

Supplementary Information

Unveiling Redox Mechanism of Cerium Doped in Nickel for Alkaline Hydrogen Evolution: A Theoretical Exploration

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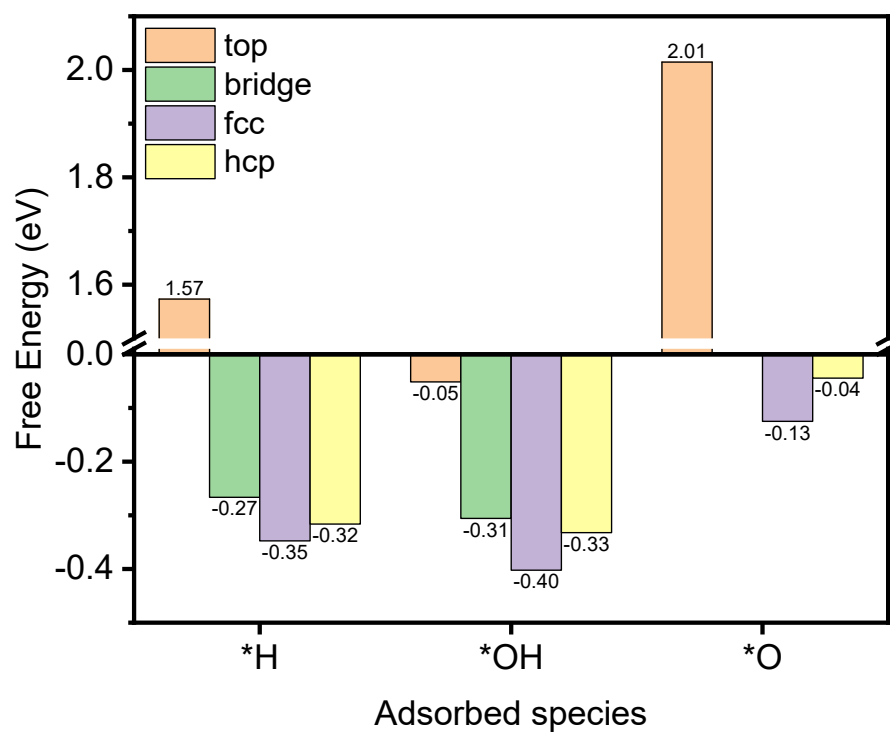


Fig S1. The Free energy of *H, *OH, and *O on the surface of Ce@Ni.

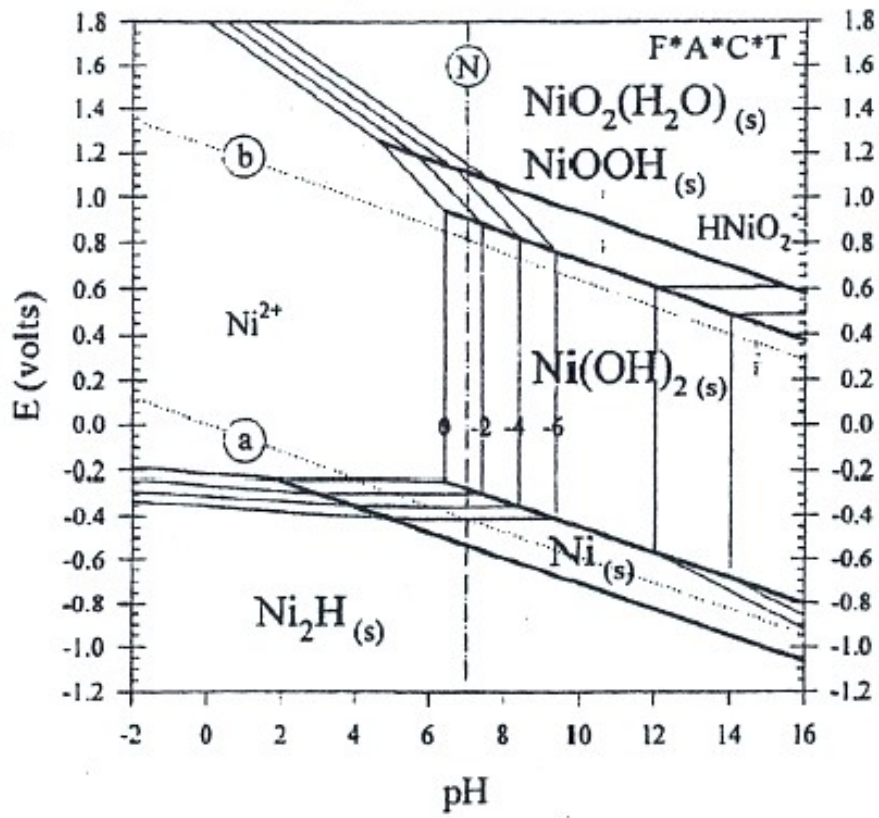


Fig S2. The Pourbaix Diagram for nickel (Ni) through experiment¹.

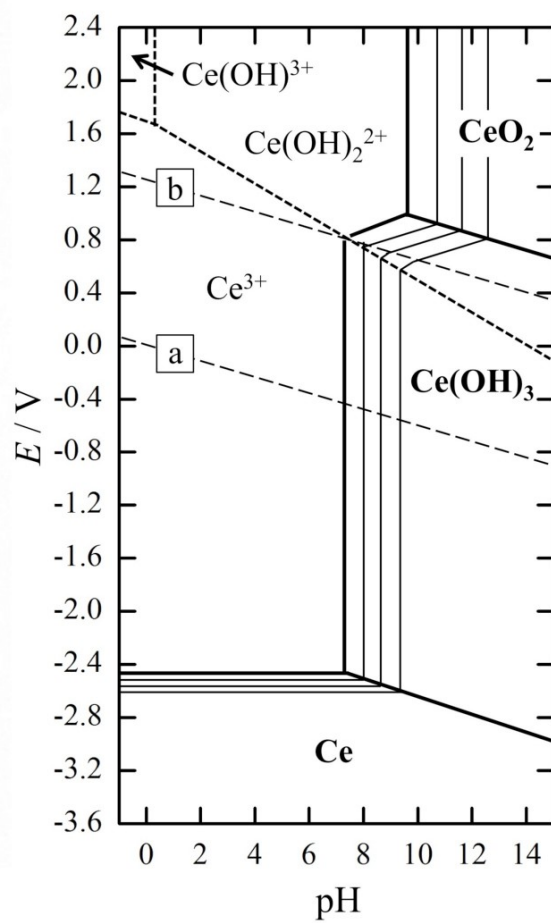


Fig S3. The Pourbaix Diagram for cerium (Ce) through experiment^{1,2}.

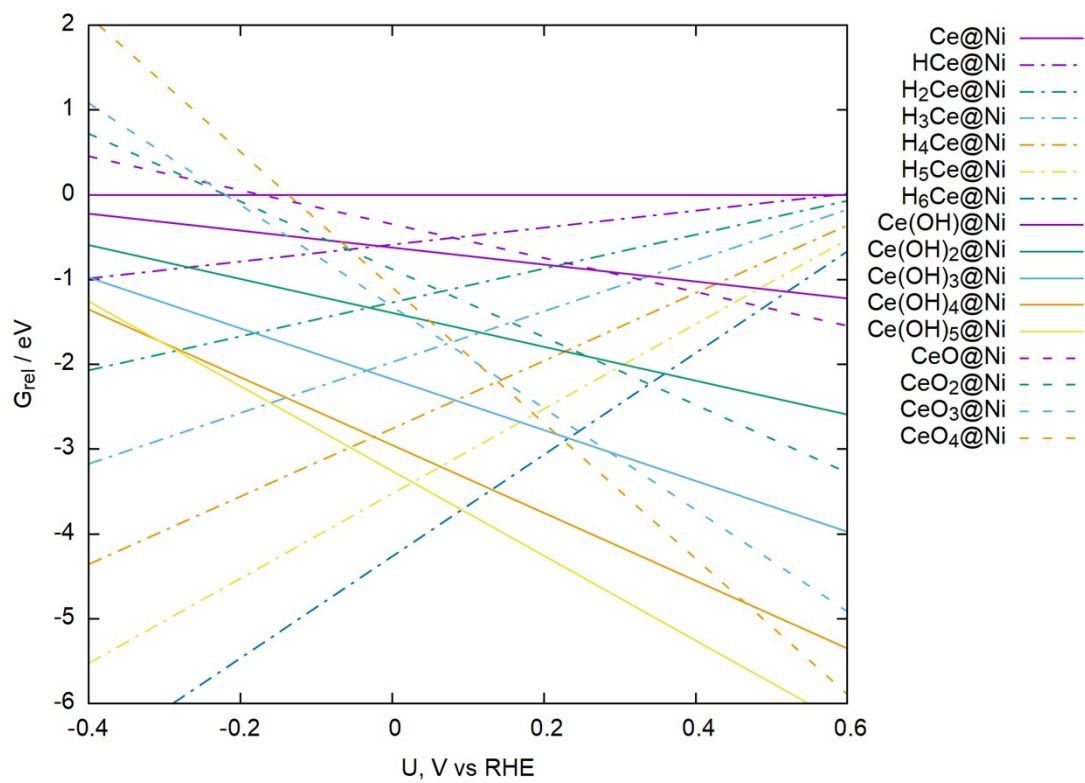


Fig S4. The Pourbaix diagram illustrating surface reactions of monodisperse Ce@Ni at pH = 0.

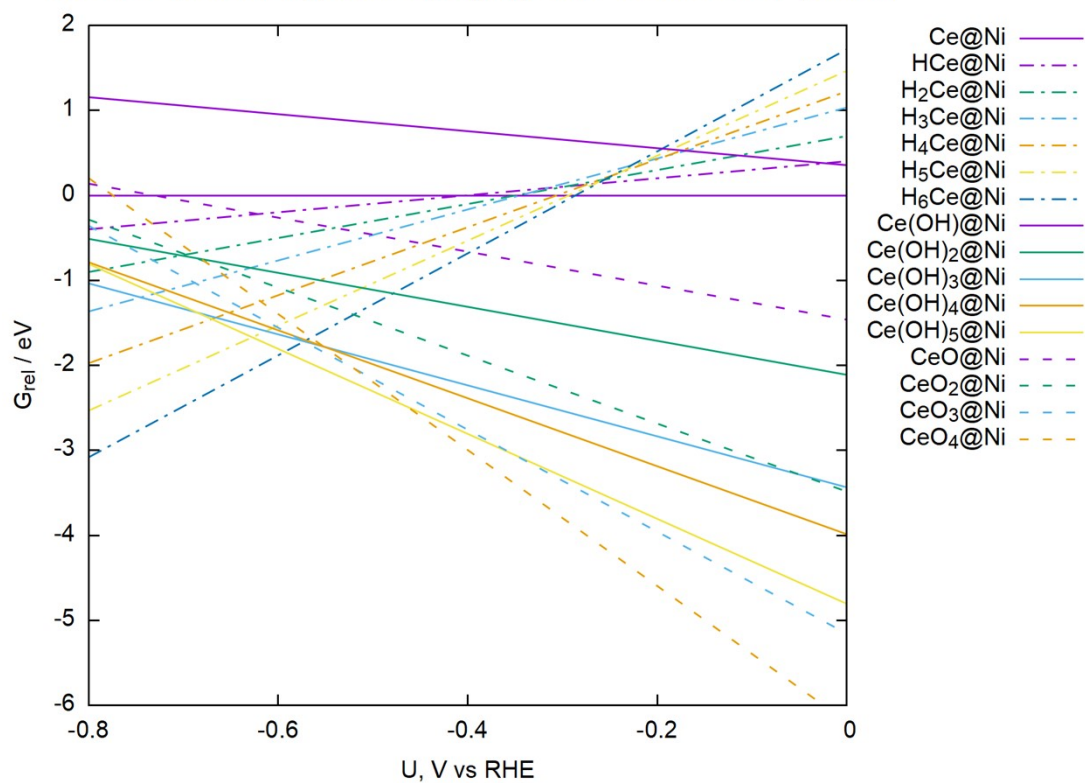


Fig S5. The Pourbaix diagram illustrating surface reactions of monodisperse Ce@Ni at pH = 14.

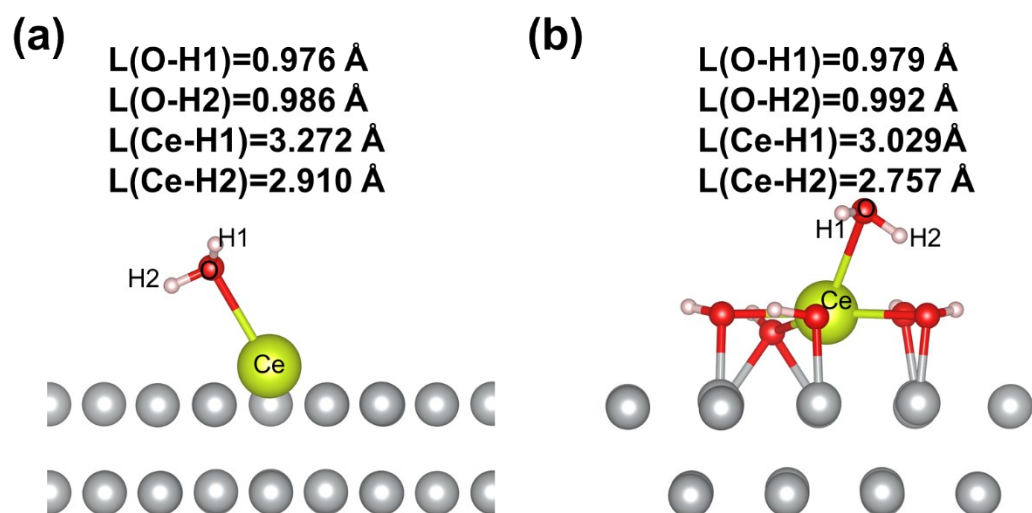


Fig S6. O-H bond length and Ce-H distance for adsorbed H₂O on (a) Ce@Ni and (b) Ce(OH)₅@Ni surfaces.

Table S1. The valence state and Bader charge of Ce in different clusters and crystals containing Ce.

	Species	Valence states	Bader charge
Ce	Cluster	0	0.000
HCe	Cluster	1	0.583
CeO	Cluster	2	1.103
H ₂ Ce	Cluster	2	1.269
Ce(OH) ₂	Cluster	2	1.369
HCe(OH)	Cluster	2	1.276
H ₂ Ce	Crystal	2	1.510
HCeO	Cluster	3	1.681
CeO(OH)	Cluster	3	1.782
H ₃ Ce	Cluster	3	1.852
H ₃ Ce	Crystal	3	1.790
H ₂ Ce(OH)	Cluster	3	1.867
CeO ₂	Cluster	4	1.969
HCe(OH) ₂	Cluster	4	1.984
H ₃ Ce(OH)	Cluster	4	2.043
HCeO(OH)	Cluster	4	2.095
Ce(OH) ₃	Cluster	3	2.097
Ce ₂ O ₃	Crystal	3	2.030
H ₂ Ce(OH) ₂	Cluster	4	2.159
CeO(OH) ₂	Cluster	4	2.207
Ce(OH) ₄	Cluster	4	2.369
CeO ₂	Crystal	4	2.450

Table S2. The calculated Bader charge of Ce in $H_xCe@Ni$, $CeO_y@Ni$, and $Ce(OH)_z@Ni$.

