

Supporting Information:

Realistic Cluster Modeling of Electron Transport and Trapping in Solvated TiO_2 Nanoparticles

Jing Zhang, Thomas F. Hughes, Michael Steigerwald, Louis Brus, and Richard A.

Friesner*

Department of Chemistry, Columbia University, New York, NY 10027

E-mail: rich@chem.columbia.edu

Contents

1	Computational Details of DFT calculations	S2
2	Figures of Bond Length Changes	S5
3	Cartesian Coordinates of Stationary Geometries	S6
3.1	555 neutral cluster in vacuum	S6
3.2	555 reduced cluster in vacuum	S12
3.3	555 I_{Li}^+ cluster in vacuum	S19
3.4	555 $\text{I}_{\text{Li}}^+/\text{e}^-$ cluster in vacuum	S26
3.5	555 O_{Li}^+ cluster in vacuum	S33
3.6	555 $\text{O}_{\text{Li}}^+/\text{e}^-$ cluster in vacuum	S39
3.7	555 neutral cluster in water	S46

*To whom correspondence should be addressed

3.8	555 reduced cluster in water	S53
3.9	555 I_{Li}^+ cluster in water	S59
3.10	555 I_{Li}^+/e^- cluster in water	S66
3.10.1	Ground State GS1	S66
3.10.2	Ground State GS2	S73
3.10.3	Transition State TS1	S80
3.11	555 O_{Li}^+ cluster in water	S86
3.12	555 O_{Li}^+/e^- cluster in water	S93
3.12.1	Ground State GS3	S93
3.12.2	Transition State TS2	S100
3.13	Solvation Corretion	S107
3.13.1	333 cluster	S107
3.13.2	444 cluster	S110
3.13.3	555 cluster	S117
4	Summary of absolute energies	S117

1 Computational Details of DFT calculations

Here we provide the detailed explanation of DFT methodology we use in this work. All calculations were performed using the DFT code Jaguar 7.7¹ with modified OpenMP/MPI hybrid parallel implementation on a 48-core workstation. Complete geometric optimization of species with up to 400 atoms can be done in several weeks. The oxygen, hydrogen and lithium atoms were treated by all-electron 6-31G basis set and the titanium was computed with LACVP basis set which uses effective core potential to represent core electrons and double- ζ basis functions for valence electrons. We employed the B3LYP hybrid functional in all calculations. The hybrid functionals, unlike the local spin density (LSD) approximation and the generalized gradient approximation (GGA), which lead to delocalization problem of unpaired electrons across several Ti sites, mix a

fraction of Hartree-Fock exchange into the exchange-correlation functional to mitigate delocalization. B3LYP hybrid functionals can give semi-quantitatively reasonable band structures, band gap energies and electron localization for TiO₂ nanoparticle, which is the goal of our study. We use restricted open-shell DFT (RODFT) method and do not consider spin-orbit coupling. Because all clusters studied in this work are with either one (doublet spin) or none (singlet spin) excess electron and have no anti-ferromagnetic effects we found that RODFT gives similar, if not completely identical, results as unrestricted DFT for absolute energies and equilibrium geometries; thus ignoring spin-symmetry breaking and using a RODFT reference function is a safe trade-off for additional 20-50% of computational speed. No symmetry is assumed for calculations in our largest clusters (explained later). No geometric constraints are imposed for all ground states, and the atoms are allowed to relax completely. For transition state (TS) searches, the atoms that are 6 Å away from the reaction center are frozen to boost the searching speed. As we will show later, because the geometrical change is located at reaction center, this constraint above has only a submillihartree effect for final results.

The continuum solvent effect was modeled by Poisson-Boltzmann continuum solvation method available in Jaguar 7.7 code. In this type of calculation, the solvated system is treated with a self-consistent reaction field method, using Jaguar's Poisson-Boltzmann solver. The process consists of Jaguar first solving the usual gas phase wave function and, from that, the electrostatic potential, and fitting that potential to a set of atomic charges. These charges are used by the Poisson-Boltzmann solver, which determines the reaction field by numerical solution of Poisson-Boltzmann equation and represents the solvent as a layer of charges at the molecular surface. These solvent point charges are then incorporated into another quantum mechanical wave function calculation. The process is repeated until self-consistency is obtained.

We also comment on the choice of initial guess of wave function. In order to converge the self-consistent total energy of a compact cluster with around 400 atoms, one needs an initial wave function that is at least qualitatively correct. Traditionally, the initial guess generators provided by Jaguar are based on atomic densities,² atomic wavefunctions³ or ligand-field theory.⁴ Although

these methods are proven to be efficient in small molecules, it is very difficult, if not completely impossible, to get converged wavefunctions for large three dimensional clusters starting from those initial guess generators. To overcome this problem, we established a new initial guess generator based on fragment orbital approach (FOA). The procedure was briefly described as follows. Firstly, the whole cluster was fragmented into several slices, each of which contains around 100 atoms. Then, each slice was converged without symmetry by the traditional protocol. Finally, an initial wave function was constructed from the molecular orbitals of all slices. The detailed implementation requires consideration of spin states and rotational symmetry, which will be described elsewhere. This FOA systematically improved the quality of the initial guess, which can then be fairly easily converged with the DIIS method.⁵

Finally, we want to point out that, as the system is compact as well as tremendously large, several cutoff and step size keywords must be carefully chosen. One important is `cut20`, which is the eigenvalue cutoff and decides the number of canonical orbitals kept in an SCF calculation. A tighter cutoff (2×10^{-3}) must be used instead of the default one (5×10^{-3}) in order to prevent resulting incorrect nonphysical MOs. Another important tuning was related to geometrical convergence. By default, a fixed step size algorithm is used for geometrical optimization, however, this method, especially when used with the Poisson-Boltzmann solver, usually resulted in large energetic fluctuation in magnitude of tens of millihartrees and no convergence for our model clusters after even one hundred optimization steps. A workable solution is to use the dynamic step size algorithm based on Culot/Fletcher heuristic⁶ (i.e. `itradj=1`) with carefully chosen minimum step size `tradm=0.07`. Based on our test, for most of our clusters, this approach can converge the geometry within 30-60 steps.

2 Figures of Bond Length Changes

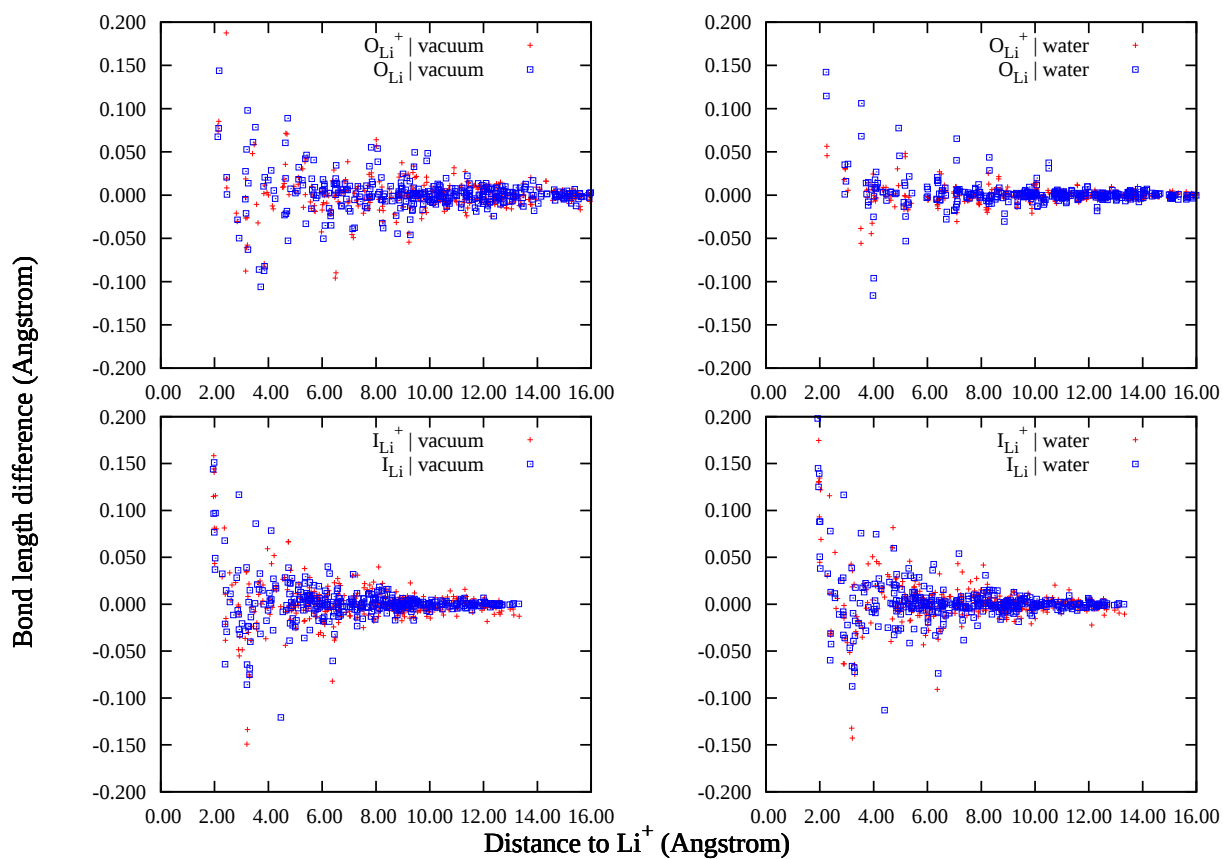


Figure S1: Bond length change of Ti-O bond in different clusters comparing to that in pure neutral TiO₂ cluster, as a function of its distance to Li⁺.

3 Cartesian Coordinates of Stationary Geometries

3.1 555 neutral cluster in vacuum

357			
555 neutral	Vacuum–Optimized	SCFE: −17166.8303471252	hartree
O1	−7.9136710244	−4.1025067080	3.1283707194
H2	−8.2262515095	−4.2257741351	4.0638825726
H3	−7.2437816361	−4.8067707533	2.9127628900
O4	−7.8652912885	−4.2539529654	5.8343932473
H5	−8.5018638301	−4.3717671969	6.5632115018
H6	−7.0592959033	−4.8819560680	5.9233223112
O7	−4.1512748906	−7.8824919763	2.9015440603
H8	−4.2822977144	−8.3586344738	2.0613707916
H9	−4.8550006730	−7.1793990176	3.0235609605
O10	−4.1846464864	−7.8540035159	6.0340082780
H11	−4.3472856050	−8.4136185847	6.8135204310
H12	−4.8829150985	−7.1400447954	5.9344872312
O13	4.1270464750	7.8654363930	3.1277317458
H14	4.2503082219	8.1835446556	4.0608571583
H15	4.8256351807	7.1858370527	2.9238354433
O16	4.2887117436	7.8153481261	5.8340266600
H17	4.4121866760	8.4485104200	6.5649559171
H18	4.9114618411	7.0022401733	5.9208188754
O19	7.8879192831	4.0972144460	2.9181516466
H20	8.3463951867	4.2293145958	2.0681437463
H21	7.1897901569	4.8028358076	3.0559625017
O22	7.8357816759	4.1418773538	6.0345729528
H23	8.4037434251	4.3081938846	6.8067767283
H24	7.1228909066	4.8423763515	5.9287938027
O25	−8.5354342243	0.9260387122	3.0022897907
H26	−9.4180151313	1.2862700074	2.7951578792
H27	−8.3382695831	0.0467393635	2.4756499596
O28	−8.2975579919	0.8917745685	5.8545479703
H29	−8.5354503074	0.6731030062	4.9192201535
H30	−8.2764027294	0.0561648842	6.4291523374
O31	0.9168827870	−8.4849036006	2.9617825766
H32	1.2646678426	−9.3839606370	2.8150382918
H33	0.0068352039	−8.3236210443	2.4835593855
O34	0.8395596079	−8.2965717773	5.8709702847
H35	0.5834969478	−8.4886697059	4.9365065881
H36	0.0218292699	−8.2670846746	6.4663444219
O37	−0.9293237865	8.4736492920	2.9338120657
H38	−1.3160425868	9.3446244365	2.7236272133
H39	−0.0562328777	8.2912198197	2.4079175282
O40	−0.7690861668	8.3410180313	5.7577351248
H41	−0.5300314315	8.5191389167	4.8128162766
H42	0.0523733650	8.3355443290	6.3620192949
O43	8.5078939071	−0.8948509692	2.9944871595
H44	9.4067085586	−1.2436572386	2.8471678931
H45	8.3371548218	0.0019092904	2.4785762886
O46	8.3255213834	−0.7975850189	5.8621922715
H47	8.4890957184	−0.4960756633	4.9338125281

H48	8.2994504482	0.0019045306	6.4943423823
O49	-3.2439513622	-1.2488752823	-1.3266045112
O50	-1.2850713213	-3.2548271327	-1.3289696114
O51	-3.3624291649	3.3950100121	-1.3333007054
O52	-1.4294902956	1.4147165866	-1.5241964289
O53	1.4503423915	-1.4479925536	-1.5131701591
O54	3.3588460355	-3.4471594774	-1.3147329294
O55	-5.6772806986	-5.6288976296	0.1520291731
Ti56	-4.7523210879	-4.7751688275	1.4622233541
O57	-5.5370723172	-1.0322926428	0.1303848568
Ti58	-4.6667614711	-0.0653404573	1.4968320559
O59	-7.8998744581	-1.1990273538	1.7600729658
O60	-5.9931491437	-3.2176196821	1.5237048504
O61	-1.0047572210	-5.5375999017	0.1257945309
Ti62	-0.1150122903	-4.5979824834	1.5197216071
O63	-3.1878899804	-5.9361219157	1.4867454338
O64	-1.3141339968	-7.9475444996	1.8118556349
Ti65	-2.3253827894	-2.2766050838	0.0356557925
O66	-0.8583898288	-0.9063187518	-0.0452028945
O67	-3.7156913972	-3.6838913003	0.0047882493
Ti68	0.0132922808	-0.0066005264	1.5421595869
O69	-3.1863843269	-1.3741069285	1.4770493854
O70	-1.3918427500	-3.1834772113	1.4787069815
Ti71	-2.3770912191	2.4179559696	-0.0870894219
O72	-3.6531946899	0.9407784058	0.0206131317
O73	-3.1868869390	3.2551754718	1.4613487002
O74	-1.4011844038	1.4092646639	1.4707995265
Ti75	2.3987046158	-2.4651151168	-0.0501782812
O76	0.8780562593	-3.6338486064	-0.0014673902
O77	1.4066377952	-1.4333166054	1.4886036597
O78	3.2011838989	-3.2767776102	1.4870753521
O79	0.8649379097	0.8753928618	-0.0340222996
O80	-5.4764997140	-5.4766211101	2.9929628229
Ti81	-6.9106409563	-2.2239696575	2.9919421027
O82	-5.5016737337	-0.8597312916	2.9836759994
Ti83	-2.2584936457	-6.8511005693	3.0585057258
O84	-0.9150186095	-5.4753369864	3.0044631457
Ti85	-2.3760588638	-2.3304482624	3.0445894344
O86	-0.8899074574	-0.8785880777	2.9683603590
O87	-3.6822943756	-3.6672432617	2.9723019934
Ti88	-2.1763321005	2.1676547218	2.9245449099
O89	-3.6511374518	0.9178499034	2.9777857137
Ti90	2.1700980497	-2.2150392633	2.9412985695
O91	0.8934554220	-3.6751874376	2.9813276151
O92	0.8718532923	0.8540026993	2.9702771016
Ti93	-4.5596124869	-4.5119538387	4.4487739094
Ti94	-4.6377580125	0.2368421633	4.4582490817
O95	-7.8532130292	-1.6945704621	4.4536528016
O96	-5.8636032181	-3.1425427589	4.4892281587
Ti97	0.1828819306	-4.6401364767	4.4878433663
O98	-3.2289541879	-5.9274998417	4.4883867085
O99	-1.6326149937	-7.7965931732	4.4953893286
Ti100	-0.0373823560	-0.0471798068	4.5015630820
O101	-3.1857953485	-1.3924719369	4.4813651293

O102	-1.4197004424	-3.1553737766	4.4816028011
O103	-3.1919367136	3.1963858690	4.4588400792
O104	-1.4132307010	1.3863891097	4.4822137311
O105	1.3689601187	-1.4309782672	4.4923097555
O106	3.1761181242	-3.1978290436	4.4871283832
O107	-5.5260896663	-5.4573743308	5.9655464510
Ti108	-4.7774729759	-4.7590582260	7.4863351660
Ti109	-6.8171142068	-2.2053252593	5.9078581723
O110	-5.5167676341	-0.8371409935	5.9573178134
Ti111	-4.6165039776	-0.0592587021	7.4516200798
O112	-7.9788215379	-1.3712581825	7.1465839271
O113	-5.9704318171	-3.1723441652	7.4241304506
Ti114	-2.2731026603	-6.8632488733	5.9404672211
O115	-0.9042209888	-5.4906041952	5.9791075668
Ti116	-0.1099860191	-4.6190456838	7.4547260684
O117	-3.2031563126	-5.9022582105	7.4648325039
O118	-1.4029241582	-7.9415278793	7.2130808091
Ti119	-2.3823779554	-2.3704692163	5.9132023929
O120	-0.8956319787	-0.8791671763	5.9909500338
O121	-3.6852344076	-3.6800707593	5.9903503919
Ti122	0.0043049920	0.0137456058	7.4299020860
O123	-3.2120418415	-1.3689171533	7.4819858648
O124	-1.4098579076	-3.1809044327	7.4940780595
Ti125	-2.1992959651	2.1980258654	6.0352457767
O126	-3.6955792012	0.9318118763	5.9724063248
O127	-3.2561229792	3.2188083068	7.4783812368
O128	-1.4384315092	1.4051583512	7.4810061637
Ti129	2.1752900698	-2.2155258474	6.0517825543
O130	0.8931632529	-3.6869591887	6.0009503873
O131	1.3856174632	-1.4298622179	7.4850567467
O132	3.1943551865	-3.2620876245	7.5030335321
O133	0.8551555920	0.8541659757	5.9928667453
O134	-5.6792758380	-5.6295041289	8.7787672339
O135	-5.5496028677	-0.9888175042	8.8210591272
O136	-1.0338626296	-5.5242526730	8.8489503596
Ti137	-2.3289889984	-2.2936839051	8.9291084272
O138	-0.9024330849	-0.8839109287	9.0202687019
O139	-3.7432518873	-3.6667264835	8.9620927493
O140	-3.2703028175	-1.2480554540	10.2923681811
O141	-1.3097984001	-3.2395776422	10.3000809823
Ti142	-2.4425461386	2.4221827748	9.0165667762
O143	-3.6585925185	0.9117422798	8.9554590573
O144	-3.4357211366	3.3572283602	10.2851731022
O145	-1.4406118516	1.4522643391	10.4657032133
Ti146	2.3891252183	-2.4560385874	9.0303932278
O147	0.8718443536	-3.6397740411	8.9776370391
O148	1.4187095078	-1.4221575134	10.4727144615
O149	3.3265510132	-3.4238812053	10.3214800650
O150	0.8453015660	0.8726281858	8.9854476644
H151	-7.7506283018	-1.2490830380	8.0906986575
H152	-4.2701893355	3.0915001925	10.7132965770
H153	-1.2680781480	-7.6676584760	8.1443932337
H154	3.0433637010	-4.2402597104	10.7777588693
H155	-5.7976826928	-2.4847523752	8.1421455422

H156	-1.6361001271	1.7901279057	11.3599090996
H157	-2.5043280224	-5.7244455902	8.1710408459
H158	1.8325181935	-1.5244867554	11.3494642425
H159	-2.7132865474	-1.0861849382	11.0996544450
H160	-1.1466493339	-2.6807003301	11.1047407084
H161	-6.2125956600	-6.0939260071	9.4332299083
H162	-4.0267351602	-3.9432630301	9.8531934428
H163	-1.2118618737	-5.0244742684	9.6862078832
H164	0.1122773547	-3.4287556742	9.6380312813
H165	-0.9416206850	-0.9352799023	12.7756081912
H166	0.8881804596	0.9432611151	12.7876017009
H167	-3.4543590953	0.1525739907	9.6260049546
H168	-5.0527592575	-1.1771782156	9.6582290275
H169	-7.5567276568	-1.0102663781	0.8583167009
H170	-1.1818192841	-7.6332318385	0.8914423382
H171	-6.5609267072	-5.6634459115	-0.2460646742
H172	-3.9528566922	-4.0112584576	-0.8835723087
H173	-1.1862419645	-5.0421152065	-0.7139530978
H174	0.1116935571	-3.4280007408	-0.6674264570
H175	-0.8811059623	-0.9749503876	-3.7984143567
H176	0.8899247530	0.9592723946	-3.8038729319
H177	-3.4715275427	0.1859469439	-0.6486916001
H178	-5.0470334572	-1.2126586511	-0.7116973296
H179	-5.8040821694	-2.5345948794	0.8067279863
H180	-2.4813245187	-5.7549955825	0.7893257348
H181	-3.0675112046	4.2101187503	-1.7796474813
H182	-1.9080664319	1.3851717571	-2.3721691565
H183	1.9120503600	-1.4790257839	-2.3711167261
H184	3.0659529102	-4.2502952579	-1.7802328389
H185	-2.6888411353	-1.1003618951	-2.1409758157
H186	-1.1283950183	-2.7006232725	-2.1343778157
O187	1.2815959767	3.2190445703	-1.3287206927
O188	3.2494910799	1.2320777789	-1.3108369520
O189	-0.8850056033	3.6235793209	-0.0209674513
Ti190	0.1144467042	4.5883367092	1.5226325638
O191	3.6481689106	-0.9710494955	0.0397746319
Ti192	4.6421655129	0.0538153369	1.5167979544
Ti193	2.3202997859	2.2701605365	0.0462914033
O194	3.7024071343	3.6771239526	0.0112353532
Ti195	4.7905755054	4.7072305379	1.4740763186
O196	1.3859443196	3.1670495092	1.4770893040
O197	3.1758941469	1.3453729363	1.4862449988
O198	1.0191261777	5.5424296142	0.1406929529
O199	1.2352649083	7.8500246097	1.7224278993
O200	3.2355653471	5.9454639164	1.5269904670
O201	5.5098797837	0.9811781134	0.1297752989
O202	5.9429459178	3.1407596431	1.5016193871
O203	7.9531486493	1.2772080758	1.8153837266
O204	5.6530395026	5.6323518470	0.1690976355
O205	-0.8995849539	3.6484801939	2.9845334971
O206	3.6477988436	-0.9395667727	3.0164529587
Ti207	2.3413006040	2.2982782691	3.0722388797
O208	3.6738891244	3.6304403108	2.9864270581
Ti209	2.2363181905	6.8859370235	2.9825277619

O210	0.8805631647	5.4747918092	2.9906899321
Ti211	6.8536187502	2.2077568651	3.0736368177
O212	5.4878345158	0.8458418896	3.0040892141
O213	5.4855743461	5.4264975451	3.0080118890
Ti214	-0.2255061675	4.6096354813	4.4789111444
Ti215	4.6032013021	-0.2552798408	4.4945043854
Ti216	4.5018250103	4.5059935055	4.4513689032
O217	1.3981128135	3.1444030566	4.4816282168
O218	3.1651576920	1.3689417217	4.4903007182
O219	1.7232931458	7.8288603999	4.4447361631
O220	3.1551656328	5.8278809735	4.4986226031
O221	5.9201167376	3.1695488500	4.4984824155
O222	7.7907787309	1.5841801791	4.5097072659
O223	-0.9283892400	3.6489404336	5.9609413106
Ti224	0.0647608066	4.6561425679	7.4750214204
O225	3.6472946520	-0.9443227255	5.9716255896
Ti226	4.6418214453	0.0611533488	7.4769195856
Ti227	2.3542981538	2.3549500505	5.9406885073
O228	3.6760181427	3.6462378517	6.0010103591
Ti229	4.7558219452	4.7353886070	7.4985111743
O230	1.3582427028	3.1711657278	7.4660855363
O231	3.1555191796	1.3591309856	7.4859886791
Ti232	2.2420799028	6.7910423284	5.9038997028
O233	0.8530509292	5.5040988538	5.9674324277
O234	1.4152066364	7.9951854378	7.1151996388
O235	3.1847591176	5.9484082112	7.4318042164
Ti236	6.8415591804	2.2326202004	5.9529921939
O237	5.4904424738	0.8453360338	5.9945365814
O238	5.8986702965	3.1526306104	7.4768178102
O239	7.9548230614	1.3753179738	7.2191761186
O240	5.4660381129	5.4742256089	5.9801680730
O241	-0.9448846784	3.6562026156	8.9312330355
O242	3.6260841883	-0.9554855551	8.9453071609
Ti243	2.2683688047	2.2769742164	8.9141648344
O244	3.6506257739	3.6957439421	8.9561110608
O245	1.2212395261	3.2311937577	10.2787625589
O246	3.2056318709	1.2550749413	10.2871015757
O247	1.0369181684	5.4880300654	8.8419310701
O248	5.4629677204	1.0113911875	8.8706047201
O249	5.6318874703	5.6204764892	8.7971377133
H250	1.2782737639	7.8285562402	8.0685460744
H251	7.7242344636	1.2495553365	8.1618499314
H252	2.5007884133	5.7782213021	8.1557231783
H253	5.7067009268	2.4608286343	8.1871418488
H254	1.0690065171	2.6818473697	11.0896730104
H255	2.6528634068	1.0943482168	11.0957515061
H256	3.4185744491	-0.2082331637	9.6108082460
H257	4.9434091419	1.1840781158	9.7004713387
H258	3.9118942029	3.9745851777	9.8533663185
H259	6.1576181571	6.0480903680	9.4821376551
H260	1.2180109217	4.9734218283	9.6729844590
H261	-0.1930538250	3.4489963561	9.6076771466
H262	3.4554674556	-0.2216641043	-0.6289460546
H263	5.0133189564	1.1530049406	-0.7127033389

H264	3.9963352685	3.9513125860	-0.8779917993
H265	5.6975919388	6.5188971136	-0.2213684135
H266	1.1995536096	5.0572353012	-0.7029738462
H267	-0.1119305053	3.4243989231	-0.6817834581
H268	1.0713495520	7.4622035388	0.8311453202
H269	2.5532840283	5.7619592704	0.8106702766
H270	5.7577248779	2.4419281486	0.7980517505
H271	7.6524395992	1.1290515749	0.8936746446
H272	1.1208024604	2.6581568116	-2.1289204338
H273	2.7090457287	1.0797611014	-2.1321705657
O274	-5.6420057928	3.6125926594	0.1753790393
Ti275	-4.5887257766	4.4598357903	1.5174030338
O276	-7.8994296585	3.2876221997	1.6176117922
O277	-5.9651785086	1.3923289773	1.5835144889
O278	-4.6442003402	6.0149208573	0.4348919908
O279	-3.3022274869	7.8251737013	1.5975310343
O280	-1.3868818334	5.9331426439	1.5441277608
Ti281	-7.0583166523	2.4773446317	2.9873693945
O282	-5.5942813830	3.8507375219	2.9832927697
Ti283	-2.5096747051	6.9620307942	2.9390679336
O284	-3.8380999176	5.5530435177	2.9989024317
Ti285	-4.4474471268	4.4176802217	4.4673335553
O286	-7.8394969926	3.1080970513	4.4774876721
O287	-5.9470292775	1.4673318815	4.4141560309
O288	-3.0599341357	7.8532026320	4.4533236445
O289	-1.4441725804	5.9394314012	4.4535916638
Ti290	-7.0374036382	2.4984262273	6.0310239591
O291	-5.5155086776	3.8115235738	5.9190343451
Ti292	-4.4438633243	4.6949435117	7.3692997826
O293	-7.7767862307	3.4152176606	7.3386857529
O294	-6.0061959538	1.3931908872	7.4310964295
Ti295	-2.3704662706	7.1376332642	5.9557770918
O296	-3.8283178567	5.6251469811	5.9172833794
O297	-3.2022259569	7.9085501552	7.3359115029
O298	-1.3792629476	5.9586782399	7.3596199827
O299	-6.0784553164	5.0106278052	8.2748375179
O300	-3.5828051178	5.6229440052	8.7810238364
H301	-7.3192112654	4.1849642304	7.8296730629
H302	-3.4935086675	7.5747969700	8.2111853645
H303	-6.3346465609	1.6083338439	8.3251977093
H304	-2.0244315373	5.8944671987	8.1241234019
H305	-3.4421094002	5.1380083140	9.6334181514
H306	-6.1415611934	5.6546992649	9.0019652540
H307	-7.5302476383	3.5632486597	0.7488794670
H308	-5.2709214173	6.0827111312	-0.3099959573
H309	-5.1572289121	3.4509455862	-0.6753048711
H310	-5.8965895011	2.0337458564	0.8173314414
H311	-3.9551697161	7.3506407661	0.9844363612
H312	-1.6655293706	6.1901717978	0.6496921991
O313	4.9163522615	-6.0891884137	0.6461585455
Ti314	4.6737819307	-4.4558168518	1.5688919034
O315	1.3304933343	-5.9972100371	1.5626582040
O316	3.3375190566	-7.8064609956	1.6465290372
O317	5.6136790284	-3.6041333208	0.1690141990

O318	5.9517192453	-1.4119606341	1.6201646125
O319	7.8902386211	-3.2727619742	1.6338579424
Ti320	2.4707623999	-6.9927050281	2.9688203230
O321	3.7938148003	-5.5264022997	3.0300746798
Ti322	7.0561053549	-2.4599149435	3.0039394706
O323	5.6254225638	-3.8713541791	3.0307043566
Ti324	4.3596998844	-4.4970008025	4.5019222665
O325	1.4131570038	-5.9236650533	4.4581150371
O326	3.0704557937	-7.7980344970	4.4926830178
O327	5.9687531436	-1.4741427522	4.4710460165
O328	7.9053506040	-3.0546908316	4.4976330931
Ti329	2.4460469332	-7.0457209545	6.0358128555
O330	3.7699506226	-5.5039853517	5.9590019773
Ti331	4.6914665862	-4.4451608945	7.4004661840
O332	1.3315628936	-6.0035944448	7.4475848552
O333	3.3648023777	-7.7769438184	7.3512725498
Ti334	7.1200144408	-2.4050348527	6.0083816112
O335	5.6259015356	-3.8526406229	5.9468050701
O336	5.9424521560	-1.4027765102	7.3851410924
O337	7.8778623309	-3.2360846307	7.3930677728
O338	5.0199716275	-6.0946428042	8.2667062582
O339	5.5761947329	-3.5895894555	8.8327138963
H340	4.1455435107	-7.3336131342	7.8279704617
H341	7.5545701096	-3.5285252882	8.2710556555
H342	1.5656815845	-6.3218887383	8.3398964847
H343	5.8642096253	-2.0301264626	8.1615728677
H344	5.6483825784	-6.1669214231	9.0066940371
H345	5.0772371554	-3.4493286874	9.6782068637
H346	4.0848310180	-7.3632671369	1.1245954084
H347	5.5410628960	-6.1634281308	-0.0989815283
H348	5.1157621289	-3.4598159282	-0.6778661126
H349	1.5376189076	-6.3525377777	0.6777069102
H350	5.8983705006	-2.0238861082	0.8304954658
H351	7.5653407790	-3.5525949725	0.7515871088
Ti352	0.0192282891	-0.0247396548	-1.4484895484
O353	-1.0536676584	-0.9296909023	-2.8417056649
O354	1.0566373894	0.8942715707	-2.8480243716
Ti355	-0.0340916167	-0.0145175808	10.4208775201
O356	-1.0366552520	-0.9757567135	11.8079158217
O357	0.9627484944	0.9587835547	11.8176353427

3.2 555 reduced cluster in vaccum

357			
555 reduced	Vacuum-Optimized	SCFE : -17166.9383199762	hartree
O1	-7.9050907674	-4.1205266292	3.1335850736
H2	-8.2102304271	-4.2360564521	4.0728387121
H3	-7.2146864461	-4.8118128525	2.9317275666
O4	-7.8531334495	-4.2676807894	5.8383075978
H5	-8.4682340711	-4.3793188780	6.5859164355
H6	-7.0337758702	-4.8858031316	5.9200916128
O7	-4.1676862925	-7.8735058279	2.8933513076
H8	-4.2928098140	-8.3088419709	2.0307298833
H9	-4.8563229214	-7.1536547133	3.0204571117

O10	-4.1983293761	-7.8441465834	6.0435852873
H11	-4.3510781322	-8.3664355276	6.8498140179
H12	-4.8824169957	-7.1129224655	5.9476036763
O13	4.1435596218	7.8578332929	3.1304798004
H14	4.2592382452	8.1701629757	4.0669920585
H15	4.8289316699	7.1579831183	2.9401301367
O16	4.3040380041	7.8049512486	5.8360492331
H17	4.4221455779	8.4184733034	6.5841849394
H18	4.9173575038	6.9788170701	5.9174688472
O19	7.8775696977	4.1131179409	2.9094613783
H20	8.2974576547	4.2367706318	2.0383359964
H21	7.1625233466	4.8046876921	3.0490151614
O22	7.8280645182	4.1548750202	6.0452189446
H23	8.3629606045	4.3071752867	6.8440808941
H24	7.0962854845	4.8427056784	5.9507125109
O25	-8.5342945052	0.9192116182	3.0008818450
H26	-9.4130498178	1.2819822562	2.7833065535
H27	-8.3328382121	0.0377693585	2.4731822998
O28	-8.3044559312	0.8924780345	5.8581467184
H29	-8.5268860637	0.6665903874	4.9210704934
H30	-8.2757782226	0.0575837080	6.4347759841
O31	0.9120969810	-8.4832260815	2.9615259762
H32	1.2606634723	-9.3812759997	2.8138925995
H33	0.0040815424	-8.3201459424	2.4773966772
O34	0.8387290690	-8.3045470888	5.8706295217
H35	0.5735012204	-8.4760094620	4.9343449616
H36	0.0240768672	-8.2730519971	6.4706824804
O37	-0.9233959138	8.4706318922	2.9308767145
H38	-1.3091503448	9.3413436432	2.7213846520
H39	-0.0510081230	8.2848126938	2.4013294910
O40	-0.7641574245	8.3462200346	5.7601332651
H41	-0.5168943578	8.5109298850	4.8148354038
H42	0.0563303909	8.3326016085	6.3674599778
O43	8.5036237171	-0.8915670294	2.9939200792
H44	9.3998983224	-1.2428376083	2.8405467823
H45	8.3308819313	0.0059840853	2.4761842694
O46	8.3300420540	-0.7975466781	5.8657460114
H47	8.4817320779	-0.4907630994	4.9367907324
H48	8.2983753539	0.0013594636	6.4993825372
O49	-3.2520427074	-1.2553506667	-1.3366143572
O50	-1.2881889577	-3.2648309967	-1.3360468296
O51	-3.3633564688	3.4013187498	-1.3244239391
O52	-1.4345330882	1.4162904180	-1.5224906289
O53	1.4539130715	-1.4485665680	-1.5082421050
O54	3.3662967144	-3.4410401014	-1.3110621811
O55	-5.6813130944	-5.6271584747	0.1538478288
Ti56	-4.7447988546	-4.7690835355	1.4638615354
O57	-5.5433571083	-1.0387263802	0.1295430995
Ti58	-4.6668056696	-0.0664627202	1.4972063732
O59	-7.9063113697	-1.2029166685	1.7589682913
O60	-5.9938902903	-3.2178751530	1.5216654957
O61	-1.0055605602	-5.5561969970	0.1279470190
Ti62	-0.1141603114	-4.5958166116	1.5211170968
O63	-3.1885239181	-5.9389923920	1.4838082676

O64	-1.3153691846	-7.9521876951	1.8058215606
Ti65	-2.3215030621	-2.2725113113	0.0296712476
O66	-0.8650651177	-0.9110898642	-0.0649294369
O67	-3.7160478699	-3.6846568276	0.0034168426
Ti68	0.0133316474	-0.0067758444	1.5466203674
O69	-3.1892346670	-1.3748783484	1.4702335703
O70	-1.3926773038	-3.1887349603	1.4708289051
Ti71	-2.3733099535	2.4146208548	-0.0750295973
O72	-3.6581031922	0.9389817192	0.0203023484
O73	-3.1942184781	3.2656104637	1.4618966901
O74	-1.4087999006	1.4211938696	1.4659228744
Ti75	2.3961695942	-2.4598638479	-0.0380377774
O76	0.8776990822	-3.6402302399	0.0017276187
O77	1.4124936957	-1.4443451612	1.4855482956
O78	3.2093104640	-3.2868896580	1.4856529655
O79	0.8702925098	0.8804434671	-0.0553378533
O80	-5.4735473710	-5.4728678651	2.9925167876
Ti81	-6.9072507659	-2.2273342454	2.9942655810
O82	-5.5083938695	-0.8659556605	2.9827720422
Ti83	-2.2586433429	-6.8526556304	3.0589439482
O84	-0.9200219421	-5.4853742559	3.0040525899
Ti85	-2.3623524607	-2.3163451392	3.0419743398
O86	-0.8964823398	-0.8845653951	2.9469525300
O87	-3.6772612264	-3.6651410124	2.9715880227
Ti88	-2.1789992156	2.1687807698	2.9272697400
O89	-3.6637461582	0.9106750407	2.9731340669
Ti90	2.1687871183	-2.2138725262	2.9480212954
O91	0.8853220405	-3.6883059557	2.9786025550
O92	0.8793696721	0.8604013412	2.9542071074
Ti93	-4.5456761980	-4.5011558150	4.4488944067
Ti94	-4.6347444476	0.2381449932	4.4572522442
O95	-7.8568652099	-1.7007654276	4.4541204207
O96	-5.8623899530	-3.1419826209	4.4881193050
Ti97	0.1858391433	-4.6410128803	4.4873884525
O98	-3.2283689502	-5.9299768784	4.4881626700
O99	-1.6410381016	-7.8070499856	4.4952353196
Ti100	-0.0397130433	-0.0467289352	4.5012068829
O101	-3.1811652915	-1.3875191299	4.4793071837
O102	-1.4151387101	-3.1521992086	4.4814912656
O103	-3.2025209138	3.2062707610	4.4586283986
O104	-1.4303179313	1.4018999766	4.4800030114
O105	1.3870642775	-1.4410211673	4.4905730282
O106	3.1876169914	-3.2062593685	4.4876524295
O107	-5.5221963130	-5.4564564211	5.9675439068
Ti108	-4.7663763327	-4.7516732992	7.4850809603
Ti109	-6.8124477341	-2.2050639489	5.9064684515
O110	-5.5195421459	-0.8414553458	5.9549904688
Ti111	-4.6112032861	-0.0581583549	7.4488384569
O112	-7.9733159751	-1.3684152490	7.1527839510
O113	-5.9671761333	-3.1730223237	7.4238022425
Ti114	-2.2723146878	-6.8617884781	5.9394654193
O115	-0.9081500446	-5.4986157618	5.9789217989
Ti116	-0.1069879262	-4.6178083370	7.4529709527
O117	-3.2000821930	-5.9044021285	7.4677912497

O118	-1.4009416249	-7.9436685500	7.2172080320
Ti119	-2.3661398383	-2.3578675225	5.9137662403
O120	-0.9032579625	-0.8853582154	6.0138602872
O121	-3.6800088821	-3.6768315316	5.9906449026
Ti122	0.0040140901	0.0131063769	7.4221086697
O123	-3.2117844124	-1.3624701490	7.4877647919
O124	-1.4084260098	-3.1828399415	7.4994888200
Ti125	-2.1952931310	2.1971729302	6.0274976963
O126	-3.7083727381	0.9275307200	5.9736782082
O127	-3.2644572713	3.2307188145	7.4772695749
O128	-1.4514649559	1.4178293672	7.4848028714
Ti129	2.1725624907	-2.2122960962	6.0436921196
O130	0.8862853513	-3.7003705597	6.0031429730
O131	1.3928381684	-1.4425511844	7.4891063599
O132	3.2042670549	-3.2687702515	7.5019352705
O133	0.8611383888	0.8605001215	6.0064041477
O134	-5.6752462187	-5.6248308167	8.7784115678
O135	-5.5630949079	-0.9922504520	8.8164627446
O136	-1.0360610426	-5.5347107330	8.8488919879
Ti137	-2.3200763900	-2.2863262760	8.9339882031
O138	-0.9086242879	-0.8880295340	9.0415304963
O139	-3.7399583982	-3.6644320152	8.9603550649
O140	-3.2801902944	-1.2505094074	10.2992797580
O141	-1.3131531154	-3.2457488858	10.3080681475
Ti142	-2.4394999734	2.4205132340	9.0041423809
O143	-3.6670315298	0.9120150837	8.9568185662
O144	-3.4346559750	3.3662123038	10.2783337457
O145	-1.4441096787	1.4587210236	10.4629992028
Ti146	2.3874430362	-2.4457158908	9.0164312536
O147	0.8729307185	-3.6469827418	8.9737302498
O148	1.4224397374	-1.4240685755	10.4707539978
O149	3.3360882330	-3.4130912005	10.3156000377
O150	0.8505893818	0.8789705288	9.0095069759
H151	-7.6986243727	-1.2317716476	8.0839466671
H152	-4.2715341077	3.0869582506	10.6916281158
H153	-1.2482750074	-7.6299356990	8.1344913366
H154	3.0375442981	-4.2265092884	10.7609162426
H155	-5.7915972471	-2.4803006443	8.1387556531
H156	-1.6360959183	1.8050134223	11.3522523935
H157	-2.4957542963	-5.7232714580	8.1705893294
H158	1.8412693413	-1.5287366846	11.3440394437
H159	-2.7177715863	-1.0850298602	11.1047535868
H160	-1.1354869595	-2.6765006909	11.1038556734
H161	-6.2164289252	-6.0753967256	9.4355161131
H162	-4.0212107536	-3.9375631332	9.8527995491
H163	-1.2143321348	-5.0243547404	9.6803034497
H164	0.1193977497	-3.4348866735	9.6378930560
H165	-0.9337117209	-0.9238940019	12.7848183090
H166	0.8845804092	0.9359627071	12.7954175506
H167	-3.4608230954	0.1556889963	9.6287230308
H168	-5.0565230060	-1.1818301352	9.6480323384
H169	-7.5411196610	-1.0107148373	0.8658589279
H170	-1.1731095354	-7.6052166100	0.8975309639
H171	-6.5785782610	-5.6270702348	-0.2153367935

H172	-3.9496073851	-4.0120906990	-0.8854901612
H173	-1.1870796696	-5.0523766688	-0.7072208420
H174	0.1154217903	-3.4349136189	-0.6674118853
H175	-0.8701729445	-0.9772168210	-3.8067691286
H176	0.8809565741	0.9563446973	-3.8119456489
H177	-3.4743593157	0.1888696692	-0.6516166775
H178	-5.0434857840	-1.2193449489	-0.7072806360
H179	-5.8011068644	-2.5305791186	0.8076217288
H180	-2.4757932661	-5.7563984273	0.7902357632
H181	-3.0652513694	4.2279749426	-1.7459921464
H182	-1.9046935086	1.4112444471	-2.3770731697
H183	1.9226021068	-1.4769856659	-2.3623388768
H184	3.0596457210	-4.2442754598	-1.7705029849
H185	-2.6909990598	-1.1014641349	-2.1466023980
H186	-1.1259816503	-2.7005746499	-2.1345838384
O187	1.2895860370	3.2270165190	-1.3389788498
O188	3.2586538028	1.2347806302	-1.3203510946
O189	-0.8793049405	3.6277487806	-0.0189601037
Ti190	0.1165822648	4.5813195977	1.5245283551
O191	3.6544933573	-0.9678725956	0.0416750144
Ti192	4.6401701227	0.0531628161	1.5193651813
Ti193	2.3169524067	2.2623673535	0.0402029728
O194	3.7027456962	3.6746951625	0.0112141331
Ti195	4.7827577156	4.7004244520	1.4769829232
O196	1.3852631133	3.1689872952	1.4702467199
O197	3.1777361116	1.3440473786	1.4810552352
O198	1.0268522527	5.5529793927	0.1432997508
O199	1.2389720569	7.8549891685	1.7165227048
O200	3.2353723584	5.9457467844	1.5257543569
O201	5.5199655381	0.9857592937	0.1325304455
O202	5.9430515804	3.1404566819	1.5008564831
O203	7.9582892213	1.2789321913	1.8114286981
O204	5.6510159953	5.6349165944	0.1718280695
O205	-0.8961917198	3.6648362103	2.9802209159
O206	3.6604793585	-0.9326180987	3.0142563523
Ti207	2.3277846331	2.2815811876	3.0735939892
O208	3.6704015171	3.6291083116	2.9879412563
Ti209	2.2365346546	6.8846360688	2.9830096738
O210	0.8880226282	5.4816730132	2.9908217961
Ti211	6.8526374463	2.2085491351	3.0750482391
O212	5.4958226279	0.8506774048	3.0033513233
O213	5.4814405319	5.4242642438	3.0082768904
Ti214	-0.2254229203	4.6106859563	4.4782345426
Ti215	4.6014935492	-0.2559384045	4.4951256185
Ti216	4.4890839298	4.4939359574	4.4512189360
O217	1.3925043012	3.1402590399	4.4809136921
O218	3.1592133353	1.3648689077	4.4913964726
O219	1.7301655740	7.8352433740	4.4448053572
O220	3.1540299109	5.8289186717	4.4975590716
O221	5.9219567622	3.1699217633	4.4981831806
O222	7.7994179834	1.5917304153	4.5101675435
O223	-0.9187526665	3.6612661372	5.9614821989
Ti224	0.0643257593	4.6548810598	7.4736255317
O225	3.6599372141	-0.9343728113	5.9733119136

