

Metal-doped ceria nanoparticles: Stability and redox processes

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Electronic Supplementary Information

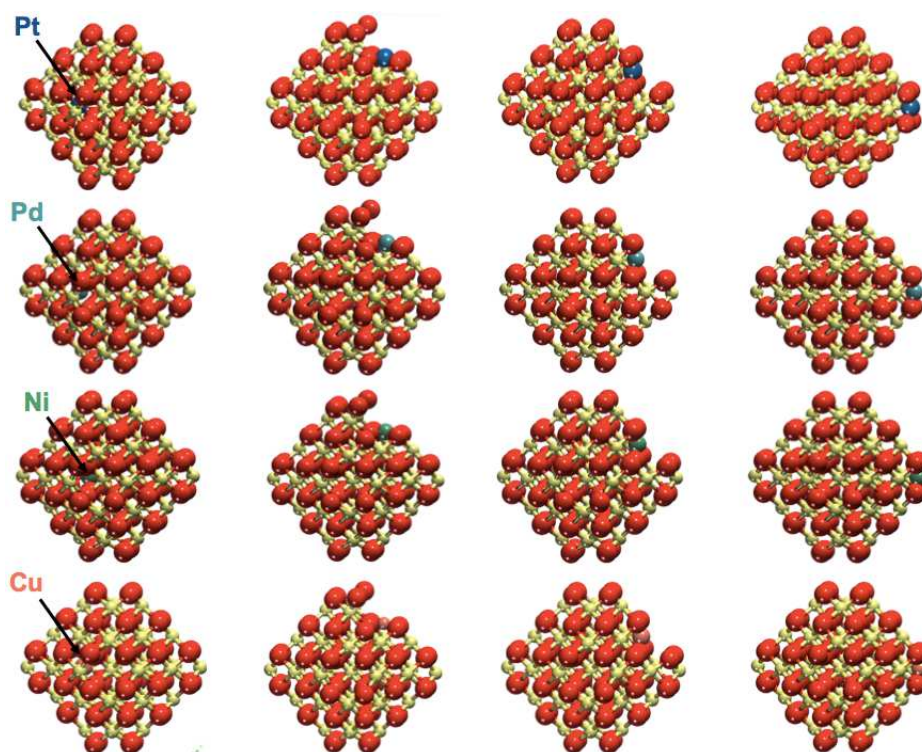


Figure S1. Stoichiometric $M_1Ce_{39}O_{80}$ structures formed by the substitution of a Ce^{4+} cation by a transition metal (M) atom. The M atoms are located in four different positions (D1, D2, D3 and D4) of the ceria nanoparticle.

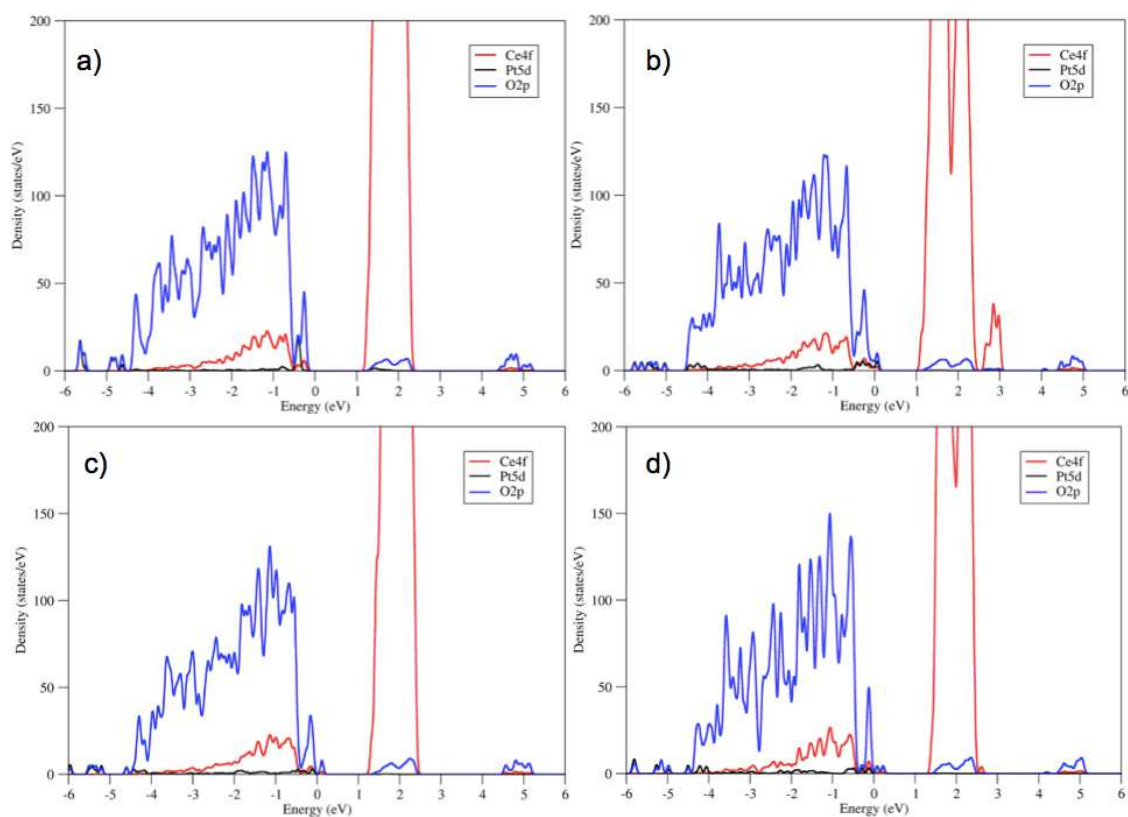


Figure S2. Density of states (DOS) plots of stoichiometric $\text{Pt}_1\text{Ce}_{39}\text{O}_{80}$. Plot a) corresponds to Pt located in D1 position, b) to D2, c) to D3 and d) to D4, respectively.

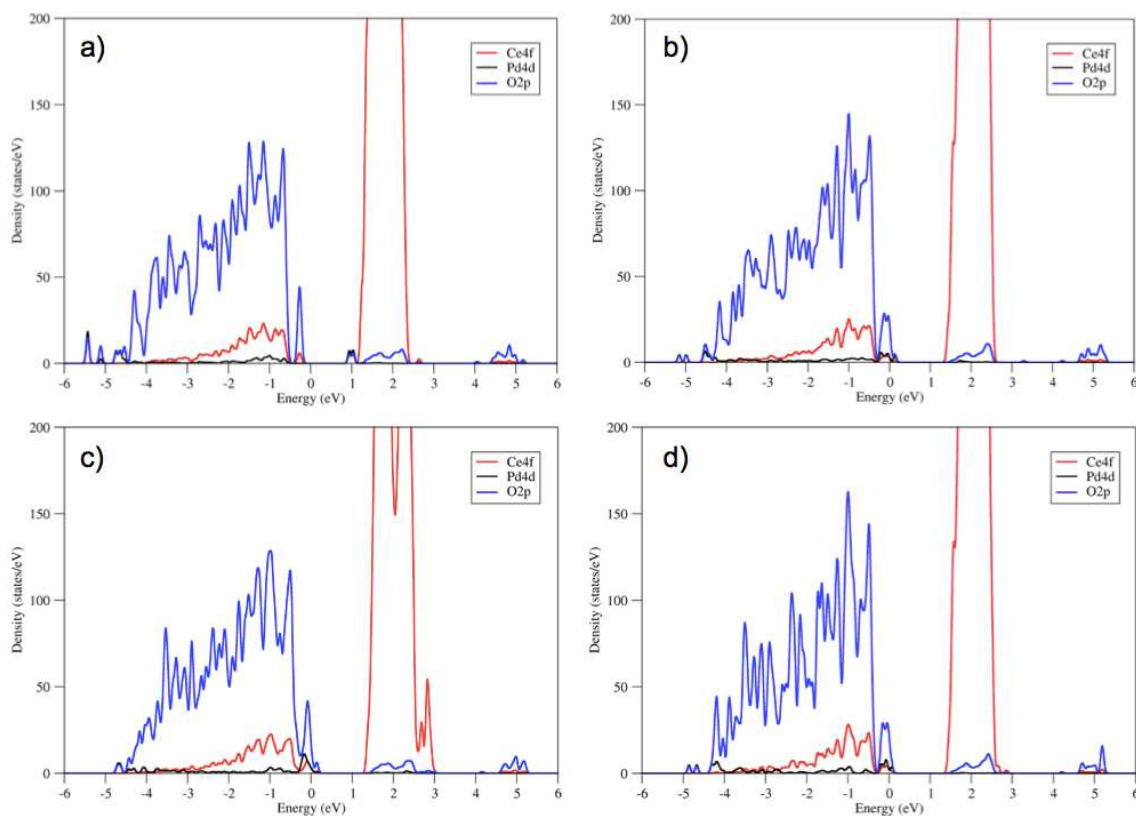


Figure S3. Density of states (DOS) plots of stoichiometric $\text{Pd}_1\text{Ce}_{39}\text{O}_{80}$. Plot a) corresponds to Pd located in D1 position, b) to D2, c) to D3 and d) to D4, respectively.

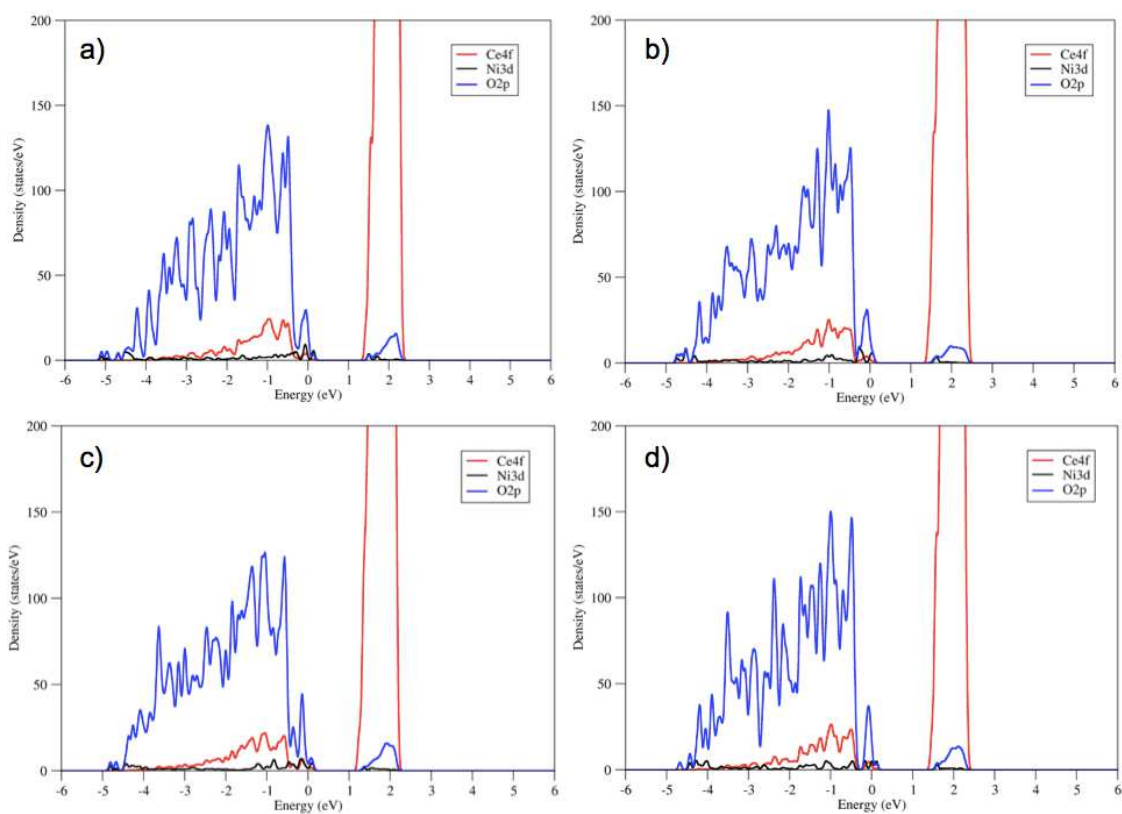


Figure S4. Density of states (DOS) plots of stoichiometric $\text{Ni}_1\text{Ce}_{39}\text{O}_{80}$. Plot a) corresponds to Ni located in D1 position, b) to D2, c) to D3 and d) to D4, respectively.

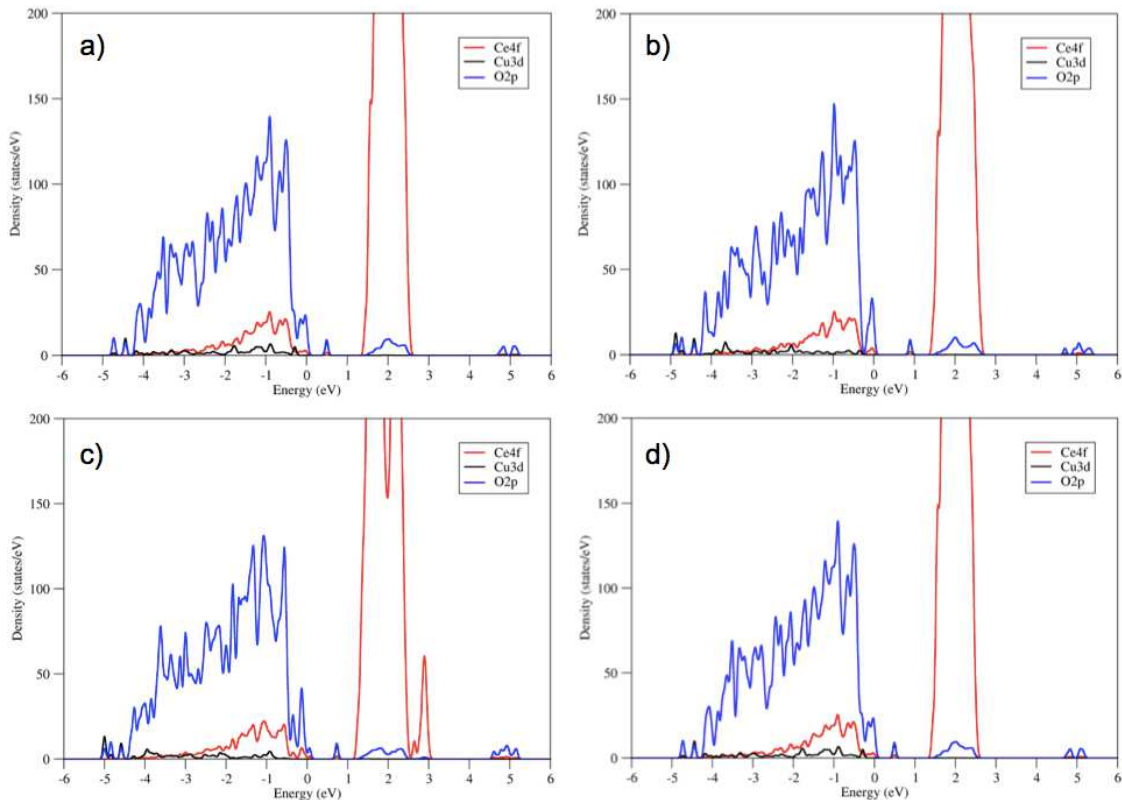


Figure S5. Density of states (DOS) plots of stoichiometric $\text{Cu}_1\text{Ce}_{39}\text{O}_{80}$. Plot a) corresponds to Cu located in D1 position, b) to D2, c) to D3 and d) to D4, respectively.

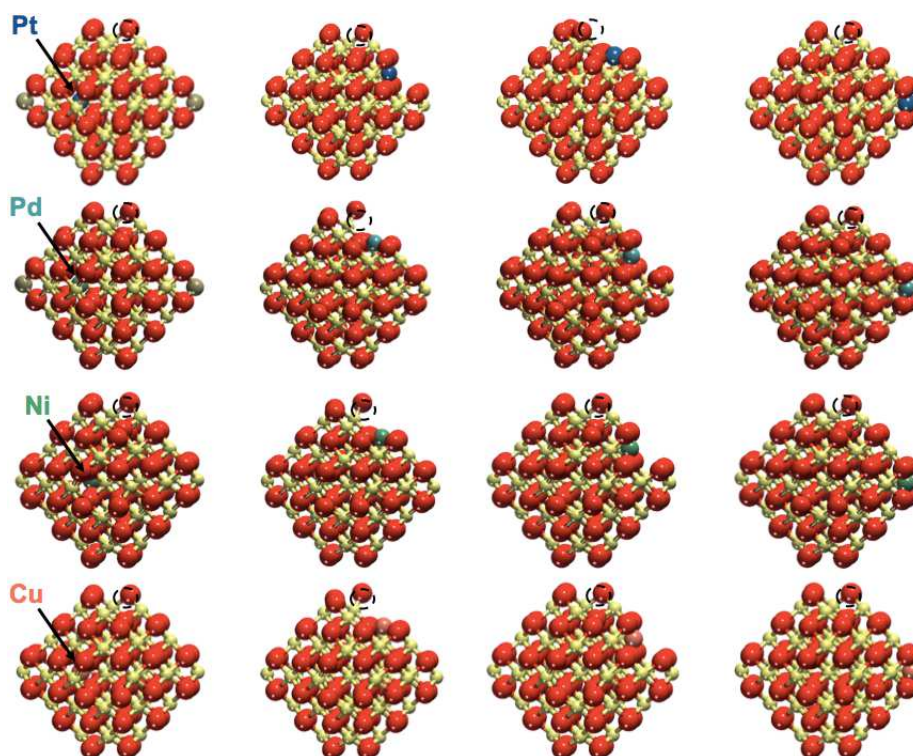


Figure S6. Most stable structures of $M_1Ce_{39}O_{80}$ systems, where an O vacancy has been created by removing an O atom from the $\{100\}$ nanofacet (denoted by a dashed circle).

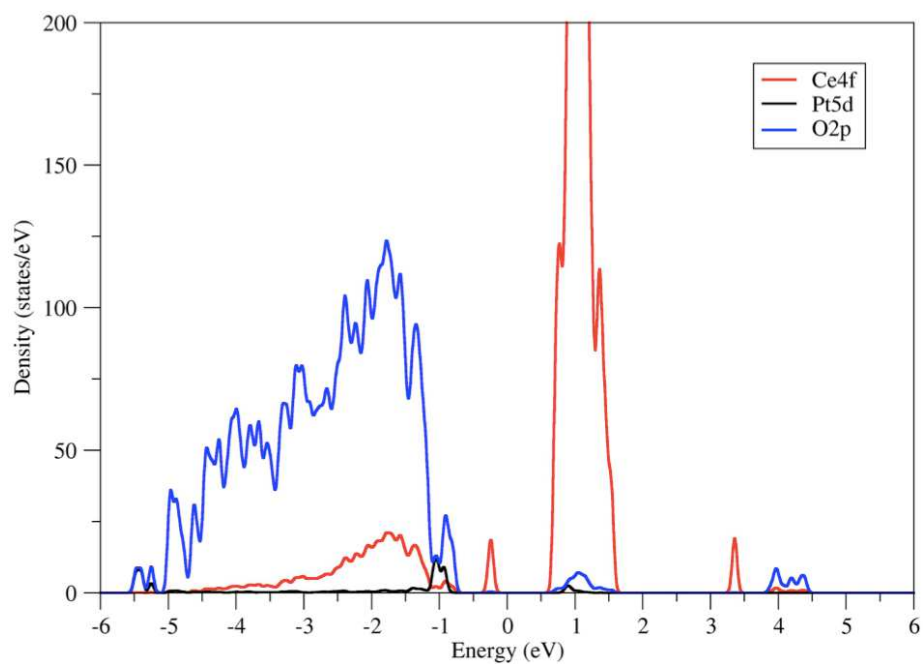


Figure S7. Density of states (DOS) plot of $Pt_1Ce_{39}O_{79}$ corresponding to Pt located in D1 position.

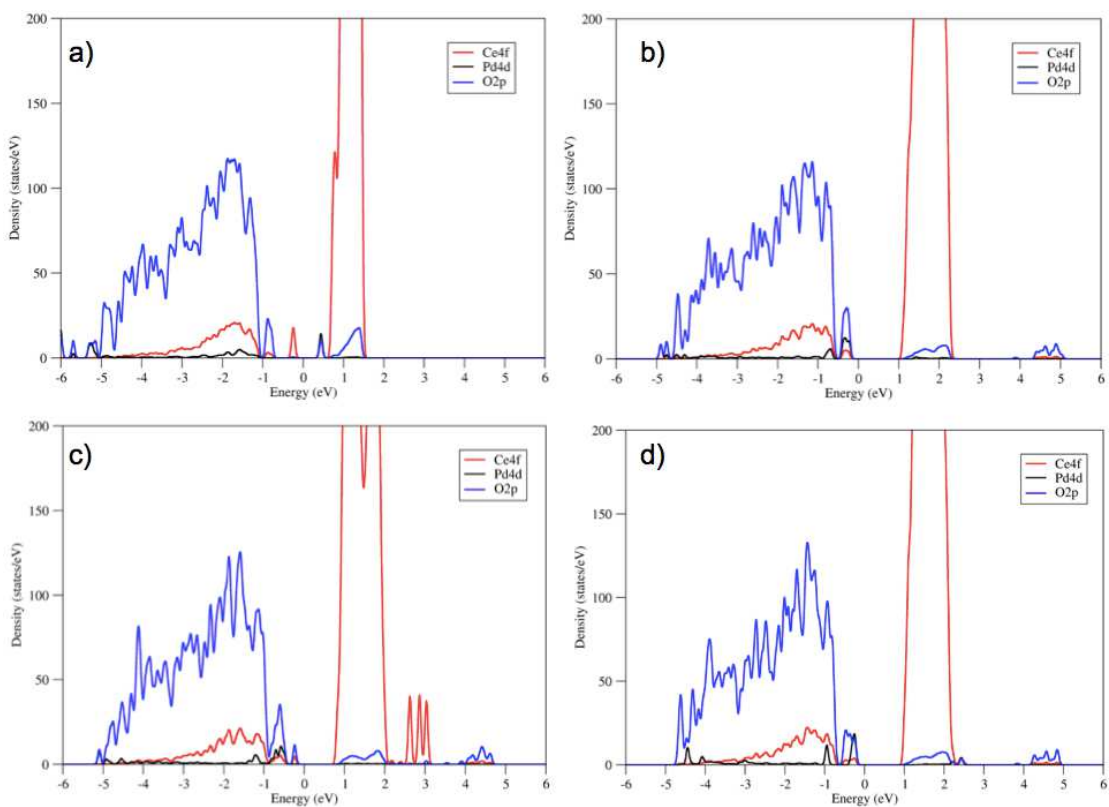


Figure S8. Density of states (DOS) plots of $\text{Pd}_1\text{Ce}_{39}\text{O}_{79}$. Plot a) corresponds to Pd located in D1 position, b) to D2, c) to D3 and d) to D4, respectively.

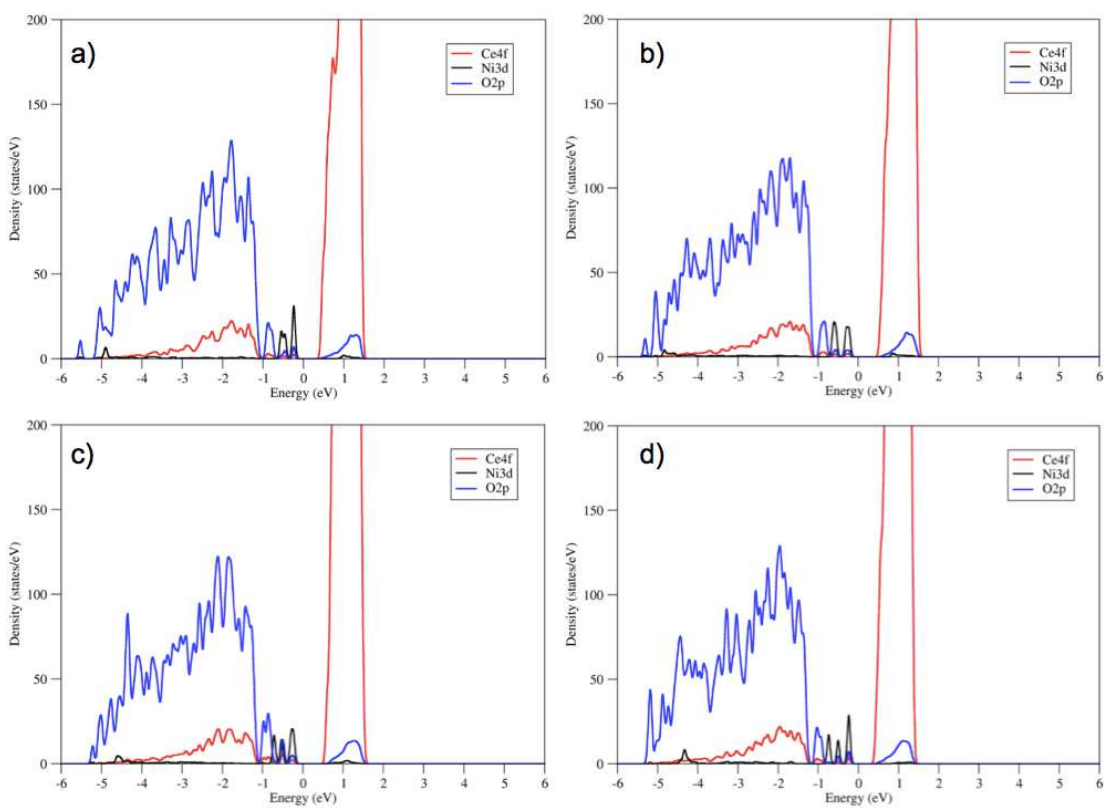


Figure S9. Density of states (DOS) plots of $\text{Ni}_1\text{Ce}_{39}\text{O}_{79}$. Plot a) corresponds to Ni located in D1 position, b) to D2, c) to D3 and d) to D4, respectively.

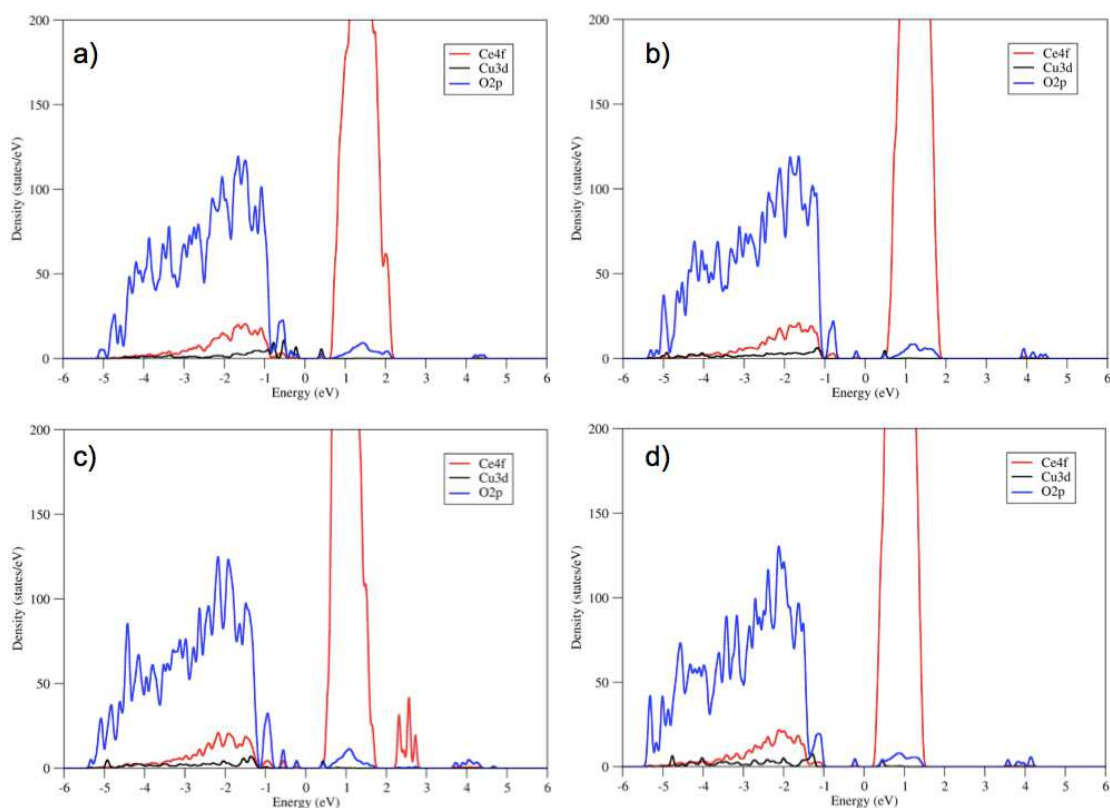


Figure S10. Density of states (DOS) plots of $\text{Ni}_1\text{Ce}_{39}\text{O}_{79}$. Plot a) corresponds to Cu located in D1 position, b) to D2, c) to D3 and d) to D4, respectively.

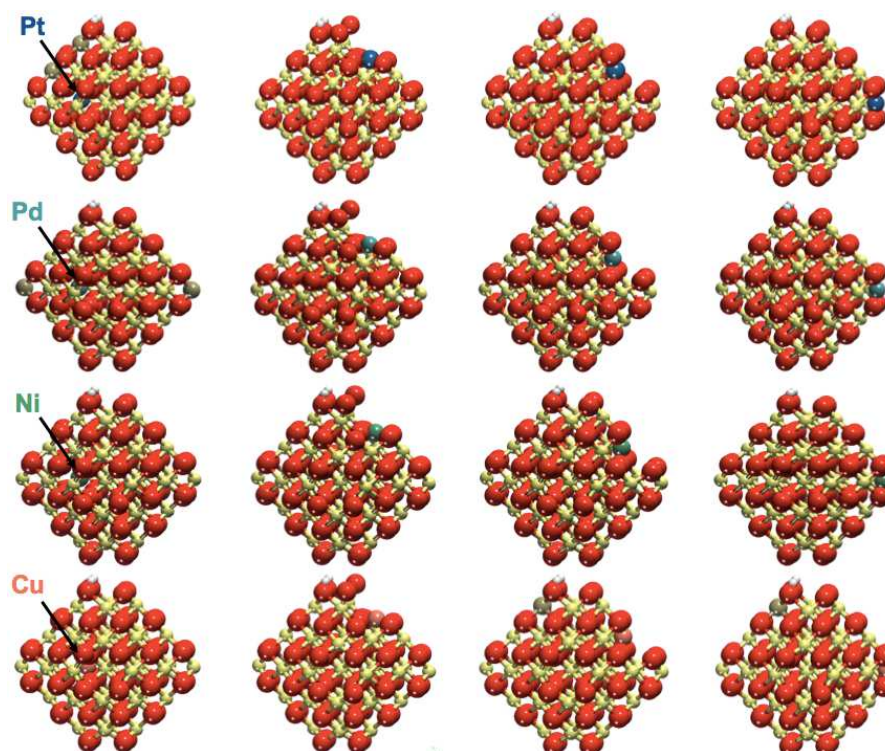


Figure S11. Overview of the most stable structures $\text{H}_2\text{M}_1\text{Ce}_{39}\text{O}_{80}$ of systems formed upon dissociative adsorption of two hydrogen atoms in two nearby oxygen atoms of one of the $\{100\}$ nanofacets.

Cartesian coordinates of atoms (Å) and total energies (eV) for the PW91+4 optimized

M-doped ceria nanoparticles

PtCe₃₉O₈₀ D1 (-943.430515 eV)

Ce	2.8923	16.2558	14.9771
Ce	-0.7479	16.3398	14.8806
Ce	2.9482	12.6163	14.9571
Ce	-0.6806	12.7044	14.9961
Ce	1.1787	10.6727	12.3068
Ce	4.9620	14.3511	12.3108
Ce	1.0413	18.2978	12.2732
Ce	4.7704	18.0831	12.2691
Ce	-2.7793	14.5938	12.2446
Ce	1.1268	14.4354	12.1867
Ce	4.8996	10.5965	12.1340
Ce	-2.6762	18.3214	12.1396
Ce	-2.5537	10.9771	12.1213
Ce	2.9357	16.2853	9.5244
Ce	-0.9273	20.1205	9.5207
Ce	6.4636	19.7460	9.5094
Ce	-4.3498	9.2738	9.4878
Ce	-0.8090	16.2979	9.5019
Ce	2.8319	20.0344	9.5056
Ce	3.0991	8.8062	9.5393
Ce	6.6897	16.1108	9.5078
Ce	6.6939	12.3338	9.4928
Ce	-0.7306	9.1014	9.4907
Ce	2.9338	12.5683	9.5714
Ce	-4.5611	16.6337	9.4827
Ce	-4.6524	12.9160	9.4258
Ce	0.9989	14.4461	6.9068
Ce	-2.6939	18.3553	6.8838
Ce	4.7943	10.6371	6.8831
Ce	4.7416	18.0718	6.7683
Ce	1.0208	18.3122	6.7430
Ce	4.8808	14.3486	6.7522
Ce	-2.9146	14.6309	6.6460
Ce	-2.7346	10.9366	6.6648
Ce	1.0413	10.6655	6.7329
Ce	-0.7753	16.3747	4.1178
Ce	2.8696	12.6085	4.1362
Ce	-0.7968	12.7471	4.0576
Ce	2.8509	16.2335	4.0825
O	1.0797	16.7192	16.0212
O	3.3247	14.4522	16.0603
O	-1.1526	14.5048	16.0101
O	1.0768	12.2225	16.0940
O	2.9919	10.6235	13.5969
O	-0.8762	10.6750	13.4870
O	-2.7677	16.4024	13.5558
O	-0.7634	18.3465	13.5782
O	4.9926	16.3668	13.5913
O	3.0367	18.3306	13.5739
O	4.9752	12.5606	13.6034
O	1.1142	16.3464	13.5051
O	3.0037	14.4501	13.5282
O	-0.8121	14.5032	13.4483
O	-2.8910	12.6569	13.4177
O	1.0856	12.6291	13.6292
O	-2.3355	20.2228	11.1333
O	4.5263	8.6534	11.1063

O	-4.5758	18.0195	11.1077
O	6.7757	10.8853	11.0844
O	-4.7025	14.4997	10.9122
O	1.3779	12.5102	11.1347
O	-4.6257	10.8957	10.8537
O	1.1507	20.2209	10.8931
O	3.0203	10.6286	10.8266
O	6.8669	14.4331	10.8863
O	1.0733	16.3678	10.8724
O	4.8761	20.1213	10.8813
O	6.8356	18.1781	10.8839
O	-2.6414	8.9982	10.8631
O	4.9109	16.3278	10.8677
O	3.0693	14.5109	10.8797
O	2.9830	18.2208	10.8623
O	-2.6333	16.3392	10.8226
O	-0.7005	11.0405	10.7443
O	-0.7751	18.2109	10.8363
O	4.8456	12.5447	10.8715
O	0.9316	8.8038	10.8693
O	-0.7146	14.2688	10.7449
O	-2.6547	12.7111	10.5068
O	0.8963	12.6052	8.4156
O	-1.0641	14.2683	8.1873
O	-1.0504	11.0539	8.1888
O	-0.7720	18.2261	8.1870
O	1.0358	16.3300	8.1708
O	4.7979	12.5501	8.1906
O	4.8580	16.2913	8.1674
O	2.9489	18.2020	8.1613
O	-2.7377	8.9443	8.1196
O	2.9555	14.4314	8.1593
O	2.8485	10.7366	8.1606
O	-2.6565	16.3832	8.1231
O	4.8540	20.1009	8.1324
O	6.7891	18.1489	8.1272
O	1.1564	20.2329	8.1228
O	6.8235	14.4240	8.1187
O	-4.8708	14.7069	8.1507
O	-4.8666	10.7084	8.1073
O	0.8336	8.8249	8.0434
O	4.4553	8.7283	7.9143
O	-2.3245	20.2517	7.9156
O	-4.5858	18.0852	7.9120
O	6.7165	10.9087	7.8985
O	-3.2074	12.7178	7.8136
O	0.9976	12.6082	5.5980
O	-0.8761	14.5483	5.5604
O	1.0596	16.3398	5.5487
O	2.8978	14.4340	5.5492
O	-0.9314	10.6166	5.4811
O	4.9320	16.3303	5.4577
O	3.0096	18.3254	5.4573
O	4.8835	12.5388	5.4497
O	-0.7790	18.3757	5.4452
O	2.8635	10.6106	5.4348
O	-2.8381	16.4579	5.3889
O	-2.8404	12.6118	5.2277
O	1.0218	12.2555	3.0397
O	1.0700	16.7446	3.0154
O	-1.1838	14.5609	2.9959
O	3.2966	14.4312	3.0168
Pt	-0.8704	12.6797	9.4567

PtCe₃₉O₈₀ D2 (-942.880255 eV)

Ce	8.43822645065107	9.41519837659231	14.98917944004698
Ce	13.50654842250059	9.39926299195997	14.95169360178226
Ce	10.99469158293129	12.01975648122118	14.96808068262991
Ce	10.95984272007359	6.80518476351292	14.87497583930558
Ce	13.63603939695620	12.22832157065686	12.29869300429424
Ce	8.32188578627956	12.25788216557826	12.38796698729025
Ce	13.60811693493489	6.67727763876506	12.25912437565491
Ce	8.29042956321764	6.70192772602955	12.26010764409762
Ce	16.12017679517979	9.43095500189377	12.24949076064773
Ce	5.80659458776523	9.45381646717615	12.27228303063595
Ce	10.95425742803422	9.50178587501742	12.15815141252418
Ce	11.17537324576890	15.03589294033721	12.44730016603975
Ce	10.93042892110260	4.06771536780498	12.09079543384357
Ce	13.52924620642010	14.97597899670033	9.54679645545894
Ce	16.12864859664559	12.20735867747814	9.52334634991916
Ce	10.97698733538321	12.30038353343762	9.50643312354192
Ce	18.50661379990441	9.43199460300429	9.50505683940765
Ce	13.55648377550681	9.50108174619706	9.50329638418041
Ce	8.34462797086608	9.57454318109324	9.50189649886250
Ce	5.67547756012470	12.14586563869519	9.54026879792959
Ce	16.10029942344193	6.71124228513126	9.49113530461545
Ce	10.94223691726906	6.85754802712635	9.48954871993237
Ce	13.46008836851093	4.02529417501410	9.48038356960242
Ce	3.38590617825645	9.40931956441201	9.49852876805973
Ce	5.81357203500649	6.74874636010450	9.46937326981048
Ce	8.40659330405481	4.04859238276062	9.46541372155642
Ce	11.17614128345753	15.06867683345552	6.62918103706545
Ce	10.94014417499609	4.10518868345713	6.85646800063712
Ce	10.97050367148563	9.52832791637486	6.84528393194964
Ce	16.12789981873129	9.45480301911983	6.75757547652279
Ce	5.81983079069546	9.52940553857953	6.72876871277095
Ce	13.65329647268780	12.26088984986658	6.73756438711036
Ce	8.34893863806392	12.29425507018235	6.65162262766062
Ce	13.61821433345604	6.70058224218195	6.72074433240716
Ce	8.29914027978802	6.75253449411521	6.70279258696744
Ce	11.02941213231972	12.08649387287530	4.07432884897049
Ce	10.97825951137082	6.86076263469221	4.09734972003474
Ce	13.52802910504268	9.44586803362301	4.05332689629870
Ce	8.46705040210109	9.48731990104218	4.00528215091437
O	9.40152682403350	10.97772881323833	16.05696847847656
O	12.55782876018491	10.97435484094427	16.04789629519392
O	12.55062774995080	7.79676872194735	15.99199129064331
O	9.38248891969696	7.80477449764062	16.01066957564807
O	9.61283814864287	13.38455230801179	13.66590666155764
O	12.47106939324404	13.49591847485635	13.68466125149246
O	15.06212695858196	10.79695478027281	13.57237601646160
O	6.86803999369208	10.84990543885111	13.58147187955738
O	15.04606738554985	8.03018403628278	13.55593562979637
O	6.84787246492044	8.06587670199368	13.56512620149938
O	12.33778344730247	5.37842226732656	13.54516364701433
O	9.53698676323086	5.38602918708175	13.53781653234893
O	9.62073268465673	10.74541815234648	13.51870082710144
O	12.29136913283492	10.77711456349402	13.50577762647321
O	12.27187193613240	8.12115496462967	13.47213419911161
O	9.62885109638888	8.11198024362439	13.47603837580329
O	10.29633881871125	16.49334118513534	13.29454301840767
O	12.73153538498368	16.05403980042153	11.16630254663052
O	12.49699240580516	2.96613495843482	11.06627297346217
O	9.34827688402079	2.98998927493658	11.05229915670309
O	15.06297770670636	13.50053129402565	10.92276574266106
O	6.73287825950825	13.56530270360633	10.94432325653798
O	17.64319670466381	10.80322894719080	10.88910493828760

O	17.62765388171928	8.05210115448143	10.87635719278290
O	15.02486676962085	5.39323008666837	10.86798301671750
O	6.85434530077765	5.43270596807366	10.85333937923780
O	4.24637243016303	10.81649801101264	10.88334177938584
O	4.26801249214058	8.06313467590702	10.86544953387413
O	9.59349050589682	11.01881731405423	10.87918228485295
O	12.29862488254498	10.88232219707265	10.84618472203829
O	14.95929051781769	10.80226797497740	10.86486669406645
O	12.30868775441767	8.14485548211211	10.85107145537193
O	9.58019920290314	8.21051129547532	10.83846953121122
O	6.93149747194923	10.83979362919719	10.87741854176390
O	14.94410137624961	8.10772664860157	10.84390667903091
O	6.96134557512939	8.15667214904368	10.84123763538696
O	9.51728637064313	13.90823162211099	10.93309648623518
O	12.25956746530989	13.50475963596261	10.89981724495666
O	12.25734574673825	5.50037229909875	10.81265860932790
O	9.61387936857504	5.52941129536024	10.81121865758939
O	12.28699059261429	13.51348705158057	8.14607689862498
O	9.54000153935234	13.89614582875170	8.13639828159443
O	9.61399543767178	5.54983548827032	8.14916022994967
O	12.26263003278426	5.51683175003335	8.15600528240478
O	14.96420600794992	10.81617762584432	8.15853536195172
O	14.94734147370037	8.12094532817835	8.15130671141416
O	9.60079030418022	11.01931634727685	8.14136026210299
O	12.30375956707888	10.89524467095819	8.17315221895980
O	6.93677394388166	10.87891374156552	8.15233582825772
O	12.31354408186620	8.15729150643900	8.14146624093415
O	6.96194649508223	8.18998663432485	8.13982984850680
O	9.58361882037063	8.22595243139115	8.14778824445208
O	15.08872544723732	13.52044555194500	8.14535586817544
O	17.64849713189543	10.81428883637572	8.13582632818472
O	17.63201586681181	8.06061644599806	8.12304637923786
O	6.76399766504882	13.59870924836062	8.13992655858911
O	4.25161263570049	10.85299444285703	8.15546044316247
O	4.26844933432104	8.09777472459761	8.10484808325442
O	15.03145417691440	5.40618890577575	8.09850827313867
O	6.85448623984920	5.45873133025702	8.07252258042860
O	10.39253227858298	16.51244231212273	5.68741249579762
O	12.70769295253321	16.08333919038201	7.99059337090153
O	12.49964992231071	2.98771492220697	7.87996067893962
O	9.35357480365388	3.00963621841521	7.87273910301445
O	12.31830154661932	10.81332763130434	5.51751930399618
O	9.64337340536710	10.79454806849055	5.50107097147530
O	12.28692975978436	8.15780146442458	5.51794408701416
O	9.64740496164761	8.16352488529798	5.50441036260593
O	12.49441223553915	13.53129907835889	5.36454238903690
O	15.08711263486608	10.83541561766597	5.44648117214237
O	9.63750301609248	13.43082073641290	5.39195404505862
O	15.06167079124200	8.06622234167422	5.43613961390786
O	6.88534931900461	10.92914300087575	5.44021548382175
O	9.54968540757588	5.44194045768600	5.42097644699955
O	6.86549831004695	8.14797426065761	5.42177233697193
O	12.35146397395021	5.41506535623030	5.42162159904379
O	12.57930790123304	11.02604744224997	2.97576065836027
O	9.43175252054193	11.06591809820324	2.96772364996409
O	12.57656975425892	7.84364780891948	2.99706780154744
O	9.40241607130050	7.88298759332724	2.97037925845810
Pt	8.14670689718782	13.86866723841805	9.54016641433821

PtCe39O80 D3 (-943.914593 eV)

Ce	8.46041167390159	9.55722759362100	14.93419315196160
Ce	13.49597065591720	9.46619641681166	14.96617834484841
Ce	11.02031139898252	12.13174262156270	14.89169542668599
Ce	10.92804007222417	6.88766499587017	14.88336680980651
Ce	13.69602638504765	12.23277017298380	12.28650026038429
Ce	8.34453916904335	12.32951977611791	12.26180830997486
Ce	13.59440908922266	6.68684398557712	12.28224122517691
Ce	8.25151069824530	6.78346907085449	12.24703338606247
Ce	16.13969035770685	9.41767404720797	12.26278586067384
Ce	5.80713340278776	9.59003905769953	12.28812555866240
Ce	10.97000626151205	9.50584680050607	12.14360268202248
Ce	11.06403044463568	14.89376375625192	12.11814816204561
Ce	10.87293002215220	4.12102170132369	12.12245127442683
Ce	13.61607621690146	14.91994449936149	9.51846322302428
Ce	16.18935924592520	12.16907240964254	9.51485033656383
Ce	8.52252857229166	14.99075623094364	9.51308906668691
Ce	11.03654848660672	12.15659733863682	9.50291267510056
Ce	18.52846479107797	9.38175550800357	9.51051557043650
Ce	13.58880693439644	9.45384447758405	9.49754818613031
Ce	8.31657018913386	9.56951800421742	9.47515748492174
Ce	5.76378693710495	12.33334013941950	9.54021647536465
Ce	16.09953019982202	6.66269413052974	9.52200577778428
Ce	10.92023417251729	6.84808167846462	9.48983997440952
Ce	13.42134251932865	3.99897882156391	9.53456202341051
Ce	3.41687662818396	9.62577324003718	9.69702387389001
Ce	5.66220520877994	6.83004843083363	9.55562600605482
Ce	8.33906750664943	4.10245830006695	9.49718248188511
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Ce	10.91525965502112	4.05702695734830	6.90745495080139
Ce	10.94011570944445	9.49539931854769	6.81463589865644
Ce	16.15090266439310	9.41085873509858	6.76513420223788
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Ce	8.39778064410928	12.39964417024199	6.76833345045540
Ce	13.61657128164942	6.67186637464594	6.74895292096997
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Ce	11.07475120513425	12.12129642462424	4.11526970428624
Ce	11.04720871616689	6.81003241115175	4.10526562552663
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O	12.57691083907648	11.07919129009930	16.01524482866854
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O	9.38081019580702	7.93801563420933	15.99441648495521
O	9.65396014342494	13.60675151229624	13.55191011823173
O	12.45482036316104	13.55237247983378	13.56534158231676
O	15.10651285203338	10.82371797317840	13.56853749470339
O	6.96590056947579	10.97470747209323	13.57702189733441
O	15.05200039266942	8.04714331639609	13.56385795494562
O	6.91518332016552	8.16627655721784	13.56032882228791
O	12.30299692384101	5.41560017961632	13.56556597292138
O	9.51058801252871	5.45833420479831	13.54120140944827
O	9.69584554114070	10.86866060740410	13.46922214263816
O	12.33615703351143	10.81571891146753	13.48334932891195
O	12.28544930657335	8.15332030124641	13.48040241321485
O	9.64279654027855	8.19347565828313	13.46176622284041
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O	12.67051409512307	15.98690967356504	11.10054393510252
O	12.45057318769956	2.96987744486543	11.12596666486147
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O	15.15197185915038	13.50521652005162	10.89454925897395
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O	17.64016032594632	8.01877668347391	10.88758673025833
O	15.00582422239988	5.37085301855844	10.90445374868924
O	6.77916151580483	5.49541404186533	10.90858735303221
O	4.38077849021369	10.96381557161958	11.14889634306554
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O	12.31829397512616	8.11973083235145	10.84410181565994
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O	9.59054808923715	10.90032037693867	8.11615347973945
O	12.34473924987736	10.82691528354472	8.13454743354334
O	6.85560389115391	10.94571290342313	8.03935538587663
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O	6.78496963466562	8.25784300768376	7.97134742888242
O	9.50187944409705	8.15552829920230	8.09493606194784
O	15.15464616187452	13.49471011801333	8.12211862128824
O	17.67614171677941	10.76830562534117	8.13110449158380
O	17.62785933233029	8.02003374673823	8.13508781757327
O	7.01218266309587	13.63499579428737	8.13964588694067
O	4.05601838654340	11.25180386323503	8.56211448863355
O	4.03973909195628	7.96978978716730	8.56048454384826
O	15.02062932661691	5.37019894747582	8.13474670512333
O	6.87314801426357	5.54916129762254	8.13003006246455
O	9.52684625747738	16.03778093125021	7.90492195050461
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O	12.46413841724256	2.93812655769684	7.93579027016142
O	9.29996610169917	3.00931585359772	7.90422156983901
O	12.31774393858864	10.79882849806912	5.52002043595993
O	9.64561359604342	10.85870440172589	5.45309090827008
O	12.31624309061683	8.13269867320388	5.51998686448327
O	9.69654451831074	8.14350917674851	5.42960908831486
O	12.46618943379500	13.53560118149289	5.43453052925968
O	15.09700988704437	10.80875448899788	5.44665454383528
O	9.66371649435517	13.60575172137814	5.44359396210296
O	15.07818997491482	8.04010260438099	5.45305064425191
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O	9.54795328029701	5.40658969420008	5.42227217762177
O	6.93785591666828	8.11881113993771	5.24316798636514
O	12.35829444960428	5.38324849140821	5.43449061896043
O	12.63933386990463	11.08584863013511	3.01359669700556
O	9.56812551332505	11.04333911968000	2.88998792035554
O	12.62119496324578	7.83802610215413	3.00260739671500
O	9.52051968884161	7.83693567149760	2.87692037992808
Pt	6.72627563215957	9.56756949961451	6.55240359561979