Species	Bader charge
$HCe@Ni$	1.293
$H_2Ce@Ni$	1.239
$H_3Ce@Ni$	1.515
$H_4Ce@Ni$	1.570
$H_5Ce@Ni$	1.575
$H_6Ce@Ni$	1.823
$CeO@Ni$	1.556
$CeO_2@Ni$	1.731
$CeO_3@Ni$	2.085
$CeO_4@Ni$	1.988
$Ce(OH)@Ni$	1.460
$Ce(OH)_2Ni$	1.911
$Ce(OH)_3Ni$	2.086
$Ce(OH)_4Ni$	2.058
$Ce(OH)_5Ni$	2.034

Calculation details

All the DFT calculations in this study were conducted using the Vienna Ab initio Simulation Package (VASP) code^{3–6}. The ion core potentials were modeled following the projector augmented wave (PAW)^{7,8} approach to describe the electron-core interaction. For electron exchange-correlation, the revised Perdew-Burke-Ernzerhof (RPBE) functional⁹ within the generalized-gradient approximation (GGA) range was applied.^{10,11} A plane wave basis set was used with a cutoff energy of 400 eV. Structural relaxations were performed until the forces on each of the atoms were below 0.02 eV Å⁻¹. The Ni(111) and Ce-doped Ni(111) surfaces were modeled with a 4 × 4-unit cell. During structural optimization and the self-consistent calculations, Monkhorst–Pack mesh k-space sampling grids¹² of 3 × 3 × 1 were used to sample the Brillouin zone (BZ). The Ni(111) and Ce doped Ni(111) surfaces were modeled as a four-layer slab, with the bottom two layers frozen. A vacuum layer of 20 Å was added perpendicular to the slab surface. Dipole corrections were included in the surface normal direction¹³. Usually, the adatom or dopant cannot change the lattice structure of the Ni(111), but causes local distortions. Thus, while optimizing the structures, the lattice structure is kept stable, and the positions of atoms are optimized. Activation barriers were calculated using the climbing image–nudged elastic band method¹⁴. The TS was identified when the forces on all the atoms and the tangent force on the highest-

energy image were below 0.02 eV Å⁻¹, and the tangent forces on the preceding images were opposite in sign to those on the images after the TS. The spin-polarization effect was considered in all cases. To better describe the dispersion interaction within water adsorption systems, vdW correction was considered by adopting the Grimme's D3 scheme^{15,16}. To treat the strongly correlated f orbitals of lanthanide metal atoms, the GGA + U scheme is adopted to describe the Coulomb and exchange corrections. The difference of the correlation energy U and the exchange energy J of the f electrons of is set to 6.3 for Ce.

The free energies (ΔG) are calculated using the following equation¹⁷:

$$\Delta G = \Delta E + \Delta ZPE + \Delta U(0 \rightarrow T) - T\Delta S$$

Where, ΔE , ΔZPE , $\Delta U(0 \rightarrow T)$, and $T\Delta S$ are the adsorption energy of adsorbed species on the given unit cell, the differences corresponding to the zero-point energy, the difference of the correction to the thermal energy, and the differences corresponding to the entropy (at 298.15 K), respectively. ΔZPE could be derived after frequency calculation by the following equation¹⁸:

$$ZPE = \frac{1}{2} \sum hv_i$$

Where h is the Planck constant, v_i are the computed vibrational frequencies.

The thermal energy correction is calculated by the following equation:

$$U(0 \rightarrow T) = \sum \frac{hv_i}{\exp(\beta hv_i) - 1}$$

The TS values of adsorbed species are calculated in the following equation^{17,19,20}.

$$TS^{vib}(T, v) = \sum kT \left(\frac{\beta hv_i}{\exp(\beta hv_i) - 1} - \ln(1 - \exp(-\beta hv_i)) \right)$$

Where $\beta = 1/kT$, $\{v_i\}$ are vibrational modes, k is the Boltzmann constant, and T is the temperature (which is set to 298 K in the present work), respectively. In the present study, the Gibbs free energy is calculated using VASPKIT²¹, and the frequencies below 50 cm^{-1} are approximately equal to 50 cm^{-1} during the calculations of the vibration contributions to the adsorbed molecular free energy correction.

Contributions from rotational and translational degrees of freedom of H_2 and H_2O molecules were also included in the ideal gas approximation at pressures of $P(\text{H}_2) = 101325 \text{ Pa}$ and $P(\text{H}_2\text{O}) = 3,534 \text{ Pa}$ in the Gibbs energy calculations. The former pressure is derived from the definition of the reversible hydrogen electrode potential, and the latter value is the vapor pressure of water at room temperature. At this pressure, the Gibbs energies of water molecules in the gas and liquid phases are equal, allowing us to estimate the Gibbs energies of liquid water molecules involved in the electrochemical reactions. The post-processing of VASP calculated data used VASPKIT²¹ and qvasp²² code.

Optimized structures

(IS: Initial state; TS: Transition state;FS: Final state; HM: The *H adsorbed at the M site.)

Ce@Ni

1.0

9.9672002792	0.0000000000	0.0000000000
-4.9836001396	8.6318486464	0.0000000000
0.0000000000	0.0000000000	26.1037006378

Ni Ce

63 1

Direct

0.000000000	0.000000000	0.000000000
0.000000000	0.250000000	0.000000000
0.000000000	0.500000000	0.000000000
0.000000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.250000000	0.000000000
0.250000000	0.500000000	0.000000000
0.250000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.250000000	0.000000000
0.500000000	0.500000000	0.000000000
0.500000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.250000000	0.000000000
0.750000000	0.500000000	0.000000000
0.750000000	0.750000000	0.000000000
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0.166667506	0.333332509	0.077940002
0.166667506	0.583332479	0.077940002
0.166667506	0.833332479	0.077940002
0.416667491	0.083332501	0.077940002
0.416667491	0.333332509	0.077940002
0.416667491	0.583332479	0.077940002
0.416667491	0.833332479	0.077940002
0.666667521	0.083332501	0.077940002
0.666667521	0.333332509	0.077940002
0.666667521	0.583332479	0.077940002
0.666667521	0.833332479	0.077940002
0.916667521	0.083332501	0.077940002
0.916667521	0.333332509	0.077940002
0.916667521	0.583332479	0.077940002
0.916667521	0.833332479	0.077940002
0.082747161	0.167090267	0.153983399
0.082754031	0.415772438	0.153991789
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0.083288267	0.916729093	0.154618293
0.333744884	0.167559206	0.153926566
0.335470974	0.417746782	0.155736312
0.333788097	0.666258156	0.153917164
0.333401263	0.916688800	0.154638365
0.584252536	0.167051002	0.153979778
0.582257688	0.417713046	0.155764371
0.582278311	0.664541066	0.155782029
0.584265411	0.917258978	0.153975204
0.833334029	0.166776150	0.154734299
0.832997203	0.415763527	0.153974757
0.832401633	0.666235447	0.153906286

0.832957983	0.917240560	0.153970495
0.249780297	0.999591589	0.231756240
0.246596560	0.244575173	0.230322599
0.246606797	0.502150893	0.230309740
0.249664202	0.750282764	0.231768414
0.500506580	0.000311701	0.232238710
0.497873485	0.244556293	0.230333909
0.497903585	0.753512621	0.230338961
0.749429405	0.998914301	0.231607124
0.749346614	0.250718802	0.231664971
0.755509794	0.502190590	0.230298519
0.755563319	0.753576040	0.230359927
0.999742568	0.000259217	0.232230499
0.001230556	0.250620574	0.231678322
0.999657691	0.499368191	0.232280761
0.000424936	0.750239611	0.231761694
0.500131309	0.500117064	0.277487397

HCe@Ni

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	H
63	1	1

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.082968466	0.167071953	0.187597677
0.000087127	0.000185432	0.284100771

0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334191948	0.167810917	0.188102901
0.249835014	0.998931110	0.283330232
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.584412217	0.166481242	0.187608272
0.501706600	0.001453152	0.283924669
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833501756	0.166543707	0.188575730
0.750137150	0.998855829	0.283079594
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0.167219996	0.333609998	0.094010003
0.083507016	0.415807545	0.187957183
0.001151355	0.249880627	0.283101171
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335474342	0.417827100	0.190459505
0.246703669	0.243882269	0.281922251
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582397640	0.417709947	0.190512195
0.498138934	0.242903367	0.281838089
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833475709	0.415559292	0.187620983
0.749818683	0.250152081	0.283222824
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001

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0.666239977	0.583119988	0.094740003
0.582230806	0.664600670	0.190465838
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832162857	0.665817678	0.188108370
0.756958425	0.501761556	0.281861842
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083405145	0.916547954	0.188543811
0.001108236	0.750210166	0.283372402
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333662987	0.916341126	0.188593268
0.249429673	0.750601232	0.284370214
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.584116757	0.916448176	0.187957138
0.499580503	0.754373312	0.283305436
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.833041430	0.917204797	0.187610880
0.756325424	0.753484607	0.281940401
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0.336913705 0.663076580 0.328235418

H₂Ce@Ni

1.0

10.0322999954	0.0000000000	0.0000000000
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0.0000000000	0.0000000000	21.1434993744

Ni	Ce	H
63	1	2

Direct

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0.999870658	0.001419648	0.283810467
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0.666630030	0.083310001	0.093910001
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0.501144826	0.001694885	0.283894449
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0.916689992	0.083310001	0.093910001
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0.167219996	0.333609998	0.094010003
0.082928464	0.415806890	0.187786505

0.000516530	0.249830112	0.282978475
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0.245118514	0.242973492	0.281599909
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0.666390002	0.333609998	0.094010003
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0.750000000	0.250000000	0.000000000
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0.748799384	0.249793470	0.283058554
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0.998184025	0.496683538	0.283306360
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0.333600342	0.665910065	0.187889740
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0.582057714	0.664460063	0.190508902
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0.166669995	0.833329976	0.094530001

0.082778782	0.916145325	0.188519955
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0.832125247	0.916211128	0.187842861
0.754411697	0.754097342	0.283183962
0.497234583	0.495460182	0.339901447
0.335590482	0.663636386	0.327697158
0.827318907	0.663625360	0.327692538

H₃Ce@Ni

1.0

10.032299954	0.000000000	0.000000000
-5.0161499977	8.6882266544	0.000000000
0.000000000	0.000000000	21.1434993744

Ni	Ce	H
63	1	3

Direct

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0.997713625	0.000044582	0.283302724

0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
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0.500000000	0.000000000	0.000000000
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0.502234936	0.000029911	0.283331394
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.832995057	0.165917948	0.188334495
0.749013126	0.997877300	0.282736480
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
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0.750000000	0.250000000	0.000000000
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0.749056816	0.249193266	0.282721847
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001

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0.333420396	0.665602326	0.187870890
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0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.581990719	0.663859844	0.190282017
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832120180	0.665504098	0.187900856
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0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083099253	0.915910184	0.188550577
0.001583978	0.750011802	0.284051448
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.332804292	0.915977955	0.188578278
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0.666390002	0.832780004	0.094010003
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0.498873651	0.752818525	0.282904834
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
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0.754161298	0.752850354	0.282893717
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0.335669905	0.662543952	0.327344358
0.335297406	0.170814797	0.327373981
0.826834917	0.662237346	0.327349126

H₄Ce@Ni

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	H
63	1	4

Direct

0.0000000000	0.0000000000	0.0000000000
0.166779995	0.083520003	0.094250001
0.082892813	0.167266011	0.187760353
0.997865856	0.001291856	0.283300817
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334321648	0.168033004	0.188190117
0.248287201	0.997815490	0.283952504
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.583330274	0.167262912	0.187856823
0.501343250	0.999773681	0.282980502
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.832491636	0.167073414	0.188460872
0.748959422	0.999098539	0.282654017
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003

0.082638763	0.415985435	0.187624216
0.000168411	0.250448287	0.282570392
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335309356	0.417762160	0.190385714
0.245331779	0.245476052	0.282810122
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582042217	0.417634100	0.190270290
0.497651339	0.244663492	0.284381837
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.832320690	0.416228771	0.187826097
0.750205576	0.249244794	0.283608675
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082897522	0.666766882	0.188468739
0.999610662	0.498154074	0.282945782
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333529294	0.666246474	0.187708274
0.244561702	0.500818253	0.282604545
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582099080	0.664484262	0.190406919
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.831911802	0.665496707	0.188167706
0.754645824	0.501689315	0.284350693
0.000000000	0.750000000	0.000000000

0.166669995	0.833329976	0.094530001
0.082870603	0.916841209	0.188502923
0.001450213	0.751066923	0.283918381
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.332889706	0.916893244	0.188481808
0.248063847	0.751604438	0.284070164
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.583757460	0.917125940	0.187578201
0.498886317	0.754965901	0.282630503
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832480490	0.916778147	0.187751204
0.753729403	0.753795266	0.282829195
0.496732473	0.502368152	0.341543555
0.335335046	0.663932323	0.327084333
0.333729535	0.171640024	0.327821553
0.827668905	0.665391505	0.327820212
0.662607908	0.336616188	0.327214867

H₅Ce@Ni

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	H
63	1	5

Direct

0.000000000	0.000000000	0.000000000
-------------	-------------	-------------

0.166779995	0.083520003	0.094250001
0.083757699	0.167493984	0.187764660
0.998173177	0.000163290	0.282876015
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334096283	0.168321192	0.188404709
0.249332130	0.998651683	0.283743441
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.583730638	0.167486608	0.187792331
0.501976550	0.000169248	0.282860518
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833852291	0.167643517	0.188579887
0.749766767	0.999508262	0.282490820
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.083457410	0.416345477	0.187657714
0.998953521	0.249824628	0.283407837
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335532278	0.417882770	0.190146402
0.247229025	0.245915949	0.284220904
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582317591	0.417854488	0.190110803
0.498491824	0.245836064	0.284199834
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.832929790	0.416347504	0.187652230

0.750823140	0.249747366	0.283374429
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.083425306	0.666805208	0.188395098
0.999625325	0.499060720	0.282634616
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333453327	0.665641427	0.188094020
0.246483549	0.502235055	0.284129947
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582284451	0.664583147	0.190343961
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832126498	0.665618896	0.188055724
0.755954504	0.502300620	0.284081936
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083502799	0.917106211	0.188358501
0.003186072	0.751868188	0.283880740
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333629042	0.917113066	0.188371360
0.248774037	0.751898468	0.283897370
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.584067523	0.917126358	0.187619284
0.499650687	0.754668295	0.282647133
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001

0.833022892	0.917123199	0.187633172
0.755315721	0.754806638	0.282637924
0.503028691	0.505515873	0.342178673
0.337149709	0.666324496	0.327614367
0.335866690	0.171652198	0.328299344
0.829188347	0.666148484	0.327616423
0.172927812	0.337032706	0.326928049
0.663991451	0.336939484	0.326863289

H₆Ce@Ni

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	H
63	1	6

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.083000861	0.167356312	0.187653244
0.998782039	0.000792956	0.282372773
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.333525628	0.168161795	0.188375026
0.248268038	0.997751772	0.283771813
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.583363593	0.167381108	0.187656015
0.500458300	0.001023545	0.282311291
0.750000000	0.000000000	0.000000000

0.916689992	0.083310001	0.093910001
0.832943857	0.166784391	0.188613608
0.750012517	0.001588805	0.283252805
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.083005756	0.416250676	0.187677190
0.997922003	0.249509573	0.283246905
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335232526	0.417970568	0.190187171
0.245904893	0.245286003	0.284079760
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.581641495	0.418075651	0.190065280
0.497651815	0.245419890	0.283946902
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.832392991	0.416388363	0.187663794
0.749916732	0.249599516	0.283153296
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082841523	0.666572988	0.188319683
0.998611808	0.499353170	0.282395065
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333770484	0.665973723	0.188353270
0.245794430	0.502180815	0.284123331
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.581782341	0.664526343	0.190199494

0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.831709743	0.666262627	0.188394234
0.754103899	0.502016902	0.283972830
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.082893662	0.916952372	0.188191965
0.001671249	0.751437247	0.283770025
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333186358	0.916909218	0.188308015
0.247983605	0.751887202	0.283840805
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.583424032	0.916756511	0.187655345
0.497627825	0.753851175	0.284058988
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832396388	0.916771889	0.187682748
0.754130661	0.753616154	0.284067392
0.499045968	0.500122845	0.343129814
0.334788799	0.664582849	0.328184247
0.827416480	0.664430916	0.328207463
0.334969014	0.171799079	0.328165412
0.171452120	0.336475283	0.326744556
0.662981033	0.828105927	0.326787502
0.662971437	0.336513966	0.326766402

Ce(OH)@Ni

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	1	1

Direct

0.0000000000	0.0000000000	0.0000000000
0.166779995	0.083520003	0.094250001
0.082242712	0.166887775	0.187664032
0.997022867	0.998007834	0.283979803
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.333170056	0.166751876	0.187703535
0.247997731	0.996825755	0.283319682
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.583862960	0.167178601	0.187693477
0.499849498	0.000272799	0.284028888
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833126843	0.166933253	0.188170284
0.748426437	0.999315619	0.282864600
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.085926756	0.417267472	0.189554885
0.996186852	0.246757269	0.282720447
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335126638	0.417703718	0.191519558
0.243425444	0.238906175	0.281105906

