.340302	-2.083173	1.952010
H	2.888170	-2.014968	2.953990
H	2.718226	-2.424247	1.246179

tsa2-3+

E_{PCM}: -1100.744419

Ir	-1.227468	0.367782	-0.272823
C	-1.038864	2.489586	-0.634793
C	-1.827824	1.925728	-1.675682
C	-3.027911	1.366006	-1.084117
C	-2.951165	1.573615	0.317817
C	-1.708558	2.238367	0.621315
H	-1.378231	2.549293	1.602587

H	-0.081183	2.977479	-0.759323
H	-1.584062	1.935210	-2.729963
H	-3.660194	1.213640	1.052312
H	-3.841156	0.892096	-1.616101
Cl	-1.774538	-1.374353	1.252000
H	3.259630	-1.074833	1.230085
N	3.394347	-0.115575	0.922809
H	4.282314	0.225120	1.275336
C	3.232681	0.050130	-0.471000
C	4.299994	0.162564	-1.360310
C	1.904425	0.161898	-0.939973
C	4.058945	0.366862	-2.717942
H	5.319050	0.079129	-0.991816
C	1.680130	0.342622	-2.308429
C	2.750612	0.446470	-3.192717
H	4.895405	0.453518	-3.404744
H	0.661537	0.416575	-2.670994
H	2.564607	0.600718	-4.251214
C	0.859875	0.176347	0.087400
C	1.055661	0.209540	1.358596
C	0.963736	0.249397	2.764657
C	0.700178	-0.926057	3.503137
C	1.160118	1.472775	3.447281
C	0.620014	-0.867894	4.888211
H	0.542196	-1.858114	2.972993
C	1.081163	1.516389	4.830251
H	1.386760	2.367689	2.875690
C	0.808985	0.347233	5.549205
H	0.408503	-1.768758	5.455631
H	1.233646	2.454485	5.354849
H	0.747675	0.385504	6.633060
C	-1.543426	-2.207998	-2.020823
O	-0.833290	-1.280124	-1.604756
C	-0.878463	-3.284065	-2.820916
H	-1.478423	-3.553105	-3.695463
H	0.126865	-2.985264	-3.117913
H	-0.812129	-4.182480	-2.194040
C	-3.013609	-2.311298	-1.789112
H	-3.524214	-2.117979	-2.741764
H	-3.275868	-3.332546	-1.496673
H	-3.353732	-1.615343	-1.025102

tsa2-o2+

E_{PCM}: -1100.743511

Ir	-1.343055	0.386944	-0.185001
C	-2.124347	-1.610826	0.310838
C	-3.171067	-0.870579	-0.356264
C	-2.754458	-0.527179	-1.664379
C	-1.407016	-1.010569	-1.825603

C	-1.047733	-1.715505	-0.617500
H	-0.102072	-2.211396	-0.442860
H	-2.172375	-2.048263	1.298142
H	-4.100604	-0.555527	0.100698
H	-0.791913	-0.912901	-2.709900
H	-3.310154	0.065636	-2.378378
Cl	-1.060541	2.483756	-1.316637
H	-0.749036	3.192612	0.958507
N	-0.777944	3.222267	1.985136
H	-0.972206	4.173124	2.285434
C	0.372439	2.687545	2.607300
C	0.893105	3.284000	3.757072
C	0.948312	1.504215	2.103739
C	1.986457	2.723813	4.409751
H	0.447383	4.202034	4.132577
C	2.055905	0.957693	2.774161
C	2.571277	1.557719	3.916324
H	2.384377	3.202957	5.298679
H	2.506797	0.051171	2.383642
H	3.427812	1.118686	4.417507
C	0.486764	0.861153	0.888152
C	0.875730	0.361755	-0.209246
C	1.754968	-0.109962	-1.242527
C	2.652297	-1.156074	-0.953340
C	1.758226	0.479048	-2.521084
C	3.543999	-1.595187	-1.926598
H	2.653479	-1.607883	0.034684
C	2.651196	0.026263	-3.485095
H	1.071306	1.293297	-2.729867
C	3.542720	-1.008445	-3.192099
H	4.239977	-2.396229	-1.696830
H	2.659055	0.488256	-4.467726
H	4.238854	-1.354917	-3.950005
C	-2.485457	2.046185	2.183613
O	-2.588490	1.626983	0.980273
C	-3.469559	3.132948	2.545354
H	-3.202597	3.631776	3.479575
H	-3.559693	3.856667	1.733160
H	-4.451848	2.666696	2.684727
C	-2.055710	1.127819	3.290699
H	-1.674447	1.668202	4.158760
H	-2.954712	0.583750	3.606912
H	-1.315247	0.402755	2.952477

i1

E_{PCM}: -1039.544316

Ir	-0.884362	0.063399	-1.278915
C	0.256774	1.809006	-1.894727
C	-0.944947	1.709690	-2.657134

C	-2.070940	1.772223	-1.760149
C	-1.537926	1.929080	-0.430283
C	-0.114685	1.945421	-0.501104
H	0.557656	2.028015	0.341135
H	1.263043	1.783576	-2.288725
H	-1.003027	1.532442	-3.722961
H	-2.122523	1.942290	0.479805
H	-3.114623	1.703594	-2.031037
Cl	-1.397073	-1.439793	-3.090796
Cl	-2.388359	-1.042345	0.250602
N	0.690675	-1.327074	-0.771692
C	1.968751	-0.674378	-0.808885
C	2.659904	-0.629899	-2.019846
C	2.513939	-0.072518	0.346377
C	3.894254	0.009573	-2.103869
H	2.204587	-1.092346	-2.891116
C	3.765042	0.567836	0.238418
C	4.446876	0.610485	-0.970708
H	4.423594	0.035259	-3.051962
H	4.188630	1.025672	1.126933
H	5.409885	1.108841	-1.029813
C	1.828024	-0.119844	1.588844
C	1.232161	-0.147742	2.650351
C	0.508165	-0.188403	3.874603
C	-0.846540	-0.573133	3.876534
C	1.131759	0.155200	5.088313
C	-1.552503	-0.611198	5.074179
H	-1.327913	-0.828819	2.936232
C	0.414189	0.111963	6.278094
H	2.176439	0.451365	5.084275
C	-0.927741	-0.271153	6.274879
H	-2.597824	-0.907257	5.068354
H	0.902979	0.377494	7.211323
H	-1.485371	-0.303621	7.206782
C	0.688451	-2.604397	-0.546407
C	1.952941	-3.368970	-0.250673
H	2.774119	-2.750722	0.108400
H	1.735337	-4.147058	0.486383
H	2.279379	-3.878891	-1.165627
C	-0.533383	-3.458650	-0.574680
H	-0.828441	-3.681302	0.457230
H	-1.370171	-2.995271	-1.086968
H	-0.277743	-4.410146	-1.054256

i2

E_{PCM}: -1039.530878

Ir	-0.564225	-0.434263	1.672971
C	0.259959	-2.092096	0.543348
C	1.072600	-1.852975	1.711016