Ti226	4.6386132776	0.0632591645	7.4739926965
Ti227	2.3377394627	2.3429530642	5.9432412771
O228	3.6710211292	3.6427736974	6.0015459233
Ti229	4.7472047935	4.7267079782	7.4972805673
O230	1.3569325948	3.1737193405	7.4714241937
O231	3.1572023153	1.3584469054	7.4914523809
Ti232	2.2443575387	6.7888725893	5.9020576090
O233	0.8567762872	5.5121140501	5.9680434650
O234	1.4189263817	7.9989220604	7.1185314282
O235	3.1840193161	5.9492664167	7.4327383488
Ti236	6.8403548901	2.2328906403	5.9521485887
O237	5.4979508896	0.8504649116	5.9946067691
O238	5.8984478295	3.1514886335	7.4785888909
O239	7.9551072368	1.3751964913	7.2254548698
O240	5.4637573625	5.4710873166	5.9823731333
O241	−0.9424768304	3.6626085914	8.9302449859
O242	3.6313283450	−0.9471436417	8.9439464018
Ti243	2.2612139402	2.2711335068	8.9203938279
O244	3.6481939889	3.6950307760	8.9558969450
O245	1.2251911752	3.2419790686	10.2870858424
O246	3.2133834582	1.2605474439	10.2974731749
O247	1.0416520811	5.4954912342	8.8411086222
O248	5.4736307821	1.0172966004	8.8676075977
O249	5.6266531190	5.6156968125	8.7985178505
H250	1.2679430851	7.7927334784	8.0628099946
H251	7.6797093442	1.2281714582	8.1540060706
H252	2.4956689267	5.7757975890	8.1540676813
H253	5.7039948439	2.4561030015	8.1872782503
H254	1.0600683932	2.6808953446	11.0888140596
H255	2.6523483098	1.1020877585	11.1025899916
H256	3.4223189782	−0.2026952313	9.6121067104
H257	4.9481177131	1.1906848953	9.6949496425
H258	3.9080777328	3.9716038878	9.8538012489
H259	6.1471302465	6.0396981156	9.4890306749
H260	1.2186355941	4.9738911694	9.6692617897
H261	−0.1950728052	3.4542641102	9.6098552277
H262	3.4620091095	−0.2235659276	−0.6317257193
H263	5.0178394108	1.1561964044	−0.7070291551
H264	3.9921298429	3.9503683555	−0.8786416864
H265	5.6635306793	6.5355493241	−0.1890697742
H266	1.2084042535	5.0585180049	−0.6950376421
H267	−0.1074441626	3.4194467003	−0.6760710729
H268	1.0726830706	7.4401330253	0.8364824057
H269	2.5471669911	5.7581191596	0.8136145669
H270	5.7546692171	2.4367132368	0.8003714562
H271	7.6276873341	1.1224339815	0.9004428949
H272	1.1246965207	2.6563057637	−2.1325416623
H273	2.7102526690	1.0785803526	−2.1365995205
O274	−5.6462609414	3.6104446324	0.1677542836
Ti275	−4.5994478605	4.4607304376	1.5193166936
O276	−7.9021396732	3.2803446603	1.6126282603
O277	−5.9685820038	1.3907620609	1.5808229618
O278	−4.6933635981	6.0328821415	0.4543329108
O279	−3.3017311837	7.8260359998	1.5917274055

O280	-1.3783802867	5.9458977109	1.5431307295
Ti281	-7.0583469984	2.4722110270	2.9909196073
O282	-5.6016014632	3.8541852956	2.9813336341
Ti283	-2.5082364594	6.9591703053	2.9360348414
O284	-3.8384781741	5.5581174472	2.9971155633
Ti285	-4.4515081616	4.4253591385	4.4682343965
O286	-7.8442680095	3.1086357646	4.4764839777
O287	-5.9541179295	1.4683662641	4.4119826141
O288	-3.0602612402	7.8582554614	4.4513439826
O289	-1.4452950682	5.9480056382	4.4534700692
Ti290	-7.0361461491	2.5009160390	6.0311987693
O291	-5.5246753231	3.8168284719	5.9206400351
Ti292	-4.4462134618	4.6976994526	7.3686272479
O293	-7.7839745168	3.4183537561	7.3388154751
O294	-6.0137542070	1.3920648061	7.4281508788
Ti295	-2.3679001979	7.1383302766	5.9502210687
O296	-3.8318237491	5.6310543365	5.9175534297
O297	-3.2003471115	7.9092242370	7.3374377764
O298	-1.3797973598	5.9626485638	7.3600965285
O299	-6.0863884547	5.0167283038	8.2754845187
O300	-3.5914218322	5.6333069796	8.7855808467
H301	-7.3184999122	4.1851407194	7.8280104431
H302	-3.4817286376	7.5412216067	8.2033337554
H303	-6.3378934069	1.6053410896	8.3236314674
H304	-2.0258902187	5.8921877079	8.1224842847
H305	-3.4440817095	5.1267292327	9.6258306921
H306	-6.1342498755	5.6628606491	9.0012615352
H307	-7.5060236843	3.5398277789	0.7492458531
H308	-5.3355625537	6.0902312513	-0.2766945935
H309	-5.1401280164	3.4446138468	-0.6710012068
H310	-5.8954373977	2.0315754440	0.8142960562
H311	-3.9691171471	7.3482938731	0.9967210980
H312	-1.6340383742	6.2261182457	0.6439812784
O313	4.9272718970	-6.0991554492	0.6497248936
Ti314	4.6747658715	-4.4600433316	1.5701266931
O315	1.3307463538	-6.0024991360	1.5652449938
O316	3.3355826745	-7.8136656346	1.6429917649
O317	5.6199775554	-3.6132725687	0.1632215662
O318	5.9522700009	-1.4141557335	1.6199900760
O319	7.8872024253	-3.2705462609	1.6295661771
Ti320	2.4723434356	-6.9912075965	2.9694178011
O321	3.7975235836	-5.5349702267	3.0270130095
Ti322	7.0516478133	-2.4599200608	3.0081120239
O323	5.6292695865	-3.8750390841	3.0319778312
Ti324	4.3642340222	-4.5035540557	4.5028452995
O325	1.4161080997	-5.9322537454	4.4585291164
O326	3.0716634646	-7.8054850581	4.4919066516
O327	5.9748679831	-1.4760379328	4.4712978071
O328	7.9085536271	-3.0570059683	4.4992740548
Ti329	2.4483239314	-7.0483386926	6.0341561704
O330	3.7756628593	-5.5148612764	5.9622081706
Ti331	4.6883873410	-4.4481477595	7.4008585813
O332	1.3329734967	-6.0090825354	7.4456223858
O333	3.3634589580	-7.7878227663	7.3536330643

Ti334	7.1167292964	-2.4058569946	6.0083957010
O335	5.6291772071	-3.8556562344	5.9495615082
O336	5.9437315011	-1.4032737178	7.3855115261
O337	7.8739087840	-3.2362679207	7.4007095167
O338	5.0104395117	-6.1009596282	8.2766129461
O339	5.5892279109	-3.6007699713	8.8376246314
H340	4.1384662999	-7.3351467936	7.8334804935
H341	7.5064419175	-3.5163303819	8.2679298106
H342	1.5701351716	-6.3207467845	8.3392281737
H343	5.8606967707	-2.0306860396	8.1610128295
H344	5.6327028883	-6.1552379027	9.0228355752
H345	5.0677624403	-3.4505788601	9.6705496996
H346	4.0833562208	-7.3643253241	1.1254350175
H347	5.5509782995	-6.1563002863	-0.0946615991
H348	5.1001597063	-3.4618003195	-0.6710089230
H349	1.5342853960	-6.3567224702	0.6787518773
H350	5.8925330099	-2.0270312912	0.8318956245
H351	7.5273680925	-3.5387408997	0.7555120496
Ti352	0.0161116146	-0.0242321641	-1.4479541624
O353	-1.0556866649	-0.9369868586	-2.8522909706
O354	1.0603036122	0.8987516582	-2.8574190433
Ti355	-0.0340168855	-0.0124744708	10.4194857793
O356	-1.0381580440	-0.9788221358	11.8191386472
O357	0.9673377893	0.9683188269	11.8266324304

3.3 $555 \text{ I}_{\text{Li}}^+$ cluster in vacuum*

358			
555	Li+ intercalation Vacuum-Optimized	SCFE : -17174.275229344	hartree
O1	-7.9276046527	-4.1050918814	3.1330133096
H2	-8.2354547159	-4.2406280484	4.0682696572
H3	-7.2791283322	-4.8190582427	2.8929297209
O4	-7.8743428794	-4.2569543457	5.8422912736
H5	-8.5315134285	-4.3838862230	6.5514129381
H6	-7.0758183508	-4.8894004593	5.9370778722
O7	-4.1344986939	-7.8868630979	2.9093233542
H8	-4.2755539124	-8.4328526653	2.1153981389
H9	-4.8556692573	-7.2021576285	3.0169818022
O10	-4.1688529481	-7.8560799141	6.0203632907
H11	-4.3425937153	-8.4906822635	6.7362208898
H12	-4.8834965153	-7.1591454350	5.9379636397
O13	4.0946210770	7.9535637646	3.1247332469
H14	4.2443241642	8.2175274868	4.0752522392
H15	4.7830020171	7.2896315251	2.8645212626
O16	4.2990158240	7.8477968272	5.8108074773
H17	4.4164738738	8.5052435543	6.5215871003
H18	4.9258187764	7.0495498095	5.9179114004
O19	7.9581198953	4.0437558517	2.9007822382
H20	8.5038778233	4.1659816607	2.1035010385
H21	7.2909137387	4.7781952104	3.0012210106
O22	7.9325520116	4.0724568577	6.0655548569
H23	8.5670944747	4.2153914998	6.7887932693

*intercalated by Li^+ cation

H24	7.2585320108	4.8042134235	5.9975247135
O25	-8.5685622469	0.9036114518	3.0221387431
H26	-9.4585310316	1.2549215434	2.8292603993
H27	-8.3733388993	0.0205308935	2.5002183971
O28	-8.3032745957	0.8840478954	5.8796783100
H29	-8.5579467448	0.6662647583	4.9494575830
H30	-8.2873406553	0.0502497442	6.4540044609
O31	0.9201417152	-8.4828400128	2.9438098607
H32	1.2681607195	-9.3827437895	2.8005421921
H33	0.0102535127	-8.3260502750	2.4708090990
O34	0.8382093418	-8.2937576578	5.8576420705
H35	0.5826822522	-8.4915232540	4.9245291788
H36	0.0231632662	-8.2798063858	6.4558871584
O37	-1.0207252538	8.5124156830	2.8994582500
H38	-1.4150887670	9.3918817923	2.7462804658
H39	-0.1728522188	8.3594763977	2.3520422069
O40	-0.7916890441	8.3428272410	5.7556171818
H41	-0.5548287457	8.5427312165	4.8176923597
H42	0.0360556222	8.3240994112	6.3577246523
O43	8.5487118096	-0.9265905825	3.0071231661
H44	9.4410684914	-1.2856006493	2.8422158463
H45	8.3827805288	-0.0433289295	2.4919222764
O46	8.3581310584	-0.8404210781	5.8667583310
H47	8.5348346644	-0.5438768403	4.9393872811
H48	8.3508008642	-0.0524771175	6.5035084548
O49	-3.2272323779	-1.2211700040	-1.3240756585
O50	-1.2832485859	-3.2141673138	-1.3323283184
O51	-3.3415274531	3.4261195874	-1.3256815003
O52	-1.4290366360	1.4419050346	-1.5031944738
O53	1.4553099069	-1.4100284569	-1.5020273837
O54	3.3436145687	-3.4281456953	-1.3244739591
O55	-5.6843803076	-5.6353383334	0.1571160084
Ti56	-4.7693461542	-4.7832920137	1.4606736425
O57	-5.5322553682	-1.0265442343	0.1109750586
Ti58	-4.6910817576	-0.0774169981	1.4902814656
O59	-7.9241603799	-1.2159237452	1.7806176605
O60	-6.0035408423	-3.2191862024	1.5228349304
O61	-1.0086225602	-5.5160954211	0.1134492110
Ti62	-0.1215103277	-4.5894229621	1.5106415795
O63	-3.1893580141	-5.9209949657	1.4849963600
O64	-1.3234350033	-7.9415287384	1.8064044958
Ti65	-2.3469070392	-2.2846652541	0.0288022804
O66	-0.8538844059	-0.8827668093	-0.0238124506
O67	-3.7328389470	-3.6779115245	-0.0090723065
Ti68	-0.0395351388	-0.0471622237	1.5262164756
O69	-3.1947990062	-1.3683975093	1.4746543563
O70	-1.4076312052	-3.1761052031	1.4716307770
Ti71	-2.4058480133	2.4364433589	-0.0645618519
O72	-3.6572316458	0.9538719464	0.0300705807
O73	-3.2079367409	3.2624536261	1.4710031319
O74	-1.4080342677	1.4199379060	1.4851632570
Ti75	2.3988312134	-2.4541448341	-0.0530605480
O76	0.8722336632	-3.6134422810	0.0010866130
O77	1.4052470866	-1.4214353789	1.4881292210

O78	3.1986684756	-3.2697205930	1.4788271937
O79	0.8622922387	0.9081923115	-0.0279114770
O80	-5.4836500950	-5.4853151081	2.9919818063
Ti81	-6.9224672984	-2.2396667833	3.0002003953
O82	-5.5059785076	-0.8734493851	2.9835735661
Ti83	-2.2591098443	-6.8453473791	3.0487278304
O84	-0.9200366757	-5.4596093690	2.9977867929
Ti85	-2.4032145920	-2.3393620232	3.0427339105
O86	-0.8949393295	-0.8654337091	2.9711876289
O87	-3.6983986240	-3.6664442466	2.9728012303
Ti88	-2.2210167394	2.1548484867	2.9291615981
O89	-3.6641698342	0.9194301329	2.9828569370
Ti90	2.1654110417	-2.2132966044	2.9380576407
O91	0.8900457703	-3.6609360717	2.9751669473
O92	0.9077489601	0.8386751151	2.9719970993
Ti93	-4.5764530832	-4.5312530080	4.4557454302
Ti94	-4.6622238524	0.2105570743	4.4652938418
O95	-7.8526771874	-1.6944283597	4.4615562499
O96	-5.8755232166	-3.1546586381	4.4976400529
Ti97	0.1730026278	-4.6365435940	4.4813707563
O98	-3.2327825818	-5.9226434239	4.4863071984
O99	-1.6171572704	-7.7747840619	4.4858837080
Ti100	-0.0458261992	-0.0378908297	4.5254864684
O101	-3.1959155460	-1.3885436092	4.4802339473
O102	-1.4258572107	-3.1480666369	4.4752882446
O103	-3.1984295114	3.2042053841	4.4657948446
O104	-1.4138492816	1.4010072221	4.4798077336
O105	1.3808184265	-1.4188548339	4.4894576925
O106	3.1816371537	-3.1899278597	4.4826557739
O107	-5.5225648644	-5.4601547361	5.9710950367
Ti108	-4.7713876503	-4.7612093702	7.4952575671
Ti109	-6.8284844943	-2.2170234013	5.9187160107
O110	-5.5210892043	-0.8448725045	5.9652757194
Ti111	-4.6277139806	-0.0710566656	7.4702912034
O112	-7.9945831925	-1.3956989453	7.1518449929
O113	-5.9691798167	-3.1774962155	7.4320026982
Ti114	-2.2733694933	-6.8613106414	5.9366050324
O115	-0.9052447477	-5.4796153134	5.9767798335
Ti116	-0.1099763780	-4.6188333694	7.4547127214
O117	-3.1923727101	-5.8963192820	7.4624986459
O118	-1.4104680485	-7.9572405042	7.1913931788
Ti119	-2.3868207638	-2.3747276308	5.9131234062
O120	-0.8913776960	-0.8698664254	5.9831007902
O121	-3.6863792776	-3.6762471036	5.9863682694
Ti122	0.0232092953	0.0221295987	7.4440185332
O123	-3.2072948229	-1.3577687860	7.4826819729
O124	-1.4060963429	-3.1660701379	7.4862283668
Ti125	-2.2331326873	2.1730785065	6.0437095138
O126	-3.7026582369	0.9313979241	5.9713902566
O127	-3.2644474374	3.2172429594	7.4834164961
O128	-1.4388739683	1.4084491534	7.4792537207
Ti129	2.1713840569	-2.2224397311	6.0440765655
O130	0.8958721013	-3.6758385063	5.9931312620
O131	1.3925469190	-1.4157942789	7.4752569347

O132	3.1953272180	-3.2579211513	7.4967601237
O133	0.8552990767	0.8705541570	5.9861981221
O134	-5.6628717217	-5.6296680024	8.7890387284
O135	-5.5327725792	-0.9978890262	8.8400075266
O136	-1.0305931881	-5.4947912028	8.8524603756
Ti137	-2.3173204299	-2.2839980907	8.9273479542
O138	-0.8890707779	-0.8684441313	9.0173238763
O139	-3.7314035624	-3.6597182419	8.9600471321
O140	-3.2591127079	-1.2421766764	10.2910404759
O141	-1.2975073057	-3.2250696270	10.2960704949
Ti142	-2.4397182946	2.4316610545	9.0181430711
O143	-3.6545492894	0.9189479747	8.9552296539
O144	-3.4150540724	3.3611129946	10.2943114130
O145	-1.4244763599	1.4656244375	10.4612948451
Ti146	2.3990663893	-2.4530341927	9.0247293038
O147	0.8776388784	-3.6230608362	8.9640163915
O148	1.4286720145	-1.4087578261	10.4646525285
O149	3.3241711130	-3.4087507874	10.3239590728
O150	0.8591951509	0.8847007237	8.9694675676
H151	-7.8436028462	-1.3078578445	8.1130902197
H152	-4.2360804387	3.1171938576	10.7585162956
H153	-1.3081267237	-7.7672261790	8.1451278146
H154	3.0558123247	-4.1945063815	10.8329019439
H155	-5.8026929470	-2.4952420260	8.1545896606
H156	-1.6080554963	1.8189728480	11.3503662966
H157	-2.4949028875	-5.7229420954	8.1709448650
H158	1.8389835516	-1.5236052958	11.3414014376
H159	-2.7105282873	-1.0794354708	11.1024946828
H160	-1.1352063673	-2.6776454246	11.1080907401
H161	-6.1883603940	-6.1023233803	9.4446172922
H162	-4.0128696372	-3.9344148708	9.8528756106
H163	-1.2091966569	-4.9976308104	9.6922045504
H164	0.1224052825	-3.4137556391	9.6290382430
H165	-0.9389057629	-0.9169472885	12.7752155557
H166	0.9250984498	0.9657383533	12.7835670624
H167	-3.4459216499	0.1640969591	9.6276461978
H168	-5.0318669310	-1.1905681516	9.6752471149
H169	-7.6348016110	-1.0370041329	0.8605021379
H170	-1.2113195775	-7.6690718182	0.8715055425
H171	-6.5318139012	-5.7520628340	-0.2971770474
H172	-3.9793668009	-4.0080830616	-0.8942471261
H173	-1.1841312532	-5.0330091432	-0.7330770544
H174	0.1086204197	-3.4023652899	-0.6651905391
H175	-0.9012560247	-0.9386281787	-3.8016239648
H176	0.9195513787	0.9750853834	-3.8017955187
H177	-3.4626912046	0.2018471155	-0.6407267393
H178	-5.0469076686	-1.2037089021	-0.7338753031
H179	-5.8236690807	-2.5472198968	0.7972362537
H180	-2.4892932866	-5.7411505380	0.7821470943
H181	-3.0758891981	4.2442628312	-1.7814813400
H182	-1.8596830810	1.4991614963	-2.3765713861
H183	1.8678880994	-1.5213305198	-2.3781011242
H184	3.0831910906	-4.2378253843	-1.8018509049
H185	-2.6676362620	-1.0623587712	-2.1330249757

H186	-1.1206153488	-2.6537225652	-2.1339497029
O187	1.2932421303	3.2349247304	-1.3296552141
O188	3.2652342575	1.2651029243	-1.2766560240
O189	-0.8866307332	3.6531447440	0.0125859914
Ti190	0.0741030257	4.5937244175	1.5465942985
O191	3.6599561416	-0.9592420138	0.0529299303
Ti192	4.7105233948	0.0035816540	1.5022235709
Ti193	2.2857745951	2.3248570897	0.0436480273
O194	3.6890270319	3.7051469136	0.0387407212
Ti195	4.7759630393	4.6973072047	1.5172243667
O196	1.4122201837	3.2059312235	1.5170741694
O197	3.1957191898	1.3411039501	1.4910141208
O198	0.9957311762	5.6026267027	0.1849214829
O199	1.1844668123	7.9174427956	1.6537932295
O200	3.1978729082	5.9404727498	1.6210910509
O201	5.5115683045	0.9873131175	0.1270235560
O202	5.9375405373	3.1330969006	1.5308532943
O203	7.9859300935	1.2672349878	1.7985322635
O204	5.5978524238	5.6334852883	0.2087596158
O205	-0.9225748173	3.6859553521	2.9740799932
O206	3.6780660382	-0.9487802230	3.0044310860
Ti207	2.3947896747	2.0665397285	3.0300776530
O208	3.7060186884	3.6351988932	3.0520205084
Ti209	2.1978461410	7.0754028037	2.9464886861
O210	0.8632618277	5.5362575025	3.0050893756
Ti211	6.8955410952	2.1722997416	3.0543475973
O212	5.5228855544	0.8302432564	2.9968633803
O213	5.5376730889	5.4416455232	3.0171735874
Ti214	-0.3388887212	4.6266394502	4.5049709980
Ti215	4.6288532344	-0.2886554450	4.4984013533
Ti216	4.6825564544	4.5199556753	4.4762916634
O217	1.4362441850	3.1606287896	4.4598679680
O218	3.1873575586	1.3290454791	4.5055663376
O219	1.7120286558	7.8921352835	4.4510456047
O220	3.1617257508	5.8618723583	4.4790857550
O221	5.9943320065	3.1818193961	4.5061531494
O222	7.8098200911	1.5468712031	4.5051722927
O223	-0.9554370949	3.6664141792	5.9767385023
Ti224	0.0548105798	4.6759518204	7.4732121063
O225	3.6730241276	-0.9514400174	5.9705090573
Ti226	4.6515772288	0.0615222262	7.4728632602
Ti227	2.3460096391	2.4079889618	5.9181543279
O228	3.6961296620	3.6658006860	5.9769973404
Ti229	4.7680141620	4.7239109606	7.5026025902
O230	1.3740104554	3.1933791078	7.4414834301
O231	3.1768388076	1.3717592975	7.4779584892
Ti232	2.2499529207	6.7746494815	5.8894908814
O233	0.8432855542	5.5069789091	5.9279382553
O234	1.3965587735	7.9801188188	7.0892724676
O235	3.1897628412	5.9566787448	7.4067719447
Ti236	6.8919359778	2.1829254202	5.9690946176
O237	5.5232666611	0.8345294223	5.9848959829
O238	5.9151774394	3.1484428493	7.4557560012
O239	7.9803400921	1.3441022500	7.2402034194

O240	5.5055762941	5.4830436424	5.9890832691
O241	-0.9337937204	3.6686005196	8.9135498828
O242	3.6345767404	-0.9431293178	8.9314304280
Ti243	2.2849813478	2.2751122245	8.8892017093
O244	3.6673617970	3.7049546644	8.9409498493
O245	1.2289691002	3.2560954344	10.2488427978
O246	3.2130149272	1.2753665385	10.2760824444
O247	1.0458816761	5.4965812807	8.8251414871
O248	5.4773569912	1.0152125429	8.8615714875
O249	5.6249794696	5.6157691846	8.7999866747
H250	1.2655067240	7.8422791175	8.0478256441
H251	7.7725576484	1.2115189120	8.1868903746
H252	2.5104853016	5.7987099538	8.1394498053
H253	5.7290289718	2.4603052487	8.1737901613
H254	1.0818417546	2.7262939541	11.0709758522
H255	2.6662401554	1.1229822586	11.0905258461
H256	3.4270562803	-0.2012456974	9.6004181545
H257	4.9625894990	1.1917366610	9.6934432999
H258	3.9139913345	3.9827270937	9.8427814609
H259	6.0916993231	6.1218975438	9.4750840386
H260	1.2275303685	4.9774353211	9.6559924877
H261	-0.1760035114	3.4594098723	9.5895481450
H262	3.4511843103	-0.2010146993	-0.6015466612
H263	4.9826886315	1.1759851757	-0.6962447296
H264	4.0189026016	3.9717081677	-0.8402557263
H265	5.7719068632	6.4678186389	-0.2497715974
H266	1.1759781539	5.1621449270	-0.6785107204
H267	-0.1433173237	3.4568248089	-0.6625317904
H268	1.0173544603	7.4411199406	0.7995071717
H269	2.5331844358	5.7670930052	0.8849213138
H270	5.7509929769	2.4426575901	0.8191986296
H271	7.7239918696	1.1303497963	0.8641693102
H272	1.1239213105	2.6721713927	-2.1313088410
H273	2.7521746819	1.1131421472	-2.1112017773
O274	-5.6317046068	3.5527007496	0.1612889270
Ti275	-4.6724778480	4.4342906453	1.5300354979
O276	-7.9318702329	3.2613200680	1.6404181702
O277	-5.9889589602	1.3735047266	1.5886123777
O278	-4.8772077741	6.0281799514	0.5353201098
O279	-3.4054760699	7.7929030600	1.5812235849
O280	-1.3976248606	5.9862338927	1.5543677286
Ti281	-7.0953547267	2.4426421586	3.0026618640
O282	-5.6241755543	3.8280582990	3.0013569855
Ti283	-2.5840469277	6.9686626319	2.9197122182
O284	-3.8683241783	5.5383267199	3.0024158519
Ti285	-4.4633956819	4.4183073964	4.4810867912
O286	-7.8491957278	3.0903909065	4.4938714797
O287	-5.9643347190	1.4412606140	4.4105843110
O288	-3.1075965661	7.8709398708	4.4464729079
O289	-1.5212479956	5.9568412540	4.4649568968
Ti290	-7.0430788544	2.4930211773	6.0529974377
O291	-5.5227615511	3.7933452047	5.9273904793
Ti292	-4.4510336021	4.7033743854	7.3842862177
O293	-7.7778908594	3.4135154306	7.3544915055

O294	−6.0181410514	1.3780889398	7.4457021850
Ti295	−2.4112759361	7.1669156338	5.9486763731
O296	−3.8570578408	5.6314646846	5.9223119423
O297	−3.2356373887	7.9281717470	7.3316645947
O298	−1.3828786319	5.9844265462	7.3490288541
O299	−6.0847972868	5.0219723068	8.2792282670
O300	−3.5757989772	5.6134971656	8.7832693244
H301	−7.3270242183	4.1903414295	7.8406784533
H302	−3.5350857257	7.6578443357	8.2218174141
H303	−6.3461600587	1.5935241229	8.3395266383
H304	−2.0266283072	5.9234200243	8.1153326375
H305	−3.4278393350	5.1428508586	9.6418622392
H306	−6.1701031743	5.6744209359	8.9955738654
H307	−7.6597189439	3.5345710761	0.7415528742
H308	−5.5059331329	6.0971720622	−0.2051867877
H309	−5.1580456414	3.4091391029	−0.6965133128
H310	−5.9294972269	2.0127868432	0.8176049065
H311	−4.1191186192	7.3311324637	1.0251255360
H312	−1.6050444298	6.3076130199	0.6557392820
O313	4.9318786062	−6.0744344876	0.6369907745
Ti314	4.6729044034	−4.4543511515	1.5634508408
O315	1.3228945201	−5.9854595666	1.5524512807
O316	3.3381066906	−7.7851133968	1.6330271239
O317	5.6069928628	−3.5741387893	0.1732520254
O318	6.0005915743	−1.4287914807	1.5977822996
O319	7.9308287350	−3.3028538815	1.6559520499
Ti320	2.4653052671	−6.9850213645	2.9548133001
O321	3.7869281756	−5.5125565744	3.0219255347
Ti322	7.0827601310	−2.4990845610	3.0167954283
O323	5.6318668451	−3.8722369431	3.0241742700
Ti324	4.3573891492	−4.4984007445	4.4999290630
O325	1.4055343275	−5.9123878179	4.4478862363
O326	3.0671715334	−7.7836128829	4.4790248061
O327	6.0009046613	−1.4936016772	4.4670784513
O328	7.9164222994	−3.0929285947	4.5083889707
Ti329	2.4400875915	−7.0436485932	6.0260361205
O330	3.7650443154	−5.4977804579	5.9518514185
Ti331	4.6949057817	−4.4473701955	7.4038944192
O332	1.3285536176	−5.9979351333	7.4416918515
O333	3.3593297755	−7.7713350091	7.3384219422
Ti334	7.1289889393	−2.4341675737	6.0211402358
O335	5.6282256822	−3.8548185227	5.9475680643
O336	5.9636807722	−1.4044496227	7.3847538238
O337	7.8833302143	−3.2630924551	7.4002335526
O338	5.0151499335	−6.0995949157	8.2582344608
O339	5.5611928187	−3.5869413847	8.8335019182
H340	4.1460155504	−7.3390991637	7.8167521952
H341	7.6218792137	−3.5671003015	8.2917048670
H342	1.5655223738	−6.3222179476	8.3314476815
H343	5.8834207017	−2.0277448921	8.1645118349
H344	5.6439343338	−6.1955442962	8.9954967940
H345	5.0687721722	−3.4416637766	9.6826744663
H346	4.0906773688	−7.3563998442	1.1090810172
H347	5.5621927121	−6.1624481651	−0.0987265244

H348	5.1226769254	-3.4315024873	-0.6800618071
H349	1.5134665954	-6.3553001842	0.6690440462
H350	5.9379315293	-2.0772076379	0.8273574013
H351	7.6859954575	-3.5908761620	0.7548322685
Ti352	0.0283833077	0.0211233033	-1.4509097595
O353	-1.0201229581	-0.9105799828	-2.8360704332
O354	1.0347976364	0.9630336625	-2.8355904852
Ti355	-0.0227375203	-0.0027836138	10.4321676868
O356	-1.0168088490	-0.9614425031	11.8062113362
O357	0.9703774780	0.9673457781	11.8118046200
Li358	2.2528922506	4.5608011298	3.6073407984

3.4 555 I_{Li}^+/e^- cluster in vacuum[†]

358			
555	Li+/e- intercalation Vac-Optimized	SCFE : -17174.4320251031 hartree	
O1	-7.9112974574	-4.1127412246	3.1330432870
H2	-8.2251944646	-4.2351092403	4.0682321692
H3	-7.2380546871	-4.8156446722	2.9217282141
O4	-7.8622952028	-4.2630292401	5.8383816741
H5	-8.4991263200	-4.3813525371	6.5669172819
H6	-7.0547139754	-4.8896227232	5.9270361107
O7	-4.1442996819	-7.8808334840	2.9016952727
H8	-4.2744647503	-8.3550855653	2.0603377213
H9	-4.8510045054	-7.1818562922	3.0272043367
O10	-4.1784799707	-7.8521456737	6.0342588526
H11	-4.3382408617	-8.4170467558	6.8104833875
H12	-4.8782586004	-7.1386941959	5.9398592138
O13	4.1062766788	7.9495837708	3.1386935054
H14	4.2499180548	8.2052953681	4.0930219288
H15	4.7834568012	7.2664784716	2.8894919471
O16	4.3033193437	7.8426225151	5.8206346612
H17	4.4130083296	8.4764444139	6.5529412589
H18	4.9245420141	7.0352637353	5.9168546707
O19	7.9600068563	4.0484831484	2.8824399810
H20	8.4181366074	4.1568732629	2.0289261981
H21	7.2845109185	4.7721777331	3.0100015140
O22	7.9239566447	4.0903534488	6.0755744741
H23	8.4878251399	4.2189771622	6.8584038933
H24	7.2326020123	4.8076245656	5.9967722247
O25	-8.5508884514	0.9060711575	3.0034952206
H26	-9.4375229850	1.2612500341	2.8044578479
H27	-8.3519465552	0.0254965834	2.4764378531
O28	-8.3098998613	0.8713681962	5.8601166802
H29	-8.5449576976	0.6481635460	4.9255357280
H30	-8.2880128619	0.0368692554	6.4375231136
O31	0.9102243951	-8.4892912352	2.9671526900
H32	1.2647135465	-9.3841106772	2.8097377963
H33	0.0029573677	-8.3279369130	2.4845879057
O34	0.8411157314	-8.2995857409	5.8742487176
H35	0.5833011422	-8.4898295780	4.9395993491
H36	0.0265084254	-8.2788464334	6.4743699495

[†]intercalated by Li⁺ cation, also reduced by an electron

O37	-1.0065102944	8.5095994081	2.9227676753
H38	-1.4050201642	9.3836067236	2.7514278796
H39	-0.1536417744	8.3494493450	2.3813726422
O40	-0.7952520456	8.3358204297	5.7777576443
H41	-0.5632020222	8.5344783375	4.8380338898
H42	0.0413885210	8.3016470641	6.3693495511
O43	8.5308775768	-0.9222180391	2.9910394188
H44	9.4105710419	-1.2999810587	2.8039690096
H45	8.3629830529	-0.0415933492	2.4708226076
O46	8.3666577474	-0.8289363598	5.8603822134
H47	8.5316272077	-0.5272020750	4.9324066422
H48	8.3588586979	-0.0424454145	6.4988402838
O49	-3.2462115640	-1.2309149601	-1.3175540259
O50	-1.2976849141	-3.2309298247	-1.3361864925
O51	-3.3703641026	3.4054016808	-1.3383355039
O52	-1.4372297552	1.4302488729	-1.5092696729
O53	1.4383147703	-1.4349121197	-1.5137680020
O54	3.3411327305	-3.4553701520	-1.3133800374
O55	-5.6808181869	-5.6339065857	0.1569865904
Ti56	-4.7554485501	-4.7797025144	1.4674958100
O57	-5.5390690862	-1.0271396472	0.1195170033
Ti58	-4.6720189193	-0.0733393868	1.4899593526
O59	-7.9076807977	-1.2113659556	1.7627913489
O60	-5.9957707003	-3.2208032116	1.5227950375
O61	-1.0023266949	-5.5340895198	0.1249482485
Ti62	-0.1091515008	-4.5881451673	1.5175293912
O63	-3.1860100766	-5.9304082218	1.4861298510
O64	-1.3142353341	-7.9428816715	1.8108029009
Ti65	-2.3362982041	-2.2863083794	0.0285790403
O66	-0.8642982027	-0.8988037818	-0.0301845297
O67	-3.7239980406	-3.6866591735	-0.0018684694
Ti68	-0.0330919789	-0.0424657728	1.5266962096
O69	-3.1975531301	-1.3742638391	1.4767858018
O70	-1.4005301341	-3.1806372505	1.4786676894
Ti71	-2.3948603251	2.4434888557	-0.0768026121
O72	-3.6550642199	0.9503698669	0.0347382664
O73	-3.2067549928	3.2690633234	1.4599650184
O74	-1.4103941647	1.4209441422	1.4788868596
Ti75	2.4067243044	-2.4416667125	-0.0569470871
O76	0.8780072555	-3.6257837001	0.0021438928
O77	1.4031852779	-1.4269433534	1.4854330563
O78	3.1997251182	-3.2669416969	1.4843039972
O79	0.8499881011	0.8917767688	-0.0300807978
O80	-5.4781191207	-5.4793239880	2.9959208597
Ti81	-6.9134485425	-2.2326097096	2.9959841849
O82	-5.5066773452	-0.8666474083	2.9857106518
Ti83	-2.2532091469	-6.8441813664	3.0577595747
O84	-0.9150259363	-5.4682908182	3.0033424294
Ti85	-2.3803110542	-2.3323486204	3.0448742275
O86	-0.9050740827	-0.8783421865	2.9705829927
O87	-3.6876565274	-3.6684658573	2.9757847376
Ti88	-2.2011350851	2.1646861518	2.9267433268
O89	-3.6585341314	0.9178876824	2.9830308204
Ti90	2.1730689994	-2.2040296558	2.9387998938

O91	0.8916852715	-3.6680283287	2.9799590117
O92	0.8733342667	0.8334754796	2.9675981669
Ti93	-4.5543132263	-4.5130560861	4.4556170032
Ti94	-4.6549081767	0.2214882639	4.4578736030
O95	-7.8556223856	-1.7007933309	4.4561569015
O96	-5.8661908230	-3.1457424031	4.4941404137
Ti97	0.1848555881	-4.6330678171	4.4868212966
O98	-3.2280967518	-5.9241470472	4.4901919635
O99	-1.6279058311	-7.7893070383	4.4945330696
Ti100	-0.0321045528	-0.0327869417	4.5105334811
O101	-3.1952166585	-1.3922431775	4.4836422838
O102	-1.4260684660	-3.1520842674	4.4825922267
O103	-3.2069782270	3.2028054422	4.4643560238
O104	-1.4166272569	1.3999360084	4.4798734038
O105	1.3754936169	-1.4228188356	4.4926715851
O106	3.1719617897	-3.1976245585	4.4821743698
O107	-5.5228083389	-5.4591512111	5.9720384938
Ti108	-4.7723798606	-4.7593460061	7.4918102020
Ti109	-6.8187373005	-2.2138930547	5.9111960986
O110	-5.5235349682	-0.8388374270	5.9640514006
Ti111	-4.6257396922	-0.0633910375	7.4668401369
O112	-7.9935783961	-1.3891182906	7.1467719824
O113	-5.9727313066	-3.1752286826	7.4299457538
Ti114	-2.2679439926	-6.8588484543	5.9412534137
O115	-0.9031698915	-5.4853791279	5.9795504995
Ti116	-0.1070129870	-4.6113280546	7.4530239135
O117	-3.1980224025	-5.9009370863	7.4678562894
O118	-1.3998341165	-7.9410743488	7.2113862107
Ti119	-2.3848615746	-2.3617813830	5.9154846052
O120	-0.8967638844	-0.8749707408	5.9863317168
O121	-3.6860234978	-3.6782406349	5.9926697417
Ti122	0.0142933723	0.0106346880	7.4335837629
O123	-3.2118782903	-1.3611295666	7.4827720438
O124	-1.4084682310	-3.1746599409	7.4920355125
Ti125	-2.2295058996	2.1750044125	6.0446516010
O126	-3.7026265246	0.9313261933	5.9720950153
O127	-3.2670279691	3.2130927161	7.4878158449
O128	-1.4410488500	1.4060173192	7.4824767667
Ti129	2.1867687363	-2.2130059466	6.0496297811
O130	0.8960110624	-3.6830072226	5.9999549045
O131	1.3908183554	-1.4215303575	7.4811841432
O132	3.1976643256	-3.2622648950	7.5066185776
O133	0.8536510435	0.8613850905	5.9835270188
O134	-5.6718115519	-5.6289537107	8.7860927174
O135	-5.5431939666	-0.9941238685	8.8349113265
O136	-1.0295156924	-5.5161129499	8.8495227287
Ti137	-2.3213356483	-2.2871147337	8.9326679339
O138	-0.8966655910	-0.8790176549	9.0180657971
O139	-3.7380228994	-3.6623432524	8.9615535302
O140	-3.2678978566	-1.2488971344	10.2938829345
O141	-1.3055716399	-3.2333580160	10.3008613441
Ti142	-2.4230966173	2.4313772034	9.0243459149
O143	-3.6596109279	0.9211058150	8.9545236108
O144	-3.4266185781	3.3577547960	10.2921325895

O145	-1.4372642195	1.4523506071	10.4680124861
Ti146	2.3982346106	-2.4502373889	9.0311480251
O147	0.8777698454	-3.6305882530	8.9743190097
O148	1.4225212559	-1.4166695484	10.4722473900
O149	3.3299319942	-3.4137445431	10.3293034045
O150	0.8468749268	0.8764767426	8.9736135766
H151	-7.7885124511	-1.2790045440	8.0967791976
H152	-4.2701024075	3.0850453214	10.6970778820
H153	-1.2661652050	-7.6718571539	8.1440605202
H154	3.0384823468	-4.2127448386	10.8040523044
H155	-5.8004296851	-2.4914300777	8.1500495488
H156	-1.6438984539	1.7786828180	11.3621413527
H157	-2.4964843882	-5.7206020955	8.1716361163
H158	1.8480089499	-1.5058749866	11.3444693621
H159	-2.7098867047	-1.0882605657	11.1015737168
H160	-1.1423806515	-2.6703008737	11.1038011610
H161	-6.1858456803	-6.1083566992	9.4450686482
H162	-4.0207785331	-3.9355733555	9.8540129948
H163	-1.2058463879	-5.0148524079	9.6864412674
H164	0.1203435431	-3.4220056293	9.6362350758
H165	-0.9301291179	-0.9366619824	12.7629672788
H166	0.8875756501	0.9551814457	12.7940424468
H167	-3.4509444292	0.1675222649	9.6246251038
H168	-5.0360394135	-1.1860684985	9.6667079793
H169	-7.5704495286	-1.0228455125	0.8591324006
H170	-1.1807926931	-7.6274884062	0.8909768970
H171	-6.5678097787	-5.6745953299	-0.2330135305
H172	-3.9653255708	-4.0216492003	-0.8862694589
H173	-1.1794272332	-5.0459950614	-0.7185079244
H174	0.1223055107	-3.4150821247	-0.6639686726
H175	-0.9109179772	-0.9556153276	-3.7836411830
H176	0.8533200018	0.9521714764	-3.8219208063
H177	-3.4647243836	0.1957857905	-0.6349125989
H178	-5.0418350604	-1.2088518205	-0.7189472545
H179	-5.8093988837	-2.5437350191	0.8022978003
H180	-2.4791715265	-5.7472113089	0.7892533031
H181	-3.0718352847	4.1714171172	-1.8595398733
H182	-1.9313390498	1.3653480301	-2.3470243803
H183	1.8830432750	-1.4964209379	-2.3790822611
H184	3.0407127814	-4.2861960583	-1.7181327791
H185	-2.6826228467	-1.0836102915	-2.1291833421
H186	-1.1303037698	-2.6587267501	-2.1294620158
O187	1.2818442630	3.2326156131	-1.3455803509
O188	3.2606595567	1.2529144855	-1.3154695000
O189	-0.8879872533	3.6461603581	-0.0196390696
Ti190	0.0790576999	4.6050026300	1.5246509554
O191	3.6601065576	-0.9678843426	0.0039214011
Ti192	4.6785035938	0.0455908881	1.4923169345
Ti193	2.3143223787	2.3111002915	0.0438030717
O194	3.6931547996	3.7127409846	0.03444440317
Ti195	4.7799580640	4.7074045114	1.5238488294
O196	1.3790555178	3.2264226203	1.4547496318
O197	3.2327890135	1.2975819300	1.3871378732
O198	0.9772282213	5.6239531003	0.1642136178

O199	1.1863275003	7.9267645153	1.6629214046
O200	3.2069123986	5.9667268612	1.6081951160
O201	5.5764541622	0.9718583768	0.1149893389
O202	5.9423418158	3.1481290205	1.5245674643
O203	7.9554550577	1.2603652958	1.7759366934
O204	5.5976838520	5.6479576764	0.1998494302
O205	-0.9248902746	3.6820004674	2.9761672514
O206	3.6553786621	-0.9378477459	3.0111442251
Ti207	2.3596794460	2.1371249136	2.9868146914
O208	3.7006785637	3.6604197344	3.0425918791
Ti209	2.1996468568	7.0736078441	2.9575061331
O210	0.8662768209	5.5384883661	2.9944104002
Ti211	6.8925749355	2.1655165605	3.0566715714
O212	5.5121444065	0.8425133831	3.0000983448
O213	5.5367497610	5.4547376179	3.0173590005
Ti214	-0.3311917358	4.6108653448	4.5108765388
Ti215	4.5847619398	-0.2450293011	4.4961198498
Ti216	4.6710902810	4.5096482331	4.4837087220
O217	1.3999015799	3.1954778253	4.5216120920
O218	3.2358287224	1.2947050778	4.5775473410
O219	1.7103281291	7.9004195813	4.4581094046
O220	3.1505784747	5.8678686343	4.4781105622
O221	5.9963317459	3.1846514019	4.5048243908
O222	7.8166346707	1.5561121919	4.5049071330
O223	-0.9671032645	3.6632612287	5.9809454259
Ti224	0.0773489171	4.6501975083	7.4807925619
O225	3.6699701303	-0.9680444162	5.9866878563
Ti226	4.6533745475	0.0592197808	7.4875616105
Ti227	2.3752739408	2.3555642330	5.8515923344
O228	3.7179069675	3.6730278039	5.9748618344
Ti229	4.7578495565	4.7162416114	7.4882829596
O230	1.3611504866	3.1938060232	7.4653837278
O231	3.1787748540	1.3557234437	7.4939467584
Ti232	2.2429606886	6.7733125501	5.8963601220
O233	0.8381218368	5.5123833617	5.9407397140
O234	1.3936162585	7.9796405639	7.1086136370
O235	3.1875637976	5.9616670736	7.4095253616
Ti236	6.8879007391	2.1826400833	5.9721956440
O237	5.5361191419	0.8348247835	6.0125621282
O238	5.9253261371	3.1497191358	7.4653247454
O239	7.9914207962	1.3535619941	7.2458223423
O240	5.5080334272	5.4929771522	5.9876187793
O241	-0.9302410031	3.6577953649	8.9345719608
O242	3.6299586373	-0.9458842215	8.9540658395
Ti243	2.2787240129	2.2762234331	8.8633421281
O244	3.6584750674	3.7024619545	8.9334306725
O245	1.2102040282	3.2541162026	10.2528242874
O246	3.2114052372	1.2751775485	10.2779402686
O247	1.0486581366	5.5106612038	8.8333092823
O248	5.4830447868	1.0141462745	8.8765796816
O249	5.6130158124	5.6059603052	8.7983807032
H250	1.2515944905	7.7844962768	8.0567890033
H251	7.7411286154	1.2010251958	8.1801942923
H252	2.5115873198	5.8014176021	8.1455340072

H253	5.7323191180	2.4627641099	8.1817995203
H254	1.0794060426	2.7205566962	11.0732000131
H255	2.6701924864	1.1339027022	11.0950920432
H256	3.4173459977	-0.1896819842	9.6121598686
H257	4.9505888792	1.1962060600	9.6967121132
H258	3.9119823468	3.9714267382	9.8354045340
H259	6.1020988231	6.0749028681	9.4838871563
H260	1.2231581117	4.9918822531	9.6633804359
H261	-0.1521363679	3.4473767750	9.6091862416
H262	3.4564398148	-0.1911877579	-0.6405845656
H263	5.0580315863	1.1611076254	-0.7110267342
H264	4.0082629793	4.0019877397	-0.8424325865
H265	5.6977234739	6.5283819254	-0.1918920052
H266	1.1736608808	5.1582086823	-0.6841596496
H267	-0.1166187311	3.4408126761	-0.6806333668
H268	1.0142403767	7.4489627452	0.8105439721
H269	2.5466109201	5.7905139054	0.8736636596
H270	5.7692363297	2.4635752851	0.8070982781
H271	7.6186595852	1.0937932656	0.8672652949
H272	1.1215012035	2.6858641405	-2.1535336689
H273	2.7525501126	1.1212677618	-2.1540555684
O274	-5.6390145169	3.5810145491	0.1688657663
Ti275	-4.6427611383	4.4546136656	1.5338556063
O276	-7.9178732486	3.2680203042	1.6180640280
O277	-5.9783540942	1.3816606004	1.5876682128
O278	-4.8136130906	6.0407495805	0.5118918649
O279	-3.3843530329	7.8216631367	1.6092870590
O280	-1.4151510674	5.9810065632	1.5583495548
Ti281	-7.0806976909	2.4567542924	2.9900353919
O282	-5.6249343889	3.8418347231	2.9943070923
Ti283	-2.5703952669	6.9742220106	2.9468373741
O284	-3.8750787275	5.5511208176	3.0124654272
Ti285	-4.4700351014	4.4164665190	4.4846530169
O286	-7.8603993571	3.0867944558	4.4805464633
O287	-5.9600154474	1.4543567401	4.4161930850
O288	-3.0994342351	7.8701514236	4.4706839565
O289	-1.5157783350	5.9524514116	4.4679055188
Ti290	-7.0558733108	2.4824516960	6.0353895414
O291	-5.5379709465	3.7990751294	5.9279308802
Ti292	-4.4585554548	4.6796717055	7.3888173396
O293	-7.8003325793	3.3899783262	7.3449275163
O294	-6.0181207226	1.3832899552	7.4373951585
Ti295	-2.4080094741	7.1461125408	5.9728501470
O296	-3.8599747333	5.6213194074	5.9342565923
O297	-3.2405444967	7.8998339724	7.3612906126
O298	-1.3833717517	5.9670331888	7.3586848706
O299	-6.0936804877	4.9617682506	8.3141407168
O300	-3.6048919105	5.6207126592	8.7913846296
H301	-7.3327892733	4.1458217437	7.8509340765
H302	-3.5317434357	7.5456643942	8.2287364805
H303	-6.3437546565	1.6073127149	8.3306383464
H304	-2.0149313774	5.9010469890	8.1299410438
H305	-3.4528286115	5.1391037728	9.6438392191
H306	-6.1576586796	5.6004833011	9.0455444992

