Supporting Information

Reactivity of Superheavy Elements Cn and Fl and of their Oxides in Comparison with Homologous Species of Hg and Pb, respectively, towards Gold and Hydroxylated Quartz Surfaces

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Coordinates of atoms (converged geometry)

(4x4)HgO/Au(111)

66 atoms

Au	-0.021887	0.087036	0.207865
Au	1.440258	0.886070	-2.252124
Au	-1.443215	-0.807447	-4.593772
Au	0.002608	0.002129	-7.057811
Au	1.435577	2.583173	0.220665
Au	2.887471	3.376241	-2.219358
Au	-0.005951	1.689276	-4.594001
Au	1.443744	2.498564	-7.056026
Au	-2.884863	-4.917466	0.255902
Au	-1.442368	-4.114178	-2.223601
Au	1.442257	4.184464	-4.582085
Au	-2.879664	-4.990739	-7.061380
Au	-1.454153	-2.427190	0.215529
Au	-0.003360	-1.617129	-2.246950
Au	-2.880647	-3.303187	-4.582255
Au	-1.438528	-2.494305	-7.059596
Au	2.909944	0.091477	0.190406
Au	4.318539	0.877233	-2.214879
Au	1.448018	-0.804150	-4.602262
Au	2.885152	0.002286	-7.056404
Au	4.327750	2.576881	0.250835
Au	5.768463	3.375190	-2.226040
Au	2.887856	1.692588	-4.592539
Au	4.326288	2.498720	-7.054620
Au	-0.005960	-4.925632	0.242256
Au	1.439336	-4.101954	-2.206648
Au	4.321409	4.187350	-4.583519
Au	0.002880	-4.990583	-7.059974
Au	1.439538	-2.444548	0.219197
Au	2.886290	-1.617927	-2.249620
Au	0.000720	-3.306193	-4.591666

Au	1.444016	-2.494149	-7.058189
Au	-5.759191	0.077043	0.249866
Au	-4.324668	0.885880	-2.225731
Au	4.330756	-0.806190	-4.594176
Au	-5.762480	0.001817	-7.060623
Au	-4.324182	2.571099	0.264178
Au	-2.887107	3.375710	-2.221959
Au	5.766907	1.689315	-4.584532
Au	-4.321344	2.498251	-7.058839
Au	-8.648687	-4.923467	0.247648
Au	-7.207194	-4.115714	-2.223944
Au	7.208474	4.189520	-4.583675
Au	-8.644751	-4.991052	-7.064193
Au	-7.198830	-2.431620	0.218982
Au	-5.761850	-1.611414	-2.219514
Au	2.880317	-3.308414	-4.593096
Au	-7.203615	-2.494618	-7.062408
Au	-2.894607	0.074978	0.244038
Au	-1.435868	0.875202	-2.207713
Au	-4.322271	-0.809518	-4.583368
Au	-2.879936	0.001973	-7.059217
Au	-1.448764	2.576005	0.249097
Au	-0.004167	3.377372	-2.225043
Au	-2.878436	1.687917	-4.581652
Au	-1.438800	2.498407	-7.057432
Au	-5.767116	-4.918369	0.265037
Au	-4.328093	-4.113975	-2.211844
Au	-1.438524	4.187208	-4.583803
Au	-5.762208	-4.990896	-7.062787
Au	-4.325745	-2.421018	0.260313
Au	-2.885131	-1.614036	-2.223650
Au	-5.766277	-3.302174	-4.582867
Au	-4.321072	-2.494461	-7.061002
Hg	1.463337	-0.721663	2.500024
O	1.503819	-0.691206	4.452456
VEC1	11.530177	0.000000	0.000000

VEC2 5.765088 9.985426 0.000000

(4x4)CnO/Au(111)

66 atoms

Au	-0.020732	0.062268	0.214846
Au	1.441629	0.876060	-2.248230
Au	-1.441880	-0.809868	-4.593281
Au	0.002608	0.002129	-7.057811
Au	1.436586	2.569950	0.210250
Au	2.888605	3.368213	-2.223137
Au	-0.004581	1.685227	-4.590099
Au	1.443744	2.498564	-7.056026
Au	-2.884289	-4.938769	0.251988
Au	-1.442603	-4.125749	-2.231895
Au	1.443774	4.181626	-4.584244
Au	-2.879664	-4.990739	-7.061380
Au	-1.462033	-2.450223	0.198988
Au	-0.004103	-1.625608	-2.247167
Au	-2.881420	-3.305271	-4.585317
Au	-1.438528	-2.494305	-7.059596
Au	2.900629	0.066158	0.205645
Au	4.314678	0.865700	-2.207226
Au	1.449296	-0.805480	-4.600356
Au	2.885152	0.002286	-7.056404
Au	4.325537	2.551969	0.246441
Au	5.768418	3.362274	-2.230725
Au	2.888338	1.690062	-4.589221
Au	4.326288	2.498720	-7.054620
Au	-0.009404	-4.951272	0.235310
Au	1.440933	-4.112821	-2.206033
Au	4.322963	4.185380	-4.586351
Au	0.002880	-4.990583	-7.059974
Au	1.435474	-2.467219	0.201953
Au	2.887114	-1.626460	-2.250360
Au	-0.000059	-3.306567	-4.592768
Au	1.444016	-2.494149	-7.058189