C	0.261232	-2.123707	2.870864
C	-1.035950	-2.468717	2.414857
C	-1.054909	-2.453904	0.971634
H	-1.900867	-2.689234	0.341686
H	0.574064	-1.949371	-0.486447
H	2.111717	-1.553574	1.714162
H	-1.898976	-2.627628	3.047420
H	0.560451	-1.997368	3.902222
Cl	0.309665	1.299528	3.077957
Cl	-2.721027	0.172542	2.530776
N	1.180780	-0.528967	-2.295497
C	2.074775	0.270200	-1.567621
C	3.421346	0.370102	-1.943228
C	1.653091	0.877339	-0.359173
C	4.332565	1.062261	-1.151554
H	3.745363	-0.121383	-2.856207
C	2.585115	1.577088	0.425532
C	3.915358	1.669030	0.033691
H	5.371662	1.125794	-1.462927
H	2.235845	2.027825	1.348822
H	4.623950	2.210945	0.652722
C	0.273037	0.795050	0.045530
C	-0.969004	0.997020	0.062595
C	-2.174015	1.665499	-0.371468
C	-2.727353	2.702724	0.394615
C	-2.779503	1.298521	-1.582583
C	-3.856469	3.373511	-0.063896
H	-2.268026	2.963050	1.341770
C	-3.912098	1.972332	-2.029698
H	-2.355310	0.485874	-2.164583
C	-4.451218	3.012431	-1.273103
H	-4.278206	4.178456	0.531278
H	-4.374564	1.685000	-2.970142
H	-5.335393	3.538033	-1.623153
C	0.812691	-0.248448	-3.488790
C	-0.078749	-1.224717	-4.204219
H	-1.025897	-0.748769	-4.484061
H	0.390765	-1.558616	-5.137188
H	-0.281848	-2.092558	-3.575369
C	1.171373	0.999061	-4.254142
H	1.754714	0.743940	-5.146577
H	0.256009	1.486660	-4.607621
H	1.742063	1.707304	-3.652525

i3

E_{PCM}: -1039.555331

Ir	-0.111944	0.297765	1.983863
C	-0.838832	-1.685518	1.594729
C	0.196946	-1.756690	2.589803

C	-0.302441	-1.071982	3.767254
C	-1.579336	-0.560048	3.486435
C	-1.919202	-0.905432	2.118693
H	-2.843390	-0.672913	1.610118
H	-0.798130	-2.115936	0.602980
H	1.131588	-2.294090	2.513360
H	-2.165660	0.075347	4.135913
H	0.267535	-0.891477	4.668641
Cl	1.820398	1.371036	2.965372
Cl	-1.083958	2.512750	1.993425
N	0.717009	1.054378	-2.151560
C	2.039358	0.653250	-1.727345
C	3.211960	0.459500	-2.443844
C	1.958234	0.446999	-0.340845
C	4.346180	0.051392	-1.729303
H	3.281495	0.556702	-3.516845
C	3.097966	0.048549	0.350560
C	4.290672	-0.143562	-0.353345
H	5.270962	-0.125312	-2.270285
H	3.043691	-0.078692	1.425490
H	5.182022	-0.457488	0.182213
C	0.555982	0.587454	0.113190
C	-0.178492	0.822394	-1.032469
C	-1.599578	0.540263	-1.330047
C	-2.660123	1.110724	-0.611678
C	-1.902146	-0.382894	-2.348723
C	-3.978074	0.769442	-0.912271
H	-2.432429	1.814682	0.185489
C	-3.221194	-0.714208	-2.650203
H	-1.093960	-0.858002	-2.901291
C	-4.268122	-0.136903	-1.931991
H	-4.785225	1.227231	-0.345942
H	-3.428903	-1.433003	-3.438586
H	-5.298134	-0.392959	-2.164309
C	0.430035	1.767085	-3.222449
C	-0.868707	2.488700	-3.343208
H	-1.243540	2.810564	-2.370603
H	-0.729114	3.357426	-3.991159
H	-1.642168	1.852992	-3.792810
C	1.408671	1.934636	-4.339367
H	1.690574	0.971953	-4.777521
H	0.967636	2.547098	-5.125773
H	2.326473	2.425623	-3.994063

i4

E_{PCM}: -1039.560623

Ir	-0.389388	0.275191	-1.772242
C	0.556232	-1.675788	-1.771590
C	-0.636636	-1.737920	-2.569187

C	-0.415217	-0.886891	-3.723881
C	0.844833	-0.283045	-3.606099
C	1.453307	-0.734923	-2.367495
H	2.429027	-0.457956	-1.995193
H	0.732665	-2.207485	-0.846261
H	-1.492247	-2.377454	-2.404727
H	1.252554	0.473243	-4.262628
H	-1.152986	-0.671189	-4.485009
Cl	-2.556265	1.208408	-2.206892
Cl	0.473357	2.522888	-1.643406
N	-0.526767	0.853861	2.455591
C	-1.721937	0.229263	2.256791
C	-2.769087	-0.050537	3.157937
C	-1.865986	-0.124262	0.874482
C	-3.890242	-0.698293	2.669689
H	-2.721182	0.230973	4.200237
C	-3.036945	-0.771484	0.414567
C	-4.035432	-1.069789	1.313839
H	-4.699105	-0.918865	3.361939
H	-3.128362	-0.986037	-0.644088
H	-4.945637	-1.561848	0.986978
C	-0.745943	0.330939	0.148431
C	0.178941	0.953336	1.165676
C	1.554099	0.305833	1.222220
C	2.674348	0.961816	0.708811
C	1.702001	-0.968867	1.780024
C	3.927673	0.350127	0.756037
H	2.557327	1.941084	0.254009
C	2.953822	-1.578382	1.826455
H	0.834410	-1.480164	2.190830
C	4.071722	-0.919119	1.313858
H	4.793897	0.873248	0.359892
H	3.057313	-2.566388	2.267021
H	5.049557	-1.390965	1.354024
C	0.016560	1.398638	3.639644
C	0.857258	2.441493	3.584840
H	1.336396	2.794068	4.490614
H	1.093726	2.963338	2.665737
H	0.276224	2.005228	0.852302
C	-0.308912	0.720680	4.944855
H	0.473682	0.947340	5.671759
H	-1.253694	1.071395	5.373412
H	-0.369375	-0.365991	4.833197

i5

E_{PCM}: -1039.577667

Ir	-0.277526	-0.453150	-1.600461
C	-1.005581	-2.136516	-0.475317
C	-1.641963	-2.106931	-1.749896