0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.581671417	0.416556597	0.189851210
0.494938880	0.242363885	0.281939954
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833047152	0.415606707	0.187430143
0.748331308	0.250134856	0.283006310
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082510158	0.665841818	0.188195467
0.996159494	0.498976052	0.283288330
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.332462788	0.664616644	0.188733011
0.241429612	0.498755187	0.287070274
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.581476450	0.663912892	0.190054402
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.831444204	0.666223884	0.188271865
0.754019499	0.500770211	0.281945288
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.082433008	0.916191041	0.188388780
0.998548448	0.749446332	0.283343464
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333737403	0.916416824	0.188289478

0.247565880	0.751526892	0.282513380
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.583842039	0.917392135	0.187273830
0.499763697	0.756817281	0.280739784
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832114816	0.916571021	0.187752753
0.751903534	0.752309561	0.282793641
0.501561403	0.497965306	0.330282778
0.307483345	0.516047835	0.379969209
0.305393547	0.605372548	0.396701187

Ce(OH)₂@Ni

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	2	2

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.082085080	0.166599602	0.186997682
0.001069052	0.000944822	0.283081234
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334500700	0.167693734	0.187804356
0.250705034	0.000472061	0.283609450
0.500000000	0.000000000	0.000000000

0.666630030	0.083310001	0.093910001
0.584459901	0.167537704	0.187480465
0.500377715	0.002326973	0.283496559
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833797574	0.166473597	0.187977076
0.749150574	0.001811632	0.282541275
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.086171538	0.416972429	0.189052001
0.998455524	0.247801840	0.282412976
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335970193	0.418658853	0.191440970
0.244758368	0.240445048	0.280260921
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.581828117	0.418362558	0.190278664
0.498136401	0.247160509	0.282078624
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833921671	0.415544748	0.186815992
0.749137700	0.250533581	0.282894731
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082981221	0.665794313	0.187827602
0.998324811	0.499990553	0.282807738
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.332629144	0.664605498	0.188590452

0.245428056	0.500923276	0.286327243
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582178473	0.663950205	0.191704020
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.831954122	0.667161345	0.188701287
0.756576240	0.498938352	0.279891014
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083261415	0.917136192	0.188104540
0.003338893	0.751162589	0.282027304
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.334048450	0.917253494	0.188033059
0.249102518	0.752943814	0.282125682
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.584140062	0.917467237	0.187059358
0.498288304	0.758171439	0.280152410
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.830834448	0.913509846	0.189463019
0.753797710	0.753954172	0.287025452
0.497291803	0.496482641	0.357143283
0.279200941	0.511278272	0.381287605
0.735519350	0.706975341	0.381268471
0.838693619	0.729734838	0.393179446
0.262006640	0.594289541	0.394916534

Ce(OH)₃@Ni

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	3	3

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.081599690	0.166880444	0.186841249
0.002232024	0.002971531	0.283293635
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.333892614	0.167856097	0.187398598
0.251198351	0.002026819	0.283634514
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.585194767	0.166758478	0.186855793
0.500878215	0.002849799	0.283323139
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833571494	0.167161852	0.188103095
0.751809478	0.003388541	0.282925457
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.086560264	0.417629600	0.189268038
0.001038059	0.250212848	0.283033490
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003

0.336748362	0.418556929	0.190486312
0.246120647	0.242851391	0.279913485
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.581936657	0.418648779	0.190520793
0.496855348	0.242950648	0.279883265
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.831113875	0.417641252	0.189214587
0.749355972	0.250215441	0.282975793
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082889013	0.665544093	0.187302694
0.000689051	0.500893593	0.282886207
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334303737	0.666156054	0.188446894
0.246846721	0.499393463	0.284756929
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.581950068	0.663890421	0.191351131
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832034349	0.666247606	0.188367769
0.753333747	0.499714047	0.284670830
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083513409	0.917943895	0.187769696
0.007748341	0.754926443	0.280813158
0.250000000	0.750000000	0.000000000

0.416740000	0.833220005	0.094250001
0.334416032	0.917804897	0.187814921
0.247817010	0.754706323	0.280962229
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.582547426	0.913583517	0.189426586
0.500338852	0.756460190	0.284929484
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.831086516	0.913640976	0.189383179
0.756802142	0.756954253	0.284825265
0.463249624	0.419604331	0.382808208
0.391132981	0.610728025	0.360756189
0.723644316	0.613848329	0.360654294
0.438722730	0.348471940	0.480442584
0.818953872	0.661264181	0.385010242
0.424313009	0.299817920	0.521329403
0.343433589	0.658022702	0.385299683

Ce(OH)₄@Ni

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	4	4

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.087377116	0.168503419	0.188646451

0.999681950	0.000165203	0.282027483
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.336311609	0.170291469	0.189972788
0.248964936	0.000026268	0.282147825
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.583740652	0.167342439	0.186854050
0.499397218	0.002054346	0.281812996
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.835252345	0.164630711	0.186539650
0.749900401	0.000364920	0.282070607
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.086348847	0.417051196	0.188553691
0.999642730	0.250196546	0.281983316
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.336400181	0.418820411	0.192385495
0.245209470	0.246697158	0.286734432
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.581409872	0.418638647	0.190263718
0.502819240	0.246392608	0.283432454
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.832661331	0.416306645	0.186823860
0.755617380	0.244547531	0.278346151
0.000000000	0.500000000	0.000000000

0.166779995	0.583260000	0.094250001
0.081135049	0.665631711	0.186749980
0.997938633	0.500636458	0.281833261
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333349496	0.666571140	0.187589824
0.242356569	0.507330954	0.283752859
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.581145406	0.663650751	0.192365408
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.829717636	0.663681924	0.189985603
0.753582656	0.497263849	0.283416510
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.082923740	0.917001009	0.187719598
0.000122385	0.751054704	0.282146692
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.334428191	0.918914974	0.186771810
0.242895171	0.757249296	0.278740525
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.583009958	0.913576663	0.188584730
0.492523819	0.757518530	0.283714920
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.831538081	0.912573040	0.188676924
0.753200054	0.754730582	0.286739767

0.498430759	0.501359344	0.367475450
0.363243163	0.636577308	0.364133835
0.738698959	0.729001760	0.381208688
0.270601928	0.261352241	0.381265074
0.635118246	0.365360409	0.363494754
0.310838014	0.688751757	0.380760550
0.241219983	0.156618997	0.393455118
0.687811494	0.313253403	0.379912615
0.843094707	0.756691992	0.393241793

Ce(OH)₅@Ni

1.0

10.032299954	0.000000000	0.000000000
-5.0161499977	8.6882266544	0.000000000
0.000000000	0.000000000	21.1434993744

Ni	Ce	O	H
63	1	5	5

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.084717974	0.167491198	0.187564775
0.003179562	0.003610583	0.281984031
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334118128	0.169433281	0.189659685
0.248074040	0.996858358	0.281241417
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.581292033	0.168693423	0.188651085
0.499249250	0.999415278	0.281942576

0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.831340671	0.165581957	0.186196551
0.751213253	0.003721417	0.280515254
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.084707655	0.417147905	0.187540382
0.991665423	0.245770603	0.279723823
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.337474883	0.418643892	0.189705461
0.247975841	0.248782724	0.283682495
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582480669	0.418318272	0.193118751
0.498292536	0.242212400	0.287721574
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.831878722	0.416948646	0.187609926
0.751177728	0.247313127	0.280528069
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082605824	0.665924191	0.187419251
0.003136818	0.499398321	0.281944603
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334038764	0.664401889	0.189636424
0.247900128	0.498712718	0.283735871
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003

0.582342207	0.663907230	0.193125591
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.830781400	0.665320992	0.189436033
0.760948181	0.501111686	0.284548104
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.082538292	0.916538537	0.187426522
0.005770641	0.752786279	0.281823516
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333847344	0.916869581	0.187239766
0.248102546	0.750796676	0.281268388
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.581192851	0.912432849	0.188653305
0.498323292	0.755667150	0.287714750
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.831823528	0.914715052	0.187634289
0.760957897	0.759741962	0.284621030
0.542010665	0.520858645	0.378360271
0.769982755	0.493726045	0.377135485
0.258525193	0.378935009	0.360851169
0.769807398	0.775090337	0.377336115
0.472288907	0.247995764	0.380524635
0.471346289	0.722446144	0.380584836
0.742613077	0.387367547	0.386216223
0.742265522	0.853960156	0.386418790
0.158510864	0.328650445	0.381654024

0.368783385	0.162681490	0.388815224
0.366928577	0.702085614	0.388532519

CeO@Ni

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O
63	1	1

Direct

0.0000000000	0.0000000000	0.0000000000
0.166779995	0.083520003	0.094250001
0.086468235	0.169206500	0.189096257
0.998726189	0.000483748	0.282990545
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334106356	0.168353260	0.188551173
0.246592298	0.993359149	0.281997442
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.582724035	0.169157431	0.189117432
0.501572907	0.000129209	0.282998800
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833948553	0.167760760	0.188163415
0.750453472	0.001214640	0.282881677
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.083359927	0.416581571	0.187655017

0.000370641	0.251676828	0.282723159
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335988432	0.418139458	0.190828890
0.242996007	0.245251641	0.285649568
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582304478	0.418089777	0.190846935
0.501660407	0.244608939	0.285573423
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833319306	0.416433245	0.187556952
0.751338899	0.251610786	0.282709420
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.083462827	0.667055964	0.188482985
0.000418132	0.500319898	0.284063011
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333679855	0.666473210	0.187708005
0.247888848	0.504887760	0.282097846
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582351208	0.664828897	0.189994067
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832624555	0.666545570	0.187673494
0.757957578	0.504707932	0.281916648
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001

0.083029628	0.917406559	0.188097239
0.000893158	0.750738204	0.283379227
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.334323734	0.917427778	0.188097164
0.249703765	0.750583649	0.283404440
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.585207582	0.918572128	0.187140524
0.497819930	0.755824268	0.281199485
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.833457887	0.918756127	0.187136844
0.757682562	0.756314993	0.281387120
0.515801907	0.525628567	0.336568445
0.393308997	0.287700921	0.351171941

CeO₂@Ni

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O
63	1	2

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.086607456	0.168933570	0.189135164
0.998736620	0.999572396	0.283067346
0.250000000	0.000000000	0.000000000

0.416740000	0.083520003	0.094250001
0.334513873	0.168229684	0.188477457
0.246663153	0.993454993	0.281942546
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.583407640	0.168485686	0.188505545
0.502529621	0.001122879	0.282018840
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.834011912	0.166852504	0.187981740
0.751358449	0.000000000	0.282576412
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.086499661	0.417520255	0.189086333
0.999667525	0.249662504	0.282557875
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335242718	0.417517513	0.191457599
0.245421141	0.243861690	0.286605477
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582083046	0.417754412	0.190500826
0.503218472	0.246189341	0.285222322
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833622515	0.415163845	0.186848968
0.751370847	0.251214683	0.282553226
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.083241016	0.666090906	0.188073233

0.998631716	0.498901844	0.282986045
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334437877	0.666223645	0.188519120
0.245232925	0.501165390	0.286540717
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582042217	0.664256513	0.190521389
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832604766	0.666280329	0.187541693
0.759127975	0.504259527	0.280359298
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083191827	0.917029381	0.188013673
0.999379277	0.749601245	0.283660620
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.334428042	0.917149127	0.187856719
0.246824831	0.753028631	0.281955153
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.583398163	0.914776385	0.188500211
0.503085792	0.756605387	0.285291940
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.833703756	0.918424606	0.186840460
0.759143651	0.754733980	0.280405611
0.552612245	0.525887311	0.370978326
0.393443793	0.611570239	0.350035071

0.393794656 0.281587809 0.350060880

CeO₃@Ni

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni Ce O

63 1 3

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.085799694	0.168200195	0.188068300
0.999009728	0.001681082	0.281619608
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334333450	0.168005899	0.188102618
0.248102129	0.995413065	0.283064574
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.583384871	0.168181419	0.188041374
0.503189743	0.000898562	0.281601727
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833485246	0.166598916	0.187642291
0.750878513	0.000765211	0.281853974
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.086016446	0.416923612	0.188189432
0.999520481	0.249319866	0.281891167

0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335809708	0.417722732	0.191060245
0.243558198	0.243406922	0.284869701
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582600176	0.417470038	0.191143721
0.501190722	0.243437514	0.284690827
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.832000792	0.416747004	0.188010931
0.750932872	0.249229446	0.281879455
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.083068967	0.666199446	0.188155577
0.999427795	0.496897608	0.281542182
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334155679	0.665900588	0.188113421
0.243822649	0.499165773	0.285071045
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582414448	0.664353430	0.191089422
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832126558	0.665797353	0.187998965
0.756689370	0.498764902	0.284540355
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083639324	0.916333854	0.188376099

0.004090831	0.751851082	0.283389628
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.334026426	0.916991830	0.188045546
0.247664094	0.752547443	0.282281250
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.583177626	0.914162338	0.188216209
0.501160264	0.756626844	0.285086125
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.831988633	0.914675832	0.188022748
0.756751060	0.756985903	0.284610063
0.506041646	0.498747349	0.379118532
0.380435467	0.620027184	0.350166291
0.755040109	0.626941919	0.349990338
0.376077354	0.250234187	0.350182444

CeO₄@Ni

1.0

10.032299954	0.000000000	0.000000000
-5.0161499977	8.6882266544	0.000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O
63	1	4

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.085025117	0.167829886	0.187605605
0.998336971	0.003930429	0.280678600

0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334603310	0.167445257	0.188895524
0.244524255	0.991454720	0.282232523
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.583031714	0.167503089	0.188988611
0.496911258	0.990496457	0.281205118
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.832356691	0.167739257	0.188605785
0.749292791	0.000742101	0.281535506
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.087256342	0.417610258	0.188378483
0.999515891	0.249676064	0.281663686
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335578501	0.416635185	0.190622106
0.240540370	0.241875365	0.284619689
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582356036	0.415806890	0.190741464
0.491697162	0.235580415	0.288062155
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.832798481	0.415205300	0.187651753
0.751915872	0.245892152	0.286676288
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001

0.081550471	0.667414606	0.188961700
0.008930711	0.499265611	0.281231761
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333809942	0.665407479	0.188783258
0.251125574	0.499801189	0.287243187
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582183242	0.663483977	0.190084189
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832166314	0.664978921	0.187757090
0.761865854	0.501903713	0.282562792
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.082021505	0.914440811	0.188690796
0.998427331	0.750155389	0.289662629
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333250999	0.916530371	0.187624797
0.245477557	0.751413047	0.282003641
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.582561016	0.913219929	0.188152313
0.503138304	0.751690328	0.286262423
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.831981242	0.916243434	0.186876014
0.755228996	0.759348035	0.281601906
0.551786900	0.494208425	0.380304903

0.409790725	0.598017395	0.347785681
0.813345194	0.668387294	0.345562547
0.362708360	0.257421494	0.352654725
0.671250880	0.333915859	0.342670500

H₆Ce@Ni-H_{Ni}

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	H
63	1	7

Direct

0.0000000000	0.0000000000	0.0000000000
0.166779995	0.083520003	0.094250001
0.083869867	0.168243140	0.187760383
0.000236824	0.001645507	0.282476485
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.333357602	0.168128833	0.188329473
0.248679951	0.998322964	0.283740312
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.583257556	0.166887373	0.187432811
0.500053108	0.998962402	0.282177001
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833731890	0.167308062	0.188458875
0.751737773	0.002394314	0.283090442
0.000000000	0.250000000	0.000000000

0.167219996	0.333609998	0.094010003
0.084228463	0.417327434	0.188262418
0.998132586	0.248919666	0.283476233
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335287571	0.419421196	0.191352710
0.247811735	0.246720418	0.284128517
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.581277311	0.417546898	0.189811587
0.497742057	0.243911028	0.283770621
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.831375301	0.415551394	0.187040821
0.749379694	0.248241097	0.282684177
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082863070	0.666100085	0.188111484
0.992234826	0.496061087	0.281802863
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334440440	0.666420639	0.188880488
0.244714290	0.503851473	0.288082272
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582623363	0.664311469	0.189816535
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.831979454	0.665974498	0.188195109
0.752389789	0.500922382	0.283035994