Au	-5.763463	0.058002	0.247411
Au	-4.326313	0.876440	-2.229555
Au	4.330406	-0.808482	-4.593204
Au	-5.762480	0.001817	-7.060623
Au	-4.321562	2.551687	0.258930
Au	-2.884254	3.366221	-2.224489
Au	5.766569	1.686109	-4.584012
Au	-4.321344	2.498251	-7.058839
Au	-8.644241	-4.946503	0.245344
Au	-7.205797	-4.125590	-2.230345
Au	7.209516	4.189471	-4.583812
Au	-8.644751	-4.991052	-7.064193
Au	-7.193663	-2.452038	0.207513
Au	-5.761746	-1.620045	-2.224693
Au	2.880805	-3.309994	-4.594006
Au	-7.203615	-2.494618	-7.062408
Au	-2.895445	0.055752	0.238909
Au	-1.434322	0.866718	-2.200592
Au	-4.322303	-0.811053	-4.587376
Au	-2.879936	0.001973	-7.059217
Au	-1.444002	2.555170	0.249624
Au	-0.003171	3.370486	-2.229064
Au	-2.875393	1.685501	-4.580502
Au	-1.438800	2.498407	-7.057432
Au	-5.764195	-4.936869	0.260632
Au	-4.326966	-4.122631	-2.214367
Au	-1.436994	4.185311	-4.586936
Au	-5.762208	-4.990896	-7.062787
Au	-4.326662	-2.439406	0.256417
Au	-2.887721	-1.622208	-2.231327
Au	-5.765986	-3.304011	-4.585427
Au	-4.321072	-2.494461	-7.061002
Cn	1.389307	-0.848539	2.619222
O	1.452629	-0.805390	4.582249
VEC1	11.530177	0.000000	0.000000
VEC2	5.765088	9.985426	0.000000

(4x)PbO/Au(111)

66 atoms

Au	-0.04040263119409	0.02715052259217	0.07561670305514
Au	1.43821383823081	0.84689561654586	-2.33319167344574
Au	-1.44127064208228	-0.82692411088840	-4.71079472336724
Au	0.00640328362484	-0.00478863670543	-7.19031373486933
Au	1.43760293787144	2.55607651162998	0.10728893670465
Au	2.88635310880850	3.34079990289714	-2.33332887385549
Au	0.01796351217818	1.66077762183955	-4.69746390171212
Au	1.45049528366271	2.48797436713964	-7.16097952190622
Au	-2.87293570038682	-4.94837740893211	0.13403691930292
Au	-1.43786638807691	-4.13875081052312	-2.33646852537391
Au	1.44929445905341	4.16462868151756	-4.68018200552574
Au	-2.87406825541942	-4.99817631581491	-7.15298707739089
Au	-1.43884198593830	-2.46596087506678	0.11006460695141
Au	0.00129107752953	-1.64998620875017	-2.38699502393021
Au	-2.87446308309224	-3.32360856770620	-4.69537068086206
Au	-1.43398458339889	-2.50131127628297	-7.17575299641572
Au	2.90327577102954	0.04318192085134	0.09465144956125
Au	4.30945633556566	0.83797053035521	-2.30776180620552
Au	1.44670370416491	-0.82405274217715	-4.72679078315787
Au	2.88971520158129	-0.00542960295285	-7.18551539989784
Au	4.34221895801218	2.54928918117456	0.12193311908889
Au	5.77028853382167	3.34010444231070	-2.33129620318277
Au	2.89176249287288	1.67187848423796	-4.69703329567691
Au	4.33533638301354	2.48909464191034	-7.16128193332270
Au	0.00740522829332	-4.97974011955803	0.14476969315081
Au	1.44523658106130	-4.15908711403500	-2.37381038692591
Au	4.33255909671415	4.16690808010754	-4.68446925413272
Au	0.00167128181833	-5.00304326454343	-7.15439907595917
Au	1.44471934298226	-2.53064928485864	0.00022377116616
Au	2.88870467756727	-1.64180142799215	-2.35299310808816
Au	0.00235308686396	-3.33180078511002	-4.71928791847400
Au	1.44899968752270	-2.50363682693124	-7.18933731615493
Au	-5.73288382106560	0.02627929818940	0.12822438450430
Au	-4.31977897577912	0.85229831149562	-2.32525809481062
Au	4.33437832879785	-0.82362473808968	-4.70798423352748
Au	-5.75677800022909	-0.00338729022881	-7.16480550584956