C	-0.612601	-2.209265	-2.764294
C	0.648613	-2.321646	-2.086969
C	0.421983	-2.277656	-0.672962
H	1.180804	-2.351012	0.092807
H	-1.511833	-2.041615	0.476145
H	-2.698893	-1.968844	-1.931249
H	1.617534	-2.346727	-2.568299
H	-0.763816	-2.182958	-3.834373
Cl	-1.679824	1.041617	-2.859293
Cl	1.589658	0.803036	-2.381710
N	-0.271659	0.279600	2.139268
C	-1.653784	0.386931	1.919419
C	-2.703435	0.042631	2.771250
C	-1.851947	0.981132	0.659624
C	-3.992933	0.312672	2.324464
H	-2.526101	-0.384212	3.753375
C	-3.158036	1.249300	0.234203
C	-4.214486	0.909718	1.072831
H	-4.838591	0.069008	2.961065
H	-3.325681	1.697574	-0.738824
H	-5.233054	1.115793	0.756278
C	-0.533179	1.179399	0.065434
C	0.406579	0.807970	1.072831
C	1.853768	1.039489	1.070984
C	2.343400	2.221163	0.493168
C	2.771522	0.131382	1.623414
C	3.707237	2.496566	0.492367
H	1.651703	2.930631	0.053655
C	4.134538	0.401676	1.606219
H	2.423894	-0.801863	2.052499
C	4.606409	1.590028	1.047726
H	4.065745	3.418214	0.044046
H	4.830795	-0.317293	2.028635
H	5.671575	1.803393	1.040999
C	0.253513	-0.217784	3.382514
C	0.700462	0.646095	4.292879
H	1.096416	0.295704	5.240416
H	0.698055	1.714619	4.107819
H	-0.310317	1.966171	-0.647171
C	0.200644	-1.707690	3.557491
H	0.557247	-1.995068	4.548880
H	-0.820558	-2.084582	3.435001
H	0.817292	-2.217948	2.808119

tsi2-3

E_{PCM}: -1039.524974

Ir	-0.115174	-0.024375	2.057563
C	0.098926	-2.160980	1.825473
C	0.731612	-1.751567	3.037876

C	-0.282214	-1.188395	3.905928
C	-1.519971	-1.244655	3.203149
C	-1.306111	-1.839759	1.912843
H	-2.061812	-2.028265	1.163371
H	0.596187	-2.610431	0.975995
H	1.784789	-1.836130	3.268392
H	-2.455677	-0.823903	3.547184
H	-0.117508	-0.761001	4.884753
Cl	1.590382	1.492210	2.828715
Cl	-1.598055	1.853000	2.142128
N	0.719612	0.809748	-2.449993
C	1.951402	0.561266	-1.838858
C	3.168484	0.408233	-2.509618
C	1.866668	0.324630	-0.449501
C	4.310764	0.068542	-1.787197
H	3.218681	0.522122	-3.587577
C	3.023088	0.005014	0.261477
C	4.240238	-0.118322	-0.406675
H	5.256827	-0.051301	-2.307523
H	2.956436	-0.116829	1.336416
H	5.136344	-0.370897	0.152797
C	0.504360	0.369914	0.085842
C	-0.499359	0.507430	-0.725880
C	-1.869898	0.601602	-1.113913
C	-2.587190	1.799494	-0.935880
C	-2.513270	-0.509435	-1.697204
C	-3.921817	1.873451	-1.325916
H	-2.090846	2.643590	-0.472615
C	-3.842386	-0.423665	-2.089469
H	-1.950117	-1.426665	-1.842870
C	-4.547686	0.769876	-1.903167
H	-4.475061	2.795670	-1.174186
H	-4.333482	-1.282728	-2.537691
H	-5.588359	0.835568	-2.209040
C	0.510466	1.657414	-3.396639
C	-0.846987	1.745037	-4.026658
H	-1.341134	2.678349	-3.731390
H	-0.740537	1.776539	-5.117158
H	-1.483389	0.907057	-3.749021
C	1.532604	2.623834	-3.932619
H	1.938406	2.269542	-4.887926
H	1.044501	3.582558	-4.136657
H	2.361847	2.777439	-3.240366

tsi3-4

E_{PCM}: -1039.496228

Ir	-0.364978	0.461381	-1.598333
C	0.496806	-1.510496	-1.873665
C	-0.754582	-1.445112	-2.579583

C	-0.580454	-0.485071	-3.652353
C	0.711929	0.054938	-3.574576
C	1.387069	-0.548001	-2.440673
H	2.398858	-0.350809	-2.117921
H	0.718533	-2.144591	-1.025613
H	-1.624149	-2.065311	-2.413665
H	1.104075	0.859291	-4.181448
H	-1.362065	-0.161814	-4.326803
Cl	-2.472230	1.591854	-1.831837
Cl	0.619177	2.626931	-1.258494
N	-0.355267	0.299946	2.651860
C	-1.659436	-0.204162	2.388568
C	-2.621623	-0.673512	3.264516
C	-1.856315	-0.199098	0.993731
C	-3.825447	-1.137371	2.712419
H	-2.453596	-0.722338	4.334196
C	-3.065670	-0.651918	0.464617
C	-4.048994	-1.124370	1.336516
H	-4.591421	-1.526245	3.377690
H	-3.225903	-0.605568	-0.606419
H	-4.993083	-1.485743	0.940640
C	-0.635767	0.257720	0.328140
C	0.327160	0.485682	1.377123
C	1.730685	-0.049946	1.309371
C	2.722479	0.581451	0.547272
C	2.062644	-1.205984	2.029581
C	4.011837	0.052677	0.496132
H	2.463645	1.481385	-0.005565
C	3.354461	-1.727818	1.979049
H	1.303504	-1.695580	2.633665
C	4.333651	-1.102348	1.208817
H	4.771480	0.556222	-0.096501
H	3.593544	-2.625623	2.542920
H	5.341168	-1.507327	1.170752
C	-0.100390	1.330623	3.515703
C	0.924662	2.195462	3.093565
H	0.976968	3.161089	3.592470
H	1.909891	1.802175	2.837201
H	0.582135	1.862198	1.727763
C	-0.992561	1.620240	4.676364
H	-0.725960	2.587093	5.104943
H	-2.051889	1.631312	4.401814
H	-0.860995	0.865235	5.461053

tsi4-5

E_{PCM}: -1039.532160

Ir	-0.327392	-0.099717	-1.810320
C	0.438865	-2.086113	-1.547882
C	-0.635949	-2.116806	-2.500756