H307	-7.5640554480	3.5385006019	0.7425497902
H308	-5.3856761696	6.0692861282	-0.2752915528
H309	-5.1474707928	3.4225068884	-0.6783439536
H310	-5.9182166452	2.0155545559	0.8142522664
H311	-4.0801894782	7.3567931712	1.0376689885
H312	-1.6388915793	6.3034465294	0.6645077777
O313	4.8725160942	-6.0882746833	0.6208199478
Ti314	4.6542739042	-4.4604758027	1.5644657072
O315	1.3293177361	-5.9913945933	1.5629637506
O316	3.3173274530	-7.8162435855	1.6459573360
O317	5.6137702652	-3.6156533249	0.1689258950
O318	5.9580113953	-1.4345904162	1.6054617043
O319	7.8911311840	-3.2873540209	1.6481723810
Ti320	2.4636801643	-6.9949134689	2.9736579310
O321	3.7876201940	-5.5314825754	3.0280458611
Ti322	7.0438688175	-2.4759078561	3.0161339587
O323	5.6137560128	-3.8785895212	3.0270255401
Ti324	4.3539534768	-4.4988387885	4.5005033241
O325	1.4090988965	-5.9226277001	4.4564758359
O326	3.0667827898	-7.7991494284	4.4952182193
O327	5.9845895562	-1.4746926443	4.4746764310
O328	7.9033036709	-3.0785084258	4.4997008600
Ti329	2.4447704859	-7.0451507802	6.0397029904
O330	3.7642618480	-5.5040854673	5.9590172169
Ti331	4.6944702173	-4.4469947015	7.3997880150
O332	1.3309511342	-6.0011629530	7.4487430560
O333	3.3643666914	-7.7781142818	7.3537998973
Ti334	7.1160979989	-2.4109089160	6.0010496189
O335	5.6186213943	-3.8555212011	5.9406383030
O336	5.9564878631	-1.4052705894	7.3982559038
O337	7.8673772896	-3.2502276852	7.3871226048
O338	5.0245756877	-6.1020916688	8.2548737844
O339	5.5718350883	-3.6025531915	8.8388776861
H340	4.1549251939	-7.3388917397	7.8215679786
H341	7.5560241017	-3.5426382205	8.2685999026
H342	1.5611341114	-6.3199109467	8.3418657841
H343	5.8833139860	-2.0322691716	8.1736788494
H344	5.6508865930	-6.1754880342	8.9964465329
H345	5.0715767489	-3.4574773152	9.6831490768
H346	4.0495668544	-7.3664751356	1.1087381729
H347	5.5000152828	-6.1622266455	-0.1122272949
H348	5.1235855223	-3.4717861752	-0.6814159828
H349	1.5179726630	-6.3653379453	0.6828166556
H350	5.9115423469	-2.0597177797	0.8244272310
H351	7.5750283291	-3.5700441859	0.7643935610
Ti352	0.0292441287	0.0118903462	-1.4477469938
O353	-1.0786094358	-0.9142105089	-2.8259223462
O354	1.0206007539	0.9047744277	-2.8649722535
Ti355	-0.0203180281	-0.0045072694	10.4226592169
O356	-1.0401700482	-0.9768977592	11.7972028555
O357	0.9571912016	0.9472620424	11.8239768506
Li358	2.2325694395	4.5606063233	3.6336365960

3.5 $^{555}\text{O}_{\text{Li}}^+$ cluster in vacuum[‡]

358			
555	Li ⁺ surface , Vacuum-Optimized	SCFE : -17174.2930342805	hartree
O1	-7.9158860101	-4.1064898630	3.1278747868
H2	-8.2274420976	-4.2398525363	4.0617300639
H3	-7.2677899893	-4.8213304264	2.8916251129
O4	-7.8676213320	-4.2575485873	5.8398486333
H5	-8.5214432453	-4.3846309541	6.5519062261
H6	-7.0703141067	-4.8913415724	5.9310112611
O7	-4.1260210091	-7.8936649275	2.9108409449
H8	-4.2639270102	-8.4376313123	2.1146229604
H9	-4.8445670458	-7.2045664058	3.0124456736
O10	-4.1608845524	-7.8667999290	6.0273341326
H11	-4.3319106157	-8.4881166187	6.7557888792
H12	-4.8754033659	-7.1705354854	5.9385310663
O13	4.0366807396	7.9433216621	3.1316863536
H14	4.1642432323	8.2404921466	4.0726625944
H15	4.7571288490	7.3113959050	2.8898191735
O16	4.2378003647	7.8604562506	5.8044012834
H17	4.3761010276	8.4877619765	6.5378093318
H18	4.8537913325	7.0470945823	5.8736753898
O19	8.0983413065	4.1182403672	2.9575711186
H20	9.0434378544	3.8706167242	2.8951924265
H21	7.7530433769	4.4626253371	2.1100629134
O22	8.0952321089	4.1363074354	6.0628285793
H23	9.0317942564	3.8910507476	6.1093491157
H24	7.7523283069	4.4273838965	6.9435077546
O25	-8.5578174314	0.8990899203	3.0245180477
H26	-9.4451413803	1.2531059687	2.8244019557
H27	-8.3625102591	0.0163827491	2.5026104040
O28	-8.2925972835	0.8839919714	5.8789103293
H29	-8.5457422612	0.6651690631	4.9486291214
H30	-8.2776047815	0.0514577410	6.4549433338
O31	0.9399490580	-8.4830017818	2.9482535251
H32	1.2860859224	-9.3858682841	2.8200357182
H33	0.0294964999	-8.3311659404	2.4740391695
O34	0.8536939232	-8.2925976987	5.8662288345
H35	0.5935004550	-8.4876351045	4.9338303212
H36	0.0419295898	-8.2834567204	6.4693745134
O37	-0.9908287132	8.4875215747	2.8992167249
H38	-1.3824331699	9.3634216306	2.7211244035
H39	-0.1214670087	8.3215250925	2.3692278167
O40	-0.8036541213	8.3588601713	5.7355214849
H41	-0.5549215737	8.5381971058	4.7944559659
H42	0.0049892342	8.3698377057	6.3509963628
O43	8.5327417337	-0.8782739105	3.0310390117
H44	9.4153444295	-1.2516027422	2.8454664731
H45	8.3658712804	0.0221523062	2.5140346158
O46	8.3382790101	-0.8079369774	5.8445834005
H47	8.5328618239	-0.5462835015	4.9088550230
H48	8.3268676888	-0.0060869938	6.4699338477

[‡]Li⁺ is adsorbed on surface

O49	-3.2233320076	-1.2549346695	-1.3371733431
O50	-1.2568864375	-3.2465356968	-1.3219234700
O51	-3.3274292516	3.4204635631	-1.3367178863
O52	-1.4212446211	1.4273047894	-1.5200267802
O53	1.4682486302	-1.4198769983	-1.5057148730
O54	3.3644149690	-3.4186673472	-1.3308526302
O55	-5.6639496325	-5.6348358044	0.1521234473
Ti56	-4.7493661400	-4.7832183871	1.4555551624
O57	-5.5160716987	-1.0382436703	0.1173366779
Ti58	-4.6813370619	-0.0728242463	1.4923763296
O59	-7.9094118090	-1.2189254985	1.7801255417
O60	-5.9870711310	-3.2228877130	1.5243960476
O61	-0.9965127648	-5.5258215753	0.1141425362
Ti62	-0.1192528120	-4.5994028881	1.5124266653
O63	-3.1763906608	-5.9327931903	1.4883590844
O64	-1.3084674318	-7.9503752026	1.8144406157
Ti65	-2.3215212038	-2.2678908080	0.0342635885
O66	-0.8504388040	-0.8855368557	-0.0470115089
O67	-3.7080337161	-3.6791720251	0.0035389929
Ti68	0.0300192298	0.0115120050	1.5112536142
O69	-3.1760811489	-1.3759286180	1.4773719147
O70	-1.3832599810	-3.1796244749	1.4751946419
Ti71	-2.3860173295	2.4312365161	-0.0792539001
O72	-3.6511097610	0.9486335403	0.0211174841
O73	-3.1909176837	3.2527424723	1.4606203714
O74	-1.3952308684	1.4132933682	1.4692270084
Ti75	2.3995590370	-2.4653300466	-0.0578143015
O76	0.8883994899	-3.6218482544	-0.0034133415
O77	1.4121184523	-1.4227789194	1.4818999867
O78	3.2062248189	-3.2644069304	1.4763232803
O79	0.8843877447	0.8867208523	-0.0273393723
O80	-5.4685769601	-5.4898406868	2.9898612820
Ti81	-6.9039267780	-2.2408469716	2.9979987946
O82	-5.4920780704	-0.8755945281	2.9799845916
Ti83	-2.2498348718	-6.8561127951	3.0549045360
O84	-0.9121971844	-5.4677344874	3.0036269214
Ti85	-2.3936180896	-2.3404625247	3.0404961117
O86	-0.8808501475	-0.8703085057	2.9712654749
O87	-3.6822356534	-3.6738053703	2.9734985892
Ti88	-2.1964448744	2.1612641617	2.9170702187
O89	-3.6492130412	0.9147576957	2.9769331646
Ti90	2.1594559973	-2.2249998633	2.9339430374
O91	0.8985523940	-3.6712591600	2.9790432413
O92	0.8860514473	0.8612849949	2.9597242862
Ti93	-4.5722132787	-4.5403653843	4.4505575487
Ti94	-4.6365961285	0.2198179333	4.4643657960
O95	-7.8404032206	-1.6997094499	4.4603447124
O96	-5.8615391771	-3.1607334737	4.4949797236
Ti97	0.1766810017	-4.6447998879	4.4858637558
O98	-3.2241114438	-5.9338930133	4.4914472046
O99	-1.6066219681	-7.7835471726	4.4925840869
Ti100	-0.0890393260	-0.0896361716	4.4957818714
O101	-3.1836886996	-1.3964467841	4.4808142840
O102	-1.4155030991	-3.1563576455	4.4803969870

O103	-3.1896301500	3.1883645898	4.4601523274
O104	-1.4119334915	1.3845906807	4.4794115996
O105	1.3695445369	-1.4292613153	4.4874731569
O106	3.1810364889	-3.1811489050	4.4868994860
O107	-5.5160272628	-5.4675532915	5.9703149173
Ti108	-4.7674843720	-4.7678171480	7.4942416333
Ti109	-6.8194620675	-2.2176036608	5.9166912211
O110	-5.5108193625	-0.8491047452	5.9590494580
Ti111	-4.6144010981	-0.0734507496	7.4545839395
O112	-7.9733920358	-1.3909853079	7.1564065170
O113	-5.9591517058	-3.1838830325	7.4291320172
Ti114	-2.2668310027	-6.8695209337	5.9415170501
O115	-0.8976576064	-5.4875548776	5.9858598447
Ti116	-0.1040879002	-4.6302758970	7.4640553715
O117	-3.1882621112	-5.9065364105	7.4677655957
O118	-1.4003427898	-7.9628329182	7.1970707577
Ti119	-2.3813055839	-2.3919769356	5.9147775933
O120	-0.8849953678	-0.8748470730	5.9895385032
O121	-3.6778491594	-3.6871772174	5.9896496857
Ti122	0.0227992722	0.0302328447	7.4510928695
O123	-3.2012804746	-1.3677318570	7.4854951284
O124	-1.3987933169	-3.1724182110	7.4937303996
Ti125	-2.1985081894	2.1929187368	6.0327817531
O126	-3.6955838479	0.9257304583	5.9718224572
O127	-3.2560556695	3.2143738212	7.4805239246
O128	-1.4317310104	1.4045132358	7.4796197215
Ti129	2.1563765530	-2.2241699787	6.0483593970
O130	0.8963946570	-3.6789093647	6.0005740823
O131	1.3942005677	-1.4206834998	7.4900837189
O132	3.1998613031	-3.2495216303	7.5028453194
O133	0.8674600292	0.8630577012	6.0009212846
O134	-5.6630099645	-5.6336802765	8.7876814888
O135	-5.5368937678	-1.0005484468	8.8259811084
O136	-1.0239501673	-5.4968373078	8.8638131224
Ti137	-2.3136567266	-2.2902234935	8.9281825717
O138	-0.8856014185	-0.8669404457	9.0218131983
O139	-3.7245383487	-3.6665537976	8.9639375759
O140	-3.2529962290	-1.2418685583	10.2943324999
O141	-1.2909369037	-3.2245332998	10.3029210988
Ti142	-2.4563354915	2.4148552912	9.0137790805
O143	-3.6505261053	0.9055725209	8.9612455174
O144	-3.4207425931	3.3554637847	10.2926994890
O145	-1.4239887141	1.4617296406	10.4625663064
Ti146	2.3984111614	-2.4478880820	9.0294583272
O147	0.8872789174	-3.6276331407	8.9751467776
O148	1.4376696947	-1.4044698048	10.4696262699
O149	3.3353227241	-3.3992884717	10.3238904747
O150	0.8683682949	0.8852266236	8.9786618959
H151	-7.7902676803	-1.2913810792	8.1118767941
H152	-4.2267150124	3.1100725521	10.7811493166
H153	-1.2980846723	-7.7736331522	8.1510855423
H154	3.0758239932	-4.1885016200	10.8319204087
H155	-5.7908247337	-2.4967804749	8.1483060155
H156	-1.5847202408	1.8393693185	11.3464289221

H157	-2.4950423990	-5.7310767012	8.1780115067
H158	1.8357482181	-1.5313493356	11.3501591678
H159	-2.7119289173	-1.0898826908	11.1114684709
H160	-1.1316557671	-2.6793942455	11.1163894787
H161	-6.2264274359	-6.0688975293	9.4377019195
H162	-4.0076012062	-3.9416994433	9.8560914548
H163	-1.2086290986	-4.9966188245	9.7003073171
H164	0.1297512749	-3.4169016115	9.6374370747
H165	-0.9327943166	-0.9128887368	12.7907838259
H166	0.9295724453	0.9656677073	12.7762538280
H167	-3.4455285217	0.1445751080	9.6337469836
H168	-5.0447554960	-1.1898147337	9.6652777826
H169	-7.6179687394	-1.0392620302	0.8607732450
H170	-1.1959322496	-7.6779703505	0.8795673703
H171	-6.5096888961	-5.7438142779	-0.3072787789
H172	-3.9461157641	-4.0023099993	-0.8864973152
H173	-1.1803047972	-5.0302401953	-0.7256851432
H174	0.1123835449	-3.4178377195	-0.6702229661
H175	-0.8739353139	-0.9635791116	-3.8162146204
H176	0.9369202320	0.9747340983	-3.8020844091
H177	-3.4624241461	0.2059738499	-0.6520221437
H178	-5.0295073165	-1.2186113795	-0.7263898984
H179	-5.8048189215	-2.5461529636	0.8018058831
H180	-2.4774522761	-5.7557124565	0.7844567306
H181	-3.0699237047	4.2418651261	-1.7927852825
H182	-1.8219772033	1.5311043306	-2.4024480013
H183	1.9074715578	-1.4873056229	-2.3733386120
H184	3.1065496177	-4.2048771901	-1.8446938781
H185	-2.6745080470	-1.0889505898	-2.1497207102
H186	-1.1092586309	-2.7063147410	-2.1372975621
O187	1.3149488387	3.2358021733	-1.3116545157
O188	3.2659362788	1.2607893229	-1.3107388523
O189	-0.8692643345	3.6292553602	-0.0060262047
Ti190	0.1152652163	4.5668388598	1.5229951600
O191	3.6791311540	-0.9481301158	0.0401841898
Ti192	4.6409591579	0.0454949585	1.4923190294
Ti193	2.3585162573	2.2971855144	0.0446908903
O194	3.7526897969	3.6916977816	0.0525613809
Ti195	4.7967380206	4.7823727522	1.5546111302
O196	1.3946502254	3.1643918983	1.4811587459
O197	3.1927190413	1.3445548076	1.4978075369
O198	1.0430558261	5.5490713757	0.1624731394
O199	1.1846165945	7.8545493737	1.7033036661
O200	3.2380098114	5.9912790958	1.5475080063
O201	5.5387721703	1.0397323971	0.1687632485
O202	6.0481971780	3.2178411014	1.5605490939
O203	7.9810187033	1.2904310701	1.8585239010
O204	5.7056265894	5.6921779164	0.2701174747
O205	-0.9055872674	3.6573819641	2.9777785429
O206	3.6552338176	-0.9377135824	3.0032794123
Ti207	2.3040616598	2.2289423172	3.0710373505
O208	3.6572930142	3.6373915012	2.9497582730
Ti209	2.1741663270	6.9117249334	2.9749113392
O210	0.8728757705	5.4757817281	3.0014014395

Ti211	6.7862639926	2.1758466732	3.0796678693
O212	5.4967985102	0.8493982677	3.0208672965
O213	5.4845122836	5.4244467855	3.0900475190
Ti214	-0.2451092027	4.6191815294	4.4719311235
Ti215	4.5777403716	-0.2851056999	4.4937512952
Ti216	4.3142135317	4.4360335983	4.4670701372
O217	1.3984031106	3.1325645922	4.4830425570
O218	3.1713793388	1.3674748347	4.4873480382
O219	1.6580867584	7.8443184664	4.4442167355
O220	3.1139525091	5.8586980465	4.4947266445
O221	5.9409593053	3.2230016247	4.5110894387
O222	7.8411416725	1.6836238202	4.5092866443
O223	-0.9332076346	3.6506224973	5.9622299504
Ti224	0.0338631049	4.6715058969	7.4762056480
O225	3.6500024216	-0.9378595345	5.9770820346
Ti226	4.6308178529	0.0583635474	7.4941699026
Ti227	2.2784944326	2.3162868185	5.9551396746
O228	3.6540738358	3.6542953664	6.0292099854
Ti229	4.7601942358	4.8070259834	7.4423459036
O230	1.3615196335	3.1652428029	7.4570225421
O231	3.1696569403	1.3585711212	7.4735197866
Ti232	2.1842460529	6.8220242807	5.9017403132
O233	0.8345625673	5.5112933160	5.9655247494
O234	1.3749011183	8.0144755928	7.1192693451
O235	3.1817759144	5.9913060018	7.4145480042
Ti236	6.7958284990	2.1644780100	5.9482171706
O237	5.5022757050	0.8366158948	5.9728553144
O238	6.0072007561	3.2429012954	7.4202411119
O239	7.9586243771	1.3586001003	7.2063321405
O240	5.4519667037	5.4938500905	5.9161839180
O241	-0.9430262088	3.6624540342	8.9236007589
O242	3.6525813494	-0.9294855526	8.9446421710
Ti243	2.2957910960	2.3019396820	8.9155121607
O244	3.6988406450	3.7088463345	8.9162445397
O245	1.2624945218	3.2445994672	10.2688356668
O246	3.2313717002	1.2764496211	10.2775390979
O247	1.0439325939	5.4861888533	8.8234951100
O248	5.4938506408	1.0654154960	8.8252824566
O249	5.6542428718	5.6909028840	8.7340909481
H250	1.2495033688	7.8841811206	8.0787570377
H251	7.7146452199	1.1940211863	8.1401118142
H252	2.4986182556	5.7989696320	8.1359723396
H253	5.8097270013	2.5766761031	8.1525880301
H254	1.1033802231	2.6995167654	11.0829718236
H255	2.6820433578	1.1262735888	11.0915369784
H256	3.4435506126	-0.1871556293	9.6182693294
H257	4.9880843963	1.2559842953	9.6588269419
H258	3.9734225609	3.9800481760	9.8127217064
H259	5.9700040002	6.2013574354	9.4900667890
H260	1.2309172391	4.9764018233	9.6560623185
H261	-0.2027605496	3.4574142209	9.5997104137
H262	3.4799656863	-0.2110879926	-0.6386403429
H263	5.0623687057	1.2204278885	-0.6817344381
H264	4.0591559390	3.9749786609	-0.8302692743

H265	5.7532055890	6.5206637249	-0.2299263246
H266	1.2224214258	5.0701841551	-0.6847524165
H267	-0.1034579905	3.4236172508	-0.6653279611
H268	1.0377310474	7.4585896496	0.8119159921
H269	2.5619728101	5.7868170086	0.8261923490
H270	5.8531211424	2.5494303801	0.8294541148
H271	7.6967883587	1.1409671575	0.9315166186
H272	1.1578988600	2.6828040033	-2.1197528938
H273	2.7184995566	1.1045362997	-2.1273799091
O274	-5.6201978299	3.5411816728	0.1554114177
Ti275	-4.6541236443	4.4260171065	1.5206084223
O276	-7.9242118154	3.2523249720	1.6389700227
O277	-5.9768786700	1.3708649259	1.5839707823
O278	-4.8610068272	6.0185774640	0.5284057198
O279	-3.3597749200	7.7680635226	1.5635576688
O280	-1.3604888263	5.9623060368	1.5367605880
Ti281	-7.0832233015	2.4393724074	3.0037074354
O282	-5.6122889155	3.8254556010	2.9909113209
Ti283	-2.5375302828	6.9404153351	2.9011368590
O284	-3.8358976913	5.5165841847	2.9899238899
Ti285	-4.4464765954	4.4082754490	4.4681473059
O286	-7.8373579137	3.0893590045	4.4922100369
O287	-5.9522381617	1.4414644133	4.4072418816
O288	-3.0950236390	7.8325129675	4.4249519866
O289	-1.4595256718	5.9415169086	4.4539562634
Ti290	-7.0279309889	2.4899982137	6.0505484159
O291	-5.5099942835	3.7894905539	5.9216199239
Ti292	-4.4469745386	4.7020248674	7.3696761570
O293	-7.7640418073	3.4140976018	7.3494641318
O294	-6.0045147973	1.3778537640	7.4438770002
Ti295	-2.3968197907	7.1446062392	5.9259252705
O296	-3.8366824839	5.6163295129	5.9061095177
O297	-3.2242192550	7.9190293202	7.3018579671
O298	-1.3922170489	5.9678964267	7.3584667201
O299	-6.0820270677	5.0499938101	8.2482468423
O300	-3.5724424111	5.6032116487	8.7778913109
H301	-7.3264921262	4.2092577015	7.8151511930
H302	-3.5204484747	7.6700798536	8.1987281053
H303	-6.3397761509	1.5796645541	8.3381889714
H304	-2.0496063666	5.9102294625	8.1165588976
H305	-3.4317879467	5.1279753006	9.6355621097
H306	-6.1596773778	5.6992765441	8.9694500005
H307	-7.6474192983	3.5228699061	0.7404759098
H308	-5.4947521768	6.0911403961	-0.2073515727
H309	-5.1488221998	3.3966273204	-0.7032694592
H310	-5.9158235257	2.0134901379	0.8144678098
H311	-4.0840532335	7.3181137562	1.0136637071
H312	-1.5691733113	6.2831329867	0.6386431523
O313	4.9888109329	-6.0741260985	0.6732436190
Ti314	4.6959079912	-4.4399811809	1.5642112013
O315	1.3261508759	-6.0001133254	1.5572437206
O316	3.3664426047	-7.7748062286	1.6391815243
O317	5.6074959452	-3.5651019494	0.1668037890
O318	5.9674890786	-1.3928210231	1.6166588706

O319	7.9167525450	-3.2427080989	1.6435987171
Ti320	2.4814015805	-6.9808167368	2.9549973544
O321	3.7912873261	-5.5002794649	3.0237371776
Ti322	7.0634034307	-2.4515202006	3.0103973176
O323	5.6364966356	-3.8557825583	3.0299315767
Ti324	4.3605117091	-4.4866699322	4.5001142185
O325	1.4142983111	-5.9144170943	4.4581831687
O326	3.0833065099	-7.7783023887	4.4829344510
O327	5.9675459700	-1.4757862379	4.4682916372
O328	7.9077591263	-3.0522101328	4.4997686555
Ti329	2.4548760129	-7.0399463680	6.0281802205
O330	3.7715576605	-5.4866010584	5.9553039137
Ti331	4.7000806653	-4.4355748549	7.4026585555
O332	1.3397676415	-5.9991893963	7.4506365686
O333	3.3777546806	-7.7633137962	7.3417139420
Ti334	7.1201437664	-2.4073273432	6.0117882009
O335	5.6303537197	-3.8407635479	5.9463741773
O336	5.9511760717	-1.3884467703	7.3874752255
O337	7.8864429997	-3.2300474229	7.3906153545
O338	5.0279813307	-6.0822138729	8.2618060987
O339	5.5774188528	-3.5710825091	8.8288333631
H340	4.1637649316	-7.3320852791	7.8194426689
H341	7.6107563104	-3.5350445270	8.2782829323
H342	1.5876808889	-6.3186054947	8.3390699386
H343	5.8799309840	-2.0217719779	8.1618760082
H344	5.6612123761	-6.1732511972	8.9958671049
H345	5.0889508553	-3.4342502469	9.6809111884
H346	4.1314857938	-7.3466999771	1.1318024303
H347	5.6213951003	-6.1633686377	-0.0616439362
H348	5.1180104711	-3.4196598013	-0.6840716110
H349	1.5169308675	-6.3677643111	0.6730400395
H350	5.9187353869	-2.0176362119	0.8331577459
H351	7.6590279812	-3.5288882499	0.7446884927
Ti352	0.0188180627	-0.0059696825	-1.4631468259
O353	-0.9996061383	-0.9283915709	-2.8520103117
O354	1.0599146112	0.9428895098	-2.8372256186
Ti355	-0.0231333757	-0.0027219161	10.4333583806
O356	-0.9914484429	-0.9581182008	11.8208946739
O357	0.9824009750	0.9948409289	11.8048976504
Li358	6.9170771530	4.9746304071	4.5404325306

3.6 555 O_{Li}⁺/e⁻ cluster in vacuum[§]

358			
555	Li ⁺ /e ⁻ Surface , Vacuum-Optimized	SCFE : -17174.4412650516 hartree	
O1	-7.9048901472	-4.1269257278	3.1336589306
H2	-8.2167522720	-4.2494581607	4.0694109640
H3	-7.2320844119	-4.8291528730	2.9192131357
O4	-7.8559725625	-4.2714786197	5.8397203610
H5	-8.4902670190	-4.3923984036	6.5699241311
H6	-7.0466263453	-4.8964462782	5.9247592552
O7	-4.1440870047	-7.8901173807	2.9046213564

[§]Li⁺ is adsorbed on surface, and one additional electron is added

H8	-4.2774227201	-8.3638796566	2.0633830327
H9	-4.8460098994	-7.1847384629	3.0276797877
O10	-4.1775905605	-7.8599244896	6.0390835020
H11	-4.3382350205	-8.4090551281	6.8266819680
H12	-4.8752131991	-7.1450529921	5.9350780790
O13	4.0611360053	7.9518632121	3.1340185771
H14	4.1908293978	8.2331871583	4.0799726917
H15	4.7735506411	7.3090230764	2.8856545576
O16	4.2537307032	7.8728081183	5.8135380404
H17	4.3620451753	8.4965568021	6.5547902975
H18	4.8788680182	7.0625100988	5.9049791513
O19	8.1023125186	4.1558423047	2.9542602879
H20	9.0276319942	3.8971745501	2.7981989492
H21	7.6798423657	4.4998900534	2.1317804283
O22	8.1058104778	4.1333032016	6.1003401199
H23	9.0434892931	3.8659960255	6.1837326068
H24	7.7123451404	4.3858505543	6.9606958401
O25	-8.5578607138	0.8876877243	3.0203926749
H26	-9.4415436788	1.2436277408	2.8093798149
H27	-8.3539406555	0.0018277865	2.4990260008
O28	-8.3014716372	0.8720995537	5.8712863177
H29	-8.5466437440	0.6547021763	4.9381975892
H30	-8.2669471493	0.0336488193	6.4398277568
O31	0.9308202880	-8.4843900519	2.9510377597
H32	1.2771346101	-9.3869270592	2.8246345717
H33	0.0226879394	-8.3302163299	2.4681434277
O34	0.8473344247	-8.3022370091	5.8666091731
H35	0.5840046862	-8.4862759700	4.9328199584
H36	0.0331217025	-8.2813070601	6.4677560544
O37	-0.9905267389	8.4683841468	2.8988315881
H38	-1.3781221163	9.3458151464	2.7231730139
H39	-0.1129890810	8.2986810789	2.3720816423
O40	-0.7997681296	8.3516505726	5.7466082990
H41	-0.5441346326	8.5199854877	4.8053516703
H42	0.0191440190	8.3572113404	6.3643811470
O43	8.5257699735	-0.8830435076	3.0326328196
H44	9.4017685345	-1.2696219596	2.8446271856
H45	8.3672968812	0.0256147728	2.5184032931
O46	8.3403034535	-0.8094433735	5.8465927004
H47	8.5243426998	-0.5447989166	4.9091493114
H48	8.3238914465	-0.0023532554	6.4698765847
O49	-3.2468177693	-1.2729295916	-1.3384093442
O50	-1.2683583097	-3.2671157649	-1.3211665469
O51	-3.3560471170	3.4082232933	-1.3344889805
O52	-1.4418782942	1.4114706861	-1.5229339722
O53	1.4524971326	-1.4404188517	-1.5080765698
O54	3.3608236285	-3.4356246194	-1.3211562758
O55	-5.6723850652	-5.6394067131	0.1547859755
Ti56	-4.7442163759	-4.7831342842	1.4614856657
O57	-5.5262742819	-1.0467316972	0.1229628679
Ti58	-4.6792419532	-0.0747206249	1.4938632225
O59	-7.9149999606	-1.2237284924	1.7787113101
O60	-5.9944043811	-3.2302655887	1.5218315111
O61	-1.0012048252	-5.5404742418	0.1220642893

Ti62	-0.1190541326	-4.5946707173	1.5149746708
O63	-3.1831900812	-5.9472640982	1.4851409409
O64	-1.3056830997	-7.9524325924	1.8085579584
Ti65	-2.3203942466	-2.2667543493	0.0330553408
O66	-0.8705816497	-0.9062047291	-0.0557941881
O67	-3.7108379454	-3.6872776843	0.0108310563
Ti68	0.0563937319	0.0416910410	1.5347543244
O69	-3.1810463705	-1.3792940338	1.4812232247
O70	-1.3875449193	-3.1883203133	1.4787006263
Ti71	-2.3836958276	2.4271920329	-0.0798308983
O72	-3.6615124623	0.9430814360	0.0215593120
O73	-3.1983968199	3.2503424925	1.4614815145
O74	-1.4002012855	1.4177626028	1.4659416105
Ti75	2.3946441876	-2.4605682634	-0.0554201843
O76	0.8844481623	-3.6319272719	0.0004175227
O77	1.4155391528	-1.4281713274	1.4775848918
O78	3.2045800306	-3.2683415625	1.4812260630
O79	0.8665006691	0.8705060660	-0.0364824461
O80	-5.4668782349	-5.4862937870	2.9947385148
Ti81	-6.9015289827	-2.2465279237	3.0010648441
O82	-5.4985766329	-0.8791439975	2.9800731334
Ti83	-2.2499123650	-6.8598489279	3.0574917028
O84	-0.9142516053	-5.4784012988	3.0054710635
Ti85	-2.3814409235	-2.3260361371	3.0395526517
O86	-0.8840619020	-0.8739694480	2.9760907781
O87	-3.6765558022	-3.6732213468	2.9733145383
Ti88	-2.1932452008	2.1665856478	2.9160277892
O89	-3.6571981387	0.9154537619	2.9752036916
Ti90	2.1600523564	-2.2204214704	2.9341936453
O91	0.8966734356	-3.6786461011	2.9786080273
O92	0.8833961395	0.8616123822	2.9559082277
Ti93	-4.5523100318	-4.5223204796	4.4504902819
Ti94	-4.6341760125	0.2228754267	4.4622044177
O95	-7.8494686028	-1.7135877522	4.4617293013
O96	-5.8581516152	-3.1562793331	4.4894397831
Ti97	0.1799762133	-4.6478866348	4.4859083806
O98	-3.2206287299	-5.9362614925	4.4912581227
O99	-1.6227672282	-7.8022837382	4.4943803513
Ti100	-0.0734279185	-0.0715321434	4.4899562933
O101	-3.1836089617	-1.3963580792	4.4792094983
O102	-1.4143706390	-3.1599560361	4.4824879204
O103	-3.1974366541	3.1849599641	4.4626886049
O104	-1.4165471299	1.3848155312	4.4773478381
O105	1.3673806850	-1.4346091346	4.4874877105
O106	3.1752438841	-3.1897369765	4.4882559894
O107	-5.5143728922	-5.4665365101	5.9680166219
Ti108	-4.7637414979	-4.7655309221	7.48944449243
Ti109	-6.8143506860	-2.2182411026	5.9151308177
O110	-5.5117349847	-0.8543932131	5.9561901758
Ti111	-4.6039814009	-0.0711502839	7.4482011627
O112	-7.9674844363	-1.3913283451	7.1647364089
O113	-5.9609708504	-3.1875227537	7.4284598750
Ti114	-2.2667248745	-6.8687158149	5.9402804579
O115	-0.8978691519	-5.4942789807	5.9836399400

Ti116	-0.1021123501	-4.6255369581	7.4618137954
O117	-3.1897382513	-5.9118131522	7.4678980175
O118	-1.3945959064	-7.9578001158	7.2057790524
Ti119	-2.3664238225	-2.3827543188	5.9128678584
O120	-0.8869871650	-0.8777420065	5.9826345016
O121	-3.6752300498	-3.6856988194	5.9896388736
Ti122	0.0376900345	0.0495763140	7.4282553648
O123	-3.2011491296	-1.3668311189	7.4814962963
O124	-1.3993978910	-3.1795943350	7.4914600712
Ti125	-2.1883982197	2.2002589647	6.0300364881
O126	-3.7022878968	0.9243853662	5.9703505928
O127	-3.2595639521	3.2140040529	7.4768896085
O128	-1.4369585265	1.4067948331	7.4824579491
Ti129	2.1561780847	-2.2186323118	6.0478337203
O130	0.8964758621	-3.6870399853	6.0018818514
O131	1.3952701592	-1.4260320697	7.4950817919
O132	3.1991876674	-3.2492248683	7.5023202335
O133	0.8665058698	0.8619026948	6.0039346422
O134	-5.6666234628	-5.6369655392	8.7819572201
O135	-5.5487234811	-1.0047486216	8.8159233497
O136	-1.0265672437	-5.5123569280	8.8581189556
Ti137	-2.3123003487	-2.2883164934	8.9301916323
O138	-0.9022665162	-0.8829392625	9.0305219361
O139	-3.7279309351	-3.6701095316	8.9572087902
O140	-3.2692424886	-1.2534677755	10.2950358077
O141	-1.3021136601	-3.2410755712	10.3037676195
Ti142	-2.4491551268	2.4154242957	9.0110691827
O143	-3.6625677039	0.9054916392	8.9576520013
O144	-3.4380804853	3.3533875189	10.2848465842
O145	-1.4418941129	1.4514475246	10.4644598596
Ti146	2.3930640135	-2.4377353172	9.0294614172
O147	0.8856859995	-3.6374828645	8.9758212485
O148	1.4259286103	-1.4184342391	10.4738892466
O149	3.3350559854	-3.4081894966	10.3178117353
O150	0.8541742082	0.8718872547	8.9869102538
H151	-7.7167765403	-1.2657094143	8.1034471022
H152	-4.2621751648	3.0757351808	10.7241770184
H153	-1.2681121524	-7.7055410494	8.1434264233
H154	3.0496825263	-4.2156414506	10.7822924647
H155	-5.7856059697	-2.4940696266	8.1423639058
H156	-1.6000001871	1.8256223256	11.3498869657
H157	-2.4926648450	-5.7305502220	8.1743504581
H158	1.8243626054	-1.5364453171	11.3550890574
H159	-2.7166181462	-1.1019765738	11.1072929126
H160	-1.1461086840	-2.6846847839	11.1129654083
H161	-6.2656390524	-6.0236031968	9.4304436081
H162	-4.0074853932	-3.9446055549	9.8503455400
H163	-1.2116889190	-5.0041407582	9.6903936563
H164	0.1279452005	-3.4285025233	9.6373074248
H165	-0.9443348782	-0.9242128490	12.7778944581
H166	0.8933646841	0.9430454713	12.7879541376
H167	-3.4584159108	0.1460536927	9.6288426314
H168	-5.0485526278	-1.1930162289	9.6512343106
H169	-7.5914194830	-1.0358837562	0.8707578731

H170	-1.1775746666	-7.6375675299	0.8878023656
H171	-6.5573865069	-5.6622834796	-0.2414204408
H172	-3.9471873619	-4.0105518339	-0.8793297898
H173	-1.1886139362	-5.0363393528	-0.7127280518
H174	0.1103326133	-3.4298908929	-0.6675380362
H175	-0.8825023046	-0.9828718725	-3.8067594129
H176	0.8930817825	0.9501659558	-3.8103295200
H177	-3.4752355967	0.2029383429	-0.6524789625
H178	-5.0295338813	-1.2301504194	-0.7153960472
H179	-5.8058867484	-2.5473173905	0.8049609312
H180	-2.4776093690	-5.7642185389	0.7874597076
H181	-3.0797492009	4.2331629469	-1.7736749195
H182	-1.8632335418	1.4813232035	-2.3987322493
H183	1.8973496401	-1.4856100096	-2.3740262475
H184	3.0778611976	-4.2381202460	-1.7956208884
H185	-2.6918286071	-1.1100380886	-2.1496054773
H186	-1.1203400990	-2.7169865323	-2.1314980909
O187	1.2842229605	3.2091392763	-1.3380810168
O188	3.2428215864	1.2284775621	-1.3316444138
O189	-0.8838905705	3.6257023269	-0.0268082637
Ti190	0.1223750451	4.5681601759	1.5165445025
O191	3.6723674602	-0.9574107413	0.0252950893
Ti192	4.6265522254	0.0611209490	1.4808473240
Ti193	2.3612977354	2.3054272596	0.0164691690
O194	3.7363353879	3.6705889275	0.0050751504
Ti195	4.7919924017	4.7763391445	1.5633745029
O196	1.3794668194	3.1598004483	1.4502445773
O197	3.1882336795	1.3318038524	1.4666158781
O198	1.0225911809	5.5594197677	0.1477126598
O199	1.1788941179	7.8595476535	1.7116401594
O200	3.2460543848	6.0203652957	1.5410596206
O201	5.5453591346	1.0213427724	0.1484608605
O202	6.0763871880	3.2129454434	1.5505651314
O203	8.0129945943	1.2896715316	1.8711889136
O204	5.6386747441	5.6263488311	0.1603470504
O205	-0.9044448685	3.6502171489	2.9797851053
O206	3.6422198632	-0.9307519130	3.0075077130
Ti207	2.3839400730	2.3235687248	3.0562000210
O208	3.6530190219	3.6291549921	2.8408145350
Ti209	2.1893056733	6.9215193785	2.9874823407
O210	0.8750185509	5.4722527619	2.9893924763
Ti211	6.7913121207	2.1770644133	3.0783372441
O212	5.4963910315	0.8607182426	3.0092734008
O213	5.5656066925	5.4797073786	3.0058736397
Ti214	-0.2248077364	4.6121259184	4.4674154149
Ti215	4.5560430644	-0.2626272612	4.4936433018
Ti216	4.4001566565	4.4950304367	4.4752489614
O217	1.4223424956	3.1649635530	4.4816040102
O218	3.2059688415	1.3928939714	4.4898556760
O219	1.6547694875	7.8629039095	4.4438767860
O220	3.1050876370	5.8872581048	4.4927260319
O221	5.9759048608	3.2365021332	4.5075106757
O222	7.8444932382	1.6687329302	4.5149489347
O223	-0.9274283763	3.6400063813	5.9563852132

Ti224	0.0555414501	4.6594744042	7.4788397266
O225	3.6364525291	-0.9331170834	5.9717001802
Ti226	4.6143924234	0.0727663664	7.5060553475
Ti227	2.3509670247	2.3774385786	5.9390413547
O228	3.6514919020	3.6502126348	6.1360833690
Ti229	4.7563369750	4.8031098912	7.4338031921
O230	1.3497771929	3.1611527116	7.4840788047
O231	3.1686134231	1.3405070079	7.5018150510
Ti232	2.2015211919	6.8174497450	5.8947875706
O233	0.8394035422	5.5074909297	5.9745682512
O234	1.3599689628	8.0308686636	7.1031407700
O235	3.1792656031	6.0191310304	7.4276023739
Ti236	6.7991814408	2.1560230061	5.9492321427
O237	5.4958038808	0.8442344596	5.9824992934
O238	6.0352689627	3.2476979561	7.4316101071
O239	7.9628915374	1.3447576306	7.2158537650
O240	5.4982449545	5.5432281003	5.9661438754
O241	-0.9518581107	3.6576079772	8.9375129625
O242	3.6487708489	-0.9330122429	8.9617169736
Ti243	2.2920715808	2.3090205587	8.9207719246
O244	3.6860026658	3.6951009259	8.9543338273
O245	1.2370119794	3.2302233289	10.2835118253
O246	3.2173802613	1.2519772459	10.2897830509
O247	1.0322018504	5.4916875593	8.8399090549
O248	5.5085408397	1.0558152305	8.8386145777
O249	5.6190148786	5.6615208305	8.7827421876
H250	1.2345321230	7.8650244525	8.0578153846
H251	7.6715363104	1.1741615994	8.1366895241
H252	2.5046091766	5.8235355545	8.1517094529
H253	5.8315866488	2.5909373203	8.1668777421
H254	1.0733469259	2.6702898512	11.0871587925
H255	2.6577730169	1.0985001287	11.0952164231
H256	3.4334984574	-0.1785999125	9.6320012976
H257	5.0009536581	1.2426835167	9.6717165595
H258	3.9801216086	3.9653151641	9.8439826604
H259	5.8531421944	6.1494091442	9.5808992486
H260	1.2152333486	4.9797376310	9.6714994028
H261	-0.2010745018	3.4460140592	9.6066289397
H262	3.4678575931	-0.2132508916	-0.6513500374
H263	5.0679619071	1.2104358298	-0.6988244603
H264	4.0855577606	3.9864076184	-0.8502454029
H265	5.6241624066	6.5098797982	-0.2404616435
H266	1.2101461975	5.0855837545	-0.6989021785
H267	-0.1095913404	3.4156965270	-0.6814066370
H268	1.0299459155	7.4473846721	0.8277338370
H269	2.5796567906	5.8134851102	0.8183084829
H270	5.8788952077	2.5568476107	0.8137948565
H271	7.7238765113	1.1453546988	0.9448105864
H272	1.1192650466	2.6356295376	-2.1314706659
H273	2.6823688155	1.0692787942	-2.1398939768
O274	-5.6315987427	3.5467254046	0.1566008939
Ti275	-4.6567354750	4.4214584764	1.5274866566
O276	-7.9278219482	3.2411032127	1.6293247302
O277	-5.9827940844	1.3655804016	1.5832036986

O278	-4.8624988034	6.0189130943	0.5359646005
O279	-3.3637077751	7.7689888569	1.5780338865
O280	-1.3729186471	5.9498828972	1.5377923524
Ti281	-7.0874196510	2.4323480359	3.0058046254
O282	-5.6226454654	3.8234986533	2.9937234348
Ti283	-2.5336623611	6.9321121366	2.9106405142
O284	-3.8430969764	5.5122822242	2.9954961469
Ti285	-4.4522873056	4.4051907837	4.4720422213
O286	-7.8539656705	3.0795073348	4.4891507549
O287	-5.9604239794	1.4398739071	4.4063009839
O288	-3.0915085144	7.8225088778	4.4349431959
O289	-1.4512756707	5.9326367956	4.4563609478
Ti290	-7.0376302388	2.4823574888	6.0479267411
O291	-5.5255239283	3.7857440114	5.9233898808
Ti292	-4.4537103530	4.6893020924	7.3707904986
O293	-7.7839715389	3.4030905152	7.3466599237
O294	-6.0213525821	1.3665875837	7.4363357358
Ti295	-2.3824988492	7.1337783487	5.9338182441
O296	-3.8459604478	5.6083926234	5.9111949938
O297	-3.2188031924	7.8970481350	7.3177527896
O298	-1.3931678761	5.9486802785	7.3578115561
O299	-6.0958263331	5.0231928515	8.2580853796
O300	-3.5978778725	5.6073371030	8.7847871029
H301	-7.3293872285	4.1866921342	7.8196657087
H302	-3.5086840138	7.5758306392	8.1967773443
H303	-6.3582420099	1.5562362294	8.3323904331
H304	-2.0396635770	5.8887061060	8.1202140435
H305	-3.4512214652	5.1187882526	9.6349531289
H306	-6.1569142392	5.6654827697	8.9867520988
H307	-7.6012933199	3.5004680864	0.7422119289
H308	-5.4910406289	6.0754447318	-0.2053658054
H309	-5.1383527328	3.3940199487	-0.6906630441
H310	-5.9184484694	2.0063158741	0.8137350542
H311	-4.0867984770	7.3138684055	1.0313539438
H312	-1.5885961368	6.2649897371	0.6396443174
O313	4.9663866235	-6.0817160543	0.6704234614
Ti314	4.6857275114	-4.4414451663	1.5686500559
O315	1.3266085960	-6.0064077624	1.5605479014
O316	3.3584212484	-7.7908632610	1.6395874582
O317	5.6119087792	-3.5852423891	0.1653759925
O318	5.9501045296	-1.3926640597	1.6215390545
O319	7.8915097532	-3.2391335631	1.6432974615
Ti320	2.4784348888	-6.9857372511	2.9575536210
O321	3.7914907104	-5.5135709103	3.0259839903
Ti322	7.0443348579	-2.4385823232	3.0175034048
O323	5.6247976912	-3.8590900494	3.0345689970
Ti324	4.3556622878	-4.4914261765	4.5023135958
O325	1.4159930926	-5.9231048616	4.4592083742
O326	3.0770597991	-7.7934255423	4.4845769938
O327	5.9550586608	-1.4628793920	4.4681871898
O328	7.8928193330	-3.0488132932	4.5028273398
Ti329	2.4513959190	-7.0482566388	6.0282740515
O330	3.7701170124	-5.4997796024	5.9579810149
Ti331	4.6871992668	-4.4364776655	7.4021202964