Au	-4.31476640071987	2.52612446635714	0.15900184355782
Au	-2.88059237008876	3.34411440192421	-2.32392403555065
Au	5.75749865581805	1.66068111354873	-4.67249927029521
Au	-4.31701351856898	2.48445560500998	-7.13582380593644
Au	-8.63250895085246	-4.97813882070726	0.14103650131251
Au	-7.20309961492033	-4.14602276386929	-2.33703755538870
Au	7.21522316788135	4.15324133597886	-4.69626914610810
Au	-8.63683006167040	-5.00038572297901	-7.13532899609477
Au	-7.18231353064483	-2.48964851069464	0.10513064832991
Au	-5.76583423595104	-1.64169218804560	-2.32900874867720
Au	2.88614766298102	-3.30721491380115	-4.71043539899952
Au	-7.19896131597915	-2.50024745778104	-7.17014595264609
Au	-2.88344925764645	0.03902101815242	0.16111010705174
Au	-1.44250255008972	0.85524311034178	-2.34686065425228
Au	-4.31595950037890	-0.82772908569233	-4.68422371846789
Au	-2.87875921521535	-0.01147982177434	-7.15887880375905
Au	-1.43744976830849	2.52776783364069	0.14432346855341
Au	-0.00092024559928	3.35003234939211	-2.33006212276865
Au	-2.87914087147142	1.66442396891700	-4.68879628596606
Au	-1.43339923387085	2.49333276303433	-7.13076222656311
Au	-5.75589847370668	-4.96223675701011	0.16621362626072
Au	-4.31873414881058	-4.14034295262420	-2.32559741686474
Au	-1.43870318504620	4.16375998909529	-4.67999804350211
Au	-5.75474189660506	-4.99802390416717	-7.13356354634891
Au	-4.30783463086648	-2.46762935070776	0.13645820205198
Au	-2.88160756196228	-1.64319392834775	-2.33235160904478
Au	-5.76106695492489	-3.31853186945312	-4.68049436686467
Au	-4.31651024476018	-2.50371746442800	-7.14836797732182
Pb	1.09464408247062	-1.31345903471731	2.61448449790964
O	2.70475133352821	-0.00075301623995	2.22938401692834
VEC1	11.53017660000000	0.00000000000000	0.00000000000000
VEC2	5.76508831000000	9.98542585000000	0.00000000000000

(4x4)FlO/A(111)

66 atoms

Au	-0.057092	0.128050	0.110694
Au	1.447517	0.885879	-2.224519

Au	-1.456405	-0.802038	-4.611503
Au	0.002608	0.002129	-7.057811
Au	1.430409	2.627948	0.209858
Au	2.882266	3.377281	-2.228162
Au	0.014712	1.685865	-4.595056
Au	1.443744	2.498564	-7.056026
Au	-2.879984	-4.878057	0.230531
Au	-1.447912	-4.104760	-2.225614
Au	1.440953	4.191629	-4.585686
Au	-2.879664	-4.990739	-7.061380
Au	-1.438667	-2.391180	0.237277
Au	-0.014387	-1.602982	-2.288750
Au	-2.886900	-3.296893	-4.593794
Au	-1.438528	-2.494305	-7.059596
Au	2.892265	0.111611	0.252960
Au	4.296289	0.876577	-2.183414
Au	1.447043	-0.796396	-4.605015
Au	2.885152	0.002286	-7.056404
Au	4.332599	2.623149	0.232291
Au	5.761778	3.386298	-2.229189
Au	2.888346	1.703184	-4.590522
Au	4.326288	2.498720	-7.054620
Au	0.003318	-4.903952	0.265976
Au	1.439631	-4.117826	-2.262895
Au	4.324897	4.196005	-4.584490
Au	0.002880	-4.990583	-7.059974
Au	1.421508	-2.452786	0.122500
Au	2.877473	-1.612256	-2.233238
Au	-0.008712	-3.301768	-4.606119
Au	1.444016	-2.494149	-7.058189
Au	-5.736899	0.102238	0.228161
Au	-4.331834	0.895966	-2.232828
Au	4.331971	-0.799048	-4.590712
Au	-5.762480	0.001817	-7.060623
Au	-4.324191	2.598833	0.252776
Au	-2.888398	3.385667	-2.237645
Au	5.752686	1.685138	-4.567973
Au	-4.321344	2.498251	-7.058839

Au	-8.643378	-4.904367	0.230598
Au	-7.207347	-4.109360	-2.237141
Au	7.201799	4.189114	-4.602683
Au	-8.644751	-4.991052	-7.064193
Au	-7.184838	-2.414333	0.209714
Au	-5.771668	-1.599916	-2.232249
Au	2.883903	-3.286012	-4.604023
Au	-7.203615	-2.494618	-7.062408
Au	-2.890518	0.111126	0.260201
Au	-1.461033	0.902222	-2.270077
Au	-4.322255	-0.802430	-4.588170
Au	-2.879936	0.001973	-7.059217
Au	-1.446470	2.609750	0.240913
Au	-0.005951	3.385261	-2.240732
Au	-2.890551	1.696724	-4.606920
Au	-1.438800	2.498407	-7.057432
Au	-5.763167	-4.888092	0.272076
Au	-4.327619	-4.105939	-2.222490
Au	-1.448597	4.186169	-4.598950
Au	-5.762208	-4.990896	-7.062787
Au	-4.309200	-2.394888	0.239348
Au	-2.886977	-1.608691	-2.229947
Au	-5.766231	-3.300363	-4.585028
Au	-4.321072	-2.494461	-7.061002
Fl	0.735462	-1.056748	2.806577
O	2.764452	-0.121671	2.343860
VEC1	11.530177	0.000000	0.000000
VEC2	5.765088	9.985426	0.000000