0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083066888	0.916927576	0.188262492
0.001743464	0.751542449	0.283750355
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.332677782	0.916122735	0.188463122
0.247905478	0.752540648	0.284232944
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.583809674	0.916632533	0.187654004
0.502732635	0.754797637	0.283275485
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.833017349	0.916998029	0.187619925
0.756651640	0.754005373	0.283926338
0.503662944	0.498182356	0.343924910
0.369849056	0.652227163	0.333081603
0.828278244	0.663361728	0.327840745
0.335687399	0.171409875	0.328193903
0.173888713	0.334661126	0.327625930
0.667300880	0.829783499	0.326389045
0.664127588	0.335296720	0.326091141
0.144084111	0.581872046	0.325666040

H₆Ce@Ni-H_{Ce}

1.0

10.0322999954	0.000000000	0.000000000
-5.0161499977	8.6882266544	0.000000000
0.000000000	0.000000000	21.1434993744

Ni Ce H
63 1 7

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.083337732	0.167217612	0.187745243
0.999072492	0.000417165	0.282716244
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.333913147	0.168218270	0.188430443
0.249073178	0.998669505	0.283802867
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.583573520	0.167195708	0.187747195
0.500803232	0.000775370	0.282811999
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833286405	0.166749120	0.188861102
0.750078857	0.000867766	0.283367366
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.083317243	0.416326284	0.187776685
0.998966336	0.249699101	0.283351302
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335561454	0.417939216	0.189941272
0.247897208	0.246691465	0.283846557
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.581922889	0.417914957	0.189826205

0.498199195	0.246927798	0.283742517
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.832645178	0.416364789	0.187772498
0.749781191	0.249761492	0.283338010
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.083167523	0.666587710	0.188365981
0.998973548	0.498911351	0.282724023
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333948344	0.665870428	0.188418165
0.247926772	0.501637042	0.283829600
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.581952393	0.664339066	0.189933404
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.831729531	0.666021347	0.188469470
0.752965510	0.501737356	0.283728421
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083189026	0.916660130	0.188411593
0.001136650	0.750725210	0.283798248
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333237469	0.916669726	0.188404977
0.248991594	0.750712752	0.283816278
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003

0.583510995	0.916570485	0.187791243
0.498071283	0.751895487	0.283846825
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832647026	0.916439176	0.187770680
0.752985179	0.751993060	0.283813179
0.499074429	0.500142694	0.360871792
0.336902589	0.662820220	0.328290343
0.824970782	0.662756205	0.328275949
0.337032735	0.174726367	0.328240544
0.174600393	0.337482452	0.326850742
0.662088752	0.825191855	0.326835066
0.662227690	0.337804705	0.326828629
0.497853220	0.500472009	0.461001724

H₆Ce@Ni-H₂O

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	H	O
63	1	8	1

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.083306499	0.167247504	0.187662736
0.999543846	0.000898354	0.282554835
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.333955497	0.168172926	0.188429773

0.248636171	0.997537732	0.283846289
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.583871484	0.167334795	0.187649921
0.501185536	0.001035419	0.282567978
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833293319	0.166739985	0.188791648
0.750723362	0.001625681	0.283389002
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.083238967	0.416219324	0.187677488
0.998653054	0.249516219	0.283364803
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335465878	0.417843223	0.190240741
0.246021628	0.244524106	0.284158885
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582232714	0.417858899	0.190214172
0.498185068	0.244580761	0.284041286
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.832765460	0.416275918	0.187670767
0.750581980	0.249532908	0.283336967
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.083219886	0.666530609	0.188292086
0.999119759	0.498925030	0.282617867
0.250000000	0.500000000	0.000000000

0.416880012	0.583119988	0.094740003
0.334063053	0.665926218	0.188408211
0.245737582	0.502067327	0.284229159
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582221627	0.664581895	0.190259278
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.831817746	0.666074872	0.188448712
0.755639732	0.502120316	0.284207135
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083229154	0.916814566	0.188293010
0.002743122	0.751570106	0.283869863
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333537370	0.916795611	0.188300818
0.248404175	0.751662374	0.283854783
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.583910584	0.916838109	0.187642157
0.498104692	0.754572988	0.284058839
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832821131	0.916740060	0.187658221
0.756019890	0.754416049	0.284181416
0.499651849	0.500717342	0.342940181
0.335169852	0.664974272	0.328281343
0.829379976	0.664864779	0.328420669
0.335388184	0.170905560	0.328235984

0.172107562	0.336327314	0.326920897
0.663889110	0.828114867	0.326776356
0.663859665	0.336316675	0.326832771
0.399251729	0.439383090	0.496060282
0.578091145	0.516144037	0.498376667
0.492265433	0.495858252	0.470835209

H₆Ce@Ni-OH

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	H	O
63	1	7	1

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.083413079	0.167332262	0.187673390
0.999556005	0.000836002	0.282521307
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334019750	0.168148413	0.188360676
0.248893738	0.997951388	0.283694983
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.583618283	0.167160481	0.187762544
0.501122952	0.000122559	0.282660425
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833349586	0.166681886	0.188837618

0.750445426	0.000846569	0.283355147
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.083385155	0.416311234	0.187698260
0.998929143	0.249526054	0.283339500
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335747629	0.418011606	0.189843938
0.248152882	0.246595711	0.283851951
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.581981897	0.417686611	0.189836219
0.497927636	0.245865539	0.283977747
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.832589924	0.416229993	0.187724248
0.750188947	0.249386057	0.283335209
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.083139315	0.666384399	0.188333973
0.998849750	0.498753905	0.282619268
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334085673	0.665927708	0.188426584
0.247840017	0.501496434	0.283959538
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582249105	0.664205849	0.189852312
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001

0.831736028	0.665923536	0.188434929
0.752932489	0.501466155	0.283947945
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083178096	0.916718483	0.188297510
0.001641962	0.750844896	0.283761084
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333425134	0.916666389	0.188362539
0.248798326	0.750742674	0.283776939
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.583706498	0.916475534	0.187764227
0.498235196	0.751335859	0.284044653
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832715333	0.916467786	0.187753737
0.753841221	0.752270162	0.284043580
0.499535948	0.499514937	0.350714445
0.335688174	0.663589239	0.328116536
0.827267230	0.663820565	0.328197151
0.335357636	0.172049984	0.328119457
0.173165575	0.336590111	0.326808274
0.663427830	0.826563418	0.326890528
0.663142383	0.336591989	0.326766819
0.481451929	0.491388589	0.496581972
0.489813864	0.493995309	0.450897902

Ce(OH)₅@Ni-H_{Ni}

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	5	6

Direct

0.0000000000	0.0000000000	0.0000000000
0.166779995	0.083520003	0.094250001
0.085275181	0.168211773	0.187559888
0.004131836	0.004843484	0.281924158
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334342688	0.169957787	0.189596742
0.248866379	0.998723388	0.281101495
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.581606388	0.169106543	0.188497230
0.499796480	0.000423530	0.281615168
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.832062185	0.166272700	0.186124384
0.751745641	0.004489173	0.280419528
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.085454166	0.417885333	0.187631622
0.992099822	0.245752186	0.279900253
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.337847084	0.419847190	0.190008879
0.248145655	0.249895245	0.283629268

0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582688034	0.418588012	0.192869872
0.499176979	0.243276700	0.287412047
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.832712948	0.417317033	0.187499762
0.751498818	0.247634381	0.280217022
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082861170	0.666171849	0.187366411
0.001012454	0.498536021	0.282468975
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334657520	0.665343344	0.189646885
0.249038562	0.499131620	0.284654856
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582971752	0.664543211	0.193059489
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.831294775	0.665555954	0.189293727
0.760843515	0.501373947	0.284120202
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083085783	0.916948795	0.187366247
0.006302525	0.754470706	0.281654954
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333729476	0.916785359	0.187353283

0.249216735	0.753221929	0.282042027
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.581755280	0.913316488	0.188448459
0.501199841	0.757753491	0.287278324
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832379043	0.915392876	0.187489927
0.762222588	0.760433197	0.284334958
0.546692431	0.524131835	0.378648132
0.772496104	0.494774818	0.376673281
0.263129741	0.376099378	0.361303717
0.775778890	0.777454495	0.377154350
0.473497838	0.250118911	0.379974842
0.476432025	0.725815058	0.379971564
0.746088386	0.388665736	0.385700166
0.752341449	0.859079599	0.386461437
0.164223045	0.331785172	0.382769018
0.367634863	0.168968573	0.387779832
0.373619050	0.709820211	0.387982517
0.162290603	0.591854870	0.325570285

Ce(OH)₅@Ni-H_{Ce}

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	5	6

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.085035861	0.167550474	0.187667668
0.002922826	0.003194424	0.281827092
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334443390	0.169283628	0.189392403
0.248486966	0.997622967	0.281339973
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.581623614	0.168800905	0.188575283
0.499851555	0.999786198	0.281896025
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.831942737	0.165958524	0.186237767
0.751724303	0.004082308	0.280563623
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.085006423	0.417343855	0.187655449
0.993166566	0.246525720	0.280216128
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.337657005	0.418733686	0.189423859
0.247982919	0.248951048	0.283469886
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582684219	0.418591201	0.192752168
0.499515861	0.243649587	0.287209541
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001

0.831932604	0.417288810	0.187789068
0.751746714	0.247619703	0.280571014
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082948901	0.666169941	0.187427461
0.003134850	0.499691129	0.281862319
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334318519	0.664923191	0.189390793
0.248067394	0.498889804	0.283419579
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582659304	0.664048135	0.192743883
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.831084788	0.665516436	0.189530015
0.759625494	0.501239061	0.285011441
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.082948595	0.916769445	0.187400624
0.006288119	0.753117502	0.281790286
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.334088922	0.917007983	0.187295333
0.248548210	0.750894964	0.281322718
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.581600964	0.912757814	0.188564375
0.499298155	0.755430043	0.287162095
0.750000000	0.750000000	0.000000000

0.916480005	0.833220005	0.094250001
0.831887782	0.914524913	0.187772393
0.759571314	0.758301318	0.284983277
0.551745296	0.525962532	0.390690237
0.768302441	0.496681720	0.377725780
0.275992543	0.387910128	0.358690202
0.768409908	0.771731555	0.377694100
0.475338787	0.259288639	0.378748655
0.475095332	0.716021597	0.378729671
0.744242489	0.391854584	0.388097584
0.744693041	0.852759361	0.388035357
0.184154242	0.342035234	0.385109186
0.369958550	0.180585936	0.389022231
0.369674921	0.689248562	0.389007777
0.500971317	0.500667989	0.485799998

Ce(OH)₅@Ni-H₂O

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	6	7

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.084542520	0.167515457	0.187495172
0.002693276	0.003407351	0.281976223
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001

0.333964765	0.169527084	0.189530000
0.247653812	0.997045517	0.281181574
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.581153631	0.168753102	0.188567817
0.498870432	0.999354601	0.281901658
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.831136107	0.165792331	0.186082095
0.750492215	0.003932266	0.280244380
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.084456757	0.417144239	0.187532261
0.991342366	0.245765790	0.279572397
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.337235957	0.418717176	0.189692661
0.247748673	0.248705208	0.283561200
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582215548	0.418536127	0.193073705
0.498514563	0.242571011	0.287494510
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.831524611	0.417101622	0.187614933
0.750985920	0.247613102	0.280365527
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082300864	0.665837586	0.187312990
0.002397635	0.499497086	0.281919658

0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333941430	0.664510965	0.189519107
0.246996805	0.498577833	0.283606350
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582288921	0.663963735	0.193179324
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.830502748	0.665583670	0.189492702
0.760494590	0.501936316	0.284660548
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.082296632	0.916734159	0.187379465
0.005372031	0.752974629	0.281611562
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333777249	0.917045295	0.187173128
0.247383967	0.751010597	0.281096816
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.580922723	0.912416458	0.188600793
0.497816533	0.755350709	0.287325770
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.831572235	0.914909601	0.187641889
0.760666013	0.759535015	0.285056680
0.540555477	0.519014418	0.382387280
0.771752954	0.493976563	0.377537131
0.258855313	0.378906608	0.360614985

0.770682037	0.782112777	0.378551096
0.471999943	0.247871593	0.380397201
0.469530642	0.721243143	0.379655093
0.703920901	0.618101597	0.491055340
0.741808474	0.386180073	0.384869963
0.734830379	0.855752945	0.384990007
0.159091607	0.328367919	0.381609082
0.369095147	0.161154822	0.388318002
0.365690470	0.702615976	0.387514830
0.769564509	0.710238874	0.464956194
0.760027707	0.561787844	0.489152223

Ce(OH)₅@Ni-OH

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	6	6

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.084908560	0.167566657	0.187756658
0.002015178	0.002895429	0.282058448
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334016800	0.169605076	0.189460069
0.247641176	0.997314930	0.281151056
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001

0.581555486	0.168962434	0.188465878
0.499353319	0.000366890	0.281607866
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.831995845	0.166181177	0.186237872
0.751471758	0.004581157	0.280426681
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.084877051	0.417501301	0.187736198
0.992747247	0.246569499	0.280125082
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.337179124	0.418717682	0.189600706
0.247557759	0.248972401	0.284266442
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582552612	0.418520778	0.192792818
0.497968972	0.242823333	0.287549466
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.831763983	0.417495072	0.187782288
0.751529515	0.247648835	0.280487269
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082446650	0.666182756	0.187410057
0.002197000	0.499847442	0.282096565
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334104687	0.665001273	0.189354777
0.248116553	0.500154078	0.284012198

0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582657635	0.664559007	0.192760572
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.830669165	0.665498257	0.189536199
0.758765697	0.500773728	0.285045475
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.082495689	0.916530907	0.187418252
0.005307807	0.752852559	0.281965017
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333764166	0.917225659	0.187097922
0.247606039	0.751371562	0.281034350
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.581626892	0.913235247	0.188312948
0.498506993	0.756887257	0.287065774
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.831899703	0.914908707	0.187651530
0.758859575	0.758671999	0.284965008
0.543506145	0.523905814	0.407987207
0.768599570	0.496093303	0.375901908
0.269439638	0.386181921	0.358184278
0.770117164	0.775879681	0.375599504
0.472410977	0.252705485	0.377560109
0.474127918	0.724639356	0.377164304
0.491861880	0.502785385	0.508121669

0.742522299	0.390599281	0.386099935
0.745457888	0.856342196	0.385676265
0.175182119	0.339461952	0.383206666
0.372162342	0.166672736	0.389479786
0.374135137	0.710893035	0.389220804
0.492567003	0.519135892	0.553243816

CeO₄@Ni-H_{Ni}

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	4	1

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.085063584	0.167810082	0.187667027
0.998551667	0.004030565	0.280662626
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334598750	0.167459413	0.188950658
0.244465038	0.991411567	0.282226950
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.583014846	0.167506158	0.189013928
0.496761888	0.990559816	0.281155348
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.832356095	0.167722464	0.188634068

0.749374688	0.000764526	0.281761348
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.087313458	0.417667568	0.188436329
0.999564350	0.249728858	0.281636178
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335620701	0.416670620	0.190658346
0.240391329	0.242012694	0.284462392
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582396209	0.415883869	0.190759510
0.491771311	0.235909626	0.288052648
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.832798958	0.415247738	0.187676817
0.752040207	0.245720729	0.286557496
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.081538357	0.667384326	0.188953981
0.008891881	0.499299437	0.281247526
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333827376	0.665426910	0.188820526
0.251014024	0.499628007	0.287139148
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582126379	0.663382828	0.190007344
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001

0.832135022	0.664970636	0.187795192
0.761292756	0.502047598	0.282731861
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.081949048	0.914428711	0.188703731
0.998639524	0.750211060	0.289531291
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333259583	0.916503429	0.187620386
0.245527968	0.751378834	0.282011420
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.582512558	0.913153708	0.188126847
0.503194809	0.751838982	0.286274880
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.831982017	0.916202247	0.186818391
0.755130470	0.758734465	0.281668425
0.551483929	0.494065642	0.379743367
0.410688132	0.596500158	0.348463833
0.812498152	0.666890264	0.345988661
0.364457399	0.259530932	0.353218347
0.670875728	0.334463060	0.342969060
0.701584399	0.841594160	0.331149161

CeO₄@Ni-H_{Ce}

1.0

10.0322999954	0.000000000	0.000000000
-5.0161499977	8.6882266544	0.000000000
0.000000000	0.000000000	21.1434993744