O332	1.3368966494	-6.0073907630	7.4479576381
O333	3.3707191673	-7.7788117003	7.3456541023
Ti334	7.1059770828	-2.3960869672	6.0128778381
O335	5.6211049037	-3.8448579333	5.9486312576
O336	5.9359910975	-1.3872329020	7.3831996736
O337	7.8665652260	-3.2235009130	7.3998689107
O338	5.0114972004	-6.0855786293	8.2718004492
O339	5.5827327450	-3.5833770947	8.8314499628
H340	4.1405740553	-7.3303373760	7.8348448890
H341	7.5268520096	-3.5126506098	8.2739755790
H342	1.5805287614	-6.3254072902	8.3379015837
H343	5.8657673434	-2.0133120276	8.1608743019
H344	5.6393297428	-6.1552368597	9.0124471444
H345	5.0784496224	-3.4356693791	9.6735866882
H346	4.1179938885	-7.3497626074	1.1327211103
H347	5.5917324464	-6.1525790217	-0.0723410208
H348	5.1107492803	-3.4362884753	-0.6789075857
H349	1.5129700443	-6.3728130933	0.6751920017
H350	5.9066489869	-2.0077363464	0.8338511665
H351	7.5788154248	-3.5188827199	0.7575015157
Ti352	-0.0022165100	-0.0268814702	-1.4484434774
O353	-1.0379134577	-0.9562988803	-2.8465439728
O354	1.0386098646	0.9112287000	-2.8491243339
Ti355	-0.0366526367	-0.0126140732	10.4200667520
O356	-1.0215193387	-0.9861619840	11.8101594475
O357	0.9546119532	0.9774786882	11.8175353907
Li358	6.9966410446	4.9667291733	4.5534866410

3.7 555 neutral cluster in water

357			
555 neutral	Water-Optimized	SCFE : -17167.2408186093	hartree
O1	-7.8794262882	-4.1329834479	3.1749403852
H2	-8.1652339205	-4.2527128493	4.1263927924
H3	-7.1956124659	-4.8307349668	2.9724643477
O4	-7.8961125401	-4.2109928890	5.8578289376
H5	-8.6625363471	-4.4112721780	6.4330077210
H6	-7.1517773427	-4.8814495198	5.9758244432
O7	-4.1370736224	-7.9161691251	2.9102363491
H8	-4.3099450128	-8.4481326030	2.1077374542
H9	-4.8559430055	-7.2377063717	3.0369155089
O10	-4.1702997165	-7.8833517714	6.0987349295
H11	-4.3523110592	-8.4261201695	6.8917786319
H12	-4.8856489957	-7.1988884990	5.9735843451
O13	4.1300756629	7.8522143997	3.1556258572
H14	4.2578423196	8.1423542682	4.1047867120
H15	4.8273210235	7.1673264757	2.9541443602
O16	4.2495749264	7.8579408276	5.8340992564
H17	4.4551584536	8.6237899764	6.4074654064
H18	4.9187690737	7.1095938389	5.9456428514
O19	7.8978054617	4.1220953737	2.8968170618
H20	8.4035043596	4.2955626214	2.0774946800
H21	7.2140330844	4.8355880912	3.0356879804
O22	7.8693000132	4.1513451698	6.0684462328

H23	8.4297504674	4.3298497417	6.8498279922
H24	7.1800651036	4.8667958366	5.9590587609
O25	-8.4848082291	0.8962915676	2.9664507288
H26	-9.4014315628	1.2087584604	2.8215171292
H27	-8.3160283040	0.0130560222	2.4528827973
O28	-8.2864519999	0.8639437534	5.8088543919
H29	-8.4656893528	0.6012634441	4.8692680019
H30	-8.2377356247	0.0439942239	6.4119434590
O31	0.9115296877	-8.4718846828	3.0066924537
H32	1.2094397842	-9.3998963550	2.9185307660
H33	0.0258922973	-8.3197425237	2.5053751484
O34	0.8313630004	-8.2651615832	5.8614836233
H35	0.5625493100	-8.4281498465	4.9208399183
H36	0.0127490535	-8.2085762323	6.4645170825
O37	-0.9105292457	8.4522131648	2.9626736214
H38	-1.2198915524	9.3724489091	2.8394789026
H39	-0.0465169701	8.2840606046	2.4301130021
O40	-0.7687267090	8.2905103255	5.7849428672
H41	-0.4984418121	8.4438929801	4.8410501396
H42	0.0480911229	8.2731708290	6.4055008080
O43	8.4734151592	-0.8768917790	2.9874508340
H44	9.3989263174	-1.1820045687	2.8973499054
H45	8.3295265534	0.0105778173	2.4750937000
O46	8.2839539501	-0.7745216636	5.8489192236
H47	8.4318066862	-0.4678261025	4.9169633016
H48	8.2542306480	0.0336283931	6.4814082804
O49	-3.1990875382	-1.2688159396	-1.3586941077
O50	-1.2450382132	-3.2421016875	-1.3311999455
O51	-3.2814280586	3.3825409851	-1.3768206799
O52	-1.4216235216	1.4084425793	-1.5494791741
O53	1.4573281683	-1.4542363237	-1.5351594651
O54	3.3042541071	-3.4425494851	-1.3506969731
O55	-5.7128522130	-5.5907194252	0.1828676375
Ti56	-4.7357561035	-4.7541156116	1.4754919514
O57	-5.4833025872	-1.0601778034	0.1039856613
Ti58	-4.6233339695	-0.0938032720	1.4729234362
O59	-7.9342610822	-1.3016906974	1.7829125087
O60	-5.9768618539	-3.2036367663	1.5301379367
O61	-1.0344618145	-5.5058806850	0.1237745346
Ti62	-0.1183152196	-4.5842228824	1.5100859760
O63	-3.1871887986	-5.9329301612	1.4869595476
O64	-1.3357449050	-7.9636823824	1.8275888409
Ti65	-2.2982201291	-2.2682492370	0.0118272902
O66	-0.8612287794	-0.8994678935	-0.0414938057
O67	-3.7027669080	-3.6724868605	0.0044860188
Ti68	0.0249824643	0.0002364675	1.5092199179
O69	-3.1701669659	-1.3771172042	1.4772983401
O70	-1.3930360108	-3.1811804591	1.4858692655
Ti71	-2.3570315945	2.4143531246	-0.1457868751
O72	-3.6401640199	0.9252480361	0.0117094422
O73	-3.1513941669	3.2319685759	1.4491360084
O74	-1.3890650137	1.4020597737	1.4549686574
Ti75	2.3912341394	-2.4687748393	-0.1165579234
O76	0.8694757806	-3.6415727472	0.0233046906

O77	1.4055298428	-1.4261676771	1.4737554378
O78	3.1763717569	-3.2630116341	1.4746162414
O79	0.8792216728	0.8659863371	-0.0302195161
O80	-5.4586696052	-5.4516673702	3.0071315537
Ti81	-6.8470592863	-2.2314024160	3.0338718637
O82	-5.4860069907	-0.8788093585	2.9722701722
Ti83	-2.2538303892	-6.8401563466	3.0570243855
O84	-0.9253899995	-5.4769664049	3.0081330299
Ti85	-2.3592018194	-2.3251179120	3.0357485888
O86	-0.8829785940	-0.8781079475	2.9730686582
O87	-3.6662994949	-3.6610458815	2.9902993216
Ti88	-2.1679652135	2.1534599203	2.9015706939
O89	-3.6277991985	0.8922359840	2.9741801411
Ti90	2.1609955931	-2.1968872741	2.9209272756
O91	0.8804081329	-3.6646445299	2.9841934587
O92	0.8810089119	0.8623429883	2.9601461673
Ti93	-4.5464285375	-4.5177389554	4.4797920258
Ti94	-4.5771519688	0.1920262599	4.4573400032
O95	-7.8351520980	-1.6918573813	4.4762658799
O96	-5.8522058228	-3.1389053205	4.5121976177
Ti97	0.1563769512	-4.5970110806	4.4860382615
O98	-3.2309171236	-5.9313718455	4.5051816128
O99	-1.6563960585	-7.7951770987	4.5093467751
Ti100	-0.0422168445	-0.0474536338	4.4982610718
O101	-3.1789200213	-1.3857915796	4.4800097470
O102	-1.4052153887	-3.1544112234	4.4819240282
O103	-3.1744099720	3.1757356997	4.4557657437
O104	-1.4032335892	1.3874148603	4.4757085241
O105	1.3743378376	-1.4216386310	4.4830763706
O106	3.1682426613	-3.1762200089	4.4837090932
O107	-5.4922847665	-5.4372005106	5.9892831159
Ti108	-4.7638911032	-4.7442203374	7.5196311763
Ti109	-6.7991851868	-2.2153453164	5.9387588935
O110	-5.4964606450	-0.8569174193	5.9618855818
Ti111	-4.5833421758	-0.0719186953	7.4544788332
O112	-7.9595653569	-1.3364481166	7.1606464738
O113	-5.9525825618	-3.1585900179	7.4491821744
Ti114	-2.2813436525	-6.8237899515	5.9592913542
O115	-0.9118893801	-5.4775659491	5.9866229527
Ti116	-0.1104385539	-4.5862618447	7.4676338389
O117	-3.1806762791	-5.8935814736	7.4920685171
O118	-1.3863587854	-7.9541175120	7.1964255073
Ti119	-2.3584770187	-2.3590017664	5.9236370089
O120	-0.8881299876	-0.8761222429	5.9822827228
O121	-3.6599604483	-3.6669994792	5.9955335348
Ti122	0.0154812782	0.0252448263	7.4595393269
O123	-3.1887697848	-1.3612404908	7.4789618568
O124	-1.4005858046	-3.1650599980	7.4896303207
Ti125	-2.1732536258	2.1793938354	6.0391435565
O126	-3.6729227881	0.9121457908	5.9612488773
O127	-3.2463044034	3.1846013037	7.4803803898
O128	-1.4266004311	1.3999696087	7.4874309562
Ti129	2.1579230634	-2.1880333224	6.0545763513
O130	0.8831006981	-3.6656170083	5.9872905757

O131	1.3852909732	-1.4142512780	7.4906105235
O132	3.1677828668	-3.2338222708	7.5044699552
O133	0.8621566351	0.8615234600	5.9942409821
O134	-5.6700596080	-5.6020823109	8.8075533595
O135	-5.5191384667	-1.0049476148	8.8210022103
O136	-1.0376101815	-5.4708661580	8.8653954828
Ti137	-2.2970939316	-2.2677470397	8.9509918202
O138	-0.8897399477	-0.8758093253	9.0129297444
O139	-3.7157681248	-3.6449674007	8.9777530791
O140	-3.2393438894	-1.2209936719	10.3050139780
O141	-1.2900514199	-3.2038439239	10.3228532132
Ti142	-2.4428595994	2.4017422022	9.0768267362
O143	-3.6502875002	0.8944938365	8.9443610302
O144	-3.4332291944	3.3155634031	10.2989979138
O145	-1.4490034549	1.4493094845	10.4920828445
Ti146	2.3789907349	-2.4325714481	9.0904864721
O147	0.8609488091	-3.6182401172	8.9656417141
O148	1.4302122341	-1.4189728650	10.5036021116
O149	3.2951286785	-3.4080714563	10.3268091170
O150	0.8565585916	0.8785968238	8.9833896262
H151	-7.7155244217	-1.1838933138	8.0988469838
H152	-4.2486766777	3.1515896782	10.8114401859
H153	-1.2634413465	-7.7280215661	8.1426869201
H154	3.1191234372	-4.2039575944	10.8661741950
H155	-5.7725616185	-2.4614017863	8.1647223441
H156	-1.6740555744	1.7314056850	11.4010688441
H157	-2.4749173294	-5.7006164544	8.1942703024
H158	1.7471552492	-1.6009397096	11.4100913920
H159	-2.6798194280	-1.0440013447	11.1100824753
H160	-1.1012731144	-2.6391724073	11.1224451740
H161	-6.2393163905	-5.9984708101	9.4882099326
H162	-4.0138531079	-3.9108825398	9.8709239549
H163	-1.2331779081	-4.9713895717	9.7002340542
H164	0.1166323463	-3.4168926807	9.6457590065
H165	-0.9604812077	-0.9379442332	12.7874598899
H166	0.9127547348	0.9809597609	12.7829786203
H167	-3.4540490708	0.1416519865	9.6328237052
H168	-5.0310633418	-1.2103852933	9.6594720336
H169	-7.6519099477	-1.1635343280	0.8529935819
H170	-1.1971167869	-7.7088311190	0.8900344453
H171	-6.6131380595	-5.5429578526	-0.1913083072
H172	-3.9930586772	-3.9653202010	-0.8828710932
H173	-1.2327646023	-5.0013472695	-0.7084217832
H174	0.1119460769	-3.4414888318	-0.6628574896
H175	-0.9073657120	-0.9968867791	-3.8113828274
H176	0.9351947824	0.9554858542	-3.8208623762
H177	-3.4460178015	0.1954473275	-0.6747242166
H178	-4.9855199698	-1.2754886888	-0.7267156470
H179	-5.7872733760	-2.5242520611	0.8070652415
H180	-2.4685448452	-5.7401074113	0.7966962781
H181	-3.1281523246	4.1644278707	-1.9436423839
H182	-1.7124602417	1.6055058381	-2.4631908057
H183	1.7756742221	-1.6365903135	-2.4422980542
H184	3.1434170699	-4.2004611482	-1.9475049781

H185	-2.6271920186	-1.0744198536	-2.1552936687
H186	-1.0688788436	-2.6803530670	-2.1348585934
O187	1.2525759466	3.1953166733	-1.3421421493
O188	3.2104538929	1.2382515920	-1.3486904682
O189	-0.8592553550	3.6215654498	-0.0000272136
Ti190	0.1248971131	4.5551743769	1.5071032952
O191	3.6479839597	-0.9645453232	0.0350151479
Ti192	4.6172412654	0.0813649132	1.4939237611
Ti193	2.3118178212	2.2571077342	0.0105200551
O194	3.6819861127	3.6791998760	-0.0088558222
Ti195	4.7578204253	4.7161587957	1.4681406327
O196	1.3887010711	3.1596520166	1.4799125477
O197	3.1764189631	1.3619993266	1.4802262142
O198	1.0482365810	5.5119901507	0.1397591712
O199	1.2775179727	7.8608621782	1.7433016786
O200	3.2103623630	5.9424578155	1.5302471910
O201	5.4617127429	1.0075212693	0.0932947603
O202	5.9268495833	3.1572525520	1.4717432982
O203	7.9995645779	1.3535711845	1.8192352568
O204	5.6003773218	5.6958661463	0.1825455230
O205	-0.8858086472	3.6422120548	2.9815338173
O206	3.6365680418	-0.9097981721	3.0030216770
Ti207	2.3316049909	2.2916486759	3.0569112077
O208	3.6623077884	3.6291281567	2.9918109859
Ti209	2.2223910371	6.8356958806	3.0204274545
O210	0.8933543975	5.4599330036	2.9994678312
Ti211	6.8363505642	2.2298687428	3.0450311752
O212	5.4887768333	0.8785771402	2.9796310180
O213	5.4536156946	5.4280012192	3.0032105178
Ti214	-0.1861994258	4.5592589518	4.4770548757
Ti215	4.5454733547	-0.1963740068	4.4851672939
Ti216	4.5000924909	4.5064511001	4.4625289540
O217	1.3895427101	3.1469260481	4.4807732986
O218	3.1663418986	1.3693955755	4.4848071801
O219	1.7114846274	7.8198371212	4.4665926739
O220	3.1462719501	5.8291653540	4.5165224515
O221	5.9268108248	3.1979636056	4.4926687402
O222	7.7849627955	1.6243771732	4.4912349568
O223	-0.9062356706	3.6335204789	5.9608624811
Ti224	0.0823477717	4.6173113329	7.4839656444
O225	3.6344145650	-0.9099295227	5.9637981654
Ti226	4.6083894136	0.1003578190	7.4766668263
Ti227	2.3368258364	2.3512475067	5.9491056524
O228	3.6666347789	3.6345249161	5.9955057529
Ti229	4.7566470594	4.7352994747	7.5133306566
O230	1.3632109519	3.1680085707	7.4646902279
O231	3.1519836514	1.3695771322	7.4848509901
Ti232	2.2544431057	6.7812396558	5.9327974594
O233	0.8649527016	5.5000343201	5.9845087308
O234	1.4203871161	8.0215463335	7.1169742895
O235	3.1783200629	5.9473485094	7.4592288139
Ti236	6.8144848992	2.2638669621	5.9443223094
O237	5.4839302321	0.8799405145	5.9935373012
O238	5.9018542791	3.1447754297	7.4839801083

O239	8.0100213791	1.4139207011	7.1611768691
O240	5.4476296138	5.4585480711	5.9872879495
O241	-0.9395384075	3.6461453943	8.9356185196
O242	3.6248992181	-0.9361681610	8.9443028505
Ti243	2.2695899861	2.2763637685	8.9501343702
O244	3.6514438169	3.6874602352	8.9721661669
O245	1.2180193294	3.2099024383	10.2940009703
O246	3.1815751823	1.2593803490	10.3120093367
O247	1.0510476709	5.4544196470	8.8589492156
O248	5.4284073686	1.0329315400	8.8860345324
O249	5.6498216030	5.5944288414	8.8116772026
H250	1.3664976240	7.9357758583	8.0899186430
H251	7.8992605681	1.3743378867	8.1322166355
H252	2.4856352851	5.7636998128	8.1784020675
H253	5.7099943656	2.4510022794	8.1975758434
H254	1.0348856571	2.6496839481	11.0975458822
H255	2.6176474772	1.0653806190	11.1120795334
H256	3.4203368908	-0.2047787939	9.6253582436
H257	4.9039834248	1.2309384876	9.7078759546
H258	3.9189375448	3.9887085837	9.8640308325
H259	6.2186464178	5.8601052380	9.5540864642
H260	1.2484102553	4.9354789332	9.6845803114
H261	-0.1976026256	3.4370361005	9.6196685725
H262	3.4484388569	-0.2434316101	-0.6554353899
H263	4.9515660611	1.2014162565	-0.7373407340
H264	3.9413698746	3.9995613790	-0.8964015905
H265	5.5662843855	6.5993199431	-0.1857456047
H266	1.2514221251	5.0403198677	-0.7066354910
H267	-0.0929623596	3.4233165592	-0.6794363908
H268	1.0907641616	7.4870210811	0.8504861408
H269	2.5189638649	5.7587959496	0.8146404075
H270	5.7296874437	2.4517959596	0.7740059861
H271	7.8219159513	1.2726952504	0.8602026663
H272	1.0702038530	2.6230022076	-2.1368510102
H273	2.6496328276	1.0403375719	-2.1513471239
O274	-5.6151834121	3.5890851461	0.1784692085
Ti275	-4.5163414074	4.4509680964	1.4765409218
O276	-7.8221733746	3.2581357100	1.5902520493
O277	-5.9199591811	1.3671760338	1.5505747584
O278	-4.2927373817	5.8813952115	0.2783537805
O279	-3.3096366732	7.7865551690	1.6200210525
O280	-1.3418117075	5.9568864230	1.5402641678
Ti281	-6.9848394555	2.4089035799	2.9631510515
O282	-5.5316097505	3.7821888155	2.9594907917
Ti283	-2.4415693932	6.9235237409	2.9370477965
O284	-3.7622262878	5.5094179058	2.9851578405
Ti285	-4.4198372771	4.4034097732	4.4534978554
O286	-7.7976065446	3.0788710075	4.4399539048
O287	-5.9252756712	1.4207977385	4.4039414208
O288	-3.0551004238	7.7951041551	4.4612926315
O289	-1.4129215971	5.9151523388	4.4520782351
Ti290	-6.9583392430	2.4411683104	5.9784328623
O291	-5.5090556781	3.7641966865	5.9141061752
Ti292	-4.4528730394	4.5769610232	7.4079781453

O293	-7.8057323095	3.3231384306	7.2811380611
O294	-5.9860645849	1.3724536107	7.4045872613
Ti295	-2.3440022116	7.0142911349	5.9389276274
O296	-3.7688250334	5.5411967339	5.9315475257
O297	-3.1748304038	7.8498932537	7.3153185587
O298	-1.3786522298	5.9062374177	7.3784271844
O299	-5.9408022513	4.3934873540	8.5617925545
O300	-3.6179908822	5.6475802447	8.7373062544
H301	-7.2323972198	3.8512625844	7.9556843697
H302	-3.4825748355	7.4076405171	8.1472714018
H303	-6.2425349780	1.6658046903	8.3009861648
H304	-2.0521802830	5.8148336837	8.1176542837
H305	-3.5308001747	5.2861499754	9.6501975754
H306	-6.0603789011	4.8268090935	9.4293626542
H307	-7.3588950778	3.5302061215	0.7559738194
H308	-4.7451196943	6.0076955282	-0.5780076239
H309	-5.2338389220	3.4834919944	-0.7257163887
H310	-5.8133097906	2.0331469025	0.8039295222
H311	-3.7968772454	7.2306434375	0.9177778563
H312	-1.6411814973	6.1819878365	0.6381896468
O313	4.4153801532	-5.9322816328	0.3720525576
Ti314	4.5894344356	-4.4495972854	1.5242770840
O315	1.3056959185	-6.0066831798	1.5661104913
O316	3.3164051655	-7.7821167007	1.6587682026
O317	5.6259638964	-3.5905167831	0.1887632028
O318	5.9302270018	-1.3804125092	1.5904337301
O319	7.8309627081	-3.2503927218	1.6345613458
Ti320	2.4297634977	-6.9508294994	2.9767717349
O321	3.7594499504	-5.5005275682	3.0159101727
Ti322	6.9849716772	-2.3933390017	2.9948767752
O323	5.5485009349	-3.7707132907	3.0078797610
Ti324	4.3688612347	-4.4513224372	4.4919497512
O325	1.3979108282	-5.9076718676	4.4605022773
O326	3.0604936987	-7.7744142313	4.4967883701
O327	5.9406852838	-1.4141502535	4.4595128465
O328	7.8252599811	-3.0469163390	4.4939518758
Ti329	2.4149765544	-6.9547297278	6.0117932035
O330	3.7537124444	-5.4866751798	5.9630941463
Ti331	4.5786643088	-4.4251973478	7.4497350569
O332	1.3367025335	-5.9554726565	7.4435597004
O333	3.2885101921	-7.7777334718	7.3363324320
Ti334	7.0019234013	-2.3517830403	5.9824427546
O335	5.5366128605	-3.7487098010	5.9706015213
O336	5.9094754714	-1.3635036565	7.3947925622
O337	7.8419533167	-3.1685829693	7.3629553787
O338	4.3804991777	-5.9134045698	8.6045076531
O339	5.6121056762	-3.5772884403	8.7924279151
H340	3.8232682723	-7.2020397540	8.0039922409
H341	7.4258624725	-3.4641237455	8.2108176093
H342	1.6366413467	-6.2086792077	8.3389960645
H343	5.8099999757	-2.0186726064	8.1486057224
H344	4.7903394910	-6.0143050779	9.4852683680
H345	5.2164551845	-3.4822008190	9.6918066294
H346	3.8401747309	-7.2165532948	0.9798686458

H347	4.8181901206	-6.0391796721	-0.5116791498
H348	5.2385490246	-3.5015216452	-0.7145471400
H349	1.5556921057	-6.3086504421	0.6701617279
H350	5.8421624643	-2.0270369071	0.8261705002
H351	7.4112376820	-3.5287986071	0.7822113301
Ti352	0.0177922588	-0.0310447293	-1.5056185119
O353	-0.9775554073	-0.9872477307	-2.8368697066
O354	0.9970163037	0.9251921603	-2.8465658571
Ti355	-0.0255540276	-0.0054836197	10.4774168852
O356	-0.9973030717	-0.9568591797	11.8113867568
O357	0.9473829249	0.9721776701	11.8069264936

3.8 555 reduced cluster in water

357			
555 reduced	Water-Optimized	SCFE : -17167.3788522449	hartree
O1	-7.8511075583	-4.1550823008	3.1953248756
H2	-8.1335444182	-4.2684560815	4.1488085399
H3	-7.1469491322	-4.8384242686	3.0006726661
O4	-7.8661517214	-4.2218987869	5.8772431970
H5	-8.6100675709	-4.4307962792	6.4768748196
H6	-7.1018163143	-4.8780632842	5.9799463046
O7	-4.1430990194	-7.8996634794	2.9055142920
H8	-4.3167056132	-8.3856666631	2.0742960529
H9	-4.8386871883	-7.1944577086	3.0379082710
O10	-4.1711272073	-7.8703531921	6.1106772014
H11	-4.3457699597	-8.3725584196	6.9315210047
H12	-4.8691244208	-7.1654478432	5.9873816895
O13	4.1417208900	7.8333163819	3.1626134484
H14	4.2658406364	8.1151497590	4.1144117835
H15	4.8252464623	7.1303680608	2.9668663783
O16	4.2526784213	7.8372363042	5.8448172977
H17	4.4615787904	8.5858311584	6.4398694426
H18	4.9084059983	7.0715239699	5.9518474036
O19	7.8783217005	4.1338856396	2.8941258573
H20	8.3433138192	4.3117625314	2.0515785954
H21	7.1753585370	4.8287451942	3.0467911632
O22	7.8483949192	4.1646253595	6.0783701727
H23	8.3660288299	4.3437505506	6.8888962265
H24	7.1363671397	4.8607056763	5.9634138690
O25	-8.4774126115	0.8894325031	2.9717267771
H26	-9.3948406139	1.1984296869	2.8264830219
H27	-8.3072545532	0.0013393013	2.4644693740
O28	-8.2840899006	0.8633012728	5.8093088400
H29	-8.4597250177	0.6004416648	4.8690467835
H30	-8.2114587005	0.0420850546	6.4127008206
O31	0.9155438498	-8.4705584586	3.0064669158
H32	1.2137159579	-9.3977888872	2.9100575637
H33	0.0319642835	-8.3136315827	2.5018483994
O34	0.8360146164	-8.2715530316	5.8544748015
H35	0.5623757611	-8.4275223746	4.9140507692
H36	0.0187312055	-8.2061784138	6.4610447890
O37	-0.9071948908	8.4572495819	2.9629655404
H38	-1.2133328862	9.3782125023	2.8365548221

H39	-0.0410928610	8.2813257808	2.4336502463
O40	-0.7728595293	8.2886349042	5.7855027493
H41	-0.5056085768	8.4410463499	4.8409502451
H42	0.0471735195	8.2589149666	6.4008275663
O43	8.4759357498	-0.8753472618	2.9902265698
H44	9.4001336196	-1.1810028523	2.8917680069
H45	8.3262491748	0.0073481804	2.4737635469
O46	8.2827448975	-0.7839399104	5.8436591648
H47	8.4254367743	-0.4826596201	4.9090239548
H48	8.2429132621	0.0270116356	6.4706070602
O49	-3.2090737873	-1.2808001330	-1.3766971760
O50	-1.2466211997	-3.2518779414	-1.3477423824
O51	-3.2948390239	3.3891411676	-1.3655094669
O52	-1.4283339940	1.4163857210	-1.5582944466
O53	1.4559265356	-1.4601357984	-1.5478440717
O54	3.3160791256	-3.4419628126	-1.3393042095
O55	-5.7123809607	-5.5849121527	0.1975602655
Ti56	-4.7181426766	-4.7473768408	1.4895845162
O57	-5.4959920972	-1.0632919609	0.1021748311
Ti58	-4.6231351579	-0.0971594313	1.4712802798
O59	-7.9366215739	-1.3136607774	1.7977048386
O60	-5.9751614565	-3.2035126393	1.5370447736
O61	-1.0219780928	-5.5391184377	0.1265851167
Ti62	-0.1098879053	-4.5773619923	1.5075867668
O63	-3.1787711324	-5.9334665871	1.4865010542
O64	-1.3226297408	-7.9557576848	1.8162451266
Ti65	-2.2977370126	-2.2721730160	-0.0049294733
O66	-0.8714614268	-0.9038771260	-0.0753513473
O67	-3.7027878619	-3.6761711568	-0.0070134672
Ti68	0.0069120208	-0.0131847857	1.5002391181
O69	-3.1797701128	-1.3860092694	1.4625899861
O70	-1.3925043948	-3.1940809503	1.4687022853
Ti71	-2.3584410315	2.4094044487	-0.1386109186
O72	-3.6467701210	0.9199038167	0.0025721589
O73	-3.1676589289	3.2418658442	1.4421824440
O74	-1.4047887150	1.4181435850	1.4362076716
Ti75	2.3843655593	-2.4552406134	-0.1136232222
O76	0.8701859869	-3.6527064103	0.0100207629
O77	1.4137379586	-1.4416737261	1.4526074192
O78	3.1819051834	-3.2642269080	1.4691684605
O79	0.8845898128	0.8690680226	-0.0751058649
O80	-5.4382752114	-5.4477920739	3.0165400983
Ti81	-6.8345771990	-2.2406420928	3.0481098963
O82	-5.4877754064	-0.8795371760	2.9753589206
Ti83	-2.2416696304	-6.8411083233	3.0593439609
O84	-0.9183530720	-5.4814667696	3.0104024393
Ti85	-2.3337845899	-2.2994013865	3.0288230418
O86	-0.8955148543	-0.8868430555	2.8868518136
O87	-3.6513850429	-3.6518197733	2.9889254450
Ti88	-2.1726198335	2.1540466729	2.9005958066
O89	-3.6422505412	0.8906745105	2.9630183145
Ti90	2.1599470435	-2.1889365291	2.9221866385
O91	0.8834446150	-3.6779352453	2.9763647255
O92	0.8873029188	0.8684017045	2.8963463263

Ti93	-4.5009358611	-4.4867747175	4.4890857130
Ti94	-4.5756773760	0.1976745310	4.4559648570
O95	-7.8370978789	-1.7083211503	4.4908882825
O96	-5.8367633222	-3.1321842050	4.5170030284
Ti97	0.1674077838	-4.5976442960	4.4846983055
O98	-3.2131389609	-5.9258493657	4.5049867702
O99	-1.6620735037	-7.8086534783	4.5112971070
Ti100	-0.0258643275	-0.0224627561	4.4783931380
O101	-3.1566608407	-1.3722829468	4.4768282921
O102	-1.3856489814	-3.1343605666	4.4802169743
O103	-3.1908638033	3.1934599316	4.4514398089
O104	-1.4354664144	1.4216191595	4.4699388110
O105	1.4033822235	-1.4459086585	4.4783327950
O106	3.1824810948	-3.1853646711	4.4852858239
O107	-5.4737868141	-5.4296847121	5.9916860958
Ti108	-4.7483578712	-4.7378310679	7.5235900622
Ti109	-6.7862555700	-2.2142901466	5.9473028648
O110	-5.4903701742	-0.8556789644	5.9574339772
Ti111	-4.5676590005	-0.0666521214	7.4527012498
O112	-7.9184717557	-1.3025550235	7.1841736159
O113	-5.9381654951	-3.1547851992	7.4565766720
Ti114	-2.2701539229	-6.8164103685	5.9598811006
O115	-0.9054229907	-5.4780137650	5.9848405474
Ti116	-0.1006160510	-4.5778385596	7.4699719881
O117	-3.1709715982	-5.8927570057	7.4941619810
O118	-1.3611080822	-7.9338610810	7.2090272018
Ti119	-2.3233200688	-2.3323953305	5.9265538585
O120	-0.9037759151	-0.8867132433	6.0665723255
O121	-3.6403396063	-3.6558142696	5.9986196185
Ti122	-0.0084475483	0.0088092156	7.4381373827
O123	-3.1953536149	-1.3641002172	7.4919041505
O124	-1.3948026896	-3.1721763760	7.5031810379
Ti125	-2.1688596237	2.1823404733	6.0297521574
O126	-3.6828642398	0.9145604767	5.9644203917
O127	-3.2537352908	3.1965866063	7.4776248474
O128	-1.4458128692	1.4186450832	7.5024802676
Ti129	2.1484843016	-2.1759027589	6.0474164457
O130	0.8810922175	-3.6719761163	5.9920786159
O131	1.3963067778	-1.4267091810	7.5126227900
O132	3.1695764814	-3.2343052739	7.5057293118
O133	0.8682534872	0.8704377315	6.0555303108
O134	-5.6716159752	-5.5970937832	8.8034134731
O135	-5.5426160594	-0.9971536798	8.8188680510
O136	-1.0311548166	-5.4949661228	8.8642746756
Ti137	-2.2885749895	-2.2643459837	8.9670815876
O138	-0.9014940165	-0.8787514866	9.0452114685
O139	-3.7079409158	-3.6500292213	8.9899060547
O140	-3.2481793213	-1.2244460919	10.3179036228
O141	-1.2842184560	-3.2072858745	10.3390367159
Ti142	-2.4301898255	2.3988323349	9.0647222071
O143	-3.6588739147	0.8949278932	8.9514637150
O144	-3.4449375167	3.3320711313	10.2690532010
O145	-1.4585092803	1.4598920377	10.5002879895
Ti146	2.3699134824	-2.4089011342	9.0865140662

O147	0.8665298549	-3.6333016261	8.9724269573
O148	1.4271381910	-1.4219383040	10.5134349991
O149	3.3014223783	-3.4023865800	10.3138509250
O150	0.8583382103	0.8870709773	9.0262570765
H151	-7.5812112040	-1.1101754894	8.0884170123
H152	-4.3012606947	3.1605008161	10.7089075075
H153	-1.2027594171	-7.6289600588	8.1296710825
H154	3.1084893631	-4.2334620953	10.7894458982
H155	-5.7541105666	-2.4527519473	8.1679025752
H156	-1.6952372109	1.7326467742	11.4087918918
H157	-2.4609086882	-5.7002220271	8.1942609053
H158	1.7207547373	-1.6304451420	11.4238743621
H159	-2.6674102902	-1.0315749993	11.1074380226
H160	-1.0986554580	-2.6248980582	11.1290753316
H161	-6.3119360886	-5.9060545075	9.4667625294
H162	-4.0161023536	-3.9117761833	9.8804443205
H163	-1.2300002804	-4.9935962168	9.6960961610
H164	0.1233140638	-3.4326978250	9.6553341942
H165	-0.9610553068	-0.9216790307	12.7961346995
H166	0.9081726993	0.9719536570	12.7986051845
H167	-3.4605699149	0.1439591137	9.6411301211
H168	-5.0526118633	-1.1957892361	9.6570461883
H169	-7.6455911495	-1.1762900619	0.8702155260
H170	-1.1644264467	-7.6483614794	0.8959959975
H171	-6.6219707407	-5.4717148236	-0.1398918457
H172	-4.0005615724	-3.9730396291	-0.8900528441
H173	-1.2214460194	-5.0375195284	-0.7055192227
H174	0.1112101209	-3.4541805073	-0.6757482824
H175	-0.9175920216	-0.9877930953	-3.8315505055
H176	0.9426892453	0.9329121376	-3.8415595859
H177	-3.4513564163	0.1913970596	-0.6835414063
H178	-4.9929187691	-1.2832243447	-0.7238846123
H179	-5.7885263845	-2.5241969576	0.8120826860
H180	-2.4563212154	-5.7428822787	0.7986717438
H181	-3.1281030035	4.1988907212	-1.8878322834
H182	-1.7188491959	1.6175119102	-2.4691288685
H183	1.7721496293	-1.6520426516	-2.4533355604
H184	3.1413028017	-4.2476977608	-1.8647262022
H185	-2.6264529911	-1.0807503944	-2.1655179206
H186	-1.0636804415	-2.6791429409	-2.1429430086
O187	1.2582215470	3.2067472474	-1.3596314085
O188	3.2250564933	1.2420109573	-1.3646112411
O189	-0.8615170309	3.6315854101	-0.0111153133
Ti190	0.1184438161	4.5459187507	1.5026937956
O191	3.6528406028	-0.9593862868	0.0203298027
Ti192	4.6169372464	0.0811297013	1.4888777637
Ti193	2.3016414168	2.2474418156	-0.0021954884
O194	3.6792759882	3.6761535886	-0.0131687164
Ti195	4.7433884838	4.6994655554	1.4805599623
O196	1.3870311680	3.1645356668	1.4650989634
O197	3.1820768278	1.3631110314	1.4678814134
O198	1.0449260128	5.5280399530	0.1406961088
O199	1.2766927130	7.8587175292	1.7454010244
O200	3.2041491482	5.9406904605	1.5327436647

O201	5.4757332831	1.0110833617	0.0890117897
O202	5.9266229439	3.1553975599	1.4715311641
O203	7.9913286292	1.3509800238	1.8081444578
O204	5.5911654177	5.7027658493	0.2014050487
O205	-0.8896199408	3.6552444461	2.9719910040
O206	3.6451408481	-0.9067921004	2.9926397722
Ti207	2.3114522001	2.2658422050	3.0512629429
O208	3.6527528641	3.6176578620	2.9906414457
Ti209	2.2206528641	6.8253332003	3.0250465638
O210	0.8946352187	5.4573689911	3.0004691955
Ti211	6.8357899133	2.2256219214	3.0464334687
O212	5.4911580592	0.8769550721	2.9778513564
O213	5.4399701756	5.4131706969	3.0130977611
Ti214	-0.1890210017	4.5608941409	4.4721088689
Ti215	4.5419563755	-0.1989613591	4.4837931218
Ti216	4.4706773264	4.4725919663	4.4689635043
O217	1.3758619818	3.1292048300	4.4769548468
O218	3.1487968308	1.3564798399	4.4821593099
O219	1.7180865320	7.8221680301	4.4716338870
O220	3.1367574905	5.8198004238	4.5200188780
O221	5.9161754266	3.1846035971	4.4932479091
O222	7.7954488876	1.6371375579	4.4929561478
O223	-0.9024279140	3.6458990116	5.9644795170
Ti224	0.0778864753	4.6187112217	7.4810383573
O225	3.6410373015	-0.9056658141	5.9700725010
Ti226	4.6043322178	0.0978874888	7.4767477815
Ti227	2.3086904244	2.3319708312	5.9572598793
O228	3.6539499962	3.6194256085	5.9995078467
Ti229	4.7427955650	4.7208773432	7.5197279993
O230	1.3605063648	3.1716677258	7.4715439076
O231	3.1547799265	1.3677346938	7.4938629264
Ti232	2.2549178142	6.7784461691	5.9341240654
O233	0.8638190555	5.5017657083	5.9849740268
O234	1.4149840027	8.0108301585	7.1289728118
O235	3.1747490698	5.9395199515	7.4636155304
Ti236	6.8062897127	2.2604153914	5.9453353043
O237	5.4833155311	0.8777825626	5.9908206936
O238	5.8986140515	3.1381289171	7.4856067687
O239	7.9922661619	1.3989014809	7.1709154736
O240	5.4347910784	5.4456485456	5.9945804070
O241	-0.9383282309	3.6560350545	8.9439233322
O242	3.6318541073	-0.9290258472	8.9567412332
Ti243	2.2515564300	2.2608850948	8.9584364612
O244	3.6434659464	3.6799742501	8.9753159957
O245	1.2190069964	3.2266182152	10.3072699998
O246	3.1935620624	1.2622728757	10.3251443215
O247	1.0506401872	5.4631838125	8.8586996944
O248	5.4393697938	1.0334644391	8.8865319418
O249	5.6485889136	5.5719744054	8.8262597432
H250	1.3353385783	7.8765475303	8.0955367197
H251	7.8209652016	1.3209553720	8.1311349662
H252	2.4762073800	5.7559898728	8.1790101684
H253	5.7046191829	2.4401994422	8.1966465535
H254	1.0290268027	2.6585819610	11.1042849221

H255	2.6205341013	1.0681482930	11.1192093280
H256	3.4316601665	-0.1933138438	9.6379072305
H257	4.9096351404	1.2379516042	9.7034616118
H258	3.9138397200	3.9728477952	9.8685103308
H259	6.2529315508	5.6912415825	9.5802043331
H260	1.2478966277	4.9338325748	9.6781569905
H261	-0.1937527905	3.4467262172	9.6260775621
H262	3.4537999204	-0.2347772617	-0.6677301115
H263	4.9596045828	1.2088714997	-0.7373937061
H264	3.9378654304	4.0046515968	-0.8972247439
H265	5.4925470991	6.6234181278	-0.1080917728
H266	1.2510444192	5.0496139098	-0.7010129783
H267	-0.0987296094	3.4350694730	-0.6925812975
H268	1.0803328642	7.4593489033	0.8644574122
H269	2.5113387336	5.7576201284	0.8166316906
H270	5.7324498419	2.4491501102	0.7724461737
H271	7.7786858978	1.2514709383	0.8567779601
H272	1.0725035338	2.6261775733	-2.1482108508
H273	2.6556455056	1.0398054663	-2.1603329231
O274	-5.6246452793	3.5974991493	0.1727053472
Ti275	-4.5277214573	4.4599234365	1.4783123871
O276	-7.8277458328	3.2523127266	1.5849576466
O277	-5.9234713786	1.3671739924	1.5472456247
O278	-4.3250268545	5.9029679778	0.2865826998
O279	-3.3042198804	7.7941494168	1.6146378805
O280	-1.3338656598	5.9716816238	1.5387821264
Ti281	-6.9808864969	2.4111933804	2.9610930803
O282	-5.5440410179	3.7938061568	2.9586290118
Ti283	-2.4390815400	6.9288207684	2.9346678387
O284	-3.7724343687	5.5242965669	2.9782611763
Ti285	-4.4235985210	4.4243108240	4.4543718872
O286	-7.8039199815	3.0762145572	4.4373002604
O287	-5.9271521459	1.4262420253	4.4054265722
O288	-3.0489183201	7.8070831199	4.4586980160
O289	-1.4161297103	5.9188746186	4.4460132215
Ti290	-6.9598621588	2.4414831651	5.9739772799
O291	-5.5172888225	3.7741408570	5.9133002577
Ti292	-4.4648812100	4.5690767996	7.4074786828
O293	-7.8104822598	3.3228462874	7.2791296609
O294	-5.9868020816	1.3772296819	7.4025415765
Ti295	-2.3557702872	7.0118621925	5.9387877140
O296	-3.7761449732	5.5522216165	5.9337033697
O297	-3.1830794269	7.8573938470	7.3151757469
O298	-1.3782299981	5.9171754579	7.3801609431
O299	-5.9457015819	4.3979836010	8.5714722890
O300	-3.6242075961	5.6635559175	8.7284416959
H301	-7.2450400183	3.8531732925	7.9563460264
H302	-3.4953355586	7.3904721224	8.1335560930
H303	-6.2266620710	1.6806913858	8.3004528532
H304	-2.0570546891	5.8194308236	8.1138779065
H305	-3.5252430680	5.2701117067	9.6282636367
H306	-6.0818524469	4.8856490852	9.4095523001
H307	-7.3521874176	3.5222272442	0.7551943786
H308	-4.7884464096	6.0228333985	-0.5662920444

H309	-5.2170344865	3.4813315079	-0.7196844958
H310	-5.8130834086	2.0332357455	0.8020193391
H311	-3.8071396742	7.2377315943	0.9208636036
H312	-1.6174768543	6.2159632245	0.6355606704
O313	4.3951368737	-5.9349692454	0.3565061961
Ti314	4.5717205601	-4.4611597055	1.5238707677
O315	1.3193509452	-6.0074879447	1.5663385343
O316	3.3196462837	-7.7888949231	1.6559211324
O317	5.6458253628	-3.6059328756	0.2002815022
O318	5.9328451258	-1.3799969676	1.5821330040
O319	7.8414714423	-3.2406771656	1.6284575578
Ti320	2.4390165790	-6.9481215603	2.9751920876
O321	3.7778916971	-5.5123532575	3.0193926863
Ti322	6.9811015252	-2.3963370468	2.9927674079
O323	5.5550053903	-3.7735232567	2.9991880285
Ti324	4.3947062606	-4.4395190697	4.4962054394
O325	1.4088499264	-5.9131198813	4.4614032484
O326	3.0693007615	-7.7829439888	4.4938924017
O327	5.9366288153	-1.4183703323	4.4588348861
O328	7.8264387769	-3.0455447954	4.4910735955
Ti329	2.4208386878	-6.9605281954	6.0026723713
O330	3.7661687889	-5.4977296597	5.9607672615
Ti331	4.5477237168	-4.4371269854	7.4588671483
O332	1.3453179445	-5.9612955039	7.4378300265
O333	3.2954233407	-7.7906185575	7.3288600259
Ti334	6.9927485043	-2.3653832389	5.9836512918
O335	5.5482549571	-3.7649177812	5.9799481515
O336	5.9120914744	-1.3650360812	7.3954129243
O337	7.8441226904	-3.1744072818	7.3651428307
O338	4.3070354631	-5.8943261114	8.6434445069
O339	5.6285638433	-3.5940181613	8.7823152004
H340	3.7994155252	-7.2167978309	8.0138956948
H341	7.3892832138	-3.4771114093	8.1937685650
H342	1.6989701380	-6.1547717953	8.3285217732
H343	5.8150456053	-2.0230794995	8.1469389252
H344	4.7443398481	-6.0078575379	9.5103465604
H345	5.2214539652	-3.4821162610	9.6751883591
H346	3.8358517279	-7.2240631644	0.9727939344
H347	4.8393124500	-6.0484244135	-0.5070310501
H348	5.2412635333	-3.5109614361	-0.6956599529
H349	1.5650182119	-6.3090445919	0.6697050060
H350	5.8357175160	-2.0367951183	0.8273087614
H351	7.3896162843	-3.5287707494	0.7938630404
Ti352	0.0160778055	-0.0273696305	-1.5191495495
O353	-0.9840875600	-0.9896898229	-2.8570110331
O354	0.9984395656	0.9290768642	-2.8665646801
Ti355	-0.0240346413	0.0068445644	10.4765909056
O356	-1.0036456094	-0.9608831100	11.8211265634
O357	0.9473352998	0.9817571038	11.8229248907

3.9 555 I_{Li}⁺ cluster in water[¶]