PtCe₃₉O₈₀ D4 (-945.716619 eV)

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Ce	11.03402071537062	12.10194780765248	14.90300400344365
Ce	10.92051280978507	6.86199114526699	14.89973150995034
Ce	13.71227630488875	12.20758339135758	12.27163088514111
Ce	8.37513845149516	12.31226353796795	12.28351675905119
Ce	13.59025514553713	6.65376918956837	12.29916271540073
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Ce	16.14886825271966	9.34702011831377	12.28849729012551
Ce	5.82984840541145	9.57801228788784	12.25510475417408
Ce	10.99441593913430	9.48425640645703	12.16179415851965
Ce	11.08870464161685	14.88140811291120	12.13300328477142
Ce	10.89149316407865	4.07969678413966	12.10474716283801
Ce	13.60794292101464	14.92845901121161	9.50504537144979
Ce	16.19586378856819	12.19202907777807	9.44161362829441
Ce	8.55092520913685	14.99111075714293	9.51922125738943
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Ce	13.63687221113184	9.44837485729107	9.50521757923628
Ce	5.87185664204150	12.33174004489845	9.51550437862673
Ce	16.10649539841305	6.63277523971829	9.56960075893970
Ce	8.37891816440608	9.54479329769390	9.50289164163624
Ce	10.95095638762262	6.83871419844679	9.50020813412495
Ce	13.43295059934780	3.99189180595926	9.49944851238842
Ce	3.44440762847167	9.61847494033357	9.50029167969260
Ce	5.78938976820725	6.82988584438669	9.49064916112483
Ce	8.37629522340915	4.07945924525141	9.48251599738602
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Ce	16.14616030298786	9.48063930549440	6.71993867472310
Ce	5.83108351414469	9.58590194988392	6.75084075861208
Ce	13.68818352710939	12.25794229073420	6.70935881493156
Ce	8.36825610718006	12.32780206406714	6.73684545097533
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Ce	11.01557694499749	12.14549591510261	4.10308728994087
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O	12.58356727758086	11.06800116552984	16.02662103209882
O	12.51649747115135	7.86700887149020	16.02527245855369
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O	9.67098591793378	13.57788908743039	13.58226552110445
O	12.47396631215637	13.51979020403277	13.56376244902921
O	15.11302941947205	10.76824031873991	13.56955263472490
O	6.92188303163528	10.94303604328656	13.57002237377632
O	15.05917744638355	8.00252661974949	13.59327438491877
O	6.86961745488606	8.17203139652595	13.56007161351719
O	12.30076767780200	5.38375702595382	13.57416569450774
O	9.51039823126352	5.44054629948394	13.55774960843376
O	12.34558701332299	10.79175067270110	13.49769619435513
O	9.69004463031203	10.84416768042776	13.49234702692282
O	12.28801854076289	8.12491153221338	13.50030232989642
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O	12.67599185890790	15.98379818205583	11.11132699103170
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O	15.16031208776744	13.48875382467796	10.84616928984155
O	6.96926898390893	13.62417141123658	10.90277311506727
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O	15.07908396343318	10.77371015643370	10.85414367571464
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O	9.66370007173800	10.86857305020816	10.85925481481147
O	7.02036871648979	10.91457579019843	10.85946024579436
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O	12.32888008772384	8.11597664069150	10.85585338865450
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O	9.60050621148645	8.15639322988449	10.85810540924775
O	12.39611075339161	13.45989096294549	10.83778527865415
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O	12.25193221486375	5.47692911665295	10.83438495425843
O	9.59964471099877	5.51927341813096	10.82168565265999
O	12.38705486294506	13.47758541120449	8.17280017752825
O	9.73628338189228	13.51503886464334	8.18332350628622
O	9.60757006605775	5.53613367489219	8.15871532496245
O	12.26337915006234	5.49453707240394	8.16553431530724
O	14.98289646128399	10.81425118410201	8.12443091351821
O	12.37817879297304	10.83223608199079	8.15360375483084
O	9.64775734872480	10.88488166619909	8.14905088414138
O	15.03526411395113	8.08477625694776	8.15568610426023
O	12.37195354358306	8.12189717472002	8.14625902725406
O	7.01005736399703	10.91721001969217	8.15669333124220
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O	6.98254387643241	8.21195794459148	8.14324267878112
O	15.16167569567365	13.52209777946651	8.07925381594944
O	17.68275577787803	10.80671356217209	8.08598789592088
O	17.72746517400831	8.04026083071544	8.16366448916194
O	6.96825154030364	13.62939355687148	8.13486429095730
O	4.34220524608507	10.98263433506104	8.12910193129460
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O	6.83880748743647	5.50033779508764	8.10311317171687
O	9.51281959968719	16.04429768721009	7.91814482794937
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O	9.32678269227069	3.01626913459843	7.88792295421380
O	12.33766227246330	10.82975027885291	5.50918736381122
O	9.69031694700160	10.86767380245006	5.51578122747783
O	12.30553932284955	8.16219692391902	5.51092572451032
O	9.64857528799406	8.20333755707261	5.51638726020319
O	12.43911101441246	13.56931529086860	5.43256484372226
O	9.64370143659727	13.60528009787829	5.44636178563308
O	15.11260720343093	10.86832764359080	5.41719984416970
O	15.07153857816729	8.09795664912457	5.43982262174192
O	6.92288226381093	10.96132356467995	5.44372944423263
O	9.54311510507641	5.46894822923479	5.42430665218226
O	6.88115999571271	8.19256987819284	5.43390066810852
O	12.35074042906607	5.43311093303761	5.43730269825225
O	12.59163734040440	11.10944151651747	2.98710067735579
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O	12.52760825866511	7.91138210726334	2.97592193689119
O	9.38597130512689	7.95219728186513	2.99437734928061
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PdCe₃₉O₈₀ D1 (-941.923496 eV)

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Ce	8.37334729077193	6.72546187803748	12.31562259120138
Ce	13.64801570722522	6.62864185421549	12.30136345468254
Ce	13.68172374764058	12.18751142915793	12.27549946950645
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Ce	5.96178533671452	9.58014335042918	12.12761947242754
Ce	11.00148657338233	9.41012694561346	12.18793295422992
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Ce	10.95004103203524	4.02902299604784	12.12403207876881
Ce	13.57646584012868	14.87658840654710	9.51847312682310
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Ce	5.85477542081840	12.41718996701751	9.43266547244317
Ce	16.16910907103884	12.15286970824170	9.50474346018996
Ce	10.96726194946991	12.09507297180535	9.50319007029510
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Ce	10.95416749007842	6.82239070340188	9.57393712757057
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Ce	3.48806071032099	9.64025167411635	9.48412396337942
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Ce	16.11924902070010	9.41782601949094	6.75907304494644
Ce	13.66731117928988	12.22359486645702	6.73847448081022
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Ce	8.26352046570581	6.83201551293291	6.74861877363178
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O	12.58702904958028	11.04679267139235	16.01727079890426
O	9.39406282887232	7.87431217622123	16.09282079921767
O	9.43400529099730	11.07815534302611	16.01499966217076
O	6.91191777429132	11.00352029195654	13.42560681865699
O	9.65751285525680	13.55418925612635	13.56143699807990
O	12.44871479499117	13.50416570403007	13.57942931828322
O	15.10817165779253	10.79588259769555	13.57219197103745
O	15.10269884224217	8.02816805477786	13.58176340497915
O	9.61856655742715	5.40401265427297	13.59869283902615
O	12.39576350727758	5.35303453324234	13.59001875373945
O	6.92452132457814	8.18059714133636	13.50224393348306
O	9.69346634322426	8.16585695725774	13.62957930581011
O	12.33583916866354	8.08466708233264	13.52764760964478
O	12.34558076721575	10.76482767392548	13.50468845030731
O	9.68366556837032	10.82860065293630	13.45175562103576
O	12.66525875572218	15.94009813078642	11.14265695565289
O	9.51445708503551	15.97458180029536	11.11997910883522
O	12.46818882568210	2.90783427510194	11.05602850520497
O	9.30316019863505	2.93194118357270	11.11293689299797
O	6.88140210218723	5.57653984797766	10.87640815641340
O	6.93827764280739	13.58204672944537	10.91787033004104
O	15.12075737552253	13.47176197391270	10.89339138201064

O	4.43338591398114	10.98723516557732	10.85048925301652
O	17.68512128629730	8.00676895040109	10.86966800650173
O	15.04665538062244	5.33387327630253	10.85988393189714
O	17.67654585872024	10.76823387974326	10.87002137683386
O	7.11477108179302	10.87555068877493	10.53692606123104
O	4.47838625800690	8.24192358543947	10.86213222398277
O	9.79931836037685	7.89703311420909	11.12144930116956
O	12.42616810063912	8.08495665893237	10.88077393175541
O	12.33704135054942	10.80675919729883	10.87302711387859
O	14.99635926146570	10.75995311413313	10.86230105813884
O	9.70589010774340	13.41752164729950	10.82797989120400
O	15.01662935326787	8.05888548250344	10.85877801303278
O	12.34086047634877	13.41699465638791	10.83604282303024
O	9.64373509760631	5.39533948348122	10.83267732550894
O	12.28716530325582	5.44482320282763	10.86046051253477
O	9.59253730722948	10.60857803030431	10.74872594118068
O	7.29012775335501	8.30622992849165	10.76162090795186
O	9.35454348463922	10.84624232014604	8.19638969486518
O	7.06683224989905	8.55087545380419	8.19175580609446
O	12.34305789758461	13.43648377412313	8.18647164533665
O	9.71014066062344	13.46303437174448	8.13078725856792
O	9.58865871498206	5.59559627971285	8.16625762643662
O	14.95690342280026	10.77717242024759	8.15985318952037
O	12.24722404721880	5.48837072174619	8.18193703287527
O	12.28841218292296	10.81613839180732	8.16867277072599
O	14.94098974417586	8.07667815812901	8.15940699076277
O	9.54449584034707	8.29017547238894	8.40918590139208
O	12.28122807322814	8.12010203759821	8.15700228307089
O	6.75971633200624	11.24074161705082	7.84789724700732
O	17.644405239251252	10.77105643140352	8.11774303112442
O	15.12320456567082	13.47807791701809	8.12142273159404
O	4.37912141094147	8.26986671949102	8.11502013072185
O	6.95664077784537	13.83809021961838	8.15348233608519
O	17.62253607559008	8.02119763784318	8.10667828442292
O	4.15298487754995	11.02195701349313	8.09991569033910
O	15.00839400132946	5.37075433569517	8.09093228852344
O	6.81576697895109	5.65993299555217	8.04933691844395
O	9.53674422440529	16.02923204214102	7.92301353971188
O	12.67257423060632	15.96698096071747	7.92538507771564
O	12.44864871761190	2.97306505182181	7.86071042926907
O	9.30431014239940	3.04115910066973	7.91877541676017
O	9.65390896330141	10.93162780747945	5.56921910928153
O	12.28587983555720	10.81910843084966	5.54375117813383
O	12.23967945545172	8.17430235628946	5.54330845486910
O	9.60442587670255	8.23304214059390	5.59472482931452
O	6.83709624348814	8.19537415112261	5.47880478704090
O	15.06985633627930	10.82546535383529	5.45376258837162
O	12.44716957066434	13.55462237992342	5.44664849513754
O	15.02199014705202	8.05582367603953	5.44699846056786
O	9.63177120045148	13.66568597046472	5.39836951973246
O	9.50139975695392	5.50155570290068	5.44014639353790
O	12.28962726885559	5.43379355432277	5.43849969134450
O	6.89369608153521	10.96351456488383	5.23954106646665
O	9.45679440344876	11.15436738878503	3.00437367677906
O	12.59585415752418	11.10976548937325	3.01715051013545
O	9.34827805252537	7.96045128359510	3.04111874200977
O	12.49610245270348	7.89230017758324	3.00901450801522
Pd	8.35498796400655	9.58990999208058	9.46230659454318

PdCe₃₉O₈₀ D2 (-941.724573 eV)

Ce	8.43543527443979	9.40543208770895	14.97455485261317
Ce	13.50703970827258	9.38550334178201	14.94722818146804
Ce	10.98343891813573	12.00665034643161	14.96727077310708
Ce	10.95602846747603	6.78707260662163	14.85829371740080
Ce	13.64191067193433	12.20844971200614	12.29807024092488
Ce	8.32091674634869	12.26226187522360	12.37152495948802
Ce	13.61320573983471	6.67038059721821	12.24534541756705
Ce	8.29416831580999	6.69371348855757	12.24323824716581
Ce	16.12739534704264	9.41872562138764	12.24626589068157
Ce	5.81274898998555	9.44258020946333	12.26993306695775
Ce	10.95702905471778	9.49365615888962	12.15412562392272
Ce	11.13080544804804	14.97886700541248	12.43937830281068
Ce	10.93770208681162	4.06152074289141	12.06928410110847
Ce	13.55623333529024	14.96978320551701	9.58308763489112
Ce	16.14677239991490	12.20359813584813	9.53263588535566
Ce	10.94964425527998	12.32987632737510	9.52708266073190
Ce	18.51034336392824	9.42794449127429	9.49907042409969
Ce	13.55707084984284	9.50483681715066	9.50136643731862
Ce	8.34803747442408	9.56900840914847	9.50371544929204
Ce	5.69388660283667	12.16578698470217	9.55752048924901
Ce	16.10310652337568	6.70700932096339	9.47599065599567
Ce	10.95002457306009	6.85996808229875	9.47478383900921
Ce	13.46354981155304	4.02587441127785	9.44618229413717
Ce	3.39661964415147	9.41117573363518	9.50174197209236
Ce	5.81609512216016	6.74374624651344	9.45753558228845
Ce	8.41820957054319	4.05237806817799	9.44083694289350
Ce	11.16469566727611	15.05325830778669	6.69622491274957
Ce	10.94167757116544	4.12781436577458	6.81908426649456
Ce	10.96789087269860	9.55347391400335	6.84905970643673
Ce	16.12224410759735	9.47387433669658	6.74802679419540
Ce	5.81733282620693	9.54881681162148	6.74044996860776
Ce	13.65272794891499	12.27216658053998	6.76852044640599
Ce	8.34107028524308	12.34307863260941	6.70978425967810
Ce	13.61630524016528	6.72931497610233	6.69860906225388
Ce	8.29706793723846	6.77099674896110	6.69887046583200
Ce	10.99053868545572	12.13058474033042	4.09959409317313
Ce	10.95474987768718	6.90042650364134	4.08432704861648
Ce	13.49837392165318	9.49745000294002	4.04997148311165
Ce	8.44093314753219	9.53282277462786	4.03352248189546
O	9.39665811235680	10.95526256040628	16.06667607837641
O	12.55381016083734	10.94724495253006	16.05523474687854
O	12.54588377713337	7.78093270180387	15.98922550666432
O	9.39135716237664	7.78813469712929	16.00320711473491
O	9.62153448235642	13.37483725102293	13.70755641071268
O	12.45762033686524	13.48663558757444	13.68940812838802
O	15.06788216471853	10.77991473289197	13.57488914611995
O	6.87622043481745	10.82045681085035	13.59284397741975
O	15.04768390720026	8.01807954336850	13.54923653189461
O	6.86096911789660	8.04130380312096	13.55953163705333
O	12.34161747966574	5.36356952296590	13.52584723264300
O	9.54848925473368	5.36731061716096	13.52098866344660
O	9.63043947425701	10.73299255154925	13.52367986787328
O	12.29994441595553	10.76476647204420	13.50950008829477
O	12.27630313922279	8.10530810620498	13.46649194106120
O	9.63083650705648	8.09891124184904	13.46789547069682
O	10.13742461247516	16.44628592957089	13.13045232116781
O	12.72335547739421	16.04225747209288	11.18636726376088
O	12.50373603097034	2.95587497220976	11.02810119001655
O	9.36602436042053	2.97835572002406	11.02146207065642
O	15.08560340163572	13.49940367274944	10.93753209777354
O	6.74515075425015	13.49355305947213	11.00049518337559
O	17.65116694798098	10.79643977690954	10.89227798232833

O	17.63365404607748	8.04442834903215	10.86744628901065
O	15.03138400925685	5.38639151931886	10.84842742533236
O	6.86982387974491	5.41488553449631	10.83099752117034
O	4.25430776134229	10.79939284256772	10.89778963707619
O	4.28099506129064	8.04712274397232	10.85835038959218
O	9.59591880358024	10.99343412567820	10.88390225605787
O	12.30483297167260	10.87293334933924	10.85532780932046
O	14.96919653442976	10.79822690707076	10.86738115718669
O	12.31672355202885	8.13564707232333	10.84262964760227
O	9.58976230634053	8.19402719862322	10.83419120800307
O	6.94125027543192	10.81556516693923	10.88540866053243
O	14.95158560092678	8.10276027124647	10.83469220855006
O	6.96803261654603	8.13665803737591	10.83644780333368
O	9.56872206168233	13.81012232532177	10.96248491201152
O	12.29718889833394	13.49236676239077	10.91868541864318
O	12.26673919220300	5.49185878248136	10.79166806760007
O	9.62468713457364	5.51973205310764	10.79281242589325
O	12.31737071047104	13.52508611769471	8.18115648511794
O	9.58361422409715	13.83862434631975	8.14110246501387
O	9.62253669047477	5.55367223919206	8.12704214485816
O	12.26866601066705	5.52495128750556	8.12860478701529
O	14.97116634516589	10.82599615493235	8.16352695904012
O	14.95331286802682	8.13237348499207	8.13866394433875
O	9.60085250955495	11.01742066216303	8.15627127308457
O	12.30903260169403	10.90581059476155	8.17735954097398
O	6.94264571544454	10.86683853599577	8.16999642440214
O	12.32007190508207	8.16750441492614	8.13078928635070
O	6.96819300604307	8.18353563043504	8.13537053653036
O	9.59274944662803	8.22633404878857	8.14275045852261
O	15.10341632816305	13.52887510019650	8.16753812949032
O	17.65106065895622	10.82136070746092	8.13851054160296
O	17.63591845649406	8.06575097921006	8.11345037041344
O	6.76286798029388	13.53946981126499	8.12664719621624
O	4.25321144246247	10.85252097968387	8.16098131807746
O	4.28151659440531	8.09920064333951	8.10166391510625
O	15.03236537035462	5.41508648804983	8.07828754675849
O	6.86644502903345	5.45626134711610	8.05570362453548
O	10.26342883707662	16.53880181764952	5.93241492402268
O	12.73521327701011	16.08832842099368	8.02211239791126
O	12.50557564454103	2.99496371889585	7.83970635443422
O	9.37136733046512	3.01503624848344	7.84257292410446
O	12.30946791314475	10.84803921643327	5.52196898767883
O	9.63839265741919	10.82641067889621	5.51308051299270
O	12.28164374791472	8.18768330072824	5.50697255553512
O	9.64157896356680	8.18849198990034	5.50465247191187
O	12.47833501596280	13.56690910955308	5.40821932642785
O	15.07512435072881	10.86288508505689	5.45163641829177
O	9.63474936739574	13.47085300350253	5.38636400672336
O	15.05047817624591	8.09684710529051	5.42097670400928
O	6.88259325331623	10.94623953218777	5.45647543072313
O	9.55007526202130	5.46259472221479	5.39855659149174
O	6.86981660812619	8.16981738677939	5.41730054443607
O	12.34596597189289	5.44777677724671	5.39263819206836
O	12.53857205854701	11.06982870845224	2.97584788595745
O	9.41232797874122	11.09242249695152	2.97220605652174
O	12.53646791034270	7.90925833138267	2.97592314397901
O	9.38230170924716	7.92647401818224	2.97009359267338
Pd	8.14881158536224	13.86891507416766	9.56002753278109

PdCe₃₉O₈₀ D3 (-942.605572 eV)

Ce	13.57945203491113	9.45128732912599	14.90724171952768
Ce	10.95962640304614	6.86900381603116	9.49292440496701
Ce	18.56176087157404	9.20818727726335	9.48927758201928
Ce	8.47697759547943	9.51665862749616	14.95148183914953
Ce	11.04760323503126	12.09472811846596	14.91313034293417
Ce	10.98382614373977	6.87446731310733	14.87997315439765
Ce	13.71990131425629	12.25958547680662	12.30667609399350
Ce	8.36452376517719	12.30625988878351	12.28653696813458
Ce	13.64836784743328	6.70479652659517	12.24264164589253
Ce	8.29363445709811	6.77358672243758	12.26882501075390
Ce	16.25573235676105	9.38844821982158	12.23140310464042
Ce	5.83176670720443	9.57331841572903	12.25928080465890
Ce	11.02521152060245	9.51183830644232	12.14416124562973
Ce	11.00403807489394	14.89599762135574	12.19035888831311
Ce	10.92355786407150	4.12938496168899	12.11849614891153
Ce	13.52217290001839	15.02633347342037	9.60974668229935
Ce	8.52519342637411	14.99077276420682	9.51810028311829
Ce	11.06944376239216	12.17949230174014	9.51027123581124
Ce	13.68596752483571	9.49100803260391	9.47855493184396
Ce	5.86728865584375	12.33824393390277	9.51631998642866
Ce	16.14531186486336	6.63282069682581	9.48184978496929
Ce	8.38336556171372	9.55825686800515	9.50375248588206
Ce	13.44110691507815	4.04373962541148	9.48390303396052
Ce	3.44899260376793	9.62107162624041	9.50172944895486
Ce	5.78880591752834	6.83159806851021	9.49981508249781
Ce	8.37764521930829	4.09430766852412	9.49929978644653
Ce	11.06639954035379	14.89968988699776	6.90521282554846
Ce	10.90661510862430	4.13512758680382	6.86086355744055
Ce	11.00087130571179	9.51069859482320	6.84998899911948
Ce	16.24902798760142	9.39085940832815	6.75251985434250
Ce	5.82985063897271	9.59491177146205	6.75122713333602
Ce	13.71164804130196	12.19546214389256	6.68551754708915
Ce	8.37476889072482	12.32715033995267	6.73852343058223
Ce	13.63452107090673	6.70209886982928	6.72351689558794
Ce	8.28163883514110	6.78187496972965	6.72710503939168
Ce	11.03718795447550	12.12324094808111	4.10177858644451
Ce	10.95565071529303	6.89558111022789	4.10463388405690
Ce	13.55644831708369	9.44878104315990	4.06828880920384
Ce	8.45686389891185	9.55934157786839	4.05604363791221
O	9.44797286660047	11.08313027608442	16.03268398198550
O	12.60223856048768	11.03546454241505	16.01463382079967
O	12.56908863649456	7.86521930323238	15.99257171114490
O	9.40482155781000	7.90328219785793	16.01173895195917
O	9.62491504752333	13.58107282602836	13.60284135739711
O	12.42232469462808	13.54013670014281	13.62096742281253
O	15.08593680202117	10.78205378076395	13.57336353804226
O	6.91718105930790	10.93154593859646	13.57419083632568
O	15.08394148295270	8.01868833889633	13.55728550532854
O	6.88994856169147	8.16801758622540	13.56500612819814
O	12.32531655575727	5.41684633882491	13.55348880236341
O	9.53997915848713	5.45082421422050	13.55818192165959
O	12.34501136316778	10.81988644245025	13.48742020242549
O	9.69204959771780	10.84728895119219	13.49385486581198
O	12.32160385356609	8.15398580706235	13.46905738141956
O	9.66675084020154	8.18610129902843	13.48298932567981
O	12.56755938596975	16.06942323680292	11.21200076166913
O	9.45791407823877	16.04079142950182	11.13459373356993
O	12.45831748960742	2.97223306169344	11.08137880950037
O	9.32998558626530	3.00973561053827	11.07796790946003
O	14.99573284167091	13.69596385708727	10.96553534558877
O	6.93443839704992	13.62530495299960	10.90447594648867
O	17.93917447145200	10.34938380023268	11.13125480971038

O	17.60574802698309	7.75401296018622	10.83743447988678
O	14.97108354253255	5.34887178322616	10.88007147070634
O	6.83565544333466	5.49711494478079	10.87986986443857
O	4.34436305098778	10.97624196955092	10.88451204690672
O	4.29508932622812	8.22518427272350	10.87826259491826
O	15.13552956201839	10.88444538393393	10.86879070031832
O	12.44847934082794	10.86861173716009	10.85614036204383
O	9.67798383779485	10.88563491300390	10.85381134449260
O	7.01838052464100	10.91561120516574	10.86246972670185
O	14.98517371641396	8.12594607716270	10.83713381095410
O	12.35725076148521	8.15561316626215	10.83105649920072
O	6.97347746586834	8.21360780793348	10.85256183710852
O	9.61160660120726	8.17987503734154	10.85490612405584
O	12.30118041240615	13.52660607912103	10.88236579479486
O	9.68857836969732	13.50804269981987	10.85438943313606
O	12.24687418159164	5.51216985956115	10.82247804723320
O	9.59950706752853	5.54187765598026	10.82630154561563
O	12.39587884545707	13.50587389658112	8.17350764069038
O	9.73718690388097	13.51880941331859	8.18843876750828
O	9.58992190818927	5.54702390100081	8.16289378147625
O	12.23941290597587	5.51317467341318	8.15364590365050
O	15.13884586288800	10.84088103697912	8.09443204383383
O	12.42291258831291	10.85698539067002	8.13213901500319
O	9.66684291035823	10.89416826271476	8.15207574613278
O	14.97484839954054	8.10805067153553	8.12935406671408
O	12.34768591412378	8.15440336603070	8.14581744295520
O	7.01593169965830	10.92568439556254	8.15582077925793
O	9.60254943086661	8.18185305634504	8.14239679790015
O	6.96804552362783	8.22194168434815	8.14952895083870
O	15.04341294038193	13.66981033453770	8.14687387005854
O	17.95307392438235	10.35379118106767	7.86025884722947
O	17.59549046242124	7.76354563108037	8.13166115911185
O	6.96824784251831	13.63653043114166	8.13623180715878
O	4.34192096235471	10.98825088753034	8.12995517221463
O	4.29047797296951	8.23441087570575	8.12149757613228
O	14.96571287798299	5.34202092511126	8.08739060023132
O	6.82498771721003	5.50568459773923	8.11240655934861
O	9.48955373173592	16.04042618941252	7.91618968573818
O	12.56586809738969	16.06259474497519	7.99399206606261
O	12.44330947221546	2.97566103530860	7.88800755192045
O	9.31759622015839	3.01558285545011	7.90539993237128
O	12.33296563801972	10.81331994595897	5.50845849015819
O	9.68419869150222	10.86554809665005	5.51215992260380
O	12.29276397806012	8.15689913426164	5.50973277028903
O	9.63874810704416	8.20006397319729	5.51362041704440
O	12.45424928583542	13.53636761669906	5.43112637206868
O	9.65543254181453	13.60022397050446	5.45151705222043
O	15.07258952985876	10.79201787045363	5.39865745448371
O	15.05350053943591	8.02746296095031	5.41483681235637
O	6.92150544307474	10.96705247442084	5.44406422859164
O	9.51782893354151	5.46755471338776	5.42693757278518
O	6.87205143280508	8.20091057708949	5.43305255392344
O	12.30224071913810	5.42299292604573	5.42109474607308
O	12.58742121374813	11.05938535950489	2.99283295605860
O	9.43887207313550	11.14494140224475	2.98178935552376
O	12.54206751058970	7.86882435462403	2.98397141719169
O	9.39310954066635	7.96980153535860	2.98051367445795
Pd	15.29665856408995	12.32308367459846	9.50990779258575

PdCe₃₉O₈₀ D4 (-944.290352 eV)

Ce	13.54651144685431	9.42601194664096	14.92802554019173
Ce	8.45900587049619	9.52927509420777	14.95743411357951
Ce	11.05355041361245	12.09232798136838	14.89495302017159
Ce	10.94798833351688	6.85751811342700	14.88349903128910
Ce	13.72979898457721	12.20062332832667	12.26398288133947
Ce	8.37170027913498	12.31068881256300	12.28124736068950
Ce	13.62279013452311	6.66936959794706	12.26934467022577
Ce	8.27002655336357	6.75635586860316	12.26699396967825
Ce	16.19579899344675	9.37727378900663	12.23547356540136
Ce	5.82085078026223	9.57762891868851	12.25205804915695
Ce	10.98530984507884	9.48395740807748	12.15750582371906
Ce	11.10087123519874	14.86822841131136	12.13801946544672
Ce	10.90994584823529	4.09862893151766	12.10548066110842
Ce	13.63815861682957	14.89092236895743	9.50977661534816
Ce	16.24030906174530	12.13991191471939	9.48324924996649
Ce	8.55545980329718	14.98667514968814	9.51627962016908
Ce	11.04412772160534	12.15066968776351	9.50794703164742
Ce	13.62305934401733	9.45037721451491	9.50693542724753
Ce	5.86191047119535	12.33673834915763	9.50817174067012
Ce	16.16100353533683	6.69414937573811	9.53876716674597
Ce	8.36368887572101	9.54947379830258	9.50162464355136
Ce	10.94422157132659	6.84535505860679	9.49846449907402
Ce	13.46682504364421	4.03569966119598	9.49804230329523
Ce	3.43365884722149	9.62022074407665	9.49516493653009
Ce	5.77938498498563	6.83280698696121	9.48557724456166
Ce	8.37412247904230	4.08536005901042	9.48125897652828
Ce	11.09096672566207	14.89956984171042	6.89610023761394
Ce	10.93049931161824	4.12702863106307	6.86904055346115
Ce	10.99811626149219	9.51192121795538	6.85214233123282
Ce	16.20843265267343	9.46052867064225	6.78943562980970
Ce	5.82561395284797	9.59348139772443	6.74415213805528
Ce	13.72557603810962	12.24276521321544	6.73857590835135
Ce	8.37013538452411	12.33042462643763	6.73564540543061
Ce	13.65141127061054	6.70608925825528	6.75343896899867
Ce	8.28797543156149	6.78056006308376	6.72090190875748
Ce	11.05558532720446	12.13437209656438	4.12342018433087
Ce	10.97971110603986	6.89694991546644	4.11571835315319
Ce	13.56479126152481	9.47085770917616	4.09249735847862
Ce	8.46926317308511	9.56126310559828	4.05255487946722
O	9.44676775391967	11.09080969908631	16.02771726141754
O	12.59698728507611	11.03067167226796	16.01536249234621
O	12.53575532699131	7.85003937610050	16.00723049255456
O	9.39011721565824	7.91489328423130	16.01896166702894
O	9.67579148680061	13.57115556840190	13.57829516316882
O	12.46135862608021	13.52205179403376	13.57316958876339
O	15.10558975770683	10.78209433647167	13.56716290564604
O	6.92185973582236	10.93853762158368	13.56746781407566
O	15.04493190402546	8.01858803961017	13.57342953299545
O	6.86671221965879	8.17244179035267	13.55850454833068
O	12.30077605978576	5.38333847389737	13.56290099452420
O	9.51717435858035	5.44029876386460	13.55432997524548
O	12.34561686829613	10.78849838480299	13.48912968250041
O	9.68649189857612	10.84059774242763	13.49952291530125
O	12.28673209388501	8.12308245036874	13.48565654805482
O	9.63146781815812	8.17195707787739	13.49037307828598
O	12.68219858899447	15.97711470144548	11.10787912126732
O	9.54055688901711	16.03089760783060	11.10930854877367
O	12.46736613424248	2.95802680034005	11.08105794162694
O	9.32099368187293	2.99145375028795	11.06303344612292
O	15.14822494188571	13.48819527650085	10.87552962986409
O	6.96926504917575	13.62756280702803	10.89273822578370
O	17.65907356402699	10.78263394036873	10.90698212605588

O	17.57717868000256	7.95321630811217	10.94393172699701
O	15.01120161962452	5.35649761508436	10.89909032015431
O	6.82874159437129	5.49244753539589	10.86523309309944
O	4.33697950022836	10.98065162772370	10.87462642529571
O	4.28711555731121	8.22826101437844	10.86548573174197
O	15.01326644748024	10.77601498295514	10.85800343141337
O	12.37407840311115	10.82376297487397	10.86243989350674
O	9.63448272380533	10.87661777335410	10.86891829624895
O	7.00177654639020	10.91732876296778	10.85562584902240
O	14.92837851957720	8.06461658924529	10.86853014404235
O	12.31208285205211	8.11491233896957	10.85505140975835
O	6.95507052588203	8.20870784943531	10.84599665513716
O	9.58410201530282	8.15914852827365	10.85592053889164
O	12.39294298249982	13.45574336333479	10.83903499666185
O	9.73384470471244	13.50218535058621	10.84692730116471
O	12.24989209260942	5.48515812308944	10.82766676868000
O	9.59266396476136	5.52055506696602	10.82326202693409
O	12.38691247742725	13.47313897766007	8.17730145465441
O	9.73303905579250	13.51548969383287	8.17728809664652
O	9.60066208073859	5.53484565322036	8.15712475728948
O	12.26195783782983	5.50090780109496	8.16671888467852
O	14.97703864788072	10.80369088019628	8.14806144001087
O	12.36543566953634	10.83583798073316	8.15448592035502
O	9.63574172545843	10.88538238923102	8.15165247406510
O	14.98007508024774	8.09184605907413	8.16111863777551
O	12.33683298756174	8.12451195839984	8.14862897752854
O	7.00146044699961	10.92418784927013	8.14985088573343
O	9.60030110671729	8.17291948975871	8.14383327243664
O	6.96692357137914	8.21711183311868	8.13851827297127
O	15.14864686598884	13.51389016223439	8.11029880002165
O	17.63032823335851	10.83562924633667	8.07825893318474
O	17.62262978232292	8.00464243743116	8.11536571787160
O	6.96793550021529	13.63591787922284	8.12907050783102
O	4.33712657858352	10.98603907540887	8.12367597766984
O	4.29881860681383	8.23503960720808	8.11453478448948
O	15.01891305666037	5.38195280264385	8.13699213097485
O	6.83656345003262	5.50300278426363	8.10018370944721
O	9.53000704679069	16.04860443317726	7.92845125866679
O	12.67246214324949	15.99654376211748	7.92767141960844
O	12.47695925464723	2.97303422329032	7.89976877846550
O	9.33622860095155	3.00959928376991	7.89503223260830
O	12.34962647848701	10.82492063561522	5.52406666190998
O	9.69235087865088	10.87012865561189	5.51436749774024
O	12.30877424569215	8.16129804825686	5.52284427824207
O	9.64871407244838	8.20025831337393	5.51042220219344
O	12.45272766423091	13.56251755167554	5.43746827005953
O	9.66505629370572	13.60366284503706	5.44672076906323
O	15.11117293686057	10.84671993910474	5.43975315824708
O	15.06614892153910	8.08403179297702	5.45194695479424
O	6.92931595375345	10.96410124010446	5.43622186376440
O	9.54475030298000	5.46966697596626	5.42682246968096
O	6.88422943423480	8.20175714852083	5.42651689974448
O	12.33301332396216	5.42733261773293	5.43766988450047
O	12.60524162449408	11.06947266718748	3.00105779898211
O	9.46439467180958	11.13818658859859	2.98406565392753
O	12.56570711378769	7.88909553139316	2.99888259077343
O	9.42063616192560	7.96902816110361	2.98045639955098
Pd	17.82822498035472	9.39069794384770	9.51163954888229

NiCe₃₉O₈₀ D1 (-942.486735 eV)

Ce	13.48903071019341	9.43925864717164	14.97489359006589
Ce	8.41175387895411	9.52163598753890	14.90509553694808
Ce	10.90342659377677	6.84634524547205	14.86837555057962
Ce	11.00094520009338	12.10706299826714	14.88934679393761
Ce	8.27942459843591	12.33485598961614	12.31160463723222
Ce	8.21354956843177	6.78757271571063	12.23430037778626
Ce	13.60679128938490	6.65822817223485	12.27580658446610
Ce	13.69522211895706	12.21014436688221	12.28983497633257
Ce	16.14068809217073	9.39867701534786	12.26876857965750
Ce	5.86568977735711	9.59004456702614	12.17583478645897
Ce	10.98047562741261	9.47370070342103	12.16889025887914
Ce	11.06003676532960	14.85680444539359	12.15093704759835
Ce	10.86845752488746	4.10314608343080	12.10221946931850
Ce	13.60135119796992	14.91907486972368	9.52468782259812
Ce	8.52399687894139	14.94430864319101	9.51833897085250
Ce	5.91150171769828	12.27271626083848	9.51565312766921
Ce	16.18928716187961	12.16548517097206	9.52170233494040
Ce	11.04087543469598	12.15927006739350	9.50495065575087
Ce	13.59834890296508	9.44595441493579	9.50939329059354
Ce	18.52431135608865	9.37578878287328	9.51134355291678
Ce	10.93754126204446	6.83028004144152	9.50122218972204
Ce	16.10015439912224	6.65310559483041	9.50461715965537
Ce	3.42202627865040	9.62773606421394	9.49849105459704
Ce	5.81761903070870	6.9055527444883	9.47386825191555
Ce	13.41521944380560	3.99137939898184	9.47318983175218
Ce	8.33116355985713	4.13655696348008	9.47227618500343
Ce	11.05868515988285	14.88663843996320	6.89453657066203
Ce	10.88034641052179	4.13909287334335	6.85016034263152
Ce	10.99004053286074	9.52025771862120	6.84001669322416
Ce	5.86954069355955	9.59668728936832	6.81989486814521
Ce	16.14771348706330	9.41775121783281	6.75595201920106
Ce	13.71176771170098	12.24020745364257	6.73716986596370
Ce	8.31771626281357	12.30644387144646	6.76144133768901
Ce	13.60956650770412	6.68843074218699	6.72573819578788
Ce	8.19193278314673	6.77053259852897	6.69658002579137
Ce	11.01795905750182	12.15122406889276	4.12923382689809
Ce	10.92523998353899	6.89358044733617	4.12204012891087
Ce	8.43540980807890	9.56745921471784	4.09204368029164
Ce	13.50570101063546	9.47902693681049	4.04415102423382
O	12.49200421965244	7.87379372368273	16.02460885683342
O	12.57154207036372	11.06382868498750	16.02839977519033
O	9.35952797468915	7.89591710746066	15.98144321350684
O	9.43327931366748	11.08727996314110	15.98853387120385
O	6.93018566341848	10.94900922335715	13.62979834359342
O	9.64419650949490	13.60073071488103	13.61371337145652
O	12.44283214012236	13.52195596452301	13.58004778100341
O	15.09849755031670	10.79894298653446	13.58012253409325
O	15.05035293231294	8.02820013600086	13.57072071211484
O	9.51906693272552	5.44024063170025	13.55090788049805
O	12.30845198899785	5.38405623750146	13.55542968118572
O	6.89823471862598	8.18581038518739	13.59018013729742
O	9.63611972762969	8.17033527288769	13.45198412414610
O	12.28794531969703	8.11826125779828	13.49344364572386
O	12.32885497710237	10.78740135416635	13.50288089159469
O	9.67152439891911	10.86301282055674	13.43172050374169
O	12.65912700008999	15.98338218041077	11.12242001790291
O	9.53174528079563	15.99658914250271	11.11615184327458
O	12.43202031900245	2.94069343223015	11.05361651964848
O	9.29208600153608	3.02500511730188	11.06999611295514
O	6.85813758735739	5.46880083103851	10.84799448112541
O	6.98480403375099	13.69056315176391	10.90593970252768
O	15.14802751647718	13.48516308154555	10.91439199699323

O	4.33944269645071	10.97912673447684	10.87349562317799
O	17.64066984041894	8.00666744657196	10.88611331710318
O	15.01957421711769	5.35339966715006	10.88014889309774
O	17.67601309975183	10.76367953697984	10.89451012480858
O	6.99573761771002	11.01426191913970	10.95165075552220
O	4.26207022600415	8.23959554995818	10.86007265974254
O	9.55903121013121	8.20307993117350	10.80449308921344
O	12.32860089854280	8.10098807565219	10.86423222277016
O	12.36064440179543	10.82381438690679	10.87174240095330
O	14.99980679543247	10.77222415590350	10.86728052549041
O	9.72622246025069	13.43926635604612	10.87433297782827
O	14.96467250833876	8.06806960086984	10.85829150293032
O	12.38605685287651	13.45919492076108	10.84693661266622
O	9.59873079036448	5.55388309930374	10.82007044644601
O	12.25227647741671	5.47453249492126	10.82206365031529
O	9.60248329185607	10.77118076659090	10.76219459855209
O	6.91809368794786	8.15161425030486	10.90597708934594
O	9.61085835375989	10.83573452045749	8.19776632899375
O	6.94504688772008	8.13520078310255	8.05230329518948
O	12.39442884920137	13.47092161335019	8.18194526133741
O	9.74291528900262	13.48110400722740	8.18020022002372
O	9.58873490602341	5.59848415848261	8.12974474057739
O	15.01252304876155	10.78460230518068	8.16417275026260
O	12.24798841765290	5.48899805284854	8.15698889981455
O	12.38268273594047	10.83847718556717	8.15006734719174
O	14.96020146049567	8.07993829054771	8.15723476488858
O	9.55949503913355	8.26538371584780	8.23520363184756
O	12.31643681471802	8.11875302839652	8.14374099512228
O	6.97421079532262	10.99272810781160	8.09539507559544
O	17.68920033299998	10.77201152837037	8.13670399202634
O	15.15855336091552	13.50382228035226	8.13932439005481
O	4.28954533162584	8.24718564258579	8.12118832807745
O	7.00285079333336	13.67449075050065	8.14388941257585
O	17.63581678128371	8.01622665727506	8.12955078638273
O	4.31730169737619	10.98671041191333	8.13528744569702
O	15.01373281303387	5.36739409979183	8.10712298852747
O	6.84066801634045	5.45743914824935	8.08510834489583
O	9.52249361916795	16.02152071801603	7.92487170809426
O	12.65514206755106	16.00095204574836	7.94810898577385
O	12.44549674039936	2.96179538951020	7.87135896527375
O	9.30673803595722	3.05069607715938	7.88586793118754
O	9.70042198488661	10.87704966068642	5.54815379532815
O	12.34672312097788	10.82582670924543	5.51829816370934
O	12.29581195917005	8.15828027070016	5.51203818527368
O	9.63764304205188	8.18564467790470	5.56884944116266
O	6.89514923940523	8.20317997604150	5.37504624489371
O	15.11199216978970	10.82618864113549	5.44907676687096
O	12.46452964928515	13.55651653925075	5.45065076303748
O	15.06034943749424	8.05149732362622	5.44527078822776
O	9.67113690353068	13.611111115782444	5.44851905788590
O	9.51493316149737	5.44977206483123	5.39821422992604
O	12.31116636864076	5.42512912096322	5.42653624116576
O	6.96166325589291	10.96362926581175	5.41163349893033
O	9.44651884404210	11.14965240409457	3.01362758787806
O	12.59356519393724	11.09781780032151	2.99469231731567
O	9.38677399766786	7.95446435249031	3.01810668303423
O	12.51276609609313	7.91314774781641	2.98040877670468
Ni	9.34388418517218	9.52308811756275	9.49970718501109

NiCe₃₉O₈₀ D2 (-943.086482 eV)

Ce	8.42999829071767	9.42269763856622	14.98195634535036
Ce	13.48794849023271	9.39872602735916	14.95809442553989
Ce	10.98015728740248	12.02527725615258	14.95785587840516
Ce	10.94364881371395	6.80534980012086	14.87202834366653
Ce	13.62166099513076	12.22423113267968	12.29533282219376
Ce	8.31578700969922	12.25890730631042	12.35481047694532
Ce	13.60285653083434	6.67823210122672	12.25886735159295
Ce	8.28614643935533	6.69770454901468	12.25640305599982
Ce	16.10623349593562	9.43463530526255	12.26094600989632
Ce	5.80127626799740	9.44548235703512	12.27470451531115
Ce	10.94990898432105	9.50107678886728	12.15625648837263
Ce	11.14180861935797	15.00255078174612	12.41276477186583
Ce	10.92818190713880	4.06523889559033	12.08551812321705
Ce	13.52618891511140	14.97590811603586	9.54683861343673
Ce	16.12422362705255	12.21110076776666	9.53193185787708
Ce	10.94415509593751	12.31947238903615	9.50201523859706
Ce	18.50081550395902	9.44222281544797	9.52420372495475
Ce	13.55180719969935	9.50515164704529	9.50261964757114
Ce	8.34610183025046	9.56073713328204	9.49990568174116
Ce	5.70189496150098	12.15784202832438	9.56223793461540
Ce	16.10129598481064	6.71993261668220	9.49846291215056
Ce	10.94336309485436	6.85573948863027	9.48690354995057
Ce	13.46153169557665	4.02641121343492	9.47959344407701
Ce	3.39421737910660	9.43459543714501	9.49835948570965
Ce	5.81199127112301	6.75205972970795	9.46161834536517
Ce	8.40725487013527	4.05127099826309	9.45577955269558
Ce	11.15601009515738	15.02791876841652	6.66944003289319
Ce	10.94408025889883	4.10620433019725	6.85149923186513
Ce	10.97555403945290	9.53077673877226	6.84365090211364
Ce	16.13130179041305	9.45705228114196	6.76311805084313
Ce	5.82935055023356	9.54533349013055	6.72769225639130
Ce	13.65755473955405	12.25396010947630	6.74214508507101
Ce	8.36985968735041	12.31922852123613	6.68456326973543
Ce	13.62158053157753	6.70207260632686	6.72119757073948
Ce	8.30189911632123	6.75662266004973	6.69731525198026
Ce	11.03473892447924	12.09079083217678	4.07624478567091
Ce	10.97834077251222	6.86606885588254	4.09469576656168
Ce	13.53324903159796	9.44816177379282	4.05294182706473
Ce	8.47621713890491	9.50183086196462	4.01089659198586
O	9.38520193096834	10.99794209251604	16.04855897204735
O	12.53203630546427	10.97389494764265	16.04863212396772
O	12.53345946717428	7.79563161541834	15.99502035625492
O	9.37372047796539	7.81502104149741	16.01047545408106
O	9.61689148810544	13.39712528479398	13.61490618300138
O	12.45499615180330	13.50361265598580	13.67048826489567
O	15.04842993034313	10.79832714002164	13.57816451329279
O	6.85919412472610	10.84187008974198	13.57788208881826
O	15.03673221619756	8.02939002773537	13.56101199501712
O	6.84571687164444	8.05746547806187	13.56465640888896
O	12.32733577013753	5.37947400648207	13.54093964044334
O	9.52834592103011	5.37957614033874	13.53639021812469
O	9.62038832191267	10.74539248478778	13.51607239556470
O	12.28445722376295	10.78044461482037	13.50686268642391
O	12.26443908848026	8.12217948355432	13.47427368921050
O	9.62251346691768	8.10926532142097	13.47449645694031
O	10.30618995187959	16.46615875539788	13.30043660216904
O	12.70438771899675	16.05619737743790	11.14189848540840
O	12.50173656682229	2.96591676699209	11.06582023128578
O	9.35099472330977	2.98665059811964	11.04047794599535
O	15.04938784133246	13.50913582687188	10.91991034628112
O	6.86846326196354	13.51751128226124	10.84629048260310
O	17.63410251055950	10.81250883090529	10.90596254610274