Ni	Ce	O	H
63	1	4	1

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.085150532	0.168296933	0.187577188
0.998195469	0.004660764	0.280837178
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334475607	0.167572707	0.188875273
0.243631274	0.991308868	0.282020509
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.582915127	0.167795479	0.189050525
0.496738762	0.990920782	0.281240314
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.832535505	0.168178350	0.188593164
0.749867320	0.002161651	0.281471670
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.087783441	0.418444753	0.188537627
0.999875844	0.251048595	0.281646639
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335885197	0.417288452	0.190358281
0.240323275	0.242933363	0.284238070
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582398057	0.415958911	0.190506399

0.490786731	0.235448778	0.287910253
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833206296	0.415617853	0.187690377
0.751687050	0.246869937	0.286658555
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.081346750	0.667799115	0.189045519
0.009688388	0.500605047	0.281387806
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333953202	0.666049242	0.188908309
0.253728807	0.501038194	0.287633300
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582219720	0.663811386	0.189859152
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832039952	0.665344954	0.187780514
0.761663318	0.502173185	0.282234401
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.081691958	0.914716482	0.188737869
0.996739268	0.750008047	0.289807200
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333244056	0.916823447	0.187600181
0.245375916	0.751860261	0.282193929
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003

0.582759142	0.913761556	0.188213632
0.503463686	0.752871156	0.286211967
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832145572	0.916765273	0.186842859
0.754248977	0.760772705	0.281489044
0.551011980	0.489076048	0.382364184
0.418645978	0.595373511	0.346067697
0.803281367	0.663891137	0.345315963
0.364750415	0.263082355	0.352072597
0.669602811	0.335233063	0.342184633
0.549369216	0.494199514	0.479459465

CeO₄@Ni-H₂O

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	5	2

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.085084975	0.168356761	0.187467650
0.998014152	0.005369280	0.280747622
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334721684	0.167955250	0.188819066
0.244920716	0.993095279	0.282775521
0.500000000	0.000000000	0.000000000

0.666630030	0.083310001	0.093910001
0.583373964	0.167920575	0.188910082
0.497143716	0.990643442	0.281234086
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.832481086	0.168054909	0.188635752
0.749490321	0.001502242	0.281570673
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.087479204	0.418241739	0.188366935
0.999581575	0.250952750	0.281654656
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335994214	0.417574435	0.190529406
0.240127832	0.243223712	0.284128070
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582800627	0.416418523	0.190729409
0.491627365	0.235645697	0.287401587
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833225429	0.415615469	0.187649310
0.751842022	0.246711329	0.286704302
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.081516057	0.667913914	0.188956037
0.009591501	0.500573397	0.281311750
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334098101	0.666264653	0.188823745

0.251676232	0.500507593	0.287191719
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582571328	0.664024591	0.190129861
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832343578	0.665535212	0.187750563
0.762720942	0.503031015	0.282444268
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.082299992	0.915091097	0.188945919
0.998789787	0.751254857	0.289980829
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333200336	0.917241335	0.187692419
0.245467216	0.752415538	0.281964839
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.582763851	0.913649380	0.188195586
0.503451586	0.752089858	0.286435723
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832244694	0.916728795	0.186831281
0.755702674	0.760610402	0.281681776
0.551028430	0.490501136	0.381605566
0.411007464	0.596808612	0.347164482
0.813120306	0.669126034	0.345445871
0.357023090	0.247510582	0.352587163
0.670077085	0.334966302	0.342593372
0.343742818	0.323680222	0.474008262

0.299307972	0.248609319	0.438622773
0.264710009	0.348915875	0.485087395

CeO₄@Ni-OH

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	5	1

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.085092820	0.167830586	0.187640518
0.998410940	0.003910083	0.280715466
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334643811	0.167487368	0.188927293
0.244626954	0.991528153	0.282178789
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.582974970	0.167528629	0.189014032
0.496970057	0.990501821	0.281228572
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.832335889	0.167739421	0.188631013
0.749279618	0.000682046	0.281538248
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.087255552	0.417634547	0.188398257

0.999530137	0.249770075	0.281640440
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335706234	0.416716069	0.190588266
0.240984663	0.242352337	0.284706801
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582393527	0.415896833	0.190714672
0.492022038	0.236355364	0.288348973
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.832840562	0.415258467	0.187703744
0.751751900	0.246069893	0.286710292
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.081545383	0.667440116	0.188953742
0.008939813	0.499327719	0.281285495
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333778024	0.665431380	0.188818127
0.252015829	0.499915600	0.287527084
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582168996	0.663476646	0.190083638
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832157731	0.665005922	0.187781915
0.761448622	0.502030194	0.282976270
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001

0.082032420	0.914463878	0.188710302
0.998354316	0.750137269	0.289702505
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333289564	0.916589200	0.187608674
0.245574549	0.751454175	0.282010138
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.582545161	0.913193762	0.188176364
0.502904534	0.750949502	0.286504865
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832011998	0.916261375	0.186895236
0.755033016	0.759055436	0.281837225
0.546568215	0.488498539	0.387515098
0.413145095	0.596536517	0.347817868
0.809154689	0.666091263	0.345431924
0.366542041	0.262642741	0.352501810
0.670350850	0.335342646	0.342557162
0.532078028	0.465603858	0.488797128
0.521774709	0.380670249	0.514574945

H₆Ce@Ni-Volmer-IS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	H	O
63	1	8	1

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.083861254	0.168027803	0.187617213
0.000242910	0.001419421	0.282418847
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.333625346	0.168227032	0.188255176
0.249338686	0.999000371	0.283577383
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.583625317	0.166933373	0.187349558
0.500093400	0.998477340	0.282167435
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833823025	0.166987017	0.188565955
0.751217067	0.000943441	0.283147722
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.084753849	0.417439491	0.188232437
0.999047160	0.248953715	0.283342600
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335445315	0.418842226	0.190900549
0.248808786	0.247023791	0.283756435
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.581348836	0.417534649	0.189729556
0.498071879	0.244528264	0.283295900
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001

0.831841707	0.415508389	0.186994553
0.749339342	0.248414904	0.282609493
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082898214	0.665936887	0.187903881
0.992693901	0.496126592	0.281895548
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334587902	0.666050792	0.188858122
0.246100292	0.502829731	0.287530631
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582208991	0.663631082	0.189757764
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.831892014	0.665725768	0.188134789
0.751856625	0.500635684	0.282738328
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083098263	0.916743875	0.188150018
0.000964348	0.751040459	0.283614218
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333326429	0.916434765	0.188140303
0.247829571	0.752333760	0.283511013
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.583707035	0.916141927	0.187703565
0.502298534	0.753149688	0.283329666
0.750000000	0.750000000	0.000000000

0.916480005	0.833220005	0.094250001
0.832831025	0.916693568	0.187536523
0.755564809	0.752372622	0.283506423
0.508300304	0.496159911	0.363832831
0.376085609	0.639214158	0.333195120
0.825153291	0.661046922	0.327878624
0.338021874	0.174591422	0.328229964
0.176951006	0.335421354	0.327530056
0.665928662	0.826580405	0.326513320
0.663142860	0.336283326	0.325936258
0.148631498	0.581259429	0.324770659
0.544202507	0.504532039	0.510301530
0.527382791	0.500066996	0.465083659

H₆Ce@Ni-Volmer-TS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	H	O
63	1	8	1

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.083176024	0.167028725	0.187625632
0.998688221	0.000097752	0.282555282
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334081560	0.168297872	0.188321158
0.248723358	0.998935223	0.283666760

0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.584302306	0.168068916	0.187390909
0.500369251	0.000830889	0.282138944
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833024561	0.166510314	0.188664049
0.750508726	0.001049955	0.283344418
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.082138956	0.415521145	0.187050968
0.998804390	0.249190420	0.283553898
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.336095423	0.417568803	0.189813897
0.246567100	0.244718298	0.284026504
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582158446	0.418087333	0.189904138
0.498401135	0.245096043	0.283635199
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.832130313	0.415795654	0.187478423
0.750496030	0.249579534	0.283295423
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082634397	0.666017294	0.187982872
0.001389972	0.499735892	0.282632411
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003

0.333734572	0.665364802	0.188336879
0.247107401	0.499163836	0.281494379
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.580638468	0.663939178	0.190738872
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.831517220	0.665796161	0.188147038
0.754832029	0.501431704	0.283455521
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.082982838	0.916807830	0.188118592
0.000462651	0.750865400	0.283650428
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.334018707	0.917301059	0.187904164
0.246259838	0.751078427	0.281655490
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.583375454	0.916250587	0.187719166
0.495661676	0.751982450	0.284952253
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832451284	0.916523278	0.187480301
0.753498971	0.752076983	0.283265591
0.505316556	0.504809856	0.360026181
0.325083137	0.673933089	0.362652123
0.825199127	0.662398636	0.327982754
0.338027239	0.175235972	0.328622282
0.176578745	0.338830173	0.326956332

0.665646732	0.827344477	0.325918853
0.662932754	0.337403029	0.326677531
0.410149425	0.748854160	0.380227596
0.577302516	0.693014026	0.480247319
0.541693568	0.602312922	0.453911215

H₆Ce@Ni-Volmer-FS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	H	O
63	1	8	1

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.083602875	0.167349383	0.187671512
0.999343395	0.000743718	0.282397270
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334136546	0.168076560	0.188364282
0.248839051	0.997619808	0.283704668
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.584120989	0.167220876	0.187612593
0.501366615	0.000072829	0.282587647
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833606720	0.166979745	0.188628286
0.751371384	0.002375457	0.283147335

0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.083579220	0.416256458	0.187591001
0.999115467	0.249800578	0.283300996
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335939825	0.417746872	0.189940363
0.247173548	0.245157078	0.284036875
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582228839	0.417545795	0.190184534
0.498439133	0.243386522	0.284004152
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.832941592	0.416148216	0.187637582
0.750763714	0.249583915	0.283320338
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.083281271	0.666369319	0.188182533
0.999880135	0.498950154	0.282449573
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334011137	0.666001916	0.188179359
0.247844920	0.501628041	0.283797175
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582158804	0.663954198	0.189898729
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.831998765	0.665729105	0.188298032

0.754907966	0.501526654	0.284063429
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083137229	0.916792154	0.188201636
0.002362809	0.751189590	0.283655852
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333859801	0.916995347	0.188146606
0.248666257	0.751616478	0.283625931
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.584170997	0.916893303	0.187461391
0.498477787	0.753594518	0.283187360
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832721293	0.916542113	0.187616482
0.754782319	0.752461731	0.283805996
0.500521481	0.501264751	0.345479012
0.333305746	0.665085316	0.326804876
0.828423500	0.664311767	0.328249007
0.336509138	0.172797397	0.328348100
0.173226804	0.336802840	0.326707363
0.667626023	0.831706166	0.324644953
0.663397014	0.336518317	0.326878786
0.429349869	0.716800988	0.423157454
0.604030192	0.797053337	0.418236822
0.516322255	0.704170465	0.436141372

H₆Ce@Ni-Heyrovsky-IS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	H	O
63	1	9	1

Direct

0.0000000000	0.0000000000	0.0000000000
0.166779995	0.083520003	0.094250001
0.083958708	0.168068662	0.187699392
0.000794327	0.001460208	0.282389343
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.333533168	0.167935789	0.188339889
0.248803392	0.997642159	0.283766329
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.582960188	0.166437238	0.187570751
0.500056982	0.998273790	0.282300353
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833688557	0.167213812	0.188455254
0.752065063	0.002282779	0.283087611
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.083005317	0.416729480	0.187696338
0.997919559	0.248432398	0.283349514
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335116535	0.419175744	0.191178486
0.248092771	0.246570513	0.284137040

0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.581012905	0.416839242	0.189871937
0.497529238	0.243176863	0.284041166
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.831116498	0.415363461	0.187072635
0.748825252	0.248040274	0.282825142
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.083001114	0.665870309	0.188124433
0.991147339	0.494441748	0.281853110
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334572375	0.666190684	0.188665152
0.242232487	0.501566947	0.286740422
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.583005428	0.663799465	0.189455718
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832097530	0.665612876	0.188217863
0.752294242	0.500471473	0.283207297
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083267257	0.916511416	0.188272446
0.002054744	0.750951052	0.283682913
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.332256228	0.915220022	0.188598633

0.248609945	0.750751197	0.285653919
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.584297717	0.917595148	0.187053114
0.506226361	0.755656958	0.281834871
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.833140314	0.916783988	0.187638968
0.757203996	0.753961444	0.283998162
0.499851555	0.500840127	0.345202982
0.356629401	0.680331528	0.324655652
0.827704728	0.662557840	0.327910334
0.335672230	0.171384111	0.328283519
0.173620731	0.334225148	0.327370226
0.667315960	0.828955770	0.326820225
0.662902534	0.336070418	0.326481164
0.139770880	0.581335902	0.326629311
0.383374512	0.677175403	0.427910149
0.248424172	0.515960753	0.415565550
0.349224627	0.568930149	0.436865836

H₆Ce@Ni-Heyrovsky-TS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	H	O
63	1	9	1

Direct

0.000000000	0.000000000	0.000000000
-------------	-------------	-------------

0.166779995	0.083520003	0.094250001
0.083547615	0.168736577	0.187572733
0.999323368	0.001161791	0.282615215
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.333470613	0.168181032	0.187990248
0.248782933	0.999082267	0.283616334
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.582619965	0.167071253	0.187450588
0.500033081	0.999169588	0.282108963
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.832620382	0.167262957	0.188246831
0.750386596	0.001558584	0.282829344
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.082934298	0.417497098	0.188435078
0.995247841	0.246282965	0.282875299
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.333764344	0.420453548	0.192410991
0.247845352	0.244992703	0.282846630
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.580433309	0.417410493	0.189778328
0.497020721	0.244002283	0.283521056
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.830420434	0.415205866	0.187126294

0.748354316	0.249053955	0.282875359
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082664259	0.666022301	0.187984258
0.990269065	0.499192625	0.281496942
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.332975775	0.665049851	0.189050227
0.236027732	0.501290798	0.294148654
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582100511	0.663530827	0.189086661
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.831560612	0.665564597	0.188172162
0.750703633	0.500882506	0.283196330
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.082841873	0.916850328	0.188131183
0.000477360	0.751504123	0.283762634
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.332644939	0.916199625	0.188142553
0.248448700	0.753997386	0.284036309
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.583864033	0.917596519	0.186663508
0.504894376	0.755362093	0.280558765
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001

0.832747757	0.916942775	0.187373534
0.755470634	0.753734291	0.283093482
0.498584151	0.504332960	0.357876003
0.364779532	0.687383771	0.326739669
0.824025393	0.662238479	0.327993691
0.337243944	0.175213858	0.328694999
0.171324596	0.322150379	0.326302677
0.664756238	0.826603234	0.326145142
0.661038697	0.336725891	0.326738209
0.129983678	0.557060778	0.336506844
0.403352290	0.625822842	0.466644168
0.186956450	0.500980794	0.362357646
0.441990405	0.563576579	0.447933316

H₆Ce@Ni-Heyrovsky-FS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	H	O
63	1	9	1

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.083497494	0.167914107	0.187588573
0.998896420	0.000288867	0.282309920
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.333971202	0.168042347	0.188289315
0.248997301	0.998458445	0.283656806

0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.584247887	0.167900458	0.187567115
0.501036823	0.000524209	0.282191217
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833587289	0.167389661	0.188829109
0.749834180	0.000410107	0.283181757
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.082942545	0.416816860	0.188039899
0.999275804	0.248537511	0.283312142
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335736871	0.417914599	0.189746946
0.247593641	0.245545238	0.283510029
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.581977963	0.418023050	0.189791366
0.497685194	0.245665297	0.283487350
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833819926	0.417003512	0.188019827
0.748930573	0.248547256	0.283188045
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082808070	0.665774703	0.188716859
0.999678373	0.499693483	0.284999013
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003

0.333714634	0.665764570	0.188309014
0.249387920	0.501238346	0.283090562
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.581912756	0.664184928	0.189657360
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.831908762	0.665914476	0.188333943
0.751585484	0.501383305	0.283145458
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083227284	0.916540861	0.188208938
0.000725803	0.751843512	0.283664554
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.332987279	0.916441560	0.188185841
0.250679106	0.751941800	0.283584565
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.583806872	0.916683853	0.187496603
0.498675734	0.752413750	0.283377677
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832618892	0.916706562	0.187498018
0.752952874	0.752548218	0.283398479
0.499440283	0.500234663	0.361471862
0.339733601	0.662260473	0.328051478
0.821691036	0.662420690	0.328056574
0.337065727	0.174501717	0.328275770
0.177359357	0.337129235	0.326599360