[¶]intercalated by Li⁺ cation

358

555	Li+ intercalation Water-Optimized	SCFE : -17174.7099929978	hartree
O1	-7.8860873873	-4.1437908847	3.1833272393
H2	-8.1656935022	-4.2728892049	4.1354544763
H3	-7.2128140807	-4.8451638108	2.9608044964
O4	-7.8953486405	-4.2152594893	5.8755931223
H5	-8.6584157557	-4.4033189696	6.4594546159
H6	-7.1569694549	-4.8898667436	5.9942089795
O7	-4.1103032886	-7.9321852757	2.9217864233
H8	-4.2850622330	-8.5118386781	2.1541937539
H9	-4.8479184450	-7.2764602836	3.0426378398
O10	-4.1421237620	-7.9007811797	6.1030844547
H11	-4.3156630295	-8.4690054447	6.8798687601
H12	-4.8731429395	-7.2356666416	5.9855213921
O13	4.0991257253	7.9136358692	3.1484569236
H14	4.2535322171	8.1670681977	4.1086861046
H15	4.7818934130	7.2322626437	2.9032738249
O16	4.2386539045	7.8947606747	5.8196807921
H17	4.4099332413	8.6671770037	6.3943037934
H18	4.9262270728	7.1740945189	5.9504081327
O19	7.9949631628	4.0519130214	2.8937487650
H20	8.5929844118	4.2020959510	2.1342120099
H21	7.3698256033	4.8130482427	3.0011148743
O22	7.9858677585	4.0716513935	6.1087644973
H23	8.5504681596	4.2261073180	6.8922873677
H24	7.3567286086	4.8263990600	5.9809911096
O25	-8.5028113733	0.8743635310	2.9851140144
H26	-9.4228068191	1.1804652542	2.8477674502
H27	-8.3341699986	-0.0099758566	2.4715965054
O28	-8.2935642971	0.8509591119	5.8345535822
H29	-8.4821214157	0.5868653223	4.8977541094
H30	-8.2493574310	0.0319350762	6.4360943316
O31	0.9125195709	-8.4658273383	2.9929229592
H32	1.2094476933	-9.3939373237	2.9011698281
H33	0.0271959421	-8.3117826290	2.4943843020
O34	0.8324348469	-8.2681369557	5.8486782866
H35	0.5581204931	-8.4319564208	4.9100408871
H36	0.0170398902	-8.2152667335	6.4559546015
O37	-0.9927877184	8.4913721701	2.9341134679
H38	-1.3006480242	9.4176058971	2.8592018529
H39	-0.1693345378	8.3375874897	2.3613846689
O40	-0.7922637497	8.2842938824	5.7767895128
H41	-0.5296133738	8.4558057472	4.8363949592
H42	0.0403352259	8.2360073456	6.3895831973
O43	8.5004899542	-0.9140862969	3.0083211067
H44	9.4233554163	-1.2267110005	2.9135514516
H45	8.3632816723	-0.0395449176	2.4918668619
O46	8.3131324387	-0.8272180045	5.8571829014
H47	8.4632898333	-0.5212787800	4.9250415780
H48	8.2977927788	-0.0315236838	6.4930682606
O49	-3.1947554390	-1.2490749621	-1.3548092414
O50	-1.2429710807	-3.2013172482	-1.3328816829
O51	-3.2771810632	3.4124608225	-1.3715745284
O52	-1.4279861004	1.4373047964	-1.5370756141

O53	1.4507122635	-1.4168335426	-1.5319534112
O54	3.2834308511	-3.4081824158	-1.3659587689
O55	-5.7139456921	-5.5832341369	0.1793925854
Ti56	-4.7434020112	-4.7598905402	1.4797168103
O57	-5.4942863236	-1.0537337431	0.0953634976
Ti58	-4.6464133459	-0.1011288426	1.4703693639
O59	-7.9535483613	-1.3209347569	1.7982361681
O60	-5.9857379890	-3.2080102516	1.5328574145
O61	-1.0253332282	-5.4973732866	0.1201751159
Ti62	-0.1176224573	-4.5717824271	1.5043694058
O63	-3.1857322231	-5.9202721954	1.4897222827
O64	-1.3330843781	-7.9522649751	1.8188752789
Ti65	-2.3234973841	-2.2791574124	0.0060401450
O66	-0.8630747503	-0.8737447116	-0.0215329934
O67	-3.7156660797	-3.6663490453	-0.0080411862
Ti68	-0.0405416965	-0.0426993035	1.4876244036
O69	-3.1812601564	-1.3705790122	1.4763347241
O70	-1.4041658442	-3.1731113174	1.4798448035
Ti71	-2.3892868987	2.4336684810	-0.1359912976
O72	-3.6484488676	0.9363064079	0.0158010812
O73	-3.1806600393	3.2445332262	1.4501507209
O74	-1.4003109928	1.4166930637	1.4673746393
Ti75	2.3861557868	-2.4442887827	-0.1210009232
O76	0.8613980942	-3.6141436914	0.0229400050
O77	1.3981920271	-1.4080381052	1.4780443218
O78	3.1663721551	-3.2375830405	1.4696835596
O79	0.8709761042	0.9006786652	-0.0323263847
O80	-5.4599689353	-5.4582192069	3.0083904106
Ti81	-6.8562398247	-2.2461613818	3.0407580217
O82	-5.4924729274	-0.8857758396	2.9738552534
Ti83	-2.2463393937	-6.8398167826	3.0530053724
O84	-0.9256329267	-5.4622487147	3.0057566618
Ti85	-2.3820802578	-2.3346525816	3.0351277312
O86	-0.8867134439	-0.8583326019	2.9682096183
O87	-3.6751590914	-3.6587547382	2.9922280307
Ti88	-2.2075441966	2.1429582671	2.9066769305
O89	-3.6463832653	0.9001818203	2.9780859448
Ti90	2.1564520294	-2.1821204953	2.9214305292
O91	0.8808969433	-3.6510904844	2.9822266209
O92	0.9162032615	0.8510574095	2.9651568359
Ti93	-4.5578479891	-4.5391025224	4.4928181243
Ti94	-4.6002103650	0.1743094261	4.4667650026
O95	-7.8329655274	-1.6959776376	4.4849177087
O96	-5.8561993311	-3.1494689771	4.5189332855
Ti97	0.1555231907	-4.5945844355	4.4802542816
O98	-3.2305587516	-5.9333920177	4.5062256105
O99	-1.6358408291	-7.7821163752	4.5043974434
Ti100	-0.0526071523	-0.0376870743	4.5290811646
O101	-3.1874768379	-1.3822140689	4.4806557652
O102	-1.4091008980	-3.1479763155	4.4777768614
O103	-3.1884388043	3.1935139569	4.4562415028
O104	-1.4093996400	1.4027465856	4.4723468321
O105	1.3844445623	-1.4064617702	4.4857645413
O106	3.1762110317	-3.1757258590	4.4805576533

O107	-5.4861346374	-5.4400691388	5.9951524162
Ti108	-4.7528273438	-4.7466071177	7.5300048677
Ti109	-6.8065200622	-2.2281274565	5.9494719734
O110	-5.5023777572	-0.8611668989	5.9712941688
Ti111	-4.5952646439	-0.0827662882	7.4742786437
O112	-7.9853343473	-1.3754495754	7.1608905169
O113	-5.9471994640	-3.1632114904	7.4606710085
Ti114	-2.2732531960	-6.8278241737	5.9596528389
O115	-0.9072546629	-5.4714165593	5.9869061893
Ti116	-0.1045343981	-4.5908210000	7.4668472873
O117	-3.1680101476	-5.8917990057	7.4927509595
O118	-1.3830553766	-7.9597850507	7.1890294214
Ti119	-2.3617351861	-2.3639546188	5.9235453349
O120	-0.8888627749	-0.8711586155	5.9732350585
O121	-3.6597189412	-3.6692945683	5.9971138274
Ti122	0.0359844052	0.0383760170	7.4751443127
O123	-3.1855208149	-1.3559258868	7.4779392718
O124	-1.3952120275	-3.1543203721	7.4832948756
Ti125	-2.2067921709	2.1638175977	6.0478446600
O126	-3.6852286493	0.9170978673	5.9628149052
O127	-3.2514947685	3.1900452002	7.4874611720
O128	-1.4286574579	1.4046158004	7.4814417649
Ti129	2.1586801314	-2.1924646219	6.0490462080
O130	0.8864077995	-3.6554927534	5.9822740537
O131	1.3953793376	-1.3990054142	7.4812431436
O132	3.1701088071	-3.2361114424	7.5054874799
O133	0.8556512155	0.8750235636	5.9859283459
O134	-5.6512607372	-5.6092617482	8.8150342404
O135	-5.4942033257	-1.0124380259	8.8464193535
O136	-1.0279053326	-5.4521079757	8.8682872970
Ti137	-2.2827564460	-2.2602510751	8.9456447179
O138	-0.8796579490	-0.8622049803	9.0081673734
O139	-3.7028789375	-3.6424690421	8.9756315823
O140	-3.2287373629	-1.2220385663	10.3048387445
O141	-1.2757362950	-3.1979532319	10.3164277459
Ti142	-2.4423776668	2.4122127266	9.0796059509
O143	-3.6432891190	0.8995526352	8.9486466945
O144	-3.4114812012	3.3203066458	10.3137943877
O145	-1.4361845248	1.4586987135	10.4892292122
Ti146	2.3904226060	-2.4322496718	9.0912923580
O147	0.8703815073	-3.6091161537	8.9552926210
O148	1.4350375722	-1.4086263011	10.4965673999
O149	3.2880400299	-3.3977343171	10.3402453209
O150	0.8674873992	0.8901329551	8.9721990077
H151	-7.8205374219	-1.2676699806	8.1203357246
H152	-4.2019417272	3.1752372846	10.8684319831
H153	-1.2717200096	-7.7713751301	8.1436842422
H154	3.1134386204	-4.1771227413	10.9023671470
H155	-5.7727845907	-2.4722265722	8.1798380734
H156	-1.6490820934	1.7591187506	11.3980088871
H157	-2.4640660384	-5.7009200772	8.1961829275
H158	1.7484639741	-1.6016262617	11.4054523316
H159	-2.6842005600	-1.0454949442	11.1176565781
H160	-1.0935205946	-2.6535689937	11.1289781982

H161	-6.2106914210	-6.0141918225	9.4991521910
H162	-4.0034744469	-3.8986666629	9.8709216492
H163	-1.2308430011	-4.9537549826	9.7029544833
H164	0.1278820627	-3.4117337758	9.6392495885
H165	-0.9500704215	-0.9296228202	12.7956478712
H166	0.9468526370	0.9958904268	12.7744199526
H167	-3.4417285978	0.1497292266	9.6373292081
H168	-4.9966654444	-1.2236064253	9.6796538792
H169	-7.7122605850	-1.1914237061	0.8564257947
H170	-1.1994157162	-7.7123987984	0.8767328319
H171	-6.6048050902	-5.5404362526	-0.2166671093
H172	-4.0275707419	-3.9513334421	-0.8908070261
H173	-1.2212527614	-5.0154871906	-0.7233719030
H174	0.1038729330	-3.4154363343	-0.6639095452
H175	-0.9300042813	-0.9623818184	-3.8015212588
H176	0.9706297551	0.9539572706	-3.8330853772
H177	-3.4475318392	0.2023851755	-0.6673435939
H178	-5.0095560605	-1.2691954771	-0.7417099152
H179	-5.8082980863	-2.5365451073	0.8026416309
H180	-2.4737106635	-5.7336764116	0.7936294067
H181	-3.1401825013	4.1985195391	-1.9353173508
H182	-1.7365999161	1.6219683890	-2.4464775260
H183	1.7440230465	-1.6382301955	-2.4398043903
H184	3.1314321822	-4.1722399140	-1.9538557643
H185	-2.6156170854	-1.0538789823	-2.1474969024
H186	-1.0643892811	-2.6314589850	-2.1318592128
O187	1.2761429325	3.2117196902	-1.3595968296
O188	3.2442110134	1.2680344130	-1.3062521706
O189	-0.8672871887	3.6501445738	0.0116910042
Ti190	0.0880222838	4.5613786020	1.5244679845
O191	3.6512019522	-0.9447284230	0.0393756208
Ti192	4.6796307644	0.0385225975	1.4807116734
Ti193	2.2643037327	2.3090122326	0.0139972038
O194	3.6701237349	3.7025487963	0.0241510902
Ti195	4.7424782945	4.6935266772	1.5089584989
O196	1.4040639714	3.2063994621	1.5067809052
O197	3.1876779261	1.3529541459	1.4766795737
O198	1.0098504621	5.5841095899	0.1742390274
O199	1.2033095259	7.8791862912	1.6369345044
O200	3.1730225585	5.9298316732	1.6245032672
O201	5.4619894157	1.0212982882	0.0989499845
O202	5.9397316599	3.1542042859	1.5014049273
O203	8.0360619454	1.3406996937	1.8136430698
O204	5.5343283908	5.6967646375	0.2206114177
O205	-0.9105182121	3.6766226547	2.9688238233
O206	3.6593718092	-0.9122853628	2.9990295141
Ti207	2.3827188546	2.0510762726	3.0300587671
O208	3.7083776380	3.6311224577	3.0465140311
Ti209	2.1789875706	7.0467927945	2.9682410245
O210	0.8713531114	5.5258788306	3.0108852111
Ti211	6.8840211176	2.1954028215	3.0318437545
O212	5.5198932052	0.8646518035	2.9766948488
O213	5.4987993806	5.4541459548	3.0137456313
Ti214	-0.2975606723	4.5855878742	4.4927616614

Ti215	4.5806867034	-0.2315394629	4.4957952704
Ti216	4.6848537591	4.5340680706	4.4742522787
O217	1.4291882750	3.1624029369	4.4510871442
O218	3.1894169239	1.3336034757	4.5078181451
O219	1.6907030058	7.8738865587	4.4735079022
O220	3.1457654192	5.8546977960	4.4826621922
O221	6.0096978832	3.2122299178	4.5077246851
O222	7.8028106095	1.5759345807	4.4960591309
O223	-0.9333516501	3.6481882983	5.9708516387
Ti224	0.0659200259	4.6321342991	7.4801941634
O225	3.6608764702	-0.9238588334	5.9697317261
Ti226	4.6183370145	0.1026878401	7.4770454961
Ti227	2.3318261021	2.4231810045	5.9367151843
O228	3.6841654912	3.6610179840	5.9776216102
Ti229	4.7709273700	4.7307841855	7.5137734256
O230	1.3721159281	3.1837037042	7.4448217391
O231	3.1738061986	1.3832191977	7.4792971078
Ti232	2.2656970311	6.7456046599	5.9070759425
O233	0.8584345713	5.4853032953	5.9412056903
O234	1.3738422783	7.9712347043	7.0964690481
O235	3.1751808754	5.9470957139	7.4288028276
Ti236	6.8766140890	2.2123756575	5.9657829628
O237	5.5193372622	0.8629768533	5.9912768561
O238	5.9202747546	3.1521337639	7.4678548600
O239	8.0330880739	1.3826065202	7.1941870756
O240	5.4783909154	5.4798472947	5.9928597530
O241	-0.9281658813	3.6546747509	8.9222696756
O242	3.6378928071	-0.9302616179	8.9420891297
Ti243	2.2933666140	2.2712353527	8.9349025258
O244	3.6645934938	3.7005877189	8.9572491789
O245	1.2280856271	3.2356951019	10.2642067721
O246	3.1838237036	1.2764070802	10.3083100296
O247	1.0523235236	5.4690655878	8.8372570721
O248	5.4503069486	1.0338363031	8.8793837034
O249	5.6093066621	5.6258073489	8.8152388578
H250	1.2830111338	7.8161763091	8.0594727414
H251	7.9711123507	1.3511696448	8.1705814293
H252	2.4919516511	5.7758878662	8.1598769162
H253	5.7357978786	2.4618996013	8.1871005448
H254	1.0504093205	2.6965043187	11.0802516639
H255	2.6191387500	1.0920141476	11.1108881549
H256	3.4361707113	-0.2039468620	9.6262659238
H257	4.9413633902	1.2384663170	9.7072236975
H258	3.9080698027	4.0128734448	9.8524246304
H259	5.9641916266	6.1004876169	9.5862458907
H260	1.2599577743	4.9453647941	9.6600263912
H261	-0.1772208684	3.4438321897	9.6033338741
H262	3.4424997313	-0.2020056401	-0.6311715402
H263	4.9088820997	1.2369440519	-0.7052705877
H264	3.9662530934	4.0035879733	-0.8587628556
H265	5.5860338057	6.5823625199	-0.1840405978
H266	1.2107575733	5.1698076656	-0.6975143674
H267	-0.1351815999	3.4695709523	-0.6860474157
H268	1.0040541820	7.3769001228	0.8006180496

H269	2.5066536271	5.7609088190	0.8854706725
H270	5.7461713402	2.4523300715	0.7975240128
H271	7.9448097417	1.2860959127	0.8409573154
H272	1.0893947226	2.6497945402	-2.1620218704
H273	2.7388034926	1.0839529105	-2.1397065874
O274	-5.6489854670	3.5741955244	0.1759711841
Ti275	-4.5781464612	4.4416265918	1.4819055102
O276	-7.8533562009	3.2331715993	1.6073016742
O277	-5.9392438303	1.3588056050	1.5574700810
O278	-4.4090057416	5.8980450358	0.3056116142
O279	-3.3878863101	7.7880693101	1.5996457703
O280	-1.3654408407	6.0045242068	1.5538694967
Ti281	-7.0145722994	2.3866384504	2.9764987208
O282	-5.5615239876	3.7728032987	2.9707404389
Ti283	-2.5182562901	6.9426531099	2.9173002101
O284	-3.8094211040	5.5182827402	2.9802173146
Ti285	-4.4451500520	4.4111361920	4.4638636859
O286	-7.8119643043	3.0618485137	4.4577790677
O287	-5.9418041691	1.4023879807	4.4095304343
O288	-3.1007282114	7.8214946636	4.4584933285
O289	-1.4894617026	5.9302899853	4.4567336098
Ti290	-6.9677226153	2.4346821938	5.9977650674
O291	-5.5181776697	3.7542957715	5.9233705057
Ti292	-4.4611099954	4.5848930124	7.4217643373
O293	-7.8096826673	3.3161225030	7.3001896892
O294	-5.9924538417	1.3621112099	7.4206126351
Ti295	-2.3897777349	7.0476866513	5.9382347229
O296	-3.7942263404	5.5513431321	5.9376408562
O297	-3.1973763510	7.8678344566	7.3317248767
O298	-1.3778654927	5.9341630188	7.3669824234
O299	-5.9394210835	4.3880398911	8.5765177623
O300	-3.6146099054	5.6455229556	8.7417944118
H301	-7.2347756812	3.8442668059	7.9734258833
H302	-3.4983573351	7.4378568421	8.1725249027
H303	-6.2551422946	1.6485400497	8.3185209492
H304	-2.0454546534	5.8470656421	8.1119957566
H305	-3.5176272044	5.2987966913	9.6589347709
H306	-6.0628269656	4.8277498943	9.4409146923
H307	-7.4183322555	3.5115974306	0.7620019362
H308	-4.8657767410	6.0188467556	-0.5498306786
H309	-5.3067357693	3.4910182042	-0.7432666885
H310	-5.8410215352	2.0241790429	0.8090004963
H311	-3.8899053683	7.2132151190	0.9124042691
H312	-1.5924673792	6.2849796153	0.6444446457
O313	4.3206220425	-5.8828946296	0.3229249652
Ti314	4.5551165232	-4.4416890302	1.5051968197
O315	1.3039191803	-5.9919705280	1.5637804944
O316	3.3116886322	-7.7694024416	1.6426976900
O317	5.6232819408	-3.5776900820	0.1917550127
O318	5.9665135787	-1.3967821164	1.5724080693
O319	7.8638125496	-3.2652260198	1.6378628186
Ti320	2.4272728574	-6.9451451450	2.9662097292
O321	3.7532629241	-5.4918042118	3.0056985463
Ti322	7.0040739348	-2.4431166387	3.0047807809

O323	5.5534161458	-3.7826755492	2.9896785982
Ti324	4.3773749171	-4.4522575327	4.4849925097
O325	1.3947449617	-5.9027309921	4.4536789665
O326	3.0611297064	-7.7713915466	4.4817499646
O327	5.9639986097	-1.4430766476	4.4608358162
O328	7.8316269626	-3.0905784891	4.5008262065
Ti329	2.4149833568	-6.9613693950	5.9984951599
O330	3.7509639686	-5.4898852886	5.9524156658
Ti331	4.5697163637	-4.4412336204	7.4505917610
O332	1.3376907965	-5.9591066791	7.4343228888
O333	3.2868046480	-7.7858289451	7.3214988359
Ti334	7.0092380361	-2.3945782957	6.0001712238
O335	5.5469896584	-3.7708157368	5.9708290844
O336	5.9256056116	-1.3766246818	7.3956411448
O337	7.8413407208	-3.2108194285	7.3792680876
O338	4.3570904705	-5.9205607779	8.6035339780
O339	5.6167866372	-3.6041475816	8.7860834645
H340	3.8133939209	-7.2170311433	7.9918259893
H341	7.4145363102	-3.5149152760	8.2203996834
H342	1.6612848973	-6.1928374460	8.3272651466
H343	5.8212869011	-2.0232508359	8.1550652938
H344	4.7732093969	-6.0395872312	9.4793228279
H345	5.2550256970	-3.5132941796	9.6996479324
H346	3.8000065999	-7.2002402519	0.9458577935
H347	4.7341313048	-6.0068907267	-0.5535529408
H348	5.2660065118	-3.4853597754	-0.7219630636
H349	1.5422686445	-6.3035580388	0.6681074321
H350	5.8736117808	-2.0720628120	0.8238932479
H351	7.4671914248	-3.5432515516	0.7771018540
Ti352	0.0319222137	0.0209948548	-1.5169799269
O353	-0.9777787604	-0.9562586372	-2.8253805475
O354	0.9799529431	0.9628339840	-2.8562467804
Ti355	-0.0216306040	0.0006628704	10.4901076272
O356	-0.9774043701	-0.9438703535	11.8190690956
O357	0.9619566171	0.9810347640	11.7976829653
Li358	2.2583360898	4.5433389190	3.5927517212

3.10 $555 \text{ I}_{\text{Li}}^+/\text{e}^-$ cluster in water^{||}

3.10.1 Ground State GS1

358			
555	Li ⁺ /e ⁻	Intercalation GS1, Water-Optimized SCFE :	-17174.8401443965 hartree
O1	-7.8712136252	-4.1343907146	3.1715434466
H2	-8.1583513623	-4.2548124628	4.1226812571
H3	-7.1841320747	-4.8308372105	2.9716772173
O4	-7.8843045371	-4.2198030544	5.8550118379
H5	-8.6503394718	-4.4197337325	6.4294455911
H6	-7.1410431346	-4.8922464682	5.9687457898
O7	-4.1431539037	-7.9078813111	2.9142884909
H8	-4.3173253470	-8.4490113590	2.1182107545
H9	-4.8574956860	-7.2213588967	3.0313458911

^{||}intercalated by Li⁺ cation, also reduced by an electron

O10	-4.1606327235	-7.8848555940	6.1060225851
H11	-4.3349429384	-8.4071995748	6.9145754555
H12	-4.8757708770	-7.2012386308	5.9740571229
O13	4.1502734019	7.8625337274	3.1570092046
H14	4.2732675677	8.1827338273	4.0916421538
H15	4.8512760913	7.1755363364	2.9732691814
O16	4.2094595549	7.9391160770	5.8813417610
H17	4.4764338798	8.7326559367	6.3900855548
H18	4.8665843436	7.1831975319	5.9788455938
O19	7.9793355761	4.0657239591	2.8571624087
H20	8.4878899550	4.2213550999	2.0361103805
H21	7.3288973962	4.8021329683	2.9977394970
O22	7.9387325950	4.1082523847	6.0762027973
H23	8.5071180537	4.2609974980	6.8569891866
H24	7.2808099675	4.8470386268	5.9762074972
O25	-8.4602244832	0.9017591439	2.9437565126
H26	-9.3827046237	1.2041315136	2.8177956117
H27	-8.2935235310	0.0213776276	2.4292693285
O28	-8.2820913321	0.8375262888	5.7968042693
H29	-8.4512229461	0.5669212191	4.8581271940
H30	-8.2399962991	0.0201648896	6.4069134879
O31	0.8959203774	-8.4796924360	3.0043444395
H32	1.1953282603	-9.4052671527	2.8995991621
H33	0.0101060419	-8.3236265880	2.5015136282
O34	0.8313521292	-8.2809547748	5.8644395871
H35	0.5582782568	-8.4433857040	4.9245605447
H36	0.0158108066	-8.2222305073	6.4722463726
O37	-0.9212436603	8.4699964364	2.9985670645
H38	-1.2230178955	9.3850906873	2.8201882062
H39	-0.0303284461	8.2806482967	2.4954900144
O40	-0.8745271458	8.3459613797	5.7841986118
H41	-0.6049511108	8.5094490817	4.8399536354
H42	-0.0953730725	8.3657837912	6.4155943555
O43	8.4814324951	-0.9156074355	2.9728987528
H44	9.3978747790	-1.2416697275	2.8659667316
H45	8.3441230529	-0.0481485302	2.4456014669
O46	8.3107662207	-0.8046425031	5.8206376740
H47	8.4497628423	-0.4958463125	4.8875358756
H48	8.2851270510	-0.0072613567	6.4576832062
O49	-3.2023373074	-1.2583386704	-1.3476916630
O50	-1.2535675336	-3.2356032231	-1.3411678495
O51	-3.2695320795	3.3300934762	-1.4370579210
O52	-1.4147474785	1.4217336171	-1.5405682063
O53	1.4475196110	-1.4522306035	-1.5440234008
O54	3.3124588836	-3.4227181932	-1.3517128743
O55	-5.7082368963	-5.5921315425	0.1822951914
Ti56	-4.7317879489	-4.7577194445	1.4776851526
O57	-5.4912704472	-1.0591539022	0.1075250714
Ti58	-4.6115639443	-0.1016159977	1.4725449614
O59	-7.9182928844	-1.3057803695	1.7627390144
O60	-5.9681388409	-3.2067987915	1.5313784879
O61	-1.0292344736	-5.4970699339	0.1160795216
Ti62	-0.1115462892	-4.5985592383	1.5109546783
O63	-3.1806741545	-5.9365325053	1.4827148597

O64	-1.3490098463	-7.9838103189	1.8307992020
Ti65	-2.2893848060	-2.2789894015	0.0138370522
O66	-0.8572342049	-0.8975563337	-0.0399044907
O67	-3.6973535818	-3.6748782139	0.0008030034
Ti68	0.0269376786	0.0052381990	1.5093523642
O69	-3.1723632722	-1.3818812719	1.4779133316
O70	-1.3891519121	-3.1812496825	1.4860873328
Ti71	-2.3792330596	2.4191681395	-0.1586700332
O72	-3.6347543540	0.9104938181	0.0207789359
O73	-3.1806716641	3.2078936134	1.4422778993
O74	-1.3952078912	1.4027124194	1.4489865120
Ti75	2.3890693223	-2.4469403241	-0.1192593720
O76	0.8784552299	-3.6404262559	0.0186105607
O77	1.4053526597	-1.4188354139	1.4791333048
O78	3.1664921753	-3.2629485920	1.4668891190
O79	0.8788283886	0.8703306124	-0.0191370990
O80	-5.4543448269	-5.4567481663	3.0056618005
Ti81	-6.8470108927	-2.2295933678	3.0286787902
O82	-5.4897874350	-0.8719898873	2.9737136072
Ti83	-2.2567925719	-6.8447544044	3.0558763377
O84	-0.9184342434	-5.4844860870	2.9979217190
Ti85	-2.3419703651	-2.3303701994	3.0377728001
O86	-0.8842555427	-0.8789727562	2.9758287553
O87	-3.6604541599	-3.6646655298	2.9906765128
Ti88	-2.1722029096	2.1365777935	2.9024278208
O89	-3.6303499037	0.8879762851	2.9798747463
Ti90	2.1660424410	-2.1942424205	2.9247556510
O91	0.8763826794	-3.6625680984	2.9869255904
O92	0.8669920810	0.8678074149	2.9797292807
Ti93	-4.5311054055	-4.5121107309	4.4797059293
Ti94	-4.5858703174	0.1924170974	4.4619114724
O95	-7.8322590597	-1.6971070746	4.4724881571
O96	-5.8459195140	-3.1367484816	4.5109170308
Ti97	0.1652286051	-4.5924106774	4.4880899801
O98	-3.2246503217	-5.9315376518	4.5015020532
O99	-1.6556260222	-7.7987515730	4.5082577079
Ti100	-0.0207618547	-0.0329671055	4.4851843632
O101	-3.1830576719	-1.3895924255	4.4802971547
O102	-1.4072802278	-3.1559730541	4.4842012339
O103	-3.1824308871	3.1928399014	4.4497439866
O104	-1.4028238727	1.3921440528	4.4807390556
O105	1.3836389418	-1.4196880470	4.4853538306
O106	3.1671953940	-3.1937916646	4.4802656496
O107	-5.4874567020	-5.4403203407	5.9891203097
Ti108	-4.7580078545	-4.7503640933	7.5160344520
Ti109	-6.7933423591	-2.2277760637	5.9362011715
O110	-5.5024095658	-0.8524256993	5.9701064201
Ti111	-4.5930383465	-0.0705198565	7.4641042306
O112	-7.9817035534	-1.3621231010	7.1431816790
O113	-5.9505909724	-3.1607420137	7.4541805652
Ti114	-2.2703898369	-6.8224584871	5.9582111902
O115	-0.9080936603	-5.4754364821	5.9847957318
Ti116	-0.1091945077	-4.5759475284	7.4661139351
O117	-3.1707529509	-5.8912598546	7.4884322068

O118	-1.3740875076	-7.9452972439	7.2014473672
Ti119	-2.3654480376	-2.3431478159	5.9239281535
O120	-0.8971165236	-0.8811314283	5.9908284134
O121	-3.6586325408	-3.6696354137	5.9956641968
Ti122	-0.0367718648	-0.0372652716	7.4847615990
O123	-3.1900994989	-1.3619888872	7.4764397227
O124	-1.3963560933	-3.1645868024	7.4916200462
Ti125	-2.1805259285	2.1770165591	6.0411088736
O126	-3.6697004041	0.9155321962	5.9579480112
O127	-3.2426731678	3.1817977059	7.4814730640
O128	-1.4218869287	1.4036329362	7.4802363414
Ti129	2.1764351308	-2.1853458964	6.0603346016
O130	0.8869094341	-3.6689676072	5.9860599007
O131	1.3919687377	-1.4184745761	7.4934473554
O132	3.1732739582	-3.2381237991	7.5069975378
O133	0.8708511334	0.8345072306	5.9879084563
O134	-5.6392647316	-5.6292109343	8.8074717378
O135	-5.5019398620	-1.0077163432	8.8348306104
O136	-1.0285272880	-5.4755168453	8.8653154986
Ti137	-2.3041962385	-2.2780292080	8.9578092643
O138	-0.8839554813	-0.8779973579	8.9980040508
O139	-3.7180756963	-3.6479202829	8.9829629634
O140	-3.2217882295	-1.2143128312	10.3007997740
O141	-1.2831531204	-3.1938914500	10.3199645515
Ti142	-2.4204802041	2.4081674578	9.0842346805
O143	-3.6436231652	0.9044071211	8.9400723824
O144	-3.4234428606	3.3194810436	10.2947331010
O145	-1.4430130570	1.4532356514	10.4969798026
Ti146	2.3971631269	-2.4325802514	9.0977878579
O147	0.8701995613	-3.6161329719	8.9668001458
O148	1.4469930551	-1.4057273279	10.5084218119
O149	3.2968791412	-3.4235297249	10.3336744091
O150	0.8388997261	0.8849956754	8.9853743539
H151	-7.7837447496	-1.2313088054	8.0938413020
H152	-4.2657418902	3.1556325515	10.7621704101
H153	-1.2381787200	-7.6909244426	8.1393725113
H154	3.1089630244	-4.2396311113	10.8368932094
H155	-5.7681873454	-2.4651944999	8.1693193699
H156	-1.7110486584	1.6923917903	11.4074973994
H157	-2.4667284039	-5.6997024064	8.1926407363
H158	1.7490716980	-1.6104341230	11.4171331833
H159	-2.6352818116	-1.0333562232	11.0919897187
H160	-1.0954064111	-2.6045948742	11.1096598055
H161	-6.0207445470	-6.1400390308	9.5405193303
H162	-4.0281934574	-3.9121763756	9.8724739995
H163	-1.2241251353	-4.9777566198	9.7001169118
H164	0.1251957658	-3.4120679591	9.6448192275
H165	-0.9554692606	-0.9321833750	12.7519576756
H166	0.9054447095	0.9931496491	12.8346022288
H167	-3.4427547213	0.1525254882	9.6265514171
H168	-5.0128727924	-1.2084265349	9.6732939368
H169	-7.6156345436	-1.1681391838	0.8384849291
H170	-1.2284513904	-7.7554477582	0.8848878923
H171	-6.6130756132	-5.5550180174	-0.1815120455

H172	-4.0038094887	-3.9510573581	-0.8863912089
H173	-1.2300204846	-4.9936806125	-0.7157097732
H174	0.1275120558	-3.4452668982	-0.6661707586
H175	-0.9210854961	-0.9597188814	-3.8087371836
H176	0.9543429890	0.9598490375	-3.8135105519
H177	-3.4365539199	0.1749740156	-0.6659383986
H178	-4.9948474904	-1.2729829177	-0.7244043429
H179	-5.7790228918	-2.5287909054	0.8076154185
H180	-2.4637040512	-5.7410336608	0.7924024956
H181	-3.2469363196	3.7476325424	-2.3193179048
H182	-1.7195227774	1.5787154162	-2.4565939480
H183	1.7703563826	-1.6320174831	-2.4503628580
H184	3.1303247747	-4.2320266724	-1.8688506796
H185	-2.6258431899	-1.0710928333	-2.1432753162
H186	-1.0691801698	-2.6738698188	-2.1421041870
O187	1.2361273188	3.2177568398	-1.3146441671
O188	3.2128048763	1.2599637772	-1.3300052132
O189	-0.8723399990	3.6390577014	0.0257724718
Ti190	0.1094662782	4.5836008222	1.4961294602
O191	3.6385530657	-0.9463371377	0.0175833857
Ti192	4.6086981383	0.0848614143	1.4918641998
Ti193	2.3031740049	2.2685486636	0.0538901430
O194	3.6716497700	3.7002285612	0.0163332802
Ti195	4.7534095927	4.7115997808	1.4808710426
O196	1.3794771786	3.1842625066	1.4927422411
O197	3.1858959268	1.3694553573	1.4748874243
O198	1.0653413941	5.5185553286	0.1461603374
O199	1.2731746187	7.8982422352	1.8290423675
O200	3.1812517781	5.9642880107	1.5643791677
O201	5.4748236986	1.0210951770	0.0981753459
O202	5.9307400415	3.1710379987	1.4828495012
O203	8.0002400561	1.3287205461	1.7651848034
O204	5.5408569595	5.7134540605	0.1813154067
O205	-0.9232725463	3.6505968013	2.9793359831
O206	3.6519658657	-0.9398720789	2.9872307865
Ti207	2.3373087601	2.3452572099	3.1162559899
O208	3.6834425639	3.6758911264	3.0187218715
Ti209	2.2479219569	6.7972472384	3.0558745741
O210	0.8603588004	5.4910872065	3.0216258308
Ti211	6.8785324796	2.1849692468	3.0191236204
O212	5.5218821015	0.8624890130	2.9617621597
O213	5.4874042411	5.4641479226	2.9920934658
Ti214	-0.2959405843	4.5900202398	4.4562574860
Ti215	4.5347698554	-0.1961402843	4.4827828852
Ti216	4.6436351014	4.5241338387	4.4689661633
O217	1.3826189037	3.2054281833	4.4544226582
O218	3.2250134838	1.2996608371	4.3914734482
O219	1.7235260886	7.9194301240	4.4822816182
O220	3.1179817641	5.8724043060	4.5585831735
O221	5.9862762869	3.2112960569	4.4758174791
O222	7.7994439111	1.5965597467	4.4803381130
O223	-0.9254925686	3.6636652958	5.9619265343
Ti224	0.0649812607	4.6449713211	7.4846904224
O225	3.6427749571	-0.9226630735	5.9656993890

Ti226	4.6517767801	0.0822491425	7.5076042282
Ti227	2.3497874576	2.1442702031	5.9928602502
O228	3.6906444564	3.6397706257	5.9469115250
Ti229	4.7331947723	4.7271126846	7.4707485996
O230	1.3536342991	3.2265564902	7.4886147071
O231	3.1895379732	1.2929126042	7.5833740178
Ti232	2.2097487498	7.0249946616	5.9728328219
O233	0.8532226205	5.5731970931	5.9765252575
O234	1.3503231255	8.0520711691	7.2519653790
O235	3.1672396536	5.9508761187	7.3884363611
Ti236	6.8336750933	2.2290205158	5.9477144970
O237	5.5000819465	0.8716933856	5.9892136984
O238	5.9113442624	3.1462107707	7.4570545070
O239	8.0084761312	1.3834565779	7.1675327629
O240	5.4696214823	5.4896480059	5.9669097168
O241	−0.9345679206	3.6674866497	8.9457743709
O242	3.6494658425	−0.9476524765	8.9744219107
Ti243	2.2498020278	2.3075755757	8.9155402663
O244	3.6427844364	3.7115511861	8.9389976284
O245	1.2159565789	3.2314996792	10.3018838643
O246	3.2202649969	1.2854214748	10.2971343391
O247	1.0232463083	5.5253674467	8.8469612833
O248	5.4781445057	1.0348662855	8.9002912381
O249	5.6304152153	5.5766352218	8.7829370967
H250	1.1853316248	7.8414259609	8.1954929503
H251	7.8758207187	1.3094533030	8.1346041786
H252	2.4910761605	5.7872660869	8.1199945049
H253	5.7301166096	2.4646005590	8.1829300754
H254	1.0515287230	2.7104852551	11.1271050388
H255	2.7329858714	1.1344415394	11.1421388314
H256	3.4220317813	−0.1868597302	9.6248353417
H257	4.8979815711	1.2526381699	9.6860670517
H258	3.9621663993	3.9621635931	9.8285664807
H259	6.2494202593	5.7364775900	9.5166982137
H260	1.2538069891	5.0051304182	9.6619358235
H261	−0.1798603302	3.4615205238	9.6277394127
H262	3.4353985805	−0.2055250271	−0.6579386407
H263	4.9492041947	1.2246212597	−0.7215548090
H264	3.9131978139	4.0281632613	−0.8731188932
H265	5.5149584277	6.6162313079	−0.1877514899
H266	1.2701397842	5.0247297944	−0.6897206189
H267	−0.1026951230	3.4379767190	−0.6596921916
H268	1.1023109498	7.5691155691	0.9178628409
H269	2.4977773526	5.7850884033	0.8331411226
H270	5.7333033916	2.4629523538	0.7838050688
H271	7.7863632833	1.2259831099	0.8144723105
H272	1.0657590949	2.6570964463	−2.1170463766
H273	2.6510367487	1.0798268852	−2.1347650058
O274	−5.6412545951	3.7170240482	0.1734101910
Ti275	−4.4828594429	4.4769985501	1.4688322060
O276	−7.8014301449	3.2930822957	1.5844987247
O277	−5.9083849510	1.3851010857	1.5420396000
O278	−3.8721265645	5.7595549091	0.2205360462
O279	−3.3312411805	7.8517621979	1.6121873295

O280	-1.3922859999	5.9430890687	1.5642176832
Ti281	-6.9675743330	2.4307612883	2.9441189759
O282	-5.5294571103	3.7882552701	2.9669124994
Ti283	-2.4830127975	6.9778014738	2.9462511691
O284	-3.8059157416	5.5475935754	2.9723475580
Ti285	-4.4366226130	4.4126963996	4.4544907192
O286	-7.8100768128	3.0714598158	4.4299020868
O287	-5.9265559658	1.4254571866	4.4108596351
O288	-3.1194465508	7.8289540765	4.4593629352
O289	-1.4925462492	5.9508398716	4.4453178956
Ti290	-6.9783680536	2.4244349466	5.9536176603
O291	-5.5206365777	3.7611811711	5.9099120426
Ti292	-4.4821223887	4.5312738191	7.4209364532
O293	-7.8309318680	3.3091109440	7.2594740907
O294	-5.9752738659	1.3860536757	7.4020139887
Ti295	-2.4375219020	7.0235998264	5.9548986109
O296	-3.8057704697	5.5517103571	5.9499464496
O297	-3.2546653835	7.8687936037	7.3285399942
O298	-1.4110221828	5.9470587274	7.3665721755
O299	-5.9064917387	4.2498813452	8.6229630439
O300	-3.6682318795	5.6690982077	8.7184703988
H301	-7.2782337031	3.7963547408	7.9648597063
H302	-3.5622244707	7.3949804228	8.1474403210
H303	-6.1369110402	1.7790446816	8.2834222996
H304	-2.0787525852	5.8479131174	8.1093851318
H305	-3.5844174190	5.3299447477	9.6396080052
H306	-6.0579420361	4.7192891137	9.4660078338
H307	-7.3147035763	3.5958701684	0.7699494919
H308	-3.8923740274	5.6547860362	-0.7517002051
H309	-5.3472935785	3.6108733798	-0.7584734147
H310	-5.8073557463	2.0256504082	0.7848247609
H311	-3.6827967167	7.3233425914	0.8331517572
H312	-1.9680420244	5.8839726337	0.7619788718
O313	4.2787256652	-5.9197163944	0.3228236535
Ti314	4.5398429869	-4.4814195412	1.5075920218
O315	1.3307856973	-5.9897003926	1.5634440287
O316	3.3072991129	-7.8188512609	1.6756488423
O317	5.6281809732	-3.6459536177	0.1930555270
O318	5.9255953435	-1.3922137999	1.5677812327
O319	7.8198069262	-3.2725990345	1.6170985076
Ti320	2.4181375562	-6.9719462303	2.9908797655
O321	3.7603490734	-5.5258926276	3.0175162624
Ti322	6.9550395003	-2.4264562852	2.9778567694
O323	5.5378378778	-3.7995433662	2.9879842412
Ti324	4.3756689623	-4.4615239028	4.4847173790
O325	1.3939400895	-5.9204101529	4.4561940525
O326	3.0533357369	-7.7922796556	4.5016443310
O327	5.9480899419	-1.4340334671	4.4485544489
O328	7.8193131465	-3.0803144582	4.4711050554
Ti329	2.4097091983	-6.9612304510	6.0193204705
O330	3.7488417895	-5.5012935286	5.9598494008
Ti331	4.5761103617	-4.4398165720	7.4439994213
O332	1.3328487201	-5.9669368939	7.4422271541
O333	3.2859182530	-7.7876504388	7.3381396242

Ti334	7.0055285546	-2.3682216712	5.9502806488
O335	5.5331087411	-3.7655227675	5.9637129721
O336	5.9341883819	-1.3848957944	7.4024415682
O337	7.8540033060	-3.1904962888	7.3281106323
O338	4.3534603333	-5.9136014465	8.6129946663
O339	5.6272774831	-3.6005340238	8.7797821890
H340	3.8090818016	-7.2084328802	8.0131345184
H341	7.4461673033	-3.4891615904	8.1779015832
H342	1.6321103486	-6.2088284341	8.3409326281
H343	5.8438645461	-2.0553308837	8.1445317219
H344	4.7675306828	-6.0159515771	9.4913730045
H345	5.2509076452	-3.5056746400	9.6872633022
H346	3.7855279765	-7.2628463690	0.9677825835
H347	4.7217035543	-6.0606132453	-0.5374987115
H348	5.2407922818	-3.5429716322	-0.7094862156
H349	1.6744111878	-6.2000978724	0.6722287966
H350	5.8321942602	-2.0406078342	0.8098100231
H351	7.3691374973	-3.5724727151	0.7861214492
Ti352	0.0237022103	-0.0233479579	-1.5012695916
O353	-0.9874232684	-0.9625512657	-2.8339556863
O354	0.9994319576	0.9338021742	-2.8382054454
Ti355	0.0240118387	0.0317217920	10.4922355573
O356	-1.0147842710	-0.9787850612	11.7774504065
O357	0.9074838459	0.9492855849	11.8591668701
Li358	2.2181220134	4.5384409219	5.3884756618

3.10.2 Ground State GS2

358			
555 Li+/e- intercalation GS2, Water-Optimized SCFE : -17174.8416835168 hartree			
O1	-7.8738950514	-4.1439894411	3.1870245192
H2	-8.1594689004	-4.2633848316	4.1383799812
H3	-7.1884610429	-4.8410790315	2.9849270605
O4	-7.8854720369	-4.2235445908	5.8701573394
H5	-8.6487874085	-4.4222256784	6.4490392065
H6	-7.1402208698	-4.8943436252	5.9837950809
O7	-4.1222438366	-7.9150731731	2.9128686852
H8	-4.2923709699	-8.4412788877	2.1060524428
H9	-4.8423798313	-7.2388162683	3.0421949362
O10	-4.1540341044	-7.8820891395	6.1083688321
H11	-4.3231676633	-8.4174139174	6.9092302627
H12	-4.8692110558	-7.1954111486	5.9930352383
O13	4.1008218232	7.9130679488	3.1661878404
H14	4.2495696337	8.1685900478	4.1260563703
H15	4.7766145715	7.2194367293	2.9333149869
O16	4.2445275806	7.8896097255	5.8373070798
H17	4.4190020988	8.6547971830	6.4226835335
H18	4.9240052092	7.1578347841	5.9657919650
O19	7.9745559307	4.0629770329	2.8836418258
H20	8.5009853335	4.2176770444	2.0736570769
H21	7.3229452380	4.8015541093	3.0129066581
O22	7.9605874447	4.0915800269	6.1072750959
H23	8.5059366407	4.2420286125	6.9050532015
H24	7.3033688491	4.8283921726	5.9978853945

O25	-8.4844605397	0.8774572174	2.9710648980
H26	-9.4033044992	1.1854954798	2.8318767250
H27	-8.3154096679	-0.0075461998	2.4582042070
O28	-8.2872035306	0.8440011172	5.8141734462
H29	-8.4608040440	0.5762410352	4.8749609265
H30	-8.2359996789	0.0256473115	6.4188256944
O31	0.9057081722	-8.4727818664	3.0024982586
H32	1.2060800175	-9.3989102281	2.9049866820
H33	0.0230661394	-8.3160501847	2.4974506855
O34	0.8328401406	-8.2706388310	5.8530755703
H35	0.5592729382	-8.4278900209	4.9125312646
H36	0.0169333076	-8.2154507786	6.4603081108
O37	-0.9835011789	8.4947512573	2.9548395570
H38	-1.3003628709	9.4173389457	2.8735045757
H39	-0.1614685539	8.3428183703	2.3777607903
O40	-0.7921449041	8.2804743499	5.7981833887
H41	-0.5285467140	8.4510596191	4.8577304738
H42	0.0400580947	8.2317391927	6.4098900219
O43	8.4852068215	-0.9032856128	2.9925795620
H44	9.4017501864	-1.2275963995	2.8816367337
H45	8.3428323888	-0.0330804801	2.4683727976
O46	8.3192317659	-0.8070778093	5.8413197059
H47	8.4551780343	-0.4929420467	4.9094710095
H48	8.3102876028	-0.0163805017	6.4815339057
O49	-3.2059778611	-1.2563764026	-1.3498965463
O50	-1.2580469256	-3.2186792278	-1.3364835771
O51	-3.2926905717	3.3838522963	-1.3814991004
O52	-1.4307875140	1.4235111719	-1.5444212474
O53	1.4409425882	-1.4372952494	-1.5418532011
O54	3.2852617191	-3.4316269130	-1.3622297137
O55	-5.7191363870	-5.5888206597	0.1954256741
Ti56	-4.7349470529	-4.7578622152	1.4890527119
O57	-5.4910614480	-1.0600138991	0.1016934882
Ti58	-4.6280654435	-0.1014652110	1.4699268707
O59	-7.9364314414	-1.3177808555	1.7946948268
O60	-5.9769297910	-3.2080093178	1.5386704247
O61	-1.0297073193	-5.5018086641	0.1236740630
Ti62	-0.1095556617	-4.5707193067	1.5063046316
O63	-3.1836493811	-5.9270726028	1.4881419134
O64	-1.3301176777	-7.9517225491	1.8164224602
Ti65	-2.3125780822	-2.2817939579	0.0047105369
O66	-0.8748141991	-0.8918672894	-0.0237281265
O67	-3.7116367024	-3.6745384469	-0.0006039824
Ti68	-0.0344392984	-0.0429384418	1.4872298538
O69	-3.1837670420	-1.3786230192	1.4823905005
O70	-1.4015768439	-3.1804598938	1.4860927668
Ti71	-2.3679369159	2.4286509607	-0.1411933841
O72	-3.6394289714	0.9293365955	0.0200065651
O73	-3.1651446113	3.2376218577	1.4487393035
O74	-1.3962687657	1.4103871177	1.4635626102
Ti75	2.3943614162	-2.4369811926	-0.1256902346
O76	0.8677131168	-3.6265306341	0.0239218996
O77	1.3986248088	-1.4139836470	1.4666713380
O78	3.1673132648	-3.2381795287	1.4678102735