C	-0.203571	-1.347522	-3.652117
C	1.077348	-0.826738	-3.386756
C	1.489156	-1.259259	-2.065329
H	2.431546	-1.040391	-1.583014
H	0.440186	-2.581003	-0.585988
H	-1.563449	-2.664671	-2.411375
H	1.624987	-0.141500	-4.019601
H	-0.811280	-1.125434	-4.518679
Cl	-2.384881	0.914560	-2.550276
Cl	0.548339	2.156589	-1.712736
N	-0.535501	0.562968	2.431953
C	-1.894376	0.385485	2.222153
C	-2.939681	0.443941	3.149325
C	-2.111650	0.169638	0.844891
C	-4.218780	0.204607	2.668781
H	-2.761078	0.670795	4.195229
C	-3.416315	-0.070521	0.388695
C	-4.454147	-0.064456	1.308347
H	-5.056630	0.228887	3.360235
H	-3.587537	-0.225684	-0.670212
H	-5.469743	-0.248737	0.970990
C	-0.823854	0.203158	0.151385
C	0.124183	0.460178	1.217911
C	1.604586	0.308996	1.203024
C	2.484462	1.352455	0.905636
C	2.119331	-0.948879	1.548000
C	3.860423	1.133103	0.937465
H	2.092572	2.321932	0.621328
C	3.495358	-1.161881	1.585296
H	1.436519	-1.760954	1.785179
C	4.369025	-0.119432	1.276571
H	4.535793	1.948158	0.694136
H	3.883029	-2.140961	1.852500
H	5.442658	-0.283653	1.301436
C	0.058283	0.925501	3.688432
C	0.493062	2.171642	3.872778
H	0.971523	2.457902	4.803560
H	0.391573	2.928466	3.102261
H	-0.301183	1.401474	0.320822
C	0.155859	-0.185971	4.690596
H	0.511386	0.187593	5.653112
H	-0.812322	-0.674803	4.841585
H	0.852857	-0.954194	4.336438

i4ass

E_{PCM}: -1232.668033

Ir	1.470114	-0.529231	-0.494024
C	2.260544	-0.168225	-2.470775
C	3.185912	-1.088464	-1.830782

C	2.472443	-2.249931	-1.481442
C	1.089290	-2.096861	-1.893415
C	0.989251	-0.818870	-2.551820
H	0.092557	-0.397138	-2.986245
H	2.504620	0.807796	-2.866885
H	4.218548	-0.877408	-1.588928
H	0.305990	-2.834372	-1.790975
H	2.857120	-3.078095	-0.901416
Cl	2.670895	1.255294	0.715466
Cl	1.456157	-1.707755	1.615645
N	-2.617110	0.846865	-0.255647
C	-2.016389	2.006344	-0.709119
C	-2.585703	3.234811	-1.062195
C	-0.616951	1.784146	-0.723767
C	-1.732591	4.231471	-1.518035
H	-3.653654	3.411139	-0.978819
C	0.217998	2.810664	-1.200947
C	-0.344789	4.016335	-1.601470
H	-2.145964	5.191827	-1.813873
H	1.292401	2.655322	-1.222071
H	0.296072	4.811165	-1.973886
C	-0.347276	0.444266	-0.211165
C	-1.617160	-0.092799	0.033896
C	-2.028293	-1.480150	0.351718
C	-1.794739	-2.070542	1.598028
C	-2.688104	-2.230412	-0.634655
C	-2.211552	-3.376413	1.850129
H	-1.268105	-1.513690	2.363608
C	-3.102722	-3.535422	-0.382694
H	-2.863263	-1.786862	-1.611708
C	-2.866786	-4.112111	0.865270
H	-2.013470	-3.821098	2.821396
H	-3.607885	-4.101828	-1.160758
H	-3.189106	-5.130246	1.066308
C	-4.019096	0.711131	-0.011690
C	-4.470034	0.540801	1.232333
H	-0.202778	0.864683	1.515981
H	-5.527742	0.390480	1.422095
H	-3.796250	0.515537	2.081563
C	-4.895210	0.724108	-1.232179
H	-4.675494	1.576567	-1.881664
H	-4.725561	-0.180982	-1.826733
H	-5.950809	0.760066	-0.953683
C	0.898847	1.841727	2.826814
O	0.112753	0.901223	2.503118
C	1.724566	1.584550	4.034314
H	1.970578	2.503944	4.568547
H	1.232939	0.857925	4.683737
H	2.652597	1.124070	3.673161

C	0.816809	3.204012	2.244632
H	0.157051	3.771369	2.921360
H	1.794475	3.686710	2.248810
H	0.394632	3.212937	1.240725

Tsi3-4ass

E_{PCM}: -1232.663252

Ir	-1.744585	-0.088669	-0.063435
C	-2.929959	-0.262401	-1.843905
C	-3.878419	-0.246225	-0.745007
C	-3.750696	0.966297	-0.047404
C	-2.700365	1.741135	-0.685800
C	-2.243711	1.004029	-1.824760
H	-1.482744	1.326943	-2.522629
H	-2.831542	-1.037275	-2.591206
H	-4.504168	-1.079778	-0.454298
H	-2.362162	2.724580	-0.391517
H	-4.267147	1.236272	0.863295
Cl	-1.750623	-2.330832	0.889650
Cl	-1.093305	0.581619	2.200559
N	2.499551	-0.061035	-0.890525
C	2.157273	-1.329288	-1.440277
C	2.924383	-2.255425	-2.142748
C	0.776135	-1.513507	-1.221894
C	2.289809	-3.406155	-2.615056
H	3.966534	-2.086718	-2.381057
C	0.164853	-2.675326	-1.704804
C	0.926859	-3.616193	-2.392970
H	2.866146	-4.130754	-3.183444
H	-0.891306	-2.834394	-1.522322
H	0.452450	-4.516409	-2.773869
C	0.209811	-0.310992	-0.594053
C	1.246770	0.593721	-0.548239
C	1.245593	2.070552	-0.566168
C	0.478088	2.862501	0.302684
C	2.017153	2.723397	-1.547939
C	0.478546	4.251645	0.182330
H	-0.100270	2.376966	1.082320
C	2.014807	4.109962	-1.661651
H	2.612326	2.129587	-2.236147
C	1.241939	4.885068	-0.797192
H	-0.118010	4.842550	0.873359
H	2.614932	4.585507	-2.433241
H	1.239812	5.968253	-0.883408
C	3.629362	0.162530	-0.145205
C	3.664107	1.037478	0.930258
H	3.008459	0.242614	2.100962
H	4.646735	1.283032	1.325293
H	2.912980	1.813560	1.035969

C	4.863099	-0.637845	-0.452197
H	5.193392	-0.459063	-1.480391
H	5.669268	-0.345093	0.221001
H	4.690673	-1.712922	-0.344157
C	1.757032	-0.973031	3.204956
O	2.528893	0.015708	3.093712
C	0.998441	-1.094249	4.473492
H	-0.037915	-0.821840	4.221783
H	0.988553	-2.126563	4.832202
H	1.380025	-0.410308	5.231516
C	1.565143	-1.979449	2.146651
H	1.683988	-2.982319	2.569680
H	0.513823	-1.925590	1.800584
H	2.230678	-1.844496	1.296063