(4x4)HgO/SiO2-2OH

322 atoms

Si	10.13011045	4.06102004	-7.19575773
Si	12.60503670	8.30152355	-7.18500472
Si	-14.27950806	-8.38365521	-8.97589976
Si	-11.83667296	-4.17357344	-8.96631273
Si	-9.42488782	0.08012452	-8.96746207
Si	-6.96164243	4.31748857	-8.97135107
Si	-9.38057605	-8.40392359	-8.98644381

Si	-6.94321024	-4.15216800	-8.98391117
Si	-4.51151426	0.08820457	-8.99103413
Si	-2.08472048	4.37961474	-9.03501429
Si	-4.48936095	-8.39462887	-8.98640611
Si	-2.03595162	-4.14019312	-8.96290700
Si	0.40014021	0.14599857	-8.92171781
Si	2.87220547	4.24115018	-9.02628228
Si	0.37854314	-8.41932963	-8.97275741
Si	2.89618118	-4.21605581	-8.98818768
Si	5.28502344	0.21649567	-9.01102321
Si	7.67634789	4.26259641	-8.98202895
O	-11.92549963	-5.13892364	-4.81053863
O	-9.49532344	-0.88714048	-4.82379714
O	-7.04260081	3.34368053	-4.84223238
O	-4.61074027	7.58105985	-4.84141592
O	-7.04253324	-5.12816802	-4.82976530
O	-4.59078420	-0.87674521	-4.81901583
O	-2.11926743	3.39706019	-4.81388697
O	0.29462172	7.57353963	-4.83676426
O	-2.13329889	-5.12934270	-4.84089317
O	0.32594112	-0.89101632	-4.85196329
O	2.69829974	3.29132588	-4.83381900
O	5.18373060	7.58823634	-4.81051860
O	2.73494926	-5.15154051	-4.83243497
O	5.16511180	-0.93422124	-4.82516756
O	7.61817835	3.33755736	-4.81822071
O	10.05889025	7.57096220	-4.83406278
O	-10.07651841	-5.78312955	-1.25271772
O	-7.64418690	-1.53862921	-1.24985006
O	-5.20971570	2.70675901	-1.25801514
O	-2.74784252	6.92929310	-1.24958348
O	-5.20063908	-5.77647025	-1.27489951
O	-2.75135943	-1.54788511	-1.27014098
O	-0.31731084	2.70484679	-1.25452241
O	2.15425305	6.93383472	-1.25133299
O	-0.32813572	-5.79913344	-1.25089900
O	2.13707605	-1.55321888	-1.25326431
O	4.57315072	2.68721509	-1.26514087

O	7.02188158	6.92782093	-1.26666049
O	4.59481132	-5.81012019	-1.23471051
O	7.02213262	-1.55497379	-1.25920939
O	9.46885596	2.67720267	-1.25658164
O	11.91976927	6.90467016	-1.26384204
O	-12.84289809	-8.05453857	-3.05991881
O	-10.39374292	-3.79394871	-3.04166568
O	-7.95643115	0.44047974	-3.04949652
O	-5.52061393	4.68789999	-3.06311498
O	-7.93516272	-8.05894720	-3.07037867
O	-5.49724755	-3.78523652	-3.07199297
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O	4.27892179	-3.84512955	-3.04914039
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O	9.17061705	4.66554812	-3.05303572
O	-11.90279555	-7.52215272	-0.59607579
O	-9.45754274	-3.28133675	-0.57265224
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O	-7.03246601	-7.50366801	-0.59799926
O	-4.57451062	-3.27747156	-0.59890464
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O	0.35175009	5.18859527	-0.54953339
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O	0.32500851	-3.30000706	-0.58790054
O	2.75419423	0.95226222	-0.58833729
O	5.16889536	5.20763714	-0.62542353
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O	5.20292155	-3.29430559	-0.58728438
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O	-10.06998888	-6.89878281	-4.13508911