0.661975443	0.824913859	0.326788992
0.659760058	0.337540179	0.326598793
0.020154839	0.550162077	0.358091652
0.498011976	0.508073568	0.508748829
0.980582118	0.451090425	0.358387232
0.498605460	0.504492462	0.462990910

Ce(OH)₅@Ni-Volmer-IS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	6	7

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.084559381	0.167499706	0.187356919
0.002574461	0.003264980	0.281809479
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334054500	0.169541866	0.189364642
0.247624099	0.996904135	0.281039834
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.581326723	0.168718576	0.188337713
0.498969257	0.999629200	0.281682044
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.831333041	0.165925264	0.185882285

0.750633180	0.004068719	0.280115902
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.084657937	0.417237192	0.187397048
0.991252482	0.245689899	0.279526800
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.337420434	0.418730736	0.189609274
0.247761890	0.248599872	0.283497125
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582386434	0.418442339	0.192785010
0.498690158	0.242400318	0.287193507
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.831745446	0.416977912	0.187403157
0.750933826	0.247422084	0.280243933
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082546607	0.665968716	0.187142462
0.002476057	0.499547571	0.281838894
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334062934	0.664547324	0.189347744
0.247473449	0.498803169	0.283571512
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582460880	0.664066374	0.192884058
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001

0.830726206	0.665552318	0.189257488
0.760230780	0.501544595	0.284495473
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.082508571	0.916698635	0.187122703
0.005317288	0.752858937	0.281538725
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333700866	0.916957676	0.186971873
0.247484431	0.750838935	0.281033725
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.581261277	0.912797391	0.188265309
0.498491436	0.756485045	0.287015945
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.831660807	0.914883733	0.187466651
0.760492504	0.759332955	0.284927636
0.539972365	0.519605041	0.381819010
0.771901429	0.493440866	0.377174109
0.258712292	0.378704429	0.360721320
0.771806419	0.781947017	0.378349811
0.472438663	0.248137593	0.379940718
0.470711023	0.722175062	0.379386663
0.704743028	0.618318319	0.490303487
0.741804838	0.385711938	0.384746641
0.736923873	0.856281638	0.384968877
0.158614382	0.327613324	0.381462306
0.369411707	0.161821693	0.388002425
0.366770893	0.703072906	0.387364417

0.770395517	0.710197568	0.464039743
0.760178089	0.561402738	0.488041729

Ce(OH)₅@Ni-Volmer-TS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	6	7

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.084629998	0.167370006	0.187350005
0.001670000	0.001960000	0.281760007
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334219992	0.169799998	0.189530000
0.248579994	0.998749971	0.281520009
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.581570029	0.168929994	0.188409999
0.499529988	0.001520000	0.281859994
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.831009984	0.164949998	0.186000004
0.750800014	0.002960000	0.280779988
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.085019998	0.416830003	0.187150002

0.990729988	0.245399997	0.279320002
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.337249994	0.418689996	0.189740002
0.246950001	0.248239994	0.284189999
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582459986	0.419140011	0.192320004
0.501850009	0.247639999	0.287070006
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.832149982	0.416599989	0.187279999
0.751640022	0.248070002	0.280809999
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082979999	0.666320026	0.186949998
0.003180000	0.500339985	0.281309992
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333939999	0.664699972	0.189349994
0.247810006	0.499579996	0.283609986
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582140028	0.664560020	0.192709997
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.831160009	0.666090012	0.188850001
0.761690021	0.501590014	0.283479989
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001

0.083350003	0.917519987	0.187050000
0.005840000	0.752759993	0.281419992
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.334060013	0.917530000	0.187089995
0.247429997	0.751680017	0.281019986
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.581489980	0.913230002	0.188250005
0.498629987	0.757480025	0.286929995
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.831420004	0.914579988	0.187680006
0.758040011	0.754230022	0.284830004
0.528110027	0.527190030	0.400420010
0.780350029	0.490940005	0.382429987
0.254909992	0.378639996	0.360610008
0.770560026	0.762350023	0.376859993
0.488970011	0.263489991	0.378800005
0.471769989	0.734279990	0.379099995
0.586189985	0.536379993	0.501339972
0.727680027	0.384869993	0.398180008
0.766550004	0.855080009	0.387510002
0.153549999	0.328379989	0.380419999
0.397020012	0.168139994	0.391020000
0.373979986	0.729929984	0.387430012
0.643949986	0.610130012	0.534259975
0.840499997	0.642250001	0.427810013

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	6	7

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.084718831	0.167589903	0.187482521
0.003076108	0.003049168	0.281743079
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334006697	0.169785902	0.189099938
0.248548329	0.997736633	0.280529499
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.581798017	0.169103175	0.188317791
0.500090301	0.000426288	0.281470567
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.831598282	0.165875658	0.186253563
0.751555681	0.004408512	0.280540794
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.084736161	0.417234302	0.187523231
0.992201269	0.246162236	0.279897720
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.337245822	0.418651193	0.189398557

0.247809350	0.248825148	0.283778816
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582551241	0.418318033	0.192861781
0.497110665	0.241979688	0.287304282
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.831675828	0.417637974	0.187981337
0.751634181	0.247541398	0.280519277
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.083054915	0.665497005	0.186575308
0.003084331	0.500225663	0.281752110
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334021121	0.664417803	0.189134747
0.247855797	0.498994827	0.283805579
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582540452	0.664274275	0.192955315
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.830347478	0.665162027	0.189674959
0.756689370	0.495305777	0.287906379
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083040088	0.917621136	0.186585858
0.012211381	0.756194949	0.280038416
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001

0.334172189	0.917113125	0.186749890
0.248427898	0.751030505	0.280570120
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.581766129	0.912748277	0.188377634
0.497100770	0.755930424	0.287369788
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.831639349	0.914076447	0.188023135
0.756711006	0.761638522	0.287941158
0.536985159	0.518433928	0.408573031
0.752469599	0.472168088	0.379363805
0.262860626	0.381365687	0.358334184
0.752285838	0.780507803	0.379452318
0.458880663	0.243775576	0.376708984
0.458220452	0.714604020	0.376667440
0.497976631	0.497849464	0.509719193
0.710794747	0.362521917	0.387850195
0.710535288	0.848471761	0.387851745
0.167261094	0.333355099	0.382505983
0.357493579	0.157933787	0.387476176
0.356489420	0.698324502	0.387317568
0.517796457	0.506003022	0.554725885
0.849334955	0.674678683	0.313907862

Ce(OH)₅@Ni-Heyrovsky-IS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	6	8

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.084528133	0.167822406	0.187258974
0.004235478	0.004767888	0.281708747
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334005207	0.169970036	0.189160362
0.248806849	0.998393238	0.280682057
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.581211150	0.169171900	0.188514143
0.499641389	0.000718084	0.281839490
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.830954909	0.166000739	0.185982019
0.750939071	0.004716221	0.280307531
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.084502771	0.417405009	0.187190920
0.991009116	0.246243998	0.279139817
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.337616533	0.419130027	0.189455777
0.247376919	0.249468267	0.283251524
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582370698	0.418762594	0.193333074

0.497088134	0.242869675	0.287507862
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.831540942	0.417858988	0.187970772
0.750632763	0.248059213	0.280414402
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082913205	0.665643990	0.186670318
0.003835311	0.500567138	0.281635016
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334112227	0.664724529	0.189174533
0.247543767	0.499090701	0.283058256
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582624912	0.664489985	0.193332776
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.830263913	0.665632308	0.190059990
0.758960783	0.497707158	0.288108438
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083017014	0.917975664	0.186652109
0.012040589	0.756799817	0.280304432
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.334161997	0.917285502	0.186858609
0.248295233	0.751621962	0.280625999
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003

0.581492901	0.912804782	0.188414216
0.497352183	0.756481588	0.287188262
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.831916630	0.914859891	0.187925667
0.758697331	0.763595462	0.287942797
0.536658168	0.520156443	0.383157879
0.755657971	0.468875110	0.382282346
0.256153464	0.379135251	0.360289305
0.755443990	0.790636301	0.381839007
0.457852155	0.243842065	0.379336715
0.457189202	0.716998816	0.379102737
0.707241058	0.605140150	0.489574939
0.708729029	0.357748777	0.388484478
0.708795428	0.855203867	0.387839168
0.156239569	0.329447985	0.381152093
0.352890253	0.159725294	0.386086613
0.351557225	0.694632709	0.385435879
0.850163341	0.676559210	0.315488517
0.765499234	0.711343050	0.473497897
0.765541077	0.558918118	0.471635073

Ce(OH)₅@Ni-Heyrovsky-TS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	6	8

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.084254809	0.166933686	0.187662303
0.999690890	0.002809482	0.281575590
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.332902640	0.169283882	0.189676493
0.247593284	0.998456895	0.280907720
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.580141783	0.168492779	0.188473165
0.497892529	0.999645472	0.281741679
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.830833972	0.165972084	0.185737237
0.748930454	0.004252125	0.279598743
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.084017590	0.417574406	0.187542394
0.990149260	0.245308280	0.279432505
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.336233884	0.418241829	0.189862743
0.245744273	0.249079108	0.285432816
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.581078708	0.417707175	0.192181677
0.495955080	0.242870033	0.288625181
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001

0.830878735	0.417291164	0.187377244
0.749171793	0.246656954	0.280155838
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.081531443	0.666387022	0.187299937
0.999694645	0.497448564	0.281493157
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.332566082	0.663936913	0.189212352
0.245799348	0.497528732	0.284913599
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.581128836	0.663803339	0.191811398
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.830804586	0.665670455	0.189448431
0.753587067	0.498326153	0.283677429
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.081703402	0.915721893	0.187361762
0.004812227	0.752675295	0.283391595
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.332681656	0.916570663	0.186885491
0.247273922	0.749653220	0.280473441
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.580209374	0.912502885	0.188072070
0.495790869	0.754163086	0.286797464
0.750000000	0.750000000	0.000000000

0.916480005	0.833220005	0.094250001
0.831291199	0.914676487	0.187094584
0.753064811	0.756612599	0.282830477
0.555932939	0.534098566	0.410115749
0.763495505	0.488980174	0.374518871
0.261440068	0.382394552	0.360636204
0.765000045	0.783319592	0.373085827
0.467279613	0.254259855	0.379233927
0.466234684	0.718530774	0.377167881
0.657703519	0.619117141	0.504252970
0.726743758	0.380821586	0.384709805
0.726523638	0.853381395	0.383200139
0.161896124	0.333180070	0.382045060
0.364708573	0.169967756	0.389249355
0.363384962	0.699057102	0.387333721
0.001225028	0.792972982	0.357530147
0.760385811	0.703451514	0.513860285
0.000018835	0.708070338	0.357507288

Ce(OH)₅@Ni-Heyrovsky-FS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	6	8

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.085112974	0.167191118	0.187579885

0.002303682	0.003840154	0.281612545
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334133059	0.169230372	0.189197242
0.249846891	0.999549568	0.280608475
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.581856847	0.168829858	0.188149706
0.500425577	0.000374098	0.281276703
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.832153022	0.166001156	0.186105639
0.751732826	0.004454578	0.280387640
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.084995128	0.417688668	0.187488735
0.992904425	0.246346876	0.280014336
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.337468177	0.418725699	0.189391926
0.248811007	0.249357194	0.283845067
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582926869	0.418633312	0.192454278
0.499403507	0.242875874	0.287123531
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.831763804	0.417653352	0.187639937
0.751714468	0.247201011	0.280431718
0.000000000	0.500000000	0.000000000

0.166779995	0.583260000	0.094250001
0.082272746	0.666431069	0.187301621
0.002177430	0.497849315	0.281304151
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334063768	0.664768577	0.189127296
0.248593554	0.499324799	0.283813596
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582854450	0.664297938	0.192466512
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.831934810	0.666074932	0.190195173
0.758153439	0.499754727	0.284993261
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.082253210	0.915835381	0.187396750
0.007955166	0.753258228	0.284032911
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333641380	0.916900933	0.186826125
0.249866113	0.750398159	0.280343860
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.581773162	0.913010657	0.188134357
0.499011874	0.756591439	0.287171572
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.831845164	0.914164484	0.187684700
0.757690251	0.758033097	0.284956038

0.541712642	0.521747947	0.408301026
0.765027583	0.492858499	0.376597434
0.267935574	0.384066701	0.358319551
0.764473975	0.774453580	0.375915378
0.471243888	0.250777632	0.377127171
0.470291346	0.721596301	0.377272874
0.504972339	0.503895760	0.509910643
0.739162505	0.387342662	0.386536151
0.733945072	0.850898147	0.385559648
0.172269583	0.335971177	0.382425994
0.370459199	0.164677516	0.388381779
0.369944513	0.707811594	0.388666749
0.051698923	0.803490758	0.357790411
0.520042777	0.513217330	0.555226147
0.981491387	0.710517645	0.359531611

CeO₄@Ni-Volmer-IS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	5	2

Direct

0.0000000000	0.0000000000	0.0000000000
0.166779995	0.083520003	0.094250001
0.084933959	0.168360919	0.187429443
0.998147070	0.005488841	0.280713141
0.2500000000	0.0000000000	0.0000000000
0.416740000	0.083520003	0.094250001

0.334604323	0.167921275	0.188610166
0.244850293	0.992989540	0.282743663
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.583330810	0.167878568	0.188796639
0.497366637	0.990770578	0.281215578
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.832523525	0.168086886	0.188608661
0.749469817	0.001395557	0.281559527
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.087441511	0.418176115	0.188294277
0.999586701	0.250937909	0.281652898
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.336063325	0.417527765	0.190356299
0.240420789	0.243320897	0.284078687
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582828462	0.416319937	0.190622523
0.491482019	0.235551149	0.287347496
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833188176	0.415582895	0.187603712
0.751761496	0.246921778	0.286720753
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.081556343	0.667938292	0.188747272
0.009557424	0.500496566	0.281268448

0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334204555	0.666253567	0.188615561
0.251692295	0.500427961	0.287167907
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582515478	0.664036155	0.189991295
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832363546	0.665751457	0.187629208
0.762628376	0.503075063	0.282391548
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.082345888	0.915114164	0.188769847
0.998795569	0.751218796	0.289979041
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333138078	0.917165458	0.187619835
0.245533869	0.752363026	0.281925529
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.582810700	0.913679600	0.188107222
0.503361046	0.751881599	0.286385030
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832254887	0.916867495	0.186797127
0.755713522	0.760319054	0.281622589
0.551151931	0.490499884	0.381639987
0.410774648	0.596840143	0.347259015
0.813329160	0.669526041	0.345585138

0.356807292	0.247349396	0.352674544
0.670219362	0.335155010	0.342787206
0.343692720	0.323741078	0.473924071
0.264565945	0.348817408	0.484992623
0.299380988	0.248596445	0.438562661

CeO₄@Ni-Volmer-TS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	5	2

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.083056822	0.167691082	0.186608896
0.995308876	0.005652517	0.280819386
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334062368	0.167913422	0.187417686
0.248611018	0.002584815	0.290110141
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.584547400	0.167068735	0.187244207
0.499789089	0.991206646	0.281024814
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.832548857	0.168038473	0.188412011
0.749168873	0.001461009	0.281534970

0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.086847566	0.418294162	0.187877730
0.999434173	0.251841217	0.281523347
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335896850	0.418633968	0.189519942
0.240788758	0.247940540	0.281324744
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.583713651	0.418064505	0.189661056
0.499125093	0.240072355	0.281656682
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833678424	0.416605264	0.187675387
0.753741503	0.248423398	0.285935074
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.081591204	0.668702304	0.188664362
0.010305811	0.501998425	0.281084359
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333172113	0.667596459	0.188587099
0.251057625	0.499535352	0.286426693
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582316816	0.664953351	0.189855963
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832858920	0.666782856	0.187931851