O79	0.8554287911	0.8781740064	-0.0389671263
O80	-5.4544814053	-5.4572632722	3.0167000896
Ti81	-6.8431782697	-2.2412264159	3.0450600929
O82	-5.4882833937	-0.8812401551	2.9789921215
Ti83	-2.2405642071	-6.8339914376	3.0550519287
O84	-0.9221042568	-5.4680297502	3.0057931383
Ti85	-2.3646993484	-2.3288874740	3.0360111383
O86	-0.8971780534	-0.8781788462	2.9667126933
O87	-3.6686211040	-3.6635964641	2.9947122801
Ti88	-2.1916330170	2.1448089959	2.9058647287
O89	-3.6373913810	0.8971263713	2.9800295178
Ti90	2.1582045677	-2.1773935226	2.9170695068
O91	0.8814047438	-3.6557231415	2.9793403141
O92	0.8766441757	0.8393527942	2.9711651830
Ti93	-4.5363817458	-4.5219267276	4.4933408063
Ti94	-4.5908529685	0.1763650338	4.4619704442
O95	-7.8301572657	-1.6994015494	4.4875887014
O96	-5.8482599340	-3.1449623283	4.5210525097
Ti97	0.1616631501	-4.5896221871	4.4827471750
O98	-3.2239369872	-5.9294186459	4.5081080105
O99	-1.6428943932	-7.7879230165	4.5064341568
Ti100	-0.0356904125	-0.0297008941	4.5069197399
O101	-3.1856673621	-1.3850693571	4.4825154548
O102	-1.4068338671	-3.1501846268	4.4829082354
O103	-3.1848376655	3.1878682909	4.4558820837
O104	-1.4081542145	1.3986520126	4.4758149212
O105	1.3803430206	-1.4102597569	4.4855995475
O106	3.1626943868	-3.1761684460	4.4767732090
O107	-5.4814630036	-5.4413784541	5.9993567270
Ti108	-4.7479479566	-4.7467965835	7.5295572446
Ti109	-6.7944024001	-2.2265283565	5.9499387979
O110	-5.4965178616	-0.8618750191	5.9725766689
Ti111	-4.5878259641	-0.0757861822	7.4721048957
O112	-7.9635429116	-1.3588191496	7.1697918648
O113	-5.9454583356	-3.1648448797	7.4628858202
Ti114	-2.2675634507	-6.8193533596	5.9593977454
O115	-0.9060794772	-5.4704218436	5.9849466330
Ti116	-0.1022613295	-4.5788133435	7.4643756857
O117	-3.1641831756	-5.8908608269	7.4933305874
O118	-1.3737823937	-7.9481938408	7.1971509142
Ti119	-2.3539383083	-2.3518389356	5.9254152782
O120	-0.8914966166	-0.8725349912	5.9802708577
O121	-3.6551676168	-3.6668350575	6.0020807123
Ti122	0.0206080380	0.0204484313	7.4627231018
O123	-3.1863946929	-1.3568311231	7.4806540223
O124	-1.3957731245	-3.1578548293	7.4876436229
Ti125	-2.2012900701	2.1596177316	6.0475757384
O126	-3.6810992370	0.9137487645	5.9630820596
O127	-3.2536045218	3.1822713112	7.4892824752
O128	-1.4279460526	1.4010692520	7.4849697645
Ti129	2.1683291603	-2.1824924043	6.0512421498
O130	0.8856459000	-3.6607937253	5.9848918990
O131	1.3884693650	-1.4045678115	7.4865077454
O132	3.1624155661	-3.2355010911	7.5094389773

O133	0.8585164624	0.8676770686	5.9820746212
O134	-5.6401808853	-5.6182680761	8.8176308037
O135	-5.5050622727	-1.0079928144	8.8423768986
O136	-1.0293766215	-5.4614610048	8.8666996962
Ti137	-2.2857183054	-2.2581861508	8.9524227564
O138	-0.8862326333	-0.8681331943	9.0094745968
O139	-3.7024424264	-3.6432392994	8.9811378941
O140	-3.2298046848	-1.2233970591	10.3102004975
O141	-1.2741671234	-3.1939048011	10.3241167089
Ti142	-2.4249946388	2.4135944003	9.0818194586
O143	-3.6459514251	0.9027421265	8.9478398472
O144	-3.4153665621	3.3246839198	10.3073148633
O145	-1.4434517743	1.4510459976	10.4956168221
Ti146	2.3824362012	-2.4273619674	9.0921000320
O147	0.8651734654	-3.6096274450	8.9629335746
O148	1.4304736907	-1.4115100452	10.5054481704
O149	3.2900527903	-3.3979233125	10.3386506464
O150	0.8574111634	0.8805442709	8.9753429870
H151	-7.7430951355	-1.2171232672	8.1148476348
H152	-4.2285387603	3.1548398799	10.8218640000
H153	-1.2451260593	-7.7206814482	8.1421429066
H154	3.1002216166	-4.1930227589	10.8738297693
H155	-5.7665599104	-2.4710999810	8.1795270022
H156	-1.6698809988	1.7316277604	11.4054149030
H157	-2.4562891601	-5.6967010599	8.1942959664
H158	1.7361378004	-1.6101317607	11.4133630071
H159	-2.6607997609	-1.0398737735	11.1090988670
H160	-1.0940519458	-2.6249289081	11.1227424093
H161	-6.1381959501	-6.0720781669	9.5172487918
H162	-3.9978223450	-3.9067083771	9.8758034240
H163	-1.2284544644	-4.9574648903	9.6981027559
H164	0.1172916044	-3.4108131465	9.6434677326
H165	-0.9439439202	-0.9306328066	12.7800882153
H166	0.9163863572	1.0036500781	12.7945854455
H167	-3.4451222890	0.1570588254	9.6373434160
H168	-5.0077256172	-1.2113880764	9.6771072932
H169	-7.6690010763	-1.1898857497	0.8589910117
H170	-1.1876496080	-7.6795183801	0.8838886001
H171	-6.6200797437	-5.5127410828	-0.1733275426
H172	-4.0111275006	-3.9692484098	-0.8845065585
H173	-1.2273238038	-5.0066173394	-0.7124874767
H174	0.1180565798	-3.4276761853	-0.6620144888
H175	-0.9447408295	-0.9612958297	-3.7818954742
H176	0.9199152691	0.9348049768	-3.8713700922
H177	-3.4405273299	0.1956039519	-0.6637096380
H178	-4.9903903790	-1.2743767506	-0.7277638935
H179	-5.7941473365	-2.5332871888	0.8111631682
H180	-2.4650286542	-5.7323624831	0.7984592851
H181	-3.1282042288	4.1521587707	-1.9626339808
H182	-1.7565270705	1.5862691258	-2.4525313522
H183	1.7233967352	-1.6638222882	-2.4509166138
H184	3.0972584315	-4.2259678682	-1.9013919562
H185	-2.6078674470	-1.0652731248	-2.1347671952
H186	-1.0756670780	-2.6309448945	-2.1260726403

O187	1.2470209212	3.2086056881	-1.3683978127
O188	3.2295215328	1.2630713940	-1.3520529771
O189	-0.8672263176	3.6437211875	-0.0079611084
Ti190	0.0868947686	4.5719925571	1.5108118353
O191	3.6558490162	-0.9564248391	-0.0061953857
Ti192	4.6491849988	0.0796526379	1.4669739168
Ti193	2.2912135512	2.2957608014	0.0132060327
O194	3.6659834841	3.7059557758	0.0189942417
Ti195	4.7360562191	4.7033399635	1.5287305671
O196	1.3768293062	3.2167069673	1.4494677495
O197	3.2075476359	1.3062679599	1.3750919985
O198	1.0005189452	5.5993003209	0.1634441527
O199	1.2009600362	7.8896020637	1.6541583268
O200	3.1748139545	5.9508876767	1.6218395181
O201	5.5148705930	1.0136623426	0.0787725985
O202	5.9307507304	3.1686415868	1.4969715082
O203	7.9844679665	1.3265907121	1.7822661304
O204	5.5181937577	5.7082879618	0.2190947996
O205	-0.9051833193	3.6664068791	2.9724357633
O206	3.6390353467	-0.9085860908	2.9971923250
Ti207	2.3378287455	2.1322097748	2.9833287486
O208	3.6883567072	3.6500661221	3.0498923557
Ti209	2.1760357710	7.0452037773	2.9825297833
O210	0.8758734840	5.5243792212	3.0048668816
Ti211	6.8688185704	2.1903087476	3.0377344166
O212	5.4977572019	0.8783955066	2.9745147664
O213	5.4961920685	5.4520460051	3.0231910119
Ti214	-0.2892917718	4.5621710681	4.5028408867
Ti215	4.5205015141	-0.1877480452	4.4864514322
Ti216	4.6672507023	4.5171413514	4.5060763382
O217	1.3862464816	3.2086849540	4.5255381857
O218	3.2338068799	1.3057982082	4.5820462691
O219	1.6890970727	7.8778787804	4.4860031960
O220	3.1431869250	5.8622261438	4.4967727374
O221	5.9979811573	3.2055185266	4.5090853964
O222	7.7992734292	1.5822111483	4.4901517073
O223	-0.9450425205	3.6463058992	5.9800694024
Ti224	0.0897255767	4.6065573197	7.4849500833
O225	3.6544984534	-0.9385083205	5.9819692496
Ti226	4.6186713209	0.0944974094	7.4915026843
Ti227	2.3544526641	2.3613262439	5.8690942736
O228	3.7003382509	3.6643869066	5.9850731651
Ti229	4.7615645330	4.7161559414	7.5177419916
O230	1.3604333114	3.1799728452	7.4688747721
O231	3.1695072960	1.3696635371	7.4947525963
Ti232	2.2607782037	6.7453596791	5.9214996831
O233	0.8543588384	5.4940492639	5.9569941138
O234	1.3734961396	7.9673963238	7.1208987820
O235	3.1793417157	5.9488208074	7.4415205806
Ti236	6.8637618719	2.2061951137	5.9734230063
O237	5.5298687391	0.8624040916	6.0204368902
O238	5.9262236229	3.1423280397	7.4812096184
O239	8.0562501658	1.3989922956	7.1890492112
O240	5.4879086414	5.4789716564	6.0037169725

O241	-0.9265290366	3.6482083167	8.9376978137
O242	3.6230063076	-0.9279494386	8.9566997759
Ti243	2.2771556232	2.2727581818	8.9009914776
O244	3.6555466946	3.6945224165	8.9573164065
O245	1.2012903611	3.2337027775	10.2685305418
O246	3.1841858146	1.2783360698	10.3041652160
O247	1.0530064594	5.4822259864	8.8453971599
O248	5.4398861583	1.0365985202	8.8978767092
O249	5.6175827498	5.5870007926	8.8306340469
H250	1.2570128068	7.7655730172	8.0726869819
H251	7.9844048808	1.3634044450	8.1641329179
H252	2.4952749463	5.7761228681	8.1726616787
H253	5.7332593746	2.4487029181	8.1976942858
H254	1.0445533868	2.6938940696	11.0856720767
H255	2.6342708459	1.1074099986	11.1148229830
H256	3.4098001750	-0.1869783921	9.6287353976
H257	4.8918382480	1.2539255835	9.7013237476
H258	3.9116343471	3.9843142472	9.8554904220
H259	6.0728499445	5.9322569992	9.6171512155
H260	1.2612291203	4.9517874410	9.6631928598
H261	-0.1554844542	3.4348398246	9.6169049313
H262	3.4386597317	-0.2020236176	-0.6645800797
H263	4.9683293096	1.2334332409	-0.7245045019
H264	3.9564372178	4.0346349841	-0.8551571007
H265	5.4812601830	6.6149006443	-0.1397398153
H266	1.2195180982	5.1571501688	-0.6916488695
H267	-0.1023141219	3.4497963528	-0.6915299317
H268	0.9973411560	7.3931610795	0.8164257003
H269	2.5103536033	5.7784248382	0.8844020023
H270	5.7506931846	2.4753603260	0.7850629622
H271	7.7747205821	1.2242208476	0.8302184751
H272	1.0679398919	2.6662055455	-2.1788439538
H273	2.7223371688	1.0886794283	-2.1839902095
O274	-5.6232479951	3.5817826512	0.1739766711
Ti275	-4.5415673426	4.4471343428	1.4818632534
O276	-7.8300934190	3.2330646070	1.5885821759
O277	-5.9195210593	1.3633979682	1.5533484375
O278	-4.3230095174	5.8829102398	0.2859155416
O279	-3.3733271143	7.7985566990	1.6261474873
O280	-1.3731209308	5.9988325570	1.5553401357
Ti281	-6.9912165180	2.3932465267	2.9630595803
O282	-5.5461232863	3.7736015421	2.9645231522
Ti283	-2.5006831852	6.9450858258	2.9441470997
O284	-3.7988575214	5.5168241436	2.9861100680
Ti285	-4.4352083854	4.4105054706	4.4636618857
O286	-7.8065550710	3.0635128121	4.4410969035
O287	-5.9335382557	1.4060473921	4.4088296098
O288	-3.0906198194	7.8152670165	4.4775375843
O289	-1.4776347760	5.9279595378	4.4589230292
Ti290	-6.9684714126	2.4307984467	5.9782531061
O291	-5.5206311077	3.7552105926	5.9165244543
Ti292	-4.4671236055	4.5657052486	7.4200577519
O293	-7.8195484123	3.3079876366	7.2820296673
O294	-5.9872535517	1.3679124699	7.4101802840

Ti295	-2.3779647102	7.0235620850	5.9570124194
O296	-3.7927264481	5.5425060657	5.9436127768
O297	-3.2024627326	7.8405520529	7.3452214185
O298	-1.3753120404	5.9206244568	7.3718731737
O299	-5.9491343592	4.3712865817	8.5737522468
O300	-3.6359879415	5.6436125465	8.7429351055
H301	-7.2514911471	3.8325767047	7.9603557211
H302	-3.5125893729	7.3826118456	8.1697832794
H303	-6.2263333777	1.6820055950	8.3056753231
H304	-2.0382736074	5.8238155258	8.1160975065
H305	-3.5347346379	5.2781161254	9.6532059803
H306	-6.0730344028	4.8124501373	9.4365997953
H307	-7.3705267175	3.5093835239	0.7535518504
H308	-4.7519724386	5.9907656095	-0.5855580284
H309	-5.2398695044	3.4787502026	-0.7294705170
H310	-5.8160576414	2.0262636395	0.8040745803
H311	-3.8504868619	7.2310085938	0.9226296674
H312	-1.6493332706	6.2488405922	0.6516602773
O313	4.3007679164	-5.9029154305	0.3318761939
Ti314	4.5454733808	-4.4520898968	1.5114548234
O315	1.3031658279	-6.0017778286	1.5691114817
O316	3.3024607003	-7.7909563827	1.6549882723
O317	5.6219962940	-3.6168328391	0.1883453806
O318	5.9327709363	-1.3954178984	1.5694544628
O319	7.8284341704	-3.2494374359	1.6377996248
Ti320	2.4240106318	-6.9542135229	2.9777307185
O321	3.7527709123	-5.5034953558	3.0101178613
Ti322	6.9650774135	-2.4094916277	3.0029869713
O323	5.5349925234	-3.7817130116	2.9951423655
Ti324	4.3697755540	-4.4440543499	4.4872368192
O325	1.3957827927	-5.9066366705	4.4563843760
O326	3.0570764040	-7.7800517808	4.4913788444
O327	5.9542387329	-1.4162781534	4.4617997356
O328	7.8148269812	-3.0736823613	4.4913691876
Ti329	2.4147561462	-6.9576230144	6.0068382543
O330	3.7493853156	-5.4917451486	5.9567030770
Ti331	4.5638101860	-4.4331271474	7.4495188112
O332	1.3349429747	-5.9584937129	7.4376694314
O333	3.2815598053	-7.7826621344	7.3336869490
Ti334	6.9890810995	-2.3571023153	5.9697418318
O335	5.5282883828	-3.7563559763	5.9666640706
O336	5.9163380372	-1.3699717011	7.4094409786
O337	7.8354463825	-3.1760193529	7.3506835486
O338	4.3222293064	-5.9025401062	8.6166212697
O339	5.6096722268	-3.5981509884	8.7890225645
H340	3.7911886809	-7.1975099616	8.0144380127
H341	7.4197085873	-3.4827499925	8.1942032006
H342	1.6476308039	-6.1985636484	8.3325923951
H343	5.8218887610	-2.0304648488	8.1578931136
H344	4.7415554533	-6.0116696372	9.4929543824
H345	5.2240834353	-3.5054103260	9.6935972088
H346	3.7840427836	-7.2163389353	0.9564409145
H347	4.7229400712	-6.0214096926	-0.5410753638
H348	5.2470435806	-3.5255834035	-0.7190897915

H349	1.5508501538	-6.3076464311	0.6734133760
H350	5.8504710845	-2.0541029085	0.8154894348
H351	7.4033177659	-3.5426093501	0.7937718373
Ti352	0.0371031533	0.0149036954	-1.5158199242
O353	-1.0166247039	-0.9937091420	-2.8078050164
O354	0.9412753790	0.9125716101	-2.8954240644
Ti355	-0.0087093842	0.0093445295	10.4814726776
O356	-0.9942490464	-0.9609396705	11.8047564822
O357	0.9398236154	0.9682991240	11.8189880826
Li358	2.2421923447	4.5519905404	3.6415382169

3.10.3 Transition State TS1

358

555 Li+/e- Intercalated TS, Water-Optimized, SCFE : -17174.8357414601 hartree

O1	-7.8792707119	-4.1431345288	3.1806974166
H2	-8.1634027123	-4.2660311337	4.1302989449
H3	-7.1903709688	-4.8368477014	2.9739539200
O4	-7.9016621349	-4.2066462961	5.8728518883
H5	-8.6624814303	-4.3940098990	6.4580365664
H6	-7.1631409253	-4.8814133307	5.9852689755
O7	-4.1320166243	-7.9152300235	2.9131710586
H8	-4.3030977538	-8.4204160817	2.0917983572
H9	-4.8439640519	-7.2338673458	3.0523167341
O10	-4.1572042431	-7.8975652480	6.1101409697
H11	-4.3237932608	-8.4265056046	6.9158017964
H12	-4.8791447106	-7.2224863210	5.9844634319
O13	4.0967737655	7.9873276096	3.1348383186
H14	4.2349985545	8.2609859850	4.0836242475
H15	4.8051478084	7.3336085356	2.9024351362
O16	4.2078233400	8.0124846388	5.8803758588
H17	4.4429280855	8.7934897075	6.4222435793
H18	4.8737442164	7.2720481305	5.9841860671
O19	7.9707847967	4.0599402467	2.8658158172
H20	8.5180803414	4.1928100236	2.0661698998
H21	7.3321857514	4.8121812985	2.9728529227
O22	7.9149892801	4.1135564125	6.1249547500
H23	8.4741161031	4.2560367764	6.9150149519
H24	7.2454061167	4.8464576230	6.0393741502
O25	-8.4742715778	0.8789383303	2.9826653376
H26	-9.3926035521	1.1926709910	2.8546419473
H27	-8.3202126230	-0.0108677063	2.4770112266
O28	-8.2872787395	0.8417026096	5.8130145992
H29	-8.4564508259	0.5693538403	4.8742675715
H30	-8.2449404241	0.0280653822	6.4247210615
O31	0.8978748521	-8.4617461043	2.9869870851
H32	1.1935821123	-9.3907085289	2.9050702008
H33	0.0167533342	-8.3071708029	2.4803708411
O34	0.8215224348	-8.2633392468	5.8658601745
H35	0.5400154756	-8.4242138822	4.9286626823
H36	0.0103088457	-8.2032452952	6.4787722462
O37	-0.9500624605	8.4976024758	2.9900904621
H38	-1.2549364773	9.4191094988	2.8592583003
H39	-0.0796248737	8.3149326359	2.4628218165

O40	-0.8501468231	8.3427652306	5.7972093683
H41	-0.5804004663	8.4980078217	4.8525603370
H42	-0.0585075316	8.3664415882	6.4201155540
O43	8.4835517050	-0.8860979400	2.9692750608
H44	9.4093869589	-1.1895604354	2.8858950092
H45	8.3386547378	-0.0168133963	2.4455059980
O46	8.2897523211	-0.7769831196	5.8604757051
H47	8.4180260004	-0.4416369155	4.9357772307
H48	8.2671279514	0.0068704540	6.5063418292
O49	-3.2079723298	-1.2659843679	-1.3511212103
O50	-1.2505508190	-3.2267206461	-1.3288162842
O51	-3.2679380448	3.4056819022	-1.3695005344
O52	-1.4071432092	1.4276448413	-1.5440524178
O53	1.4514758916	-1.4563059026	-1.5405570794
O54	3.2880072842	-3.4802449473	-1.3168961641
O55	-5.7175163417	-5.5475301860	0.1817292094
Ti56	-4.7286631097	-4.7430181660	1.4963545787
O57	-5.4688383217	-1.0677188870	0.0965373410
Ti58	-4.6309643378	-0.1041081237	1.4688251926
O59	-7.9607186068	-1.3205066544	1.8083492554
O60	-5.9847340598	-3.1963622785	1.5371980157
O61	-1.0293508765	-5.5030463498	0.1184138398
Ti62	-0.1140948707	-4.5741631298	1.5072278712
O63	-3.1923284963	-5.9266336559	1.4897718088
O64	-1.3451585987	-7.9607690541	1.8163861919
Ti65	-2.2950346633	-2.2643128904	0.0089568029
O66	-0.8682105631	-0.8888129844	-0.0315967797
O67	-3.7038605272	-3.6593268336	0.0129562697
Ti68	-0.0015850258	-0.0245059661	1.4867609529
O69	-3.1750053140	-1.3746060215	1.4894315266
O70	-1.3951966511	-3.1791959653	1.4942518755
Ti71	-2.3553377678	2.4289169816	-0.1383928804
O72	-3.6307312475	0.9323541697	0.0169123274
O73	-3.1667729952	3.2285075876	1.4530848371
O74	-1.3859296832	1.4042101512	1.4625870732
Ti75	2.3973055118	-2.4502517911	-0.1162126462
O76	0.8670213743	-3.6362931745	0.0291081517
O77	1.4044646307	-1.4246685825	1.4738018628
O78	3.1811920658	-3.2545264817	1.4765913881
O79	0.8813781574	0.8568727923	-0.0352568602
O80	-5.4586422511	-5.4503620645	3.0202447912
Ti81	-6.8426477566	-2.2371729988	3.0465519294
O82	-5.4951244761	-0.8769205757	2.9731584410
Ti83	-2.2453018356	-6.8386768996	3.0572040800
O84	-0.9242446646	-5.4752677654	3.0059370128
Ti85	-2.3669441551	-2.3338772903	3.0371557105
O86	-0.8863255165	-0.8799888190	2.9718591900
O87	-3.6729379913	-3.6587158935	3.0011241359
Ti88	-2.2015105583	2.1260310695	2.9014205081
O89	-3.6338954388	0.8919515897	2.9845467956
Ti90	2.1649005947	-2.1920876350	2.9197510769
O91	0.8855434992	-3.6660616425	2.9837550663
O92	0.8759958160	0.8485066254	2.9742732906
Ti93	-4.5479945344	-4.5256834211	4.5057231634

Ti94	-4.5820091144	0.1682823598	4.4781986612
O95	-7.8300838157	-1.6883847787	4.4930958094
O96	-5.8537054942	-3.1411162590	4.5221411432
Ti97	0.1581237594	-4.5870699289	4.4872982847
O98	-3.2311393782	-5.9298373508	4.5086966674
O99	-1.6535371510	-7.7913468241	4.5094281885
Ti100	-0.0272194525	-0.0297557259	4.4728692410
O101	-3.1867761577	-1.3859826327	4.4852420451
O102	-1.4069174508	-3.1564008510	4.4867999969
O103	-3.1756868397	3.1867027880	4.4519982260
O104	-1.3970312639	1.4016207986	4.4787948379
O105	1.3830831043	-1.4221983579	4.4815765597
O106	3.1746166448	-3.1885995234	4.4778066141
O107	-5.4924202028	-5.4391341787	6.0100697428
Ti108	-4.7533891540	-4.7381808692	7.5369088703
Ti109	-6.8044854823	-2.2214359268	5.9516266301
O110	-5.5011202791	-0.8570971478	5.9761651498
Ti111	-4.5890685766	-0.0760290044	7.4813081886
O112	-7.9741107450	-1.3563443462	7.1702545317
O113	-5.9486381957	-3.1587685739	7.4663230908
Ti114	-2.2760026102	-6.8181579772	5.9619021252
O115	-0.9055204152	-5.4809336168	5.9880029534
Ti116	-0.1041979024	-4.5858256036	7.4730707471
O117	-3.1738628933	-5.8905264837	7.4927980179
O118	-1.3830596689	-7.9429972462	7.2037346349
Ti119	-2.3516058104	-2.3547926805	5.9312465276
O120	-0.8990914286	-0.8819273875	5.9849668503
O121	-3.6629645494	-3.6675059057	6.0083062083
Ti122	-0.0138438776	-0.0201784841	7.4590830163
O123	-3.1868242024	-1.3626571710	7.4811834703
O124	-1.3955224719	-3.1688135795	7.4875411241
Ti125	-2.1862287945	2.1671110092	6.0502032242
O126	-3.6731436777	0.9105594116	5.9642198023
O127	-3.2537695864	3.1716254105	7.4859811777
O128	-1.4209127933	1.3989632271	7.4840048352
Ti129	2.1646693015	-2.1854594066	6.0562104404
O130	0.8811651925	-3.6650046291	5.9824872395
O131	1.3828923878	-1.4286799052	7.4951070322
O132	3.1643105371	-3.2472159091	7.5061427100
O133	0.8743885966	0.8218570221	5.9980518264
O134	-5.6315754192	-5.5889311807	8.8572610250
O135	-5.5011879948	-1.0094983435	8.8495624006
O136	-1.0336498995	-5.4708624977	8.8709742060
Ti137	-2.2869534633	-2.2613043024	8.9590887137
O138	-0.8901030420	-0.8808712904	9.0094862412
O139	-3.7053510463	-3.6439593132	8.9844007576
O140	-3.2210490186	-1.2296508271	10.3187860652
O141	-1.2806688821	-3.2096268643	10.3243902651
Ti142	-2.4187747458	2.4200029879	9.0831400087
O143	-3.6424200745	0.8990304142	8.9462590042
O144	-3.4367782623	3.3175939860	10.2944438009
O145	-1.4422963735	1.4541787433	10.4968497167
Ti146	2.3823424838	-2.4306927411	9.0989420868
O147	0.8611390865	-3.6228089395	8.9660975459

O148	1.4339396087	-1.4229760875	10.5133491015
O149	3.2880198642	-3.4378641203	10.3103653368
O150	0.8476818907	0.8653159449	8.9835884620
H151	-7.7703171495	-1.2208776995	8.1198907508
H152	-4.2892699940	3.1494877174	10.7430174525
H153	-1.2620352102	-7.7104204377	8.1484053319
H154	3.1380727193	-4.2832816944	10.7780694146
H155	-5.7698916653	-2.4655560734	8.1830592481
H156	-1.7028142435	1.7006984726	11.4089571038
H157	-2.4664263073	-5.7009207786	8.1952181672
H158	1.7066742446	-1.6513623875	11.4253953182
H159	-2.6358484764	-1.0509687492	11.1110004100
H160	-1.0927811033	-2.6287610424	11.1152647208
H161	-5.9324888690	-5.8499140034	9.7443452260
H162	-3.9968903051	-3.9032673580	9.8809449732
H163	-1.2287723798	-4.9656504099	9.7024231573
H164	0.1181335849	-3.4204973237	9.6509688808
H165	-0.9530353537	-0.9162335552	12.7704039347
H166	0.9380527479	0.9708084686	12.8166231946
H167	-3.4414777726	0.1570557042	9.6352413605
H168	-5.0018312622	-1.2160449136	9.6822856938
H169	-7.7347834649	-1.2130452280	0.8608764953
H170	-1.2071387012	-7.6956182967	0.8811269743
H171	-6.5876094963	-5.3497346017	-0.2163469994
H172	-3.9977152954	-3.9648110974	-0.8689491320
H173	-1.2202682687	-5.0019379978	-0.7154132156
H174	0.1169116436	-3.4382762699	-0.6611529461
H175	-0.9386189335	-0.9587205387	-3.7887408963
H176	0.9567033674	0.9276522213	-3.8763561530
H177	-3.4290319378	0.1989157760	-0.6639310873
H178	-4.9597467157	-1.2879362474	-0.7282151887
H179	-5.8029452077	-2.5253261867	0.8061473821
H180	-2.4694446817	-5.7333153908	0.8041924083
H181	-3.1134136561	4.2425652277	-1.8491878541
H182	-1.6969527216	1.6417161367	-2.4538099987
H183	1.6925887485	-1.7280056464	-2.4496602002
H184	3.1319163057	-4.3430140453	-1.7471498452
H185	-2.6191250817	-1.0756522155	-2.1412883473
H186	-1.0766309743	-2.6485134971	-2.1267506807
O187	1.2313881392	3.2173497579	-1.3502624015
O188	3.2275258935	1.2612202358	-1.3716613626
O189	-0.8593149696	3.6489054137	0.0120757684
Ti190	0.1235152511	4.5677329639	1.5166395643
O191	3.6555377104	-0.9605646277	0.0033971852
Ti192	4.6354914382	0.0942632882	1.4768042492
Ti193	2.3122474806	2.2635993358	0.0074578742
O194	3.6602359402	3.7069029362	0.0141496557
Ti195	4.7064486418	4.7385948030	1.5020029936
O196	1.3601037351	3.2007011951	1.4154904716
O197	3.2089286555	1.3456620082	1.4044558281
O198	1.0266951932	5.5825410682	0.1605218193
O199	1.2209814690	7.8843278660	1.7981833220
O200	3.1762291376	6.0094057095	1.5569546889
O201	5.5111917178	1.0059995462	0.0790152624

O202	5.8860902578	3.1955984292	1.5067154894
O203	7.9595762028	1.3517274632	1.7654305533
O204	5.4922967386	5.7178878673	0.1727026064
O205	-0.9256089486	3.6698835326	2.9544009377
O206	3.6399173727	-0.9153343185	2.9949517588
Ti207	2.3096177647	2.2847766624	3.0056015822
O208	3.6323688578	3.7401670743	3.0838744674
Ti209	2.2116847846	6.8644425015	3.0549016284
O210	0.9324436151	5.4373122060	3.0902128246
Ti211	6.8547241391	2.2033593232	3.0391664307
O212	5.4883135314	0.8808768183	2.9778391844
O213	5.5039493222	5.4817857689	2.9914229582
Ti214	-0.3202407432	4.5363423059	4.4691464472
Ti215	4.5271953323	-0.2020366304	4.4811511901
Ti216	4.6775919526	4.5765406440	4.4591196805
O217	1.2936701192	3.1167588220	4.5867984086
O218	3.2345287525	1.3049332051	4.5551618847
O219	1.6592768955	7.9059428794	4.4834603453
O220	3.2101014991	5.9990038908	4.5551736455
O221	5.9717620920	3.2271487229	4.5010973461
O222	7.7743227685	1.5998766785	4.4861229770
O223	-0.9562387222	3.6735292796	5.9935344670
Ti224	0.1170326230	4.6368908033	7.4631156382
O225	3.6489308903	-0.9449473319	5.9770293140
Ti226	4.6322813163	0.0747890022	7.4981417764
Ti227	2.3477019907	2.2159993921	5.8827478283
O228	3.5818590961	3.7136571002	5.9229019854
Ti229	4.6812623454	4.7413002932	7.4833750484
O230	1.3297824464	3.1698320023	7.4872356022
O231	3.1551063115	1.3552259863	7.4886098909
Ti232	2.2333086709	6.9935416919	5.9734459608
O233	0.9237906844	5.5301987496	5.9605630700
O234	1.4049425192	8.1323258653	7.1877090855
O235	3.1738178849	6.0272370585	7.4511177792
Ti236	6.8238334718	2.2305622248	5.9750901929
O237	5.5182662504	0.8530785076	6.0152405365
O238	5.8377955715	3.1394658231	7.4357739736
O239	8.0181607819	1.4271422555	7.1895961895
O240	5.4698165274	5.4883873855	6.0088326133
O241	-0.9415757452	3.6660957289	8.9402032020
O242	3.6171956493	-0.9331531953	8.9536392529
Ti243	2.2388981755	2.2784619319	8.9019293601
O244	3.6075142135	3.6966422900	8.9433811811
O245	1.2057369928	3.2134685836	10.2903811894
O246	3.1918393595	1.2577805607	10.2911996261
O247	1.0508441203	5.4771638141	8.8555531551
O248	5.4181721057	1.0445742142	8.8938648590
O249	5.5839728836	5.5160217621	8.8468481099
H250	1.3720170180	8.1681377045	8.1634006794
H251	7.9769803459	1.4185163560	8.1657255222
H252	2.4749817045	5.8444564533	8.1637548221
H253	5.6518519784	2.4617141968	8.1644165738
H254	1.0419098051	2.6811666199	11.1103021904
H255	2.6716730355	1.0886435131	11.1165518725

H256	3.4004850153	-0.1820503697	9.6222785842
H257	4.8510284277	1.2542513902	9.6919745057
H258	3.8803576874	3.9809409978	9.8378701180
H259	6.0178638612	5.4704252681	9.7180197082
H260	1.2680968584	4.9395697025	9.6654013489
H261	-0.1862723967	3.4556951481	9.6168239588
H262	3.4498401210	-0.2279563736	-0.6743975161
H263	4.9920382176	1.2140182338	-0.7419091982
H264	3.9005218359	4.0693374900	-0.8620737808
H265	5.3324610615	6.5963002829	-0.2243207933
H266	1.2435973641	5.1032039919	-0.6776431948
H267	-0.0874012891	3.4451320655	-0.6721874502
H268	1.0334482588	7.5129417889	0.9038888723
H269	2.4857363526	5.8401077478	0.8326402458
H270	5.7141362199	2.5078160503	0.7913858690
H271	7.7236130055	1.2473386649	0.8183413133
H272	1.0590122725	2.6975635107	-2.1723786647
H273	2.7166304200	1.0744716170	-2.1974548755
O274	-5.6388276336	3.6111382853	0.1966133054
Ti275	-4.5135633827	4.4712005004	1.4849970194
O276	-7.8269277525	3.2340435573	1.5937220361
O277	-5.9065455029	1.3717176753	1.5506388573
O278	-4.2970383724	5.8748561710	0.2616708688
O279	-3.3379797347	7.7913039238	1.6159785794
O280	-1.3153671816	6.0202824791	1.5835094863
Ti281	-6.9757594400	2.3966659451	2.9625473806
O282	-5.5347442353	3.7770105466	2.9640674084
Ti283	-2.4675517028	6.9664320287	2.9536217226
O284	-3.7823209807	5.5200426255	2.9826305032
Ti285	-4.4257068697	4.4091616465	4.4562372636
O286	-7.8021795767	3.0617461693	4.4417219158
O287	-5.9265906223	1.4055228155	4.4177879715
O288	-3.1023031858	7.8170574482	4.4749364120
O289	-1.4704971478	5.9423691050	4.4553779817
Ti290	-6.9632968089	2.4195257694	5.9693747722
O291	-5.5098707259	3.7476462521	5.9138921141
Ti292	-4.4723491057	4.5422418056	7.4151262982
O293	-7.8099414991	3.3055552480	7.2752422861
O294	-5.9799697307	1.3716871553	7.4181536519
Ti295	-2.4080000529	7.0169602136	5.9617939922
O296	-3.7899728655	5.5397164705	5.9446789838
O297	-3.2351503253	7.8472977751	7.3420177119
O298	-1.3626334021	5.9493874097	7.3624787322
O299	-5.9381510975	4.3632961683	8.5852096886
O300	-3.6385142404	5.6596887228	8.7157939404
H301	-7.2545129524	3.8270639496	7.9606828202
H302	-3.5330570142	7.3590210698	8.1574207709
H303	-6.2071822510	1.7051819569	8.3098351212
H304	-2.0209318991	5.8358570078	8.1087038728
H305	-3.5499568194	5.3166865137	9.6346420780
H306	-6.0984265565	4.8807909457	9.4001170014
H307	-7.3438651993	3.5211979955	0.7701544972
H308	-4.7861519435	6.0146355354	-0.5732073822
H309	-5.2905485729	3.5279966254	-0.7212603537

H310	-5.7929598181	2.0467205747	0.8107229215
H311	-3.8078347696	7.2263979301	0.9080976571
H312	-1.5425295811	6.3207808906	0.6808370487
O313	4.3912069529	-5.9262189072	0.3363792518
Ti314	4.5580314101	-4.4759610354	1.5233532157
O315	1.3081755702	-6.0004362667	1.5624436195
O316	3.3047848783	-7.7851774065	1.6517159637
O317	5.6663163945	-3.6164107621	0.2211942007
O318	5.9366791969	-1.3820847099	1.5772344833
O319	7.8444290156	-3.2529778175	1.6371983016
Ti320	2.4226485980	-6.9483948806	2.9754138264
O321	3.7694488906	-5.5131306780	3.0157328668
Ti322	6.9850157697	-2.3956465599	2.9903162587
O323	5.5546082910	-3.7852854113	2.9958490226
Ti324	4.4048051577	-4.4345740148	4.4878757125
O325	1.3999412472	-5.9107239015	4.4593486725
O326	3.0537471893	-7.7872307897	4.4863687579
O327	5.9545496972	-1.4190991040	4.4530252463
O328	7.8360447152	-3.0496674002	4.4876683972
Ti329	2.4101345874	-6.9578530910	5.9933342710
O330	3.7628606725	-5.4983424332	5.9502872375
Ti331	4.5513356694	-4.4539900110	7.4399612574
O332	1.3494692762	-5.9530463193	7.4408642122
O333	3.2899906325	-7.7930897761	7.3119849668
Ti334	6.9935702654	-2.3640318797	5.9655281221
O335	5.5398257896	-3.7556232374	5.9683061460
O336	5.9197254110	-1.3770660020	7.4156863015
O337	7.8460445439	-3.1851580572	7.3411095192
O338	4.3980287386	-5.9226590745	8.6041560853
O339	5.6564374928	-3.6043026357	8.7521326626
H340	3.8215510593	-7.2401141529	7.9898194392
H341	7.3862615097	-3.4982045201	8.1647353949
H342	1.6713550816	-6.1866445621	8.3334028385
H343	5.8235714024	-2.0613521911	8.1472554042
H344	4.9221274455	-6.0849716907	9.4097372816
H345	5.3198386285	-3.5480115211	9.6736336030
H346	3.8273547587	-7.2262360827	0.9727443788
H347	4.9310073235	-6.1018587443	-0.4574706511
H348	5.3317473466	-3.5579905802	-0.7023986057
H349	1.5433106174	-6.3172368620	0.6659002725
H350	5.8426846162	-2.0488091965	0.8296297228
H351	7.3755912181	-3.5495087430	0.8125147406
Ti352	0.0456237215	0.0039155049	-1.5273923484
O353	-0.9983135022	-1.0014870715	-2.8143262069
O354	0.9479053828	0.8986668863	-2.9008783460
Ti355	0.0052118131	0.0210975720	10.4850981375
O356	-1.0080127371	-0.9719275198	11.7963680561
O357	0.9236766797	0.9472227163	11.8406879488
Li358	2.2078600627	4.5893243240	4.8894439031

3.11 555 O_{Li}^+ cluster in water**

**Li⁺ is adsorbed on surface

358

555 Li+ Surface , Water-Optimized

SCFE : -17174.7209298565 hartree

O1	-7.8723994633	-4.1406042173	3.1765078784
H2	-8.1575485710	-4.2649117345	4.1278242361
H3	-7.1900473933	-4.8384237819	2.9677947442
O4	-7.8888232466	-4.2152620291	5.8626820159
H5	-8.6552127647	-4.4128666653	6.4385641747
H6	-7.1461183759	-4.8868015648	5.9803483949
O7	-4.1285858990	-7.9158079706	2.9059893720
H8	-4.2963816478	-8.4379742153	2.0956791255
H9	-4.8490346502	-7.2395097183	3.0329658793
O10	-4.1614661982	-7.8827650065	6.1009695257
H11	-4.3376226698	-8.4276162621	6.8942306135
H12	-4.8811559808	-7.2023916244	5.9784272436
O13	3.9740364115	8.0348553020	3.1422103435
H14	4.1501952941	8.2349116102	4.1069986562
H15	4.7297114067	7.5511787733	2.7448109827
O16	4.1665643791	7.9650395698	5.8393224922
H17	4.3015999632	8.7714170945	6.3787891179
H18	4.8344580539	7.2579775690	6.0604256418
O19	8.0297469158	4.0027053540	2.8399942157
H20	8.6399344167	4.0617985084	2.0764607854
H21	7.3784499833	4.7468144660	2.8177953247
O22	7.9827487339	4.0445751140	6.1324864078
H23	8.6352240157	4.1116703315	6.8588077419
H24	7.3289337485	4.7863407145	6.1764918042
O25	-8.4902395527	0.8782134825	2.9829706033
H26	-9.4069499948	1.1910442364	2.8398583612
H27	-8.3251723953	-0.0066739057	2.4720647392
O28	-8.2892638457	0.8517229302	5.8212506954
H29	-8.4765365330	0.5868770697	4.8837968454
H30	-8.2380617404	0.0344204390	6.4274159319
O31	0.9090973088	-8.4755277327	3.0002373818
H32	1.2074046955	-9.4036344986	2.9174278105
H33	0.0246243276	-8.3257115817	2.4988249526
O34	0.8265289588	-8.2711387761	5.8579402383
H35	0.5578147553	-8.4424953537	4.9191644849
H36	0.0076045412	-8.2153286798	6.4605497841
O37	-0.9432814629	8.4622146886	2.9563758515
H38	-1.2629502647	9.3798987660	2.8388763440
H39	-0.0933533938	8.2983522693	2.4065085682
O40	-0.8015088699	8.2986476987	5.7826762093
H41	-0.5253844895	8.4539290088	4.8415228424
H42	0.0096577006	8.2719517168	6.4082022330
O43	8.4768697826	-0.9019954792	2.9836732610
H44	9.4023120931	-1.2074309914	2.8915039405
H45	8.3261486770	-0.0267948811	2.4551121801
O46	8.2874762878	-0.8070372136	5.8441096539
H47	8.4447213923	-0.5003613688	4.9140696601
H48	8.2442929904	-0.0028281657	6.4807873395
O49	-3.1876581133	-1.2680496388	-1.3649809812
O50	-1.2306748839	-3.2336178264	-1.3299923347
O51	-3.2671805688	3.4085900265	-1.3573981257
O52	-1.4170241858	1.4170296269	-1.5470593529

O53	1.4634744075	-1.4442014658	-1.5317377849
O54	3.3061312315	-3.4374690780	-1.3428440354
O55	-5.7054511539	-5.5676123220	0.1733411762
Ti56	-4.7251059425	-4.7475073490	1.4738574366
O57	-5.4723519488	-1.0661779998	0.0990443246
Ti58	-4.6306600182	-0.1002570412	1.4709915867
O59	-7.9431229072	-1.3180872118	1.7911174200
O60	-5.9752500461	-3.2029177908	1.5307371981
O61	-1.0307740456	-5.4977918782	0.1197364869
Ti62	-0.1195275980	-4.5815727197	1.5073397903
O63	-3.1831919530	-5.9314136563	1.4822629067
O64	-1.3385546764	-7.9651819080	1.8275673684
Ti65	-2.2861224731	-2.2548253592	0.0126599816
O66	-0.8499814057	-0.8857015590	-0.0418537993
O67	-3.6909191427	-3.6600400942	0.0067174097
Ti68	0.0479309367	0.0224570370	1.4995146983
O69	-3.1604205214	-1.3712681553	1.4780854818
O70	-1.3855866710	-3.1741169253	1.4865420038
Ti71	-2.3590200855	2.4082588101	-0.1386957467
O72	-3.6383245467	0.9271945148	0.0050663247
O73	-3.1586832506	3.2279730298	1.4516641144
O74	-1.3854781929	1.4053453447	1.4551136271
Ti75	2.3888061421	-2.4618607215	-0.1112774058
O76	0.8738295848	-3.6336711338	0.0220251794
O77	1.4098738020	-1.4186125186	1.4752606724
O78	3.1764441293	-3.2609342512	1.4754358672
O79	0.8956202065	0.8791766688	-0.0250104218
O80	-5.4476438992	-5.4489769507	3.0052388292
Ti81	-6.8468381081	-2.2412481751	3.0356446738
O82	-5.4830031929	-0.8845261089	2.9693115669
Ti83	-2.2508724973	-6.8402522535	3.0553709726
O84	-0.9266032423	-5.4712808507	3.0066588722
Ti85	-2.3590947277	-2.3224823150	3.0343073386
O86	-0.8718906264	-0.8656985241	2.9753567953
O87	-3.6595424444	-3.6557257728	2.9910140333
Ti88	-2.1792503942	2.1449400271	2.9020926251
O89	-3.6309401849	0.8916847743	2.9717341562
Ti90	2.1584525784	-2.2017428958	2.9216756862
O91	0.8826922658	-3.6642140237	2.9839570103
O92	0.8962302685	0.8767596429	2.9577581838
Ti93	-4.5437334665	-4.5216625479	4.4813427063
Ti94	-4.5789083431	0.1839520306	4.4608214927
O95	-7.8296497351	-1.6954902065	4.4824006704
O96	-5.8477925841	-3.1434603992	4.5136410261
Ti97	0.1524834530	-4.5994886144	4.4860869149
O98	-3.2280486786	-5.9300277347	4.5053223237
O99	-1.6524279578	-7.7908784190	4.5088187252
Ti100	-0.0581588522	-0.0605461584	4.4945238929
O101	-3.1762727899	-1.3832435588	4.4803601151
O102	-1.4012439213	-3.1502251120	4.4819331338
O103	-3.1809465038	3.1729703235	4.4531432303
O104	-1.4081851292	1.3846806828	4.4756645349
O105	1.3736613263	-1.4203798951	4.4810162311
O106	3.1672459130	-3.1763326655	4.4860319640