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Si	-2.12277492	-4.05940083	-3.60067771
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O	7.45977687	2.97584704	-9.99451471
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O	1.96491831	-0.03928365	-8.52697601
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O	1.95268271	-8.26662335	-8.52493367
O	4.45577843	-4.07611685	-8.50931347
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O	-9.52998813	-3.21885949	-6.03570406
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O	2.70079069	0.99883909	-6.11157220
O	5.13786347	5.24644455	-5.98823237
O	2.70333831	-7.47955254	-6.04318165
O	5.17039861	-3.26482748	-6.02459100
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O	10.00553381	5.25996821	-6.07700020
O	-9.61810145	-6.92734015	-9.67024756
O	-7.18892160	-2.69259588	-9.68777812
O	-4.84134520	1.47983363	-9.76963625
O	-2.24763168	5.94909886	-9.52405239
O	-4.72867260	-6.91316459	-9.65927225
O	-2.23398938	-2.63240988	-9.63900761
O	0.27158674	1.50777407	-9.78736574
O	2.56025023	5.65222920	-9.81654457
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O	2.57725505	-2.76931184	-9.73563649
O	4.97755993	1.60217179	-9.71049697
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O	5.03636332	-6.90722583	-9.64710114
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O	9.83489087	1.52151591	-9.67844244
O	12.35556075	5.78052254	-9.66824790
O	-7.84302028	-4.51676190	-7.65646226
O	-5.42789555	-0.31011911	-7.68927693
O	-2.94736249	3.92799519	-7.69259619
O	-0.49797697	8.20919255	-7.65064374
O	-2.94614594	-4.47884250	-7.64794734
O	-0.53627519	-0.15812025	-7.62730596
O	1.92863150	3.96870211	-7.69104098
O	4.39965906	8.19351330	-7.65601949
O	1.96221034	-4.54221957	-7.68062408
O	4.42994263	-0.33793465	-7.68726190
O	6.82722650	3.97606399	-7.60155248
O	9.27459029	8.16109718	-7.64162198
O	6.86195853	-4.58065483	-7.63083156
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O	14.15846633	8.16391276	-7.67157333
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Si	1.28418540	-2.11086239	-5.36995497
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Si	6.13448171	6.38133861	-5.36835566
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Si	-9.40121604	-4.39060288	-7.17632307
Si	-6.97823925	-0.14882358	-7.19246507
Si	-4.49334233	4.07272846	-7.19187567
Si	-2.05459824	8.32564844	-7.17235610
Si	-4.51257775	-4.37152243	-7.17255982
Si	-2.10615451	-0.06687098	-7.15369528
Si	0.37219999	4.08771383	-7.23105164
Si	2.83920384	8.32041238	-7.18402270
Si	0.41130042	-4.40455237	-7.18421455
Si	2.89011936	-0.23360988	-7.17575292
Si	5.26005984	4.09639560	-7.15799834
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Si	5.30751375	-4.44560077	-7.14909867
Si	7.71047631	-0.17616904	-7.16369200
H	-7.95795163	2.57706550	-9.97153633
H	-3.12061488	2.69794288	-10.07945028
H	1.30437599	-2.08067037	-14.04694575
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H	9.17126464	6.77622075	-9.95447889
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H	-0.62426659	6.81144062	-9.92941273
H	-5.45125680	6.81435453	-9.98599900
H	-10.36259020	-1.69714120	-9.94845486
H	-5.35425447	-1.74282112	-9.97320575
H	-0.96802564	-1.68508062	-9.74275516
H	5.13894584	-0.84057038	-10.98144090
H	-12.81142212	-5.91903344	-9.97282128
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H	3.38078695	-2.19430311	-9.76605692
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H	8.91508917	1.85912281	-9.83374726
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(4x4)CnO/SiO_2-2OH

322 atoms

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Si	-11.85658070	-4.22276380	-8.99934339
Si	-9.38987389	0.05320655	-9.00361189
Si	-6.95088252	4.29476311	-9.00533458
Si	-9.40584043	-8.43072483	-9.00502499
Si	-6.94454919	-4.19054954	-9.01059229
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Si	-2.07863533	4.29185072	-9.01619472
Si	-4.49132385	-8.42016822	-9.01236532
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Si	0.39754321	-8.41863174	-9.00263631
Si	2.84776389	-4.17403760	-8.97484569
Si	5.25917491	0.11364915	-8.93862706
Si	7.73186929	4.29752452	-9.00104701
O	-11.93979738	-5.17899859	-4.84133505
O	-9.49839248	-0.94532948	-4.85612224
O	-7.05250200	3.29803944	-4.84970187
O	-4.60855633	7.53862397	-4.83999450

O	-7.04982345	-5.17978906	-4.86016411
O	-4.60165987	-0.93816141	-4.85118507
O	-2.14933585	3.30556621	-4.85902258
O	0.28667913	7.52796804	-4.87417622
O	-2.14870283	-5.17642503	-4.84627000
O	0.28551347	-0.93828920	-4.83170926
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O	5.20193269	7.55277704	-4.85067897
O	2.73022433	-5.17811335	-4.83705763
O	5.19171799	-0.93483293	-4.83862479
O	7.62414577	3.30227256	-4.85707500
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O	-10.07718843	-5.83512109	-1.27523578
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O	-5.19542755	2.64840190	-1.28498641
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O	-5.19737203	-5.81975598	-1.28179037
O	-2.75219031	-1.57291536	-1.27470569
O	-0.30674262	2.66368361	-1.28400972
O	2.13885334	6.89386271	-1.28392531
O	-0.30666001	-5.81066703	-1.26625546
O	2.14377460	-1.57026438	-1.27406735
O	4.58586919	2.66508305	-1.28372601
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O	4.58229786	-5.83131476	-1.26265543
O	7.03365363	-1.58573392	-1.27871816
O	9.48820924	2.64371683	-1.28135872
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O	-12.83905400	-8.07740834	-3.08090871
O	-10.39197112	-3.85483368	-3.07332652
O	-7.95088629	0.39704955	-3.09775149
O	-5.49259196	4.62859187	-3.09035206
O	-7.94454704	-8.09653719	-3.10610264
O	-5.49705004	-3.84810520	-3.09615842
O	-3.05393573	0.39889356	-3.08588572
O	-0.60594233	4.64157779	-3.09173159
O	-3.05265127	-8.06909922	-3.07341376
O	-0.60391782	-3.83982721	-3.08169366