O	17.62407407551201	8.05730315201881	10.88960206503366
O	15.02442920833615	5.40009219646110	10.87395820365373
O	6.85073949705377	5.42797619947656	10.84105740749002
O	4.25102598379340	10.83206793933695	10.89569954234656
O	4.26655820457555	8.07280690545032	10.85794765842670
O	9.58069304359488	11.00003985843502	10.87213212703996
O	12.29282459981364	10.88185178838096	10.84985620463432
O	14.95302193594787	10.80835291313974	10.86841786330837
O	12.30558707725407	8.14298207557093	10.84978859975807
O	9.57868677800497	8.20117794375242	10.83734327377024
O	6.92617549536640	10.82310851454811	10.87906399516962
O	14.93890758514842	8.11437950585217	10.84660719729305
O	6.95845617469213	8.14626381529697	10.83986102810913
O	9.46359252311203	13.79794993077951	10.81349282246332
O	12.24767027762884	13.50956242285940	10.90083010683230
O	12.25621907488065	5.49800528132433	10.80922359796034
O	9.61261259616833	5.52608120786741	10.80825103130196
O	12.28592591421458	13.51851813072214	8.14287331332634
O	9.52729964950756	13.82096847157503	8.19519588939164
O	9.61675576205365	5.54667501419007	8.14456824484438
O	12.26538087696042	5.51719092663282	8.15261883623338
O	14.96716961815306	10.82061107365142	8.16313636266800
O	14.94817723340780	8.12562062190922	8.15299326462136
O	9.59642842410950	11.00018761805945	8.14317193119494
O	12.30680926575912	10.89820128261103	8.16728176572882
O	6.93830358482403	10.88589454000473	8.16670888441374
O	12.31586116123399	8.15756997541705	8.14035013906641
O	6.96426181798932	8.19141298608744	8.13643697119512
O	9.58743709184909	8.21759246736881	8.14349424630298
O	15.08041898038258	13.52758104059678	8.15180618661686
O	17.64865685282412	10.82455468744205	8.15205771514181
O	17.63175264161905	8.07062539050111	8.13676205300084
O	6.94022099015785	13.56156195829157	8.23436070307448
O	4.26193231082039	10.88536149142995	8.16712531343428
O	4.27296075580600	8.12630155168653	8.09663194650124
O	15.03414371486651	5.41111019508650	8.10507029812987
O	6.85527950065064	5.46379887530687	8.06318252355812
O	10.32993196985545	16.50165568018473	5.77842275654568
O	12.68568315757056	16.08317335283061	7.98465586196039
O	12.50171868074780	2.98801770924982	7.87885168876052
O	9.35463188565734	3.00929598551390	7.86159135516248
O	12.32925276433446	10.81630917056620	5.51599573405292
O	9.65934897543149	10.80600604156502	5.49855447018717
O	12.29266826182376	8.15968929904622	5.51621854442611
O	9.65284073087359	8.16984955302286	5.50377049200545
O	12.49148480291417	13.54092002059274	5.37968467548709
O	15.09383567828267	10.83982303438945	5.45245784580652
O	9.66206175767879	13.45286161458853	5.40756479234516
O	15.06882562134608	8.06959739245316	5.43958698186394
O	6.89060224543624	10.94393790579456	5.45320766206446
O	9.55226003183560	5.44683570992941	5.41474476663568
O	6.87475425741791	8.16104898905744	5.41859493941069
O	12.35416371080906	5.41763377916572	5.41933344731042
O	12.58962896177558	11.03220896594946	2.97742080632546
O	9.44406540616216	11.07633023464718	2.96435098224170
O	12.57868675551284	7.84993583867901	2.99548238932662
O	9.40157114333325	7.89178070233588	2.97351200935890
Ni	8.19306446889459	13.85099489508759	9.52081680125364

NiCe₃₉O₈₀ D3 (-944.010170 eV)

Ce	13.54952841620229	9.43424138098483	14.93463959161246
Ce	10.95465132181939	6.86338927848944	9.49734371930168
Ce	18.56929340893003	9.23289742475958	9.51967684104677
Ce	8.46719305390283	9.51393189450882	14.96151482782696
Ce	11.03556470416339	12.08930496036818	14.91900530264716
Ce	10.96969524525250	6.86545019229591	14.88902604583297
Ce	13.69426118248132	12.20631722177236	12.31608328827537
Ce	8.36436471660743	12.30705816118739	12.28374603594328
Ce	13.63736646171656	6.70151346154797	12.26475954696197
Ce	8.27921713377380	6.75979139861215	12.27107637449101
Ce	16.23922655550473	9.41672786087557	12.22427182153479
Ce	5.82967455883932	9.57406403763713	12.25828275444210
Ce	10.99283042569149	9.49579592026695	12.15569873580669
Ce	11.03706281944901	14.88510863380583	12.15508546999464
Ce	10.91558878797573	4.12009330977087	12.11619878624560
Ce	13.52451458201690	15.02591770827654	9.50287559132744
Ce	8.53298604688719	14.98630250667800	9.50807501955313
Ce	11.05671413205872	12.17728305448730	9.50488463274327
Ce	13.66079390577316	9.48897825500993	9.51010327195683
Ce	5.86380100171918	12.33566941591666	9.50726357350130
Ce	16.14273258384818	6.65588992370221	9.50547368615209
Ce	8.37525110550038	9.55380482831883	9.50126879827568
Ce	13.43946391964098	4.04225701833965	9.49348841361726
Ce	3.44903676338776	9.62004716245750	9.50021226950326
Ce	5.78781042816147	6.82822305125220	9.49505218070978
Ce	8.38161833929058	4.08725925754739	9.49210064945247
Ce	11.03342190710402	14.89430134493177	6.85811308988970
Ce	10.91863038805951	4.14023527956215	6.86383828651766
Ce	11.00055987326759	9.51389531785393	6.85152523726781
Ce	16.25211523337553	9.43419953033118	6.80278249439916
Ce	5.82956583760526	9.58651619365214	6.74320677668783
Ce	13.70126467542384	12.22701107735843	6.70296162382176
Ce	8.36236177464884	12.32075629747276	6.72688553605573
Ce	13.64663044796409	6.72315892541025	6.73860797206037
Ce	8.28710485453148	6.77867941019794	6.72246797602258
Ce	11.04155270349360	12.10876376123496	4.09086930792355
Ce	10.97949580201584	6.89446581428697	4.10846573069708
Ce	13.56640396488808	9.45845094083584	4.08210570983685
Ce	8.46958621127129	9.54231185681027	4.04389669194446
O	9.44529386523554	11.08892071586969	16.02905563874054
O	12.59893872914914	11.04177895292177	16.01147905613169
O	12.56060994872416	7.84870108686889	16.00146425832274
O	9.39449416083737	7.90528069775170	16.01235309925828
O	9.64009348980899	13.58196736996595	13.58025302389840
O	12.43998142114238	13.53202190182567	13.59201390741183
O	15.06617623732115	10.80658695753512	13.54276299394327
O	6.91031844520540	10.93730135472296	13.56862081234753
O	15.07367439437689	8.04142153224872	13.56416605936448
O	6.87483365660697	8.16607066085379	13.56387059631692
O	12.31953780143956	5.41302583362715	13.56146488662255
O	9.52716810029990	5.44234447398781	13.55739777533135
O	12.32369404569969	10.80356128364005	13.49574993205076
O	9.67600917160060	10.84316786586077	13.49531290747542
O	12.29945623685888	8.14644053831556	13.48273299672295
O	9.64766829401916	8.17695285173581	13.48621434185673
O	12.61821690083651	16.04715399812451	11.12941692887176
O	9.49766167261785	16.02850554138774	11.11901592832814
O	12.46082932947020	2.97341915437300	11.08543082316250
O	9.32625145170714	3.00626061017256	11.07554256139576
O	15.03264640518134	13.52266765083460	10.78391739365219
O	6.95675125995092	13.62763136195999	10.89063810048805
O	17.94825380257365	10.37840632677716	11.15249935741045

O	17.59569176041697	7.78965378747537	10.86449937571280
O	14.97822377341872	5.36968081303859	10.89876364168181
O	6.82859945607882	5.49432445960282	10.87769315302767
O	4.34055451573697	10.98119771119388	10.87948408062731
O	4.28889664579485	8.22529810494710	10.87547352601114
O	15.13251501249711	10.92864665465857	10.80541320809809
O	12.42476825478789	10.85926196828602	10.87257846038441
O	9.66458280205925	10.88416000711354	10.85468745686393
O	7.01236297468814	10.91592960200504	10.85655044358089
O	14.97187030816217	8.14515268730876	10.85647131179210
O	12.34166765447953	8.15011455321542	10.84784920309060
O	6.96618087421807	8.21076589793024	10.84940672222069
O	9.59819725018382	8.17314326794461	10.85624895896314
O	12.35684388258144	13.51335555633521	10.85478317108208
O	9.71867686802904	13.50488861352912	10.84124836277966
O	12.24486707383321	5.51094155416242	10.83011997661569
O	9.59555130429439	5.53702319133350	10.82540756045998
O	12.34834271665216	13.52107144462406	8.15687786195342
O	9.71491492934456	13.51022917071360	8.17145402249253
O	9.59549268102374	5.54815309752953	8.16275055043112
O	12.24854727941014	5.52025844981413	8.16170496519945
O	15.13420328311959	10.94183527837839	8.22107656054530
O	12.43121742374822	10.86794586753768	8.14298013233727
O	9.66688655365148	10.89126494630362	8.15250298869552
O	14.97828007117941	8.15545538514069	8.15692079383390
O	12.34615380811064	8.15910869529632	8.15758339994799
O	7.01317327095623	10.92147322773592	8.14918131636658
O	9.60218250971831	8.18216601156270	8.14305350416226
O	6.96737205303510	8.21860791286557	8.14514031133622
O	15.03135728576969	13.53363828857978	8.23402875743848
O	17.94072566514299	10.39240501319615	7.89778595966131
O	17.60553247882040	7.79821882432406	8.16098623169167
O	6.95557699920905	13.63372795240576	8.12471529892338
O	4.34188068923286	10.98675253169609	8.12631601094543
O	4.28997401819758	8.23208592276202	8.11678802279368
O	14.98146615203595	5.38084252231168	8.10209436620779
O	6.82811908705545	5.50427212626660	8.10696521921438
O	9.49793356219470	16.03560840270228	7.90346200571595
O	12.62152999358447	16.05411687686024	7.88383480547451
O	12.46121758032751	2.98470910164098	7.89366959760579
O	9.32820383746064	3.02019230999377	7.89811317743602
O	12.33365479051096	10.82147295045960	5.51777456875817
O	9.68216306300313	10.86070839849137	5.51028336830121
O	12.31018502984139	8.16841556961386	5.52417731874055
O	9.65489171887372	8.19725525373478	5.51482973746787
O	12.44326091677340	13.54949765876485	5.42358476886535
O	9.64108504555415	13.59948807020636	5.43410305652346
O	15.08336807839719	10.83092336697613	5.48320195038592
O	15.08854674582505	8.06823885208572	5.45002138036616
O	6.91352087287048	10.96005774491738	5.43800531517871
O	9.53534985510265	5.46474883447971	5.42880476113275
O	6.88135207281208	8.19150180360080	5.43035640902295
O	12.32839514590612	5.43812926485292	5.43198303351170
O	12.61618550728109	11.06562419742616	3.00430745574738
O	9.45351618210006	11.112521967616451	2.97646191186750
O	12.58144030621124	7.87223501184931	3.00784839819982
O	9.40772707392370	7.94670633243449	2.98705732288172
Ni	15.24437898514813	12.27191743345103	9.51142772866095

NiCe₃₉O₈₀ D4 (-945.668054 eV)

Ce	13.53725493796239	9.43690649367558	14.94300281963918
Ce	8.46056452335415	9.52799958430221	14.95817213472051
Ce	11.04193266382296	12.09830978326580	14.89964648718069
Ce	10.95011506308018	6.86534067981311	14.89140964893512
Ce	13.71340568803103	12.21468050784094	12.27666138626164
Ce	8.36926068277434	12.31259024466337	12.28152902975447
Ce	13.61943549852075	6.66884695012483	12.27370872565112
Ce	8.27559888785574	6.75602907138854	12.26955336050097
Ce	16.17563667737665	9.39067995767947	12.24266930248261
Ce	5.82540423729816	9.57659322795770	12.25315377636302
Ce	10.98796558558718	9.48716152731686	12.15852279572478
Ce	11.08506144571251	14.87933580375110	12.13543960245325
Ce	10.91129572014930	4.09665283181990	12.10891674126886
Ce	13.62443954799172	14.90428247000185	9.51471600289573
Ce	16.22064126758516	12.15296669083005	9.49525625397877
Ce	8.54977394736259	14.98701129224536	9.51281511860953
Ce	11.04297469515198	12.15299144768297	9.50831041958663
Ce	13.61529148919433	9.45207492672746	9.50466711603909
Ce	5.86409321293229	12.33212286921672	9.50654770317337
Ce	16.13985606515387	6.68297591734134	9.52363347657654
Ce	8.36955969320938	9.54680739097957	9.50036652714489
Ce	10.94664389182613	6.84283242652832	9.49704208127554
Ce	13.45443245007574	4.02126808017690	9.49736954763125
Ce	3.44035553904572	9.61663177259122	9.49681949016301
Ce	5.78742427706061	6.82832635391206	9.49238130194299
Ce	8.38159427770143	4.08091135915851	9.48650590362710
Ce	11.08667143100977	14.90316786204458	6.90162706643911
Ce	10.92433432533648	4.11644107689483	6.86998646339827
Ce	10.99852105676236	9.50852172460391	6.84806958909418
Ce	16.18373409211746	9.44771435722351	6.77337038592171
Ce	5.83035368147056	9.58755951559652	6.74365487617899
Ce	13.72010651046037	12.24401675924206	6.73413114003251
Ce	8.37335189579827	12.32685946827200	6.73397994499719
Ce	13.63715024325675	6.69116816677411	6.73317623620122
Ce	8.28845961357525	6.77668018361866	6.72025777831668
Ce	11.05405315868470	12.13173706085447	4.11961990079377
Ce	10.96267812417931	6.89714949718305	4.10380739362012
Ce	13.54576255174154	9.46323454015426	4.06846778187376
Ce	8.47077646803545	9.56257929516026	4.04569485151488
O	9.44324017306545	11.09367292920208	16.02459531083123
O	12.59550210527627	11.04495671512577	16.01448732635251
O	12.54254599339315	7.85776272513929	16.01056332978852
O	9.38978836696729	7.91110881705056	16.01621066205883
O	9.66093485003184	13.57683772088644	13.58029646067664
O	12.45525975645310	13.52914497770294	13.57680420170943
O	15.11326555168885	10.79522452048655	13.56813952138870
O	6.91960545572036	10.93995567165041	13.56756278926331
O	15.06294269381553	8.02368726547716	13.56915156228254
O	6.87342500670032	8.17218276055863	13.56146792797741
O	12.31467966612395	5.39171625644825	13.56495754653360
O	9.52484349976300	5.44261385438589	13.55721692364465
O	12.34427778641525	10.79624715012208	13.49093106566595
O	9.68690367315232	10.84491040960371	13.49487333502152
O	12.29544003845695	8.13154381763259	13.48807943941225
O	9.63970060269422	8.17645842632259	13.49045547985878
O	12.67236723952954	15.98025479752930	11.11171886881033
O	9.52498428161091	16.02960039644153	11.10968969391300
O	12.47209820404983	2.96011214386357	11.08690873318959
O	9.32485165630230	2.99620781643439	11.07302455338743
O	15.15473853643902	13.48952538192878	10.89073121921622
O	6.96440630951587	13.62516837129425	10.89162889093945
O	17.65117438117652	10.67447889905638	10.79253014769821

O	17.58540678050430	8.08201335309593	10.81899010136153
O	15.02626252711007	5.36145406750796	10.89689236663937
O	6.83375857017617	5.49123150431590	10.87419190935035
O	4.33989424959703	10.97840334449666	10.87594566460004
O	4.29606625476463	8.22612385258779	10.87138282147848
O	15.01643040837607	10.78286438343878	10.86232418612892
O	12.38152224569404	10.82630705068925	10.86278035772006
O	9.64548498589462	10.87144628077887	10.85910350077135
O	7.00707972946943	10.91455470201726	10.85533285342062
O	14.94338756396638	8.06492962822184	10.86580607155467
O	12.32299408149818	8.11775677381200	10.85348675846593
O	6.96515261623622	8.20621507838258	10.84940120806679
O	9.59427841523169	8.15894001456561	10.85538166402420
O	12.38790326961708	13.46006495515653	10.84360081012864
O	9.73086162081534	13.50120322437908	10.84701806619698
O	12.25565535831301	5.48743498176000	10.82850209875430
O	9.59948359332253	5.52256919395541	10.82419970417212
O	12.39135131988071	13.47248565094874	8.18048879543606
O	9.73557685673691	13.51408016703169	8.18150926130638
O	9.60594026912479	5.53377421037990	8.15776672856291
O	12.26392200637900	5.49752856269060	8.16402978597407
O	14.98954127758662	10.80431127090294	8.14692296872593
O	12.37270689683943	10.83497701386117	8.15458142551315
O	9.64160158450702	10.88405914256276	8.14858938832177
O	14.98353885327339	8.08616001705571	8.15141892995865
O	12.34387474106495	8.12376251166159	8.14459933535506
O	7.00548359285964	10.91991861456771	8.15008846458398
O	9.60554859947565	8.17130882849198	8.14300145545003
O	6.97179381384146	8.21277964249965	8.14154718169293
O	15.16191006136419	13.50955167876270	8.11558776062793
O	17.63176537153192	10.71353789233852	8.20038252505546
O	17.61695415584276	8.11985794203601	8.22706341549562
O	6.96838871574057	13.63142426382022	8.12667600735707
O	4.33937925393561	10.98271176938601	8.12419580113592
O	4.30130525065631	8.23050594064319	8.11883521593226
O	15.03033219721257	5.38049740233749	8.12516606343581
O	6.84045765496829	5.49940204089251	8.10661762516888
O	9.52508737096993	16.04353761077171	7.92149954133291
O	12.67285628521211	15.99720351143679	7.93170041306313
O	12.47691290713199	2.97050748858301	7.89917905531240
O	9.33243254390684	3.01057084607432	7.89205229054396
O	12.35414210561582	10.81930751364200	5.52343681788784
O	9.69740594296208	10.86671173014408	5.51448992781710
O	12.30525324953832	8.15441010163634	5.51551358912733
O	9.64829384612202	8.20005839356436	5.50871555145966
O	12.46028256252504	13.55880963401052	5.44183223212536
O	9.66774183325599	13.60123883777267	5.44969186122850
O	15.12452430716054	10.84465572203005	5.44482158070062
O	15.07500099529102	8.07018383081359	5.44563794875837
O	6.93052629194900	10.96098641580379	5.43722937349873
O	9.54045174552460	5.46762203839939	5.42532537363972
O	6.88219243029197	8.19502504648451	5.42981902648971
O	12.33615526158329	5.41991511104058	5.43208440339660
O	12.61291893738002	11.07493178924192	3.00265317681463
O	9.46244517491102	11.14408828393030	2.98831024603606
O	12.55316985337908	7.88637539205805	2.99084218292100
O	9.40471193150977	7.95978031913645	2.98082662638685
Ni	17.77840855906685	9.39487243843545	9.50944535195103

CuCe₃₉O₈₀ D1 (-939.640859 eV)

Ce	13.49583830233832	9.46539135929283	14.94761058629699
Ce	8.43371609366972	9.53506093346801	14.93269621404985
Ce	10.94743948337012	6.86682650454977	14.91706312067473
Ce	11.00725449354240	12.10760988888482	14.86180549026043
Ce	8.27508528239061	12.35108735661980	12.29488649839423
Ce	8.35532804320531	6.80247586099285	12.25515842304845
Ce	13.62403937667466	6.65886152348002	12.28236137321505
Ce	13.65760755994870	12.18812348310284	12.26009665203719
Ce	16.14666200089327	9.40509655719384	12.25975576484990
Ce	5.88311906049538	9.66363430437007	12.20300943402865
Ce	10.94579855983168	9.42778543119313	12.12367490992443
Ce	11.05552193833223	14.83950465521709	12.13503353144410
Ce	10.93056433607209	4.07360750003742	12.12277920399931
Ce	13.55701563754460	14.84656366459064	9.50391536821451
Ce	8.50184265531659	14.96668177757119	9.50767967986746
Ce	5.81425515292019	12.46184062895587	9.51354278035151
Ce	16.16521876932295	12.14990085595047	9.50710311841366
Ce	10.90824617189442	12.04246192229976	9.50923020393113
Ce	13.59967732232824	9.42020958721117	9.50459957131112
Ce	18.52849473531066	9.38443673319866	9.50383429528928
Ce	10.95941726345828	6.79976664721952	9.49887914430702
Ce	16.13070579766591	6.64616399970710	9.49818342367055
Ce	3.46647946489715	9.65107401365270	9.50257928384867
Ce	5.99329670854353	7.06141215070435	9.49927449162431
Ce	13.46208617302553	3.99605972384758	9.49201586738786
Ce	8.41281608237332	4.04822921320442	9.49481013961635
Ce	11.05392324459897	14.84678103044480	6.88331961083205
Ce	10.92867609195170	4.07839387314471	6.86432359906764
Ce	10.94299960295466	9.43526179339340	6.88373466304103
Ce	5.88427445612325	9.66840919874038	6.80109957170298
Ce	16.14545535952742	9.41644417255851	6.74705040503949
Ce	13.65540062498139	12.19325367370124	6.75260685967368
Ce	8.27508126264754	12.35678124082669	6.72469333194116
Ce	13.62294402690500	6.66725106236294	6.71552222756053
Ce	8.35530995415412	6.80888731192482	6.74348472951623
Ce	11.01272564747552	12.12894576915789	4.15646483593899
Ce	10.94765900362348	6.88183360248488	4.08084227065400
Ce	8.44053427451353	9.55205553198005	4.06968287672914
Ce	13.49652605236656	9.47410449389494	4.06125999962137
O	12.50728938803903	7.89655241886815	16.04077536750035
O	12.57397483309994	11.07653471372830	16.01365804521111
O	9.35516828152493	7.90615096980381	16.02836962429361
O	9.44272627041711	11.09027760459073	15.98724404679346
O	6.91887839640642	10.97381793845451	13.64006486492222
O	9.63610820094091	13.61034504807954	13.59757696143246
O	12.43403510459166	13.51677520925007	13.56699657276303
O	15.07733180113146	10.80735974966493	13.56274434912824
O	15.06497409071984	8.04667002009216	13.57401208147520
O	9.59868888141232	5.45248588216715	13.56765824896950
O	12.36195892524129	5.37481989571640	13.57376166462332
O	6.90376146476649	8.20045491840952	13.48942347814807
O	9.65310618584380	8.20761448370560	13.54859441505567
O	12.29218300635691	8.11099785746401	13.49592843079130
O	12.30943287889446	10.77749024386323	13.48320217850275
O	9.65957004449373	10.88568196840489	13.40466265514324
O	12.65060189377598	15.94208028189690	11.10745489986709
O	9.53318007749254	15.98940494906938	11.10457051148216
O	12.46734856143831	2.91919986761556	11.07297969250944
O	9.32295874492721	2.93477085503427	11.08214128007759
O	6.89998257295015	5.65979442688082	10.89667665390107
O	6.93869187347860	13.80289974123091	10.88485168507252
O	15.10859244301253	13.46576431374484	10.89069690450161

O	4.22051633214678	11.01666071357390	10.88618693605642
O	17.67552638172383	8.01729645157558	10.88438622305654
O	15.04219674619304	5.34365730998869	10.87337629862176
O	17.65533622321432	10.77359949571026	10.88127054549468
O	6.85120272787294	11.18011430800109	10.93347846034269
O	4.47837867638772	8.28276549583624	10.86981526079824
O	9.74567894190797	7.96905164211806	10.95401468784701
O	12.39921603098188	8.08752943292510	10.86053207654015
O	12.29111254869221	10.79237653954247	10.85324079882531
O	14.97342369790312	10.76389926980759	10.85706052982777
O	9.67559739581912	13.40464593306396	10.86057665235443
O	15.01071393900108	8.06202279367857	10.85395513195786
O	12.31732781813322	13.40482591091494	10.82765979287855
O	9.63368456418462	5.41803599624687	10.81960610805003
O	12.28939000870803	5.44887688150633	10.84247784435710
O	9.41134607997327	10.64554074092988	10.74972291430086
O	7.25462658162891	8.52791229055575	10.76794265579710
O	9.40751962827646	10.65112150570869	8.25995456810315
O	7.25495633700683	8.53207902564363	8.23603846974728
O	12.31371227491416	13.40794819755887	8.18529632809106
O	9.67566097422735	13.40957114697600	8.15968193396288
O	9.63323912858229	5.42086796479596	8.17318528146795
O	14.97141866072323	10.76976370971331	8.15347769830778
O	12.28781335660310	5.45160095820042	8.14887890873989
O	12.28790505087966	10.79405935949722	8.16524904694510
O	15.01059540329219	8.06717632762025	8.14854293001023
O	9.74507151513136	7.97334875179983	8.04853562218181
O	12.39937715626300	8.09120760613394	8.14289273639110
O	6.84435497385269	11.18516841966646	8.07827728109736
O	17.65441196310638	10.77778702699122	8.12918098597178
O	15.09894652397764	13.47718163461380	8.13125134768061
O	4.47874342956246	8.28539159071713	8.13280123757748
O	6.94054215660502	13.80777666304305	8.13921116071135
O	17.67654565158208	8.02008772722501	8.12154127126568
O	4.21371112792793	11.02032803383009	8.12602726729748
O	15.04091745967592	5.34785789611748	8.11791489151102
O	6.90004472333527	5.66353465728266	8.09673943473608
O	9.53140214878485	15.99549379331759	7.91742822270155
O	12.65006461051838	15.94751505721257	7.91014974356801
O	12.46944390180102	2.92240505940233	7.90792248885339
O	9.32486169064386	2.93752316177809	7.90259743068035
O	9.66108505626533	10.90016410846135	5.60756647303844
O	12.30953137804379	10.78817639778489	5.53377507475399
O	12.29001030430733	8.12157555952072	5.50826627771178
O	9.65313852953059	8.21984690028085	5.45382255809984
O	6.90273332561823	8.20858734762904	5.51402757821813
O	15.08055933206694	10.82177380097637	5.45059256695298
O	12.43729177183897	13.52986362119802	5.44796757139728
O	15.06459332732800	8.05993875331965	5.42827248717416
O	9.63952956534521	13.62488068468276	5.42343980588543
O	9.59829516445402	5.46328759754467	5.42558098842217
O	12.36072966915011	5.38644451046552	5.41951852656966
O	6.92204281137640	10.98329175580412	5.37011373096984
O	9.45420609087166	11.11506493330290	3.02571113711444
O	12.58696531987139	11.09117923373037	3.01060042294452
O	9.35551028640684	7.93191103545622	2.97098827491672
O	12.50816551094460	7.90690649129343	2.96289952634599
Cu	8.37678785191532	9.60342839886030	9.50369963123745

CuCe₃₉O₈₀ D2 (-940.979302 eV)

Ce	8.43230407237548	9.42367773859766	14.97991814102747
Ce	13.49284702019871	9.39839309817009	14.96193421615927
Ce	10.98790161009896	12.02368068488899	14.96313080363696
Ce	10.94482394632880	6.80621474648586	14.87317760055499
Ce	13.62677852724600	12.22742413678938	12.30896627744038
Ce	8.33305011667189	12.26071053195293	12.35768565939969
Ce	13.60418185256804	6.67743166771071	12.25964775409887
Ce	8.28840279916009	6.69697392711542	12.25192113021531
Ce	16.10793239392207	9.43511305890762	12.26154322205741
Ce	5.80443640338303	9.45047024082436	12.26911020127689
Ce	10.95369542149485	9.49622154471588	12.15776500631513
Ce	11.14104239520702	15.00822534740958	12.41819834392628
Ce	10.92934621087849	4.06462600626446	12.08389465207990
Ce	13.52369581444684	14.97394626148169	9.54673851965840
Ce	16.12258156704104	12.21259270954993	9.53529271874328
Ce	10.94580107258486	12.31414681080683	9.52304650422130
Ce	18.50013903677463	9.44229267057908	9.52260633952922
Ce	13.55242993963719	9.50594833788343	9.50513181994334
Ce	8.34213518270092	9.55250124332820	9.49802989908362
Ce	5.70048950209292	12.14995563451412	9.52917505589179
Ce	16.10328232998407	6.72084422228172	9.49617125255433
Ce	10.94514380043203	6.85355426218146	9.48409794437717
Ce	13.46425216396438	4.02856577115697	9.47901114584525
Ce	3.39172651813380	9.42971962403614	9.49128018343676
Ce	5.81208001116067	6.74500716671209	9.45674662021052
Ce	8.41106540059929	4.04674248247965	9.45185805260507
Ce	11.16283984206778	15.04828256014984	6.66012826602080
Ce	10.94990434320431	4.10537676308816	6.84664890884767
Ce	10.96821843205671	9.53522775499295	6.84708541528548
Ce	16.12602036050457	9.46501693357204	6.76446956172944
Ce	5.82040988078082	9.52381987599703	6.71152731235742
Ce	13.64578556729330	12.26028428211436	6.74942971826340
Ce	8.34417260615359	12.30967537308873	6.68838332700166
Ce	13.62185668135563	6.71199664484815	6.72081352998769
Ce	8.30332267603960	6.74714816089216	6.69223152099646
Ce	11.01669062667623	12.10299263754388	4.08713407805698
Ce	10.98104684102699	6.86774845124047	4.09305108079708
Ce	13.51859230135661	9.46443602730322	4.05363633232713
Ce	8.47330466777315	9.49414957760515	4.00995771501444
O	9.38735609065633	10.99331008158087	16.05005349833466
O	12.54130917146709	10.97214347805229	16.05435841176796
O	12.53302429196470	7.79623117500139	15.99656323722750
O	9.37602053054203	7.81461329168195	16.00940390904523
O	9.62417666944043	13.39308873853436	13.63284544792656
O	12.45932069664661	13.49965601793811	13.67926944684697
O	15.05352487204815	10.79853148515565	13.58407544280487
O	6.86449643749185	10.84194280085424	13.57273035080337
O	15.03919492985286	8.02972815758345	13.56051327714915
O	6.84605224061791	8.06006490228910	13.55783751788899
O	12.32913355797395	5.37800196552104	13.53985906879998
O	9.53025500565067	5.37953780100780	13.52959472806403
O	9.62822084950860	10.74405885194822	13.51775824392238
O	12.28953140878076	10.77664804427853	13.51222370866881
O	12.26719349806594	8.11968276441331	13.47556432621808
O	9.62364000036475	8.10779930113664	13.47396940816674
O	10.31847752271649	16.45769277620375	13.35202487187112
O	12.68874796068432	16.05896647130150	11.14769507870018
O	12.50331329648273	2.96586892362293	11.06295333878855
O	9.35150129910152	2.98437154952893	11.04021519122714
O	15.05451057031971	13.51326109228618	10.92398880874935
O	6.89001642304305	13.52561200283705	10.84978403608483
O	17.63383405481849	10.81284000546050	10.90474376853699

O	17.62519102350602	8.05688654810212	10.88686612776084
O	15.02568811873117	5.39900756596072	10.87025684101166
O	6.85186662435808	5.42831991572921	10.83962873802420
O	4.25171792281509	10.83500018350089	10.87773275159074
O	4.26596491447152	8.07585209335653	10.85513567586362
O	9.57909645788831	10.98786445310969	10.87297220828209
O	12.29326602833726	10.88073047996815	10.85731462806769
O	14.95295238619308	10.81039013865238	10.87396768944239
O	12.30751355330132	8.14157641469306	10.85003443404541
O	9.57994361737349	8.19561531529017	10.83689395116847
O	6.92530670511975	10.83041626653392	10.86597756561829
O	14.94100275541119	8.11513862341425	10.84661237791431
O	6.95752840044435	8.14688904158038	10.83339872191648
O	9.50468401668038	13.79985213126391	10.85775068628340
O	12.25735955482476	13.50727387379196	10.91164202987978
O	12.25745290245462	5.49844464734067	10.80888323869791
O	9.61375470776667	5.52275961851526	10.80115653698694
O	12.26570456394507	13.52490309632333	8.15007913654803
O	9.50225180530704	13.82589275418413	8.21432499853523
O	9.62247836528483	5.54518594196002	8.13379868223314
O	12.26948283678554	5.51824784120795	8.15130049897490
O	14.96460830836208	10.82539081865597	8.16890247978007
O	14.94720504283187	8.13071647611232	8.15447584455225
O	9.58797750386543	11.01002459551896	8.15065540464893
O	12.30408180521017	10.89936699397123	8.17342020851216
O	6.93226074060516	10.86126424320344	8.15283090137635
O	12.31356788576895	8.16088954153769	8.14085547491515
O	6.96180572690216	8.17701755814855	8.12590552562725
O	9.58527526812606	8.21755635615905	8.14297606555412
O	15.06643077301212	13.53010977993364	8.15840766190175
O	17.64595869452719	10.82718819660616	8.15140565593843
O	17.63062910244955	8.07329107225324	8.13384110243508
O	6.88873188018396	13.54612062221716	8.22690448253830
O	4.25621682675142	10.87483876649195	8.15054416817921
O	4.26848029741906	8.11291845710009	8.09335908865834
O	15.03749203049998	5.41685086270811	8.10102417149166
O	6.85866524651621	5.45260493106269	8.06291649070786
O	10.44426329293949	16.50602917081165	5.66949832039356
O	12.69778906019991	16.08901866414623	7.99144994107695
O	12.50700658283598	2.98927438133274	7.87532516944862
O	9.36014531389197	3.00769774483808	7.86037411676722
O	12.31149967757185	10.82630557809374	5.52087201593564
O	9.64264570987016	10.80414346078380	5.50507007403992
O	12.28881254315570	8.16842902295331	5.51753555531531
O	9.65182018199517	8.16648543572287	5.50366136191163
O	12.48377176767973	13.54569579242200	5.38600047682172
O	15.07999244633922	10.84810777736403	5.45844876028100
O	9.64327088898421	13.45494876369574	5.43186649040845
O	15.06347672947182	8.07925751813471	5.44119751549719
O	6.87640023499520	10.93027713046435	5.44157617357599
O	9.55383543974284	5.44010395129924	5.40811276361914
O	6.87360014680819	8.14796472678408	5.40614776717434
O	12.35575371119180	5.42511074668498	5.41705020276874
O	12.57261348198807	11.04874024664604	2.98416594680456
O	9.44072266096062	11.07274622621613	2.96983064315456
O	12.57567559707938	7.86196527004353	2.99432727672464
O	9.40412444618187	7.88675059648322	2.97121641010660
Cu	8.19344849314298	13.87227876831627	9.53833544634355

CuCe₃₉O₈₀ D3 (-941.79981 eV)

Ce	13.55676922682033	9.43768892047436	14.91262113521522
Ce	10.95449368910699	6.86480340283913	9.49347072705265
Ce	18.58145208211499	9.23801572794030	9.53002435189559
Ce	8.46350387445586	9.51306991628812	14.94877973620841
Ce	11.03854175542657	12.09272386762607	14.90446332856872
Ce	10.96559759248393	6.86244796115786	14.88068088364220
Ce	13.70172554974701	12.22076421530292	12.28902933515837
Ce	8.35409004755706	12.30864685061129	12.28109160791162
Ce	13.63792743854561	6.70317686628747	12.25670889765665
Ce	8.27709025249423	6.75758150420600	12.26446204686855
Ce	16.24417108347384	9.41684275069777	12.22294262580986
Ce	5.82315424023340	9.57130647795044	12.25135181196524
Ce	10.99378358106818	9.49645891405935	12.14953275575206
Ce	11.03743910007747	14.88631783602607	12.15819703778442
Ce	10.91882706107267	4.11914041431664	12.10923104340351
Ce	13.55584074855733	14.95434319792692	9.53356490538728
Ce	8.51752468811069	14.99255121847899	9.51171312677466
Ce	11.03359011355760	12.17487655337011	9.51041707736033
Ce	13.65992284553425	9.49109476930522	9.50694061032579
Ce	5.85275459554539	12.33468589977933	9.50100342130701
Ce	16.14797072326405	6.65900643304802	9.50404751111580
Ce	8.36851296849224	9.55240294897373	9.49709387394434
Ce	13.44480107405994	4.05014724874456	9.48246711364293
Ce	3.44260788141159	9.61694085652150	9.49602430010535
Ce	5.78329407514851	6.82648580012424	9.48526578413447
Ce	8.38034880555332	4.09087756933172	9.48636895453367
Ce	11.05660320156482	14.90514419543101	6.88685460150316
Ce	10.92014177695764	4.14234077908459	6.85775611709986
Ce	11.00739188386274	9.52374702989310	6.85484928990800
Ce	16.26634060487222	9.43920688867912	6.81075058710016
Ce	5.82870069472291	9.58916032275362	6.73882570091609
Ce	13.72412460367214	12.24618930752395	6.74045157295452
Ce	8.36457184059029	12.32860474268592	6.73005941167447
Ce	13.65123333863559	6.73191931777442	6.73673900151964
Ce	8.29009547887211	6.78508497895884	6.71876849086761
Ce	11.06390472519533	12.13191303738533	4.11990052870702
Ce	10.98657103786627	6.90748445353124	4.11019381786345
Ce	13.58805785016940	9.48260873742787	4.10160869931418
Ce	8.47728835526535	9.55808815974768	4.04770678363247
O	9.44567643348461	11.08214605824946	16.02682420097381
O	12.59595020925671	11.03512080275605	16.00995896114447
O	12.55287873643369	7.85371398881855	15.99681523375297
O	9.39621984357065	7.90743724531525	16.01261893626405
O	9.63541002830151	13.57418418442578	13.58538084406297
O	12.43348466559415	13.53039511741074	13.59686360837177
O	15.06881921569524	10.79496684609246	13.54485840900193
O	6.90757890622849	10.93011104704536	13.56727760677581
O	15.06061703814664	8.03510952047804	13.56434297096926
O	6.87549404586366	8.16455908497244	13.55796010331456
O	12.31364337356915	5.40959323248533	13.55617111713403
O	9.52569124194366	5.44099832424533	13.55403229917508
O	12.32627456043252	10.80317398654691	13.48922673624920
O	9.67306521046992	10.84095762943148	13.49158249178771
O	12.29639192899700	8.14301271031751	13.47695349122023
O	9.64425832496614	8.17332242428516	13.48326964120169
O	12.61604264501736	16.01641225601529	11.16074862701686
O	9.48646808506556	16.03953595182433	11.11301872811320
O	12.45935623640569	2.97316154235211	11.07211654026607
O	9.32671823278220	3.00366555097692	11.06660033999514
O	15.02491639409104	13.53415360603202	10.82617006907807
O	6.93285020928003	13.62324721270231	10.89167362353591
O	17.95278559184022	10.38462564291991	11.15411448152782

O	17.59804971352736	7.79372880487733	10.87072188364323
O	14.97824258448083	5.36175367560165	10.88849757442350
O	6.82949454947835	5.49045742787104	10.86919570566555
O	4.32976541762806	10.97689999971773	10.87633231664932
O	4.28487748706238	8.22159591971635	10.87065328163383
O	15.12424334617339	10.89919778865661	10.82003393290577
O	12.41332890706508	10.85244943560933	10.86622216202140
O	9.64929374376931	10.87885062579564	10.85586394785165
O	7.00088640167662	10.91096466205772	10.85337276726263
O	14.97270852836671	8.13522566246549	10.85584670403322
O	12.34006424595347	8.14544854554443	10.84512389293607
O	6.96122784121331	8.20608831053464	10.84321631718888
O	9.59568419540986	8.17052715377518	10.85174592694659
O	12.31845976722100	13.49193363622265	10.86150377699724
O	9.68603083590970	13.50846262136146	10.84578449570524
O	12.24585075705280	5.50945714363552	10.82240450305914
O	9.59569246623583	5.53409134265621	10.82198433670832
O	12.32959090622306	13.50059061642848	8.17745481425514
O	9.69582543984927	13.51950781101130	8.17933402788113
O	9.59516130297640	5.54737779896880	8.15801359439074
O	12.24809815251534	5.51976266684399	8.15482031268872
O	15.13262438507065	10.91022132851010	8.20732125157419
O	12.42249620104815	10.86532241166816	8.15120316893054
O	9.65324841149286	10.89138816836125	8.14901738244371
O	14.98100464137909	8.14784743991529	8.15320661337159
O	12.34496864251657	8.15670895804700	8.15485225602020
O	7.00451378089975	10.92030007207708	8.14586427529302
O	9.60189045177453	8.18306080501294	8.13811787620014
O	6.96478686069931	8.21657493242578	8.13792446425668
O	15.03387766813361	13.54502220504540	8.22094410604998
O	17.95762200647603	10.39676767009828	7.91241927485212
O	17.60887308375122	7.80295372539459	8.16838305035056
O	6.93938692296097	13.63379595724386	8.12082100856280
O	4.33262018281742	10.98217869839967	8.11943955167041
O	4.28885458239996	8.22802077748874	8.11411307057689
O	14.98112548588043	5.37859924500082	8.09713740172401
O	6.82913268136488	5.50330768404194	8.10134809041449
O	9.49573618477249	16.05115063382503	7.92671785342783
O	12.62875237036170	16.02709441362559	7.90538623885113
O	12.45949197035071	2.98389840392092	7.88238896466184
O	9.33201182103861	3.01834563071583	7.89375063153427
O	12.34670086423042	10.83340332770088	5.52802120166692
O	9.69010621471652	10.87146748486090	5.51465320995450
O	12.31522341233849	8.17731577730863	5.52460880327329
O	9.65636450274653	8.20601017425082	5.50995405849201
O	12.45794344682803	13.56056093651594	5.43991627154918
O	9.65567674969510	13.60213509694545	5.44155415004302
O	15.09664345850092	10.82661759698515	5.48317160010774
O	15.08570687404463	8.07184776509061	5.44798189931567
O	6.92438489459971	10.96068354081580	5.43202510629143
O	9.53673143009832	5.47281567480360	5.42439813348105
O	6.88459157395979	8.19853183497873	5.42408577111472
O	12.32360642993224	5.44676682953054	5.42185601069158
O	12.62931220063141	11.08545399608457	3.01016712237910
O	9.48168988304392	11.12424494993281	2.98024325479362
O	12.58395078323674	7.90392657725035	3.00666873357080
O	9.42181599447036	7.96093056850557	2.97717362185912
Cu	15.27945454363652	12.25233302030579	9.51970057828350

CuCe₃₉O₈₀ D4 (-943.488306 eV)

Ce	13.54752529800871	9.43878612053726	14.92569148009735
Ce	8.45747614803562	9.52511390759581	14.95578871173762
Ce	11.04137162841034	12.09842395986247	14.89760215878457
Ce	10.95942787081057	6.86296497570939	14.88111897157719
Ce	13.71603414306064	12.21243699617685	12.27810710757795
Ce	8.36008059326497	12.31087619428488	12.27797948666048
Ce	13.63378065821036	6.68202377090690	12.26401483262314
Ce	8.27263632263227	6.75482380261592	12.26704658447948
Ce	16.19405668694496	9.41081191410044	12.21878065472950
Ce	5.81848092114183	9.57219785235042	12.24868065195845
Ce	10.97886480328801	9.48898171774364	12.15918532951911
Ce	11.08640501307694	14.87306138303883	12.13651904664924
Ce	10.92331748960861	4.10319685310585	12.10821106177088
Ce	13.63921136001743	14.88304737165610	9.52068772868255
Ce	16.23988710061456	12.12538059207257	9.52156623560623
Ce	8.54974244187610	14.98397272886608	9.50626001362020
Ce	11.03696481727196	12.15231178852189	9.51104412127819
Ce	13.60281636418608	9.45424585896010	9.51048525031517
Ce	5.85639328763378	12.33225644721743	9.49884927707520
Ce	16.15963268402798	6.71441971854077	9.50741758257722
Ce	8.36134207709936	9.54719161850009	9.49898290287897
Ce	10.94283544790034	6.84528003064307	9.49692608826837
Ce	13.47463144189534	4.04327816717945	9.49728391240725
Ce	3.43257779355146	9.61246668476057	9.48808082727409
Ce	5.78205563268565	6.82652727276438	9.48415388257271
Ce	8.38287002004302	4.08223611729628	9.48748105061933
Ce	11.09822080494309	14.89405957549790	6.89566305029489
Ce	10.93040488045020	4.12033712437597	6.87254730916988
Ce	10.99506902114087	9.50782705039013	6.84908518354835
Ce	16.20630763554817	9.42711009944519	6.81268465000478
Ce	5.82762890077815	9.58817391223822	6.73786679660289
Ce	13.73280743306648	12.22997604179125	6.75379479001461
Ce	8.37223871023667	12.32554797620482	6.73096655843269
Ce	13.64283306451818	6.69819735272816	6.74197431059796
Ce	8.28854447693685	6.77603634808830	6.71821715621996
Ce	11.06957766906961	12.13161697144933	4.12639308543333
Ce	10.98320895042194	6.89327778091832	4.11038905823532
Ce	13.57357865989691	9.46804509887453	4.09260974284929
Ce	8.47904345651087	9.55811030370453	4.04541378761195
O	9.44510208298747	11.09084098257693	16.02785884192357
O	12.59386220863926	11.04125927628112	16.01270781637962
O	12.54508538310456	7.85725795974057	16.00469859457630
O	9.39322509375677	7.91651716286778	16.01650901867552
O	9.65412092840119	13.57521687096491	13.57568133648233
O	12.44073591567473	13.53436591156223	13.58218120857214
O	15.10267749739604	10.80790463406800	13.56891301253099
O	6.91233820753817	10.93331602799067	13.56399386990091
O	15.05519378262435	8.03566487395541	13.56193489246718
O	6.86841723423994	8.16724728719709	13.55701109017549
O	12.31620243464817	5.39466984170489	13.56258452771812
O	9.52847931091737	5.44216023792516	13.55556227124746
O	12.33721289088123	10.79749330943187	13.49065663428024
O	9.67715890414973	10.84305506511189	13.49947473888751
O	12.29204198721511	8.13455552697015	13.48454551819961
O	9.63363500156278	8.17289332537929	13.48968407206757
O	12.67239198406133	15.97685056750269	11.11065681686313
O	9.53135130144664	16.03402235577413	11.09772018525351
O	12.48006602198454	2.96607889910584	11.08301053248683
O	9.33558770757461	2.99317637139193	11.06727414226361
O	15.14592707847942	13.48933849674755	10.90780201243470
O	6.96053102549877	13.62424754842056	10.88414492149605
O	17.63530925398782	10.71787934706916	10.84026980459925