Tsi4-5ass

E_{PCM}: -1232.667708

Ir	1.454944	-0.482228	-0.555008
C	2.083013	0.005496	-2.559259
C	3.050966	-0.943955	-2.038541
C	2.364402	-2.131900	-1.711499
C	0.958166	-1.964768	-2.020178
C	0.809825	-0.647089	-2.583103
H	-0.116696	-0.202994	-2.922553
H	2.295472	1.006300	-2.908898
H	4.097052	-0.741327	-1.854245
H	0.184936	-2.711579	-1.907998
H	2.792255	-2.991405	-1.212897
Cl	2.765422	1.216411	0.641004
Cl	1.582042	-1.789427	1.474959
N	-2.625872	0.825639	-0.226547
C	-2.041094	2.024312	-0.613136
C	-2.638117	3.241891	-0.952306
C	-0.639756	1.846371	-0.569591
C	-1.798545	4.282460	-1.330450
H	-3.714175	3.379503	-0.914218
C	0.182120	2.913538	-0.968618
C	-0.402996	4.114765	-1.353090
H	-2.229831	5.239038	-1.612287
H	1.260687	2.787910	-0.949319
H	0.227616	4.942505	-1.666614
C	-0.347551	0.496880	-0.079980
C	-1.621456	-0.088319	0.072401
C	-1.993921	-1.484713	0.383180
C	-1.665410	-2.090146	1.601131
C	-2.699323	-2.232666	-0.573363
C	-2.039213	-3.408529	1.855018
H	-1.104225	-1.534622	2.342120
C	-3.066688	-3.550787	-0.319675

H	-2.942777	-1.780187	-1.531097
C	-2.739578	-4.142327	0.900695
H	-1.768968	-3.864754	2.803088
H	-3.606257	-4.115936	-1.075082
H	-3.025903	-5.170837	1.103009
C	-4.036293	0.656076	-0.041514
C	-4.529639	0.469564	1.183279
H	-0.107892	0.730122	1.436686
H	-5.591710	0.305369	1.332816
H	-3.886935	0.447522	2.056354
C	-4.863121	0.675091	-1.295480
H	-4.636077	1.545248	-1.918573
H	-4.654870	-0.213259	-1.902781
H	-5.928961	0.685308	-1.057158
C	0.903451	1.630986	2.990635
O	0.163294	0.732884	2.525189
C	1.713295	1.267936	4.182589
H	1.910283	2.124424	4.830323
H	1.254738	0.441577	4.727334
H	2.668896	0.905947	3.778084
C	0.903648	3.032618	2.497528
H	0.296964	3.605203	3.216346
H	1.913557	3.445906	2.513718
H	0.472884	3.128618	1.502395

i1+

E_{PCM}: -1217.457232

Ir	1.171928	-0.338263	-0.556309
C	1.185699	1.170836	-2.135109
C	2.353016	0.370214	-2.244803
C	1.948911	-1.003494	-2.461509
C	0.521682	-1.025660	-2.483358
C	0.033557	0.301596	-2.243659
H	-1.005692	0.595249	-2.189483
H	1.162553	2.237045	-1.957982
H	3.371619	0.728484	-2.165417
H	-0.092647	-1.913250	-2.562380
H	2.599893	-1.852597	-2.612240
Cl	0.142732	-2.278713	0.379061
N	0.396755	0.901611	1.032597
C	-0.005859	2.195970	0.537038
C	0.936624	3.224631	0.512274
C	-1.321609	2.414469	0.077581
C	0.592762	4.484168	0.027131
H	1.940692	3.026885	0.878103
C	-1.645353	3.697548	-0.413030
C	-0.703297	4.716831	-0.439375
H	1.331183	5.280042	0.018569
H	-2.656416	3.873589	-0.765937

H	-0.979667	5.695790	-0.818420
C	-2.302453	1.388114	0.103956
C	-3.175394	0.537245	0.102904
C	-4.204834	-0.444425	0.097023
C	-3.910223	-1.790796	0.384492
C	-5.530119	-0.072665	-0.198821
C	-4.926381	-2.739352	0.375083
H	-2.886514	-2.076627	0.605873
C	-6.536541	-1.030722	-0.204228
H	-5.756426	0.965969	-0.419126
C	-6.238221	-2.363635	0.082447
H	-4.694534	-3.777034	0.596883
H	-7.557144	-0.737682	-0.431575
H	-7.028132	-3.108974	0.077715
C	0.236580	0.704808	2.307238
C	-0.418861	1.742820	3.181018
H	-1.485556	1.798870	2.935353
H	-0.324306	1.470379	4.232994
H	0.000180	2.739654	3.027621
C	0.662636	-0.525605	3.029856
H	-0.206873	-0.945114	3.548722
H	1.085289	-1.290856	2.390601
H	1.374460	-0.228248	3.809700
C	3.662226	-1.454218	0.997418
O	2.814967	-0.560506	0.838352
C	3.681930	-2.722030	0.209455
H	4.082236	-3.544451	0.807766
H	2.685697	-2.970223	-0.159420
H	4.367672	-2.586845	-0.637844
C	4.725333	-1.240451	2.027336
H	4.558087	-1.939641	2.856299
H	5.710480	-1.482020	1.614346
H	4.711108	-0.218431	2.405912

i2+

E_{PCM}: -1217.444642

Ir	-1.102136	-0.348695	-0.613731
C	0.231978	-1.191124	-2.088909
C	-0.522892	-2.260855	-1.502897
C	-1.911271	-2.066385	-1.846291
C	-2.012708	-0.857949	-2.572423
C	-0.692187	-0.281676	-2.706236
H	-0.443686	0.622791	-3.243683
H	1.306952	-1.041038	-1.999613
H	-0.113004	-3.091185	-0.943399
H	-2.932297	-0.390506	-2.900055
H	-2.733284	-2.712362	-1.568210
Cl	-2.708785	1.399869	-0.428822
N	3.177383	-0.581787	-0.870369

C	2.912892	-1.361118	0.257597
C	3.769478	-2.399524	0.650473
C	1.680780	-1.199895	0.946559
C	3.430544	-3.245032	1.701223
H	4.698929	-2.542311	0.107737
C	1.359392	-2.062920	2.011294
C	2.225054	-3.078887	2.388761
H	4.113984	-4.039151	1.987633
H	0.421764	-1.908265	2.534400
H	1.969461	-3.735875	3.213884
C	0.794017	-0.135961	0.584032
C	0.291484	1.000546	0.355675
C	0.325536	2.426600	0.602121
C	0.797667	2.877602	1.847186
C	-0.035847	3.359642	-0.379715
C	0.909898	4.240733	2.096873
H	1.072950	2.154342	2.608959
C	0.088895	4.721049	-0.124631
H	-0.421709	3.012595	-1.331566
C	0.557931	5.164298	1.112051
H	1.272780	4.582808	3.061601
H	-0.189757	5.438794	-0.890289
H	0.645418	6.228547	1.309866
C	4.162431	0.235291	-0.954877
C	4.381805	0.952029	-2.254612
H	4.254393	2.032133	-2.117227
H	5.408463	0.800760	-2.606469
H	3.685887	0.601593	-3.017732
C	5.124470	0.566642	0.153519
H	6.131071	0.220265	-0.108185
H	5.192285	1.653671	0.268415
H	4.840341	0.122806	1.108411
C	-2.886938	-1.014722	1.893347
O	-1.765813	-0.791066	1.411190
C	-3.010812	-1.038786	3.384720
H	-3.663827	-1.849888	3.718762
H	-2.032885	-1.106765	3.861301
H	-3.484871	-0.098278	3.694567
C	-4.117575	-1.265336	1.089161
H	-4.929513	-0.622924	1.444665
H	-3.957592	-1.084849	0.029036
H	-4.437776	-2.300514	1.263496

i3+

E_{PCM}: -1217.474772

Ir	1.310261	-0.431210	-0.278613
C	0.932566	-1.138727	-2.260691
C	2.172071	-0.429028	-2.280943
C	3.113309	-1.175597	-1.463181