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O	4.28666044	4.65557374	-3.07607152
O	1.84425705	-8.08429443	-3.07746439
O	4.29005826	-3.85686947	-3.07608975
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O	9.18960269	4.61439164	-3.09270482
O	-11.89661540	-7.57593279	-0.61181541
O	-9.45697990	-3.32724857	-0.61007441
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O	-4.57416381	5.15208721	-0.61934307
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O	-4.58385349	-3.30903042	-0.62675255
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O	-2.13107203	-7.54550176	-0.60519154
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O	2.75791572	0.93730796	-0.61067431
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O	5.21247761	-3.32342324	-0.60992736
O	7.66048886	0.91604564	-0.60967662
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Si	2.75877891	-0.15611866	-1.83895073
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Si	7.65495017	-0.17351325	-1.84133941
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Si	-14.36626171	-8.34402034	-3.60377918
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Si	-4.57520749	-8.33558392	-3.60989135
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Si	2.76025157	-4.10476273	-3.60049284
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O	10.06013650	7.26692887	-10.06815989
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O	7.18947715	6.87317314	-6.56991774
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O	-10.28748281	-4.05132506	-8.55144823
O	-7.81993362	0.18535895	-8.54132090
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O	-7.83226541	-8.29396377	-8.54901139
O	-5.37741732	-4.05402359	-8.53749806
O	-2.92492088	0.18921621	-8.53566333
O	-0.50413153	4.41703694	-8.56121644
O	-2.92273922	-8.28788635	-8.54001281
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O	-9.52874073	-3.26637510	-6.07046814

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O	-4.63150208	-3.27172472	-6.05339903
O	-2.18486054	0.96594265	-6.04963270
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O	2.69728217	0.98759955	-6.02235891
O	5.16651553	5.21030740	-6.02329819
O	2.69910682	-7.50703534	-6.04681566
O	5.16354950	-3.26784966	-6.04212268
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O	10.04787283	5.20704418	-6.04547794
O	-9.66415907	-6.96145216	-9.68732300
O	-7.19871297	-2.72352923	-9.69601147
O	-4.76245508	1.51821470	-9.68104896
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O	-4.74474651	-6.95053651	-9.69237704
O	-2.29885619	-2.72017910	-9.68123152
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O	0.14420704	-6.94842628	-9.68146644
O	2.60640150	-2.68846604	-9.62765987
O	5.10903851	1.61103958	-9.57111506
O	7.47346255	5.75607486	-9.70107463
O	5.02525149	-6.94221742	-9.66459086
O	7.42965589	-2.75000537	-9.68247184
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O	12.36205796	5.76366946	-9.68596926
O	-7.86220169	-4.57625406	-7.69957427
O	-5.40012670	-0.33886654	-7.68212276
O	-2.96288359	3.90943927	-7.67845981
O	-0.52022058	8.14735237	-7.67837965
O	-2.95379595	-4.57303488	-7.68060843
O	-0.50581501	-0.34957289	-7.66690074
O	1.92072273	3.85968124	-7.74858527
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O	1.94626514	-4.56422754	-7.65726286
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O	6.81989655	3.92057817	-7.68319349
O	9.28042787	8.14943554	-7.67985510
O	6.83297904	-4.59678533	-7.66237930
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Si	-1.18879366	-6.37394618	-5.40719876
Si	1.24597648	-2.13247402	-5.39622439
Si	3.70194339	2.12499156	-5.40730813
Si	6.16082315	6.35150270	-5.40279497
Si	3.68868806	-6.37624082	-5.39891976
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Si	8.58125740	2.10609072	-5.42780595
Si	11.03807945	6.34214042	-5.40485664
Si	-9.41443669	-4.43754553	-7.21318691
Si	-6.95470628	-0.20147194	-7.20256113
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Si	0.38418167	-4.43567377	-7.18791474
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H	4.18109715	-1.68278263	-9.80465693
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(4x4)PbO/SiO_2-2OH

322 atoms

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Si	-9.40590724185149	0.04266860314953	-9.00475953277927
Si	-6.93570292974233	4.28419011811948	-9.00645514708579
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Si	-4.49496852333072	-8.42040564807040	-8.99857049062356
Si	-2.04227477062916	-4.18805021026030	-8.99462988029393
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Si	2.82742525709292	4.28310832948345	-8.99565468752182
Si	0.40468485265004	-8.43880984970198	-9.02815594299026
Si	2.97422127311224	-4.07756614645815	-9.08049164400160
Si	5.25543997954113	-0.04307230279233	-9.04443285989700
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O	-9.48717279395240	-0.92871991324535	-4.84973927040997
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O	-2.13565758973723	3.35385865105169	-4.80951080700351
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O	2.75432233332273	-5.17094930563585	-4.86447234255299
O	5.18707903027878	-0.95176025527645	-4.84150676717068
O	7.62169048075721	3.30694011511887	-4.86958148834454
O	10.08606557580369	7.55770303297072	-4.87391568458548
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O	-7.64931211023976	-1.55182138908975	-1.26368899617396