O	17.59320026434598	8.07897617314396	10.83173643805998
O	15.02181918951706	5.37410440604555	10.88586401479454
O	6.83507625970054	5.48883935391307	10.86721106991932
O	4.32937818635921	10.97511586313019	10.86701792894396
O	4.28894301642123	8.22167067637969	10.86043238404196
O	14.98458330361827	10.78434143134554	10.86593432729088
O	12.35694435667281	10.82678481632984	10.86449207222531
O	9.62690794181855	10.87716487311801	10.86777252195962
O	6.99373281048726	10.91337122436008	10.85045109303264
O	14.94314542737840	8.07880770324313	10.85991652164634
O	12.31413211636192	8.11775745932101	10.85764651768026
O	6.95708073983050	8.20385970524972	10.84461549697137
O	9.58527426195282	8.16046162398943	10.85412240904355
O	12.38348026990063	13.45793727016919	10.84560390650769
O	9.72453739993349	13.50396804560845	10.84447043715207
O	12.25769867597934	5.49234569326344	10.82705731902310
O	9.59862118873333	5.52187053604940	10.82570525044809
O	12.38998126011360	13.46791903112760	8.18457218963016
O	9.73306438631028	13.51284765763773	8.17457416432386
O	9.60337320092954	5.53110647022854	8.15872741464496
O	12.26349678182221	5.50129078509139	8.16533290921737
O	14.99057639611943	10.79404427176521	8.16436794625901
O	12.36651825573852	10.83654424019707	8.15501365434668
O	9.63583360653607	10.88250873073152	8.15067687713979
O	14.95011151588976	8.08851075257450	8.16089252724174
O	12.32124242240067	8.12658161239424	8.14837571086421
O	7.00110601770985	10.92140567404452	8.14432552797960
O	9.59336364191583	8.17012204223011	8.13999382790285
O	6.96369916420968	8.21304239324123	8.13634586084911
O	15.15306345239597	13.50048760941000	8.13499844066295
O	17.64242779062576	10.72618327187921	8.20210127221277
O	17.60082224291765	8.08727914849711	8.19401496525332
O	6.96773935455135	13.63260919344961	8.12186966785736
O	4.33678082151995	10.98116728691948	8.11623206803301
O	4.29725030881065	8.22940754247345	8.10845652729822
O	15.02729638587872	5.38626962702653	8.11498514696430
O	6.83960999649452	5.49801565573108	8.10173810173925
O	9.53308236325897	16.04462898427625	7.92135908360771
O	12.68027826515645	15.98892905965691	7.93265894901336
O	12.48276430335772	2.97647536845538	7.90199010850452
O	9.33932554092206	3.00545329385283	7.89740677444240
O	12.35593078012114	10.81847590793595	5.52796246802440
O	9.69653542799718	10.86630316425410	5.51254224663251
O	12.30940819095709	8.15741958623106	5.52001028922881
O	9.65043398581760	8.19682258326115	5.50479217671086
O	12.46255749374719	13.55576449184652	5.44566533450238
O	9.67620169023716	13.59800163376238	5.44558191393457
O	15.12025007629162	10.83212861851294	5.46084503253078
O	15.07401817409712	8.06024135581600	5.45674189863991
O	6.93422540456652	10.96108350368660	5.43165547479316
O	9.54365019673837	5.46730484715810	5.42695696118082
O	6.88676916188138	8.19785068467891	5.42229598311613
O	12.32804700709468	5.42038308360010	5.42871871375231
O	12.62583106593357	11.07525808070215	3.00690645915159
O	9.48164638773171	11.12972422869156	2.98217777930973
O	12.57968362043790	7.88964274661901	2.99973614635909
O	9.43033369951300	7.96195449887569	2.97344650253195
Cu	17.79742963193778	9.40026306636226	9.51767890503274

PtCe₃₉O₇₉ D1 (-937.481770 eV)

Ce	18.68499244493549	9.31965434329075	9.48927473428097
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Ce	13.55346972211607	9.43345242784176	14.94379142156586
Ce	8.44271744622814	9.39529619971715	14.98616661834524
Ce	10.99769684506859	6.82946883248785	14.93014932664334
Ce	10.98623397976719	11.99399590907787	14.94750896017712
Ce	8.26268052613583	12.19573224726089	12.22904140490252
Ce	8.34404043272140	6.72789028044718	12.28837738218802
Ce	13.65746159374772	6.65923716506019	12.29267809891871
Ce	13.69949175935865	12.22233276509257	12.27726806883125
Ce	16.19578099456702	9.41417755926226	12.19548008554970
Ce	5.86552576532978	9.54796013566917	12.08801851751319
Ce	10.98814838048692	9.43541985839649	12.19318598701238
Ce	10.82429378615970	14.71403432697675	12.33068052873171
Ce	10.93610182684897	4.05502765900231	12.11373469483032
Ce	13.80746159513114	14.70284914261712	9.27660096518301
Ce	8.52355242732552	14.91476995510623	9.48235724159902
Ce	5.77484792427105	12.34192445780376	9.41975840516290
Ce	16.28394757620975	12.02298655836596	9.46409959973364
Ce	10.96932643820519	12.11931218088078	9.50711689787722
Ce	13.59095844582181	9.45126385792201	9.50500805807341
Ce	10.94764076717958	6.84434833638589	9.56946089573457
Ce	16.14610793910174	6.69133513991289	9.51215359686331
Ce	5.86540439739232	6.99650200034212	9.46572989842746
Ce	13.45433793694721	4.03389307890913	9.48521790387110
Ce	8.38419648673568	4.08576418331841	9.52809841780463
Ce	11.08137348171125	14.83463364867002	6.88101487854582
Ce	10.88998221932966	4.15747646259364	6.88993879797107
Ce	10.91342467771333	9.51611254966641	6.90772901866787
Ce	5.74542490822062	9.69722827958868	6.73497872583471
Ce	16.17735430259682	9.35083468203488	6.78983305553651
Ce	13.71721881256993	12.14220569018484	6.66472730824573
Ce	8.26607625323841	12.39150748360097	6.65668672264860
Ce	13.59673587424118	6.69226649360911	6.75410843902235
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Ce	10.91437636923185	6.89181979703693	4.15219114354718
Ce	8.41007749655494	9.59124907827785	4.09634108287023
Ce	13.49751095337258	9.42144786785963	4.07253103733874
O	12.57556932495467	7.87273264428450	16.02967760877765
O	12.57790192327662	11.03403147826102	16.03156715723363
O	9.34527490211197	7.81813941746665	16.07194032632144
O	9.42853058566797	10.98932848499468	16.03955639080317
O	6.85402099136873	10.97376899688486	13.41773843945185
O	9.50922154677454	13.55250407839314	13.62244788902924
O	12.31980469891259	13.52108937218644	13.58729026013966
O	15.07312561003232	10.90528786316806	13.51200231028565
O	15.10284355969464	8.10102709598970	13.58059280354917
O	9.61761162551567	5.41459020429137	13.58490440959728
O	12.39425472683018	5.38558653034912	13.59950593822476
O	6.91494944279091	8.15960704291081	13.49011172562592
O	9.69605684459383	8.17807444333334	13.62783123456230
O	12.33394350092633	8.10803303845708	13.50913876014434
O	12.34046077165644	10.78630859836260	13.50500795276576
O	9.64502511303929	10.82334994141159	13.46459787771582
O	9.59706336811731	15.95693033917263	11.17110989235535
O	12.48147654979796	2.94296035387784	11.08063493534866
O	9.29537985946168	2.95904610844070	11.10889565156038
O	6.95992856611632	13.56636165120200	10.88906749480636
O	6.87830472710399	5.58698326483707	10.84960850330152
O	15.12525436478923	13.48076243917637	10.77683116971548
O	4.46775906397196	11.01555576133006	10.88470319676796

O	17.61373124702390	7.97869359232752	10.92466973395136
O	15.04298674063931	5.36937777683987	10.90354859511572
O	17.64383385926110	10.80256735819778	10.87403012795123
O	7.10807289089895	10.84979054663630	10.53211906617019
O	4.48875986690950	8.18946976880478	10.88627382958906
O	9.81311828790432	7.89660468487008	11.14926667068281
O	12.40011664176722	8.17984049621566	10.86939061676471
O	12.34477013983199	11.00795881995937	10.89611044948827
O	14.97817034991104	10.78052855201939	10.83471916699148
O	9.70084918628162	13.36583768287535	10.89559342881979
O	14.97579307461603	8.09076283104685	10.85405560432226
O	12.38488778019864	13.91728383811219	10.87024222089129
O	9.63863307086115	5.41424904819027	10.81534482599431
O	12.28778494868056	5.49673064542509	10.86935532310235
O	9.59828695094729	10.60845138447415	10.74567468394946
O	7.29743373185908	8.31661544157034	10.74018588759213
O	9.37789477797549	10.86430544885783	8.22031056653892
O	7.08425353498449	8.57190882111067	8.20293773771106
O	12.41716949001685	13.38549674813332	8.16907750661237
O	9.74842246552712	13.46030264373865	8.16300789354589
O	9.58525067910531	5.61017389881237	8.16034065144231
O	14.96031703732828	10.75990527102837	8.13646671376368
O	12.24369650709938	5.50938311339620	8.19385984090618
O	12.27299526049184	10.81691725759723	8.18423835272966
O	14.92578436571964	8.08718108316512	8.17364198512868
O	9.55010671433138	8.30531496595546	8.42209058066391
O	12.28791925101197	8.13138142806200	8.15514018363765
O	6.80354946608940	11.24831823042578	7.86125444676691
O	17.62610432879080	10.76493560599734	8.07642207717841
O	15.19134090928794	13.46289879812957	8.02003846516869
O	4.42143824921570	8.25371650359765	8.06162018394063
O	7.00354759734179	13.85055581808713	8.15227904275829
O	17.58347696331061	7.94603651357404	8.07832014603080
O	4.23917973573366	11.08513833866280	8.07816412214794
O	15.00365601557492	5.37889754327146	8.12579866894855
O	6.80949884182796	5.66506454589163	8.03112591417910
O	9.58969428519760	15.99173237242432	7.96009257499691
O	12.77573628710556	15.94719513536653	8.00172507042987
O	12.46572879622085	2.99956776224757	7.89047434506626
O	9.30165003914596	3.05126482858356	7.91807483521995
O	9.66955256463615	10.92881338739754	5.57504329525934
O	12.30475322656141	10.79577245986365	5.54173017928594
O	12.24627531118276	8.16325019585922	5.54570281430912
O	9.60585204152771	8.22958765405204	5.61506218914501
O	6.83879743358486	8.21737555751339	5.49310859877124
O	15.08300684185740	10.78328659570439	5.43234199989380
O	12.45670886409613	13.55419332390827	5.45444884884626
O	15.03640561981708	8.01618522284281	5.45639956808709
O	9.67010728648387	13.68815649865657	5.44022175802495
O	9.50382967306087	5.50070851865608	5.43414209446177
O	12.29259689393287	5.42391433648993	5.45147499170403
O	6.91793231032299	10.98811069976618	5.26500191094274
O	9.44778245292866	11.16956162797156	3.01831230712634
O	12.60228152134567	11.07133733381731	3.02261914295174
O	9.34625837565858	7.97643742679559	3.06829277159703
O	12.51694954021230	7.85080970075662	3.01391106343184
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PtCe₃₉O₇₉ D2 (-939.357797 eV)

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Ce	11.05358386124627	12.12276365001102	14.89833266481980
Ce	10.94147676671333	6.89384679277128	14.89908559465238
Ce	13.70616794968510	12.22339745313438	12.27599759995054
Ce	8.38512732689294	12.33490868953469	12.28254111468100
Ce	13.59572482288501	6.68381464424578	12.27338270316412
Ce	8.27391708941990	6.78182921017302	12.28463676757509
Ce	16.13885833133816	9.40732491429916	12.24207006798924
Ce	5.84405705181168	9.60800674880191	12.28731422451291
Ce	10.98143986530835	9.50857289321187	12.13182907698157
Ce	11.09786019847858	14.88903027878798	12.15078159415080
Ce	10.88723146756320	4.11962367118929	12.15126300889020
Ce	13.63597616608052	14.92282520155301	9.56125876698863
Ce	16.20939119413662	12.16086302052597	9.52767725345994
Ce	8.55944085140518	15.02722374819501	9.55501493054670
Ce	11.03476155208751	12.15979986667070	9.46721046191700
Ce	18.52498115231070	9.37177391476522	9.49729374382622
Ce	13.57307436229877	9.45444443534994	9.46560990675998
Ce	8.35722057302239	9.55387166970373	9.45439678316899
Ce	5.87674443766310	12.37136143965715	9.55247216153609
Ce	16.08037405088053	6.65611085031825	9.50363109990280
Ce	10.92598463726509	6.84671704976097	9.48134183599051
Ce	13.40729157021569	3.99756576562299	9.53919753406613
Ce	3.40918712817564	9.66952228545595	9.63018745877969
Ce	5.77864452392965	6.84470940292620	9.52869120065881
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Ce	11.10253366455887	14.97721147818229	6.96021601250751
Ce	10.88252634758607	4.08329806067853	6.92215070236168
Ce	10.92865912725865	9.46921633937202	6.69104884736610
Ce	16.14270711134547	9.41092077209251	6.74165015163800
Ce	5.69581781709815	9.62406377662353	6.86080136799471
Ce	13.74290146985548	12.23505870090857	6.78677085870121
Ce	8.35063742304498	12.36524055419529	6.74056723323756
Ce	13.58815500580782	6.68145743622275	6.72497337542806
Ce	8.27085765330875	6.73462156104387	6.70584734538544
Ce	11.19833855356985	12.34593548683119	4.22359600588822
Ce	11.07538319130331	6.60963474854432	3.93736338976669
Ce	13.49584997208298	9.49717137797427	4.02695955988630
O	9.45789319089129	11.15534447919621	16.00885110953323
O	12.61282425199097	11.08040579664901	16.00510746648407
O	9.39315488681841	7.97159188713242	16.00613841999881
O	9.67514532331402	13.60642420376242	13.57610524177323
O	12.47027952395794	13.54803514158137	13.57235473591528
O	15.11101047677774	10.81785542347864	13.55786998286438
O	6.94562286642230	10.98399458822941	13.58689271918265
O	15.05344826792456	8.04617493838348	13.55839176776342
O	6.87519175190250	8.20875697827369	13.59146307273158
O	12.30683367947936	5.42841758889491	13.58023841827086
O	9.51016178080009	5.47954015409270	13.59350722799724
O	9.69977333269201	10.87211304834489	13.46666548020976
O	12.34342351753183	10.81201862314582	13.47386857760181
O	12.28364342063896	8.15812646908278	13.47360242311787
O	9.63626686640140	8.20776995648989	13.46671321022026
O	9.53309525549823	16.04814789210158	11.14317688266665
O	12.71219390085908	15.98534173090269	11.15724886208196
O	12.45528359629958	2.97429100338858	11.15479588005766
O	9.29529058713707	3.02587270816985	11.14407227136194
O	15.16685546329508	13.50141546563401	10.91524505819546
O	6.97141746818057	13.66938530829990	10.92088858751116
O	17.68631490643753	10.77424859290550	10.88019606636696
O	17.63631638155952	8.01876063044541	10.88019221396329

O	15.00490959503521	5.37505984748461	10.91249641501372
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O	4.33682933069383	11.03105646973922	10.97002465897327
O	4.27285152960410	8.27702796636919	10.96594688066996
O	9.64097824197620	10.88598743174454	10.79244559220424
O	12.36899576311908	10.84154595825957	10.83111635343307
O	15.00224345106668	10.78533812406598	10.84710407814782
O	12.31808367332404	8.12910786106634	10.83061700072545
O	9.58516078870322	8.19064033153417	10.80312254340554
O	7.01660666891198	10.94279601806973	10.87039008066484
O	14.95083197800575	8.08629265161754	10.83935900351706
O	6.96266089297856	8.23996560026632	10.86788279148555
O	9.74320272156134	13.51606683200367	10.84217844811835
O	12.38634883055622	13.46750483473365	10.83274645700008
O	12.22905594436758	5.50206695317326	10.84324262653174
O	9.58408757607451	5.55339745127725	10.86497703685522
O	12.40004692222041	13.49214451106690	8.18363202390556
O	9.72743300392110	13.54227430714873	8.18264840635435
O	9.56715142660790	5.53038207733678	8.22550545145471
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O	15.01491777983638	10.79303266445517	8.16216495723546
O	14.94747909663880	8.08574331009864	8.14090187613275
O	9.63192345569256	10.90185106928824	8.00519707837503
O	12.35014877168324	10.82732276076854	8.10454466699294
O	6.97665912495269	10.95902995619480	8.19680989431502
O	12.27788840687750	8.14440064640605	8.09570970661625
O	6.91020036102728	8.24072157554545	8.19114857091486
O	9.57433462958050	8.16726666144088	8.02718938345776
O	15.16920233692296	13.50381728079643	8.14900065667499
O	17.68869975979209	10.77428886048112	8.12936475753988
O	17.63028438501292	8.02093240533812	8.11927962679351
O	6.97819773877965	13.65385420891683	8.13824244906517
O	4.29095967856109	11.03504388475853	8.22574385795294
O	4.21921974435584	8.29228980324635	8.20787647958261
O	15.01067551372924	5.36986049529626	8.14113049527957
O	6.79682974800349	5.52825786569278	8.13303717920218
O	9.53767317656082	16.08524894010985	7.96381829845755
O	12.68552257589485	16.03203642984510	7.98465880653678
O	12.42617191206527	2.94523815842261	7.97608896075712
O	9.27647212050208	2.99778870132081	7.96450432581779
O	12.31219940210776	10.88590404733207	5.51857506589857
O	9.60729594132320	10.96910521688172	5.15281649122186
O	12.29338598009500	8.14789967646138	5.47137013469220
O	9.53357717932054	8.13553012873864	5.19176596060028
O	12.54451617123377	13.62777933062876	5.45466440090816
O	15.08106678100162	10.86157820396028	5.45588844235714
O	9.75245097599087	13.67505308762188	5.46107958659908
O	15.07123878508914	8.08926211002974	5.42894170726512
O	6.76971724624920	11.10457048092164	5.50561499709271
O	9.52485502905184	5.38628616542259	5.58315330443665
O	6.69348053077705	8.17141654471903	5.49335625186832
O	12.40486026398634	5.34733811997592	5.48492543895843
O	12.41879364787098	11.28688206479471	2.96866650473755
O	12.66988942697637	8.09937589748888	2.88635109211170
O	10.50521723429896	5.59711106221860	2.48554492730690
O	12.53848346658522	7.88751194837526	16.00205705717529
Pt	8.13401305904336	9.58806190900564	5.24090504510926

PtCe₃₉O₇₉ D3 (-939.165507 eV)

Ce	13.48104351127457	9.46909224165447	14.96311675457174
Ce	8.45033388377152	9.55473933413727	14.91592950993119
Ce	11.00993619805779	12.13198984543464	14.87856186652898
Ce	10.91348355411347	6.88365683729006	14.86410928506601
Ce	5.80304771207495	9.58871488627437	12.28809468007337
Ce	13.68570028056073	12.23011929683591	12.27229844000714
Ce	13.58238436594659	6.69002336287453	12.29153042446288
Ce	16.13671665837699	9.42415186896702	12.27530190265893
Ce	8.34056218002572	12.32141285872114	12.25540656892613
Ce	8.23116157453038	6.78897725991316	12.22636538802450
Ce	10.96113040056066	9.50438937820264	12.12144500246687
Ce	10.83689743562151	4.12147685888351	12.12252163279691
Ce	11.05722399744373	14.88766633358907	12.10278892565628
Ce	3.40170428802337	9.63834082101303	9.68971956418943
Ce	5.65695941090572	6.87389165711395	9.50289034511299
Ce	5.74800029214692	12.33632263698356	9.57192756858688
Ce	13.42542973818358	3.97858008400414	9.59007327103928
Ce	16.12875835264305	6.66140984224774	9.57742339539733
Ce	13.59929147766350	14.91308922486580	9.49851380682088
Ce	16.18594971211426	12.16510204065158	9.50195199348059
Ce	8.50542987382128	14.98072344574457	9.51221094298240
Ce	18.53676790031900	9.38656850317146	9.51548915800051
Ce	11.01428277012266	12.14211237408077	9.48060272738890
Ce	13.59040683872254	9.44791784645762	9.49854910568077
Ce	8.30118671296315	4.13566626144209	9.48365320525976
Ce	10.92228165273819	6.83870474841566	9.47380825467673
Ce	8.28851670553601	9.56192265928680	9.43883699694777
Ce	10.91035485385332	4.02436515726590	6.96992955930225
Ce	11.05888753453112	14.92192211287381	6.89198381278459
Ce	10.95144654844263	9.47695843975768	6.78578294770018
Ce	8.31973923690292	12.39556799598217	6.77947956435494
Ce	16.16873674515719	9.40591405191774	6.76305609750771
Ce	13.69986714373363	6.64516010594381	6.82867840917271
Ce	13.70221986933438	12.21379549260654	6.74155676682524
Ce	8.21913911596629	6.75598734106718	6.68846219868583
Ce	11.07537402566206	12.14810528499680	4.14211656192359
Ce	11.20700000099002	6.66742479271230	4.25293459030926
Ce	13.53101438557982	9.44368541339645	4.07337613553692
Ce	8.34489486231847	9.79840380011593	4.12594459235413
O	12.57173703694589	11.07987659210027	16.01333917885520
O	12.50730149045599	7.87923753678783	16.00226751181038
O	9.43064775636413	11.14264074563437	15.99058949208329
O	9.37431071011430	7.92742624985222	15.98251314018298
O	6.97021108530217	10.96448157877721	13.59626526942295
O	15.10697034218630	10.83098997885186	13.56408432524452
O	12.28768503473008	5.41788072254106	13.56811871568829
O	12.46014580578562	13.54978882245943	13.55106243254903
O	15.04503515784616	8.05305252155402	13.57077299175059
O	6.90839162561869	8.15707149414162	13.57374876675630
O	9.66438827022519	13.60281229758460	13.55202990838425
O	9.49411724459468	5.45044628012466	13.53661490934637
O	12.33278297220418	10.81430151694118	13.47082805546469
O	12.27484540120366	8.15549094203401	13.47178483366823
O	9.69857564277618	10.85969264076252	13.46108360473546
O	9.63104475554948	8.18732606362860	13.43008827909743
O	4.33369938113456	8.25499938634977	11.12595147601838
O	4.37403809473059	10.96561492523956	11.16311041345099
O	12.44892550133094	2.95905528940275	11.16357579482520
O	12.66978712714572	15.98346293195947	11.07304912138818
O	9.50725039020635	16.03056140103385	11.09515155933820
O	9.25634411808177	3.04912439431327	11.07099910495192
O	6.79400732620698	5.49655947895961	10.85182791095773

O	6.94563122695995	13.64640991547958	10.93889614637243
O	15.01362937681568	5.36761631678140	10.94032787513977
O	15.15087398522010	13.50063056109508	10.86676735942073
O	17.64727553656262	8.01893807308209	10.90538340440462
O	17.69033927546521	10.78004153004515	10.87607902588019
O	15.00729742203405	10.78170376466473	10.84930243049735
O	14.96483333585589	8.08141393229748	10.86815767108162
O	12.37141330623717	10.82731793923392	10.83109020827424
O	12.32376389673541	8.10949427423261	10.83978771242668
O	12.37295775177662	13.45716020768772	10.81300517508784
O	12.21809765719203	5.48613932565169	10.83646813255252
O	9.62288293966117	10.87064624049117	10.81460168614124
O	9.71971237285838	13.50106911647247	10.81508284072536
O	9.58834663727012	8.19049843195549	10.74808078629762
O	9.56632204977763	5.55876614511469	10.80429061894753
O	7.00504991553677	10.92435330033187	10.83020486301764
O	6.95955473599416	8.21603478628004	10.80278989329953
O	4.03325702882884	11.27803947429379	8.57968745361338
O	3.99504791134361	7.99120751055830	8.53591364120267
O	12.38157842836224	13.45346042131768	8.14670308376156
O	12.27603642955155	5.46156593240853	8.18908402807399
O	9.72971836066061	13.51309158529350	8.16457170159080
O	14.98760906453809	8.06500067868725	8.18277227852954
O	15.00209297925306	10.77075501670556	8.14359845254099
O	9.59870332261691	5.52064250711412	8.14300479230340
O	6.98440733640541	13.68070343474893	8.17144747922740
O	12.31386149774025	8.11301221911407	8.14285659276135
O	17.65040467200517	8.01473486801087	8.15226254105932
O	15.05794706424802	5.35374768244044	8.17750761211357
O	12.34586369483668	10.80134564269788	8.10584693140042
O	17.67932694180602	10.76240361136645	8.11846331020439
O	6.86749417980517	5.51321403073934	8.05640778510053
O	15.14934793259724	13.47540962084189	8.08981164033128
O	9.61152347430489	10.87107329264162	8.11598284774561
O	9.55184740176928	8.13371637537530	7.95571526145941
O	6.85213783443649	10.98650180525500	8.13057805467943
O	6.83169591571873	8.18939153784005	8.07515150419938
O	12.44862503039283	2.91074214635937	8.00290900685487
O	12.66816460272891	15.98713594878306	7.88952068203506
O	9.50897468514975	16.02881194847524	7.88613122268630
O	9.29132362156590	2.99783331780038	7.89045267668392
O	12.33164929408066	10.75902637894002	5.49840452884971
O	12.36784772118042	8.05721874863234	5.56764016157623
O	9.69819030759258	10.91551682816059	5.51361368191270
O	15.09966248895349	8.02284814901211	5.46311829564593
O	15.09008794079932	10.77779250725323	5.42603183947611
O	9.69332064752155	13.60898955031948	5.41677037763202
O	12.47981580617794	13.49166587876434	5.39115559075308
O	12.47306852943861	5.31907706916741	5.45519508304444
O	9.74780668893643	8.22325581040933	4.99788724115112
O	9.65425933478080	5.46556796180844	5.41131334258552
O	6.98042034608301	11.13144247981667	5.29192969324641
O	7.02139874147155	8.17314183854278	5.23319648738323
O	12.63811916351309	11.01769801686303	3.00094535332212
O	12.46282059018933	7.80528256933763	2.99207654015623
O	9.47932972720868	11.09199948100752	2.94695291493926
Pt	6.81807725067466	9.61372597427189	6.64906370943655

PtCe₃₉O₇₉ D4 (-941.024797 eV)

Ce	8.40204597334469	9.52613087375035	14.90138833715285
Ce	13.52420674487085	9.51467269648511	14.98547899636866
Ce	10.98419069271521	12.10750152638935	14.88343954698001
Ce	10.95076322331753	6.94728321606070	14.97283812948790
Ce	13.69688217280122	12.23274758311309	12.28499081151130
Ce	8.32571946216674	12.27718765478369	12.26084441707025
Ce	13.70182190159899	6.76081878072623	12.30030593171367
Ce	8.24304000834340	6.74490569031946	12.25712582096144
Ce	16.19471062543325	9.45755528244226	12.25673210997387
Ce	5.74794887132296	9.55980592977188	12.16799916413740
Ce	10.99640450200978	9.46390176222084	12.16764754722396
Ce	11.04758813094297	14.86403025606949	12.12983203278057
Ce	11.13455754477825	4.24351215879649	12.30430657931974
Ce	13.59390480132586	14.92444811766652	9.52410978526192
Ce	16.19966279311478	12.18355000649442	9.50538442027968
Ce	8.51189133324664	14.92901117495280	9.51210275601867
Ce	11.04115179475651	12.13374353093971	9.51059203222295
Ce	18.55983543406144	9.38263516675832	9.49716702482483
Ce	13.61886409091924	9.45611411563825	9.50706557049936
Ce	8.35140379089334	9.53341537684694	9.48444064752286
Ce	5.79943880492057	12.27856993448197	9.51494488153857
Ce	16.13389399700037	6.67651601482266	9.49618131801651
Ce	10.93328956934633	6.81706266788216	9.50986135308980
Ce	13.42205408809494	4.04214535954841	9.49493286762748
Ce	5.64518312031257	6.97711692631622	9.44315079481921
Ce	8.13954010181029	4.28285973490645	9.23781957273429
Ce	11.05602402789016	14.89629289602837	6.91105742541909
Ce	10.88657354243812	4.16715202926988	6.86247719239316
Ce	10.99327821949458	9.51010183030260	6.85413912398374
Ce	16.15965703776059	9.42201818833119	6.74827536956359
Ce	5.74547417945695	9.64723240825649	6.79245094392314
Ce	13.70508889783971	12.24377890886865	6.73301336661330
Ce	8.33958367474825	12.32417038572399	6.74709560144070
Ce	13.61059698484378	6.70356311031997	6.72325069058986
Ce	8.22992327230000	6.8645666970453	6.64864121809399
Ce	11.01601840165731	12.14391491107873	4.12816963893101
Ce	10.92520843961364	6.92635075222254	4.07110373398187
Ce	13.50897954019050	9.48819758136995	4.04098677742447
Ce	8.42270810291457	9.59904514976424	4.06645544845357
O	9.39026934996660	11.09168137012731	15.97890025772610
O	12.58560021591933	11.09092596593554	16.02395721880222
O	12.51827751774715	7.94316418619374	16.06473099213245
O	9.36425134052396	7.90899322831187	16.01973749700455
O	9.63946300403607	13.55431231301364	13.58711755614916
O	12.43677245460159	13.52310339504355	13.57857128273881
O	15.11996545817922	10.83396400714387	13.57640984486934
O	6.91010020627560	10.87312572373087	13.56545678998284
O	15.10730402841061	8.06752626058529	13.57201348821981
O	6.91254394952766	8.06053271765391	13.50718528895323
O	12.46176473385561	5.39942348847736	13.63062686736747
O	9.64773535767878	5.42375263110965	13.55819970042170
O	9.67798005951792	10.81787510318266	13.46843901578517
O	12.33196501634775	10.79429723122269	13.49959514559272
O	12.32771713133516	8.13901545685684	13.51789476004610
O	9.64777293276948	8.15910539535911	13.49191430667273
O	9.49817805606135	15.99038369482336	11.12226934826658
O	12.65424198194189	15.97707654732561	11.12522302121935
O	12.35349746689038	2.97110243892415	11.14376595118883
O	15.15214539983918	13.49703107676890	10.90009764405207
O	6.97113282706124	13.60013855911898	10.91781875947122
O	17.70744268566040	10.77060985259641	10.88604041606978
O	17.65738666952156	8.02148403358498	10.87382160531768

O	15.02741185341308	5.37899063582567	10.88564498119780
O	6.85996727482438	5.48091973608426	10.75134347712255
O	4.39058478988678	11.04163977526681	10.95797182032817
O	4.31784014257784	8.16075761920945	10.92025753715509
O	9.67800205525961	10.78333376291442	10.84623814661823
O	12.39936288215629	10.81525729235688	10.87554237543565
O	15.03062934995506	10.79093651340573	10.86264603510914
O	12.34678773872594	8.11715429077764	10.86147919214848
O	9.60135226954890	7.98208161395115	10.88052288127471
O	7.05345935918275	10.89439854465580	10.85284158496329
O	15.00499534280931	8.09711920598942	10.86351231122501
O	6.99627966553916	8.18151524125575	10.82909006081278
O	9.72394396231879	13.44826450282858	10.84854976582654
O	12.38050297229953	13.45231044221077	10.84569218528071
O	12.28994326310062	5.53662691390638	10.89945139372714
O	9.59760328758383	5.06739458625502	10.82416213105513
O	12.39328665267846	13.45839312096580	8.18373482034858
O	9.74190963540329	13.48900254001677	8.18753982337748
O	9.53849777469721	5.59549945840567	8.13299953269188
O	12.21441936478855	5.48756945309553	8.20076068528352
O	15.02757501744197	10.78576499765565	8.15612152657284
O	9.66647823776842	10.86850327405026	8.15157870069992
O	14.97903523345986	8.07592302590278	8.15724888153393
O	12.39993391996452	10.81896201234539	8.15462629526777
O	7.05179196538321	10.92024971979308	8.15051000854915
O	12.33707630821847	8.09445169562394	8.16567008009675
O	6.99005484508531	8.22306020248026	8.10973519449351
O	9.62917106163075	8.17251241335931	8.15960521468544
O	15.16830673160987	13.50088547822559	8.12310889543073
O	17.70077070475596	10.75957821784288	8.12589588407671
O	17.64227695898381	8.00451181316775	8.13307240195274
O	6.98086317061052	13.62746263041609	8.13525378293668
O	4.38581466039259	11.08271323790643	8.05502903209477
O	4.31619018948317	8.19771082663585	8.01796162541498
O	14.98021351183606	5.35708643565979	8.14328434518408
O	6.78161178040415	5.51426296976762	7.98594070524761
O	9.49660846283070	16.01218522162020	7.92247681919385
O	12.65727652220881	15.99424963487128	7.94108274835501
O	12.43757356953233	2.99076208757237	7.94195792683823
O	9.23061382782679	3.04703744714889	7.96273387187098
O	12.34384281681701	10.81833257765980	5.52333789048310
O	9.69098244903639	10.86547531659597	5.52300756263797
O	12.29588395606270	8.14467897735136	5.51288228219165
O	9.64429623492203	8.21737945946237	5.50550917791620
O	12.46651076631580	13.54810882463012	5.44873037517592
O	15.11814081504322	10.81190856111700	5.43932450054847
O	9.67050508193941	13.60540653584045	5.44573159345308
O	15.05798942292347	8.03603358415173	5.45535680853528
O	6.92341756774700	10.99276193755531	5.44018549491137
O	9.54334775879008	5.45184221163754	5.43129564985375
O	6.88934663955805	8.22273945275587	5.40182355629697
O	12.31678924740684	5.38856016418961	5.48028597511274
O	12.59530740873819	11.08628897277816	2.99944859432844
O	9.42214399255798	11.16864609603230	3.00452227616482
O	12.52430730144698	7.89713524833461	2.97819617756093
O	9.37343471188497	7.95338964620798	2.99578881310990
Pt	4.24719147025547	9.63129280576061	9.48725285224300

PdCe₃₉O₇₉ D1 (-936.214605 eV)

Ce	18.68727581487535	9.31104084953923	9.48945628861467
Ce	3.33028783335942	9.65135142823345	9.47028292986826
Ce	13.55260454692721	9.43244237601720	14.94223350470709
Ce	8.44007875265288	9.39896274531963	14.97827258638337
Ce	10.99460413975372	6.82983799337691	14.92767661795249
Ce	10.98689519901176	11.99397748614320	14.94554968650058
Ce	8.26519575840145	12.18658686630818	12.22102017003721
Ce	8.34102012694461	6.74060340982655	12.28266919312987
Ce	13.65819364553793	6.65872131253205	12.29319920126604
Ce	13.70227801001894	12.22220688960908	12.27587483906717
Ce	16.19708303093836	9.41454482842561	12.19285569379976
Ce	5.85881391275179	9.55156242046040	12.08059721418723
Ce	10.98798739527040	9.43526424055404	12.18877819886550
Ce	10.82363442409516	14.71246629781865	12.33102312064234
Ce	10.93051078893050	4.06001296904273	12.12202093446716
Ce	13.80782673624174	14.70102224716769	9.27587304974841
Ce	8.52607506037921	14.91275960131490	9.48395693469383
Ce	5.78692297966766	12.34139219786395	9.41113091969698
Ce	16.28787218590603	12.02095765084502	9.46131500921754
Ce	10.97012748576448	12.11449018197926	9.50535083527193
Ce	13.59192572994513	9.44972091173033	9.50426488655446
Ce	10.94593455217450	6.84666206114499	9.57401280480476
Ce	16.14578467388108	6.68811662370740	9.51077460941790
Ce	5.85805108487310	7.00097815474939	9.46880687245213
Ce	13.44968579607406	4.03117813740369	9.49136301535503
Ce	8.37983332792196	4.09320961134159	9.53287884951836
Ce	11.08326095561863	14.83233368094010	6.88085426021294
Ce	10.88780649839302	4.15774242771603	6.89484489722405
Ce	10.91256431956780	9.51374609589467	6.91023970187447
Ce	5.75302929683297	9.70092320132176	6.74264555620390
Ce	16.17877904050599	9.34877046962212	6.78799642830679
Ce	13.71694050289657	12.14000835160824	6.66455673342822
Ce	8.26574521610159	12.39071929351729	6.65690683019094
Ce	13.59678120484299	6.68888580616977	6.75525498096793
Ce	8.23829121504490	6.84110299535689	6.75542654924905
Ce	11.02834923118927	12.11513377103214	4.10123457772651
Ce	10.91293142516150	6.88859238837912	4.15685597025677
Ce	8.40987339590966	9.58813034247885	4.10033513299215
Ce	13.49840489221274	9.41828739979619	4.07347887102688
O	12.57542782580449	7.87285338613908	16.02744604702573
O	12.57612117083558	11.03224161749418	16.03094324231100
O	9.34383012977108	7.82056873630151	16.06363615811062
O	9.42550874387665	10.99067311656414	16.03421330479127
O	6.85698431410894	10.97269912990701	13.41789572143615
O	9.51309703712134	13.54785480474670	13.62098559123408
O	12.32202680906728	13.52005771436758	13.58715660711531
O	15.07594171017998	10.90581244152786	13.50863685022388
O	15.10303994359220	8.10221890077985	13.57743295362516
O	9.61497391863515	5.41944816294488	13.58541901115063
O	12.39182811206520	5.38496544968611	13.60114379785007
O	6.91537199510092	8.16340592682315	13.48885464031127
O	9.69584109759097	8.17595763619288	13.61621659859219
O	12.33273577337568	8.10786104247281	13.50753198966643
O	12.34173196342254	10.78589321085970	13.50308417904119
O	9.64768834838953	10.82094551595078	13.46095107958894
O	9.58925800945241	15.95487296069056	11.17539103356772
O	12.47826150765490	2.94464065711980	11.08631887781191
O	9.29267218392184	2.96716456327148	11.11429497013652
O	6.96951214864507	13.57247272256980	10.87597692814463
O	6.87736064108149	5.58807892260266	10.85158922641611
O	15.12665447902748	13.47656715879973	10.77557568724837
O	4.46475849513129	11.02312747595553	10.87506851938596

O	17.61561032880888	7.97614896007772	10.92234156090999
O	15.04194123515159	5.37043177336955	10.90739896792217
O	17.64758756832219	10.80178940024788	10.87151503856976
O	7.10353003782154	10.85328929152059	10.54944307906021
O	4.47175077891120	8.19904237563291	10.88312261587130
O	9.79067696259953	7.92715475780738	11.12181277924849
O	12.39769354455402	8.17717452926849	10.87152557224828
O	12.34673152885513	11.00457051197623	10.89422737707596
O	14.98140865777467	10.77751602780516	10.83218911101172
O	9.70555551907942	13.36784642852377	10.89341993246510
O	14.97723430549767	8.08979300840631	10.85268229131489
O	12.38779961897782	13.91974095364393	10.87102739773008
O	9.63744176107467	5.42568237297371	10.82369909186046
O	12.28545276651878	5.49760917691011	10.87269743999465
O	9.59967460951675	10.62115980278073	10.74744215908260
O	7.27063045128701	8.31226704328563	10.74501261145054
O	9.39736882559474	10.86103105114935	8.22057314392393
O	7.08271651267711	8.55306181135006	8.20141582372542
O	12.41665728888756	13.38418078074212	8.16905225254997
O	9.74711898179579	13.45689334896746	8.16191000654769
O	9.58548666073564	5.61317867365134	8.16795301866143
O	14.96360790864804	10.75602237048706	8.13560659479957
O	12.24302772248051	5.50887676848189	8.19815150204640
O	12.27915077230615	10.81476759757503	8.18183179542044
O	14.92664167742528	8.08391211710139	8.17240328231882
O	9.54886703145713	8.30269532304368	8.41375599264424
O	12.28574530747283	8.12905094928494	8.15875121336885
O	6.83509741458679	11.21897119850359	7.88812619205955
O	17.62548539225754	10.76425379161422	8.07377663889897
O	15.19092103392564	13.46042900151452	8.01905237744502
O	4.42302325074638	8.26315249738772	8.06251137343009
O	7.00149391285666	13.83846998303668	8.13593741158873
O	17.58456200538044	7.94113490110316	8.07563566787443
O	4.25060935562447	11.09430387883773	8.06906255369944
O	15.00400151859406	5.37674024746474	8.12923720105261
O	6.80940709280786	5.66473985314614	8.03636328332168
O	9.59345225676343	15.98989277273323	7.96673564711991
O	12.77742255452355	15.94464698078205	7.99738411875434
O	12.46196731293466	2.99808066203338	7.89507885903345
O	9.29581885765212	3.05578321168251	7.92371891522306
O	9.66794160813737	10.92824171267615	5.57801515094923
O	12.30349765172453	10.79304975025899	5.54069271080026
O	12.24816765930139	8.15876193493674	5.54868520985570
O	9.60731987826004	8.23035753895168	5.61453133527766
O	6.84383092082601	8.22637890388384	5.49230074137332
O	15.08198339875573	10.78006481124226	5.43124988217709
O	12.45724419115136	13.55175063456468	5.45447939964540
O	15.03707318172166	8.01396589035373	5.45648389366107
O	9.67190320787928	13.68783377670156	5.44028636471034
O	9.50556066426316	5.50478470977087	5.44243780589832
O	12.29310398064890	5.41885269244768	5.45449378809829
O	6.91489326225615	10.99965365214833	5.27803859652443
O	9.44784129840960	11.16477835558911	3.02115554577747
O	12.60310540049572	11.06951422696870	3.02269029906591
O	9.34395462685472	7.97486934653423	3.07039580840981
O	12.51426799452861	7.84874762948754	3.01619163482798
Pd	8.35742333517845	9.58888127752246	9.46659847095713

PdCe₃₉O₇₉ D2 (-938.570007 eV)

Ce	8.43323462630234	9.40653667237406	14.97761165053726
Ce	13.48617117098827	9.37871600596283	14.97214286500930
Ce	10.97682763246125	12.00584365058289	14.96889701446993
Ce	10.94583809477481	6.78420893616584	14.86456447200731
Ce	13.63812416108778	12.21258680114496	12.33292284510502
Ce	8.32380547089207	12.27348309505247	12.37079337445475
Ce	13.60401603861627	6.66321412976587	12.24778773380418
Ce	8.28755219682259	6.68880558926514	12.23855347974757
Ce	16.11123202501655	9.41217578470387	12.27100669115381
Ce	5.81023916639384	9.44483528830471	12.26471001933189
Ce	10.95327718694271	9.48182095949873	12.16626560937763
Ce	11.13848266008084	15.00874035284290	12.47965102783196
Ce	10.93143264256535	4.05917451988224	12.05441715218535
Ce	13.53487865674100	14.94757975434550	9.56792587134754
Ce	16.14308985107868	12.20840005192541	9.56724917802003
Ce	10.93566004684241	12.30423858307059	9.59028739537822
Ce	18.50434280901365	9.42699576332240	9.52662980452544
Ce	13.55643613418726	9.50219533018562	9.50843251744410
Ce	8.34141311598372	9.55980827569537	9.50743902021131
Ce	5.70471563191997	12.17779368033913	9.54335993287001
Ce	16.09587215201132	6.70324454277992	9.47847215004223
Ce	10.94530509728747	6.86081790988889	9.47244284193840
Ce	13.45373540263588	4.02301122032611	9.43219906166146
Ce	3.39515089324586	9.42422302553620	9.49203221668468
Ce	5.80896636885396	6.74100455344856	9.44631358128113
Ce	8.41510275602309	4.05354151104288	9.41959726183212
Ce	11.19018379134261	14.81773557074503	6.75350433269963
Ce	10.93760907206121	4.13886154047814	6.81025264762189
Ce	10.97187136298710	9.56940756257520	6.85579255537043
Ce	16.14514179382673	9.45055862045752	6.76965530509394
Ce	5.80957386607562	9.55072421682510	6.73923258098997
Ce	13.70387845591745	12.22181413282290	6.77520964789559
Ce	8.31629598911731	12.33828802144397	6.74845612871403
Ce	13.61111330523706	6.73196112010628	6.69705384065079
Ce	8.29293154230793	6.78472879422967	6.69070784129244
Ce	11.01564858486905	12.12754304815518	4.07608670628105
Ce	10.94528306505016	6.93484647160201	4.08231113219064
Ce	13.51525021681260	9.49058998015880	4.04728482969259
Ce	8.44113547149738	9.57389152905423	4.04279801454772
O	9.38288837643394	10.95616314189980	16.06328393331172
O	12.53914735531974	10.93442595536749	16.06589836574143
O	12.53352870421153	7.75747793838993	15.99316121518865
O	9.37925113795603	7.77900254023610	15.99765623053196
O	9.60239782015925	13.37058014306312	13.71673184524297
O	12.48209589364555	13.44374598498761	13.70412403254532
O	15.07437572887088	10.77300309953221	13.59789856199390
O	6.86293608169569	10.81516768662375	13.58366036110749
O	15.04161212023589	8.00443538967546	13.55337451216564
O	6.85219300520539	8.03354491905549	13.54478320720776
O	12.33366318905281	5.34879797365752	13.51153232508239
O	9.53492633445440	5.35760971523557	13.50335093467426
O	9.62986505636803	10.73031825335810	13.52367477469886
O	12.29837273393745	10.74596370849148	13.51781247996353
O	12.27018857424053	8.09210305386440	13.47133066974788
O	9.62479789121749	8.09391205497021	13.46561255992413
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O	12.49818182665077	2.95526143230604	11.00376480054972
O	9.36049481857409	2.97433335448560	10.98685973206601
O	15.11110844612405	13.51736853622245	10.92680290323018
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O	9.58726495600708	10.96174871865147	10.88929478332866
O	12.29156695635016	10.86796663127289	10.86582029529430
O	14.95783789279898	10.80243896902177	10.88332924229169
O	12.31457568045907	8.13169190475802	10.84156082841439
O	9.58542549205232	8.18249675886493	10.83084061911959
O	6.93001021438503	10.80734901183957	10.86995026512703
O	14.94850401870523	8.10054440846843	10.83728184202334
O	6.96224972491922	8.12816431197860	10.82458790280254
O	9.58806856654306	13.76637586992504	10.97672964184539
O	12.33617440939402	13.49379150131253	10.90642603121532
O	12.26037219840972	5.49031107238185	10.78063019469793
O	9.61783651782779	5.51516042448773	10.77760591069040
O	12.31683141680459	13.48582571634422	8.17290723002048
O	9.61503546451135	13.84944254546914	8.13009650421868
O	9.62016242604438	5.55834779596509	8.11112595747266
O	12.26394861466693	5.52795548603395	8.12007347318498
O	14.98796090122815	10.81523122791715	8.17646227353747
O	14.94806344331621	8.12938159789709	8.14200114513901
O	9.60278413528013	11.02499729795379	8.16373142912750
O	12.32317872379200	10.89695626842325	8.18057706616899
O	6.95484898775401	10.85853917756049	8.15699584530941
O	12.31524790414953	8.17119677697181	8.12708775391882
O	6.96285524862918	8.18278464749303	8.12149480299840
O	9.59178919452949	8.23265550720940	8.13607688362012
O	15.08156019904466	13.52389688379624	8.15303739710514
O	17.65874408771622	10.81386207915264	8.15431459420850
O	17.62991883117735	8.06353394446507	8.12165897110909
O	6.76197319467344	13.52637073108034	8.07280400475286
O	4.26476361271238	10.85565313998609	8.13978736110912
O	4.27838813446397	8.11011787472470	8.08037190823599
O	15.02676499510208	5.41884614801363	8.06500569553610
O	6.86512148078960	5.46414664703744	8.02906249979234
O	12.43464818205830	16.04451958046754	7.81053906140386
O	12.49825348183106	2.99774323167377	7.80808059676299
O	9.35613888992014	3.01869349368878	7.79721630797152
O	12.32327629455244	10.85811672661538	5.51813095159245
O	9.65403385534871	10.90158565845401	5.51903955239147
O	12.27918223956937	8.20665665051549	5.50366055268575
O	9.63678265725600	8.23705587190084	5.50441273205741
O	12.49926413419150	13.58761649949982	5.42830280664055
O	15.09277459899946	10.85955498341573	5.46659299897572
O	9.70745388042993	13.62454927810688	5.42357830716623
O	15.06053218792406	8.09515603252549	5.42726520393132
O	6.90092177138840	10.98064267606508	5.46210691604993
O	9.53796832185758	5.50113715559193	5.37295760981661
O	6.86503335433115	8.20079411032848	5.40051957418297
O	12.33394941017678	5.46793209666483	5.38003371585716
O	12.56748276541122	11.09521607210256	2.98026125829722
O	9.41769985400994	11.16513173265682	2.98181617265069
O	12.55790496965169	7.92105055936009	2.97812351545983
O	9.37979723139882	7.98968876963068	2.97413603631920
Pd	8.16079929503160	13.83159231326485	9.55007388949935

PdCe₃₉O₇₉ D3 (-938.423214 eV)