0.760700345	0.503484607	0.283396840
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.084139563	0.916308045	0.190447569
0.998205245	0.752411544	0.291222006
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.332001269	0.919106245	0.188617349
0.245317370	0.756566525	0.282303274
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.582305312	0.913541198	0.187882453
0.501783788	0.749957860	0.286753297
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832642019	0.916837752	0.186885864
0.752723694	0.759365439	0.282692224
0.518467784	0.447953105	0.389105886
0.411985815	0.588817418	0.343274713
0.811119974	0.666576862	0.343806446
0.335256964	0.191485047	0.342608631
0.667822957	0.332374990	0.341581792
0.424323112	0.354879797	0.482649595
0.197733328	0.351069123	0.461760461
0.350720316	0.255246431	0.496999323

CeO₄@Ni-Volmer-FS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000

	0.0000000000	0.0000000000	21.1434993744
Ni	Ce	O	H
63	1	5	2
Direct			
	0.0000000000	0.0000000000	0.0000000000
	0.166779995	0.083520003	0.094250001
	0.083407201	0.167394266	0.187002733
	0.993503094	0.002428893	0.280954391
	0.250000000	0.000000000	0.000000000
	0.416740000	0.083520003	0.094250001
	0.333214015	0.167512789	0.188131869
	0.248457581	0.001161271	0.291069567
	0.500000000	0.000000000	0.000000000
	0.666630030	0.083310001	0.093910001
	0.583773911	0.166266814	0.187341899
	0.498815745	0.990068078	0.281025916
	0.750000000	0.000000000	0.000000000
	0.916689992	0.083310001	0.093910001
	0.832151473	0.166907474	0.188037366
	0.748427033	0.000177973	0.281281382
	0.000000000	0.250000000	0.000000000
	0.167219996	0.333609998	0.094010003
	0.087082848	0.417792112	0.188068241
	0.995898724	0.249471962	0.281445920
	0.250000000	0.250000000	0.000000000
	0.416880012	0.333759993	0.094740003
	0.335100174	0.417152554	0.190213755
	0.240558282	0.243952289	0.283915967
	0.500000000	0.250000000	0.000000000
	0.666390002	0.333609998	0.094010003

0.583222091	0.416610569	0.189739332
0.498019665	0.239335954	0.282700270
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833830714	0.415887803	0.187380224
0.752679467	0.246217936	0.284867764
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.081347741	0.668087363	0.188790739
0.009521968	0.501093149	0.281107813
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.332484603	0.665982842	0.189029247
0.253129095	0.500488818	0.289267629
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.581615210	0.663710356	0.189727694
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832427323	0.665981650	0.187857002
0.760518551	0.501156211	0.282802135
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083942369	0.915751696	0.190659955
0.996825695	0.750912309	0.291321218
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.331370711	0.918098927	0.188766837
0.244148195	0.754561543	0.282424927
0.500000000	0.750000000	0.000000000

0.666390002	0.832780004	0.094010003
0.581695735	0.912940919	0.187855542
0.501508534	0.750034273	0.286326349
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832444668	0.916223645	0.186818853
0.751518011	0.757255554	0.282441705
0.535313547	0.459563047	0.390899271
0.421826303	0.593267739	0.343819410
0.805422604	0.661798656	0.344286233
0.338972867	0.187947720	0.344620407
0.669457495	0.330023944	0.341253132
0.518786430	0.457880586	0.492212385
0.151929468	0.324161828	0.325776368
0.506485701	0.450982124	0.537670135

CeO₄@Ni-Heyrovsky-IS

1.0

10.032299954	0.000000000	0.000000000
-5.0161499977	8.6882266544	0.000000000
0.000000000	0.000000000	21.1434993744

Ni	Ce	O	H
63	1	5	3

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.085386813	0.168591291	0.187358156
0.000917370	0.007027836	0.280648708
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001

0.334981263	0.168117613	0.188612655
0.246483684	0.994256198	0.282927483
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.583737075	0.167847842	0.188682288
0.498046249	0.992000282	0.281111717
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.832951546	0.168258443	0.188318253
0.751524270	0.005092443	0.281788319
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.087308817	0.418055803	0.188046247
0.000325113	0.251052320	0.281430244
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.336660117	0.417903036	0.190212324
0.242550105	0.244805068	0.284205496
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.583366632	0.416574419	0.190561548
0.492730409	0.236347407	0.287322313
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833410323	0.415995687	0.187454253
0.753456950	0.248606786	0.286080658
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082403772	0.668064177	0.188571081
0.009767939	0.500704288	0.280997992

0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.335003793	0.666629314	0.188721403
0.250122845	0.499615461	0.286030143
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.583289683	0.664634645	0.190305561
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832939386	0.666479826	0.187618762
0.763257086	0.504668236	0.282215923
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.082926437	0.915521204	0.188694552
0.001959105	0.752780557	0.288886279
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333656162	0.917453170	0.187626138
0.247289672	0.752768695	0.281798184
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.582982659	0.913481474	0.188256398
0.500684083	0.749754488	0.288318276
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832543612	0.917104125	0.186959028
0.758468688	0.760242760	0.282722175
0.550047159	0.492079854	0.379784226
0.400059283	0.589755714	0.348244190
0.823418677	0.669170558	0.345689386

0.359021008	0.248814866	0.352208823
0.671953857	0.335986197	0.342123002
0.711973369	0.755667925	0.450013757
0.677446783	0.846827865	0.324798763
0.676640391	0.827656806	0.439535111
0.799826324	0.785015702	0.421242774

CeO₄@Ni-Heyrovsky-TS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	5	3

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.084133677	0.166690499	0.187073737
0.996857166	0.002781429	0.280218899
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334840059	0.166815177	0.188241169
0.248418614	0.995830715	0.289875478
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.583986819	0.165830433	0.188441560
0.498904645	0.988510609	0.280913770
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.831748724	0.165796816	0.189190477

0.748767078	0.998199999	0.282771736
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.087570444	0.416038245	0.188012168
0.999659657	0.248795897	0.281786382
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335996836	0.415777028	0.189933047
0.242978409	0.243292823	0.284178257
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582733333	0.414574653	0.189858571
0.498460710	0.240624323	0.286516458
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833776712	0.413543910	0.187185958
0.752849102	0.247405633	0.287834078
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082772985	0.665873051	0.188032508
0.010833555	0.497964263	0.280710459
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333644301	0.664962649	0.188549429
0.251855075	0.492629021	0.287214994
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582876265	0.663016737	0.189196795
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001

0.833536208	0.664452791	0.186446071
0.760862350	0.499551237	0.280691564
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.085061677	0.915715396	0.189272702
0.005613592	0.750340402	0.286450595
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.332531303	0.916822076	0.188360184
0.248279572	0.750649035	0.281808943
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.582186520	0.911787927	0.188105926
0.501658857	0.741585493	0.285420984
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832770705	0.916505873	0.186648801
0.758028924	0.756197214	0.279420435
0.587072313	0.519338250	0.393091381
0.418961883	0.575799346	0.342026919
0.828527510	0.670290053	0.340575606
0.327011168	0.171599850	0.343290001
0.669812441	0.338117748	0.344046414
0.713416457	0.732142866	0.450074732
0.628132463	0.931756616	0.376150131
0.657970369	0.882912219	0.393043041
0.820573092	0.805590272	0.439040333

CeO₄@Ni-Heyrovsky-FS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	5	3

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.083411604	0.166866094	0.186899498
0.997489512	0.003678225	0.280541420
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334169596	0.167213053	0.187875435
0.248822272	0.002289192	0.291193932
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.584200561	0.165332675	0.187485352
0.496624947	0.988707364	0.280914217
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.832583427	0.166172326	0.188636124
0.749076843	0.999926746	0.284570247
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.086816736	0.417365402	0.188064232
0.001447791	0.251911521	0.281376719
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.336113274	0.417808354	0.189747602
0.243099391	0.247957602	0.282307357

0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.583653092	0.416026145	0.189826161
0.499132961	0.238560125	0.282973826
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833883405	0.415573955	0.187371656
0.754120648	0.248491898	0.284502476
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.081496209	0.668054879	0.188670725
0.010292329	0.501027822	0.281080872
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333272070	0.666743815	0.188874334
0.251091540	0.497567952	0.287232608
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.581899822	0.663817346	0.189626649
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832867622	0.666064262	0.187731639
0.760964811	0.500823379	0.283064336
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.084046811	0.915551960	0.190476045
0.997381032	0.750951529	0.291359574
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.331972629	0.918160856	0.188606277

0.243922785	0.754752576	0.282203466
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.583553493	0.913408339	0.188610449
0.498490036	0.745949805	0.286596596
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832085371	0.916591465	0.187340707
0.751250207	0.754299104	0.281164020
0.538621306	0.463013202	0.390613586
0.412319392	0.585385382	0.344092518
0.806213200	0.662675679	0.344313323
0.337823272	0.193643108	0.344208747
0.669548154	0.330010116	0.341840774
0.543099701	0.475362182	0.492311895
0.803748310	0.044904519	0.356439352
0.709590614	0.966729879	0.358075827
0.549467504	0.480381995	0.537951887

Ni(111)

1.0

10.0492000580	0.0000000000	0.0000000000
-5.0246000290	8.7028625379	0.0000000000
0.0000000000	0.0000000000	24.1026000977

Ni

48

Direct

0.166669995	0.083329998	0.000000000
0.083330803	0.166669190	0.084129207
0.000002350	0.999997675	0.168073788

0.416669995	0.083329998	0.000000000
0.333330810	0.166669190	0.084129207
0.250002354	0.999997675	0.168073788
0.666670024	0.083329998	0.000000000
0.583330810	0.166669190	0.084129207
0.500002325	0.999997675	0.168073788
0.916670024	0.083329998	0.000000000
0.833330810	0.166669190	0.084129207
0.750002325	0.999997675	0.168073788
0.166669995	0.333330005	0.000000000
0.083330803	0.416669190	0.084129207
0.000002350	0.249997646	0.168073788
0.416669995	0.333330005	0.000000000
0.333330810	0.416669190	0.084129207
0.250002354	0.249997646	0.168073788
0.666670024	0.333330005	0.000000000
0.583330810	0.416669190	0.084129207
0.500002325	0.249997646	0.168073788
0.916670024	0.333330005	0.000000000
0.833330810	0.416669190	0.084129207
0.750002325	0.249997646	0.168073788
0.166669995	0.583329976	0.000000000
0.083330803	0.666669190	0.084129207
0.000002350	0.499997646	0.168073788
0.416669995	0.583329976	0.000000000
0.333330810	0.666669190	0.084129207
0.250002354	0.499997646	0.168073788
0.666670024	0.583329976	0.000000000
0.583330810	0.666669190	0.084129207
0.500002325	0.499997646	0.168073788

0.916670024	0.583329976	0.000000000
0.833330810	0.666669190	0.084129207
0.750002325	0.499997646	0.168073788
0.166669995	0.833329976	0.000000000
0.083330803	0.916669190	0.084129207
0.000002350	0.749997675	0.168073788
0.416669995	0.833329976	0.000000000
0.333330810	0.916669190	0.084129207
0.250002354	0.749997675	0.168073788
0.666670024	0.833329976	0.000000000
0.583330810	0.916669190	0.084129207
0.500002325	0.749997675	0.168073788
0.916670024	0.833329976	0.000000000
0.833330810	0.916669190	0.084129207
0.750002325	0.749997675	0.168073788

Ni(111)-H

1.0

10.0492000580	0.000000000	0.000000000
-5.0246000290	8.7028625379	0.000000000
0.000000000	0.000000000	24.1026000977

Ni

48

Direct

0.166669995	0.083329998	0.000000000
0.083330803	0.166669190	0.084129207
0.000002350	0.999997675	0.168073788
0.416669995	0.083329998	0.000000000
0.333330810	0.166669190	0.084129207
0.250002354	0.999997675	0.168073788

0.666670024	0.083329998	0.000000000
0.583330810	0.166669190	0.084129207
0.500002325	0.999997675	0.168073788
0.916670024	0.083329998	0.000000000
0.833330810	0.166669190	0.084129207
0.750002325	0.999997675	0.168073788
0.166669995	0.333330005	0.000000000
0.083330803	0.416669190	0.084129207
0.000002350	0.249997646	0.168073788
0.416669995	0.333330005	0.000000000
0.333330810	0.416669190	0.084129207
0.250002354	0.249997646	0.168073788
0.666670024	0.333330005	0.000000000
0.583330810	0.416669190	0.084129207
0.500002325	0.249997646	0.168073788
0.916670024	0.333330005	0.000000000
0.833330810	0.416669190	0.084129207
0.750002325	0.249997646	0.168073788
0.166669995	0.583329976	0.000000000
0.083330803	0.666669190	0.084129207
0.000002350	0.499997646	0.168073788
0.416669995	0.583329976	0.000000000
0.333330810	0.666669190	0.084129207
0.250002354	0.499997646	0.168073788
0.666670024	0.583329976	0.000000000
0.583330810	0.666669190	0.084129207
0.500002325	0.499997646	0.168073788
0.916670024	0.583329976	0.000000000
0.833330810	0.666669190	0.084129207
0.750002325	0.499997646	0.168073788

0.166669995	0.833329976	0.000000000
0.083330803	0.916669190	0.084129207
0.000002350	0.749997675	0.168073788
0.416669995	0.833329976	0.000000000
0.333330810	0.916669190	0.084129207
0.250002354	0.749997675	0.168073788
0.666670024	0.833329976	0.000000000
0.583330810	0.916669190	0.084129207
0.500002325	0.749997675	0.168073788
0.916670024	0.833329976	0.000000000
0.833330810	0.916669190	0.084129207
0.750002325	0.749997675	0.168073788

Ni(111)-OH

1.0

9.9672002792	0.000000000	0.000000000
-4.9836001396	8.6318486464	0.000000000
0.000000000	0.000000000	26.1037006378

Ni	H	O
64	1	1

Direct

0.000000000	0.000000000	0.000000000
0.000000000	0.250000000	0.000000000
0.000000000	0.500000000	0.000000000
0.000000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.250000000	0.000000000
0.250000000	0.500000000	0.000000000
0.250000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000

0.500000000	0.250000000	0.000000000
0.500000000	0.500000000	0.000000000
0.500000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.250000000	0.000000000
0.750000000	0.500000000	0.000000000
0.750000000	0.750000000	0.000000000
0.166669995	0.083329998	0.077940002
0.166669995	0.333330005	0.077940002
0.166669995	0.583329976	0.077940002
0.166669995	0.833329976	0.077940002
0.416669995	0.083329998	0.077940002
0.416669995	0.333330005	0.077940002
0.416669995	0.583329976	0.077940002
0.416669995	0.833329976	0.077940002
0.666670024	0.083329998	0.077940002
0.666670024	0.333330005	0.077940002
0.666670024	0.583329976	0.077940002
0.666670024	0.833329976	0.077940002
0.916670024	0.083329998	0.077940002
0.916670024	0.333330005	0.077940002
0.916670024	0.583329976	0.077940002
0.916670024	0.833329976	0.077940002
0.083463669	0.167203575	0.154920295
0.086314164	0.418369710	0.156391487
0.083464958	0.666498840	0.154926538
0.083526291	0.916964829	0.155254304
0.333925337	0.167235717	0.154946044
0.333994806	0.417643666	0.155692726
0.333900601	0.666599989	0.155581772

0.334012300	0.917061269	0.154925078
0.583594203	0.166996688	0.154858500
0.582242370	0.418290198	0.156396389
0.582917869	0.666611493	0.155604944
0.582257152	0.914508820	0.156269103
0.833573759	0.167051822	0.154810205
0.833639205	0.416911483	0.154851109
0.833242118	0.666511893	0.154926240
0.833292186	0.917060673	0.154889539
0.250297070	0.000517439	0.231937602
0.247426644	0.244815230	0.231093302
0.242298096	0.496681958	0.234775633
0.247443631	0.753468513	0.231044203
0.500743449	0.002795652	0.231730998
0.500508964	0.248862341	0.231824532
0.504487693	0.496783257	0.234718665
0.504535913	0.758943379	0.234462902
0.752213478	0.002687937	0.231694117
0.750374675	0.250551164	0.231610566
0.752113640	0.500251770	0.231796354
0.756170869	0.753434837	0.231016204
0.000378249	0.000500350	0.231892556
0.998305798	0.248820588	0.231774509
0.998279929	0.500289142	0.231795773
0.000315101	0.750519156	0.231929943
0.420124590	0.588780522	0.320294440
0.417835891	0.585329056	0.283004314

Ni(111)-H₂O

1.0

9.9672002792	0.0000000000	0.0000000000
-4.9836001396	8.6318486464	0.0000000000
0.0000000000	0.0000000000	26.1037006378