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O	-2.74753429138115	6.91196623580130	-1.25214996841369
O	-5.18607362673455	-5.83598034720264	-1.30340117813536
O	-2.74157619702472	-1.58154121399624	-1.27321490747956
O	-0.30795244248429	2.67573004543392	-1.26803419655650
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O	2.14348568292678	-1.57922997708149	-1.27600851935187
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H	-3.19035583913968	-2.31429273040317	-9.82648267718334
H	-8.10372964206598	-2.35443068999394	-9.88079538541236
H	-12.82101190663190	-5.95705042758592	-9.97467293996861
H	-7.93126381555557	-5.93617305656045	-9.99139778445599
H	-3.08528762497906	-5.90609849286181	-9.99028649872633
H	2.01571816060568	-5.88267100139152	-10.03772245737213
H	4.17752170303433	-6.52806120876813	-9.87488739791548
H	-0.80041735848577	-6.65094271675678	-9.90693851161989
H	-5.65801618204930	-6.59466855172479	-9.87422653245499
H	-10.55663104688226	-6.58718472879772	-9.85721669565775
Pb	0.33467583757514	-1.16954399153398	-12.31569148943507
O	2.06323808059320	-2.26463476962044	-12.18744899143250
VEC1	19.57131164000000	0.00000000000000	0.00000000000000
VEC2	9.78369180000000	16.95531931000000	0.00000000000000

(4x4)FlO/SiO_2-2OH

322 atoms

Si	10.20789531	4.07084417	-7.19511183
Si	12.66158819	8.30276033	-7.19187434
Si	-14.24081843	-8.41128178	-9.00030720
Si	-11.78349666	-4.17083261	-9.00079389
Si	-9.34735304	0.08419073	-9.00218910
Si	-6.90516055	4.34707225	-8.98967318
Si	-9.35189791	-8.40908129	-9.01020316
Si	-6.87822957	-4.14833674	-9.00089971
Si	-4.56156716	0.17571833	-8.95424740
Si	-2.02874514	4.29956320	-9.00173697
Si	-4.45654144	-8.40938260	-9.02586771
Si	-1.91032335	-4.14893402	-9.01500428
Si	0.38876295	-0.00609224	-9.03329683