Ce	13.58459593475366	9.44959665757884	14.90547652043796
Ce	10.96340523197138	6.88374722793621	9.49927234877514
Ce	18.57091725835325	9.20147816767880	9.47621610198525
Ce	8.45613555044595	9.45004270867443	14.98293703904448
Ce	11.02176932172677	12.01761112506505	14.98392082588133
Ce	11.00250269816274	6.86917155655224	14.88140748137526
Ce	13.76153395106844	12.25185300266767	12.29478505975425
Ce	8.27831878146182	12.22530623630503	12.31492826650261
Ce	13.65364399503603	6.71771691434940	12.24646072612710
Ce	8.29914748597287	6.75996842338383	12.27225101983236
Ce	16.27134951444614	9.40578124814957	12.20047638231625
Ce	5.79915035453087	9.52698382828599	12.25475609953395
Ce	11.01021708843437	9.53065881366979	12.16351993600482
Ce	10.81433935680895	14.75151107998517	12.33562804197579
Ce	10.92628399337326	4.13062675483039	12.11366571705470
Ce	13.75270028780715	14.81872139220102	9.26257384715785
Ce	8.54663714914009	14.97273034204750	9.51194199459499
Ce	11.06797002863363	12.21620436852792	9.53301698137802
Ce	13.69249309664281	9.51163423596755	9.48116320245791
Ce	5.85496274490842	12.33249748147449	9.51156797006964
Ce	16.13735062493293	6.62558709633911	9.48054300829215
Ce	8.38452563026011	9.55344236369162	9.51053302819605
Ce	13.43526189332684	4.04680835965258	9.48544808929674
Ce	3.44331794775757	9.61889902272281	9.49917088178940
Ce	5.79635540804031	6.81736453004030	9.49324318130603
Ce	8.39099617079926	4.08713764651792	9.49791414262998
Ce	11.06385955600390	14.86161398166138	6.86688135256655
Ce	10.91170314695910	4.13644047589430	6.87175635778317
Ce	11.01168714720168	9.52689278972648	6.86301977853293
Ce	16.26282334376949	9.34589440824309	6.74312673877100
Ce	5.83299102109220	9.59315199026072	6.75164833522273
Ce	13.76273662277751	12.17453802742425	6.65874358990440
Ce	8.37482771132072	12.31513833711187	6.74474617890816
Ce	13.63117456643718	6.69639726052053	6.72635477517537
Ce	8.28892562466792	6.78419230256149	6.72366159113214
Ce	11.06392838798738	12.11689987497459	4.08802904675794
Ce	10.95597107851611	6.90765939578272	4.11096068178454
Ce	13.55992719672633	9.43887593587910	4.06185324534088
Ce	8.46948760971967	9.56576628237095	4.05042485222081
O	9.44867752806578	11.01599925985147	16.07138958372006
O	12.60281277122449	11.05297052747656	16.03235865091822
O	12.59249302266251	7.87478441649745	15.97828543376711
O	9.38623093226101	7.85715588190451	16.01623795682376
O	9.50446511465117	13.57195232105553	13.66140682861110
O	12.32198505487279	13.55350939683193	13.56249027270184
O	15.07131743528638	10.86635032536889	13.55316744490294
O	6.87250084313831	10.90532700976809	13.58102520520235
O	15.08693215692843	8.07076989662586	13.55921849391117
O	6.87231986310717	8.14130407498737	13.56901007779746
O	12.34752479788429	5.43296809244137	13.56686963696921
O	9.54645016942914	5.45490066496166	13.56155521632182
O	12.33984535131726	10.82401442203754	13.50367689617588
O	9.65698316438015	10.83474001650766	13.52304254213566
O	12.31545514565164	8.16516539927268	13.46494390152879
O	9.6660005594809	8.18781612522553	13.49491534740271
O	9.59667441842522	16.03147176217764	11.17614367180201
O	12.46532035829085	2.99069073136435	11.09821972178274
O	9.32296119010704	3.02673966087234	11.09814903363728
O	14.98771187341755	13.67842212519774	10.88502047965831
O	6.92407129874970	13.61220335684768	10.91075140865247
O	17.95784163035874	10.36278613685738	11.11018734613617
O	17.60058236539778	7.77286606201589	10.83603085565464

O	14.97587419562646	5.35264555110588	10.89369983388330
O	6.83159933551555	5.49594537355018	10.87955897280966
O	4.32877294171800	10.97223922388812	10.88415082359190
O	4.28229385906513	8.22105966887094	10.88481559330176
O	15.11949690907847	10.83736429646171	10.88395212838627
O	12.42622808245010	11.02561770747832	10.89201224638229
O	9.66113878068371	10.88454358908612	10.87098000047173
O	6.98829193581419	10.89379988997383	10.87054775962207
O	14.98087210575777	8.11571246913214	10.83716659928168
O	12.34842065941230	8.22885753173684	10.83531062839193
O	6.96800038212867	8.20404723191589	10.85600137180477
O	9.60767855025386	8.18800803846973	10.87104764077983
O	12.28373780285385	13.98266267300019	10.80658916604463
O	9.65226523568029	13.45913124977419	10.92465744084264
O	12.25128927166532	5.54655877041439	10.83274256816613
O	9.60501757377954	5.55395999052510	10.82510239476544
O	12.38726578383481	13.45969399434851	8.12570282596913
O	9.74510875322935	13.52881480304984	8.22313129135579
O	9.59346227642828	5.56560134035173	8.16657678430803
O	12.23523427878093	5.52566882398998	8.16658669923448
O	15.14406191266300	10.78398434759726	8.07551593045308
O	12.41278990372557	10.86518135961741	8.16715447943813
O	9.67577774266525	10.92314544137025	8.18129375077889
O	14.97186764411921	8.09434277011435	8.13549692033794
O	12.35207463236184	8.16554177507397	8.15218493515517
O	7.01883415453664	10.93426000354010	8.16507537762269
O	9.60505095557928	8.20210845140961	8.15348699188430
O	6.96785655480552	8.22857589101034	8.15389910003334
O	15.09089679449552	13.62831302218543	7.94926337423832
O	17.96816129305617	10.32929842635846	7.84199930975020
O	17.59880552707426	7.74332303614111	8.12563867858855
O	6.98852315172659	13.65376958390202	8.15593652589717
O	4.34604576853365	10.99917723734052	8.13629860855403
O	4.28356635577144	8.24182432489662	8.12001548034771
O	14.96809824155453	5.33405733576584	8.09038125030127
O	6.81679428568050	5.51162682823868	8.10191845292675
O	9.50260747599786	16.02990097410089	7.96235681512783
O	12.66569002687182	16.02395882014812	7.95236645057338
O	12.45576228862205	2.99288304181950	7.88387302380581
O	9.31150793018471	3.03092370995309	7.89884965656866
O	12.34576154830556	10.81576588514378	5.51486301719823
O	9.69496247126591	10.88918566045143	5.52992904132230
O	12.29287757173257	8.16725944065895	5.51933497272080
O	9.64220884125865	8.22014006401867	5.52511599803381
O	12.44221072265618	13.56472341564901	5.42698344746977
O	9.65557244227257	13.64005031846583	5.49102629098561
O	15.09191702672934	10.76529208490657	5.37930658406290
O	15.06211251107819	7.99927602552587	5.41527910370176
O	6.92869718852683	10.98491674841179	5.46099312499526
O	9.50872175727737	5.48349177838209	5.42624380457934
O	6.86275400075829	8.21191157063947	5.43659313665479
O	12.30011394255412	5.42977143429115	5.42655353861588
O	12.60464729772997	11.08275521865298	3.00046090525935
O	9.44745646406700	11.15893161296335	2.99576266661260
O	12.54895639750002	7.86825634538439	2.99510311635255
O	9.38332797420043	7.97445079873499	2.99226501935801
Pd	15.27376571330893	12.26062356569770	9.45775143743165

PdCe₃₉O₇₉ D4 (-940.213754 eV)

Ce	13.77262329293715	9.69731970499932	14.76339425979201
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Ce	11.07064645073243	12.12136154940939	14.83893967049191
Ce	10.71029591759610	6.68550178554146	14.74089805040700
Ce	13.76375427498701	12.30089234515633	12.19104838307231
Ce	8.37640892945298	12.31217893146045	12.26089597943954
Ce	13.64996166174652	6.68767880657839	12.28786874373088
Ce	8.18381624032902	6.73502660573092	12.17866391901552
Ce	16.30492017816285	9.46183926215416	12.11463977245228
Ce	5.81318463543286	9.57925357618000	12.24132857447573
Ce	11.00298037981589	9.46962524926496	12.18953009365060
Ce	11.09741918648114	14.92273363949314	12.10046827647124
Ce	10.89348394891356	4.02455766261993	12.03225548646672
Ce	13.64859674937054	14.90015966585451	9.47668432565665
Ce	16.28876452432354	12.11962841431634	9.45040772922952
Ce	8.55123006253848	14.99035302582873	9.49986582646937
Ce	11.03804462632085	12.14560845820644	9.50807706625714
Ce	13.62440651967039	9.46852144495264	9.52461732581854
Ce	5.85787199195798	12.33158272899331	9.50169203793967
Ce	16.19347571608782	6.75530388675960	9.52213275148772
Ce	8.36331895284786	9.54227237117571	9.49813993023283
Ce	10.93490482240664	6.83162489993374	9.51746912548162
Ce	13.48331697726829	4.05801976559064	9.49534510244474
Ce	3.42144235390277	9.61979301152727	9.49501705807202
Ce	5.74224360890981	6.82939303550755	9.43173478689007
Ce	8.36263397000749	4.05620896232505	9.42153395256178
Ce	11.09545478391819	14.87904252089577	6.88943623987349
Ce	10.94953079011336	4.12768769273420	6.86871248508241
Ce	10.99267203260716	9.50292277351516	6.87014574411534
Ce	16.23152326012569	9.41209968837572	6.82120018142177
Ce	5.82797146165604	9.58980062034373	6.72912314262810
Ce	13.73780919619313	12.22122745075998	6.74736069438703
Ce	8.36904400224722	12.32448148877001	6.72489550305653
Ce	13.65948315801730	6.70533566762459	6.76514005040865
Ce	8.29222860914919	6.77283072584808	6.70763499258440
Ce	11.07245427419824	12.11283367197256	4.12756326847151
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Ce	13.58044485587520	9.47044173191880	4.11938705938674
Ce	8.49260791044067	9.54405783497777	4.03588298749107
O	9.48698615826098	11.06754170160566	15.99627216882580
O	12.69081966655684	10.99121365066531	15.98206996299407
O	9.50450647518204	7.87315156647000	16.00512732387747
O	9.67164682621177	13.52833875161677	13.60344907476060
O	12.44696711707242	13.53465486474149	13.58749367343878
O	15.17021771002936	10.93144288935647	13.56125487108729
O	6.97265700601600	10.91079782954753	13.58561626436314
O	15.03763576316217	8.16931440224428	13.58092093441890
O	6.85785527192411	8.16567033735866	13.54315701775882
O	12.19459492059557	5.40750949893040	13.58225322618807
O	9.38376898326856	5.38438144473666	13.55652635473686
O	12.41104107126516	10.82682571843766	13.43074822515650
O	9.73441199907917	10.80766990001997	13.50123184308023
O	12.28685780728300	8.13737776992641	13.94780099407533
O	9.59285591035168	8.11153029123129	13.43860195230311
O	12.67975465846135	15.98029414041727	11.10735832154482
O	9.51891683927185	16.03266495486493	11.11633428365393
O	12.47333208846437	2.95121348543196	11.08994958574689
O	9.31452240094301	2.96113783893849	11.01392834164406
O	15.14027850520553	13.52981891698980	10.86499650184934
O	6.96657066850342	13.60665913813929	10.90787099592245
O	17.64925117197295	10.86534199325043	10.91918326844398
O	17.59682611569966	7.97423083236395	10.94965349187020

O	14.97949301651515	5.42673568614711	10.99308112768944
O	6.78659086320469	5.49153632787355	10.84020866824667
O	4.34009968770894	10.96813975896686	10.89146437401660
O	4.27868699100532	8.22729755313627	10.85975593771417
O	14.99669725859751	10.81783541785350	10.85041378297514
O	12.35229957596301	10.81354761482575	10.86081106629764
O	9.64507164683453	10.84936611504630	10.89369292711821
O	7.00304667323307	10.90764764847314	10.86293507725610
O	14.94367074945604	8.10645559959171	10.88174838060168
O	12.33155501061170	8.08929730258880	11.03714150740165
O	6.93266065204977	8.19975100787980	10.82449782722359
O	9.58811839562138	8.15417360352304	10.85437983621768
O	12.38369967710704	13.47267517790078	10.82511987239800
O	9.73033655588412	13.50073451122587	10.85180353715716
O	12.24511406105786	5.48520913722509	10.84783131996340
O	9.56581404567314	5.50006164103425	10.81815685972275
O	12.38291944819521	13.46347949198188	8.18345705243475
O	9.72472508781854	13.49797565127988	8.18102012133838
O	9.60243085718385	5.52589204285604	8.16636011900693
O	12.25491231304160	5.51546998327634	8.18659634605556
O	14.97520979614339	10.78759371529454	8.16552941055108
O	12.36297462364955	10.83441198830492	8.16597519706174
O	9.62841718677788	10.87243067239406	8.16902014571498
O	14.92619236337304	8.09099957598994	8.18080941601070
O	12.30056923710965	8.13667048221313	8.23720483794657
O	6.99416435199373	10.91486694542595	8.15362599309700
O	9.58354155805987	8.15430634511946	8.15419908573367
O	6.95332542551650	8.21088220481272	8.13212716411862
O	15.15392286605944	13.50114967757742	8.09403212514262
O	17.62763107088632	10.84628595100896	8.03707435192573
O	17.56794589747524	7.93991960794651	8.06905471813077
O	6.94871193941799	13.63020833838078	8.13690641828234
O	4.32285788141233	10.98484778590600	8.13710810477343
O	4.27523803764594	8.22536019388789	8.10958570330012
O	15.02027361327094	5.37571106996893	8.18319444717487
O	6.81382202561094	5.49715095152942	8.07313983750269
O	9.52241238732546	16.02753745988167	7.92759344545341
O	12.68987081368752	15.98030705074596	7.90016923518872
O	12.50278485276387	3.00188324178854	7.91057123531285
O	9.31087209518199	3.00813136638605	7.85396596478693
O	12.34008095980647	10.80748706296778	5.54482238364412
O	9.68626726631367	10.85821351215353	5.53099643743281
O	12.31148053088673	8.15025346294272	5.57254877982216
O	9.65486691753602	8.19479239132928	5.52194952267863
O	12.45030739978290	13.54972043604486	5.44705328132020
O	9.65202035772091	13.59439688467212	5.45299673574649
O	15.10239494295906	10.81542576235178	5.45685072192447
O	15.06275010826970	8.03293917720958	5.47186879117607
O	6.90902339763129	10.96340208901486	5.44035014566768
O	9.55251440476648	5.46256989126889	5.43707718981743
O	6.88193380794076	8.18841709065169	5.42805604112634
O	12.34950730299902	5.40956663998685	5.45495599766942
O	12.63889173950968	11.07815210319024	3.02985699206386
O	9.47907248933981	11.11894124872797	2.99308826082777
O	12.59046525038316	7.87389128982765	3.03582049857368
O	9.42896736992608	7.94224591067853	2.99309559059767
Pd	17.79459656733443	9.40353377978625	9.48218867536902

NiCe₃₉O₇₉ D1 (-937.987436 eV)

Ce	13.47961362311371	9.41989998110181	14.97710143651081
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Ce	10.90622469724575	6.84246551850592	14.86210211274366
Ce	10.95285253870463	12.01573817458233	14.97856581130759
Ce	8.23152851465827	12.19113028198386	12.26726173263884
Ce	8.22513406973758	6.77898048331862	12.22309536945772
Ce	13.59227292573306	6.68092521227646	12.26852827361276
Ce	13.67708298261949	12.25392893144592	12.30963706814467
Ce	16.13171756293607	9.43303226082448	12.25352651620776
Ce	5.80924323117284	9.51825973611327	12.17425218367690
Ce	10.95505910317116	9.50713009669722	12.15625579495130
Ce	10.80472390722029	14.74017437930219	12.34090195517270
Ce	10.87432472681254	4.11701365030480	12.09648636357536
Ce	13.79944483306281	14.75816691713792	9.27545290625219
Ce	8.53294070202186	14.92523931362447	9.51251902437778
Ce	5.88875598753444	12.26341859795250	9.50080162073714
Ce	16.25051582171404	12.08926391702739	9.47200170856975
Ce	11.03197979406743	12.16961286660785	9.52892340458438
Ce	13.59700128602240	9.46217654840491	9.49255165533391
Ce	18.55117648323727	9.33762106681525	9.51272918475092
Ce	10.92106027587710	6.87309897857018	9.49343315844926
Ce	16.08699505443178	6.64429489270812	9.50589299547263
Ce	3.40008069680961	9.61870794522523	9.48715947901857
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Ce	8.34399559249402	4.12285494052631	9.47844793963062
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Ce	10.96843473620695	9.50848741229955	6.86588268506363
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Ce	16.16063464930239	9.36971372221553	6.72969428597750
Ce	13.71693077245230	12.16120536905208	6.65472946808208
Ce	8.32826083199435	12.28222895923867	6.77626499255077
Ce	13.59402500927398	6.67883306683728	6.71625326309744
Ce	8.21934957118701	6.81226501841397	6.75238329163888
Ce	11.00980084903797	12.12762846887172	4.09941976845761
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O	9.39832216451956	11.03136175032969	16.04202379203100
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O	15.08358222491277	10.90969523215053	13.52515051384081
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O	12.34001745046691	5.41018725809605	13.55698709284583
O	6.87631709417714	8.13837417517926	13.59458048587639
O	9.63336213622951	8.17156967435897	13.45540077701278
O	12.27769881464817	8.14093104542573	13.48350583549809
O	12.32867880940199	10.81249507066315	13.50908999646304
O	9.65363412900012	10.83076916241536	13.49383632188048
O	9.60828057251652	16.00870188206573	11.17979710853166
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O	7.00352945531266	13.65318649394677	10.88277418395748
O	15.14787528221055	13.50702403941603	10.77810641269505
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O	17.65606711859934	8.02289067384227	10.89951465336363
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O	6.91965419819796	10.95814761106451	10.92440368442592
O	4.24174884025934	8.22215561179549	10.86453379274517
O	9.56080347512918	8.22217459508488	10.81681275963363
O	12.34135236568984	8.18190721824520	10.85916465772690
O	12.40179529956696	11.00387670259546	10.89651832052520
O	15.01460794886501	10.80013293341462	10.83828199830855
O	9.71493043755422	13.43485889172542	10.92397071622968
O	14.97500606154354	8.09557881993247	10.85248174046291
O	12.40982166125631	13.93014607622254	10.87884360904508
O	9.60145480750482	5.56350676941110	10.81938644764022
O	12.25302527563473	5.52160294645457	10.82408794029811
O	9.60888188567899	10.84396105995510	10.82408188292660
O	6.89950349061479	8.12665054548397	10.91645989788393
O	9.63573279809041	10.87649323452695	8.21699594245007
O	6.90636334111770	8.15351649992283	8.07859267107357
O	12.44755662964323	13.42798319390459	8.15811674426389
O	9.77661775023650	13.49475989086580	8.21413901489710
O	9.59393820721191	5.58025158648499	8.15186625502173
O	15.03601127946037	10.77406405617805	8.12928255782225
O	12.23868269658556	5.50805867017342	8.15316009536565
O	12.39481348366472	10.84418677691361	8.15697758254030
O	14.97894607723995	8.08688441609841	8.15238823137973
O	9.56153925019836	8.23548098454507	8.18890486402709
O	12.35085677208655	8.13129646760140	8.14072661285551
O	6.97474275047634	11.01207709468544	8.09560286147511
O	17.71161250395225	10.75241447786583	8.13309718390216
O	15.21300948227538	13.49042930200966	8.03739743995256
O	4.24750108318249	8.24846996638534	8.11458141896761
O	7.04149586740153	13.69939047322147	8.15628987857160
O	17.66672799683099	7.99461956120528	8.13138036460074
O	4.32374032121978	10.99531972631404	8.13361510269759
O	15.01730983748718	5.36979478300316	8.11420835674975
O	6.84634943055317	5.47304596640113	8.09907248537988
O	9.56156052618847	16.00179162046722	7.94946576039499
O	12.76421444058702	15.99289481893757	8.02664571355706
O	12.44937678405987	2.97340964543120	7.87465575630434
O	9.29512011232265	3.04449613653566	7.87389880846580
O	9.70007636997753	10.88956700936687	5.55064222997092
O	12.34189444482267	10.80977230956834	5.50508664800113
O	12.29239698171923	8.15438065310782	5.50809337531293
O	9.63916450875289	8.20847342982636	5.54506150354743
O	6.89475415171396	8.22197339199900	5.39627166617711
O	15.12202975917643	10.79459533504400	5.41973746531797
O	12.46934277396830	13.56257136085944	5.45291733549031
O	15.08608640803240	8.02287855914159	5.43546702023771
O	9.69733920978944	13.64793992470486	5.49111762315469
O	9.52270958379378	5.47491548304074	5.41673169016468
O	12.31647167856970	5.42493984330318	5.42095206977111
O	6.96881758031986	10.97780358247082	5.42367243870205
O	9.44267544227269	11.17529067054806	3.01478278325542
O	12.59870685604612	11.09309117329127	2.98853176301430
O	9.36406659168978	7.96057165303092	3.01545146830737
O	12.51266675098504	7.88436266523433	2.96807337309524
Ni	9.42714846884146	9.54302417394109	9.50879146957800

NiCe₃₉O₇₉ D2 (-939.491058 eV)

Ce	8.42142705128871	9.42542986739190	14.97159653944795
Ce	13.45809008174412	9.40062882985067	14.98850808888998
Ce	10.95356489478047	12.03384060336202	14.95455926542738
Ce	10.93271753816004	6.79581453643226	14.87555917920449
Ce	13.61542061656169	12.23225976207462	12.33214443983790
Ce	8.31907363825560	12.27850219519769	12.32636038823073
Ce	13.59870684563577	6.67482101266436	12.26473304063447
Ce	8.27828913153064	6.69989390832470	12.24857775230798
Ce	16.09064739735244	9.43535838406482	12.28771229807219
Ce	5.79725048877495	9.46387912276030	12.25358689692841
Ce	10.94556280089822	9.48639132184698	12.17116158661557
Ce	11.09039874970735	15.02082996940872	12.43181487517487
Ce	10.92515391779252	4.06524185993415	12.07670560194328
Ce	13.51369944746168	14.94819077855543	9.56282495268341
Ce	16.13235424807310	12.21791842946983	9.56561600016781
Ce	10.92332992253015	12.29301221118413	9.58351386660769
Ce	18.49948815903420	9.44534194965424	9.54776489460532
Ce	13.55295406443543	9.50514770084827	9.51326517473312
Ce	8.33802723751068	9.54874460312023	9.50406921082874
Ce	5.74344216822704	12.19607523499376	9.50677361765530
Ce	16.09856497034389	6.71839178647242	9.50617529040668
Ce	10.94307406236294	6.85591225435863	9.48783432632857
Ce	13.45533822403307	4.02410044935320	9.46606737726731
Ce	3.39900411316326	9.46072381147856	9.47294144796139
Ce	5.80061997639355	6.74980108349049	9.45038380344151
Ce	8.40899853046822	4.05602603309771	9.44250127017797
Ce	11.15358867345580	14.78669757819547	6.77643732598039
Ce	10.93932496604221	4.12566047716795	6.83591453565397
Ce	10.97920108011373	9.54907070042628	6.85734740434198
Ce	16.15199887942335	9.44386753556454	6.78289806794764
Ce	5.81107937411858	9.54218955444754	6.72547253247068
Ce	13.70397032407891	12.21200009029633	6.77079788876510
Ce	8.33241435118851	12.31591743836881	6.74790909919879
Ce	13.61837446224939	6.71095059685741	6.72480214342484
Ce	8.29730868845786	6.77349853240711	6.69891497186898
Ce	11.04811146248173	12.08978846006389	4.07201526125685
Ce	10.96148534338860	6.90872839361344	4.09564119431682
Ce	13.54555519533122	9.44817215310609	4.05972974309550
Ce	8.45683387430166	9.55126106618290	4.04035383753042
O	9.36275967672461	10.98725363439841	16.05187036893554
O	12.50909105156359	10.96453236119686	16.06634582802350
O	12.51193079794037	7.78150694145195	16.01202151239776
O	9.36539891504570	7.80372455694558	16.00172431872262
O	9.59070853216079	13.39282392245663	13.65578013441382
O	12.45161451332319	13.46939370743969	13.68843596005827
O	15.04817713062006	10.79684109533811	13.60334932171651
O	6.84332068109217	10.84016797180073	13.56132736611796
O	15.02862992142408	8.02204065591932	13.56633450552920
O	6.84597938786914	8.05749816308712	13.54337404005165
O	12.32624650851112	5.36441693687701	13.53244543669401
O	9.52664172703400	5.36810837894583	13.51943736226481
O	9.61634438864444	10.74156428404215	13.51761455335044
O	12.27825196285110	10.76531018775743	13.52279240939770
O	12.26053242225844	8.10627363664130	13.48627497995551
O	9.61859083433848	8.10064605663201	13.47029498010155
O	10.50703999907363	16.47001698362299	13.44156801215692
O	12.70839695243865	16.08528812732746	10.97487106916743
O	12.49382748963036	2.95802127522727	11.03669534985616
O	9.35157085583177	2.98003913174410	11.01319096483927
O	15.08352873422675	13.53149351096166	10.91787778663386
O	6.89449120264963	13.51676739826154	10.82673613090742
O	17.63234118356190	10.81956293984140	10.92275787105019

O	17.62200147891922	8.05819341001846	10.90033983235015
O	15.02562302544334	5.39548052402864	10.86806595978519
O	6.84833269364208	5.41911806178817	10.81830810117650
O	4.24058875873077	10.84601955031510	10.85613172025228
O	4.26630574060040	8.08369149934356	10.83005382738409
O	9.58051234840528	10.94664983192229	10.88402782732823
O	12.28703574763547	10.87182698643029	10.87184030052702
O	14.94812281282266	10.81629261656626	10.88644774528696
O	12.30779831813411	8.13580728588752	10.85291895849822
O	9.57736510686092	8.18018752241959	10.83690397295780
O	6.92276961582326	10.81672899294136	10.85308582352264
O	14.93967008979140	8.11450453104168	10.85125171293067
O	6.95453063354953	8.13599426630356	10.82441782373409
O	9.51931892060192	13.74521127336235	10.86372031382770
O	12.30324019551193	13.50549029125391	10.90271826664317
O	12.25644278838474	5.49273803012595	10.80376893124206
O	9.61188225713017	5.51748136739768	10.79524924232504
O	12.30634421735537	13.47261591545990	8.17098297400407
O	9.56786480476779	13.81565177859223	8.19657669232106
O	9.61848236497726	5.55056635097661	8.12788756462147
O	12.26410461849172	5.51872419346698	8.14638040587743
O	14.98921579759966	10.81497160929286	8.17989319365276
O	14.94958124178756	8.12746992941412	8.15708434968880
O	9.60690400751984	10.99791676843759	8.15708744122043
O	12.32653764553937	10.88581653247675	8.17772874413488
O	6.95858853019328	10.85378303311354	8.13853815788661
O	12.31762940773525	8.15901731470860	8.13997901454764
O	6.96127602636775	8.17871009989564	8.12095902612495
O	9.59182977427158	8.21842444443733	8.13987990300768
O	15.07337336496554	13.52500422714919	8.14584379487824
O	17.66073726665231	10.82433466497802	8.16726560902758
O	17.63154797799016	8.07244334136412	8.14457249873833
O	6.92256498229078	13.53792971811837	8.15172741851237
O	4.27844979834390	10.87613949282257	8.10662385150752
O	4.27810874984411	8.12702766383032	8.07274260710962
O	15.02972522812926	5.41650288138694	8.09746610751706
O	6.85942293478833	5.46404545566548	8.04244375978400
O	12.39004730406295	16.03490184686340	7.81505774757067
O	12.50337274168061	2.99232009058576	7.84332023692953
O	9.35486527694492	3.01153306561308	7.82594084988307
O	12.34487569443898	10.82866848991700	5.51899154033936
O	9.67548465438773	10.87508383092828	5.50991635233550
O	12.29147576953689	8.18150260836755	5.51519660620228
O	9.64764206408218	8.21482001152091	5.50834471831150
O	12.48932718549785	13.56486195998792	5.43330730613982
O	15.10847658635923	10.84194418932642	5.46954876037781
O	9.70777978541230	13.60186204861558	5.44928391600518
O	15.07463505204414	8.07661165975211	5.44336774305345
O	6.90951232680505	10.96068520673788	5.44559767409837
O	9.54760173797975	5.48193096529441	5.38815875933140
O	6.87699943802187	8.18273583176540	5.39728472086585
O	12.34327523206153	5.44511002625159	5.40893767384049
O	12.60100260076752	11.05389266999834	2.98376765614301
O	9.45283995001859	11.14174171309966	2.97614282132165
O	12.58566215433807	7.87214758715574	2.99406459626061
O	9.39891347934420	7.96911879221249	2.97852449040950
Ni	8.21943401946742	13.77350197195771	9.51661976872667

NiCe₃₉O₇₉ D3 (-939.412179 eV)

Ce	13.57103721082008	9.45660365550045	14.90708714384027
Ce	10.96365619844406	6.88435236034500	9.50066382555607
Ce	18.58658008521783	9.22657193314653	9.50555104823369
Ce	8.44281818087370	9.44487343617094	14.97679948813503
Ce	11.00844067745087	12.01945947782071	14.97726660142228
Ce	10.99521244836365	6.86994289399014	14.88314897001795
Ce	13.74369942915699	12.26323131642378	12.26993426109704
Ce	8.26790879224513	12.22331086150539	12.30926253885209
Ce	13.64934077941346	6.74163067959850	12.26050994550500
Ce	8.28965510410352	6.75530290823572	12.26760158371449
Ce	16.24747713674578	9.47026125445846	12.18501827733744
Ce	5.78912280698953	9.52147262833113	12.24222322730538
Ce	10.99339507930927	9.53212714771071	12.16291685987269
Ce	10.80733788430785	14.75366784020623	12.33658499277620
Ce	10.92734636423394	4.13740063982089	12.11781398878574
Ce	13.76113731521560	14.78998202775782	9.25190394520311
Ce	8.54863364994675	14.97334649180010	9.50409457801373
Ce	11.05076100793718	12.21383402926694	9.52409392495213
Ce	13.68093061121685	9.52741872867525	9.49203777557102
Ce	5.85232115292224	12.33238207449292	9.49995066013083
Ce	16.14116631220316	6.65585973011143	9.51150710804111
Ce	8.37759592549357	9.55090235157801	9.50339151538026
Ce	13.44157343961364	4.06096911087073	9.49837876778517
Ce	3.43756180317344	9.61349104664522	9.48290021441809
Ce	5.79346537401691	6.81393588922109	9.48425544269325
Ce	8.39506190896513	4.08435861299069	9.49689943156930
Ce	11.07106918624482	14.85244345076315	6.85153212995071
Ce	10.92469005130367	4.13554837574242	6.88003983228893
Ce	11.00908749552152	9.51721776787507	6.86030154614622
Ce	16.27102909898162	9.38861035657790	6.80072422674305
Ce	5.83599980854141	9.58771895822039	6.74003498292041
Ce	13.75881807540653	12.15621372476506	6.67897543414177
Ce	8.37171426811856	12.31065458832250	6.73285539991762
Ce	13.64880353493640	6.71282178816103	6.74156074480451
Ce	8.29366895043668	6.77578922023691	6.71793470162560
Ce	11.07358081506934	12.10263386459591	4.08575500578998
Ce	10.98631682176052	6.88926853243685	4.11591804755653
Ce	13.57823578517854	9.43357211795398	4.07501901818352
Ce	8.48968725556483	9.54134843458133	4.03856569512190
O	9.43949807836743	11.01404744137460	16.06357299441607
O	12.59539040085552	11.05513050581061	16.03014504715454
O	12.58548906286839	7.87661925668549	15.97882255961463
O	9.37385399413502	7.85891710183465	16.01608704296526
O	9.49068161505098	13.56977665820555	13.65583948078051
O	12.30410499750111	13.56416313847809	13.56655002879091
O	15.06367943665891	10.90781228323061	13.51522897810779
O	6.86131435163443	10.89962193579592	13.57244891973466
O	15.06747365224644	8.11523816555076	13.56731304261522
O	6.85985775538084	8.13507634027085	13.55990282081933
O	12.34086719521440	5.44413677007010	13.57469192065253
O	9.54124430369288	5.45345820649179	13.55969488021031
O	12.32656681928243	10.82901627008719	13.50024657907636
O	9.64160408201970	10.83354626246730	13.51661482410990
O	12.29825669020370	8.17329131382470	13.47122867181339
O	9.65272307765867	8.18527208059855	13.49345979173692
O	9.58615071053766	16.03157841345001	11.17209464001110
O	12.47101836515294	3.00041530999198	11.10770113306009
O	9.32544433191958	3.02812251629092	11.09901021467144
O	14.98004619435307	13.53005321135379	10.74767404459062
O	6.92339716242104	13.60921895389852	10.90122567905433
O	17.97207984829415	10.39363466938702	11.13491211123516
O	17.59397716641949	7.80867141113777	10.85941611503057

O	14.98007788368012	5.38450084630330	10.92140414300124
O	6.82923839304840	5.49405611099583	10.87506505091725
O	4.32026422271172	10.96603561276014	10.86999155106152
O	4.27397303431194	8.21468254253659	10.87085853807112
O	15.11743590423953	10.90355268543626	10.80704420558330
O	12.40834327584555	11.02901603336917	10.89049571308437
O	9.64864467902031	10.88505319284742	10.86352663165303
O	6.98011367537445	10.89169778741910	10.86216264458583
O	14.97122423822392	8.15108827159165	10.85387405101055
O	12.33698558165886	8.23241274120438	10.84369188998527
O	6.96047506063270	8.20146130031303	10.84751374171528
O	9.59745624885064	8.18741057790449	10.86742956525249
O	12.29976396389100	13.99741098200529	10.82180438457140
O	9.65485638450586	13.46090253255211	10.91707639792655
O	12.25292323491483	5.55495619188804	10.83958248420060
O	9.60434766235944	5.55399848665116	10.82412528402141
O	12.37318206268827	13.45429715269307	8.13060103012285
O	9.73595995067969	13.52453331691255	8.21101305830521
O	9.59827691512662	5.56273169196468	8.16699578828616
O	12.24280907862591	5.53015478271104	8.17215071847588
O	15.14515801752767	10.83769381221004	8.16444905900905
O	12.40186535658967	10.86367501425886	8.16305605212667
O	9.67006901809667	10.91957229251938	8.17537610734420
O	14.97546318841352	8.12068192698458	8.15974980321147
O	12.35113813765281	8.16601942998710	8.15484632503351
O	7.01484273633079	10.93171278873179	8.15622898471999
O	9.60169268945588	8.19789522579942	8.15000545498317
O	6.96605134705148	8.22382976214243	8.14514893112504
O	15.08713184516134	13.47570650846029	8.06621228383489
O	17.98846723534079	10.36075796188300	7.87242469559437
O	17.60639415570526	7.77733347839377	8.15673038898480
O	6.98277153839673	13.65251509277484	8.14541487275768
O	4.34308209352175	10.99392000843781	8.12279690054265
O	4.28331634288061	8.23589163080411	8.10674500517871
O	14.97978339397575	5.35790816104523	8.11788329795646
O	6.82040131680396	5.50767403136448	8.09680561985144
O	9.52378262127139	16.02830568883031	7.96251633284054
O	12.71556823177862	15.99446574297484	7.90167455990587
O	12.47091169139567	2.99811317391566	7.90028086635503
O	9.32412891793567	3.02757932653742	7.90165192870244
O	12.34877333043821	10.80138299040686	5.51420611332481
O	9.69640003122170	10.87685798388254	5.52394151409574
O	12.30582949024599	8.16222575280387	5.52440511860418
O	9.65584244640075	8.20467147917131	5.51931951046319
O	12.43898257348382	13.55432860319810	5.42944324458710
O	9.65505565202666	13.62919098430102	5.47900503301658
O	15.10417374644067	10.77996852334124	5.43169966381975
O	15.07788850586097	8.02214138910427	5.44792270100921
O	6.93050452287510	10.97661386585457	5.45229425033810
O	9.52505142643651	5.47216782426331	5.42868579318271
O	6.87629828748987	8.20242147709232	5.42798407143594
O	12.31906899867642	5.42998565029648	5.43383888059120
O	12.62983318702701	11.07217287744354	3.00626562629491
O	9.47031924841115	11.13685832723107	2.98609061209479
O	12.58441868046135	7.85712036861813	3.00616497451800
O	9.41038710193533	7.95335801077817	2.98841422262524
Ni	15.21077725202551	12.20229747278066	9.45480299758479

NiCe₃₉O₇₉ D4 (-941.075020 eV)

Ce	13.78137457451066	9.69501423652122	14.75914883556546
Ce	8.48815237710111	9.54181829260997	14.92701575509041
Ce	11.07552326943515	12.12070599245525	14.84172069248241
Ce	10.71015156843192	6.68261156682708	14.73865642059377
Ce	13.76257248200331	12.30566709563940	12.19535991973660
Ce	8.37808644856299	12.31248869026312	12.26319779123811
Ce	13.64888672132633	6.68552316134934	12.29177283923842
Ce	8.18306676035115	6.73411794982217	12.17748072865530
Ce	16.30532917625474	9.46954938092105	12.09552359061362
Ce	5.81429353104066	9.57891058447393	12.24271758183245
Ce	11.00337778567068	9.46909799233995	12.19134165856372
Ce	11.09955154738554	14.92556222747355	12.09724821403231
Ce	10.89237309439834	4.02329920037275	12.02946710026261
Ce	13.65246453151624	14.89584245239828	9.47183137614901
Ce	16.28644964799514	12.10906964246367	9.45041106587658
Ce	8.55149282788194	14.99028104562091	9.49995223886409
Ce	11.03639889681794	12.14497814410490	9.50907325903134
Ce	13.61705579711553	9.46960880367970	9.52657166251796
Ce	5.85898177112827	12.33116881233401	9.50347191022332
Ce	16.19256192456072	6.77096315935327	9.52227756503207
Ce	8.36284253318531	9.54176469654099	9.49886256373821
Ce	10.93342943166375	6.83076999149768	9.51732668347777
Ce	13.48619483763382	4.06122471226889	9.49713235337186
Ce	3.42217593568231	9.61998172888878	9.49487320627537
Ce	5.74179418301632	6.82960407455298	9.43110786565641
Ce	8.36049291193881	4.05469203643692	9.41952009646278
Ce	11.09607941353944	14.87774628658891	6.88885983123433
Ce	10.95120163656006	4.12633128576342	6.86987657658940
Ce	10.99110608161107	9.50204644805716	6.87055880635483
Ce	16.23086337792666	9.41356962520249	6.83864407685210
Ce	5.82841202627007	9.58956181575085	6.72880866302110
Ce	13.73795875141662	12.22316171807400	6.74468025927857
Ce	8.36955662375447	12.32393785962064	6.72487665294755
Ce	13.66070933624585	6.70154267575500	6.76366681434421
Ce	8.29245464536383	6.77206598833960	6.70655599139710
Ce	11.07381354774256	12.11247493064011	4.12755442459180
Ce	11.00366170338449	6.90121177542101	4.12912376426325
Ce	13.58728754641580	9.47227268655451	4.12607392916799
Ce	8.49453623949108	9.54252025292761	4.03535673780733
O	9.49136792944361	11.06611256295530	15.99820600520457
O	12.69841277865423	10.98959693142521	15.97973002898867
O	9.50405630005878	7.87002226321309	16.00462297246130
O	9.67413806858513	13.52769200600098	13.60381193821908
O	12.45006880380874	13.53786422453576	13.59004497257826
O	15.17544891445557	10.93892001469979	13.55868084382411
O	6.97458983032089	10.91000978181874	13.58705985348880
O	15.04120756313444	8.16906756384905	13.57969303390096
O	6.85782373288606	8.16436873346747	13.54247202397194
O	12.19228398657367	5.40244245134832	13.58324959928362
O	9.38253097375534	5.38276562054289	13.55445253058133
O	12.41313104106918	10.82647280071701	13.43090217106100
O	9.73692586922254	10.80745195960988	13.50335115018454
O	12.28959203612766	8.13326363743342	13.94751580715398
O	9.59335761448526	8.11044248648773	13.43838754684116
O	12.68202858956959	15.97919051502090	11.10418211456852
O	9.52102010296168	16.03565770554290	11.11373374944849
O	12.47364518763072	2.95150531275666	11.08860756341942
O	9.31252717527156	2.95908137826581	11.01043932205898
O	15.14534638220790	13.52946437318205	10.86691653138394
O	6.96768448550158	13.60676164737367	10.90891485051762
O	17.64468909303817	10.75944191003435	10.80387055248790
O	17.59459637318244	8.08709604284036	10.83580692623149

O	14.98297185585027	5.42814887319024	11.00117746405180
O	6.78480937042842	5.49059178188964	10.83849607544903
O	4.33975768371280	10.96849925139021	10.89193842831533
O	4.27778315428893	8.22633137351094	10.85889058623053
O	14.99207752425948	10.82369764339168	10.85184933367371
O	12.34994689890574	10.81310312036655	10.86296615710309
O	9.64419854830688	10.84956388608621	10.89520533603598
O	7.00309666526250	10.90735208207647	10.86477454123041
O	14.94100335795682	8.10392501891660	10.88568098560290
O	12.33036248563021	8.08887621676252	11.03773011587315
O	6.93189522048489	8.19918482914531	10.82389182796356
O	9.58759353840688	8.15375473692131	10.85484384254389
O	12.38478714439399	13.47249084170752	10.82462338776578
O	9.73081336951328	13.50207374561374	10.85209862950374
O	12.24506704457619	5.48500259068016	10.84813576803606
O	9.56408079050911	5.49858848982051	10.81724440695016
O	12.38395414662817	13.46205648498482	8.18360930460337
O	9.72563996554546	13.49727653376811	8.18099468087427
O	9.60282037510715	5.52457809219527	8.16597077985628
O	12.25648356833817	5.51609291831497	8.18725760290595
O	14.96775911505076	10.79053409085045	8.16426620695239
O	12.35954747770411	10.83297475743787	8.16888023329532
O	9.62668224484223	10.87225134294555	8.16941849428971
O	14.91779549871630	8.08854993560623	8.18024084796950
O	12.29668825332390	8.13763389989720	8.23988037064298
O	6.99331739307084	10.91472092601877	8.15506729788243
O	9.58156115297290	8.15370627349889	8.15383610727532
O	6.95275792786054	8.21025629015218	8.13140390419995
O	15.15905978523429	13.49838101343114	8.08564372749950
O	17.61725322126643	10.73608363406281	8.14555755698627
O	17.56165088387940	8.05500897034327	8.17883355897028
O	6.94912731706411	13.63037811742152	8.13767760858658
O	4.32189234278912	10.98471070969289	8.13620303524885
O	4.27461700679235	8.22533508864773	8.10785163153171
O	15.02491855563799	5.37821301148030	8.18094530909084
O	6.81305728642278	5.49600389100296	8.07133299692634
O	9.52432218202325	16.02696491486628	7.92754835195103
O	12.69672768046089	15.97692232595346	7.89637623919131
O	12.50632770145810	3.00302112859466	7.91281632469337
O	9.31133372622131	3.00689884593137	7.85233762561695
O	12.33965118129039	10.80751239243000	5.54755451698164
O	9.68583584240327	10.85703286785090	5.53075714319453
O	12.31383069342830	8.14964048485594	5.57496185499870
O	9.65603670744746	8.19338574430508	5.52038604236711
O	12.44907085470561	13.55120237403427	5.44529995341570
O	9.65225103744298	13.59346053712049	5.45316995224479
O	15.10544642961379	10.82233630306431	5.45927977094125
O	15.06924026514939	8.02914324615637	5.47676375376320
O	6.90933116978155	10.96444817770207	5.44134318231859
O	9.55334297887877	5.46248562074231	5.43683726915711
O	6.88307790003120	8.18955250846556	5.42645580809175
O	12.34993234093972	5.40573264691456	5.45352468427588
O	12.64611381367220	11.08120383453511	3.03506229900266
O	9.48079720052363	11.11769330876876	2.99232867847940
O	12.59836421809370	7.87544335686827	3.03982249244679
O	9.43766406202295	7.94485008860345	2.99002088155548
Ni	17.7265499580482	9.40721788598734	9.48222344310353

CuCe₃₉O₇₉ D1 (-935.130619 eV)

Ce	13.48707423609177	9.45488278389974	14.93804184999984
Ce	8.44267159586737	9.54813416184506	14.94475417991870
Ce	10.92716249245540	6.88453972352113	14.90785138289201
Ce	11.00817822188254	12.10854009281521	14.86799854346683
Ce	8.31984076221395	12.30762453802068	12.27364819232637
Ce	8.32185763101804	6.81606337341567	12.24819572586085
Ce	13.59506946079463	6.66330055911277	12.29888975302374
Ce	13.65580897977415	12.20214579086294	12.25152260151135
Ce	16.13723103492092	9.41826190254862	12.26937534270840
Ce	5.88779309198243	9.61273527852337	12.20406108711977
Ce	10.93062497217315	9.46255734682567	12.10389574856496
Ce	11.05940156789869	14.85103740722136	12.13496603175650
Ce	10.88732001994257	4.09421205543456	12.13716749927447
Ce	13.56381207329089	14.86952375647856	9.50692978197449
Ce	8.46863417529682	14.98642919269320	9.58552171394859
Ce	5.80333732426014	12.39849403073191	9.56514720496410
Ce	16.15752878856647	12.14398058840569	9.47331421690718
Ce	10.91353342314156	12.07983558845997	9.48652279188086
Ce	13.60175080173837	9.41417730730577	9.49506240880223
Ce	18.54340372540994	9.38039807658101	9.53884880955293
Ce	10.93467463011560	6.82742119210783	9.50429399021053
Ce	16.12129765398530	6.61523595369313	9.56147989443222
Ce	3.45210105967611	9.63511766694273	9.49656215994317
Ce	5.95782414386226	7.02509807949770	9.49758606515359
Ce	13.42101602275149	3.94393590597705	9.54814966665869
Ce	8.38322714099266	4.07432301532332	9.50818259836942
Ce	11.00422193255960	14.94993447035436	6.97433921515715
Ce	10.89579634405989	4.04541395552431	6.90435551617461
Ce	10.93247069479751	9.46868458426190	6.86321994481701
Ce	5.88903865163469	9.61957041528120	6.81742558201902
Ce	16.19796623788454	9.35488182888639	6.82600975201464
Ce	13.63868631063932	12.20795743684265	6.70856440251800
Ce	8.23952563873207	12.33688125550336	6.84242633105310
Ce	13.61532688718775	6.57950516863382	6.80002482829663
Ce	8.32480532632170	6.81353397146976	6.75775251819087
Ce	10.77577790327040	12.32393671312045	4.26306535500400
Ce	10.92861746430988	6.86070780959228	4.13626223399513
Ce	8.45508229190940	9.54640453107322	4.08349188464729
Ce	13.69112935150170	9.20059756917807	4.21037792780674
O	12.52441082507741	7.88873024024821	16.02142532750216
O	12.59307027473017	11.07513853331167	15.99024171612746
O	9.36444306241887	7.92306518881647	16.02187410389338
O	9.44055173423013	11.13721327236832	16.00156576917209
O	6.94759781035859	10.95348010806812	13.61777598057809
O	9.67699732926802	13.59938674002592	13.57830434227807
O	12.47143367615114	13.53337454143377	13.54910071063674
O	15.10228365338506	10.83307835252662	13.54385527154077
O	15.06359315118173	8.06006707499669	13.57434777627429
O	9.57274303265916	5.45734142018290	13.56281848314479
O	12.34621858034435	5.38939251778389	13.58221922472825
O	6.89300442867259	8.18192734145713	13.53106597493232
O	9.64291357642521	8.21143555878577	13.52001200831836
O	12.27709662274475	8.12721531512824	13.48036404048173
O	12.32726017142551	10.79743923656374	13.43956783528333
O	9.68442146907792	10.86461833371568	13.45661256488933
O	12.67940370070642	15.94143203368233	11.09383742011720
O	9.50046279877269	16.00744187924302	11.15984269969645
O	12.45477697854788	2.91575709809686	11.11854125209727
O	9.29204352507483	2.97993083497952	11.09334105256900
O	6.89523592077380	5.60389929896531	10.87390280406115
O	6.93812573546531	13.75480015984862	10.92540595552293
O	15.13528718223585	13.48713343740101	10.81672599707301