C	2.446622	-2.277859	-0.909038
C	1.062523	-2.246432	-1.351151
H	0.303693	-2.981764	-1.123432
H	0.034198	-0.860117	-2.794389
H	2.397635	0.445886	-2.875261
H	2.855558	-2.982893	-0.197426
H	4.144631	-0.899308	-1.286697
Cl	1.056030	-1.131838	1.993980
N	-2.701917	1.095001	0.098347
C	-2.017816	2.303738	-0.293307
C	-2.535749	3.539407	-0.663032
C	-0.662074	1.984337	-0.451364
C	-1.640543	4.506187	-1.131877
H	-3.591751	3.770116	-0.645608
C	0.210731	2.954340	-0.937519
C	-0.283334	4.220304	-1.258938
H	-2.021715	5.480592	-1.419962
H	1.256798	2.715261	-1.081552
H	0.391639	4.980700	-1.640282
C	-0.469745	0.547216	-0.193637
C	-1.709614	0.014438	0.020411
C	-2.095172	-1.412254	0.126125
C	-2.024923	-2.115701	1.334885
C	-2.521710	-2.086868	-1.029835
C	-2.384580	-3.461941	1.386764
H	-1.665905	-1.610820	2.224445
C	-2.884520	-3.431995	-0.974988
H	-2.578652	-1.548564	-1.973245
C	-2.818126	-4.120953	0.236973
H	-2.319390	-3.998071	2.329041
H	-3.217482	-3.940355	-1.875393
H	-3.100322	-5.168770	0.282824
C	-3.924511	1.042096	0.587550
C	-4.672754	-0.229235	0.809597
H	-4.373184	-0.689748	1.759222
H	-5.737921	0.002544	0.878689
H	-4.506785	-0.969575	0.029336
C	-4.650306	2.273226	1.021755
H	-5.331600	2.626746	0.236575
H	-5.281589	2.005614	1.873869
H	-3.986888	3.087471	1.310838
C	3.027094	1.508829	1.481881
O	2.085229	1.349250	0.692807
C	3.201303	2.861447	2.102231
H	4.145988	3.302940	1.763696
H	2.372278	3.519229	1.842311
H	3.275425	2.762049	3.190647
C	4.000157	0.441096	1.855275
H	5.010643	0.853721	1.930425

H	3.721925	0.057289	2.843679
H	3.966365	-0.395171	1.158677

tsi2-3+

E_{PCM}: -1217.440671

Ir	1.478327	-0.337857	-0.339944
C	1.497484	-0.096718	-2.487476
C	2.696475	0.460927	-1.963413
C	3.442430	-0.600869	-1.315103
C	2.685549	-1.795164	-1.436200
C	1.456882	-1.495198	-2.127452
H	0.683557	-2.205114	-2.385454
H	0.725181	0.446295	-3.016229
H	3.007845	1.492942	-2.056408
H	2.938174	-2.753784	-1.001460
H	4.411055	-0.503668	-0.844228
Cl	1.170889	-1.809288	1.502742
N	-3.116030	1.157408	-0.333488
C	-2.220751	2.213758	-0.462185
C	-2.611961	3.526134	-0.761104
C	-0.839528	1.894641	-0.431769
C	-1.659177	4.516895	-0.977554
H	-3.668585	3.757880	-0.849190
C	0.102250	2.908458	-0.635443
C	-0.299971	4.213216	-0.903559
H	-1.980830	5.528228	-1.208102
H	1.156093	2.661878	-0.584070
H	0.442957	4.987366	-1.069199
C	-0.495149	0.487992	-0.241155
C	-1.269122	-0.528523	-0.172042
C	-1.934271	-1.756119	0.003129
C	-2.119704	-2.290477	1.297930
C	-2.442417	-2.452487	-1.118345
C	-2.786764	-3.497995	1.457733
H	-1.723853	-1.752569	2.151221
C	-3.110754	-3.654226	-0.944776
H	-2.318303	-2.023530	-2.107886
C	-3.279612	-4.177379	0.342273
H	-2.922501	-3.913527	2.451365
H	-3.504268	-4.187596	-1.804538
H	-3.802424	-5.120450	0.473934
C	-4.163751	1.165345	0.410084
C	-5.083525	-0.017825	0.348759
H	-5.156066	-0.501422	1.329782
H	-6.096742	0.312253	0.089949
H	-4.744084	-0.742843	-0.390491
C	-4.561804	2.257296	1.367375
H	-5.429296	2.804944	0.980024
H	-4.877650	1.812042	2.316620

H	-3.757690	2.970780	1.552460
C	2.617831	1.154649	2.162485
O	1.808569	1.109350	1.223835
C	2.441744	2.243114	3.175297
H	3.394370	2.736622	3.390671
H	1.699644	2.968016	2.840933
H	2.101665	1.788975	4.114378
C	3.753239	0.203752	2.340714
H	4.694268	0.765408	2.292614
H	3.704428	-0.242045	3.339598
H	3.736677	-0.590044	1.597298

o1

E_{PCM}: -521.246743

Ir	-0.062627	-0.465085	-0.185325
C	0.211928	1.372521	-1.287574
C	1.246873	0.446722	-1.603879
C	0.642091	-0.754493	-2.138663
C	-0.785277	-0.521310	-2.194470
C	-1.055208	0.769118	-1.656010
H	-2.034186	1.208932	-1.521323
H	0.346818	2.342847	-0.828972
H	2.299113	0.576237	-1.387842
H	-1.527655	-1.246525	-2.500530
H	1.161919	-1.641120	-2.473491
Cl	1.762919	-1.049062	1.236686
O	-1.011576	0.468216	1.552450
C	-1.190780	0.211546	2.748810
Cl	-1.229546	-2.473969	0.372589
C	-1.940289	1.224379	3.568358
H	-2.915998	0.805086	3.842348
H	-1.408405	1.425195	4.504294
H	-2.087957	2.148756	3.009146
C	-0.710093	-1.018117	3.442797
H	0.276940	-0.796583	3.866602
H	-1.382059	-1.276449	4.266219
H	-0.595040	-1.847713	2.745698

o2

E_{PCM}: -1115.974558

Ir	2.262402	-0.024712	0.140702
C	4.099822	0.443250	1.137183
C	3.534143	-0.758485	1.686381
C	3.419515	-1.738518	0.648046
C	3.939430	-1.144462	-0.571170
C	4.344823	0.186935	-0.266947
H	4.711752	0.911140	-0.982125
H	4.313790	1.358884	1.670137
H	3.166733	-0.874767	2.697823