O107	-5.4820476900	-5.4367067476	5.9922766105
Ti108	-4.7569083361	-4.7435652781	7.5246166132
Ti109	-6.7982732546	-2.2207628374	5.9423611950
O110	-5.4908245905	-0.8620267935	5.9640972748
Ti111	-4.5824421553	-0.0778530761	7.4585859668
O112	-7.9472417522	-1.3449710242	7.1732075787
O113	-5.9456463702	-3.1615002988	7.4524473895
Ti114	-2.2809441317	-6.8258650520	5.9614403532
O115	-0.9139411694	-5.4740676371	5.9898715511
Ti116	-0.1107747594	-4.5896114575	7.4704742776
O117	-3.1769724038	-5.8948911789	7.4987352332
O118	-1.3890673861	-7.9573915133	7.1938822751
Ti119	-2.3541957312	-2.3613290683	5.9251393897
O120	-0.8784172058	-0.8663609984	5.9795349462
O121	-3.6524699555	-3.6641283776	5.9962425357
Ti122	0.0306122826	0.0439512080	7.4634380681
O123	-3.1815759841	-1.3578507050	7.4798206569
O124	-1.3958868068	-3.1574634523	7.4904387313
Ti125	-2.1801091327	2.1785206556	6.0376224000
O126	-3.6767757827	0.9120217973	5.9619128938
O127	-3.2511013981	3.1882553317	7.4796937025
O128	-1.4252423431	1.4037161961	7.4839679617
Ti129	2.1501457158	-2.1897724022	6.0525392079
O130	0.8800471491	-3.6624173416	5.9873546648
O131	1.3861804804	-1.4047950276	7.4896878314
O132	3.1619495675	-3.2303434100	7.5053080434
O133	0.8754945567	0.8771037901	5.9923633732
O134	-5.6764394013	-5.5909046220	8.8099541460
O135	-5.5147008493	-1.0056106492	8.8286680362
O136	-1.0350382998	-5.4579965359	8.8728445566
Ti137	-2.2852904511	-2.2593330936	8.9515040635
O138	-0.8811715086	-0.8596070292	9.0112259215
O139	-3.7034640267	-3.6388226918	8.9796647354
O140	-3.2295870656	-1.2106392126	10.3058109856
O141	-1.2777520582	-3.1886639660	10.3261931795
Ti142	-2.4486377422	2.4008571150	9.0731705083
O143	-3.6491273618	0.8956550267	8.9484547387
O144	-3.4357162331	3.3180636649	10.2928826124
O145	-1.4425360356	1.4618798736	10.4886033751
Ti146	2.3756862482	-2.4262223526	9.0898500960
O147	0.8644962384	-3.6131406380	8.9645477415
O148	1.4344728691	-1.4058408490	10.5012923027
O149	3.2855636387	-3.4010203104	10.3290335756
O150	0.8702742987	0.8947453863	8.9745785278
H151	-7.6991375458	-1.1919111453	8.1104753640
H152	-4.2526861678	3.1596834850	10.8057788174
H153	-1.2728924317	-7.7577030684	8.1464767551
H154	3.1091536595	-4.2053810528	10.8557197257
H155	-5.7700800094	-2.4676115798	8.1702387337
H156	-1.6557176859	1.7568161632	11.3973121147
H157	-2.4731781251	-5.7026756087	8.2023012558
H158	1.7382035959	-1.6041684683	11.4103570984
H159	-2.6753855177	-1.0384472094	11.1142524673
H160	-1.0920168601	-2.6305174088	11.1303956593

H161	-6.3260408544	-5.8838656572	9.4718647345
H162	-4.0070357340	-3.8964794994	9.8735934638
H163	-1.2319354058	-4.9640182806	9.7104704457
H164	0.1215773748	-3.4156678440	9.6499454580
H165	-0.9408998900	-0.9227006927	12.7906586111
H166	0.9265239406	1.0070659654	12.7696567711
H167	-3.4535684663	0.1414492993	9.6415409336
H168	-5.0348506830	-1.2090865874	9.6715399210
H169	-7.6948806019	-1.1875522041	0.8511407346
H170	-1.2048317893	-7.7289607386	0.8847458285
H171	-6.6021541666	-5.4717106551	-0.2008565205
H172	-3.9842800223	-3.9440272508	-0.8826043231
H173	-1.2321215282	-4.9968119976	-0.7136855794
H174	0.1137580261	-3.4371226216	-0.6677528019
H175	-0.8857357423	-0.9903715001	-3.8169334002
H176	0.9482178885	0.9735985034	-3.8096172381
H177	-3.4492258732	0.1982809372	-0.6838404166
H178	-4.9791076298	-1.2869974402	-0.7324580503
H179	-5.7940419404	-2.5276195163	0.8023654881
H180	-2.4657324970	-5.7423110260	0.7905583661
H181	-3.0987025318	4.2353857897	-1.8506595846
H182	-1.7083029296	1.6137482897	-2.4608025782
H183	1.7800262475	-1.6319977137	-2.4388799499
H184	3.1435069622	-4.2330628767	-1.8864375016
H185	-2.6220908478	-1.0742020918	-2.1647808782
H186	-1.0567862044	-2.6810083522	-2.1387709622
O187	1.2787916358	3.2059664622	-1.3318767870
O188	3.2276834348	1.2622002213	-1.3455176782
O189	-0.8473819933	3.6237102360	0.0053341163
Ti190	0.1204695548	4.5435419805	1.5011551744
O191	3.6573288962	-0.9513151689	0.0332693499
Ti192	4.6225685649	0.0774999266	1.4902845945
Ti193	2.3491598817	2.2867090850	0.0101283046
O194	3.7137617654	3.7096250296	0.0285827813
Ti195	4.7976830066	4.7600327718	1.5356167587
O196	1.3987728169	3.1647844613	1.4876906880
O197	3.1852430134	1.3690129612	1.4903575538
O198	1.0645692039	5.5282836979	0.1618419382
O199	1.2355496329	7.8429751664	1.7216216166
O200	3.2387365939	5.9808425448	1.5675426629
O201	5.4904916417	1.0270430836	0.1161182549
O202	5.9437522978	3.1906956926	1.5071130230
O203	7.9558116618	1.3038443953	1.7891920678
O204	5.6142113575	5.7342774390	0.2313318236
O205	-0.8857538035	3.6374578765	2.9785121840
O206	3.6369726934	-0.9127383626	2.9990372263
Ti207	2.3270825170	2.2795176874	3.0544381785
O208	3.6833642299	3.6644123225	2.9842705202
Ti209	2.1729296823	6.8478988770	3.0167681551
O210	0.8878255247	5.4557371123	3.0056322132
Ti211	6.8452696101	2.1939178319	3.0518947149
O212	5.4886763007	0.8666524713	2.9865382585
O213	5.5456804352	5.4592339689	3.0729214725
Ti214	-0.2038964945	4.5590626451	4.4706407970

Ti215	4.5484175859	-0.2170454125	4.4827814467
Ti216	4.4509109785	4.4673056538	4.4754421064
O217	1.4027319971	3.1489655205	4.4781553641
O218	3.1757508392	1.3826716158	4.4816362228
O219	1.6473763068	7.8106581110	4.4754420381
O220	3.1622658554	5.8647302090	4.5133033034
O221	5.9416907677	3.1854784570	4.4941546507
O222	7.8013590480	1.5952372552	4.4938119251
O223	-0.9091945532	3.6284724622	5.9576956951
Ti224	0.0711591015	4.6172754139	7.4819123540
O225	3.6285507309	-0.9107736608	5.9629854970
Ti226	4.6065971584	0.0893511309	7.4758237909
Ti227	2.3205533946	2.3373770382	5.9503638621
O228	3.6823384873	3.6628367876	6.0014581881
Ti229	4.7877194718	4.7643453258	7.4700664521
O230	1.3693529144	3.1694261528	7.4492663042
O231	3.1606758374	1.3775874917	7.4716070351
Ti232	2.2120113790	6.7826608931	5.9237225499
O233	0.8578718684	5.4867515672	5.9730118525
O234	1.3626024541	7.9702688281	7.1452598813
O235	3.2074285078	5.9642177118	7.4279322193
Ti236	6.8178791040	2.2208603551	5.9376204058
O237	5.4804291837	0.8641630422	5.9834111312
O238	5.9052102052	3.1642196575	7.4522465639
O239	7.9541930190	1.3478113940	7.1937486738
O240	5.5179646397	5.5136522514	5.9379938336
O241	-0.9354837086	3.6527209092	8.9299622603
O242	3.6294771648	-0.9247881122	8.9419472214
Ti243	2.2923056287	2.3021428378	8.9456721704
O244	3.6764015244	3.7166751909	8.9407244745
O245	1.2412701643	3.2281655384	10.2810550489
O246	3.1941611291	1.2810814617	10.3021853770
O247	1.0576878057	5.4702507674	8.8313771910
O248	5.4468324971	1.0433913362	8.8622189398
O249	5.6749332247	5.6077069532	8.7792353718
H250	1.2589302153	7.8087799270	8.1051990864
H251	7.7472296065	1.2497317864	8.1458362799
H252	2.5274957858	5.7747775794	8.1537546173
H253	5.7058898176	2.4801187867	8.1723032655
H254	1.0552925050	2.6671247537	11.0849886307
H255	2.6296488592	1.0917491536	11.1038933678
H256	3.4281668309	-0.1949766100	9.6243830322
H257	4.9407333695	1.2398475450	9.6945497095
H258	3.9511579842	4.0157824756	9.8314608511
H259	6.1540951750	5.8297900390	9.5966965700
H260	1.2611153159	4.9665535496	9.6645981709
H261	-0.1978505627	3.4483184340	9.6146350822
H262	3.4595522687	-0.2313594130	-0.6568906652
H263	5.0074199392	1.2186575725	-0.7289649040
H264	3.9692706700	4.0538898203	-0.8517700327
H265	5.5122565390	6.6010300634	-0.2057056464
H266	1.2719129714	5.0742380078	-0.6919309105
H267	-0.0864640447	3.4278911689	-0.6771214131
H268	1.0417802824	7.4332024653	0.8437972624

H269	2.5634288147	5.7803153501	0.8417994576
H270	5.7366857583	2.4979679745	0.8020557202
H271	7.7038728918	1.1877141095	0.8483842488
H272	1.1001982402	2.6292399208	-2.1260887143
H273	2.6616046191	1.0645366198	-2.1460747686
O274	-5.6251150270	3.5739156126	0.1749031983
Ti275	-4.5367490958	4.4390163578	1.4764181095
O276	-7.8274347938	3.2327279145	1.5911002930
O277	-5.9227972594	1.3568505749	1.5487070460
O278	-4.3394132029	5.8793976959	0.2862157186
O279	-3.3234824538	7.7710398559	1.6059061265
O280	-1.3366435379	5.9617547218	1.5424851086
Ti281	-6.9918993776	2.3910337939	2.9668923429
O282	-5.5410120487	3.7695406898	2.9608381897
Ti283	-2.4613629354	6.9170551863	2.9284574846
O284	-3.7750113491	5.5003873540	2.9802446194
Ti285	-4.4304337670	4.3975502091	4.4537773780
O286	-7.8016285363	3.0659855524	4.4437372204
O287	-5.9294028487	1.4078269219	4.4052743288
O288	-3.0731596230	7.7885317722	4.4544357971
O289	-1.4261264156	5.9097990023	4.4496633306
Ti290	-6.9662082260	2.4289173074	5.9829658156
O291	-5.5130909829	3.7530104288	5.9154842734
Ti292	-4.4693445626	4.5736834613	7.4073067638
O293	-7.8092315293	3.3105694017	7.2858734203
O294	-5.9895341338	1.3636232219	7.4098962033
Ti295	-2.3675046972	7.0109918830	5.9346258111
O296	-3.7823823023	5.5368661445	5.9283956843
O297	-3.1912123236	7.8413286946	7.3155564786
O298	-1.3829588494	5.9062450128	7.3707141082
O299	-5.9518759647	4.4072001412	8.5641624157
O300	-3.6215027604	5.6475354794	8.7296841737
H301	-7.2456562170	3.8525483182	7.9566981981
H302	-3.4936124724	7.3934638864	8.1480827593
H303	-6.2516163542	1.6504134458	8.3072522300
H304	-2.0557626764	5.8188041879	8.1119310579
H305	-3.5335695699	5.2915757751	9.6447239698
H306	-6.0848935321	4.8749977194	9.4122764412
H307	-7.3753945460	3.5076086499	0.7521720493
H308	-4.8190352418	6.0183488212	-0.5543551511
H309	-5.2492159342	3.4789067127	-0.7319168438
H310	-5.8232064346	2.0220949106	0.8001410938
H311	-3.8200933576	7.2102429550	0.9094712776
H312	-1.6149662859	6.2106214483	0.6381273530
O313	4.4042695517	-5.9345307434	0.3634321522
Ti314	4.5792991520	-4.4607053773	1.5245557199
O315	1.2997948134	-6.0080039552	1.5669520954
O316	3.3080041902	-7.7828986877	1.6548337594
O317	5.6224748625	-3.5966724516	0.1945373216
O318	5.9309647641	-1.3834385794	1.5897998781
O319	7.8255425532	-3.2587582327	1.6240092165
Ti320	2.4227271269	-6.9537809841	2.9733932900
O321	3.7514905447	-5.5020593790	3.0162201183
Ti322	6.9825649253	-2.4145876373	2.9894367292

O323	5.5459123293	-3.7830527693	3.0066533505
Ti324	4.3660435569	-4.4525248119	4.4962873615
O325	1.3912453082	-5.9085399990	4.4622824002
O326	3.0546302516	-7.7760083367	4.4937912270
O327	5.9317753285	-1.4348003978	4.4595598512
O328	7.8207255897	-3.0658581398	4.4884996710
Ti329	2.4073986612	-6.9638797010	6.0077164927
O330	3.7409000075	-5.4879865565	5.9640776414
Ti331	4.5610537973	-4.4329012276	7.4559304366
O332	1.3290494484	-5.9628809894	7.4420227458
O333	3.2817914921	-7.7838198423	7.3322732366
Ti334	6.9974900441	-2.3779306692	5.9811688564
O335	5.5363113270	-3.7677440904	5.9726093791
O336	5.9048180191	-1.3742936884	7.3884968866
O337	7.8341351555	-3.1892300967	7.3632423513
O338	4.3598021925	-5.9105994880	8.6121691595
O339	5.6125710619	-3.5839599498	8.7851843951
H340	3.8093528601	-7.2126768534	8.0033571484
H341	7.4089357778	-3.4899619045	8.2061578480
H342	1.6384258749	-6.2087159590	8.3365651913
H343	5.8131839115	-2.0280217253	8.1459041912
H344	4.7899670969	-6.0323229717	9.4815402301
H345	5.2398699014	-3.4901567477	9.6930934016
H346	3.8332816929	-7.2213104893	0.9744644078
H347	4.8535174996	-6.0627240050	-0.4951660674
H348	5.2337956409	-3.4988277491	-0.7075824571
H349	1.5377657863	-6.3241532477	0.6724600899
H350	5.8419079034	-2.0326807641	0.8271577072
H351	7.3997069418	-3.5369996089	0.7738233036
Ti352	0.0264054878	-0.0200131939	-1.5054781410
O353	-0.9524312348	-0.9677178574	-2.8424783738
O354	1.0149634072	0.9500230035	-2.8351041143
Ti355	-0.0181953959	0.0089346459	10.4750863549
O356	-0.9741488042	-0.9399718120	11.8143170488
O357	0.9608481759	1.0000740358	11.7933487322
Li358	6.5624081149	6.4231036970	4.4685642289

3.12 555 O_{Li}⁺/e⁻ cluster in water^{††}

3.12.1 Ground State GS3

358			
555	Li ⁺ /e ⁻ Surface, Water-Optimized	SCFE :	-17174.8471324545 hartree
O1	-7.8697417132	-4.1448055444	3.1849056667
H2	-8.1459698746	-4.2692269299	4.1385890435
H3	-7.1815289250	-4.8365181108	2.9711516992
O4	-7.8891446495	-4.2142026900	5.8703733297
H5	-8.6509246078	-4.4125031057	6.4517160118
H6	-7.1390098350	-4.8789039643	5.9907923055
O7	-4.1491808873	-7.8971674967	2.9139753206
H8	-4.3248495236	-8.4111882337	2.1003747208
H9	-4.8575492651	-7.2059452610	3.0448144607

^{††}Li⁺ is adsorbed on surface, and one additional electron is added

O10	-4.1756778920	-7.8709649255	6.1084759521
H11	-4.3500005630	-8.3953358277	6.9157597656
H12	-4.8850432740	-7.1776729236	5.9888049808
O13	4.0183363194	7.9879492148	3.1349091440
H14	4.1710463320	8.2061973593	4.0988226293
H15	4.7362974010	7.3952176175	2.8065287121
O16	4.1843839481	7.9565806888	5.8375255910
H17	4.3168850523	8.7668369053	6.3717634245
H18	4.8530352721	7.2461540348	6.0666479982
O19	8.0023824807	4.0417651060	2.8415555301
H20	8.5740012787	4.1078270121	2.0493901289
H21	7.3085039137	4.7574512063	2.8268711487
O22	7.9623946518	4.0799465072	6.1569294164
H23	8.5660553712	4.1390795829	6.9251814849
H24	7.2755632565	4.7998136665	6.1955853208
O25	-8.4934872384	0.8813926664	2.9816109266
H26	-9.4085865774	1.1972483573	2.8348542512
H27	-8.3285637217	-0.0030119300	2.4655611626
O28	-8.2907503475	0.8548854836	5.8164244281
H29	-8.4681293811	0.5882738077	4.8772966896
H30	-8.2399905347	0.0381294002	6.4247256340
O31	0.9008582590	-8.4729849576	3.0020564856
H32	1.1956980586	-9.4028637320	2.9277556163
H33	0.0140542509	-8.3237860530	2.5024485423
O34	0.8173558419	-8.2680809700	5.8587016381
H35	0.5429106645	-8.4267391431	4.9192876365
H36	0.0016694633	-8.2109381319	6.4666456520
O37	-0.9484670553	8.4499249715	2.9458876628
H38	-1.2685066265	9.3672766510	2.8291792281
H39	-0.0889827883	8.2849598334	2.4045137556
O40	-0.7952202957	8.2885295850	5.7760519960
H41	-0.5193670070	8.4381467285	4.8339062440
H42	0.0292733183	8.2520706446	6.3996758817
O43	8.4709518685	-0.8998688554	2.9817183994
H44	9.3971270465	-1.2048666117	2.9007016974
H45	8.3234830686	-0.0189229382	2.4516013582
O46	8.2787483182	-0.7962499461	5.8499565326
H47	8.4285154174	-0.4836545792	4.9207564527
H48	8.2316046779	0.0136883171	6.4887404234
O49	-3.2046557688	-1.2770445820	-1.3658206517
O50	-1.2421617304	-3.2433678633	-1.3335479341
O51	-3.2888610357	3.3913000137	-1.3617686413
O52	-1.4287788857	1.4043975419	-1.5526811736
O53	1.4550478696	-1.4603392790	-1.5374017703
O54	3.3042252447	-3.4542589720	-1.3392635136
O55	-5.7150749292	-5.5618076540	0.1783422833
Ti56	-4.7285798970	-4.7409468825	1.4787760764
O57	-5.4770582115	-1.0683878130	0.1015341129
Ti58	-4.6281178651	-0.0995071807	1.4733861146
O59	-7.9546409569	-1.3174565233	1.7997808260
O60	-5.9826137831	-3.1987306805	1.5343986617
O61	-1.0366460603	-5.5042529579	0.1224133256
Ti62	-0.1202832506	-4.5783199386	1.5082387297
O63	-3.1897396419	-5.9298273115	1.4850553046

O64	-1.3471613279	-7.9646519149	1.8273016176
Ti65	-2.2872007729	-2.2551154021	0.0121687488
O66	-0.8653638739	-0.9012257901	-0.0493837781
O67	-3.6984011679	-3.6632113951	0.0095172226
Ti68	0.0557380583	0.0294923721	1.5150436394
O69	-3.1654556462	-1.3736755289	1.4799873131
O70	-1.3902996046	-3.1786591289	1.4868939280
Ti71	-2.3557706233	2.4046812685	-0.1443748037
O72	-3.6421038944	0.9217358790	0.0069067469
O73	-3.1567602753	3.2220948580	1.4489719201
O74	-1.3869084296	1.4044793442	1.4508180632
Ti75	2.3884159417	-2.4632336822	-0.1139709086
O76	0.8682332980	-3.6389837365	0.0211869620
O77	1.4108155696	-1.4246169426	1.4704022529
O78	3.1775983906	-3.2625889684	1.4770421361
O79	0.8810264660	0.8625471797	-0.0383451534
O80	-5.4531744045	-5.4476706677	3.0087080021
Ti81	-6.8467018098	-2.2379405224	3.0423324665
O82	-5.4877692451	-0.8847494354	2.9716121352
Ti83	-2.2548968414	-6.8349648508	3.0583536215
O84	-0.9293759794	-5.4748781478	3.0073419657
Ti85	-2.3530976470	-2.3143372294	3.0340504632
O86	-0.8792125169	-0.8739526346	2.9766194826
O87	-3.6636013832	-3.6540718795	2.9909640204
Ti88	-2.1720194628	2.1444056511	2.8999700109
O89	-3.6296770436	0.8873657267	2.9724293361
Ti90	2.1606783657	-2.1971444398	2.9190701873
O91	0.8813130238	-3.6674698369	2.9821357425
O92	0.8888042875	0.8666461699	2.9508776026
Ti93	-4.5378824560	-4.5095880303	4.4825326893
Ti94	-4.5745624954	0.1857084365	4.4596524701
O95	-7.8354187742	-1.6959672094	4.4873875200
O96	-5.8507894283	-3.1387558242	4.5173841645
Ti97	0.1538995298	-4.5966047436	4.4841913502
O98	-3.2307481736	-5.9258806279	4.5075430971
O99	-1.6618107857	-7.7908704456	4.5120303394
Ti100	-0.0404130605	-0.0459373640	4.4912401924
O101	-3.1768294920	-1.3831850092	4.4803457898
O102	-1.4011849270	-3.1522271162	4.4806752287
O103	-3.1800604097	3.1669171083	4.4532487866
O104	-1.4030275071	1.3862381757	4.4730551429
O105	1.3765337499	-1.4213815271	4.4792235970
O106	3.1650817160	-3.1795032025	4.4848745494
O107	-5.4870388745	-5.4331545900	5.9928608867
Ti108	-4.7585072867	-4.7382099837	7.5235115509
Ti109	-6.7953255403	-2.2151226715	5.9458747548
O110	-5.4913166670	-0.8599657412	5.9628796466
Ti111	-4.5735080426	-0.0740946665	7.4541199014
O112	-7.9423035510	-1.3280901054	7.1770233759
O113	-5.9469542368	-3.1563062119	7.4546471429
Ti114	-2.2841123063	-6.8159737585	5.9619230187
O115	-0.9158764231	-5.4739961498	5.9867882909
Ti116	-0.1094970635	-4.5859102988	7.4675793004
O117	-3.1804714418	-5.8914117415	7.4993886492

O118	-1.3893856725	-7.9466262900	7.2005255779
Ti119	-2.3466698738	-2.3553674033	5.9228070924
O120	-0.8823553317	-0.8732409500	5.9745224964
O121	-3.6540331719	-3.6621963378	5.9962194069
Ti122	0.0384750444	0.0463572127	7.4473948936
O123	-3.1820609875	-1.3596757172	7.4767402227
O124	-1.3953526386	-3.1618131373	7.4880881382
Ti125	-2.1685201066	2.1769806064	6.0365639056
O126	-3.6747271941	0.9101412181	5.9600225502
O127	-3.2401728684	3.1796174122	7.4784549967
O128	-1.4229779273	1.3999619578	7.4862731363
Ti129	2.1530898993	-2.1860410014	6.0512316050
O130	0.8811038527	-3.6664761345	5.9858094221
O131	1.3870789838	-1.4125357465	7.4913548812
O132	3.1644424201	-3.2327269580	7.5007572380
O133	0.8707887504	0.8667215677	5.9951145224
O134	-5.6820760643	-5.5872002336	8.8092941016
O135	-5.5139202576	-1.0083127164	8.8232963158
O136	-1.0395964135	-5.4650258780	8.8686861086
Ti137	-2.2840599723	-2.2596644748	8.9503501906
O138	-0.8922917001	-0.8757517639	9.0159603882
O139	-3.7078328054	-3.6409146574	8.9775903607
O140	-3.2370830850	-1.2169808491	10.3072747425
O141	-1.2854159483	-3.2008025506	10.3276837862
Ti142	-2.4359872390	2.3971369279	9.0751096252
O143	-3.6465804504	0.8925141305	8.9465264501
O144	-3.4304354755	3.3157771393	10.2947013389
O145	-1.4475156464	1.4491591498	10.4927465954
Ti146	2.3761440564	-2.4268933770	9.0886496256
O147	0.8617837508	-3.6192360916	8.9636551662
O148	1.4277828640	-1.4229208958	10.5038639679
O149	3.2877973301	-3.4177748013	10.3181992694
O150	0.8577663523	0.8756938107	8.9846455049
H151	-7.6668565802	-1.1595092282	8.1045345123
H152	-4.2539128181	3.1403272115	10.7908750247
H153	-1.2621992330	-7.7168266109	8.1453320672
H154	3.1034524889	-4.2297896871	10.8296074941
H155	-5.7636226324	-2.4577897086	8.1689508172
H156	-1.6605004116	1.7379378369	11.4032244814
H157	-2.4729194366	-5.6964690845	8.1999039747
H158	1.7207135566	-1.6259573811	11.4153006260
H159	-2.6691302672	-1.0385287330	11.1073640188
H160	-1.1004083738	-2.6292599832	11.1251982214
H161	-6.3335428020	-5.8766952459	9.4694830180
H162	-4.0105820679	-3.8993051768	9.8710690954
H163	-1.2370254464	-4.9601101503	9.7002821624
H164	0.1183223169	-3.4171332670	9.6455690593
H165	-0.9506528904	-0.9291059636	12.7834721159
H166	0.9033141579	0.9840143820	12.7835531186
H167	-3.4514144125	0.1385921259	9.6376405856
H168	-5.0227133586	-1.2064582524	9.6615738334
H169	-7.6969533327	-1.1878704770	0.8622882408
H170	-1.2098451878	-7.7115784184	0.8890886808
H171	-6.6125074869	-5.4544576974	-0.1904320806

H172	-3.9927844197	-3.9480348004	-0.8788790056
H173	-1.2368249697	-4.9933612911	-0.7059875908
H174	0.1083972910	-3.4377906140	-0.6652687193
H175	-0.9035358646	-0.9864047753	-3.8121255425
H176	0.9291022067	0.9437312742	-3.8241325742
H177	-3.4498165491	0.1910443715	-0.6787872899
H178	-4.9720701711	-1.2887898727	-0.7241671029
H179	-5.7975981020	-2.5189969308	0.8089689442
H180	-2.4691890186	-5.7360971448	0.7966759511
H181	-3.1195199357	4.2190260499	-1.8529758723
H182	-1.7261962891	1.5852182837	-2.4670855891
H183	1.7593988322	-1.6552688740	-2.4466418434
H184	3.1229421404	-4.2527111262	-1.8726439972
H185	-2.6263729932	-1.0834352936	-2.1590634533
H186	-1.0687724410	-2.6760934567	-2.1350688535
O187	1.2552358321	3.1920926876	-1.3519401167
O188	3.2099395228	1.2382954605	-1.3649552010
O189	-0.8568310964	3.6185509732	-0.0129078289
Ti190	0.1209018504	4.5349507763	1.4942805017
O191	3.6545968774	-0.9629874703	0.0210802155
Ti192	4.6111859934	0.0849596671	1.4874603495
Ti193	2.3467965891	2.2822834798	-0.0081717894
O194	3.6964695204	3.6851204837	-0.0083368349
Ti195	4.7860693036	4.7463430193	1.5551451935
O196	1.3833701187	3.1572188566	1.4591655382
O197	3.1839621343	1.3568396119	1.4589681157
O198	1.0516860732	5.5317430780	0.1518107981
O199	1.2272834723	7.8521349989	1.7197524021
O200	3.2307551702	5.9920734887	1.5687721521
O201	5.4966539551	1.0068894588	0.1030222985
O202	5.9641286843	3.1862044040	1.4914219120
O203	7.9773712289	1.3028936128	1.8033562024
O204	5.5302505728	5.7038522418	0.1586204411
O205	-0.8866287590	3.6325272641	2.9773943517
O206	3.6319044732	-0.9056296486	3.0015464058
Ti207	2.3831039013	2.3435029145	3.0440655758
O208	3.6650280788	3.6447294762	2.8734417905
Ti209	2.1702019011	6.8513386181	3.0200409313
O210	0.8813038166	5.4543105396	2.9929917958
Ti211	6.8476297129	2.2039262304	3.0555199382
O212	5.4864821532	0.8771334481	2.9793320773
O213	5.6151485327	5.5111433137	2.9982057907
Ti214	-0.1880068292	4.5502853772	4.4665530346
Ti215	4.5376686901	-0.1931300296	4.4823125861
Ti216	4.4994321477	4.5078699616	4.4870111856
O217	1.4197372845	3.1752440058	4.4767321994
O218	3.2025288043	1.4085862030	4.4861789076
O219	1.6470678161	7.8276902542	4.4709324260
O220	3.1464716671	5.8844220752	4.5081369551
O221	5.9641538960	3.1928448730	4.4954578125
O222	7.8093367635	1.6015370565	4.4974582655
O223	-0.9055188774	3.6225502368	5.9527513946
Ti224	0.0805465985	4.6064888606	7.4797156909
O225	3.6234561375	-0.9045702727	5.9583771208

Ti226	4.5937315974	0.1010871548	7.4783775196
Ti227	2.3680580146	2.3872401261	5.9460425647
O228	3.6619585953	3.6617062321	6.1154282994
Ti229	4.7721813706	4.7606193781	7.4741632689
O230	1.3494173093	3.1604080608	7.4766550971
O231	3.1557865874	1.3663288082	7.4946862042
Ti232	2.2268590919	6.7757422381	5.9133785365
O233	0.8617411439	5.4809391110	5.9764367683
O234	1.3443573896	7.9832022361	7.1282419745
O235	3.1963141631	5.9893863814	7.4404112726
Ti236	6.8131783456	2.2363719363	5.9398895048
O237	5.4794260711	0.8732801327	5.9908111612
O238	5.9166298999	3.1618398716	7.4661712427
O239	7.9636004921	1.3476507708	7.1922185899
O240	5.5723705368	5.5596430465	6.0203183509
O241	-0.9392579011	3.6497608532	8.9398217794
O242	3.6238926894	-0.9313889590	8.9524873166
Ti243	2.2843587330	2.2983232298	8.9507671394
O244	3.6470371670	3.7010636389	8.9736945968
O245	1.2113615834	3.2094951656	10.2943601568
O246	3.1792049918	1.2604821888	10.3132153111
O247	1.0543941930	5.4757990425	8.8365154524
O248	5.4461957483	1.0358977166	8.8752836699
O249	5.6103045190	5.5591104101	8.8657086043
H250	1.2258700208	7.7753216436	8.0781891164
H251	7.7221983742	1.2547314099	8.1375277672
H252	2.5117513791	5.7867887509	8.1594938376
H253	5.7116753485	2.4814467580	8.1846857870
H254	1.0286471349	2.6381654064	11.0914647430
H255	2.6097809137	1.0719235423	11.1108246615
H256	3.4161519597	-0.1932387915	9.6298751419
H257	4.9277889375	1.2385223903	9.6989647697
H258	3.9229926762	4.0178182584	9.8568606654
H259	5.9918841633	5.6834640138	9.7514554744
H260	1.2619884926	4.9635022826	9.6619430212
H261	-0.1907730919	3.4405769845	9.6203599735
H262	3.4540231252	-0.2382535847	-0.6666784391
H263	5.0057675696	1.2086201471	-0.7345309518
H264	3.9600703247	4.0659798081	-0.8700397192
H265	5.3255498417	6.5829597617	-0.2137268640
H266	1.2684083149	5.0710509778	-0.6954560894
H267	-0.0857000585	3.4191065451	-0.6915951737
H268	1.0395369418	7.4264623786	0.8479580143
H269	2.5616777740	5.7834486011	0.8436698683
H270	5.7455188341	2.4973644539	0.7893082288
H271	7.7108033106	1.1922021968	0.8657102496
H272	1.0730459800	2.6084513137	-2.1399326494
H273	2.6337374860	1.0344689099	-2.1566006351
O274	-5.6262755926	3.5656771231	0.1787207317
Ti275	-4.5283171356	4.4309236770	1.4776884890
O276	-7.8306290287	3.2346965868	1.5943581770
O277	-5.9250544266	1.3544034502	1.5512702353
O278	-4.3153332780	5.8598327504	0.2731732113
O279	-3.3287410484	7.7635398251	1.6101357627

O280	-1.3501001370	5.9463397385	1.5359367575
Ti281	-6.9902086462	2.3920041169	2.9701266691
O282	-5.5412430670	3.7658056724	2.9606747920
Ti283	-2.4567334569	6.9049511948	2.9295454629
O284	-3.7749323940	5.4914155431	2.9817344942
Ti285	-4.4277316228	4.3907908654	4.4558494531
O286	-7.8008703240	3.0677376899	4.4452475901
O287	-5.9304910636	1.4076443604	4.4043349073
O288	-3.0702667343	7.7789272881	4.4519261789
O289	-1.4197338570	5.9035433858	4.4472493511
Ti290	-6.9610575086	2.4298134874	5.9834201863
O291	-5.5127136582	3.7484979043	5.9176469512
Ti292	-4.4559235527	4.5578901065	7.4126620544
O293	-7.8108467298	3.3118332655	7.2855208055
O294	-5.9850395549	1.3662895826	7.4078291730
Ti295	-2.3535107362	7.0028547179	5.9303559492
O296	-3.7843221792	5.5294090328	5.9298344920
O297	-3.1785620593	7.8372200787	7.3121584214
O298	-1.3800581520	5.8992983594	7.3685756862
O299	-5.9261489518	4.3347433180	8.5829238893
O300	-3.6245075715	5.6386402213	8.7361138238
H301	-7.2356767730	3.8335197731	7.9627085063
H302	-3.4936162457	7.3870925169	8.1381600404
H303	-6.2244100311	1.6712737453	8.3054309476
H304	-2.0501045621	5.8115485082	8.1098193405
H305	-3.5239185450	5.2699974128	9.6453586848
H306	-6.0455542751	4.7733562811	9.4481943344
H307	-7.3675859112	3.5057678573	0.7597408898
H308	-4.7873485834	5.9899722045	-0.5730385825
H309	-5.2384860619	3.4615382217	-0.7230116797
H310	-5.8227211871	2.0231462293	0.8056030673
H311	-3.8181623633	7.2050179597	0.9107779408
H312	-1.6538987068	6.1685474835	0.6331890243
O313	4.4166858017	-5.9413364287	0.3749153717
Ti314	4.5831114929	-4.4567980425	1.5281670085
O315	1.2968272491	-6.0112377162	1.5649599396
O316	3.3043134093	-7.7873750019	1.6526243448
O317	5.6258035784	-3.6019688104	0.1915665098
O318	5.9265677118	-1.3817118031	1.5923011071
O319	7.8155110891	-3.2612700405	1.6314437977
Ti320	2.4206540315	-6.9543321453	2.9721664397
O321	3.7528239919	-5.5089344028	3.0150827192
Ti322	6.9769073502	-2.3998397820	2.9949099477
O323	5.5402454018	-3.7820231887	3.0111215563
Ti324	4.3614540451	-4.4569721197	4.4949380366
O325	1.3915985078	-5.9108994758	4.4605314946
O326	3.0467055011	-7.7841505546	4.4923738505
O327	5.9268956044	-1.4223398273	4.4598018926
O328	7.8151640169	-3.0576969590	4.4924450766
Ti329	2.4044990568	-6.9627503260	6.0051395638
O330	3.7407023607	-5.4958626336	5.9626194661
Ti331	4.5637357970	-4.4341961454	7.4511079463
O332	1.3258841368	-5.9656913323	7.4416168843
O333	3.2753185007	-7.7895541810	7.3304229249

Ti334	6.9885244128	-2.3628672209	5.9807373360
O335	5.5333289989	-3.7722206811	5.9685443823
O336	5.8911113299	-1.3737834668	7.3888589061
O337	7.8238124205	-3.1773439053	7.3660445604
O338	4.3556514602	-5.9190483057	8.6052531819
O339	5.6116091881	-3.5960277755	8.7895116888
H340	3.7934263594	-7.2124835899	8.0076737513
H341	7.3861210187	-3.4789513036	8.2026108930
H342	1.6287512271	-6.2165339458	8.3366489494
H343	5.7958035063	-2.0251938218	8.1452769004
H344	4.7744973368	-6.0272440077	9.4817134616
H345	5.2226576877	-3.4985040349	9.6916264969
H346	3.8351647531	-7.2203395891	0.9795228252
H347	4.8548433126	-6.0569866271	-0.4906260587
H348	5.2290773090	-3.5079937321	-0.7078956108
H349	1.5283890141	-6.3268619183	0.6690203971
H350	5.8373144411	-2.0249450552	0.8270752439
H351	7.3787944207	-3.5392946896	0.7862747324
Ti352	0.0170185464	-0.0329024331	-1.4972391424
O353	-0.9799203352	-0.9921197769	-2.8382310119
O354	0.9934695648	0.9251427823	-2.8498961154
Ti355	-0.0230061407	-0.0043216797	10.4659580754
O356	-0.9935720742	-0.9654349446	11.8082422906
O357	0.9425543999	0.9745511192	11.8078181919
Li358	6.5996030023	6.4174615841	4.4820203203

3.12.2 Transition State TS2

358			
555	Li+/e- Surface , Water-Optimized	SCFE : -17174.8380171877	hartree
O1	-7.8697417132	-4.1448055444	3.1849056667
H2	-8.1459698746	-4.2692269299	4.1385890435
H3	-7.1815289250	-4.8365181108	2.9711516992
O4	-7.8891446495	-4.2142026900	5.8703733297
H5	-8.6509246078	-4.4125031057	6.4517160118
H6	-7.1390098350	-4.8789039643	5.9907923055
O7	-4.1491808873	-7.8971674967	2.9139753206
H8	-4.3248495236	-8.4111882337	2.1003747208
H9	-4.8575492651	-7.2059452610	3.0448144607
O10	-4.1756778920	-7.8709649255	6.1084759521
H11	-4.3500005630	-8.3953358277	6.9157597656
H12	-4.8850432740	-7.1776729236	5.9888049808
O13	4.0149766546	7.9673079395	3.1499700521
H14	4.1750551557	8.1454392080	4.1255324311
H15	4.6723271678	7.3177886946	2.8178138205
O16	4.2400626598	7.8884615936	5.8099795346
H17	4.4209933274	8.6646414650	6.3725499708
H18	4.8952762599	7.1352909286	5.9783357108
O19	7.9895591786	4.0276143992	2.8404261623
H20	8.5095874301	4.1038036631	2.0142819224
H21	7.2611875625	4.7109591268	2.8550423275
O22	7.8855215871	4.1537929386	6.0939167240
H23	8.4298989331	4.2831115998	6.8948793142
H24	7.1687560673	4.8551572113	6.0411266702

O25	-8.4934872384	0.8813926664	2.9816109266
H26	-9.4085865774	1.1972483573	2.8348542512
H27	-8.3285637217	-0.0030119300	2.4655611626
O28	-8.2907503475	0.8548854836	5.8164244281
H29	-8.4681293811	0.5882738077	4.8772966896
H30	-8.2399905347	0.0381294002	6.4247256340
O31	0.9008582590	-8.4729849576	3.0020564856
H32	1.1956980586	-9.4028637320	2.9277556163
H33	0.0140542509	-8.3237860530	2.5024485423
O34	0.8173558419	-8.2680809700	5.8587016381
H35	0.5429106645	-8.4267391431	4.9192876365
H36	0.0016694633	-8.2109381319	6.4666456520
O37	-0.9484670553	8.4499249715	2.9458876628
H38	-1.2685066265	9.3672766510	2.8291792281
H39	-0.0889827883	8.2849598334	2.4045137556
O40	-0.7952202957	8.2885295850	5.7760519960
H41	-0.5193670070	8.4381467285	4.8339062440
H42	0.0292733183	8.2520706446	6.3996758817
O43	8.4709518685	-0.8998688554	2.9817183994
H44	9.3971270465	-1.2048666117	2.9007016974
H45	8.3234830686	-0.0189229382	2.4516013582
O46	8.2787483182	-0.7962499461	5.8499565326
H47	8.4285154174	-0.4836545792	4.9207564527
H48	8.2316046779	0.0136883171	6.4887404234
O49	-3.2046557688	-1.2770445820	-1.3658206517
O50	-1.2421617304	-3.2433678633	-1.3335479341
O51	-3.2888610357	3.3913000137	-1.3617686413
O52	-1.4287788857	1.4043975419	-1.5526811736
O53	1.4550478696	-1.4603392790	-1.5374017703
O54	3.3042252447	-3.4542589720	-1.3392635136
O55	-5.7150749292	-5.5618076540	0.1783422833
Ti56	-4.7285798970	-4.7409468825	1.4787760764
O57	-5.4770582115	-1.0683878130	0.1015341129
Ti58	-4.6281178651	-0.0995071807	1.4733861146
O59	-7.9546409569	-1.3174565233	1.7997808260
O60	-5.9826137831	-3.1987306805	1.5343986617
O61	-1.0366460603	-5.5042529579	0.1224133256
Ti62	-0.1202832506	-4.5783199386	1.5082387297
O63	-3.1897396419	-5.9298273115	1.4850553046
O64	-1.3471613279	-7.9646519149	1.8273016176
Ti65	-2.2872007729	-2.2551154021	0.0121687488
O66	-0.8653638739	-0.9012257901	-0.0493837781
O67	-3.6984011679	-3.6632113951	0.0095172226
Ti68	0.0557380582	0.0294923722	1.5150436394
O69	-3.1654556462	-1.3736755289	1.4799873131
O70	-1.3902996046	-3.1786591289	1.4868939280
Ti71	-2.3557706235	2.4046812687	-0.1443748037
O72	-3.6421038944	0.9217358790	0.0069067469
O73	-3.1567602753	3.2220948580	1.4489719201
O74	-1.3869084296	1.4044793442	1.4508180632
Ti75	2.3884159422	-2.4632336826	-0.1139709086
O76	0.8682332980	-3.6389837365	0.0211869620
O77	1.4108155696	-1.4246169426	1.4704022529
O78	3.1775983906	-3.2625889684	1.4770421361

O79	0.8810264660	0.8625471797	-0.0383451534
O80	-5.4531744045	-5.4476706677	3.0087080021
Ti81	-6.8467018098	-2.2379405224	3.0423324665
O82	-5.4877692451	-0.8847494354	2.9716121352
Ti83	-2.2548968414	-6.8349648508	3.0583536215
O84	-0.9293759794	-5.4748781478	3.0073419657
Ti85	-2.3530976470	-2.3143372294	3.0340504632
O86	-0.8792125169	-0.8739526346	2.9766194826
O87	-3.6636013832	-3.6540718795	2.9909640204
Ti88	-2.1720194628	2.1444056511	2.8999700109
O89	-3.6296770436	0.8873657267	2.9724293361
Ti90	2.1606783657	-2.1971444398	2.9190701873
O91	0.8813130238	-3.6674698369	2.9821357425
O92	0.8888042874	0.8666461700	2.9508776026
Ti93	-4.5378824560	-4.5095880303	4.4825326893
Ti94	-4.5745624954	0.1857084365	4.4596524701
O95	-7.8354187742	-1.6959672094	4.4873875200
O96	-5.8507894283	-3.1387558242	4.5173841645
Ti97	0.1538995298	-4.5966047436	4.4841913502
O98	-3.2307481736	-5.9258806279	4.5075430971
O99	-1.6618107857	-7.7908704456	4.5120303394
Ti100	-0.0404130606	-0.0459373639	4.4912401924
O101	-3.1768294920	-1.3831850092	4.4803457898
O102	-1.4011849270	-3.1522271162	4.4806752287
O103	-3.1800604097	3.1669171083	4.4532487866
O104	-1.4030275071	1.3862381757	4.4730551429
O105	1.3765337499	-1.4213815271	4.4792235970
O106	3.1650817160	-3.1795032025	4.4848745494
O107	-5.4870388745	-5.4331545900	5.9928608867
Ti108	-4.7585072867	-4.7382099837	7.5235115509
Ti109	-6.7953255403	-2.2151226715	5.9458747548
O110	-5.4913166670	-0.8599657412	5.9628796466
Ti111	-4.5735080426	-0.0740946665	7.4541199014
O112	-7.9423035510	-1.3280901054	7.1770233759
O113	-5.9469542368	-3.1563062119	7.4546471429
Ti114	-2.2841123063	-6.8159737585	5.9619230187
O115	-0.9158764231	-5.4739961498	5.9867882909
Ti116	-0.1094970635	-4.5859102988	7.4675793004
O117	-3.1804714418	-5.8914117415	7.4993886492
O118	-1.3893856725	-7.9466262900	7.2005255779
Ti119	-2.3466698738	-2.3553674033	5.9228070924
O120	-0.8823553317	-0.8732409500	5.9745224964
O121	-3.6540331719	-3.6621963378	5.9962194069
Ti122	0.0384750445	0.0463572126	7.4473948936
O123	-3.1820609875	-1.3596757172	7.4767402227
O124	-1.3953526386	-3.1618131373	7.4880881382
Ti125	-2.1685201067	2.1769806064	6.0365639056
O126	-3.6747271941	0.9101412181	5.9600225502
O127	-3.2401728684	3.1796174122	7.4784549967
O128	-1.4229779273	1.3999619578	7.4862731363
Ti129	2.1530898994	-2.1860410016	6.0512316050
O130	0.8811038527	-3.6664761345	5.9858094221
O131	1.3870789838	-1.4125357465	7.4913548812
O132	3.1644424201	-3.2327269580	7.5007572380