O	4.24027871215107	11.01156733256916	10.87771855025983
O	17.68738321380551	8.01978818695202	10.90895420650375
O	15.05644725956894	5.34336861465453	10.92797473723897
O	17.67407180430233	10.78522561329753	10.86644446459785
O	6.89114474475678	11.10616563838283	10.92058230127908
O	4.40964294099285	8.26328739391922	10.85891719271052
O	9.70113026701318	8.03818006901545	10.90380323271027
O	12.38987333809503	8.09741498170616	10.85093125719733
O	12.31696113118244	10.79476401492137	10.76731708042027
O	14.98745641828492	10.77200597130754	10.83450081409459
O	9.69644456566295	13.46004862539879	10.84115866314686
O	15.00570732739192	8.06796877048271	10.85507232625005
O	12.33260418864937	13.41370919411141	10.81499998802300
O	9.62599833923813	5.46202132283344	10.81639029655076
O	12.27336495580990	5.45536726669702	10.85146232055577
O	9.50118624120635	10.77582583238742	10.80600010015309
O	7.15540602156381	8.40921759006309	10.81290467391713
O	9.50104333202815	10.75336733329859	8.19651255532243
O	7.17744988218054	8.41032481804231	8.16977244841968
O	12.32493105205080	13.43330298157938	8.15876424086815
O	9.66690537720202	13.48465901711143	8.18450643439458
O	9.62248148596959	5.45635133541313	8.16451983638943
O	14.98639696429534	10.74387481006398	8.12651544684327
O	12.26796288967773	5.44064223836870	8.17934298469664
O	12.34058154773494	10.82946502719017	7.97919904074200
O	15.01277257775193	8.03069607253637	8.16687802042978
O	9.73621570905831	8.03539546654103	8.02547136764391
O	12.38861299067183	8.10536983980827	8.14873144534813
O	6.86077569080316	11.10793115352324	8.12945240848147
O	17.66355412227750	10.74345884595628	8.11510174200157
O	15.086574562211559	13.42419774950525	8.02001573538787
O	4.43481009505977	8.26905872652768	8.11341959456375
O	6.92964142685181	13.75208608146529	8.18101289173970
O	17.67921533441763	8.00973945101280	8.14319455576190
O	4.23271211804190	10.99949123004840	8.12431025571554
O	15.03561288005591	5.31857670808851	8.16389301201455
O	6.89637063854015	5.62226223415947	8.07941474664234
O	9.49852321340712	16.05393454731327	7.97891955101408
O	12.64467476599807	15.98599128017410	7.91598566926046
O	12.46022936016647	2.91979668043734	7.92430732029014
O	9.30867627479834	2.96406275280499	7.88257940467799
O	9.67287055433317	10.94575164615087	5.58992884265922
O	12.36071522075530	10.83903551387177	5.03412350213105
O	12.33924801814477	8.10404270921529	5.55312760878848
O	9.68484457795492	8.24400580299534	5.45145615764205
O	6.95410610671665	8.22122485151813	5.43120765134082
O	15.08845439859916	10.67700714538629	5.43069261713590
O	12.33363085964882	13.54482799098035	5.43673089531891
O	15.10897696549718	7.93909597416959	5.44392108312529
O	9.52654872471515	13.68063714673479	5.43692920301725
O	9.59410733177242	5.49977435103854	5.38739242476328
O	12.35152963183934	5.39760206323225	5.42232524125786
O	6.96667212600108	10.96371378024707	5.40934672949087
O	9.53849838198749	11.17433205764134	3.00255786950769
O	9.40876422382263	7.94891970997509	2.98859139261111
O	12.61472375211680	7.96726358749633	2.97819226725659
Cu	8.44081256597914	9.61045004034944	9.51252013291601

CuCe₃₉O₇₉ D2 (-937.027003 eV)

Ce	8.42143069011368	9.41786848459689	14.97285359789922
Ce	13.46914616544812	9.39320250019642	14.97949966405988
Ce	10.96113286728532	12.02233062918057	14.96172525738982
Ce	10.93405645075040	6.79509032500111	14.87462002768427
Ce	13.61999984602595	12.23124114124017	12.33239886587398
Ce	8.31993429537073	12.28058087916952	12.35079004060426
Ce	13.59815407200352	6.67342244552708	12.26314698408566
Ce	8.28144711439203	6.69474936726981	12.24567072414936
Ce	16.09601102725008	9.43382154168284	12.28195526085281
Ce	5.80250065492719	9.45610988244076	12.25898944389638
Ce	10.94586993308812	9.48873177253769	12.16877182373820
Ce	11.09611453401926	15.01350201224160	12.44196028138622
Ce	10.92734644577637	4.06359317004758	12.07435403121341
Ce	13.51980417964708	14.95477138540058	9.55986689188800
Ce	16.13378267272478	12.21790311989875	9.56644163864394
Ce	10.93165215421499	12.30360132969260	9.58562991026539
Ce	18.49917394811875	9.43869160513140	9.54151597641614
Ce	13.55312984484738	9.50446223940104	9.51165454789361
Ce	8.33682603393018	9.54989919941769	9.50571397391882
Ce	5.72868339713695	12.19618289870188	9.52498717621073
Ce	16.09399472938965	6.71113047126444	9.50297526668009
Ce	10.94284809039593	6.85718990841749	9.48611886088579
Ce	13.45375527681125	4.02154720990595	9.46148573737878
Ce	3.39787286993021	9.44835890194100	9.48258284715699
Ce	5.80167546278113	6.74667714753487	9.44963092677959
Ce	8.40927519916977	4.05654592315126	9.44027425611964
Ce	11.16364321455970	14.78952916885117	6.76416288031469
Ce	10.93754984457549	4.12928579439685	6.83229575909935
Ce	10.97453511059379	9.55503641718514	6.85930891729789
Ce	16.15162043962186	9.44344321777658	6.78261451958474
Ce	5.80852672232694	9.54806367033806	6.73423340757431
Ce	13.70584556320216	12.21212148090330	6.77128082784028
Ce	8.32352980315133	12.32851757451164	6.74020560360480
Ce	13.61454850748538	6.71419539930160	6.72036460036998
Ce	8.29324428557667	6.77571958694508	6.69583417484465
Ce	11.04096607954946	12.09240870698379	4.07186652373225
Ce	10.95690068655243	6.91387679615995	4.09490696005634
Ce	13.54070856343562	9.45230020848861	4.06187217843707
Ce	8.44954097733806	9.55592602229611	4.04344379555071
O	9.36746147454858	10.97417330620219	16.05537023705801
O	12.5217535998349	10.95687812561904	16.06477743434756
O	12.51694342066802	7.77820663082335	16.00641841671403
O	9.36513003725893	7.79339962790698	16.00143615686985
O	9.58429767632408	13.38632006503302	13.69095425577204
O	12.45582865218813	13.46192049603806	13.69252812544573
O	15.05725424186137	10.79384682483934	13.60180232077598
O	6.85253417518247	10.82370444278459	13.57565606082211
O	15.03069264228717	8.02058288362863	13.56378459452181
O	6.84540540455474	8.04385403567762	13.54370972375836
O	12.32705004906516	5.36125754992936	13.52922245798881
O	9.52852398789721	5.36505156046171	13.51648071303135
O	9.62077913027597	10.73927796236124	13.51894473711251
O	12.28473477730016	10.76093898964529	13.51991709628114
O	12.26128832342408	8.10428192944581	13.48145959966136
O	9.61956293436372	8.09945419254308	13.46931837356779
O	10.49217067228298	16.47330566119179	13.42663948541469
O	12.71118798636047	16.08187852197199	10.97773215206047
O	12.49603664876345	2.95625682133986	11.03365297995230
O	9.35392319515126	2.97951857063110	11.00925836749544
O	15.09361037623097	13.52968420081607	10.92034370893453
O	6.81311211299597	13.48837768701120	10.90159290232301
O	17.63423006922014	10.81422725445302	10.91888409800670

O	17.62378247761242	8.05313359141980	10.89487806956399
O	15.02488545698662	5.39113009699573	10.86608241205249
O	6.85215032992870	5.41345784407054	10.81524811570083
O	4.24123979637192	10.83059466781429	10.86952962079847
O	4.26905860198699	8.06980584292825	10.83437228008234
O	9.57767375440449	10.96029868863626	10.88220929288999
O	12.28586850664627	10.87338862750634	10.86933823331482
O	14.94823285001584	10.81427889630687	10.88559038111640
O	12.30793677484521	8.13614463014525	10.85047614264437
O	9.57914528429037	8.18233016938581	10.83642993497202
O	6.92811148953159	10.81366951703473	10.85933111813382
O	14.94008713594286	8.11154556276241	10.84926513862885
O	6.95677014582901	8.13207802258728	10.82499102583823
O	9.55389240578380	13.74316418442729	10.91977092496358
O	12.31994782537542	13.50357618554420	10.89903430962349
O	12.25696563709198	5.49161756364028	10.80000534866901
O	9.61422907742234	5.51678172052164	10.79229473425643
O	12.31784798295354	13.47580282488819	8.16966811487194
O	9.60015265942626	13.82053992909109	8.16263644334785
O	9.61751995473734	5.55464048489439	8.12420944663002
O	12.26292964276912	5.51976577779455	8.14291802796178
O	14.98752772192337	10.81373178981329	8.17965543009742
O	14.94716083871512	8.12499556310524	8.15439660525807
O	9.59689447019526	11.02086192258873	8.16448156840845
O	12.32266244482322	10.88862631438822	8.17923720236474
O	6.95652375437377	10.85528722255092	8.14872856476682
O	12.31494132750162	8.16185783142205	8.13791520177140
O	6.96076620430609	8.17943634176424	8.12234420468774
O	9.59162068937238	8.22561259922885	8.14058072452545
O	15.08008058433819	13.52470285650016	8.14471313749136
O	17.65807168883057	10.81769130752008	8.16108238582790
O	17.62945463429774	8.06834102295140	8.13826681576377
O	6.86288358412398	13.51269893552116	8.12249438233020
O	4.26963783084646	10.87008177138851	8.12133760885390
O	4.27818605661307	8.12282760744142	8.07586098826867
O	15.02729686003744	5.41357259029851	8.09392421704895
O	6.85942803536206	5.46333164272204	8.04044219925984
O	12.39592558832205	16.03749772972057	7.81671821212523
O	12.49951439026083	2.99200604681371	7.83936257161507
O	9.35222014282880	3.01508393582424	7.82019655289623
O	12.33998748038400	10.83158978563546	5.52164897069290
O	9.66806891210987	10.87857941076829	5.51524434313996
O	12.28558805197637	8.18491673809456	5.51608036530617
O	9.64144685643800	8.21974567427772	5.50984907943120
O	12.49022234588491	13.56338684614096	5.42753316331811
O	15.10563494753495	10.84384316825212	5.47001092667562
O	9.69967825117477	13.60033853233148	5.43155849449926
O	15.06951204763697	8.07853878472684	5.44115224228299
O	6.90615681777977	10.96735410384255	5.45006103545489
O	9.54216107432689	5.48634125506099	5.38458828309512
O	6.87023095093129	8.18922795670357	5.40092158297291
O	12.33980194183046	5.44779273882032	5.40565573860985
O	12.59434078118998	11.05486322976856	2.98527833064268
O	9.44205729473138	11.14462080414755	2.97866268012883
O	12.58117755432061	7.87693752276497	2.99419018952703
O	9.39415913226007	7.97361538055287	2.98032915654285
Cu	8.19284240249084	13.90677599873195	9.54464687096951

CuCe₃₉O₇₉ D3 (-937.020362 eV)

Ce	13.55938684021830	9.44625663305277	14.91472301618731
Ce	10.96548052954529	6.88508317524315	9.49922990365168
Ce	18.58287648181056	9.22746622187461	9.51251229904950
Ce	8.43606256644519	9.43540582954924	14.97426769543746
Ce	10.99769211005878	12.01414651861830	14.97642204585785
Ce	10.98627612192769	6.86020031383517	14.87967587358965
Ce	13.74642027611278	12.25205833721956	12.28963328668782
Ce	8.26188609949809	12.21862792820332	12.31225078981505
Ce	13.64735960334082	6.72773067071329	12.25855913398073
Ce	8.28617823792075	6.74871787088328	12.26111863890536
Ce	16.24482320474902	9.44816312283733	12.20008602139002
Ce	5.78580837851120	9.51203189877261	12.23535017385402
Ce	10.99234844223516	9.52595263120569	12.16303691087056
Ce	10.80145434623975	14.74939952895308	12.33549759540079
Ce	10.92689552808654	4.13056050521125	12.11192327338350
Ce	13.76026230464644	14.79822006932119	9.25636682407958
Ce	8.54435589077847	14.97630206813209	9.50542449400895
Ce	11.05171778891942	12.21846340038667	9.53095512380852
Ce	13.69111354921093	9.51665541648538	9.49256483158757
Ce	5.85252263080453	12.33179475377602	9.50046118839758
Ce	16.14709469881138	6.64763847821174	9.51074157010077
Ce	8.38217827220763	9.55302010580105	9.50069681093291
Ce	13.44518030319398	4.05780420897347	9.48949438208287
Ce	3.43837735016534	9.61139789296114	9.47635590935529
Ce	5.79500161157747	6.81685616041237	9.47497076354121
Ce	8.39569333609169	4.08437703629428	9.49191830557641
Ce	11.07015402676435	14.85982531546653	6.86147153918644
Ce	10.92522842602965	4.13998362197891	6.87448350741712
Ce	11.01907988189952	9.52809908547347	6.86282895226840
Ce	16.26978297425586	9.38788476353652	6.79152996433815
Ce	5.83961559066899	9.59248346930862	6.73632695688980
Ce	13.76746025384432	12.17253778339617	6.66771507410774
Ce	8.37755615264230	12.31612862587408	6.73527803330776
Ce	13.65277458287923	6.71448035771513	6.74100087829345
Ce	8.29862510009841	6.78330432675790	6.71578462426393
Ce	11.07609958087985	12.11227079219002	4.08480250471611
Ce	10.98890630178402	6.90046952708019	4.12153286663031
Ce	13.58279151865434	9.44191534829498	4.07291521607424
Ce	8.49037240816255	9.55342321688163	4.04357773885816
O	9.42311724781176	11.00775543293438	16.05961007262982
O	12.57646225604913	11.04523970820782	16.03433537621271
O	12.57114408494355	7.86694098193760	15.98284297049349
O	9.36431543140197	7.84881733796784	16.01279629205857
O	9.48700644554463	13.56406657079724	13.65919511070437
O	12.29830018665888	13.55470473136534	13.56546754951438
O	15.05576145227640	10.89608756377757	13.54134597234972
O	6.85471295209016	10.89038187496313	13.56896534561610
O	15.05882666455959	8.09900161363902	13.57201103335403
O	6.85398331734241	8.12413827116456	13.55175775776877
O	12.33561176613328	5.43245710134147	13.57053547027810
O	9.53679426801103	5.44742787904998	13.55601519196057
O	12.32053967911711	10.81958635792160	13.50321624546802
O	9.63753961020640	10.82707526022855	13.51435888154258
O	12.29312913313348	8.16260369126064	13.47134409679619
O	9.64830676431272	8.17928549834444	13.49031411314147
O	9.57885570150664	16.03080291212618	11.17489268851397
O	12.46956572127901	2.99687963331101	11.09783211128238
O	9.32293449589251	3.02474692427954	11.09324079712512
O	14.94248584257872	13.57499043054983	10.80687449770394
O	6.91098241320896	13.60472076076557	10.90643478183803
O	17.96154577364042	10.39555021054806	11.13738604424064
O	17.59425789571755	7.80531242609373	10.86618643937683

O	14.98301785326777	5.36919504456455	10.91596433455506
O	6.83057247433311	5.49102648211576	10.86537372639845
O	4.31863945455241	10.95968088622251	10.86725000642418
O	4.27484038325103	8.20873659400264	10.86195374935231
O	15.10896921130585	10.85319401282113	10.84515630622547
O	12.42281621066810	11.03716446736068	10.88871971965388
O	9.65427931573577	10.88223213675082	10.86405972861987
O	6.98081384564129	10.88748365495588	10.85935122612761
O	14.97143248420045	8.12564331193104	10.85388491860167
O	12.33800388524272	8.23232681151265	10.84304468039921
O	6.96139148174163	8.19843766994726	10.83853649633732
O	9.59775238634198	8.18477092942922	10.86588650259073
O	12.27306341907948	13.99437833097417	10.80882192329966
O	9.63959483997238	13.45843996275308	10.92166094274557
O	12.25411982909104	5.55192985296716	10.83601203291642
O	9.60633936685864	5.55086788442654	10.82077560643797
O	12.38404447938724	13.45247435295281	8.13005233879538
O	9.74166017868792	13.53073112556680	8.21697680351834
O	9.59988755989676	5.56676127494179	8.16432632703304
O	12.24547908947670	5.53161965856359	8.16932659307052
O	15.12184008262758	10.81016721148232	8.12323882351154
O	12.41066966558261	10.86927673882104	8.17312988040994
O	9.67297546562534	10.92504779613177	8.17508746603191
O	14.98386148418899	8.10925299960379	8.16053320305414
O	12.35813793811078	8.16729025977343	8.15527427492124
O	7.01754605835450	10.93446867133415	8.15412675257597
O	9.60968161634313	8.20389425334542	8.14992837281724
O	6.97152921731230	8.22856489068655	8.13936153164541
O	15.07659150778834	13.54695082167285	8.01047762542496
O	17.96394799846831	10.37908206134785	7.89935683789339
O	17.61635402090464	7.78073616078420	8.15894266309626
O	6.98815784446903	13.65538006874864	8.15062434760008
O	4.34427448691314	10.99527634274232	8.11995550560673
O	4.28681442976515	8.23868653343562	8.09746379492816
O	14.98341593507599	5.35273466170432	8.11340845711612
O	6.82213324597401	5.51360669552215	8.08642337619864
O	9.51443168539914	16.03173124831243	7.96114010373011
O	12.69284776692527	16.00936974194256	7.93400340647309
O	12.47168770612647	2.99964519069183	7.88865784913509
O	9.32523952513063	3.03066483733407	7.89561163399692
O	12.35546218911022	10.81363947564127	5.51628823835819
O	9.70368356569647	10.88625150401841	5.52535316087668
O	12.31266602511985	8.17214507311558	5.52659507008868
O	9.66122954817626	8.21485484008640	5.52391964398308
O	12.44015330206184	13.56763188353744	5.42866719339003
O	9.65642352279480	13.63919532335472	5.48622222166275
O	15.10932426906527	10.78675307724860	5.40925640513804
O	15.08066881429010	8.02386626659149	5.44607445371050
O	6.93661708244240	10.98296567772777	5.45049322253867
O	9.52867474858461	5.47926371594735	5.42610495828444
O	6.87982509194714	8.20980572378453	5.42354917072195
O	12.32196053266979	5.43850865806411	5.43187069501117
O	12.62868914842950	11.08354940432360	3.00658766677887
O	9.46876974635611	11.14956286468982	2.98880551975837
O	12.58964568027090	7.86640060288573	3.00707060148684
O	9.41556205561471	7.96610191733897	2.99425076193011
Cu	15.36352402273002	12.22792992199401	9.45901896214007

CuCe₃₉O₇₉ D4 (-938.522610 eV)

Ce	13.55719872421701	9.43198474306259	14.88804198109373
Ce	8.47060703363175	9.52110442487744	14.96830635398067
Ce	11.05688533281225	12.08319393264183	14.88895484640510
Ce	10.96661874422945	6.87120335536376	14.88052675459939
Ce	13.73724998080954	12.19927017973023	12.25341164173345
Ce	8.36996595260868	12.30605139685849	12.29664767457995
Ce	13.63773182662240	6.68207035873527	12.26730920493191
Ce	8.27125487062714	6.75179179619079	12.26998327171275
Ce	16.22259397026015	9.41342907398160	12.19101009193514
Ce	5.82064524847040	9.56723424876560	12.26161029237223
Ce	10.97688574205397	9.48636187935440	12.13885983662891
Ce	11.11960225209356	14.85973825226151	12.15080993485277
Ce	10.91657011831674	4.11184470419551	12.10795426339722
Ce	13.66871491637722	14.85322843368646	9.53721177025118
Ce	16.29183229976266	12.06642300241059	9.50274325889290
Ce	8.53956548012802	15.02094421933258	9.59657578301710
Ce	11.02848286806015	12.16558186192294	9.48995375977628
Ce	13.61267876155117	9.44089281428169	9.49088880445457
Ce	5.83171704874779	12.33202094542942	9.55635455288658
Ce	16.20272424999864	6.71937018917887	9.57298109560803
Ce	8.36364450641497	9.55002849846511	9.49908717096485
Ce	10.94065512920028	6.85031509492793	9.49420524307872
Ce	13.47571143680094	4.02467797920322	9.52880602364641
Ce	3.42626642320391	9.60832554389516	9.48775032070976
Ce	5.78094513992066	6.8283375222399	9.48033147784116
Ce	8.38033782143075	4.07732684960120	9.48696961588646
Ce	11.07825204633166	14.98604644575413	6.99744707739321
Ce	10.93586557223288	4.08540110937023	6.89367235615537
Ce	11.01185659982737	9.53306074147376	6.81364578835708
Ce	16.32071087278862	9.36807231400420	6.91912864134701
Ce	5.82189452854185	9.59311307189923	6.74610054150983
Ce	13.75355510023444	12.22687428259428	6.72951343012386
Ce	8.28575643624223	12.35990459394989	6.82115667265440
Ce	13.67716540999719	6.61894524965765	6.82029339291530
Ce	8.29419760908599	6.78336333504131	6.72659650941642
Ce	10.82485828754453	12.33941624484082	4.27100005936428
Ce	10.99450302600296	6.89219942422069	4.15220070434874
Ce	13.77998540563001	9.20862906815557	4.25405245786604
Ce	8.50082583376293	9.55981941747488	4.06737021083536
O	9.44328797451941	11.09137557335023	16.02173026361072
O	12.60898236618698	11.05518552162853	15.97859926117103
O	12.56398391346126	7.85473390483877	15.97791249244820
O	9.39386702206514	7.90960593038205	16.00959507536467
O	9.67292946287132	13.56576295265544	13.57713916236141
O	12.46678522465504	13.53491562607520	13.56339692104399
O	15.09425236395004	10.82750174386837	13.54508591693365
O	6.90607899750671	10.93425266292423	13.56538152824401
O	15.03630901424300	8.04055431694903	13.55789044047145
O	6.85239349964458	8.15716777897306	13.54998420426853
O	12.30158112655646	5.39539076109127	13.56117298683016
O	9.50973364862485	5.44135310013195	13.54493748146054
O	12.33728252038533	10.79726761271122	13.44030777123045
O	9.67901445082170	10.83543879544509	13.48797299851552
O	12.27662196664297	8.13830433235878	13.46421435775587
O	9.62678465420725	8.17394126394789	13.47397630927582
O	12.71945471544544	15.93807196638094	11.11882056618762
O	9.51464576900266	16.03090518965237	11.17292224970036
O	12.47809842024279	2.96833819482652	11.10030614212463
O	9.31185038530400	3.00943950313709	11.05878602957147
O	15.15377026711315	13.48875754375626	10.83675001560321
O	6.94848017924395	13.62681707609584	10.92771803005510
O	17.58848258960305	10.79510046748175	10.90072723202016

O	17.54795448904637	7.99570614597211	10.94373860368040
O	15.01906491428303	5.36958195171758	10.92645811557646
O	6.81520540452777	5.49058715425680	10.84727646307093
O	4.31743446268935	10.97732480951093	10.87548257190520
O	4.27642397006700	8.21620537053836	10.84574142323240
O	14.96467547116222	10.77572892380154	10.83575214305581
O	12.33819749083012	10.81413771657503	10.77805019603570
O	9.62235098752427	10.88562120057473	10.84895556006239
O	6.99129408908757	10.91391069049690	10.85970149471876
O	14.92021808915442	8.08505953390748	10.84735721388555
O	12.30529426853584	8.11681569725140	10.84196120761522
O	6.94961438165639	8.20900682759295	10.83499833458349
O	9.57477730311636	8.16516959820941	10.83430866842472
O	12.38560966340831	13.43562368239854	10.83052996119813
O	9.73480263069071	13.50758932455106	10.84795790931917
O	12.24805050816331	5.49341234452640	10.82265455822195
O	9.59097779536743	5.53283920808986	10.81501033877703
O	12.38296309428201	13.47394422946293	8.17405601631780
O	9.69986462225077	13.54522118244229	8.19400669879514
O	9.60043126339273	5.53971380996259	8.14325331640496
O	12.25499841255563	5.49101793707628	8.17948257933988
O	14.99514991566553	10.76028029810163	8.14435707366178
O	12.38345928777708	10.86653595818664	7.97434806255335
O	9.63931581132856	10.89425520664053	8.14883060937809
O	14.95451932028783	8.05741987240613	8.17149154772004
O	12.30881995493984	8.14417435961784	8.14584576697609
O	6.98391206564577	10.93391326752255	8.16522679152650
O	9.60629374884365	8.19719685388072	8.10524791077922
O	6.96726668130924	8.22715367869385	8.12435830259458
O	15.11960064058896	13.44080807272863	8.02170469099575
O	17.63081019336348	10.75855676650092	8.12705354220336
O	17.58251846632451	7.98070295615981	8.16974686765794
O	6.92063082210049	13.64277129383693	8.16349452409981
O	4.33151053360583	10.98098403795282	8.12537794569025
O	4.30049985108656	8.24029990480316	8.08715718744580
O	15.01111006889794	5.34384893354878	8.15345216402448
O	6.83846539633205	5.52481973929241	8.06875924211202
O	9.53012241039911	16.09360829515644	8.01351746994543
O	12.68750770169277	16.00144621923622	7.94396377154167
O	12.48613161716724	2.97973883597969	7.88684330274375
O	9.32754246833665	3.01124532762628	7.87614771334181
O	12.35089509147263	10.82460194410745	5.05802311710994
O	9.65762279511451	10.94477840327586	5.56411117721905
O	12.37508572911777	8.13187822150241	5.57606724849364
O	9.70262765834678	8.24617349159292	5.49215642217833
O	12.34269945479413	13.55708382718336	5.43772175738577
O	9.53089969021894	13.67519732437364	5.45364806849724
O	15.09708503935936	10.69763502218956	5.44218287666631
O	15.13002933298471	7.92656512447554	5.45709146562048
O	6.92015178579030	10.97449936130196	5.44763301878493
O	9.54865749242013	5.52791349299926	5.38743033556036
O	6.94000166879424	8.22905114033092	5.40258167005862
O	12.32093029782031	5.42934990086242	5.41788452479231
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O	12.66020288679965	7.95286797130680	3.02317540248952
O	9.45394700326591	8.00223921397723	2.99455591175945
Cu	17.85578728920411	9.37671013141755	9.55616056235061

H₂PtCe₃₉O₈₀ D1 (-953.212824 eV)

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Ce	10.99655999964419	6.81152509612352	14.94148347839028
Ce	11.02947516536522	12.02809165931841	14.90398073104158
Ce	8.37561226336132	6.71218396012194	12.30108010739066
Ce	13.64886952475025	6.61972189574015	12.29393001247673
Ce	13.71035914618118	12.14407903261406	12.28471734307712
Ce	16.17555550409098	9.37161017004182	12.26467389888544
Ce	11.15691669909166	14.75763689381542	12.23635748186390
Ce	8.32179741745931	12.29330974376597	12.21137663942426
Ce	10.99429790627491	9.41779244970493	12.18264561795909
Ce	5.93425741627259	9.56325148922146	12.11623113477587
Ce	10.94926377420838	4.01937114766763	12.09961647192827
Ce	10.96417581922243	6.82833812328406	9.56091415985762
Ce	13.57436996415667	14.84489135792868	9.52674581860599
Ce	13.58447217701940	9.43950740005531	9.52263114258699
Ce	8.40770790716723	4.06801405158759	9.51654935913962
Ce	16.18156164489389	12.15054711727252	9.51037665397667
Ce	10.93288179168313	12.13665241692183	9.50648962537868
Ce	8.38582209028905	14.95068105515748	9.51532960475776
Ce	3.44016005749008	9.54075220848797	9.49584996094888
Ce	18.53355276526974	9.37508956660250	9.49781447600524
Ce	16.11262176221354	6.64112313685502	9.48336529331413
Ce	5.91669807219062	6.94429659849899	9.49056985121527
Ce	13.44702527724561	3.98014306966285	9.45382258195398
Ce	5.68624166005657	12.41273799429100	9.43047005392525
Ce	10.89939564529806	9.54701322302943	6.91046069168819
Ce	10.89741698382795	4.15680784904819	6.86216218319588
Ce	11.14106239321891	14.82024415628921	6.81945095227231
Ce	16.13256883779504	9.40783204252100	6.76356660123717
Ce	8.27170804916575	6.83630328558427	6.73930199640730
Ce	13.69389747067573	12.20021569731114	6.73796259625016
Ce	13.57897162210785	6.71106920419083	6.73191628468195
Ce	8.21437658377136	12.44664698891235	6.69460838525675
Ce	5.77616969110115	9.66990021949145	6.66936709313806
Ce	10.92089141332609	6.92085641913054	4.12579405607799
Ce	11.01146865299139	12.14147547735804	4.11607090680199
Ce	13.47896755517617	9.47675031717390	4.06836588784341
Ce	8.42229155160618	9.60741134488087	4.07584320561145
O	9.38829356547289	7.83801309666983	16.07133130820065
O	12.57766462355545	7.81822836081360	16.05091503337059
O	12.59594036132719	11.00060573763763	16.02925065903394
O	9.45736002796232	11.02544938512067	16.01932806490647
O	9.70521168390749	8.15531176840201	13.62013283617062
O	12.50937135085086	13.48479702221053	13.60173375346411
O	15.11516175910744	8.00853585777610	13.58148264103781
O	9.73343990977187	13.56223346411104	13.57446826542345
O	12.40234996262180	5.33916521637561	13.57479679066420
O	9.62758526341662	5.38423580670952	13.58055358040772
O	15.12407825216344	10.77513225904500	13.57190263496368
O	12.34089420783995	8.07431543112237	13.51971857531938
O	12.35855041597134	10.74541355053582	13.50870745836105
O	6.94315017796737	8.15862902123188	13.49481396245306
O	9.67817857969739	10.82293597943135	13.45358805088195
O	6.90181924010055	10.98662657515648	13.41264492345377
O	12.62268181242502	15.92911398021312	11.15484824232108
O	9.54822367510512	16.25337282087683	11.30389433252419
O	9.82534420445744	7.88123639898942	11.12991337721295
O	9.31675338303855	2.91764802886321	11.08610614445680
O	12.48096096573144	2.89357475207554	11.03434637821902
O	6.98643043305107	13.59884188004771	11.00402715420510
O	15.12886428897762	13.47182039066626	10.89697770654272

O	4.30930749242602	10.85755512736402	10.90984145504739
O	12.37139276095174	13.39877365593378	10.84833341905999
O	17.68522422891161	10.76575987598989	10.87395258605142
O	17.70212514018426	8.00443369999301	10.87463957613594
O	12.32666679439695	10.81430899275416	10.86996935411210
O	12.43583605325930	8.09167483405808	10.87596287439980
O	4.50728317412220	8.15069725738697	10.87221017709343
O	15.06290613098293	5.32926072559560	10.85437030215421
O	15.00645266536104	10.75429500627781	10.86378131527844
O	6.90846355712412	5.54398943423842	10.86811664564449
O	15.02559098914581	8.05682026657874	10.85706176770280
O	12.30048610208846	5.44060797557376	10.84602242099773
O	9.73792379491200	13.52763808305941	10.86746701744056
O	9.65869472717657	5.38681126105004	10.81140937119297
O	7.31710266088735	8.29678104297949	10.74685586409842
O	9.56513978160874	10.65213751728194	10.75411622451210
O	7.06582493378520	10.84559352104750	10.53806385387434
O	9.55829998435225	8.32099670318938	8.41913951367800
O	9.31261123375765	10.90729182342967	8.21863933346577
O	7.07533982801763	8.55616139807807	8.19997075813500
O	12.26385980702064	5.49236446769870	8.17089336335008
O	12.26789991804638	10.83442217333427	8.18365770488531
O	14.95139005414878	8.08343473863479	8.16164275242223
O	14.96275768003430	10.78445165259070	8.16193638073822
O	12.29165535782157	8.13301904938536	8.15138149716077
O	9.61034437418556	5.59850096548138	8.15317993223446
O	12.36470852540359	13.42503619523677	8.18411152144522
O	4.39500219081772	8.17506183901511	8.13412372703537
O	17.64824158294843	10.77367927940099	8.12803083025392
O	9.72730732016763	13.58025710051519	8.11765540065945
O	6.97968802151660	13.83599773005141	8.01330764889172
O	17.63810652827864	8.02375122053609	8.10804612408434
O	15.12520701289141	13.50012184095153	8.14443361343431
O	15.02201619969615	5.37424176465766	8.08581129208942
O	4.02410781976482	10.90128929973980	8.08124241682861
O	6.85715007921593	5.63153683732713	8.05107706237868
O	9.55531700454692	16.31241676213295	7.81593118600964
O	9.32140902740000	3.03483751677773	7.89633741598248
O	12.46132890480041	2.97063188350265	7.84985154184530
O	12.61693485272351	15.96213077122171	7.93972175325762
O	6.68242806671408	11.22162727280183	7.78259186338686
O	9.61480713233742	8.24414439438385	5.60149296201407
O	9.64799822002571	10.94823153979222	5.57943237437217
O	12.29811710880172	10.82990482878795	5.55261371789099
O	12.24442030515683	8.18883535695813	5.54197888594060
O	6.85734503829834	8.16877414302560	5.48235372586763
O	15.09070064293429	10.83175264556671	5.46081748947176
O	15.03703837087275	8.06003669052836	5.44877336793901
O	12.50236234621750	13.56651670494038	5.44375190387113
O	12.30573435965812	5.44104949691394	5.43100152194992
O	9.52006425996735	5.50662075251252	5.42768761583746
O	9.71175205878312	13.70444957462075	5.40321780671321
O	6.88440483676233	10.93417940269423	5.19836572054932
O	9.36120090268102	7.97721094965904	3.04523997840457
O	12.59778196358426	11.10101414651731	3.01850114516574
O	12.51715354134252	7.89503689692964	3.00499812924500
O	9.46017854450419	11.17014897655241	3.00501724141473
Pt	8.33280706502331	9.60455104341559	9.47214918796602
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H₂PtCe₃₉O₈₀ D2 (-954.823204 eV)

Ce	8.41811525582148	9.41287186550935	14.97320497480367
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Ce	13.48206191226635	9.38394345703057	14.97771696654350
Ce	10.93642512988785	6.79902466392435	14.87541693777592
Ce	11.04829055351090	14.96420084867144	12.52954217743030
Ce	8.30644669678592	12.26703250942172	12.34158436789762
Ce	13.62302739260495	12.21168903539775	12.32948445246743
Ce	5.79844693875726	9.45663474904560	12.26219514537603
Ce	8.27850538122020	6.70536998395191	12.25596426199589
Ce	13.59544834318938	6.68194201070276	12.26445865973493
Ce	16.10751384220664	9.42325912281523	12.26375342585042
Ce	10.94438062353644	9.50614565138216	12.16173787871886
Ce	10.92137541482411	4.07218525440560	12.08492827801055
Ce	13.67212938548897	14.78189476411612	9.53812322908189
Ce	5.69957832938181	12.17687705561010	9.52563236815159
Ce	16.18541716844258	12.15711301583849	9.52088415938989
Ce	10.92371536944019	12.35917035729551	9.51962230880752
Ce	18.51671372968912	9.40422540793874	9.50993383007470
Ce	13.54221371657142	9.52806944250117	9.50640374039716
Ce	8.34109189125017	9.57266163111078	9.50304703208189
Ce	3.38819189780639	9.42781538551436	9.49791271986601
Ce	16.08504898383453	6.71242534316967	9.49430971317938
Ce	10.93672616853939	6.86710042100348	9.48902983236064
Ce	13.45393533347000	4.03816602001080	9.47903823450124
Ce	5.80254753467037	6.74791727126923	9.46955860380081
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Ce	10.93428816236744	4.11017656511091	6.85501527955902
Ce	10.95438858410705	9.53974064743643	6.84812796069679
Ce	16.11884552683408	9.44928140483072	6.75098191187327
Ce	13.63405583870869	12.23850535193584	6.71013973342413
Ce	5.80229815966434	9.51197021118317	6.74176678241144
Ce	13.60337287192153	6.71554314691417	6.71402496977367
Ce	8.28806871532009	6.74472964432618	6.70797645558386
Ce	8.30920896567583	12.30602045432074	6.70012726874208
Ce	11.06023645416880	14.99552851995563	6.54796710570873
Ce	10.95419901913037	6.86149830208084	4.09524955699689
Ce	10.95914529563806	12.06367269457094	4.05987179399371
Ce	13.49505086885331	9.45072922815962	4.02932879971461
Ce	8.42374717311175	9.46547901987802	4.03275698176591
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O	9.36730761782641	7.79765995780789	16.00408593370410
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O	9.59444508534046	13.40474832503050	13.71126621056886
O	6.86239107107303	10.83480179665567	13.57659922737635
O	15.06036400496367	10.79960339776385	13.57508693080415
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O	15.04511063112908	8.02601144685048	13.56034038415322
O	12.33295196161597	5.37383453972295	13.53844869123244
O	9.53372491962873	5.37783784877268	13.53372278296355
O	9.61985753658129	10.74906126204547	13.52051388996854
O	12.29339414596308	10.76187592079803	13.51699759692109
O	9.62497154153442	8.11099615819094	13.47504818030895
O	12.26480140093334	8.11282366894706	13.48036282924532
O	10.56510329159853	16.57028884157775	13.34385902973231
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O	12.50429094811801	2.96304888513960	11.05837517273657
O	9.35518025875195	2.98549931901549	11.04307358712685
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O	12.36158350941947	13.59395788733412	10.88780591254254
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O	4.24159813112600	10.81565513415920	10.88313427066085
O	9.60325244284484	10.98843150239787	10.87501606509465
O	6.93160608050954	10.81560190933751	10.87296953232428
O	17.63055456618250	8.04500805070106	10.88094731115942
O	15.02222947990033	5.40025239447744	10.87324547743672
O	4.27020447939752	8.06376166609160	10.86189848941759
O	14.96969010272318	10.81782642315437	10.86719719914775
O	6.85393039112909	5.42285768456847	10.84923461864793
O	12.30907018891237	8.16693140155615	10.84968054252803
O	12.29959343008609	10.93064512896118	10.86115286554447
O	14.93795233903283	8.12287314938231	10.84579648206127
O	6.95958844639275	8.14180474646879	10.83978501898297
O	9.58191818117974	8.19956300036681	10.84292710336552
O	12.25429634356994	5.50929986365156	10.81141014035978
O	9.61217267412741	5.52774775894146	10.80717539091640
O	12.30570132641033	10.94755012701386	8.16621908370335
O	14.97532639441896	10.83049526509397	8.15912206069106
O	12.26048665146225	5.52810350881174	8.15256517076730
O	4.24504301442309	10.84054770737504	8.13802240172382
O	6.93569435630392	10.83690639935993	8.15300885445082
O	14.94279682176972	8.13766404513512	8.15284783877161
O	9.61598265491150	5.54674754917990	8.15056944930492
O	9.58642725564543	8.21818397829911	8.14749260181500
O	12.36811157756303	13.60935535151215	8.17143047481072
O	15.11606175359391	13.54620251817596	8.17345172444140
O	12.31349925473783	8.18449127808288	8.14465201337034
O	9.60669570431659	11.00659967039904	8.15169170678864
O	6.74294192512127	13.52941005299566	8.06342283044794
O	6.96393365764333	8.16451142141355	8.13954794725728
O	9.59042725976540	13.82743156482771	8.10540545661659
O	17.65818356513228	10.81341280608401	8.14860405511835
O	17.63505125151746	8.05805448693792	8.12425665099314
O	4.27347975273824	8.08995045479288	8.10626404942056
O	15.02864392112288	5.41610512408415	8.10042750948407
O	6.85662960075808	5.44240224898801	8.07409301928918
O	12.81128829318104	16.22615234079711	7.97559005181406
O	12.50575304689006	2.98639790133808	7.88100110634806
O	9.35742745155087	3.00785170958456	7.86835748927857
O	10.57409364129057	16.60073958454767	5.73527019155438
O	12.27820791858772	8.16064913003157	5.51220876001886
O	12.30416477328211	10.80709284809534	5.50882522493048
O	9.64102024606803	8.16192300107290	5.51180555159329
O	9.62410051678962	10.79717031279412	5.50447958947747
O	15.07524502124473	10.84571829243448	5.45084731239522
O	6.86609250345596	10.89835193115523	5.44606113042834
O	15.06242314521970	8.07280384173802	5.43594466763663
O	6.86340381325181	8.12012761344858	5.42125008379150
O	12.35038636314125	5.42145117762526	5.42212093467121
O	9.55034461822264	5.43249807602398	5.42157164203830
O	9.60680407775926	13.45326820396486	5.34444082609280
O	12.46872755935998	13.49669320497063	5.36312261104361
O	12.55554284975270	7.85065532892837	2.98387824683349
O	12.53432107580712	11.01830340682274	2.96224402575304
O	9.37422074712040	7.85865421603402	2.98427476777127
O	9.38521694249707	11.03043620704098	2.95964482184285
Pt	8.15123115221952	13.76760102055169	9.52967380005013
H	12.70722765756205	17.16533644247470	11.19553472535090
H	12.69165636896269	17.19127547128119	7.93671743535535

H₂PtCe₃₉O₈₀ D3 (-955.176395 eV)

Ce	13.48090188646027	9.47267862234606	14.95807447251084
Ce	8.45260910422187	9.56304206106958	14.92948805403950
Ce	11.01015598999055	12.13926857872234	14.87733080340691
Ce	10.91216192076709	6.89209825315489	14.88082663778695
Ce	5.79955115977069	9.59637323737157	12.29434782053585
Ce	13.67645205112233	12.23536221291887	12.26938970360786
Ce	13.57863422792609	6.68305708570198	12.28682705729599
Ce	16.13069197358002	9.41481195072390	12.27838799408625
Ce	8.33521435815759	12.31908802115190	12.25071391537572
Ce	8.22744794283224	6.79388302144601	12.25644665461209
Ce	10.95767398594995	9.50817744068089	12.12853466827254
Ce	10.83933755306448	4.12139548004230	12.13318294223112
Ce	11.04126932735177	14.89573754899729	12.09840786212183
Ce	3.39726242708699	9.63076082653746	9.69633550647343
Ce	5.65241255365693	6.86269793774840	9.53958638343087
Ce	5.75587271921903	12.31783923360124	9.53433671346817
Ce	13.39069889459623	3.97192665842456	9.54928168041059
Ce	16.09699767153882	6.64403410785639	9.54213349282618
Ce	13.58927979596232	14.93322133602055	9.50501534678775
Ce	16.19140362039959	12.17332904570314	9.51857022072984
Ce	8.48875534062464	14.95033150338042	9.50045807757831
Ce	18.55372792753678	9.37237096459121	9.56852838344810
Ce	11.00426057397776	12.14879127925605	9.47462043659957
Ce	13.59891402957688	9.45055067026200	9.49373710519619
Ce	8.28709760889882	4.13751648865075	9.53151999521199
Ce	10.90898971914996	6.84780363320272	9.49586013631628
Ce	8.28689791748042	9.54651099784703	9.45434675706409
Ce	10.84395028428825	4.05663149341709	6.94081256190886
Ce	11.03523536811170	14.93023996231494	6.90364596866636
Ce	10.97266330473781	9.49087810737345	6.82196223066079
Ce	8.30258405216514	12.31316554437880	6.73609208521304
Ce	16.22708392185712	9.40064790625021	6.83374137385295
Ce	13.60524599826392	6.63732922981921	6.77282209328101
Ce	13.70199918429983	12.25123960943558	6.75248545039535
Ce	8.20651377306788	6.7666243254502	6.75385954530196
Ce	10.97805514135895	12.20865939097031	4.16804981804657
Ce	10.88899217727724	6.76386300773809	4.18590685561556
Ce	13.70939016806461	9.43808193574396	4.22079080490471
Ce	8.53376348856503	9.52289114107049	4.03737255577765
O	12.57895510932267	11.08290573834973	16.01542997584666
O	12.51941972145900	7.89331771001537	16.01449144848933
O	9.44986081230161	11.15528423863713	16.00163250163108
O	9.38420529432794	7.94064806574944	16.00342980896457
O	6.97479896153252	10.98160138614503	13.59463630960823
O	15.10256635393209	10.82712194592496	13.55893058802798
O	12.30684189527517	5.42237640417053	13.57106288044736
O	12.46180025661146	13.55295706360636	13.54832238416474
O	15.04918490828964	8.04582840741478	13.56641854331342
O	6.91432775304118	8.18131223586948	13.60054770180109
O	9.66410034007803	13.61153628764408	13.54527722982449
O	9.51328348591279	5.46095709461989	13.56363793341609
O	12.33256619615241	10.82161506155845	13.46708886045728
O	12.28031891346801	8.15531701901061	13.47041504411761
O	9.69774882643466	10.86925176492395	13.46715852841432
O	9.64037050501999	8.20232766914141	13.46760944207091
O	4.33252645208346	8.26237135106484	11.15335901302597
O	4.37658696474823	10.96733257421011	11.15507842443159
O	12.43403971695342	2.95688700412511	11.13143815389758
O	12.66729303983754	15.99638685177160	11.07822753814094
O	9.49500152740587	16.01743186597114	11.08350229295569
O	9.25569669985969	3.04490677910018	11.12197004586293
O	6.80441582516025	5.49901276612024	10.92699489281213

O	6.95961062600072	13.64810591557187	10.91089932552465
O	15.01701340933271	5.36087128443065	10.90170741948525
O	15.16094774814939	13.50415527209138	10.86814715248486
O	17.65141413804223	8.01034239626252	10.91586494672213
O	17.70157031798761	10.77201449744306	10.90556174640479
O	15.01354655960079	10.78231091180698	10.84100621768919
O	14.96595264217480	8.07872153508094	10.85090394021792
O	12.37687169645363	10.83201527957466	10.81571150252699
O	12.32908565958928	8.12401774991458	10.82258510511136
O	12.37054420123278	13.46718575739649	10.81208542172441
O	12.22504614349397	5.49125196693508	10.83955497052762
O	9.63130070036519	10.87152071233082	10.81610573481025
O	9.72105704189898	13.49601313840082	10.80467327547624
O	9.58425283435982	8.18274719933279	10.82315165632096
O	9.57126541364149	5.55501360669445	10.82629603834089
O	7.00509240876338	10.92689390203399	10.82570226498075
O	6.95865776739704	8.21493411013399	10.82861057369063
O	4.03660070803087	11.26281942395847	8.56679333535109
O	3.96539353130208	7.96829117871499	8.57008095301539
O	12.38231056661626	13.46581268883356	8.15157214101504
O	12.24266055482451	5.47662690182838	8.17818364391887
O	9.72104584396467	13.50098418149645	8.14037722192669
O	14.98195664984422	8.07185761226678	8.15378769816934
O	15.02469684494183	10.77837120678981	8.14249724943609
O	9.57715926467381	5.53540173929228	8.16936437027825
O	6.97778179756972	13.64445029591510	8.14285626808771
O	12.33077891860338	8.11047366880272	8.08928802966042
O	17.65499718502178	8.02245019293547	8.16007680467022
O	15.01175449569057	5.37243686582236	8.12129886340249
O	12.37854707004095	10.82800677475540	8.07949090381633
O	17.70112536890214	10.74953410736470	8.15193332901527
O	6.82875680837132	5.48533797818719	8.15943260199235
O	15.15032315108801	13.47785726984963	8.08731606860196
O	9.61693946003131	10.87161804010328	8.11388561377569
O	9.56878251568986	8.16516738681648	8.12201160214725
O	6.85806140779310	10.95495166848408	8.09538302392792
O	6.80560990733469	8.18196678466285	8.10346286344572
O	12.42614088710866	2.93684583267748	7.94912879154863
O	12.65770121702016	15.99671257996136	7.89908672748081
O	9.50457390655188	16.03239681340625	7.89101020254007
O	9.27064422888356	3.01478434305790	7.92789785843046
O	12.42058262730024	10.80426737834979	5.39381168065349
O	12.37877185891777	8.12263130341973	5.40677037936821
O	9.77300487097423	10.86891795535746	5.49452165129712
O	15.10883579448835	8.06146437735173	5.43505597749534
O	15.15028059549945	10.76918546223288	5.42591805696160
O	9.64353594158486	13.59825963516545	5.39144840005052
O	12.44111244600911	13.52358750783874	5.41607744718478
O	12.30227021608587	5.40719605887693	5.44211536421273
O	9.72902531135937	8.15077518224693	5.50343951586954
O	9.50852835488027	5.42760606819624	5.42054189093456
O	7.10098343402125	10.99005863047942	5.20354486636554
O	7.05044007820787	8.11512153493027	5.21663665156905
O	12.80025385216342	11.05134277096683	2.78075763658561
O	12.73087562058351	7.84891219935882	2.79086136685768
O	9.64621330022314	11.13668078761156	2.94320707852305
O	9.58409554338049	7.86542368058410	2.95535352625983
Pt	6.86225448382203	9.56253375554683	6.61520098508854
H	12.49892593050143	10.85505723585005	1.87480339771646
H	12.43279009166786	8.05365246060620	1.88598096254107