H	3.962105	-1.611398	-1.546107
H	3.008995	-2.733626	0.749029
Cl	0.630211	-1.155393	-1.272795
H	-0.181203	1.630954	-0.445281
N	-0.959768	1.219272	0.115963
H	-1.019807	0.244445	-0.218877
C	-2.188843	1.942848	-0.084989
C	-3.410312	1.241293	-0.184083
C	-2.155373	3.330381	-0.195894
C	-4.591405	1.986929	-0.354824
C	-3.337047	4.046659	-0.368201
C	-4.556311	3.372751	-0.437960
H	-5.532426	1.452206	-0.431705
H	-3.301110	5.128204	-0.455430
H	-5.480085	3.927454	-0.572332
C	-0.290792	1.064647	1.607178
O	0.667461	0.142373	1.475490
C	-1.394067	0.540993	2.522508
H	-2.242024	1.229352	2.583225
H	-1.740045	-0.436574	2.181945
H	-0.969520	0.426004	3.523227
C	0.181101	2.455775	2.027241
H	-0.645598	3.166180	2.118863
H	0.642397	2.349665	3.013321
H	0.930854	2.843454	1.334866
Cl	1.748576	2.054725	-1.050301
H	-1.200229	3.845212	-0.161302
C	-3.447740	-0.177409	-0.148066
C	-3.467441	-1.395146	-0.142905
C	-3.487490	-2.817653	-0.132836
C	-4.702591	-3.509990	0.023267
C	-4.717070	-4.899724	0.031020
C	-3.527766	-5.614755	-0.116808
C	-2.320222	-4.933372	-0.273368
C	-2.290287	-3.543084	-0.282229
H	-5.624314	-2.947528	0.136835
H	-5.659084	-5.427217	0.151884
H	-3.543085	-6.701128	-0.111963
H	-1.393539	-5.487637	-0.393232
H	-1.354588	-3.006507	-0.412903

o3

E_{PCM}: -1115.974449

Ir	0.423399	0.235636	1.585943
C	-0.687432	-0.860704	3.045151
C	0.368994	-1.687160	2.565667
C	1.624728	-1.022355	2.860818
C	1.326676	0.205002	3.518113
C	-0.112497	0.338838	3.611410

H	-0.653487	1.161973	4.056816
H	-1.745601	-1.049790	2.921201
H	0.252465	-2.638293	2.065087
H	2.047432	0.956990	3.811111
H	2.611464	-1.380845	2.600225
Cl	1.386795	2.346265	1.012943
H	-0.543809	0.444892	-1.845725
N	0.325505	0.197119	-2.316678
H	1.743433	0.657126	-0.584714
C	0.175700	0.119757	-3.725657
C	1.158404	0.682524	-4.578319
C	-0.969828	-0.444001	-4.297116
C	0.983957	0.597975	-5.972497
C	-1.141898	-0.493549	-5.678554
C	-0.152061	0.014723	-6.518991
H	1.746315	1.025861	-6.616099
H	-2.042565	-0.935373	-6.095455
H	-0.272513	-0.027814	-7.597589
C	0.976288	-0.869931	-1.577849
O	1.451883	-0.244139	-0.335929
C	2.209245	-1.410715	-2.291270
H	1.927891	-1.920763	-3.216389
H	2.904848	-0.605927	-2.536555
H	2.709872	-2.128475	-1.637048
C	0.041743	-2.008201	-1.180265
H	-0.294943	-2.518348	-2.087818
H	0.562866	-2.740989	-0.556102
H	-0.831365	-1.627743	-0.645294
Cl	-1.543121	0.821969	0.357785
H	-1.735585	-0.845156	-3.637986
C	2.285838	1.376402	-4.057966
C	3.249111	2.010282	-3.666257
C	4.365716	2.751578	-3.187791
C	4.367666	3.275093	-1.880614
C	5.463341	3.996772	-1.419544
C	6.568067	4.208904	-2.245173
C	6.573315	3.694998	-3.542429
C	5.483374	2.972595	-4.014317
H	3.504864	3.115934	-1.240773
H	5.451614	4.397843	-0.409807
H	7.420795	4.774637	-1.880127
H	7.430399	3.858969	-4.189911
H	5.482754	2.571373	-5.023261

o4

E_{PCM}: -1115.985509

Ir	-0.173100	0.147198	-1.055149
C	0.733104	-1.007623	-2.642768
C	0.475831	-1.861756	-1.529114

C	-0.941652	-1.859422	-1.259941
C	-1.552549	-0.989326	-2.229271
C	-0.534235	-0.452462	-3.073482
H	-0.678353	0.265268	-3.869083
H	1.698378	-0.792224	-3.079953
H	1.226722	-2.372739	-0.941472
H	-2.598120	-0.711818	-2.253001
H	-1.460901	-2.422987	-0.498080
Cl	-1.972185	1.386604	-0.084569
H	0.967387	1.489381	0.819509
N	0.840917	0.472153	0.901282
H	1.835840	-1.789510	1.970969
C	-0.001499	0.240676	2.056913
C	-0.507429	-1.031716	2.315463
C	-0.279612	1.299012	2.951005
C	-1.260325	-1.278974	3.461263
H	-0.340560	-1.820028	1.590452
C	-1.048975	1.032331	4.097478
C	-1.527798	-0.244961	4.357074
H	-1.649984	-2.276414	3.643080
H	-1.267129	1.851967	4.774407
H	-2.121120	-0.429780	5.247485
C	2.253023	-0.113308	1.101719
O	2.177149	-1.516023	1.109643
C	2.846415	0.393382	2.419290
H	2.871394	1.485629	2.451044
H	2.273518	0.044617	3.283514
H	3.868576	0.016639	2.507751
C	3.145854	0.280692	-0.061261
H	3.228717	1.365005	-0.149431
H	4.136745	-0.146730	0.112151
H	2.752866	-0.100700	-1.002697
Cl	0.863943	2.264528	-1.574022
C	0.193607	2.612944	2.690643
C	0.577455	3.741320	2.440132
C	0.999122	5.062950	2.120934
C	1.277862	5.992262	3.139502
C	1.679822	7.282853	2.814876
C	1.808543	7.662593	1.478284
C	1.532081	6.745379	0.463634
C	1.128928	5.451228	0.774149
H	1.174061	5.690974	4.177522
H	1.891932	7.995666	3.606923
H	2.121203	8.672705	1.228329
H	1.626590	7.039709	-0.577898
H	0.903596	4.732530	-0.008403