Si	2.86841932	4.29542221	-9.02191472
Si	0.44788640	-8.41149784	-9.01392577
Si	2.89680786	-4.20200179	-8.96804585
Si	5.31863505	0.05974125	-9.01860320
Si	7.78073820	4.31135200	-9.01399246
O	-11.88750363	-5.15323505	-4.85359642
O	-9.47593381	-0.92764017	-4.83072367
O	-7.00525404	3.34934537	-4.82089197
O	-4.54702024	7.57514251	-4.83832767
O	-6.96788324	-5.15004948	-4.87492641
O	-4.57777380	-0.94041659	-4.83314067
O	-2.13247331	3.32630333	-4.85666856
O	0.33349937	7.56244798	-4.85626675
O	-2.09614160	-5.15666821	-4.86416286
O	0.32345088	-0.94798352	-4.85961094
O	2.77281064	3.32225439	-4.87880645
O	5.22749423	7.56324908	-4.87481357
O	2.79452357	-5.15422240	-4.83380802
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O	7.67704234	3.33237407	-4.85986340
O	10.11812975	7.57128246	-4.84968869
O	-10.03781840	-5.81461783	-1.29184139
O	-7.60097566	-1.56026340	-1.27271977
O	-5.16037284	2.68302726	-1.27636890
O	-2.69729394	6.91171739	-1.27257804
O	-5.14913505	-5.80968070	-1.29665316
O	-2.71537257	-1.56658404	-1.28722391
O	-0.25588891	2.66335112	-1.29573487
O	2.19215164	6.90823977	-1.30302801
O	-0.25258544	-5.80058678	-1.26924652
O	2.16332343	-1.54928631	-1.30297413
O	4.62832352	2.67309570	-1.30920713
O	7.05652864	6.90437451	-1.26940594
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O	7.06631808	-1.54378217	-1.27614150
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O	-7.89541136	-8.05802220	-3.09799625
O	-5.45094277	-3.81721622	-3.08844167
O	-3.01633569	0.41159494	-3.09562499
O	-0.55795743	4.63893940	-3.09975053
O	-2.99735552	-8.08547308	-3.09514849
O	-0.55631630	-3.82976659	-3.08646793
O	1.85769160	0.42745282	-3.11502296
O	4.33067282	4.65090551	-3.11637388
O	1.87386621	-8.06962258	-3.06399196
O	4.34312918	-3.82205582	-3.07046417
O	6.76099678	0.42338918	-3.09298814
O	9.22203893	4.66844434	-3.09145366
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O	5.22037305	5.17853747	-0.63403706
O	2.81235644	-7.52942017	-0.60236247
O	5.26701546	-3.29763939	-0.60376314
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O	-10.03869792	-6.91161218	-4.16534129
O	-7.60924325	-2.68654178	-4.15624057
O	-5.15762976	1.55945888	-4.16246460
O	-2.69633326	5.81027372	-4.14882697
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O	-2.70105500	-2.68153905	-4.16698511
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O	-0.31024227	-6.93984774	-4.09213323
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O	4.61791701	1.56054186	-4.19033269
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O	-3.00606928	3.81030551	-2.37419394
O	-0.55340014	8.05181792	-2.37911976
O	-2.99944892	-4.67541714	-2.38693567
O	-0.56945380	-0.43797803	-2.38886706
O	1.89303044	3.79624563	-2.39753849
O	4.33802178	8.04947901	-2.39763654
O	1.89558279	-4.66021758	-2.36359043
O	4.31154605	-0.42055676	-2.40004519
O	6.77953303	3.82613187	-2.38698775
O	9.22355195	7.99478114	-2.35566292
O	6.79369520	-4.67012613	-2.37203611
O	9.21493093	-0.40534480	-2.36079584
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Si	-11.21909261	-6.07693673	-0.09923499
Si	-8.79631258	-1.84756226	-0.10113359
Si	-6.36377055	2.41766034	-0.10536691
Si	-3.88395009	6.64384623	-0.08661179
Si	-6.34240471	-6.07911852	-0.11764271
Si	-3.90206447	-1.84404576	-0.10402039
Si	-1.45146912	2.39960390	-0.11657615
Si	1.00483365	6.63194177	-0.11957653
Si	-1.46755920	-6.07193746	-0.11374778
Si	0.96994347	-1.81255582	-0.12284263
Si	3.42799823	2.41309120	-0.13320965
Si	5.84365873	6.64126251	-0.11089698
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Si	10.74904894	6.66622368	-0.09653097
Si	-9.41627163	-4.40355897	-1.85686163
Si	-6.99060950	-0.14542779	-1.83920174
Si	-4.53209471	4.09610237	-1.82955498
Si	-2.08016256	8.32696942	-1.83342048
Si	-4.52961266	-4.39420746	-1.85394244
Si	-2.09813362	-0.15494199	-1.85402886
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Si	2.80856964	8.32476412	-1.86140014
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Si	2.77927355	-0.13794939	-1.87359570
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Si	-14.31729561	-8.31517102	-3.59435984
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Si	-9.42338778	-8.31965935	-3.61934003
Si	-6.97131011	-4.09232766	-3.62674966
Si	-4.54571742	0.14988752	-3.61283065
Si	-2.09033719	4.39232483	-3.61473158
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Si	2.80232812	4.38931289	-3.63764330
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O	-2.57449563	-1.56461062	-6.55946464
O	-0.13499098	2.65959966	-6.58116015
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O	-0.03238293	-5.89025627	-6.48974871
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O	-0.46467454	8.15757452	-7.68517199
O	-2.86099445	-4.53697948	-7.70913623
O	-0.52157261	-0.26937152	-7.69160486
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O	4.42413844	8.14251673	-7.71158407
O	2.06103869	-4.60368286	-7.60612482
O	4.39528012	-0.31095570	-7.71018644
O	6.86317071	3.92412725	-7.70534136
O	9.31215824	8.16600637	-7.70373905
O	6.89825355	-4.55559880	-7.67009753
O	9.31276519	-0.29615409	-7.68775884
O	11.76436098	3.93805517	-7.67704882
O	14.21626489	8.15922434	-7.67590433
Si	-10.92519540	-6.34632536	-5.42081948
Si	-8.50956216	-2.11698437	-5.39853961
Si	-6.06067685	2.14768162	-5.39330398
Si	-3.59064591	6.37539499	-5.39886302
Si	-6.00363993	-6.34229069	-5.44412703
Si	-3.60374372	-2.12016224	-5.41364233
Si	-1.19505645	2.12447247	-5.44823225
Si	1.29118307	6.36799917	-5.42750282
Si	-1.14169535	-6.37660856	-5.38644313
Si	1.30510768	-2.13351051	-5.40793729
Si	3.72724519	2.12194277	-5.44464351
Si	6.18674144	6.36653450	-5.43807184
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Si	-6.95164585	-0.14657249	-7.15517054
Si	-4.47845627	4.07898942	-7.18439933
Si	-2.01912243	8.29996734	-7.20165963
Si	-4.41529489	-4.41259185	-7.23626622

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Si	0.49321673	-4.48944516	-7.14382421
Si	2.83877769	-0.18551859	-7.22692256
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Si	7.75923297	8.30752570	-7.21872750
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H	-5.44677679	6.79888763	-9.99530477
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H	1.70388919	6.12259591	-9.90027240
H	6.62780244	6.14232177	-9.90134884
H	11.50621159	6.17285944	-9.87878293
H	6.82336798	2.54732274	-10.01384508
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H	4.36040485	-1.71498717	-9.98901339
H	-0.59987225	-1.88151459	-9.81504394
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H	-10.30609010	-1.68327037	-9.99280332
H	6.63231496	-2.34421819	-9.87903354
H	1.68801894	-2.39613938	-9.81522413
H	-4.42572909	-4.59963971	-11.67644576
H	-8.04251445	-2.31110594	-9.85835304
H	-12.78433306	-5.91412805	-9.99607996
H	-7.90138369	-5.88199182	-9.99399124
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H	1.89494063	-5.94322620	-9.97511115
H	4.16738628	-6.58465942	-9.87129669

H	-0.69849645	-6.55908402	-9.88615473
H	-5.64366792	-6.59122967	-9.89031326
H	-10.51993866	-6.58613186	-9.88796971
Fl	-3.20303915	-2.06902599	-11.75313153
O	-4.50607588	-3.85317162	-12.29790294
VEC1	19.57131164	0.00000000	0.00000000
VEC2	9.78369180	16.95531931	0.00000000