H₂PtCe₃₉O₈₀ D4 (-956.938970 eV)

Ce	8.48380434729433	9.50501709839874	14.98915961890818
Ce	11.09899674897854	12.04750630932853	14.95244888074115
Ce	13.58009374938277	9.38877736798132	14.90850333421675
Ce	10.97084161080452	6.84796042835661	14.87739622584435
Ce	13.78498385165729	12.14766114076990	12.28509451000372
Ce	8.38945763327069	12.28682646664999	12.32541668453359
Ce	8.27432376266909	6.75577391999979	12.27201704101398
Ce	13.64218450052531	6.66502278373962	12.25594658452795
Ce	5.82146260694322	9.57814096795389	12.26593510432978
Ce	11.21597033477165	14.79208205552694	12.21912448573877
Ce	16.24339434047769	9.36706035881502	12.18414121197154
Ce	10.99378619835231	9.48367341320759	12.16103371195674
Ce	10.91855121926606	4.09903269141779	12.09005046557762
Ce	13.68112876574706	14.78366123929568	9.52309439121231
Ce	16.30335400113083	12.06556904912019	9.50852791587063
Ce	8.42876987617430	14.83457188314317	9.51596263691738
Ce	11.04910024243514	12.14671216957632	9.51067169985442
Ce	13.62609335342816	9.43237556805748	9.50489812823445
Ce	5.81853575656303	12.29161032695487	9.51111980705624
Ce	8.35917430909453	9.55998198645470	9.50178521764524
Ce	16.17849142550446	6.69609195571682	9.50233930886136
Ce	3.41511723259087	9.61144312108241	9.49958764402794
Ce	10.93756960759599	6.85254104871706	9.49680308213733
Ce	13.46440024064541	4.04763223924467	9.48728536255438
Ce	5.77870647997717	6.83696048682684	9.48971474587499
Ce	8.37144495026082	4.08387402180074	9.48272460719634
Ce	10.92305410151887	4.12457854124178	6.87763330271957
Ce	11.00550857157828	9.50822366746187	6.84627091863559
Ce	16.25504879195548	9.37815177625993	6.83095764175773
Ce	11.23040355044620	14.80819857038585	6.81975616999669
Ce	13.65156720950720	6.68263405072952	6.74153739242736
Ce	5.83049459225663	9.59959271191686	6.73469963031641
Ce	13.79849421838740	12.16736937131719	6.73782319687701
Ce	8.39802632660150	12.30887312000096	6.69573436344319
Ce	8.28667199458610	6.78418980540979	6.71347231816825
Ce	10.98962222023288	6.88632931888033	4.11403481633296
Ce	13.60257085099278	9.42005633513295	4.10480673784528
Ce	11.11946053413926	12.07971942811321	4.06788707437714
Ce	8.49950431191500	9.54521066510791	4.01444884781411
O	9.48105418453644	11.08623860130411	16.04238475561553
O	12.63251216461451	11.02190244550475	16.01828668680117
O	9.38806045605333	7.90809085437287	16.02061523204913
O	12.56383864287968	7.82296389799857	15.98377866970385
O	9.72343564458246	13.58495811303200	13.55869610076829
O	12.50511358478565	13.54240684172535	13.59213011210759
O	15.04250357501016	8.01391928059273	13.56256536571464
O	6.93315808587858	10.97620892283699	13.55784805425834
O	15.11000253523789	10.78927357548430	13.56368208488289
O	6.84970122455223	8.19439054168072	13.56688178278670
O	12.29928199800792	5.38482114972348	13.55968950355952
O	9.50494403447957	5.45088680141810	13.55297334731566
O	9.69180262524483	10.84672597902876	13.50916614997358
O	12.35335655318665	10.78207384203837	13.49422746973722
O	9.63133113942396	8.17802678689032	13.49167320724011
O	12.28309124495360	8.12482074232102	13.47428305952498
O	12.62463307808920	15.93632642198019	11.13192179177724
O	9.42822740280410	16.23978045426761	11.12186689330899
O	12.46131901991664	2.96850007246018	11.08303883536462
O	9.29871202603698	3.00109838602818	11.06414732515191
O	17.64601022493564	10.82019045850316	10.95454238647454
O	17.58974488545908	7.91708523423442	10.95062737841710
O	15.12244738589117	13.49561027123702	10.88883960361387

O	14.99526432137282	5.35182842535573	10.88461208406721
O	6.97663915655489	13.66316796333002	10.86575222463555
O	4.26763722794708	8.24657719279692	10.87650344066853
O	4.33373964833793	11.00077173919320	10.86738061059614
O	6.80597102289119	5.51557011237855	10.87635701232053
O	12.35009645497051	10.81936111044740	10.85637421772241
O	14.98611033049460	10.77078143899285	10.86148352170567
O	9.57184366584989	8.19321369724679	10.85340043539531
O	6.99301623305964	10.93968101548349	10.85912809470986
O	9.62469844055348	10.93512665281068	10.86975049944876
O	9.71602054928221	13.62149182476358	10.85171240753454
O	12.39150009585065	13.41590391372292	10.85610834710531
O	14.92411902283394	8.05724680382924	10.85559685588023
O	12.30028394739530	8.11838451975785	10.85459174823840
O	6.94555143100501	8.23312600474234	10.84951160357457
O	9.57943503266170	5.54034672811917	10.82461553445074
O	12.23640997930888	5.49560323081012	10.81775743352008
O	12.39919455761909	13.42487588245072	8.17635628705224
O	9.72215324860158	13.63044207080955	8.17616155418441
O	12.24137611216610	5.50825873087972	8.16614391965565
O	9.58275579783153	5.55306566618882	8.15721086828172
O	14.99200709342582	10.77628602709725	8.15411073965488
O	15.13246475366454	13.50187180809900	8.14300531974565
O	9.62918925699044	10.94463718990388	8.14345743967407
O	12.30420353029039	8.13012042968756	8.14816864974560
O	12.35804375731202	10.83140642908100	8.16006629636454
O	14.92974081075029	8.06428942800003	8.15074502027506
O	6.99849501621222	10.95312979055247	8.15049435681478
O	6.98189178170012	13.67477004569615	8.16123363069401
O	9.57767271177124	8.20643115422007	8.14396544498073
O	6.95039941780920	8.24742246277556	8.14289229240677
O	4.33856915163782	11.01239460429705	8.14564109088350
O	4.27256166191066	8.25764645682431	8.11360901636161
O	14.99837254950254	5.35862751288142	8.10685042114942
O	6.80842429401889	5.53195183714498	8.09607825375673
O	17.65365222679150	10.82608504684836	8.07100829373860
O	17.59598422153846	7.92359167510424	8.06303345891832
O	9.43473642980498	16.24431489629934	7.92067362985506
O	12.63882844354896	15.94502958117944	7.91661552463375
O	9.29766792960207	3.01713429500975	7.89283648418669
O	12.46189689829373	2.98411179301666	7.88090668479932
O	12.30018749928813	8.15544212496741	5.52813255980594
O	12.36901338768871	10.80911601255334	5.52202252837372
O	9.64635985195993	8.20707629169195	5.50668657511438
O	9.70675023166523	10.87613372471220	5.50222449294227
O	12.52422623100003	13.56778653925904	5.43908930595322
O	15.12424555078030	10.80828941451437	5.45426720431511
O	9.74094683193460	13.61375769441548	5.47219386437406
O	6.94671892693846	11.00416300686028	5.45190558201150
O	15.05969340651045	8.03173019913469	5.44332855657817
O	9.51548947953154	5.48086703669584	5.42763348835784
O	6.86270560477783	8.22554092712527	5.42532026476203
O	12.30810474297159	5.41522065473616	5.42425282466057
O	12.58852802627979	7.85709306601742	3.01884599145322
O	12.65232969492611	11.05566410526854	2.99933500773482
O	9.41036999945780	7.95708001768800	2.97562193340563
O	9.49841649995134	11.13220880072499	2.96999886168602
Pt	17.72220278449296	9.36709679706285	9.51048311453131
H	9.71598165791224	17.15107737476636	10.93070073270058
H	9.71199655657483	17.15951188921894	8.10801574818603

H₂PdCe₃₉O₈₀ D1 (-952.217706 eV)

Ce	3.33244267161071	9.58892599076360	9.49531759134462
Ce	18.67395371724297	9.37712346260773	9.48180404003558
Ce	8.50323060196624	9.42609585418757	15.00182811248466
Ce	13.57983099340832	9.39077678461735	14.94380713285290
Ce	11.01428440755491	6.80668008174261	14.92751334159367
Ce	11.06971126584192	12.02347746317360	14.91981163622938
Ce	8.36035213182550	6.73134167456424	12.29077991218041
Ce	13.67532771617797	6.62500845861840	12.28402618908740
Ce	13.73899108792972	12.12797521660218	12.29225456977232
Ce	16.22404725774712	9.36275137452458	12.20389722859836
Ce	11.16451309082811	14.74823366401845	12.21943413681817
Ce	8.36598216458496	12.23192058505262	12.24543901853141
Ce	11.00505424120425	9.39977139212889	12.18429174043887
Ce	5.91654769345177	9.57329867467900	12.09602049341363
Ce	10.94872569371930	4.03649379310623	12.10493389644837
Ce	10.95709356795978	6.82976866517052	9.56836083641040
Ce	13.59664992776435	14.78339196196235	9.52845262334015
Ce	13.58882065092083	9.42576472762046	9.52219598714544
Ce	8.39450763183465	4.08448302458778	9.51824237329160
Ce	16.23082163142728	12.08577566089524	9.52692628019641
Ce	10.95820548769223	12.08887132186346	9.51239327252559
Ce	8.35921330686460	14.79354160974418	9.49583135254363
Ce	16.16122200959974	6.69218289921174	9.49078813171682
Ce	5.88577001787842	6.99658286962714	9.47721379270236
Ce	13.46600779032610	4.01818862725971	9.47421886160811
Ce	5.73236603990769	12.28005497660920	9.41622077989256
Ce	10.92804656978068	9.52031231785527	6.90377226285485
Ce	10.90667196299036	4.15933642485616	6.87708223574110
Ce	11.16085285537932	14.80305700326853	6.82476064309343
Ce	16.18248227059851	9.40575857244889	6.81348583133265
Ce	8.26314824792862	6.84079022746693	6.74587185079124
Ce	13.72358804676207	12.18098182337048	6.74967037726513
Ce	13.61313481012370	6.70067985193265	6.75152618644119
Ce	8.27737883454325	12.37083475121681	6.62899182798710
Ce	5.75733961464187	9.67542197445550	6.73361373298622
Ce	10.93485326373851	6.90717223082096	4.14427620552866
Ce	11.06572875926580	12.10953870396662	4.08829937992125
Ce	13.52600134027730	9.44479488430406	4.10377302147859
Ce	8.42686631880777	9.59325216717997	4.07397837094769
O	9.38694694105488	7.84455002226604	16.07985282689247
O	12.58987632297776	7.82317599949303	16.03099392097303
O	12.62168908890134	11.01424110487162	16.01957413047309
O	9.47906361881063	11.03314582355756	16.01954310093936
O	9.70620570238433	8.15711822885713	13.62163106526473
O	12.49399010812584	13.50590780123657	13.59460197006074
O	15.11009288681706	8.01314164982568	13.56842402894087
O	9.72084520058249	13.56018713629921	13.53470829794961
O	12.38962367437700	5.34513588243048	13.58333207155648
O	9.61546535278746	5.40242385007274	13.57987736710411
O	15.11389549173991	10.78127084810810	13.56142035674368
O	12.34553849554785	8.07542885323450	13.51025918842235
O	12.35980257221089	10.74637409221097	13.50758647103409
O	6.93586382996231	8.19651723697765	13.49215198743666
O	9.68835667932675	10.82546585583449	13.45786688090786
O	6.91348657358690	11.03852510579909	13.39463372715381
O	12.58126786855514	15.91616247965942	11.14104514175960
O	9.41063855130410	16.16750909637598	11.13474644549092
O	9.78909375917619	7.91924872443519	11.10792387504736
O	9.30078951073082	2.93698349151355	11.07743872374787
O	12.48100410484956	2.91717019812946	11.05612242416409
O	6.96468682204108	13.59980673598026	10.85177441789991
O	15.09148088952051	13.46928654578612	10.90025190927036

O	4.45812102677747	11.01418465108080	10.87682255556090
O	12.34159732087653	13.38547420342413	10.85161474938536
O	17.62886252568222	10.80789328163789	10.90805984569120
O	17.62962445336946	7.97071074080951	10.90115282653747
O	12.31632271485339	10.80864745034816	10.87063038036120
O	12.41069381348220	8.08993697109828	10.87649280350869
O	4.51269716704867	8.19555023198902	10.89850727070078
O	15.04921090690702	5.34356855355796	10.86296447065639
O	14.98180054962838	10.74629386530714	10.86100490861272
O	6.88804878146719	5.58894106319546	10.85863662733281
O	14.98891840953699	8.06106560352745	10.84877797144189
O	12.28900124750225	5.45404338602311	10.85406531570394
O	9.68668885449404	13.51789195746916	10.83071086834961
O	9.64323299223398	5.40901377745999	10.82066014619465
O	7.29655056364767	8.32576233003925	10.74426346004284
O	9.58056183559167	10.66360788520211	10.77076536781587
O	7.11066182484695	10.87541139192775	10.53941483243356
O	9.55688976215436	8.31343252753193	8.41086463775744
O	9.37983017006054	10.88764440294390	8.20398543116564
O	7.09254222686737	8.56785089352988	8.20118027423877
O	12.26040317735939	5.50262479749017	8.18338456006280
O	12.27574717904531	10.82675361113836	8.17974539226413
O	14.93222130659521	8.08703041815187	8.16952113211359
O	14.94822100999380	10.77630637667691	8.17479995438432
O	12.28136134362151	8.12697156461438	8.15435395698524
O	9.60063000396231	5.60814852844068	8.15517780875829
O	12.32923790901685	13.41003884201533	8.18837501803134
O	4.42749812200711	8.23457148883608	8.06698590666526
O	17.60234004244103	10.82726810469562	8.10176173839238
O	9.66588628457970	13.56906646198884	8.13895617997956
O	6.92910280527813	13.85053862366677	8.13539938217375
O	17.58754861394150	7.99906210319849	8.06152928646421
O	15.08420441173758	13.49575929113169	8.15872068839861
O	15.01715976703698	5.38367767787059	8.09433913607035
O	4.23741835232862	11.05645806895238	8.09397085372320
O	6.83433127227535	5.66903395979737	8.03786200088305
O	9.43457196427089	16.23259670425449	7.93212644371523
O	9.30318773454228	3.04935004969705	7.90001717814855
O	12.46303782145279	2.98919176494663	7.86715222781443
O	12.59253458638371	15.93820117552715	7.92944497193308
O	6.81207694524511	11.23221386282927	7.86602422998105
O	9.61280553140119	8.24224871387931	5.59998524562332
O	9.67634827446960	10.93292923916320	5.56571901760635
O	12.31665971505399	10.81838430444328	5.54972441671382
O	12.25315144964460	8.17617141881737	5.55107366168748
O	6.83810480973915	8.22041609719496	5.49287773408386
O	15.08798155824220	10.83204727665144	5.47283297153617
O	15.03418355930624	8.05890968102929	5.45652432432512
O	12.49528332799558	13.57293791713874	5.45449229813217
O	12.29974499476318	5.43623810584212	5.43792736186031
O	9.51435988302129	5.51706436342430	5.42955262066731
O	9.70817007740742	13.68052281508435	5.42624803860728
O	6.93262325984686	10.99704067176244	5.26730336833999
O	9.35165382100426	7.98208257417041	3.05188944423447
O	12.62510043364185	11.08431795718096	3.01704148277695
O	12.52999099166206	7.88491842317111	3.02628371215352
O	9.47095330688041	11.16357122954443	3.00832365545605
Pd	8.35982539718782	9.60419538927149	9.46491287380601
H	9.71938730251377	17.06854740321894	10.92952569725943
H	9.75971607769635	17.12172926395299	8.16349369789195

H₂PdCe₃₉O₈₀ D2 (-954.031402 eV)

Ce	8.41686721824965	9.41207644213063	14.97246525315405
Ce	10.95993184599184	12.00436705132836	14.98253169774766
Ce	13.48109697080746	9.38509671566694	14.97816848821323
Ce	10.93584736803464	6.79922772501219	14.87493717509913
Ce	11.03843436003585	14.95975136381046	12.51907520299950
Ce	8.30813751054786	12.26929107759895	12.33982617641673
Ce	13.62106928901349	12.21345666700394	12.32995206343522
Ce	5.80075985535584	9.45751606214742	12.26079032849879
Ce	8.27867903351040	6.70471125905011	12.25575337134372
Ce	13.59476424400943	6.68253370022746	12.26423164164996
Ce	16.10604728815954	9.42368971032148	12.26430606749344
Ce	10.94385590486968	9.50686639926766	12.16135366004020
Ce	10.92144956785443	4.07146692607307	12.08478985197692
Ce	13.67443610398277	14.78471439174799	9.53868306833431
Ce	5.70534803375181	12.18348365659321	9.52857578935759
Ce	16.18502876311572	12.15721739733202	9.52204299746929
Ce	10.92301038507513	12.36139131747413	9.51825964295864
Ce	18.51594104793609	9.40247209675982	9.51155145756081
Ce	13.54168360487795	9.52833585235930	9.50680734400848
Ce	8.34322858680201	9.56788914481363	9.50217848122176
Ce	3.39269891963687	9.43134105764024	9.49872969292633
Ce	16.08497449668016	6.71232888719934	9.49481998129880
Ce	10.93733243170513	6.86555290475807	9.48888417106742
Ce	13.45359159993907	4.03821933089416	9.47900169759112
Ce	5.80260332133676	6.74852592145321	9.46831459204258
Ce	8.39884793339743	4.05692146468233	9.46016948024887
Ce	10.93287208484626	4.11024819753246	6.85423481277390
Ce	10.95543331332149	9.54000481302521	6.84773653890131
Ce	16.11974478288996	9.44911632569078	6.75248077004553
Ce	13.63504554518635	12.23993726251063	6.71178435124765
Ce	5.80686052283558	9.51882124204805	6.74166536026322
Ce	13.60422285054691	6.71483571551714	6.71480807924470
Ce	8.28907949458775	6.74592522329042	6.70594727820537
Ce	8.31158124543506	12.31193933845895	6.70314716910752
Ce	11.05268197556505	14.99101831563872	6.55499916476451
Ce	10.95790448805260	6.86072362737938	4.09389489316145
Ce	10.96397394645964	12.06274778085253	4.06151993601948
Ce	13.50046299143642	9.45000903836583	4.03143109293612
Ce	8.42788552702122	9.46586222143143	4.03278305809222
O	9.37910422374389	10.96421926867131	16.06455953467174
O	12.53196089243956	10.95037803251506	16.06581127515998
O	9.36559414298355	7.79574070278427	16.00315285141318
O	12.53283336706700	7.78233102278240	16.00478051085446
O	12.45561087541392	13.45387402763706	13.69358084905084
O	9.58981518779001	13.40621109813115	13.71526392341594
O	6.86346417013298	10.83261830045646	13.57678177662989
O	15.05895553021889	10.80011032628615	13.57577928084608
O	6.85096093436755	8.05414533101130	13.56052626569361
O	15.04402776347997	8.02644543229940	13.56040493183205
O	12.33216056105255	5.37395794893463	13.53843505780985
O	9.53375117912698	5.37772923618873	13.53364026598221
O	9.61999345570060	10.74978782137979	13.51942296600431
O	12.29219424779269	10.76317653168878	13.51719204285088
O	9.62465965851919	8.11116278569266	13.47472374142794
O	12.26395924062509	8.11385955635999	13.47985678194618
O	10.52613046996020	16.57693151599065	13.29451844467786
O	12.81783697132479	16.19958478522809	11.13717487511868
O	12.50393575652871	2.96238401169805	11.05817890491033
O	9.35511736143756	2.98501727347849	11.04300871975174
O	6.74917715986537	13.49271220835104	10.98870209138386
O	9.59843107980695	13.78034967920575	10.95882964470055
O	15.11226485914148	13.53348583714339	10.88736145367364

O	12.36653525701002	13.59392410499797	10.88523062579295
O	17.65031007480482	10.79781037359892	10.88465397504085
O	4.24633720320042	10.81807818800102	10.88568419481618
O	9.60055729347953	10.98826576228151	10.87069268666542
O	6.93769985371074	10.81454115794501	10.87034735148998
O	17.62992111075984	8.04350497001503	10.88221425880735
O	15.02136292180612	5.40049773688502	10.87378388560555
O	4.27214489623436	8.06504638120577	10.86192904140782
O	14.96730806018672	10.81911330728754	10.86827320638752
O	6.85376926325602	5.42174646726276	10.84748692102145
O	12.30893279992662	8.16721715707753	10.84983449895439
O	12.29785218738743	10.93163766993400	10.86123937495597
O	14.93760188637486	8.12347585157213	10.84592740442496
O	6.96080859207328	8.13988122511312	10.83880755638589
O	9.58318092660560	8.19752261472940	10.84332325843171
O	12.25431623715163	5.50866408692633	10.81149884658309
O	9.61216597884974	5.52677576552922	10.80701020520493
O	12.30514556727072	10.94853492656181	8.16593300635309
O	14.97511783404630	10.83106471429294	8.16006825277937
O	12.26078974263827	5.52795585174132	8.15235353142085
O	4.24984260759559	10.84593589697945	8.14089597485804
O	6.94259691491546	10.84028656153381	8.15394890212608
O	14.94264326676417	8.13786088973856	8.15391233911932
O	9.61574108582825	5.54628807274667	8.15038358674764
O	9.58799414222164	8.21650513817793	8.14613492949903
O	12.37159117431115	13.61078213941777	8.17259680049355
O	15.11710636986268	13.54671775167240	8.17340555008533
O	12.31401619829838	8.18467723043863	8.14534388175475
O	9.60453314389443	11.00779618149194	8.15470438961138
O	6.74727254236339	13.51162912492827	8.07771609590687
O	6.96450340757525	8.16590090904671	8.13827668645531
O	9.59552118680596	13.80055848478534	8.10157496952420
O	17.65827079100744	10.81142035625836	8.14984791009854
O	17.63481825837037	8.05625217047816	8.12547628237367
O	4.27497682496921	8.09445767232384	8.10632138744117
O	15.02849011115260	5.41539613784751	8.10068249791831
O	6.85680982839693	5.44467370741179	8.07215967326229
O	12.80301937056073	16.22777404483844	7.98017703334253
O	12.50402742732036	2.98641830724434	7.88128005845436
O	9.35611524501786	3.00758408574556	7.86760731909052
O	10.55495648564419	16.60130686415785	5.75742841888260
O	12.28027742025782	8.16052760333641	5.51357549019994
O	12.30688756662531	10.80687963471870	5.50927106679005
O	9.64339039277900	8.16215802426633	5.51125831389804
O	9.62685987469168	10.79802885841360	5.50564349833247
O	15.07719140419345	10.84526717190085	5.45172748328051
O	6.86846524799993	10.90212786692144	5.44546699023289
O	15.06504832545191	8.07164356489088	5.43776879974252
O	6.86685831981656	8.12452525565405	5.42014310804538
O	12.35114460075940	5.42105217391021	5.42190769685954
O	9.55085703120910	5.43279309978837	5.42098689061212
O	9.60567537044625	13.45466121965076	5.34223358103573
O	12.46708770614753	13.49632060999903	5.36520478765505
O	12.56337655302917	7.84755686063351	2.98620396252535
O	12.53879896048851	11.01597545304419	2.96243791309283
O	9.37897303539176	7.85870852623864	2.98391535216794
O	9.39188456755629	11.02847622105955	2.95930432234202
Pd	8.15541756366034	13.82334462552460	9.53291473906841
H	12.69274066168093	17.16306595822055	11.19138810955063
H	12.68071904305580	17.19222087260369	7.94108305627104

H₂PdCe₃₉O₈₀ D3 (-954.416995 eV)

Ce	13.47858433806194	9.47275316707368	14.95736295195499
Ce	8.44785785460322	9.56050649011421	14.92919164801597
Ce	11.00482344677267	12.13748800674052	14.87767532855159
Ce	10.90972185364526	6.89255551803465	14.88217914948852
Ce	5.79558599153259	9.59501058295459	12.29327795135212
Ce	13.67491695362406	12.23524808891763	12.26911716447445
Ce	13.57616062470308	6.68191975674026	12.28704015645971
Ce	16.12901860463577	9.41320235458680	12.28097835340337
Ce	8.33185143861793	12.31691026343517	12.25044995616703
Ce	8.22669920936097	6.79418970725720	12.25560668739908
Ce	10.95591458472020	9.50759398895186	12.12849164249755
Ce	10.83672118458561	4.12063987618631	12.13303477028752
Ce	11.03992431211726	14.89535460119676	12.09868799862538
Ce	3.39667005976723	9.63140691251192	9.69260866262042
Ce	5.65685776805813	6.86878957974039	9.53396034591602
Ce	5.75820481605546	12.31635028562125	9.52793818763934
Ce	13.38728825440696	3.97229488153015	9.54797676688243
Ce	16.09678152463033	6.64387939631246	9.54165300674676
Ce	13.58688621217342	14.93461793879492	9.50375777816492
Ce	16.19261149413220	12.17330043970071	9.52021379683847
Ce	8.48740668280870	14.95110286136361	9.49846766392731
Ce	18.55363339273287	9.37220567038603	9.56867436804702
Ce	11.00364274990160	12.14887621296571	9.47564937465003
Ce	13.60190746624081	9.45010677972559	9.49586554977072
Ce	8.28408677634496	4.13912480479320	9.53042371240788
Ce	10.90884025880996	6.84834273468335	9.49486147021427
Ce	8.28576936522401	9.54867803231033	9.45365375101878
Ce	10.83960572817284	4.06012425170976	6.93858210984266
Ce	11.03400387860289	14.92882181422945	6.90206814010620
Ce	10.98484715546640	9.49084629932311	6.82440255955671
Ce	8.30007868373003	12.31225235448041	6.73851595600921
Ce	16.22946613442000	9.39903078896628	6.83310513980929
Ce	13.60717311435385	6.63360120427406	6.77044467322346
Ce	13.70511430585350	12.25329896255518	6.75424190041912
Ce	8.20328195771519	6.77160944827713	6.75559249745038
Ce	10.97850850008718	12.20484505856962	4.17070472135242
Ce	10.88697289075873	6.76601773533514	4.18486156599294
Ce	13.71254474679441	9.43575137756599	4.22103203080708
Ce	8.52900903188446	9.52288970394349	4.04779271375618
O	12.57699800737455	11.08250201654187	16.01494856960000
O	12.51745083963490	7.89255147064631	16.01437996742299
O	9.44547053821286	11.15516374329673	16.00110859422425
O	9.38223068271629	7.94197234908550	16.00474521630110
O	6.96971806566516	10.97971582187919	13.59549838048623
O	15.10077000679673	10.82551051253584	13.56066123544017
O	12.30487256268044	5.42136399577435	13.57070603135926
O	12.45994909812041	13.55287118004059	13.54741039237641
O	15.04732536780706	8.04429187661714	13.56693978292891
O	6.91146031276615	8.18075416224044	13.60107536414652
O	9.66185049091562	13.60904087284901	13.54493464536241
O	9.51156975438152	5.46194877246629	13.56419855750227
O	12.32917568704673	10.82112349467098	13.46695127414779
O	12.27833360293256	8.15442434725000	13.47090267226585
O	9.69298545451792	10.86674454475252	13.46648870774791
O	9.63849577798314	8.20165626774348	13.46845719351348
O	4.32810978140562	8.26047344445511	11.14674123804060
O	4.37096543055566	10.96648785283340	11.14885690784344
O	12.43098277187854	2.95715518427579	11.13151950212588
O	12.66421460334037	15.99792060871540	11.07659724292879
O	9.49423962476898	16.01736567482071	11.08178542487821
O	9.25062002516320	3.04601552808236	11.12285466540102
O	6.80463942889619	5.50287255638725	10.92343795813069

O	6.95737194173299	13.64498787175175	10.90732781502278
O	15.01387779973722	5.36076113032743	10.89953608394292
O	15.15956056279270	13.50311839129731	10.86883701538147
O	17.64965447874966	8.00900411840981	10.91475584653344
O	17.70080202880989	10.77186336367376	10.90572259908995
O	15.01336196593281	10.78198455464931	10.84374832195165
O	14.96501088041107	8.07757021566750	10.85136220996010
O	12.37614435025114	10.83210708955615	10.81700985382910
O	12.32782716745326	8.12424393173052	10.82284732743110
O	12.36920456785096	13.46806137616941	10.81218617991453
O	12.22147673288840	5.49130309926533	10.83873595393497
O	9.62963463749217	10.87187724063950	10.81616410187209
O	9.71908936068354	13.49610907375493	10.80517909300423
O	9.58225378839377	8.18276919967276	10.82243915662703
O	9.57033780352699	5.55523657038110	10.82615120928162
O	7.00162326565367	10.92537516912188	10.82874317491112
O	6.95569593531754	8.21877004432889	10.83139395140624
O	4.04660609475457	11.25439323230407	8.55504236527732
O	3.98323479388553	7.98266070369956	8.55505584760020
O	12.38168961354071	13.46585100138371	8.15206360275242
O	12.24087325799198	5.47807585799608	8.17613325420227
O	9.72017806225586	13.50104422354373	8.14208645294774
O	14.98424962334202	8.07125732812116	8.15293037094018
O	15.02972221862836	10.77776045430432	8.14495010275390
O	9.57473414637096	5.53792438228656	8.16984716230315
O	6.97483630462138	13.65105353416442	8.13937773686959
O	12.33700184854218	8.10939602014683	8.09053236371407
O	17.65681065642194	8.02154363464060	8.15938271359754
O	15.01081762159297	5.37113896194950	8.11909584828268
O	12.38448990407604	10.82908930001207	8.08249140653183
O	17.70451162174944	10.74950146024421	8.15190227475753
O	6.82490556300457	5.48481481964191	8.15596721674511
O	15.15051854721685	13.47842647379598	8.08845866817805
O	9.62159639097135	10.86928819527191	8.11184001679354
O	9.57344759179413	8.17132227956237	8.11909174174117
O	6.88651572588765	10.96402649303832	8.10267960744932
O	6.83662808293444	8.17700077689342	8.10964215008416
O	12.41984914270193	2.93778550789090	7.95054797570376
O	12.65750905265408	15.99631342238907	7.89643454763346
O	9.50177783440964	16.03195684899849	7.88644628093723
O	9.26695399077973	3.01684397334116	7.92658574176327
O	12.42590941417161	10.80329163896652	5.39614613097112
O	12.38208253047629	8.12076616937329	5.40569949866800
O	9.77548338959161	10.86439113105087	5.50108758984977
O	15.11167779583664	8.05862416200134	5.43332422094465
O	15.15386487114794	10.76718368567584	5.42815701347281
O	9.64384978818066	13.59634724821019	5.39286053134209
O	12.44162587697373	13.52215668733320	5.41748060277962
O	12.29957941894035	5.40601454992587	5.44051511011364
O	9.73155211139519	8.15407000760347	5.50747890895801
O	9.50598039966216	5.43020293225838	5.42135237260027
O	7.12377007373089	10.99203023681130	5.21564091698239
O	7.07188309280705	8.12064002542498	5.22618918460916
O	12.80342076177310	11.04743455435656	2.78112270580330
O	12.73365783875462	7.84681785367877	2.79137077495906
O	9.64801398793929	11.13342779177048	2.94810712749320
O	9.58154023221813	7.86644072341361	2.95845774387589
Pd	6.80848908196402	9.56729275376450	6.61806887255673
H	12.50547651163408	10.85595508292759	1.87350550619247
H	12.44476725554811	8.04941722961542	1.88268811815188

H₂PdCe₃₉O₈₀ D4 (-956.115961 eV)

Ce	8.48287029685613	9.50516158181131	14.99081286790523
Ce	11.09689427894443	12.04773770708521	14.95177473714681
Ce	13.57892587335244	9.38967595407310	14.90885910472698
Ce	10.97169394199755	6.84813227799288	14.87771510345612
Ce	13.78443907783871	12.14585841028126	12.28458499686019
Ce	8.38772979663526	12.28606493681599	12.32390949526475
Ce	8.27375173816124	6.75449423499224	12.27225382218262
Ce	13.64407913400404	6.66660450866711	12.25593042430043
Ce	5.82081940331893	9.57659608821288	12.26473143380701
Ce	11.21737358709490	14.79148228980231	12.21952901520505
Ce	16.24630593321094	9.36807806635098	12.18032725997985
Ce	10.99097958725630	9.48303775730066	12.16295298090193
Ce	10.92227216096733	4.09934224512306	12.09231951107700
Ce	13.68178160057329	14.78423046963955	9.52346417008204
Ce	16.30517383186814	12.06421104194631	9.50897929886663
Ce	8.43528316519688	14.83738943891316	9.50914957863392
Ce	11.04770111048713	12.14717379928052	9.51160593672553
Ce	13.61948055011025	9.43314594754661	9.50534032353244
Ce	5.82109792372549	12.29062940273066	9.50826040680827
Ce	8.35854597727314	9.55824469685566	9.50185503239546
Ce	16.18307535630290	6.70171991363576	9.50358627022807
Ce	3.41431864682108	9.61002501725136	9.49717160026170
Ce	10.93642839170665	6.85154404197540	9.49744806163044
Ce	13.46779769897131	4.04904728466945	9.48801957845451
Ce	5.77826001257081	6.83448228526574	9.48797792295103
Ce	8.37576477228396	4.07986186838690	9.48487462322289
Ce	10.92546829225172	4.12459394453275	6.87897099558723
Ce	11.00405164859382	9.50770760094545	6.84597329377424
Ce	16.25934281200947	9.38078598428494	6.83651582669084
Ce	11.23385793921618	14.80873011723965	6.81746842161413
Ce	13.65259015321824	6.68538800909413	6.74460862922073
Ce	5.83053690745958	9.59878608374019	6.73392747570342
Ce	13.79724624261832	12.16617344231859	6.74043731765454
Ce	8.39824342183202	12.30813382347927	6.69388917866576
Ce	8.28642578734120	6.78250246215999	6.71373561924548
Ce	10.99133358582233	6.88686963467474	4.11492607227457
Ce	13.60552429015230	9.42110772571765	4.10776206255813
Ce	11.12047916037911	12.07939261632632	4.06789693872228
Ce	8.50139792044428	9.54466092477845	4.01335031065493
O	9.47394609875828	11.09016681318310	16.04104243160488
O	12.62647832486781	11.01963694597116	16.02020864476564
O	9.38939775003610	7.90974212139576	16.02199791792151
O	12.56465834991667	7.82304593275803	15.98408034508041
O	9.72330109848561	13.58307359658129	13.55753055221565
O	12.50437875751706	13.54041162501632	13.59252003502384
O	15.04200667219752	8.01539547228264	13.56072562287362
O	6.93038158740106	10.97668280680496	13.55585432199392
O	15.10820966828523	10.78971637560776	13.56215905701207
O	6.84833383141492	8.19329807711738	13.56616213132127
O	12.30076642683020	5.38518864648566	13.56066938882732
O	9.50609812881167	5.45052014816164	13.55409354771823
O	9.68949825331795	10.84503245928964	13.50972705206442
O	12.35170419817048	10.78230837131175	13.49439631593186
O	9.62996391983397	8.17671194184793	13.49257250812702
O	12.28279458041785	8.12518767540159	13.47532616067070
O	12.63233656216918	15.93450051186512	11.13876895159705
O	9.42868041501259	16.23954620731836	11.12212311501777
O	12.46413102723161	2.96928406955332	11.08357193926685
O	9.30373817617210	2.99828236137067	11.06451894602648
O	17.62169271034262	10.82004912900908	10.95299020092325
O	17.56833157812009	7.92035554911074	10.95110420398801
O	15.12275622675658	13.49404699499662	10.88898227235695

O	14.99727084464543	5.35510222667511	10.88534648107835
O	6.97804579148347	13.66147031385833	10.86048016835146
O	4.26620748267701	8.24290766817212	10.87203958010715
O	4.33406356411596	10.99725786934181	10.86430055011491
O	6.80736847855562	5.51409001892524	10.87508437974064
O	12.34680768333080	10.81934750610492	10.85818532046426
O	14.98350638441498	10.76676781464059	10.85715170506248
O	9.56979267842646	8.19185047235724	10.85382672363475
O	6.99277956425602	10.93813507085016	10.85789314242647
O	9.62319683157824	10.93417247044511	10.86934758608781
O	9.71654428125247	13.62267505422819	10.84962772697885
O	12.39171925112763	13.41578608627423	10.85532540340952
O	14.92384479796386	8.06257614263616	10.85184221135545
O	12.29776753596432	8.11748479080634	10.85643338002395
O	6.94417239309286	8.23200822037168	10.84851413044795
O	9.58080829554693	5.53779782578237	10.82616190444872
O	12.23816784997648	5.49592717577629	10.81861860275904
O	12.39927986393853	13.42565424421483	8.17647713191013
O	9.72439415120219	13.63149909680999	8.17400388491916
O	12.24210085747460	5.50865106532446	8.16741360781385
O	9.58340752237734	5.55085295825347	8.15817415866495
O	14.98997765646700	10.77369479886586	8.16084318973089
O	15.13246237718609	13.50237202342300	8.14442198597924
O	9.62816674390913	10.94464393127674	8.14326781364000
O	12.30209002807860	8.12961425832059	8.14848509663804
O	12.35516630524531	10.83214126613123	8.16009581439263
O	14.92924810199741	8.06985543998335	8.15692147833336
O	6.99893778135265	10.95177686428872	8.14949389829228
O	6.98480293627253	13.67444451532048	8.15669584329502
O	9.57755213189068	8.20504618504121	8.14359251935065
O	6.95028371778931	8.24524536204505	8.14182784048706
O	4.33920516091097	11.00941732215781	8.14155709460710
O	4.27227548662940	8.25603340306246	8.11014329928131
O	14.99977717135132	5.36205090432443	8.10935719945475
O	6.80918082040091	5.53042004450579	8.09416014818435
O	17.63088077339199	10.82763252832919	8.07337902674613
O	17.57425390456905	7.92741315575028	8.06276878825478
O	9.43463467836802	16.24522860196495	7.91665218229064
O	12.63889539461616	15.94642091601236	7.91759111537094
O	9.30325624049479	3.01384378883457	7.89528326141233
O	12.46539220770726	2.98526685486539	7.88080038646848
O	12.30134449855287	8.15707208560743	5.52954901142707
O	12.36942436489702	10.81026576171502	5.52369691687559
O	9.64664180092851	8.20638082961176	5.50588672600933
O	9.70724327214550	10.87546100393292	5.50133436435668
O	12.52612539623276	13.56843911443418	5.43948191289732
O	15.12488765704990	10.80903047555897	5.45866203716542
O	9.74224337864155	13.61311033879154	5.47036708306638
O	6.94760052516053	11.00404889998267	5.45087434778840
O	15.06128311164928	8.03406232202715	5.44807308076924
O	9.51681491455160	5.48054103823794	5.42795429749147
O	6.86363314631283	8.22531526436374	5.42462869096467
O	12.30958305635589	5.41776168282424	5.42607910663038
O	12.59241269676498	7.85779502070982	3.02098060703425
O	12.65481056225575	11.05631818032547	3.00109695735154
O	9.41416552543137	7.95821032263391	2.97404993662962
O	9.50055186013041	11.13143729875351	2.96947640361541
Pd	17.77765988977849	9.36724227161368	9.51074106617422
H	9.70678498993196	17.15566934965704	10.93890022467610
H	9.70350859428876	17.16419501452758	8.09623010576459

H₂NiCe₃₉O₈₀ D1 (-952.907850 eV)

Ce	8.52628994268788	9.43948391233739	15.01381721378266
Ce	13.56954721883313	9.36951402841997	14.97931423025423
Ce	10.99755117539416	6.80054036095768	14.89549748266411
Ce	11.07574253627703	12.00632289475509	15.00864265331748
Ce	8.35933986760064	6.75689989744708	12.21374219479595
Ce	13.63177660775901	6.63518889851717	12.25413972587705
Ce	13.74021907148755	12.15404641147096	12.32194869804239
Ce	16.18916416500885	9.36839492733426	12.26038979274477
Ce	11.19260989603948	14.78338241740374	12.27411539810911
Ce	8.44062913058372	12.24782438263050	12.29663419374417
Ce	11.00898737217061	9.46002413029141	12.19548108361868
Ce	6.04212414515274	9.54124392408821	12.03420724108460
Ce	10.92590078744334	4.06241018448919	12.07754155206905
Ce	10.89016906123059	6.88389256471684	9.51972157170150
Ce	13.57643985821364	14.83124966388597	9.54820385521752
Ce	13.59334481985410	9.44368014982685	9.52623906814401
Ce	8.37308974850147	4.08869314116204	9.46917294404424
Ce	16.19046849755414	12.15733112223344	9.51445079690405
Ce	10.96314739559745	12.11303656371242	9.56772176838483
Ce	8.38960927991336	14.82736897593478	9.55773231514037
Ce	3.45187381352208	9.57266720176894	9.47764988978133
Ce	18.53509794263584	9.38441299663249	9.48407322524296
Ce	16.10068172164256	6.65004550879339	9.45870589086690
Ce	5.86432257106982	6.86762677146768	9.43508367783635
Ce	13.40645197410080	4.00792352883420	9.43713331695988
Ce	5.89386063720166	12.19411169625070	9.45770951093710
Ce	10.85500316825815	9.52146066494127	6.94956875355985
Ce	10.87393552827567	4.16141931339159	6.83975187419412
Ce	11.13183185687060	14.81249900485573	6.85842663610348
Ce	16.12861120490052	9.42559836311463	6.75355730995884
Ce	8.21532576226797	6.80991372309080	6.71045023580821
Ce	13.66897076717011	12.18816934606521	6.75700610726486
Ce	13.55659183145871	6.72458900650752	6.72679490721028
Ce	8.30496268459935	12.29670803428749	6.73014265592424
Ce	5.77168984036386	9.58845211242496	6.63562399693001
Ce	10.90548506770156	6.92599991431502	4.12335035890401
Ce	11.01746117790044	12.13917929187640	4.11558270772191
Ce	13.46422257271383	9.48259044190329	4.08248179523060
Ce	8.41125165097954	9.58571567002362	4.05240466717729
O	9.41536931069531	7.83367746523009	16.06407554073989
O	12.59411060957643	7.80127949438681	16.02926519845954
O	12.63813281131249	10.97535904665335	16.07929278454958
O	9.49509299967915	11.02428435957510	16.11796678423340
O	9.71109198156239	8.14719440854144	13.58043649836413
O	12.55538439674206	13.52909187817190	13.62103512574846
O	15.12121460540697	8.00665253436128	13.56563232595260
O	9.79468963182824	13.56280550429041	13.60287699895271
O	12.39087020413427	5.35381131999442	13.55389638856732
O	9.61778682521249	5.41075572908222	13.53524476907509
O	15.14759512233027	10.77110406279948	13.58279898451404
O	12.35229960942939	8.08827079681840	13.50826627637069
O	12.38538809799784	10.77231912166321	13.54652509634138
O	6.96928945707204	8.14598406766838	13.43225876325441
O	9.72610873591248	10.79295129265979	13.61838911461354
O	6.99044644841764	10.95947876749261	13.42577198723936
O	12.60075827652525	15.95435662110394	11.16314875192761
O	9.41294635864261	16.23669090475887	11.18694665916122
O	9.72608145533393	8.10001381341786	11.00408342297936
O	9.31686158235903	2.97132976977897	11.05488222570833
O	12.46956695431161	2.92646641386999	11.03222701402352
O	7.00407443778324	13.60692751401047	10.87186480193404
O	15.12607350403390	13.49713492993709	10.89683678217886

O	4.50242608898208	10.94308753361176	10.83575837137571
O	12.37265707170418	13.41819188479992	10.89657367868024
O	17.72225291122108	10.77631262086281	10.86738351769680
O	17.69217410467847	8.01104651230842	10.85562590416866
O	12.43124496155347	10.81308794766652	10.88831067486251
O	12.39771997435585	8.10094133942157	10.86743806279708
O	4.44750349671411	8.20798769242156	10.82382496521640
O	15.03641129754566	5.34896919362755	10.83226392038910
O	15.05749026368457	10.76958812685963	10.87141079107587
O	6.87706171903224	5.52310837671371	10.85187592628366
O	15.01679289592261	8.06743253027837	10.84600295502664
O	12.25461458820644	5.47691874465507	10.81484514622538
O	9.72120610135833	13.66316691002812	10.87334020656297
O	9.62073894121218	5.47555026984331	10.78572310923014
O	7.20951405103035	8.25004562477487	10.58671743019103
O	9.78987802656820	11.01578486933384	11.06613243082589
O	7.26096568465602	10.85293308978433	10.60231531186083
O	9.41144129760541	8.26575864460697	8.29527576628904
O	9.44644180484450	10.88332328028990	8.31830787178228
O	6.80315976453921	8.17815518060576	7.91613692901508
O	12.23140678750623	5.51943902145405	8.15110052117132
O	12.29346038791438	10.83306109648276	8.19420877956704
O	14.93896266976614	8.09415350656940	8.14576253494603
O	14.97794077799744	10.79628098678996	8.16794830214112
O	12.26252964256060	8.15025685655324	8.16240394217376
O	9.58637071045778	5.59102457178708	8.11972541290813
O	12.34174663865902	13.43701292547876	8.20831889420297
O	4.15542440786142	8.22436160736646	8.07841079001104
O	17.65148071492913	10.79195199845074	8.12219410247051
O	9.67788511300876	13.60038076132579	8.19670966042866
O	6.97902411919249	13.70261292052850	8.15566798204523
O	17.62754729523717	8.03846881337037	8.08945201185083
O	15.09521194106867	13.51347600327872	8.16409062891640
O	15.00712686386986	5.39097134204607	8.06631294076106
O	4.24346744791733	10.98085661853789	8.12447119454525
O	6.85326897554714	5.46530286018984	8.07184717698657
O	9.43955661631635	16.25916532992210	7.98730802052028
O	9.30721922666821	3.03315007613930	7.85689634514848
O	12.44407562028806	2.98490093352275	7.83587272369324
O	12.56460496321913	15.96939157160851	7.96846815407324
O	6.87007786245012	10.98754869977484	7.93149956678471
O	9.58484428113904	8.22859066322505	5.56683203919148
O	9.64505491904667	10.90917397588527	5.58326417977796
O	12.27610103190313	10.83877444769114	5.56231020230604
O	12.22394850996634	8.19499504563827	5.54994978799127
O	6.83502236176208	8.24213154278442	5.27213460214069
O	15.06975784087440	10.85318695340801	5.46624192897050
O	15.02483537233126	8.09116178326114	5.43623838472906
O	12.48059098018098	13.59226217794769	5.47561861613848
O	12.29992354620815	5.45639041872332	5.41222445856915
O	9.50920880003498	5.49463215919763	5.38757571963514
O	9.70526280955027	13.66303405368119	5.48844175055299
O	6.91706979384022	10.99776530513808	5.31296940983803
O	9.37721432978600	7.99540077641246	3.00367658631078
O	12.58505893224068	11.13288196924448	3.02262692811416
O	12.51860270551198	7.92214481481499	3.00988831539760
O	9.44455370514713	11.19932564683890	3.02091588239480
Ni	8.39422077874339	9.54387699788251	9.42576747392902
H	9.68702833326015	17.15460877448698	11.00942600377298
H	9.81269268248729	17.12220266164167	8.24485148319653