O133	0.8707887505	0.8667215676	5.9951145224
O134	-5.6820760643	-5.5872002336	8.8092941016
O135	-5.5139202576	-1.0083127164	8.8232963158
O136	-1.0395964135	-5.4650258780	8.8686861086
Ti137	-2.2840599723	-2.2596644748	8.9503501906
O138	-0.8922917001	-0.8757517639	9.0159603882
O139	-3.7078328054	-3.6409146574	8.9775903607
O140	-3.2370830850	-1.2169808491	10.3072747425
O141	-1.2854159483	-3.2008025506	10.3276837862
Ti142	-2.4359872391	2.3971369280	9.0751096252
O143	-3.6465804504	0.8925141305	8.9465264501
O144	-3.4304354755	3.3157771393	10.2947013389
O145	-1.4475156464	1.4491591498	10.4927465954
Ti146	2.3761440567	-2.4268933772	9.0886496256
O147	0.8617837508	-3.6192360916	8.9636551662
O148	1.4277828640	-1.4229208958	10.5038639679
O149	3.2877973301	-3.4177748013	10.3181992694
O150	0.8577663522	0.8756938108	8.9846455049
H151	-7.6668565802	-1.1595092282	8.1045345123
H152	-4.2539128181	3.1403272115	10.7908750247
H153	-1.2621992330	-7.7168266109	8.1453320672
H154	3.1034524889	-4.2297896871	10.8296074941
H155	-5.7636226324	-2.4577897086	8.1689508172
H156	-1.6605004116	1.7379378369	11.4032244814
H157	-2.4729194366	-5.6964690845	8.1999039747
H158	1.7207135566	-1.6259573811	11.4153006260
H159	-2.6691302672	-1.0385287330	11.1073640188
H160	-1.1004083738	-2.6292599832	11.1251982214
H161	-6.3335428020	-5.8766952459	9.4694830180
H162	-4.0105820679	-3.8993051768	9.8710690954
H163	-1.2370254464	-4.9601101503	9.7002821624
H164	0.1183223169	-3.4171332670	9.6455690593
H165	-0.9506528904	-0.9291059636	12.7834721159
H166	0.9033141579	0.9840143820	12.7835531186
H167	-3.4514144125	0.1385921259	9.6376405856
H168	-5.0227133586	-1.2064582524	9.6615738334
H169	-7.6969533327	-1.1878704770	0.8622882408
H170	-1.2098451878	-7.7115784184	0.8890886808
H171	-6.6125074869	-5.4544576974	-0.1904320806
H172	-3.9927844197	-3.9480348004	-0.8788790056
H173	-1.2368249697	-4.9933612911	-0.7059875908
H174	0.1083972910	-3.4377906140	-0.6652687193
H175	-0.9035358646	-0.9864047753	-3.8121255425
H176	0.9291022067	0.9437312742	-3.8241325742
H177	-3.4498165491	0.1910443715	-0.6787872899
H178	-4.9720701711	-1.2887898727	-0.7241671029
H179	-5.7975981020	-2.5189969308	0.8089689442
H180	-2.4691890186	-5.7360971448	0.7966759511
H181	-3.1195199357	4.2190260499	-1.8529758723
H182	-1.7261962891	1.5852182837	-2.4670855891
H183	1.7593988322	-1.6552688740	-2.4466418434
H184	3.1229421404	-4.2527111262	-1.8726439972
H185	-2.6263729932	-1.0834352936	-2.1590634533
H186	-1.0687724410	-2.6760934567	-2.1350688535

O187	1.2552358321	3.1920926876	-1.3519401167
O188	3.2099395228	1.2382954605	-1.3649552010
O189	-0.8568310962	3.6185509730	-0.0129078289
Ti190	0.1209018504	4.5349507763	1.4942805016
O191	3.6545968768	-0.9629874699	0.0210802156
Ti192	4.6111859935	0.0849596678	1.4874603493
Ti193	2.3467965906	2.2822834792	-0.0081717902
O194	3.6964695212	3.6851204874	-0.0083368291
Ti195	4.7826133029	4.7466756308	1.5473080189
O196	1.3833701184	3.1572188565	1.4591655383
O197	3.1839621337	1.3568396116	1.4589681157
O198	1.0516860732	5.5317430780	0.1518107981
O199	1.2272834746	7.8521349967	1.7197524045
O200	3.2263878932	5.9935202068	1.5661233617
O201	5.4966539551	1.0068894588	0.1030222985
O202	5.9594551642	3.1862427203	1.4900938699
O203	7.9836788532	1.3020363296	1.8009372518
O204	5.5131832919	5.6895314038	0.1254458950
O205	-0.8866287590	3.6325272641	2.9773943517
O206	3.6319044733	-0.9056296488	3.0015464058
Ti207	2.3831038990	2.3435029118	3.0440655781
O208	3.6714381367	3.6545255570	2.8755452699
Ti209	2.1601269292	6.8494830755	3.0267241524
O210	0.8763758856	5.4551149519	2.9943826486
Ti211	6.8509241982	2.1921625514	3.0598505735
O212	5.4878390118	0.8712332914	2.9780533408
O213	5.6462061579	5.5683864901	2.9487204682
Ti214	-0.1880068301	4.5502853774	4.4665530350
Ti215	4.5376686893	-0.1931300300	4.4823125862
Ti216	4.5383916512	4.5478537190	4.4846160743
O217	1.4197372845	3.1752440058	4.4767321995
O218	3.2025288043	1.4085862029	4.4861789075
O219	1.6443463523	7.8248717591	4.4779071885
O220	3.1491052394	5.8871796326	4.5036506727
O221	5.9648213896	3.1970080123	4.4815855670
O222	7.8070604606	1.6033749223	4.5035314815
O223	-0.9055188773	3.6225502368	5.9527513946
Ti224	0.0805465985	4.6064888606	7.4797156909
O225	3.6234561374	-0.9045702726	5.9583771208
Ti226	4.5937315968	0.1010871547	7.4783775198
Ti227	2.3680580144	2.3872401270	5.9460425631
O228	3.6628922643	3.6631415402	6.0981676951
Ti229	4.7579619704	4.7558175836	7.4934131399
O230	1.3494173094	3.1604080607	7.4766550972
O231	3.1557865874	1.3663288083	7.4946862043
Ti232	2.2352113478	6.7688974880	5.9200099641
O233	0.8617411438	5.4809391107	5.9764367682
O234	1.3443573897	7.9832022334	7.1282419724
O235	3.1842761792	5.9932639396	7.4546519810
Ti236	6.8027446758	2.2553612707	5.9452870789
O237	5.4778234036	0.8790444005	5.9920426871
O238	5.9179465411	3.1553943949	7.4754642492
O239	7.9613510177	1.3607535296	7.1914613639
O240	5.5287692816	5.5482278090	6.0697000494

O241	-0.9392579010	3.6497608531	8.9398217794
O242	3.6238926890	-0.9313889587	8.9524873166
Ti243	2.2843587326	2.2983232302	8.9507671406
O244	3.6470371673	3.7010636380	8.9736945895
O245	1.2113615834	3.2094951656	10.2943601568
O246	3.1792049918	1.2604821888	10.3132153111
O247	1.0543941930	5.4757990425	8.8365154524
O248	5.4461957483	1.0358977166	8.8752836699
O249	5.6192347465	5.5554165837	8.8919942342
H250	1.2258700220	7.7753216443	8.0781891167
H251	7.7221983737	1.2547314109	8.1375277655
H252	2.4978605709	5.7953439564	8.1738858176
H253	5.7097676665	2.4711692463	8.1900907720
H254	1.0286471349	2.6381654064	11.0914647430
H255	2.6097809137	1.0719235423	11.1108246615
H256	3.4161519597	-0.1932387915	9.6298751419
H257	4.9277889375	1.2385223903	9.6989647697
H258	3.9229926772	4.0178182604	9.8568606644
H259	5.9632137180	5.5347833204	9.8015280145
H260	1.2619884926	4.9635022826	9.6619430212
H261	-0.1907730919	3.4405769845	9.6203599735
H262	3.4540231252	-0.2382535847	-0.6666784391
H263	5.0057675696	1.2086201471	-0.7345309518
H264	3.9600703247	4.0659798081	-0.8700397192
H265	5.2855861103	6.5606336916	-0.2520980580
H266	1.2684083149	5.0710509778	-0.6954560894
H267	-0.0857000585	3.4191065451	-0.6915951737
H268	1.0395369416	7.4264623787	0.8479580143
H269	2.5523641652	5.7817843348	0.8462676590
H270	5.7390062541	2.4943479094	0.7926367848
H271	7.7108033100	1.1922021977	0.8657102516
H272	1.0730459800	2.6084513137	-2.1399326494
H273	2.6337374860	1.0344689099	-2.1566006351
O274	-5.6262755926	3.5656771231	0.1787207317
Ti275	-4.5283171356	4.4309236770	1.4776884890
O276	-7.8306290287	3.2346965868	1.5943581770
O277	-5.9250544266	1.3544034502	1.5512702353
O278	-4.3153332780	5.8598327504	0.2731732113
O279	-3.3287410484	7.7635398251	1.6101357627
O280	-1.3501001369	5.9463397386	1.5359367575
Ti281	-6.9902086462	2.3920041169	2.9701266691
O282	-5.5412430670	3.7658056724	2.9606747920
Ti283	-2.4567334569	6.9049511948	2.9295454629
O284	-3.7749323940	5.4914155431	2.9817344942
Ti285	-4.4277316228	4.3907908654	4.4558494531
O286	-7.8008703240	3.0677376899	4.4452475901
O287	-5.9304910636	1.4076443604	4.4043349073
O288	-3.0702667343	7.7789272881	4.4519261789
O289	-1.4197338570	5.9035433858	4.4472493511
Ti290	-6.9610575086	2.4298134874	5.9834201863
O291	-5.5127136582	3.7484979043	5.9176469512
Ti292	-4.4559235527	4.5578901065	7.4126620544
O293	-7.8108467298	3.3118332655	7.2855208055
O294	-5.9850395549	1.3662895826	7.4078291730

Ti295	-2.3535107362	7.0028547179	5.9303559492
O296	-3.7843221792	5.5294090328	5.9298344920
O297	-3.1785620593	7.8372200787	7.3121584214
O298	-1.3800581520	5.8992983594	7.3685756862
O299	-5.9261489518	4.3347433180	8.5829238893
O300	-3.6245075715	5.6386402213	8.7361138238
H301	-7.2356767730	3.8335197731	7.9627085063
H302	-3.4936162457	7.3870925169	8.1381600404
H303	-6.2244100311	1.6712737453	8.3054309476
H304	-2.0501045621	5.8115485082	8.1098193405
H305	-3.5239185450	5.2699974128	9.6453586848
H306	-6.0455542751	4.7733562811	9.4481943344
H307	-7.3675859112	3.5057678573	0.7597408898
H308	-4.7873485834	5.9899722045	-0.5730385825
H309	-5.2384860619	3.4615382217	-0.7230116797
H310	-5.8227211871	2.0231462293	0.8056030673
H311	-3.8181623633	7.2050179597	0.9107779408
H312	-1.6538987068	6.1685474835	0.6331890243
O313	4.4166858017	-5.9413364287	0.3749153717
Ti314	4.5831114929	-4.4567980425	1.5281670085
O315	1.2968272491	-6.0112377162	1.5649599396
O316	3.3043134093	-7.7873750019	1.6526243448
O317	5.6258035784	-3.6019688104	0.1915665098
O318	5.9265677119	-1.3817118030	1.5923011071
O319	7.8155110891	-3.2612700405	1.6314437977
Ti320	2.4206540315	-6.9543321453	2.9721664397
O321	3.7528239919	-5.5089344028	3.0150827192
Ti322	6.9769073502	-2.3998397820	2.9949099477
O323	5.5402454018	-3.7820231887	3.0111215563
Ti324	4.3614540451	-4.4569721197	4.4949380366
O325	1.3915985078	-5.9108994758	4.4605314946
O326	3.0467055011	-7.7841505546	4.4923738505
O327	5.9268956044	-1.4223398273	4.4598018927
O328	7.8151640169	-3.0576969590	4.4924450766
Ti329	2.4044990568	-6.9627503260	6.0051395638
O330	3.7407023607	-5.4958626336	5.9626194661
Ti331	4.5637357970	-4.4341961454	7.4511079463
O332	1.3258841368	-5.9656913323	7.4416168843
O333	3.2753185007	-7.7895541810	7.3304229249
Ti334	6.9885244128	-2.3628672209	5.9807373360
O335	5.5333289989	-3.7722206811	5.9685443823
O336	5.8911113300	-1.3737834667	7.3888589061
O337	7.8238124205	-3.1773439053	7.3660445604
O338	4.3556514602	-5.9190483057	8.6052531819
O339	5.6116091881	-3.5960277755	8.7895116888
H340	3.7934263594	-7.2124835899	8.0076737513
H341	7.3861210187	-3.4789513036	8.2026108930
H342	1.6287512271	-6.2165339458	8.3366489494
H343	5.7958035063	-2.0251938218	8.1452769004
H344	4.7744973368	-6.0272440077	9.4817134616
H345	5.2226576877	-3.4985040349	9.6916264969
H346	3.8351647531	-7.2203395891	0.9795228252
H347	4.8548433126	-6.0569866271	-0.4906260587
H348	5.2290773090	-3.5079937321	-0.7078956108

H349	1.5283890141	−6.3268619183	0.6690203971
H350	5.8373144411	−2.0249450552	0.8270752439
H351	7.3787944207	−3.5392946896	0.7862747324
Ti352	0.0170185464	−0.0329024331	−1.4972391424
O353	−0.9799203352	−0.9921197769	−2.8382310119
O354	0.9934695648	0.9251427823	−2.8498961154
Ti355	−0.0230061408	−0.0043216796	10.4659580754
O356	−0.9935720742	−0.9654349446	11.8082422906
O357	0.9425543999	0.9745511192	11.8078181919
Li358	6.9381794756	6.9580768406	3.4498545303

3.13 Solvation Corretion

3.13.1 333 cluster

171			
333	SolvCorr D2h, Reduced–Optimized		
Ti1	0.0000000000	0.0000000000	0.0000000000
Ti2	0.0000000000	3.1060000000	0.0000000000
Ti3	0.0000000000	−3.1060000000	0.0000000000
O4	−1.2934000000	1.4945000000	0.0000000000
O5	1.2934000000	1.4945000000	0.0000000000
O6	−1.2934000000	−1.4945000000	0.0000000000
O7	1.2934000000	−1.4945000000	0.0000000000
O8	−1.3697000000	4.3866000000	0.0000000000
O9	1.3697000000	4.3866000000	0.0000000000
O10	−1.3697000000	−4.3866000000	0.0000000000
O11	1.3697000000	−4.3866000000	0.0000000000
H12	−1.4136000000	5.3606000000	0.0000000000
H13	1.4136000000	5.3606000000	0.0000000000
H14	−1.4136000000	−5.3606000000	0.0000000000
H15	1.4136000000	−5.3606000000	0.0000000000
O16	0.0000000000	0.0000000000	1.9110000000
O17	0.0000000000	0.0000000000	−1.9110000000
O18	0.0000000000	2.8825000000	1.8973000000
O19	0.0000000000	2.8825000000	−1.8973000000
O20	0.0000000000	−2.8825000000	1.8973000000
O21	0.0000000000	−2.8825000000	−1.8973000000
Ti22	0.0000000000	1.4092000000	3.2953000000
Ti23	0.0000000000	−1.4092000000	3.2953000000
Ti24	0.0000000000	1.4092000000	−3.2953000000
Ti25	0.0000000000	−1.4092000000	−3.2953000000
H26	0.0000000000	3.7503000000	2.3749000000
H27	0.0000000000	3.7503000000	−2.3749000000
H28	0.0000000000	−3.7503000000	2.3749000000
H29	0.0000000000	−3.7503000000	−2.3749000000
O30	0.0000000000	0.0000000000	4.4542000000
O31	0.0000000000	0.0000000000	−4.4542000000
O32	0.0000000000	2.7688000000	4.8169000000
O33	0.0000000000	2.7688000000	−4.8169000000
O34	0.0000000000	−2.7688000000	4.8169000000
O35	0.0000000000	−2.7688000000	−4.8169000000
H36	0.0000000000	3.6917000000	4.4729000000
H37	0.0000000000	3.6917000000	−4.4729000000

H38	0.0000000000	-3.6917000000	4.4729000000
H39	0.0000000000	-3.6917000000	-4.4729000000
Ti40	-3.1313000000	1.4935000000	0.0000000000
Ti41	-3.1313000000	-1.4935000000	0.0000000000
Ti42	3.1313000000	1.4935000000	0.0000000000
Ti43	3.1313000000	-1.4935000000	0.0000000000
O44	-3.2825000000	0.0000000000	1.2195000000
O45	-3.2825000000	0.0000000000	-1.2195000000
O46	3.2825000000	0.0000000000	1.2195000000
O47	3.2825000000	0.0000000000	-1.2195000000
O48	-3.1926000000	2.9663000000	1.3665000000
O49	-3.1926000000	2.9663000000	-1.3665000000
O50	-3.1926000000	-2.9663000000	1.3665000000
O51	-3.1926000000	-2.9663000000	-1.3665000000
O52	3.1926000000	2.9663000000	1.3665000000
O53	3.1926000000	2.9663000000	-1.3665000000
O54	3.1926000000	-2.9663000000	1.3665000000
O55	3.1926000000	-2.9663000000	-1.3665000000
H56	-2.5867000000	3.7011000000	1.0532000000
H57	-2.5867000000	3.7011000000	-1.0532000000
H58	-2.5867000000	-3.7011000000	1.0532000000
H59	-2.5867000000	-3.7011000000	-1.0532000000
H60	2.5867000000	3.7011000000	1.0532000000
H61	2.5867000000	3.7011000000	-1.0532000000
H62	2.5867000000	-3.7011000000	1.0532000000
H63	2.5867000000	-3.7011000000	-1.0532000000
Ti64	-3.3596000000	0.0000000000	3.1933000000
Ti65	3.3596000000	0.0000000000	3.1933000000
Ti66	-3.3596000000	0.0000000000	-3.1933000000
Ti67	3.3596000000	0.0000000000	-3.1933000000
O68	-1.8999000000	1.4480000000	3.2774000000
O69	-4.3617000000	1.5130000000	3.2956000000
O70	-1.8999000000	-1.4480000000	3.2774000000
O71	-4.3617000000	-1.5130000000	3.2956000000
O72	1.8999000000	1.4480000000	3.2774000000
O73	4.3617000000	1.5130000000	3.2956000000
O74	1.8999000000	-1.4480000000	3.2774000000
O75	4.3617000000	-1.5130000000	3.2956000000
O76	-1.8999000000	1.4480000000	-3.2774000000
O77	-4.3617000000	1.5130000000	-3.2956000000
O78	-1.8999000000	-1.4480000000	-3.2774000000
O79	-4.3617000000	-1.5130000000	-3.2956000000
O80	1.8999000000	1.4480000000	-3.2774000000
O81	4.3617000000	1.5130000000	-3.2956000000
O82	1.8999000000	-1.4480000000	-3.2774000000
O83	4.3617000000	-1.5130000000	-3.2956000000
Ti84	-3.0760000000	2.9384000000	3.3777000000
Ti85	3.0760000000	2.9384000000	3.3777000000
Ti86	-3.0760000000	2.9384000000	-3.3777000000
Ti87	3.0760000000	2.9384000000	-3.3777000000
Ti88	-3.0760000000	-2.9384000000	3.3777000000
Ti89	3.0760000000	-2.9384000000	3.3777000000
Ti90	-3.0760000000	-2.9384000000	-3.3777000000
Ti91	3.0760000000	-2.9384000000	-3.3777000000

O92	-1.7691000000	4.3237000000	3.2248000000
O93	-4.1925000000	4.1724000000	4.1863000000
O94	-1.7691000000	-4.3237000000	3.2248000000
O95	-4.1925000000	-4.1724000000	4.1863000000
O96	1.7691000000	4.3237000000	3.2248000000
O97	4.1925000000	4.1724000000	4.1863000000
O98	1.7691000000	-4.3237000000	3.2248000000
O99	4.1925000000	-4.1724000000	4.1863000000
O100	-1.7691000000	4.3237000000	-3.2248000000
O101	-4.1925000000	4.1724000000	-4.1863000000
O102	-1.7691000000	-4.3237000000	-3.2248000000
O103	-4.1925000000	-4.1724000000	-4.1863000000
O104	1.7691000000	4.3237000000	-3.2248000000
O105	4.1925000000	4.1724000000	-4.1863000000
O106	1.7691000000	-4.3237000000	-3.2248000000
O107	4.1925000000	-4.1724000000	-4.1863000000
H108	-1.9474000000	5.2735000000	3.3673000000
H109	-4.0215000000	4.9346000000	4.7716000000
H110	-1.9474000000	-5.2735000000	3.3673000000
H111	-4.0215000000	-4.9346000000	4.7716000000
H112	1.9474000000	5.2735000000	3.3673000000
H113	4.0215000000	4.9346000000	4.7716000000
H114	1.9474000000	-5.2735000000	3.3673000000
H115	4.0215000000	-4.9346000000	4.7716000000
H116	-1.9474000000	5.2735000000	-3.3673000000
H117	-4.0215000000	4.9346000000	-4.7716000000
H118	-1.9474000000	-5.2735000000	-3.3673000000
H119	-4.0215000000	-4.9346000000	-4.7716000000
H120	1.9474000000	5.2735000000	-3.3673000000
H121	4.0215000000	4.9346000000	-4.7716000000
H122	1.9474000000	-5.2735000000	-3.3673000000
H123	4.0215000000	-4.9346000000	-4.7716000000
O124	-3.1544000000	0.0000000000	5.2871000000
O125	3.1544000000	0.0000000000	5.2871000000
O126	-3.1544000000	0.0000000000	-5.2871000000
O127	3.1544000000	0.0000000000	-5.2871000000
O128	-2.4192000000	2.5599000000	5.5136000000
O129	2.4192000000	2.5599000000	5.5136000000
O130	-2.4192000000	2.5599000000	-5.5136000000
O131	2.4192000000	2.5599000000	-5.5136000000
O132	-2.4192000000	-2.5599000000	5.5136000000
O133	2.4192000000	-2.5599000000	5.5136000000
O134	-2.4192000000	-2.5599000000	-5.5136000000
O135	2.4192000000	-2.5599000000	-5.5136000000
H136	-2.7602000000	0.8540000000	5.6214000000
H137	2.7602000000	0.8540000000	5.6214000000
H138	-2.7602000000	0.8540000000	-5.6214000000
H139	2.7602000000	0.8540000000	-5.6214000000
H140	-2.7602000000	-0.8540000000	5.6214000000
H141	2.7602000000	-0.8540000000	5.6214000000
H142	-2.7602000000	-0.8540000000	-5.6214000000
H143	2.7602000000	-0.8540000000	-5.6214000000
H144	-2.7622000000	3.1470000000	6.2165000000
H145	2.7622000000	3.1470000000	6.2165000000

H146	-2.7622000000	3.1470000000	-6.2165000000
H147	2.7622000000	3.1470000000	-6.2165000000
H148	-1.3821000000	2.6320000000	5.4038000000
H149	1.3821000000	2.6320000000	5.4038000000
H150	-1.3821000000	2.6320000000	-5.4038000000
H151	1.3821000000	2.6320000000	-5.4038000000
H152	-2.7622000000	-3.1470000000	6.2165000000
H153	2.7622000000	-3.1470000000	6.2165000000
H154	-2.7622000000	-3.1470000000	-6.2165000000
H155	2.7622000000	-3.1470000000	-6.2165000000
H156	-1.3821000000	-2.6320000000	5.4038000000
H157	1.3821000000	-2.6320000000	5.4038000000
H158	-1.3821000000	-2.6320000000	-5.4038000000
H159	1.3821000000	-2.6320000000	-5.4038000000
O160	-5.2535000000	1.5970000000	0.0000000000
O161	-5.2535000000	-1.5970000000	0.0000000000
O162	5.2535000000	1.5970000000	0.0000000000
O163	5.2535000000	-1.5970000000	0.0000000000
H164	-5.7936000000	1.5408000000	0.8103000000
H165	-5.7936000000	-1.5408000000	0.8103000000
H166	5.7936000000	1.5408000000	0.8103000000
H167	5.7936000000	-1.5408000000	0.8103000000
H168	-5.7936000000	1.5408000000	-0.8103000000
H169	-5.7936000000	-1.5408000000	-0.8103000000
H170	5.7936000000	1.5408000000	-0.8103000000
H171	5.7936000000	-1.5408000000	-0.8103000000

3.13.2 444 cluster

348			
444	SolvCorr C2h, Reduced-Optimized		
O1	-5.5684678964	-3.3545618735	-4.3052940377
Ti2	-4.5394458766	-2.2337542509	-2.9813485871
O3	-5.4091719422	-3.1652314737	-1.4746294120
Ti4	-4.5840485955	-2.3067895469	0.0000000000
O5	-5.4091719422	-3.1652314737	1.4746294120
Ti6	-4.5394458766	-2.2337542509	2.9813485871
O7	-5.5684678964	-3.3545618735	4.3052940377
O8	-7.9635629369	0.4497634035	-5.8306214602
O9	-5.6707126620	-0.9476810702	-5.7544637448
Ti10	-6.9548013122	-0.0333931390	-4.4244089227
O11	-5.6024954183	1.3954974725	-4.3747551423
O12	-7.7770543915	-1.9687567127	-4.2233284669
Ti13	-4.4295182999	2.2132877674	-2.9483440640
O14	-7.8263594275	0.5452136295	-2.9419144614
O15	-5.8109018936	-0.8792739974	-2.9008626979
Ti16	-6.7594520454	0.0829483707	-1.4654102821
O17	-5.5823854922	1.5491393150	-1.4592353585
O18	-7.7838943498	-2.0076357546	-1.5908108339
Ti19	-4.3369950606	2.1776670638	0.0000000000
O20	-7.8151959528	0.4941122608	0.0000000000
O21	-5.7522279141	-0.8322633666	0.0000000000
Ti22	-6.7594520454	0.0829483707	1.4654102821
O23	-5.5823854922	1.5491393150	1.4592353585

O24	-7.7838943498	-2.0076357546	1.5908108339
Ti25	-4.4295182999	2.2132877674	2.9483440640
O26	-7.8263594275	0.5452136295	2.9419144614
O27	-5.8109018936	-0.8792739974	2.9008626979
Ti28	-6.9548013122	-0.0333931390	4.4244089227
O29	-5.6024954183	1.3954974725	4.3747551423
O30	-7.7770543915	-1.9687567127	4.2233284669
O31	-7.9635629369	0.4497634035	5.8306214602
O32	-5.6707126620	-0.9476810702	5.7544637448
O33	-5.5662788350	4.1554983040	-2.8184499650
O34	-5.6372850055	4.5574185669	0.0000000000
O35	-5.5662788350	4.1554983040	2.8184499650
O36	-0.9163043051	-7.9116572559	-4.2552986981
Ti37	-0.2079681456	-6.8856374220	-2.9388059414
O38	-0.6105877926	-7.8290224404	-1.4245225382
Ti39	-0.2117525227	-6.7072517658	0.0000000000
O40	-0.6105877926	-7.8290224404	1.4245225382
Ti41	-0.2079681456	-6.8856374220	2.9388059414
O42	-0.9163043051	-7.9116572559	4.2552986981
O43	-3.1629415067	-3.7294231310	-5.9918084653
O44	-1.5125830234	-5.8260458170	-5.6786622357
Ti45	-2.3786804028	-4.4965877112	-4.5793561817
O46	-0.8644130714	-3.3588673002	-4.4569688316
O47	-4.1975180204	-5.6082175242	-4.2774262357
Ti48	0.1063596876	-2.2634606000	-3.0351010774
O49	-3.1047050630	-3.6103735687	-3.0039509502
O50	-1.5875221600	-5.5913810302	-2.9042774680
Ti51	-2.2245827408	-4.3834512569	-1.5309178775
O52	-0.8841638332	-3.1415140449	-1.4863753351
O53	-4.2546188006	-5.5601928899	-1.6550169516
Ti54	0.0858648104	-2.1662864590	0.0000000000
O55	-3.1447126283	-3.6674752468	0.0000000000
O56	-1.6232803303	-5.5461484766	0.0000000000
Ti57	-2.2245827408	-4.3834512569	1.5309178775
O58	-0.8841638332	-3.1415140449	1.4863753351
O59	-4.2546188006	-5.5601928899	1.6550169516
Ti60	0.1063596876	-2.2634606000	3.0351010774
O61	-3.1047050630	-3.6103735687	3.0039509502
O62	-1.5875221600	-5.5913810302	2.9042774680
Ti63	-2.3786804028	-4.4965877112	4.5793561817
O64	-0.8644130714	-3.3588673002	4.4569688316
O65	-4.1975180204	-5.6082175242	4.2774262357
O66	-3.1629415067	-3.7294231310	5.9918084653
O67	-1.5125830234	-5.8260458170	5.6786622357
O68	-3.4073814568	1.0799188001	-5.7643693477
O69	-1.4965284222	-0.8269690271	-6.1410544390
Ti70	-2.2523148948	-0.1810072344	-4.6805074143
O71	-1.0325044900	1.4126216098	-4.4845862340
O72	-3.7055649774	-1.3302747264	-4.4608663717
Ti73	-0.1063596876	2.2634606000	-3.0351010774
O74	-3.2306564349	0.8850803090	-2.9355652433
O75	-1.3815643015	-0.8935677894	-3.1054330577
Ti76	-2.2147716604	-0.1365235207	-1.5700920784
O77	-0.8594483596	1.3395168431	-1.5445556124

O78	-3.5490888784	-1.4361414095	-1.5008346155
Ti79	-0.0858648104	2.1662864590	0.0000000000
O80	-3.1551444683	0.8376268416	0.0000000000
O81	-1.3326451223	-0.8366270679	0.0000000000
Ti82	-2.2147716604	-0.1365235207	1.5700920784
O83	-0.8594483596	1.3395168431	1.5445556124
O84	-3.5490888784	-1.4361414095	1.5008346155
Ti85	-0.1063596876	2.2634606000	3.0351010774
O86	-3.2306564349	0.8850803090	2.9355652433
O87	-1.3815643015	-0.8935677894	3.1054330577
Ti88	-2.2523148948	-0.1810072344	4.6805074143
O89	-1.0325044900	1.4126216098	4.4845862340
O90	-3.7055649774	-1.3302747264	4.4608663717
O91	-3.4073814568	1.0799188001	5.7643693477
O92	-1.4965284222	-0.8269690271	6.1410544390
O93	-3.1832867241	5.5175703694	-5.8958776013
O94	-1.2465236789	3.5760369594	-5.7991034084
Ti95	-2.3670163973	4.7040454077	-4.5050567664
O96	-0.8244880813	5.9062634816	-4.3916750515
O97	-3.6149545959	3.1561912836	-4.4167266027
Ti98	0.2079681456	6.8856374220	-2.9388059414
O99	-3.1047686550	5.4373019623	-2.9752601162
O100	-1.3676322078	3.6077336774	-2.9841259023
Ti101	-2.1806920060	4.5823181535	-1.4771156624
O102	-0.7840168347	5.7688606195	-1.4034804038
O103	-3.6413081277	3.1144811517	-1.4528336375
Ti104	0.2117525227	6.7072517658	0.0000000000
O105	-3.1067265081	5.4084145714	0.0000000000
O106	-1.3999022871	3.5331431502	0.0000000000
Ti107	-2.1806920060	4.5823181535	1.4771156624
O108	-0.7840168347	5.7688606195	1.4034804038
O109	-3.6413081277	3.1144811517	1.4528336375
Ti110	0.2079681456	6.8856374220	2.9388059414
O111	-3.1047686550	5.4373019623	2.9752601162
O112	-1.3676322078	3.6077336774	2.9841259023
Ti113	-2.3670163973	4.7040454077	4.5050567664
O114	-0.8244880813	5.9062634816	4.3916750515
O115	-3.6149545959	3.1561912836	4.4167266027
O116	-3.1832867241	5.5175703694	5.8958776013
O117	-1.2465236789	3.5760369594	5.7991034084
O118	1.7638050799	-7.7986906191	-2.7402653032
O119	2.2819871088	-7.9228664438	0.0000000000
O120	1.7638050799	-7.7986906191	2.7402653032
O121	1.2465236789	-3.5760369594	-5.7991034084
O122	3.1832867241	-5.5175703694	-5.8958776013
Ti123	2.3670163973	-4.7040454077	-4.5050567664
O124	3.6149545959	-3.1561912836	-4.4167266027
O125	0.8244880813	-5.9062634816	-4.3916750515
Ti126	4.4295182999	-2.2132877674	-2.9483440640
O127	1.3676322078	-3.6077336774	-2.9841259023
O128	3.1047686550	-5.4373019623	-2.9752601162
Ti129	2.1806920060	-4.5823181535	-1.4771156624
O130	3.6413081277	-3.1144811517	-1.4528336375
O131	0.7840168347	-5.7688606195	-1.4034804038

Ti132	4.3369950606	-2.1776670638	0.0000000000
O133	1.3999022871	-3.5331431502	0.0000000000
O134	3.1067265081	-5.4084145714	0.0000000000
Ti135	2.1806920060	-4.5823181535	1.4771156624
O136	3.6413081277	-3.1144811517	1.4528336375
O137	0.7840168347	-5.7688606195	1.4034804038
Ti138	4.4295182999	-2.2132877674	2.9483440640
O139	1.3676322078	-3.6077336774	2.9841259023
O140	3.1047686550	-5.4373019623	2.9752601162
Ti141	2.3670163973	-4.7040454077	4.5050567664
O142	3.6149545959	-3.1561912836	4.4167266027
O143	0.8244880813	-5.9062634816	4.3916750515
O144	1.2465236789	-3.5760369594	5.7991034084
O145	3.1832867241	-5.5175703694	5.8958776013
O146	1.4965284222	0.8269690271	-6.1410544390
O147	3.4073814568	-1.0799188001	-5.7643693477
Ti148	2.2523148948	0.1810072344	-4.6805074143
O149	3.7055649774	1.3302747264	-4.4608663717
O150	1.0325044900	-1.4126216098	-4.4845862340
Ti151	4.5394458766	2.2337542509	-2.9813485871
O152	1.3815643015	0.8935677894	-3.1054330577
O153	3.2306564349	-0.8850803090	-2.9355652433
Ti154	2.2147716604	0.1365235207	-1.5700920784
O155	3.5490888784	1.4361414095	-1.5008346155
O156	0.8594483596	-1.3395168431	-1.5445556124
Ti157	4.5840485955	2.3067895469	0.0000000000
O158	1.3326451223	0.8366270679	0.0000000000
O159	3.1551444683	-0.8376268416	0.0000000000
Ti160	2.2147716604	0.1365235207	1.5700920784
O161	3.5490888784	1.4361414095	1.5008346155
O162	0.8594483596	-1.3395168431	1.5445556124
Ti163	4.5394458766	2.2337542509	2.9813485871
O164	1.3815643015	0.8935677894	3.1054330577
O165	3.2306564349	-0.8850803090	2.9355652433
Ti166	2.2523148948	0.1810072344	4.6805074143
O167	3.7055649774	1.3302747264	4.4608663717
O168	1.0325044900	-1.4126216098	4.4845862340
O169	1.4965284222	0.8269690271	6.1410544390
O170	3.4073814568	-1.0799188001	5.7643693477
O171	1.5125830234	5.8260458170	-5.6786622357
O172	3.1629415067	3.7294231310	-5.9918084653
Ti173	2.3786804028	4.4965877112	-4.5793561817
O174	4.1975180204	5.6082175242	-4.2774262357
O175	0.8644130714	3.3588673002	-4.4569688316
O176	1.5875221600	5.5913810302	-2.9042774680
O177	3.1047050630	3.6103735687	-3.0039509502
Ti178	2.2245827408	4.3834512569	-1.5309178775
O179	4.2546188006	5.5601928899	-1.6550169516
O180	0.8841638332	3.1415140449	-1.4863753351
O181	1.6232803303	5.5461484766	0.0000000000
O182	3.1447126283	3.6674752468	0.0000000000
Ti183	2.2245827408	4.3834512569	1.5309178775
O184	4.2546188006	5.5601928899	1.6550169516
O185	0.8841638332	3.1415140449	1.4863753351

O186	1.5875221600	5.5913810302	2.9042774680
O187	3.1047050630	3.6103735687	3.0039509502
Ti188	2.3786804028	4.4965877112	4.5793561817
O189	4.1975180204	5.6082175242	4.2774262357
O190	0.8644130714	3.3588673002	4.4569688316
O191	1.5125830234	5.8260458170	5.6786622357
O192	3.1629415067	3.7294231310	5.9918084653
O193	5.5662788350	-4.1554983040	-2.8184499650
O194	5.6372850055	-4.5574185669	0.0000000000
O195	5.5662788350	-4.1554983040	2.8184499650
O196	5.6707126620	0.9476810702	-5.7544637448
O197	7.9635629369	-0.4497634035	-5.8306214602
Ti198	6.9548013122	0.0333931390	-4.4244089227
O199	7.7770543915	1.9687567127	-4.2233284669
O200	5.6024954183	-1.3954974725	-4.3747551423
O201	5.8109018936	0.8792739974	-2.9008626979
O202	7.8263594275	-0.5452136295	-2.9419144614
Ti203	6.7594520454	-0.0829483707	-1.4654102821
O204	7.7838943498	2.0076357546	-1.5908108339
O205	5.5823854922	-1.5491393150	-1.4592353585
O206	5.7522279141	0.8322633666	0.0000000000
O207	7.8151959528	-0.4941122608	0.0000000000
Ti208	6.7594520454	-0.0829483707	1.4654102821
O209	7.7838943498	2.0076357546	1.5908108339
O210	5.5823854922	-1.5491393150	1.4592353585
O211	5.8109018936	0.8792739974	2.9008626979
O212	7.8263594275	-0.5452136295	2.9419144614
Ti213	6.9548013122	0.0333931390	4.4244089227
O214	7.7770543915	1.9687567127	4.2233284669
O215	5.6024954183	-1.3954974725	4.3747551423
O216	5.6707126620	0.9476810702	5.7544637448
O217	7.9635629369	-0.4497634035	5.8306214602
O218	5.5684678964	3.3545618735	-4.3052940377
O219	5.4091719422	3.1652314737	-1.4746294120
O220	5.4091719422	3.1652314737	1.4746294120
O221	5.5684678964	3.3545618735	4.3052940377
O222	0.9163043051	7.9116572559	-4.2552986981
O223	-1.7638050799	7.7986906191	-2.7402653032
O224	0.6105877926	7.8290224404	-1.4245225382
O225	-2.2819871088	7.9228664438	0.0000000000
O226	0.6105877926	7.8290224404	1.4245225382
O227	-1.7638050799	7.7986906191	2.7402653032
O228	0.9163043051	7.9116572559	4.2552986981
H229	-8.2712399715	0.3039616773	6.7437192840
H230	-3.2900677721	5.6800016056	6.8502692180
H231	-5.7191315130	-0.8158270730	6.7174830322
H232	-1.3757011234	3.7407476991	6.7512027440
H233	-3.3757282451	1.0053003684	6.7366180448
H234	1.6808434550	5.8355487975	6.6419984480
H235	3.0962612434	3.1224946986	6.7490115890
H236	-0.9298375534	-1.0009734178	6.9012374231
H237	0.9298375534	1.0009734178	6.9012374231
H238	-3.0962612434	-3.1224946986	6.7490115890
H239	3.3757282451	-1.0053003684	6.7366180448

H240	-1.6808434550	-5.8355487975	6.6419984480
H241	5.7191315130	0.8158270730	6.7174830322
H242	1.3757011234	-3.7407476991	6.7512027440
H243	8.2712399715	-0.3039616773	6.7437192840
H244	3.2900677721	-5.6800016056	6.8502692180
H245	5.2943381014	3.1633757276	5.2299699649
H246	1.2794284512	7.3893634463	5.0332670391
H247	0.1415494991	3.5125544464	5.1815177130
H248	-1.2066909125	2.1158430146	5.2047403519
H249	-4.6634309439	-1.1183440673	5.2935445132
H250	-5.2943381014	-3.1633757276	5.2299699649
H251	-4.9389612402	1.2386338862	5.1289245281
H252	-3.4468695608	2.4473358687	5.1591160428
H253	-0.1629346174	5.8356037523	5.1368844801
H254	4.9389612402	-1.2386338862	5.1289245281
H255	3.4468695608	-2.4473358687	5.1591160428
H256	0.1629346174	-5.8356037523	5.1368844801
H257	-1.2794284512	-7.3893634463	5.0332670391
H258	1.2066909125	-2.1158430146	5.2047403519
H259	-0.1415494991	-3.5125544464	5.1815177130
H260	4.6634309439	1.1183440673	5.2935445132
H261	-3.2900677721	5.6800016056	-6.8502692180
H262	-8.2712399715	0.3039616773	-6.7437192840
H263	-5.7191315130	-0.8158270730	-6.7174830322
H264	-1.3757011234	3.7407476991	-6.7512027440
H265	-3.3757282451	1.0053003684	-6.7366180448
H266	1.6808434550	5.8355487975	-6.6419984480
H267	3.0962612434	3.1224946986	-6.7490115890
H268	-0.9298375534	-1.0009734178	-6.9012374231
H269	-3.0962612434	-3.1224946986	-6.7490115890
H270	-1.6808434550	-5.8355487975	-6.6419984480
H271	5.7191315130	0.8158270730	-6.7174830322
H272	3.3757282451	-1.0053003684	-6.7366180448
H273	0.9298375534	1.0009734178	-6.9012374231
H274	1.3757011234	-3.7407476991	-6.7512027440
H275	3.2900677721	-5.6800016056	-6.8502692180
H276	8.2712399715	-0.3039616773	-6.7437192840
H277	1.2794284512	7.3893634463	-5.0332670391
H278	-0.1629346174	5.8356037523	-5.1368844801
H279	0.1415494991	3.5125544464	-5.1815177130
H280	-1.2066909125	2.1158430146	-5.2047403519
H281	-4.6634309439	-1.1183440673	-5.2935445132
H282	-5.2943381014	-3.1633757276	-5.2299699649
H283	1.2066909125	-2.1158430146	-5.2047403519
H284	-0.1415494991	-3.5125544464	-5.1815177130
H285	5.2943381014	3.1633757276	-5.2299699649
H286	4.6634309439	1.1183440673	-5.2935445132
H287	4.9389612402	-1.2386338862	-5.1289245281
H288	3.4468695608	-2.4473358687	-5.1591160428
H289	0.1629346174	-5.8356037523	-5.1368844801
H290	-1.2794284512	-7.3893634463	-5.0332670391
H291	-3.4468695608	2.4473358687	-5.1591160428
H292	-4.9389612402	1.2386338862	-5.1289245281
H293	6.3939329159	-5.1819565650	0.0000000000

H294	4.7494635719	-5.0496101222	0.0000000000
H295	5.8242321302	-4.2960932851	-1.8698040988
H296	4.8453368328	-4.8169039967	-3.0168223267
H297	5.8242321302	-4.2960932851	1.8698040988
H298	4.8453368328	-4.8169039967	3.0168223267
H299	-2.9243272244	8.6638711707	0.0000000000
H300	-2.7577375408	7.0219307726	0.0000000000
H301	-1.9324018869	8.0653478319	-1.7960510765
H302	-2.4344143031	7.0955335843	-2.9754277172
H303	-1.9324018869	8.0653478319	1.7960510765
H304	-2.4344143031	7.0955335843	2.9754277172
H305	2.7577375408	-7.0219307726	0.0000000000
H306	2.9243272244	-8.6638711707	0.0000000000
H307	2.4344143031	-7.0955335843	-2.9754277172
H308	1.9324018869	-8.0653478319	-1.7960510765
H309	2.4344143031	-7.0955335843	2.9754277172
H310	1.9324018869	-8.0653478319	1.7960510765
H311	-4.7494635719	5.0496101222	0.0000000000
H312	-6.3939329159	5.1819565650	0.0000000000
H313	-4.8453368328	4.8169039967	-3.0168223267
H314	-5.8242321302	4.2960932851	-1.8698040988
H315	-4.8453368328	4.8169039967	3.0168223267
H316	-5.8242321302	4.2960932851	1.8698040988
H317	4.4902854056	6.3358335575	-1.1121319770
H318	4.8944974998	4.7825230734	-1.5257957069
H319	4.2122060536	5.9003531930	-3.3162562661
H320	4.9139884663	4.8882094866	-4.3485538012
H321	4.4902854056	6.3358335575	1.1121319770
H322	4.8944974998	4.7825230734	1.5257957069
H323	4.2122060536	5.9003531930	3.3162562661
H324	4.9139884663	4.8882094866	4.3485538012
H325	8.5642674817	2.2970797335	-1.0818522023
H326	6.9891364499	2.6371069020	-1.4859549579
H327	8.0626736528	2.0564229612	-3.2638666774
H328	7.0227056523	2.6485426034	-4.3574690304
H329	8.5642674817	2.2970797335	1.0818522023
H330	6.9891364499	2.6371069020	1.4859549579
H331	8.0626736528	2.0564229612	3.2638666774
H332	7.0227056523	2.6485426034	4.3574690304
H333	-8.5642674817	-2.2970797335	-1.0818522023
H334	-6.9891364499	-2.6371069020	-1.4859549579
H335	-8.0626736528	-2.0564229612	-3.2638666774
H336	-7.0227056523	-2.6485426034	-4.3574690304
H337	-8.5642674817	-2.2970797335	1.0818522023
H338	-6.9891364499	-2.6371069020	1.4859549579
H339	-8.0626736528	-2.0564229612	3.2638666774
H340	-7.0227056523	-2.6485426034	4.3574690304
H341	-4.4902854056	-6.3358335575	-1.1121319770
H342	-4.8944974998	-4.7825230734	-1.5257957069
H343	-4.2122060536	-5.9003531930	-3.3162562661
H344	-4.9139884663	-4.8882094866	-4.3485538012
H345	-4.4902854056	-6.3358335575	1.1121319770
H346	-4.8944974998	-4.7825230734	1.5257957069
H347	-4.2122060536	-5.9003531930	3.3162562661

H348

−4.9139884663

−4.8882094866

4.3485538012

3.13.3 555 cluster

The geometry is identical to that of 555 reduced cluster in water.

4 Summary of absolute energies

Table S1: Summary of absolute energies for all 555 clusters

cluster	Li ⁺	e [−]	sol	SCFE * [hartree]
(5,5,5)	/	NO	v	-17166.83035
(5,5,5)	/	YES	v	-17166.93832
(5,5,5)	YES,I	NO	v	-17174.27523
(5,5,5)	YES,I	YES	v	-17174.43202
(5,5,5)	YES,O	NO	v	-17174.29303
(5,5,5)	YES,O	YES	v	-17174.44126
(5,5,5)	/	NO	w	-17167.24082
(5,5,5)	/	YES	w	-17167.37885
(5,5,5)	YES,I	NO	w	-17174.70999
(5,5,5)	YES,I,GS1	YES	w	-17174.84014
(5,5,5)	YES,I,GS2	YES	w	-17174.84168
(5,5,5)	YES,I,TS1	YES	w	-17174.83574
(5,5,5)	YES,O	NO	w	-17174.72093
(5,5,5)	YES,O,GS3	YES	w	-17174.84713
(5,5,5)	YES,O,TS2	YES	w	-17174.83802

* calculations are performed at ROB3LYP/LACVP level

References

- (1) *Jaguar*, version 7.7, Schrödinger, LLC, New York, NY, 2010.
- (2) Langlois, J.-M.; Yamasaki, T.; Muller, R. P.; Goddard, W. A. I. *The Journal of Physical Chemistry* **1994**, *98*, 13498–13505.

- (3) Van Lenthe, J. H.; Zwaans, R.; Van Dam, H. J. J.; Guest, M. F. *Journal of Computational Chemistry* **2006**, 27, 926–932.
- (4) Vacek, G.; Perry, J. K.; Langlois, J.-M. *Chemical Physics Letters* **1999**, 310, 189 – 194.
- (5) Pipek, J.; Mezey, P. G. *The Journal of Chemical Physics* **1989**, 90, 4916–4926.
- (6) Culot, P.; Dive, G.; Nguyen, V. H.; Ghuysen, J. M. *Theoretical Chemistry Accounts: Theory, Computation, and Modeling (Theoretica Chimica Acta)* **1992**, 82, 189–205, 10.1007/BF01113251.