tso1-2

E_{PCM}: -1115.974663

Ir	0.037443	0.126067	1.622674
C	0.180292	-1.500310	3.020084
C	1.315399	-0.615133	3.171915
C	0.833412	0.682083	3.521848
C	-0.612948	0.628676	3.585342
C	-0.996084	-0.720305	3.278271
H	-2.015008	-1.070994	3.177017
H	0.210175	-2.550324	2.765790
H	2.350712	-0.875346	2.994913
H	-1.277223	1.449812	3.814280
H	1.438393	1.569231	3.652371
Cl	0.326488	2.331081	0.675651
H	-0.655404	0.286323	-1.504248
N	0.231500	0.367160	-2.025231
H	0.691356	1.216249	-1.685607
C	0.069443	0.342453	-3.430975
C	0.924901	1.111513	-4.256875
C	-0.913549	-0.465359	-4.006284
C	0.774740	1.020230	-5.652074
C	-1.045470	-0.537058	-5.389912
C	-0.195315	0.200686	-6.214793
H	1.429266	1.614117	-6.282015
H	-1.817924	-1.166091	-5.822330
H	-0.296644	0.146173	-7.294449
C	1.258592	-0.945699	-1.078865
O	1.391525	-0.401726	0.081907
C	2.541805	-0.965999	-1.885662
H	2.357733	-1.188797	-2.939547
H	3.066257	-0.014151	-1.794990
H	3.182514	-1.755031	-1.476410
C	0.396387	-2.180035	-1.241967
H	0.219114	-2.412726	-2.294995
H	0.952971	-3.017705	-0.805185
H	-0.551639	-2.074913	-0.713633
Cl	-1.930678	-0.127066	0.218340
H	-1.583582	-1.025286	-3.360102
C	1.889525	1.977872	-3.677495
C	2.691899	2.721456	-3.141193
C	3.633240	3.582464	-2.510935
C	3.550683	3.828334	-1.126903
C	4.476112	4.668316	-0.517033
C	5.487872	5.270101	-1.266123
C	5.573547	5.030479	-2.638208
C	4.654860	4.193902	-3.261201
H	2.758724	3.362634	-0.546729
H	4.403267	4.855587	0.550684
H	6.206855	5.925860	-0.782899
H	6.359022	5.498290	-3.225222
H	4.716152	4.004390	-4.328514

o1+

E_{PCM}: -699.155277

Ir	-0.253462	-0.271190	-0.121417
C	0.312288	1.503129	-1.256453
C	1.237147	0.458628	-1.519379
C	0.513760	-0.679648	-2.051111
C	-0.866976	-0.292007	-2.156809
C	-1.006791	1.028217	-1.626435
H	-1.933541	1.578909	-1.533725
H	0.541294	2.471890	-0.832092
H	2.302085	0.492786	-1.328704
H	-1.678604	-0.933751	-2.475492
H	0.936015	-1.625797	-2.361519
O	-1.037579	0.826107	1.584626
C	-1.538074	0.610389	2.701325
Cl	-1.743562	-2.024784	0.371102
C	-2.154205	1.770641	3.420118
H	-3.173024	1.514679	3.731727
H	-1.592595	1.974296	4.339489
H	-2.167202	2.661602	2.792598
C	-1.568763	-0.719815	3.373473
H	-1.372792	-0.603968	4.443962
H	-2.585004	-1.122613	3.278461
H	-0.893411	-1.436929	2.912136
C	2.029904	-0.946263	1.924749
O	1.033693	-1.300717	1.276979
C	2.532671	0.461413	1.944432
H	3.470272	0.511155	1.376473
H	1.806922	1.150176	1.510254
H	2.781331	0.764337	2.966326
C	2.757172	-1.980095	2.722301
H	3.832349	-1.931995	2.518746
H	2.635258	-1.763995	3.790865
H	2.373131	-2.977041	2.506689

o2+

E_{PCM}: -1100.745862

Ir	-1.332776	0.397888	-0.177056
C	-2.188419	-1.583132	0.222049
C	-3.212838	-0.778079	-0.398588
C	-2.794080	-0.389056	-1.692763
C	-1.472837	-0.924249	-1.897915
C	-1.127325	-1.691844	-0.728726
H	-0.201676	-2.234351	-0.588546
H	-2.242278	-2.061775	1.189483
H	-4.115519	-0.435164	0.089853
H	-0.865876	-0.811048	-2.785585
H	-3.333881	0.257874	-2.371133

Cl	-0.943776	2.570596	-1.177733
H	-0.862933	3.062064	0.968211
N	-0.937048	3.027573	2.010249
H	-1.153814	3.974439	2.322227
C	0.296891	2.584174	2.621173
C	0.802260	3.269874	3.720030
C	0.943948	1.452277	2.102083
C	1.976072	2.832836	4.328411
H	0.287791	4.150315	4.097866
C	2.126280	1.028161	2.731339
C	2.635317	1.709424	3.830970
H	2.372813	3.370458	5.183279
H	2.641704	0.156840	2.341368
H	3.552303	1.364725	4.298284
C	0.469637	0.762806	0.921756
C	0.852422	0.274530	-0.187589
C	1.757702	-0.184417	-1.205278
C	2.660425	-1.222412	-0.905397
C	1.775718	0.408866	-2.481654
C	3.570462	-1.650514	-1.866675
H	2.646215	-1.681455	0.079174
C	2.689650	-0.029885	-3.432353
H	1.088383	1.220890	-2.698217
C	3.585025	-1.058306	-3.129497
H	4.268151	-2.447993	-1.629764
H	2.709885	0.437217	-4.412406
H	4.295859	-1.395864	-3.877695
C	-2.288650	2.087423	2.224871
O	-2.550303	1.558775	1.022924
C	-3.384194	3.091860	2.580625
H	-3.186485	3.593110	3.533690
H	-3.500274	3.830432	1.782314
H	-4.330377	2.553980	2.672386
C	-2.016641	1.101155	3.349093
H	-1.670733	1.586556	4.265219
H	-2.964718	0.601883	3.567611
H	-1.292310	0.341828	3.049989

$CpIrCl_2$

E_{PCM}: -328.103569

Ir	-0.845409	0.249305	-1.555822
C	0.635989	1.738756	-1.258380
C	0.401378	1.634372	-2.662060
C	-0.995162	1.893209	-2.874642
C	-1.600742	2.265772	-1.613946
C	-0.599282	2.151333	-0.611882
H	-0.737926	2.301623	0.450367
H	1.572070	1.535623	-0.754690
H	1.113422	1.312843	-3.409328

H	-2.642424	2.508875	-1.455334
H	-1.511108	1.825191	-3.823815
Cl	0.017993	-1.761674	-2.268975
Cl	-2.469845	-0.878629	-0.382754