H₂NiCe₃₉O₈₀ D2 (-954.949912 eV)

Ce	8.41613042209287	9.41264270044436	14.96746183140847
Ce	10.95606667297185	12.00679969728206	14.97488531129932
Ce	13.47738078897490	9.38744616284067	14.98237118562713
Ce	10.93609733365995	6.79845437955288	14.87552694877057
Ce	11.01105113072607	14.95153551349158	12.47713057253413
Ce	8.31108623545883	12.26316849915535	12.31668709318746
Ce	13.61463239843387	12.21414336568253	12.33016375781949
Ce	5.79539349334114	9.45721929533535	12.26208769642906
Ce	8.27770289543329	6.70232093936613	12.25724986031666
Ce	13.59581968182150	6.68210558436156	12.26499442621756
Ce	16.10313298059010	9.42670168312348	12.26740048069488
Ce	10.94504370194620	9.50238573142880	12.16255227320931
Ce	10.92195490198869	4.06883399090401	12.08506597327162
Ce	13.66489042275953	14.77994606929286	9.53803610181551
Ce	5.74264335446987	12.19207407205624	9.51763009370588
Ce	16.18320680063062	12.15686621102969	9.52175205818655
Ce	10.91257610582204	12.35531906667869	9.51975953933526
Ce	18.51548770921637	9.40466572281199	9.51228656518025
Ce	13.54228544928123	9.52802378005166	9.50817066403740
Ce	8.34289817654300	9.55628981732100	9.50273004272807
Ce	3.39787058398038	9.45452977843525	9.49408348427875
Ce	16.08589172127974	6.71348479258134	9.49546349675640
Ce	10.93779214959348	6.86086654565289	9.49130829500913
Ce	13.45562240743388	4.03509071485572	9.47879523360425
Ce	5.79801496820497	6.75218225724590	9.46855533379762
Ce	8.39876345430505	4.05628984038274	9.46057047755419
Ce	10.93455971143415	4.10933907361125	6.85540627043672
Ce	10.95764306705001	9.53651479370047	6.85061568454807
Ce	16.11846585662997	9.45004956991774	6.75180595693463
Ce	13.63039469990651	12.24194808365506	6.71185868426371
Ce	5.80205525127603	9.51787148042525	6.73509654152699
Ce	13.60496665520778	6.71500091090697	6.71564598847327
Ce	8.28519426456618	6.74464301077089	6.70781479579733
Ce	8.32119761585952	12.30780576585292	6.72850661663474
Ce	11.03207612782616	14.99013749171377	6.58388195340320
Ce	10.95302672410178	6.86576378135587	4.09856170193985
Ce	10.95671391157040	12.07088946746240	4.07173132037889
Ce	13.49536164074371	9.45726257889786	4.03163835643269
Ce	8.42308673113533	9.47605706385857	4.03797227237543
O	9.37566421524656	10.97448127118851	16.05737642097360
O	12.52682538398957	10.95640433834569	16.06452532203033
O	9.36663986965016	7.80096202735778	16.00257761032795
O	12.53121500930541	7.78368484965703	16.00831466815476
O	12.43838642536529	13.45603345467523	13.67897952330072
O	9.58733882139327	13.40806105251726	13.67450308540564
O	6.85609018000458	10.83232044273536	13.57227243781148
O	15.05512531725864	10.80185695192593	13.57757248755453
O	6.85125057716849	8.05401624100302	13.56072360541964
O	15.04314506179217	8.02771877213420	13.56201332793542
O	12.33274887798952	5.37422396791164	13.53994983490782
O	9.53414522336329	5.37605529845241	13.53470418262309
O	9.62108577211499	10.74633790173530	13.51784472840291
O	12.29059478728078	10.76197402831495	13.51943420556193
O	9.62417758124749	8.10784066412839	13.47412767651941
O	12.2638729779072	8.11303467594501	13.48380373262222
O	10.50977756658693	16.56571684425206	13.26349826602262
O	12.81056053047965	16.19481915411027	11.13268977140932
O	12.50461293322641	2.95926182404936	11.05766344616191
O	9.35503924913012	2.98320636649750	11.04273181249152
O	6.90187640086884	13.50770494065944	10.86426867323346
O	9.53690798815575	13.76127494288558	10.87089390815595
O	15.10140268670344	13.53159383096437	10.88640102555766

O	12.34798976944926	13.59359833094545	10.88447972410232
O	17.64943479188111	10.80165632708044	10.88441748584188
O	4.25129787196603	10.83326064442189	10.88293683569842
O	9.59999681484213	10.97193298584282	10.87112682377580
O	6.93447231325594	10.81408796669438	10.86893175628113
O	17.63013416601798	8.04682314895528	10.88351012791814
O	15.02188161035763	5.40083972544581	10.87415201411929
O	4.26889834838988	8.07768734988278	10.85797480683040
O	14.96760141767739	10.81957266355197	10.86874417258014
O	6.85131474906308	5.42293354232926	10.84620359385172
O	12.30892587401258	8.16260162299075	10.85234482058374
O	12.30044182835672	10.92697440679870	10.86571457106176
O	14.93781675540365	8.12372578068117	10.84730834057223
O	6.95857547162017	8.13883628044481	10.83937493447972
O	9.58226165699872	8.19063608122161	10.84484246817886
O	12.25478622950017	5.50449405180447	10.81278984748261
O	9.61165500728166	5.52341260352826	10.80804875703404
O	12.30999915057022	10.94492687566192	8.16476673415172
O	14.97637276780604	10.83138282204463	8.16044568495430
O	12.26194696660350	5.52447060101878	8.15385356864590
O	4.25935244286503	10.86143363695534	8.13051791662278
O	6.94396201875818	10.83945057352893	8.14971031523971
O	14.94308329793828	8.13797551563256	8.15464393005924
O	9.61563019309851	5.54271780759546	8.15103714982098
O	9.58816672666237	8.20991338112563	8.14877701289306
O	12.35589942407950	13.61201526324122	8.17112041238607
O	15.10929585688503	13.54649552886959	8.17277317773712
O	12.31483144149860	8.18103809223070	8.14831695988516
O	9.60681947551337	10.99043982595896	8.15685603283250
O	6.90308742182061	13.52528154874397	8.18950929227262
O	6.96287902185021	8.16508695836020	8.13778699219971
O	9.54080829264543	13.78172395912248	8.18948945142678
O	17.65831394202204	10.81393817244264	8.15059092783922
O	17.63486243674706	8.05762903319213	8.12632496298389
O	4.27511228052096	8.10734872386109	8.10376923313554
O	15.03001743365782	5.41581207276685	8.10115540052905
O	6.85352365110679	5.44598338418997	8.07287777495589
O	12.79415537396403	16.22830882215519	7.98821889691205
O	12.50649985117475	2.98369392564192	7.88129019774157
O	9.35636692838898	3.00612249870588	7.86771215436196
O	10.55565206110965	16.59723130893927	5.76997188552413
O	12.28021683117698	8.16192942628737	5.51569329435911
O	12.30602754111221	10.80934454671622	5.51127009407066
O	9.63982965603630	8.16458708668995	5.51597117707890
O	9.63137642997703	10.80062210360088	5.50872378324311
O	15.07547476062818	10.84687792712767	5.45107148060813
O	6.86600862844876	10.90128554789760	5.44662723622676
O	15.06358439201257	8.07324565770287	5.43797445708550
O	6.86478832536290	8.12384642884350	5.41870221423605
O	12.34980665862620	5.42192976266315	5.42387085317109
O	9.55004165233179	5.43439186553909	5.42152522464667
O	9.60196094761234	13.46553477483143	5.38052721332409
O	12.45409626167169	13.50287775861538	5.37561775836485
O	12.55739290446764	7.85378037188120	2.98867636783158
O	12.52786352667021	11.02341995769665	2.96819992268777
O	9.37549339757394	7.86999106618612	2.98863879813173
O	9.37807504986200	11.05112750457609	2.96851649341676
Ni	8.21328497390056	13.76622155625819	9.52922229811830
H	12.68405648875601	17.15742988403564	11.19423961402232
H	12.67754806230311	17.19346980330496	7.94330988136975

H₂NiCe₃₉O₈₀ D3 (-955.367340 eV)

Ce	13.47642479710926	9.46939732846742	14.96015120275890
Ce	8.44508245938998	9.55681672157247	14.92044419943229
Ce	11.00207969784427	12.13402392755401	14.87576314097089
Ce	10.90522198561278	6.88709502703214	14.87519517796131
Ce	5.79278705521184	9.59549703451334	12.27329645426048
Ce	13.67915075995941	12.23456929126785	12.27262306270873
Ce	13.57815629636347	6.67843603538164	12.28973985972308
Ce	16.13141288833428	9.41297267089574	12.28405696510965
Ce	8.33307419996209	12.31681423963169	12.23957664482440
Ce	8.22488447435005	6.79223064000169	12.24819558139258
Ce	10.95952030271849	9.50587213054357	12.12848252402322
Ce	10.83091078371943	4.11449989041436	12.12982899855037
Ce	11.04234134243779	14.89460232324989	12.09774181693199
Ce	3.39197383767314	9.63692356240905	9.65494215987471
Ce	5.67191732833939	6.90506122026981	9.50040379734025
Ce	5.77147790042533	12.28690635609706	9.49186329410724
Ce	13.38681243121570	3.97022588318231	9.54804531275060
Ce	16.09823854485465	6.63761192915501	9.54410559506272
Ce	13.59148295541898	14.93630331801959	9.49991370474534
Ce	16.19750713114382	12.17151466324588	9.52352094130016
Ce	8.49224396036941	14.94766130536527	9.50022258980702
Ce	18.55409989034379	9.36331115987531	9.57612858579133
Ce	11.01827559168326	12.15013599060302	9.47927475048405
Ce	13.61090883063246	9.44823674262497	9.49871005098142
Ce	8.27923598803080	4.14833556730145	9.52507813602514
Ce	10.91675274656132	6.84640524524683	9.49818949806724
Ce	8.30203290288199	9.54850691658161	9.45003473133401
Ce	10.83519868748715	4.06565002883472	6.93874575331628
Ce	11.03210686663043	14.92299074628544	6.89883299245363
Ce	11.00358962432521	9.49194067839307	6.82710080066635
Ce	8.30811815135231	12.29139696345580	6.75561941431768
Ce	16.22982526364094	9.39774204180416	6.83333676884402
Ce	13.60732704663283	6.63106001700113	6.76804920053224
Ce	13.71176261384046	12.25707487700524	6.74917831828026
Ce	8.21053249825485	6.79610849757424	6.76441239824895
Ce	10.96515287184517	12.20995137301947	4.16585732133851
Ce	10.87069775034512	6.77276779927252	4.18150996541230
Ce	13.70861764013991	9.43746195022328	4.21919895062545
Ce	8.50602292633791	9.53715384597912	4.09320865019328
O	12.57486093585037	11.08236532064739	16.01453717586493
O	12.51109866894406	7.89197757280104	16.01379790016215
O	9.44109176358954	11.15091045726178	15.99617512933633
O	9.37597515320092	7.93787805484639	15.99785993799950
O	6.96565873271026	10.97723325481329	13.57792747855978
O	15.10199650724165	10.82560706682402	13.56313419403028
O	12.30130897999235	5.41808984466857	13.57082043540015
O	12.46024385439935	13.55179654412676	13.54749930718778
O	15.04648949427644	8.04386655582258	13.57038436270778
O	6.90627892660171	8.17862239579392	13.58395756549622
O	9.66221759195472	13.60697776311090	13.54036828188572
O	9.50779757212679	5.45702081603384	13.56019135429091
O	12.33007064973557	10.81943179570011	13.46781517523486
O	12.27764467284640	8.15064582595962	13.47030439792282
O	9.69144825901144	10.86344155634502	13.46348217709658
O	9.63621930499075	8.19858856954500	13.46413925960648
O	4.33596910711447	8.26474411772602	11.11341555671629
O	4.37597198006237	10.96517587980496	11.11354223642104
O	12.42639785804750	2.95375915635382	11.13120431393409
O	12.66722694053667	15.99761994715175	11.07218393331993
O	9.49559670249912	16.01690675566344	11.08301976430425
O	9.24108119178617	3.04833810087342	11.11637307499953
O	6.80647777716281	5.51223742417604	10.90203642895948

O	6.96744400252321	13.63784971481302	10.88462760246771
O	15.01492870706132	5.35583857944207	10.90364646523445
O	15.16826772469835	13.50101841619895	10.86976378373205
O	17.65084064390960	8.00239425550379	10.92224227897815
O	17.70563425446204	10.76625503623004	10.91381803182208
O	15.01914220164116	10.78111137816562	10.84582702291583
O	14.96978813566370	8.07514272837631	10.85480685661593
O	12.38484015137743	10.82969663681061	10.81876876899287
O	12.33572770685706	8.12283694550561	10.82352054084173
O	12.37996857899516	13.46804539729743	10.81269920436180
O	12.22485688150450	5.48761198173787	10.84080010582369
O	9.64056520779465	10.87560210037424	10.81748988664763
O	9.72835998402340	13.49778604099497	10.80508422696725
O	9.59141775764276	8.17811418112977	10.82486844794392
O	9.57244454180170	5.55364977805713	10.82440900329814
O	7.00975158611863	10.92362895173222	10.81131389234284
O	6.96498775926501	8.22309028190341	10.81555783794678
O	4.04220981678457	11.25725936909676	8.51988147959035
O	3.97718078958880	7.99153528774051	8.52288652923409
O	12.38893192918534	13.46503988778011	8.14988861944761
O	12.24357737064931	5.47736469512471	8.17698494186654
O	9.72789481694745	13.50102160713421	8.14999613792649
O	14.98933880790815	8.06786592232180	8.15428049582030
O	15.03471853895167	10.77729052489999	8.14330709242727
O	9.57733520739513	5.54033320529806	8.17343855884987
O	6.9768077763711	13.61063996224275	8.12348286311095
O	12.34543365764503	8.10817230285507	8.09005236260720
O	17.65864534085570	8.01372443321818	8.16531462442484
O	15.01067163916614	5.36644991323529	8.12261945363020
O	12.39633528279773	10.82875483588780	8.08306199654529
O	17.70567505246869	10.74154449022585	8.15791695937016
O	6.82395799634157	5.52697614368086	8.13950452005142
O	15.15577547887097	13.47760696067217	8.08738164421338
O	9.63726748019181	10.87282399147674	8.11527125608805
O	9.58908706925662	8.17179466820757	8.12257184647852
O	6.89311968404631	10.88586423319000	8.05489591638552
O	6.84517189810427	8.25513105657369	8.05937771847300
O	12.40954082615190	2.93789104285520	7.95442109485095
O	12.65469298790771	15.99438586141200	7.89414511353794
O	9.49301410232509	16.02617758700128	7.88566211137280
O	9.25392436131097	3.02459950606254	7.92183115538520
O	12.43043372434978	10.80659643568421	5.39260359921615
O	12.38345552984831	8.12319777607263	5.40368694932805
O	9.78340141350966	10.86371349435119	5.50601000061532
O	15.10915077785863	8.05935419327751	5.43261062101943
O	15.15721348633082	10.76644361748771	5.42246366030745
O	9.64961441433036	13.59565673700822	5.39194262402945
O	12.44203498047973	13.52300926391150	5.41483936588403
O	12.29454231093458	5.41010721239886	5.44260868099561
O	9.73498376788109	8.16250124456533	5.51453212163078
O	9.50459108040778	5.43847840164669	5.41719418464740
O	7.10973108802658	10.87870008944842	5.39034981137759
O	7.06314796669777	8.24779838799386	5.39242901145542
O	12.76305081744442	11.03868495529771	2.77511125109024
O	12.70876834168628	7.85528029584074	2.78596878227937
O	9.58318019562720	11.16356244961287	2.97251558299217
O	9.53283207919515	7.86733667172900	2.98196239551887
Ni	6.85839859164851	9.56841484928889	6.69441185105826
H	12.47307855727007	10.83919301891845	1.86651738947087
H	12.41344614276348	8.06513029759827	1.88139491647721

H₂NiCe₃₉O₈₀ D4 (-956.889427 eV)

Ce	8.47064822499086	9.51456594837469	14.97644056005734
Ce	11.07986215731511	12.05593495633735	14.94034161708943
Ce	13.56339548299318	9.39231825880690	14.92219771545979
Ce	10.95673804365140	6.85275677137853	14.87951456534821
Ce	13.77489885616847	12.14727450170024	12.28775373143291
Ce	8.37854665060801	12.30196117416383	12.30547854121237
Ce	8.27037938319415	6.75607105560678	12.26863718034989
Ce	13.62378241104019	6.65600940195928	12.26467297134270
Ce	5.82156653661867	9.57978907122171	12.25734740764548
Ce	11.21034222896778	14.79478149563394	12.21954115294744
Ce	16.21871445019702	9.34057579312691	12.19516046903865
Ce	10.98445868594218	9.48775198648246	12.16121374372178
Ce	10.90760386820031	4.09437653186385	12.09012061583201
Ce	13.67148471804260	14.80070303987610	9.52253958723727
Ce	16.28486427140717	12.06217522639852	9.50328313514579
Ce	8.42730769191938	14.90256652180283	9.52163791311961
Ce	11.03075308164614	12.16642079868985	9.51471071790829
Ce	13.60238799912450	9.43843488577716	9.50719941284035
Ce	5.83389494334563	12.30526644008867	9.50717588299352
Ce	8.35734713553669	9.55651772914981	9.49866985234291
Ce	16.15659374131728	6.69435460837028	9.52154346520773
Ce	3.42113890747850	9.60679193582596	9.48973590798379
Ce	10.93479376441714	6.85114480898420	9.49592866152774
Ce	13.45287904896041	4.03585774516416	9.48802034450270
Ce	5.77912479342098	6.83270070373578	9.48537571257493
Ce	8.37083797459576	4.08446430435329	9.47705711080539
Ce	10.91915986453126	4.12874693166076	6.86992869492620
Ce	10.99968702728927	9.51701671355379	6.84630476051521
Ce	16.23155606480606	9.39918510027043	6.82899221082634
Ce	11.21284526801330	14.81458215266129	6.82270696010316
Ce	13.64521818531403	6.68792348558754	6.74122740899591
Ce	5.82982064679439	9.59764173698509	6.73605394585655
Ce	13.77818157295242	12.18141338478009	6.74006692499163
Ce	8.38697919005372	12.32499260017841	6.71356478173346
Ce	8.28434630084589	6.78507663963987	6.71016316853731
Ce	10.98315973563785	6.89484240041304	4.11076818156480
Ce	13.58695749093253	9.43367280844172	4.09188600694034
Ce	11.09868675652333	12.09183971941701	4.07578445372528
Ce	8.48955028806145	9.55510503401544	4.02563350495588
O	9.44779490083730	11.09210447857238	16.03221617227450
O	12.61296086513744	11.01819704461574	16.01874592482676
O	9.38989182474042	7.90872597052683	16.01392277689786
O	12.56102659216250	7.82642284179517	15.98921935379031
O	9.73098936993651	13.58245630555852	13.57498476470321
O	12.51353626542831	13.52918216193820	13.59530529608215
O	15.05087739338114	7.99411079773282	13.56207882340598
O	6.92966571106932	10.97051527030722	13.55531095121121
O	15.11709691570439	10.77287275685829	13.56161320376087
O	6.85305766339447	8.18968928321766	13.56273123365678
O	12.29423178378135	5.37960954123464	13.55976259331730
O	9.50329061066811	5.44776638040535	13.55067910524938
O	9.69051237780396	10.84764729609695	13.50256423914773
O	12.35305784495517	10.78058754953987	13.49384184816458
O	9.62942380073744	8.17777453270677	13.48729821440266
O	12.28265451145697	8.12410269428040	13.47740937586487
O	12.66006894457130	15.93200029414198	11.14103991121469
O	9.49793671081980	16.26281641375617	11.19841939330226
O	12.45876496197106	2.96268820621837	11.08177529830245
O	9.29947582557995	2.99675689617752	11.05997873464650
O	17.63423907124886	10.66250130299792	10.81972900345856
O	17.56240597165681	8.02036376605272	10.85051544900655
O	15.14268234656716	13.46546907807723	10.88818617373445

O	15.00186645157280	5.35188613921210	10.89654939744054
O	6.95015163187080	13.62776309215044	10.89488041495569
O	4.27488024925830	8.23283065812590	10.86553876733900
O	4.33065490321854	10.98435138782113	10.86537330138980
O	6.81215891348244	5.50493177417003	10.86919165686176
O	12.35334792506746	10.82220942896571	10.85863493808952
O	15.00011965182147	10.75500684845360	10.86259473285907
O	9.57471275089578	8.18795599801094	10.85237178891021
O	6.99877918529162	10.92292704198750	10.85665995035907
O	9.62688755349972	10.93166338169383	10.86510445868632
O	9.72605176880244	13.62255785214854	10.87083273640767
O	12.40065788649066	13.41812708863628	10.85547767792877
O	14.91332275086945	8.05249007127162	10.85896452134507
O	12.29633874524795	8.11663537070062	10.85546344905595
O	6.94919485667817	8.22123641261017	10.84525137436570
O	9.58104890308594	5.53531601441967	10.82088607258961
O	12.23525934485812	5.48960235053757	10.81786647994351
O	12.40347688280464	13.43061942897486	8.17840923763903
O	9.72941593586204	13.63462213378233	8.16354528330609
O	12.24634419188863	5.50818506643138	8.16452980112829
O	9.58789842491991	5.55202030715975	8.15277121158489
O	14.98478476253812	10.77485846139257	8.15997402594717
O	15.14864540424167	13.48745728704746	8.13784667811023
O	9.62864409864584	10.94527826098829	8.14582670951026
O	12.31251378186043	8.13006714135869	8.14631946336789
O	12.35233079146516	10.83609113585204	8.16284916718595
O	14.94298712480336	8.07212632601692	8.15850956002592
O	7.00080536387357	10.93311386297824	8.14848435584600
O	6.95403938426752	13.63897649131244	8.13318147569827
O	9.58654390470828	8.20353209691924	8.14292540381457
O	6.95845508816322	8.23329204055710	8.13807261020290
O	4.33516144060807	10.99063638274379	8.12662075423484
O	4.28361268705561	8.23976435695871	8.10804585317548
O	15.01039267057021	5.37023110575782	8.11448437352525
O	6.81810072670745	5.51996298344459	8.09000624414189
O	17.62620209113100	10.70990851908112	8.18626495702105
O	17.58491028690776	8.06335984501334	8.21191833948120
O	9.49372710460724	16.27494478988325	7.85184666205016
O	12.65327437696760	15.94637086148391	7.92392740760426
O	9.30514630962215	3.01809305813045	7.88437546244534
O	12.46401460862084	2.98323520546876	7.88125773275490
O	12.30382704847117	8.16186792535560	5.52564273173925
O	12.36861662399797	10.81455689218154	5.52243437374318
O	9.64851393181974	8.21027768441748	5.50858342365486
O	9.70636138236156	10.88019080877427	5.50562352732609
O	12.51952053946062	13.56590487195970	5.43741326392836
O	15.13575243020192	10.82337623304673	5.46338063984174
O	9.73710212180078	13.61436166491496	5.45871605364313
O	6.94966643635998	10.99274353419195	5.44777572274245
O	15.07410943886572	8.04285815208905	5.45541112641063
O	9.52311192444702	5.48017161177008	5.42140706852094
O	6.86964350835966	8.21722208125061	5.42133252706332
O	12.31601448066239	5.42276028205762	5.42582535791044
O	12.59166646922696	7.86369847767451	3.01374976327460
O	12.64450623932298	11.05874693815566	2.99951926375627
O	9.41142726881625	7.96381329942603	2.98053705813140
O	9.48803853286688	11.14047690932852	2.97366230785616
Ni	17.75439998803921	9.35883585328065	9.51673443560702
H	9.78773710446877	17.17881223824152	11.03843762705628
H	9.77431922315840	17.19504121694386	8.00414241970240

H₂CuCe₃₉O₈₀ D1 (-951.761365 eV)

Ce	8.45915909145402	9.47526422191605	14.95436368390070
Ce	13.53336502415017	9.37209921971980	14.96346013317597
Ce	10.93484408841491	6.82029416570999	14.85185818830031
Ce	11.05860459880356	12.03104333749805	14.96900041876849
Ce	8.25160757640309	6.77409789246662	12.22445650798250
Ce	13.60666739703614	6.64187885561352	12.24422140701730
Ce	13.73006792943040	12.15505839655250	12.31381256624602
Ce	16.16394375353718	9.36662481446879	12.24925147460461
Ce	11.14995786824132	14.77027308744360	12.26867719601765
Ce	8.34321834560150	12.23470340646089	12.31520946045834
Ce	10.97843544116390	9.47173701828298	12.15535182776417
Ce	5.87757756253923	9.53861171769556	12.20085878370610
Ce	10.88187053148368	4.08930272096996	12.06864892006394
Ce	10.92151124923119	6.85385729482525	9.47806705525537
Ce	13.57374874947124	14.85665868810124	9.55368386876404
Ce	13.59792193127043	9.44181451623042	9.49794157455162
Ce	8.35242977487958	4.11321358538657	9.45271073802851
Ce	16.19190343999303	12.15765920758882	9.51786084614159
Ce	11.00015978868601	12.14933112153211	9.53442293790518
Ce	8.37736052651446	14.82092451191178	9.56240213866045
Ce	3.41100049106039	9.57051907780001	9.50446603495037
Ce	18.53344892415789	9.37762943763002	9.49377768178074
Ce	16.09730217805684	6.64367653721986	9.46558328785128
Ce	5.83521483195559	6.87470501680458	9.48054047884677
Ce	13.40062451779496	3.98517947584806	9.44400277970116
Ce	5.86242842832868	12.18803293827611	9.53435764431236
Ce	10.96331067696159	9.51726502483830	6.84996010911384
Ce	10.87536641484140	4.13971979829201	6.82996256068852
Ce	11.13876473608707	14.81962418868209	6.84504690734883
Ce	16.15795514092912	9.41517260508727	6.74104075770868
Ce	8.24276904699753	6.81622114852935	6.72760062684582
Ce	13.70982732327158	12.19992580473164	6.73965931534520
Ce	13.59747652999161	6.69135202294261	6.69954805692939
Ce	8.33406714308230	12.28470101626173	6.75941523634722
Ce	5.87151023472844	9.58347499168605	6.80848846350329
Ce	10.91809880525128	6.91314729352815	4.09520583436193
Ce	11.03409087475502	12.12232711103943	4.08787202579106
Ce	13.50996530930606	9.46388863065853	4.03432106653487
Ce	8.44019204057144	9.57109215697334	4.05459857015636
O	9.38794280472884	7.85989551504689	15.99501326473507
O	12.55007151691208	7.81030310513965	15.99505095733928
O	12.63033505133538	10.99460761695258	16.04313843577191
O	9.48435679332844	11.06403601701222	16.04495754587992
O	9.65534033232123	8.16315878404266	13.47440823376075
O	12.52191817293119	13.52441236094859	13.61395438162551
O	15.08400062168457	8.00410779954787	13.55169943335608
O	9.74667462734061	13.58213085663833	13.59791638792911
O	12.33670909838902	5.37031944801816	13.53096075132484
O	9.54553316437596	5.42895984864671	13.53504487698369
O	15.13220411210478	10.77740736013783	13.56812600406836
O	12.30428848647793	8.10391841211064	13.46967195646151
O	12.36176112265424	10.76996072001415	13.50865635434541
O	6.90672331055581	8.16271041704401	13.59490649839080
O	9.71180885834536	10.83028331186431	13.51116273566650
O	6.98282465849876	10.92551840288561	13.61506406904859
O	12.57605572037586	15.95312299637227	11.16007176173910
O	9.42299552062456	16.22468057002460	11.18302534083745
O	9.58257341338823	8.18895549325763	10.84151628520974
O	9.30454833553722	3.00019030046141	11.04485279098519
O	12.44615214282226	2.93580939830739	11.03404122977301
O	6.99205312027733	13.67235359599924	10.90554740612327
O	15.12120751612672	13.49480747940096	10.90499688383296

O	4.32657289380276	10.94867197665579	10.87540201674669
O	12.37230728840058	13.42385823452875	10.88739962763608
O	17.68896121931841	10.76965933152312	10.87502713109823
O	17.65854538156819	8.00997487762406	10.86720300794425
O	12.37197039280522	10.82057310119632	10.86505947629763
O	12.33690296600162	8.10889815496608	10.84190317496276
O	4.26491769484116	8.20674646206365	10.87140932210218
O	15.02515090040893	5.35278654314746	10.84416491459051
O	15.01947597627536	10.76917456641081	10.86153386253364
O	6.86456792224904	5.45839107192960	10.84810838312541
O	14.97774507759304	8.06527033221814	10.83467893568577
O	12.24958838005040	5.47766639085894	10.79513256578721
O	9.70740242590766	13.60175142760704	10.88751953541634
O	9.60300545371035	5.53637445115402	10.79948581419101
O	6.93190729364115	8.14692212073270	10.90510128188593
O	9.61961516960158	10.91735923036810	10.87618907282707
O	6.98180595830016	10.97667594094150	10.94288198184143
O	9.57423831396537	8.21213408326130	8.14259810664121
O	9.61749784050860	10.94188097375248	8.16041497113855
O	6.92635787574786	8.16468490493113	8.07217474402436
O	12.24542338665275	5.50149046390356	8.12920605602013
O	12.36461600576003	10.84564689889539	8.16422208880288
O	14.97303961201600	8.08754047246485	8.13264643668670
O	15.01476639430756	10.79185802773147	8.15924379269669
O	12.33101323978650	8.13482796812282	8.13031961468942
O	9.59875875532781	5.56349442793622	8.13032307862095
O	12.36535470058903	13.45071448856840	8.19792785172341
O	4.25828584092204	8.22347947303839	8.11737096699112
O	17.68282286926989	10.78677595823250	8.12979322165340
O	9.70066505036430	13.62654906851925	8.20847522245552
O	6.98994426693642	13.69411046989746	8.19097521713168
O	17.65425016390488	8.02746688694287	8.10107075543471
O	15.11367666231180	13.51676067514557	8.16642099546168
O	15.02086650506254	5.37660392385333	8.06897744916524
O	4.32295197691882	10.96563683810974	8.15754197125388
O	6.85835979066740	5.47652820564309	8.08658408821169
O	9.42692035048720	16.25703812408318	7.97397343432579
O	9.30018498995022	3.03200264347974	7.83740256521561
O	12.44493337089816	2.96452399532492	7.84030660886797
O	12.56703389955637	15.98186698020245	7.97012633189174
O	6.97694876696201	10.99766334803031	8.10268466268261
O	9.64115100067174	8.22556326288531	5.50631004614434
O	9.69462417044099	10.89675633428189	5.52054222065733
O	12.34281236246274	10.83423988951186	5.51748886409680
O	12.28797835743350	8.17105897935349	5.50394903299278
O	6.89459126620733	8.23187044026649	5.38248388600186
O	15.11244123654341	10.84575108905252	5.45421942187217
O	15.07287704877630	8.07378905496420	5.41797419798229
O	12.50205056165623	13.58964796029940	5.46959312835916
O	12.32460564485846	5.43937182483364	5.39286934661235
O	9.53132035338660	5.49382381810869	5.38971392847567
O	9.73026351664154	13.65373894683133	5.49597915239604
O	6.96924326827141	10.99494176174740	5.42909637775444
O	9.37332150007125	7.97999133380656	2.97851335464228
O	12.60136508855965	11.10543394542512	2.98696485861102
O	12.53114691960877	7.91859826372515	2.97203067419874
O	9.45534935952432	11.18393783573372	2.99088760188902
Cu	9.18202652259924	9.55733136327586	9.50541226277620
H	9.75307203487874	17.11572742720108	10.96542609904130
H	9.77065125558805	17.13789108762195	8.20889445841897

H₂CuCe₃₅O₈₀ D2 (-952.479926 eV)

Ce	8.41457086267117	9.40932215469421	14.96689746777007
Ce	10.95908009806919	12.00106879087197	14.98235973684347
Ce	13.48153065217295	9.38320909738093	14.97998992420618
Ce	10.93605643215455	6.79751786419107	14.87504048633830
Ce	11.02168649859887	14.94805435364749	12.49546595657304
Ce	8.30921075286250	12.27081368932703	12.33571602288190
Ce	13.61853265232800	12.21252129536592	12.32957663311047
Ce	5.79889666928980	9.46103291265621	12.25654412509885
Ce	8.27757003079020	6.70289596175117	12.25701538676519
Ce	13.59608438718852	6.68170639845721	12.26508095063884
Ce	16.10574089718128	9.42435747842607	12.26526959146398
Ce	10.94545935391124	9.50513221605822	12.16171230843212
Ce	10.92188166309876	4.07016813460101	12.08484448299024
Ce	13.67438760855335	14.78573116567401	9.53954176146662
Ce	5.73058702832582	12.19644327226053	9.52344153043098
Ce	16.18420474298712	12.15819073361612	9.52233807584177
Ce	10.92206247788111	12.36511664541961	9.51881427989662
Ce	18.51642318575413	9.40486449550313	9.51148016132523
Ce	13.54228093751445	9.52826678062348	9.50686287370300
Ce	8.34452425186079	9.55920819389164	9.50195120630895
Ce	3.39686666641650	9.44574520683889	9.49287263493803
Ce	16.08614558549554	6.71297282262350	9.49547432481934
Ce	10.93855828882617	6.86315714505957	9.48950588449182
Ce	13.45494429452895	4.03616251000064	9.47901011888575
Ce	5.80036839445873	6.75019488260200	9.46723156806515
Ce	8.39863518580872	4.05708610736718	9.46037779415944
Ce	10.93459551415505	4.10975899040622	6.85534285452327
Ce	10.95522735984263	9.53960833468169	6.84873826735047
Ce	16.11839162702940	9.45100065504097	6.75282473021994
Ce	13.63073028667674	12.24021531756876	6.71078945427905
Ce	5.80616742493084	9.52004115923683	6.73930061145372
Ce	13.60478649546545	6.71539264283632	6.71514111632107
Ce	8.28661222859260	6.74349332660801	6.70646834542708
Ce	8.31412990151304	12.31555084672136	6.71162104902981
Ce	11.03305107684703	14.98327961720542	6.57471275396764
Ce	10.95520422214343	6.86235777577812	4.09594420395733
Ce	10.95578655334974	12.06362164064552	4.06287838506890
Ce	13.49610497405394	9.45323705613205	4.03130926282105
Ce	8.42339740753340	9.46617802266467	4.03653621600232
O	9.37889536721529	10.96471848588534	16.06163305833880
O	12.53161167317391	10.94924464754284	16.06700260210625
O	9.36420616359774	7.79572443107470	16.00169862944241
O	12.53312312177858	7.77991415465687	16.00590038519719
O	12.44316855506011	13.44891853568867	13.68724122112289
O	9.58294246338937	13.40802822907356	13.70270931289160
O	6.86044674424416	10.83026500102972	13.57612894323023
O	15.05881713253732	10.79960234937012	13.57672488808153
O	6.85193238699684	8.05378323371123	13.55849594957389
O	15.04436042864035	8.02586414789596	13.56192023921681
O	12.33279568870703	5.37238542714975	13.53869143852001
O	9.53331753261297	5.37539708618467	13.53404190657147
O	9.62228208736559	10.74790106360024	13.51831856198093
O	12.29348889395276	10.75899128678283	13.51912892690462
O	9.62540028321015	8.10860426892715	13.47414354337032
O	12.26467274843019	8.11165784343775	13.48118771978102
O	10.50332145231925	16.56970545277025	13.26012394041459
O	12.81559661670108	16.19603855042621	11.13670396923632
O	12.50409011371969	2.96060288796477	11.05675007892793
O	9.35527660868854	2.98371495606912	11.04331609842753
O	6.83198140176238	13.47768963951798	10.92521751129163
O	9.57372260102135	13.75826657772977	10.91800247348493
O	15.11044400269175	13.53294741008331	10.88819953995822

O	12.36359195494142	13.59315987149972	10.88293568094683
O	17.65112194950510	10.80017609947218	10.88461796654456
O	4.25114350493602	10.82533158439628	10.88330795734071
O	9.59585162039926	10.98746174009664	10.86604362956667
O	6.94100772161879	10.81418222633313	10.86705566931925
O	17.63056287999175	8.04635225758463	10.88319509673856
O	15.02313368955892	5.39975780964467	10.87423313722590
O	4.27411940128826	8.07229899971131	10.85627525866812
O	14.96796465307592	10.81916085177747	10.86840847919010
O	6.85253519056142	5.42176570846417	10.84649750540891
O	12.30981664722441	8.16533514417842	10.85030595808745
O	12.29881299369692	10.92892411559261	10.86461923173629
O	14.93801856855743	8.12310081190829	10.84681368445623
O	6.96178522954512	8.13821152878187	10.83757542397352
O	9.58494373453986	8.19440732317607	10.84428987573315
O	12.25585414563124	5.50708165100913	10.81238158819584
O	9.61242295530217	5.52502509369020	10.80735949919651
O	12.30541122820643	10.94613063580286	8.16432607922532
O	14.97405068207559	10.83160886234882	8.15955148784394
O	12.26215929731525	5.52624914478393	8.15299399553023
O	4.25623988849202	10.85478602733638	8.13390780864165
O	6.94686279176621	10.84069446254041	8.15393265341558
O	14.94350126910464	8.13825294574131	8.15479412501601
O	9.61597951735825	5.54502330758296	8.15104191678577
O	9.58951718962395	8.21404114360354	8.14641532738333
O	12.37000930368702	13.61017690587581	8.17373504978623
O	15.11589513370601	13.54744696929520	8.17373078313256
O	12.31463564279125	8.18320270055136	8.14570754959303
O	9.60048136240208	11.00800750693761	8.15887662265486
O	6.83433634642551	13.50131743586279	8.14442974865536
O	6.96525474068865	8.16412080294780	8.13759120111717
O	9.57582963150410	13.78012869034402	8.14159241219270
O	17.65722365638315	10.81414184539781	8.15027691431491
O	17.63578925694715	8.05847630843852	8.12621816568587
O	4.27755840651477	8.10232951049201	8.10203077283711
O	15.02959898654846	5.41667050467834	8.10138492236687
O	6.85531309961046	5.44374333571676	8.07196938979098
O	12.79583295728073	16.22766371271624	7.98852185026818
O	12.50671092760383	2.98489134906998	7.88078349894908
O	9.35694708808906	3.00692236910260	7.86835542321018
O	10.54198328965822	16.60140036347890	5.78621404138417
O	12.27933045938890	8.16163593653114	5.51410524728979
O	12.30445339954192	10.80694595375048	5.50922798163587
O	9.64212184960403	8.16237299960329	5.51328056668638
O	9.62750471060504	10.79905735563814	5.50750659125790
O	15.07394100825165	10.84680264593472	5.45044205105847
O	6.86523599599717	10.89903561010415	5.44378004637087
O	15.06363569875219	8.07339458764194	5.43781568352761
O	6.86727740130500	8.12246516939689	5.41961284439319
O	12.35131033750208	5.42152290716105	5.42301669492738
O	9.55104299099819	5.43195370331028	5.42152601570408
O	9.58597461982086	13.46172494963129	5.35167108932083
O	12.45040965418655	13.49550969808193	5.37025248335931
O	12.56061544342183	7.84974405679973	2.98754114976840
O	12.52925898655064	11.01922586358133	2.96468127120831
O	9.37447893833439	7.85849236039712	2.98629005633626
O	9.38538821671399	11.03187819346285	2.96114994909446
Cu	8.19040680877810	13.90088802985120	9.53518440852570
H	12.68636705714945	17.15866293662602	11.19869238092070
H	12.66878040653405	17.19154602352531	7.94354263056722

H₂CuCe₃₉O₈₀ D3 (-952.979058 eV)

Ce	13.48722027459622	9.47344127155021	14.95841484873933
Ce	8.45513603994033	9.56295202956366	14.92918823628752
Ce	11.01315353820693	12.13750134493490	14.87734861863478
Ce	10.91866589206159	6.89444056884663	14.88203687818847
Ce	5.81107148997962	9.58929776235123	12.27329820663090
Ce	13.68912499018239	12.23143404093356	12.27539303351857
Ce	13.59331018665988	6.68523388719378	12.28898033404080
Ce	16.14089004678829	9.41858284132197	12.28656456531847
Ce	8.34369156906092	12.32147173842114	12.24522155016645
Ce	8.24046699697440	6.78468883760005	12.24978030467253
Ce	10.96646453492304	9.50542793428883	12.13273490906007
Ce	10.86120731474140	4.12290098061419	12.13351069963438
Ce	11.05572133162534	14.89088653042429	12.09995023200489
Ce	3.40378083233674	9.63337266843411	9.66416403688216
Ce	5.66918689624889	6.88387152817201	9.52137114007902
Ce	5.76974766196273	12.30050069249290	9.51422678468026
Ce	13.40765183897447	3.99102339884621	9.54387787048845
Ce	16.10484904444442	6.65270464443216	9.54244286259011
Ce	13.60476876397092	14.91602904099927	9.50362873575013
Ce	16.19743384818966	12.16858646690834	9.52182937790520
Ce	8.50398325041940	14.96007483920933	9.50447120116036
Ce	18.54819149473132	9.37533032386503	9.56954443022562
Ce	11.02556877482479	12.14739213460758	9.47591451768902
Ce	13.61297399121591	9.45002269670247	9.50279397957242
Ce	8.31103790618094	4.12502899015223	9.53240571930285
Ce	10.92876114015587	6.84708720798896	9.49176187170195
Ce	8.32732110555590	9.54768844781235	9.45993939068564
Ce	10.87112730346741	4.06113927289461	6.93610910522069
Ce	11.05485054177404	14.92613625803330	6.90939966672979
Ce	11.03548950618050	9.49132616499314	6.79550668771079
Ce	8.33256508690044	12.31647964006882	6.75032409694488
Ce	16.20645560185599	9.40351896565153	6.81088894755191
Ce	13.62923672296668	6.65648295318204	6.74869531621255
Ce	13.72251169444194	12.23481809354077	6.73119168059927
Ce	8.24067411265326	6.76496959397120	6.76971392985856
Ce	10.98844365076357	12.20669279865101	4.17657725127338
Ce	10.90167110079960	6.76277714089516	4.18963250656193
Ce	13.72231567120660	9.43469253529300	4.09187515528133
Ce	8.54086881345483	9.52248564335738	4.03733454009344
O	12.57680280759613	11.08608273391365	16.01549870874374
O	12.51450256100109	7.89312590695600	16.01781186745168
O	9.44221968894600	11.15394776332243	15.99933464759288
O	9.38023591269218	7.94809757329710	16.00230342023849
O	6.96689839076602	10.97843152915971	13.56846721364242
O	15.10024738138251	10.82920776473250	13.57768752438871
O	12.30873731806470	5.42140927800494	13.57469549478227
O	12.45759367351366	13.55284214412555	13.55306551704601
O	15.04685918154279	8.05082690569047	13.58073524336167
O	6.90775177664329	8.17685737960869	13.57413495031520
O	9.65827050981386	13.60651854646050	13.54065355414228
O	9.51435351403277	5.46213096385007	13.55884662675012
O	12.33214474757146	10.81954518067202	13.47292203463471
O	12.28168099794416	8.15533151220755	13.47604288254908
O	9.69401131918671	10.86800816938211	13.46515218034555
O	9.63889326386473	8.20018257360775	13.46702945281816
O	4.33943051693221	8.25523200768678	11.11421465372144
O	4.37972223899043	10.96333013718077	11.11894544891562
O	12.44302588922851	2.96665196583673	11.13283766734665
O	12.66947764299702	15.98504466283093	11.08280657679854
O	9.49510155436224	16.01778861236853	11.08544308743568
O	9.26309255025450	3.04141995565757	11.12004560243856
O	6.79738481914790	5.51091452785080	10.90900399190664

O	6.94614827160493	13.63547121806590	10.89019434477271
O	15.01224986786895	5.36595942679572	10.91421150585191
O	15.15482256115700	13.50518954388686	10.88071203684918
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O	17.69338924228967	10.77250149263787	10.92406951037071
O	15.01314853957935	10.78541426470920	10.86512888520443
O	14.97036717002315	8.08171204878628	10.87030514668085
O	12.37880692029236	10.83064706043694	10.82526444196666
O	12.33226584701302	8.12269860836208	10.82894399647439
O	12.37481086982066	13.46071066529003	10.81626074015288
O	12.23101022933031	5.49658254583319	10.84037820775601
O	9.64055549731430	10.87262903173778	10.81834552958652
O	9.72300930898544	13.49590677747110	10.80506036823742
O	9.59322938883755	8.17818392495363	10.82377620872914
O	9.57949368458483	5.55092530944766	10.82437658171389
O	7.01472406342288	10.92252660870634	10.79372943342061
O	6.97034313143089	8.21804655007073	10.79666528574636
O	4.06816909220351	11.24493539704411	8.52128010950320
O	4.01068102117941	8.00064912281190	8.51768243887478
O	12.38891306830974	13.46219750830917	8.15394565627406
O	12.25136924818328	5.48196127302012	8.17622751108916
O	9.72930652531059	13.50217209928653	8.15107164533381
O	14.97766474238333	8.07083975881934	8.18076678425050
O	15.02260460312655	10.78162492390937	8.17362373523575
O	9.59063838403253	5.53338340194767	8.17432934908980
O	6.98226018095427	13.59448069057924	8.12724959174261
O	12.34040753300195	8.11521402709029	8.09280321780773
O	17.65967914730995	8.01399253723894	8.18233609758640
O	15.01598409751979	5.36804948702382	8.13674601353736
O	12.38832944351633	10.82471462056170	8.08696484679753
O	17.70685862605311	10.76193441640146	8.17389357562426
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O	9.50048354599216	16.02999562819090	7.90038905092352
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O	9.74835932790592	10.85745073543142	5.50157232351802
O	15.14666486454346	8.01077784499309	5.49064710225803
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O	12.29357889519114	5.37860990148659	5.44258406678513
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O	9.49644785805757	5.43062844725028	5.43426928128754
O	7.05993386682365	10.86139936897233	5.37986093788968
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H₂CuCe₃₉O₈₀ D4 (-954.665425 eV)

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Ce	13.55441629520609	9.40033728185404	14.93689481231089
Ce	10.95640099510043	6.85315532768409	14.87760504286842
Ce	13.75043476634937	12.15951113344345	12.29617962982844
Ce	8.36701912429320	12.31272491374967	12.29011030324931
Ce	8.27113165609641	6.75290169375507	12.26658467323253
Ce	13.62419024594806	6.66284877054760	12.26123195727995
Ce	5.82158575232143	9.57443852891460	12.25078126611423
Ce	11.18583292529267	14.79953579011404	12.22705234835830
Ce	16.20167641891101	9.36974851042159	12.21016291364326
Ce	10.98236844108436	9.49132153848905	12.15913859403093
Ce	10.90968396528852	4.09488375751820	12.09046051891179
Ce	13.64523577383511	14.83495006368093	9.53935284674110
Ce	16.25374448986471	12.09596504893599	9.52821380096714
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Ce	13.59284729527009	9.44604050918666	9.50654044770183
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Ce	3.42138066846113	9.59349216942319	9.48775949605866
Ce	10.93728843191244	6.84894358901463	9.49312732431693
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Ce	13.63208173289691	6.68345414904413	6.73080015001511
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Ce	8.37626222254887	12.33252326756013	6.72800077374331
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O	9.64463268204756	8.20526944177799	5.51049019907372
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O	12.52278482246556	13.55348392831239	5.44433824084130
O	15.13831010344972	10.81250200228609	5.47069342394779
O	9.73428048022161	13.60330855023318	5.44393809656067
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