Ni	O	H
64	1	2

Direct

0.0000000000	0.0000000000	0.0000000000
0.0000000000	0.2500000000	0.0000000000
0.0000000000	0.5000000000	0.0000000000
0.0000000000	0.7500000000	0.0000000000
0.2500000000	0.0000000000	0.0000000000
0.2500000000	0.2500000000	0.0000000000
0.2500000000	0.5000000000	0.0000000000
0.2500000000	0.7500000000	0.0000000000
0.5000000000	0.0000000000	0.0000000000
0.5000000000	0.2500000000	0.0000000000
0.5000000000	0.5000000000	0.0000000000
0.5000000000	0.7500000000	0.0000000000
0.7500000000	0.0000000000	0.0000000000
0.7500000000	0.2500000000	0.0000000000
0.7500000000	0.5000000000	0.0000000000
0.7500000000	0.7500000000	0.0000000000
0.166667506	0.083332501	0.077940002
0.166667506	0.333332509	0.077940002
0.166667506	0.583332479	0.077940002
0.166667506	0.833332479	0.077940002
0.416667491	0.083332501	0.077940002
0.416667491	0.333332509	0.077940002
0.416667491	0.583332479	0.077940002
0.416667491	0.833332479	0.077940002

0.666667521	0.083332501	0.077940002
0.666667521	0.333332509	0.077940002
0.666667521	0.583332479	0.077940002
0.666667521	0.833332479	0.077940002
0.916667521	0.083332501	0.077940002
0.916667521	0.333332509	0.077940002
0.916667521	0.583332479	0.077940002
0.916667521	0.833332479	0.077940002
0.083364956	0.166882098	0.155027032
0.083128318	0.416441858	0.154925108
0.083298869	0.666645050	0.155203149
0.083261132	0.916704476	0.155179769
0.333342344	0.166759431	0.155044496
0.334672421	0.417378783	0.156046882
0.333355874	0.666734397	0.154916018
0.333348125	0.916683733	0.155195877
0.583368540	0.166925177	0.155086875
0.582501113	0.417492032	0.156245485
0.582690299	0.665428519	0.155970171
0.583511829	0.916728795	0.154975846
0.833281159	0.166653946	0.155141205
0.833065152	0.416571617	0.155058473
0.833290756	0.666620672	0.154958695
0.833203077	0.916808128	0.154926851
0.249701887	0.999535501	0.231863022
0.248188570	0.248115227	0.231419787
0.247992039	0.500366867	0.231147096
0.249822035	0.750096977	0.231940046
0.500126719	0.999945343	0.231894866
0.499626458	0.248058259	0.231567353

0.499928355	0.499824971	0.236716017
0.499573797	0.751675069	0.231277213
0.749986053	0.999997377	0.231844470
0.750065029	0.249945477	0.231809005
0.752077699	0.500560343	0.231474176
0.752164364	0.751865923	0.231182516
0.999766767	0.000078417	0.231874168
0.999867320	0.250074327	0.231835127
0.999958098	0.499875754	0.231909513
0.000304388	0.750219703	0.231913775
0.497871131	0.508066952	0.319146186
0.404083729	0.513493955	0.326220989
0.584516287	0.611708522	0.326838493

Ce@Ni-H_{top}

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	H
63	1	1

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.082959861	0.167101353	0.187563896
0.999879003	0.000160004	0.284015030
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334000379	0.167902663	0.188030154
0.250428379	0.000212882	0.283419907

0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.584310353	0.167058930	0.187447518
0.500709713	0.000000000	0.283940703
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833406329	0.166525677	0.188678786
0.749345601	0.998291433	0.283342779
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.082971260	0.415675759	0.187560067
0.001674469	0.250618786	0.283373624
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335765690	0.417827427	0.190166667
0.248169184	0.245886058	0.282071441
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582178652	0.417823583	0.190152302
0.498359531	0.245692894	0.281994611
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.832865238	0.415602118	0.187458411
0.749378145	0.250630319	0.283318430
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.083238818	0.666403830	0.188237116
0.999928653	0.499297291	0.283957571
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003

0.333934128	0.665945232	0.188092738
0.247950792	0.501659811	0.282128870
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582192063	0.664252996	0.190172821
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832204700	0.666069508	0.188009053
0.754440606	0.501793683	0.281984925
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083233856	0.916771531	0.188290626
0.999913394	0.749737859	0.283399343
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333520591	0.916639149	0.188294128
0.250284165	0.749542475	0.283485562
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.584245622	0.916956604	0.187551647
0.498246789	0.751933038	0.282109648
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832884610	0.917085946	0.187530532
0.754325151	0.752034426	0.282027215
0.500657678	0.499932587	0.357935756
0.502430856	0.495588422	0.458124191

Ce@Ni-H_{bridge}

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	H
63	1	1

Direct

0.0000000000	0.0000000000	0.0000000000
0.166779995	0.083520003	0.094250001
0.082303122	0.167558283	0.187302843
0.999574780	0.000453051	0.284172684
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.333706647	0.167828247	0.187822819
0.249415025	0.999579191	0.283394039
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.584515154	0.167601481	0.187553123
0.500496626	0.000985139	0.283956796
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833267987	0.167635649	0.188494459
0.749515831	0.000274818	0.283235162
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.082808442	0.416100889	0.187543437
0.999951303	0.249221236	0.283049494
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335274458	0.418042302	0.190600961
0.244555041	0.242512405	0.281582296

0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582347989	0.418136537	0.190253988
0.496879816	0.244085789	0.281764716
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.834036529	0.416817635	0.187790528
0.749210656	0.251454175	0.283260822
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.083369710	0.666402221	0.188221887
0.998487949	0.498889983	0.284869105
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334084064	0.666400313	0.187830716
0.248108074	0.501174927	0.282549232
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.581716299	0.664415538	0.190345511
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832269132	0.666393101	0.187812388
0.755662799	0.503417730	0.281901419
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083063014	0.916706562	0.188225821
0.999932051	0.751064062	0.283218414
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333026856	0.916138887	0.188548952

0.250321031	0.751921356	0.284327805
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.584139466	0.917869210	0.187319934
0.500043690	0.756459534	0.281686366
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832747638	0.917668343	0.187510043
0.756403208	0.755224526	0.281903028
0.499428958	0.500284076	0.339238882
0.169174597	0.583553612	0.327574819

Ce@Ni-H_{hcp}

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	H
63	1	1

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.083734907	0.167607665	0.187554151
0.000169635	0.999584198	0.283992678
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334174424	0.168223485	0.188173696
0.250572681	0.999496043	0.283349514
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001

0.585196018	0.167300373	0.187604129
0.501141489	0.000574224	0.284167141
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.835192382	0.167561889	0.188747689
0.750721276	0.999769151	0.283186078
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.083829314	0.416108310	0.187596351
0.000380231	0.250118762	0.284013331
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.336309582	0.418039560	0.189881966
0.248808339	0.244671553	0.282931864
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582770526	0.418033272	0.190275177
0.499249101	0.244243264	0.281924456
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833803892	0.415757000	0.187276155
0.750800133	0.250940472	0.283172518
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.083865456	0.666383505	0.188215971
0.000350684	0.500456512	0.283948690
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333998382	0.665776670	0.188226640
0.248984322	0.503971279	0.282925695

0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582636952	0.664623141	0.190260723
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832723618	0.666406989	0.187692404
0.757992506	0.502254486	0.281584978
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083856709	0.917378485	0.188284904
0.001653174	0.750692070	0.283457875
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.334281206	0.917067349	0.188269481
0.250748456	0.750954568	0.283364803
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.585132539	0.917728424	0.187603891
0.499252737	0.755076170	0.281959355
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.833871841	0.918067217	0.187321588
0.757841825	0.755466163	0.281504542
0.506375134	0.502919376	0.339758992
0.175562114	0.337571084	0.326374769

Ce@Ni-H_{fcc}

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000

	0.0000000000	0.0000000000	21.1434993744
Ni	Ce	H	
63	1	1	
Direct			
	0.0000000000	0.0000000000	0.0000000000
	0.166779995	0.083520003	0.094250001
	0.082899764	0.167159468	0.187429994
	0.999894381	0.000011209	0.284096658
	0.250000000	0.000000000	0.000000000
	0.416740000	0.083520003	0.094250001
	0.333930582	0.167472541	0.187782675
	0.249784693	0.998792470	0.283369541
	0.500000000	0.000000000	0.000000000
	0.666630030	0.083310001	0.093910001
	0.584472239	0.166355118	0.187383175
	0.501702309	0.001425616	0.283938259
	0.750000000	0.000000000	0.000000000
	0.916689992	0.083310001	0.093910001
	0.833492875	0.166404739	0.188546851
	0.750123978	0.998836517	0.283159465
	0.000000000	0.250000000	0.000000000
	0.167219996	0.333609998	0.094010003
	0.083631434	0.415813327	0.187816083
	0.001119017	0.249778658	0.283161432
	0.250000000	0.250000000	0.000000000
	0.416880012	0.333759993	0.094740003
	0.335654318	0.417789966	0.190369457
	0.246177137	0.243228987	0.281849116
	0.500000000	0.250000000	0.000000000
	0.666390002	0.333609998	0.094010003

0.582325995	0.417644739	0.190386623
0.497885555	0.242513061	0.281546414
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833528757	0.415419847	0.187372386
0.749707222	0.250071317	0.283144802
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.083788022	0.666227520	0.188375726
0.998537481	0.498250663	0.283952951
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333973855	0.665883839	0.187808260
0.245666832	0.500109911	0.283264935
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582192540	0.664322734	0.190344647
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832455039	0.665984869	0.187785611
0.757557929	0.501989603	0.281577349
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083414182	0.916589797	0.188322574
0.001232669	0.750246108	0.283373713
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333686441	0.916129351	0.188349098
0.249483347	0.750443220	0.284458429
0.500000000	0.750000000	0.000000000

0.666390002	0.832780004	0.094010003
0.584180832	0.916302562	0.187787190
0.499818265	0.754239976	0.283239961
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832801402	0.917041481	0.187424600
0.756702065	0.753699601	0.281840235
0.503038645	0.497294813	0.339625210
0.337642133	0.662460029	0.328330576

Ce@Ni-OH_{top}

1.0

10.032299954	0.000000000	0.000000000
-5.0161499977	8.6882266544	0.000000000
0.000000000	0.000000000	21.1434993744

Ni	Ce	O	H
----	----	---	---

63	1	1	1
----	---	---	---

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.082859308	0.167173341	0.187517345
0.999794602	0.000361790	0.283973813
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.333792835	0.167927653	0.188073039
0.250083625	0.000492928	0.283644527
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.584214211	0.167145386	0.187495172
0.500482261	0.000382603	0.283998877

0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833284795	0.166745678	0.188686863
0.749290764	0.998650789	0.283340603
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.082885161	0.415852576	0.187539861
0.001439154	0.250816196	0.283350497
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335598737	0.417903095	0.190288052
0.247663230	0.246084481	0.282128334
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.581960917	0.417869866	0.190235838
0.497993261	0.245710716	0.281998992
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.832879663	0.415760726	0.187475920
0.749214828	0.250806481	0.283353299
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.083252832	0.666584730	0.188349143
0.999770999	0.499618441	0.284000903
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333930641	0.666169405	0.188031077
0.247761503	0.502262235	0.282067686
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003

0.582018018	0.664193571	0.190251604
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832165658	0.666151762	0.187987119
0.754217982	0.501878142	0.281926066
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083259098	0.916756034	0.188294172
0.999472857	0.749844193	0.283566236
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333385974	0.916785061	0.188348576
0.249936596	0.750146151	0.283658743
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.584282517	0.917201579	0.187456787
0.498007774	0.752845705	0.281935394
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832889378	0.917252302	0.187453568
0.754273236	0.752554476	0.281887174
0.502821743	0.501980662	0.360215187
0.522086382	0.513689101	0.461301714
0.543763459	0.526956618	0.506205082

Ce@Ni-OH_{bridge}

1.0

10.0322999954	0.000000000	0.000000000
-5.0161499977	8.6882266544	0.000000000
0.000000000	0.000000000	21.1434993744

Ni	Ce	O	H
63	1	1	1

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.082814604	0.167226627	0.187084109
0.998960435	0.999212086	0.283930182
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334201634	0.167718723	0.187641814
0.250049323	0.999215364	0.283406258
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.584710300	0.167785078	0.187567681
0.500900507	0.001159188	0.283756316
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833629131	0.167333320	0.188200533
0.749720454	0.999428809	0.283099711
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.086002536	0.417291015	0.189006805
0.998230696	0.247727245	0.282335371
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335982770	0.418179125	0.191284642
0.244336426	0.239532128	0.280809999
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582424521	0.417908549	0.190323055

0.497161031	0.245457008	0.282037556
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833913684	0.415505260	0.186947376
0.749306440	0.250708193	0.283326834
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.083446488	0.666231632	0.188096777
0.998646855	0.499486029	0.283571422
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333072990	0.664841592	0.188826680
0.246490881	0.501458526	0.286416411
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.581824243	0.663517654	0.190142289
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832442582	0.666559219	0.187749922
0.758767605	0.502336681	0.280759513
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083213121	0.916668653	0.188239142
0.000445289	0.750555217	0.283535480
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.334106177	0.916899562	0.188030452
0.250084728	0.752233148	0.282686561
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003

0.584354222	0.917621017	0.186927870
0.502094686	0.757481217	0.280581713
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.833034515	0.917530298	0.187287375
0.755072773	0.753235519	0.281729102
0.503949046	0.500365555	0.347252518
0.277875304	0.490451813	0.380927473
0.177174479	0.410352409	0.395569801

Ce@Ni-OH_{hcp}

1.0

10.032299954	0.000000000	0.000000000
-5.0161499977	8.6882266544	0.000000000
0.000000000	0.000000000	21.1434993744

Ni	Ce	O	H
63	1	1	1

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.084127143	0.167238355	0.188004062
0.998888969	0.999051511	0.283740908
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.332546055	0.168148682	0.189152315
0.249815583	0.998796403	0.283316493
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.583253801	0.166482791	0.187393159
0.500000954	0.999456108	0.283966422

0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.831920147	0.165824741	0.187598214
0.747498393	0.997016430	0.283171982
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.084038243	0.416174918	0.188073039
0.990509748	0.244583279	0.280413985
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.336026430	0.417674571	0.190574750
0.246615812	0.244452074	0.284831196
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582177520	0.417678773	0.190363154
0.499449283	0.244653359	0.281997144
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833135843	0.414690524	0.186820045
0.748037338	0.249446794	0.283167958
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082918197	0.665867269	0.188151389
0.999119222	0.499019831	0.283798486
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.332243145	0.663378298	0.189259216
0.246738762	0.500559866	0.285087913
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003

0.582086980	0.663818717	0.190177605
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832452536	0.666124761	0.187521100
0.759487152	0.501755297	0.280685514
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.082998395	0.916673303	0.188208207
0.001205369	0.750226796	0.283646017
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333220840	0.916236877	0.188184440
0.249473631	0.749705255	0.283295363
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.583083272	0.916005135	0.187427387
0.499004662	0.752645731	0.281982243
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.833146632	0.918183208	0.186818615
0.758930266	0.756348550	0.280634046
0.522025526	0.509800196	0.345454097
0.253655076	0.374768227	0.364276946
0.152597368	0.322701752	0.384286106

Ce@Ni-OH_{fcc}

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	1	1

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.082974531	0.167385593	0.187456623
0.999616146	0.000273160	0.284142166
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.333535492	0.167989299	0.187554404
0.249329492	0.000919708	0.283510089
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.585361063	0.166835591	0.186982423
0.500360012	0.001869753	0.283806294
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833686173	0.166271210	0.188238159
0.750718057	0.000165219	0.283224195
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.086487241	0.417612523	0.189326033
0.999651611	0.249206647	0.283206046
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.336140424	0.418433130	0.191333488
0.246039078	0.243416771	0.281974405
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.582389891	0.417736024	0.190020621

0.496945024	0.240889639	0.280389965
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833186388	0.414613217	0.186968535
0.749498904	0.250459701	0.283066481
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.081806570	0.665445387	0.187607944
0.998228490	0.499651253	0.283808500
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333799720	0.666072786	0.188197792
0.243232593	0.501441360	0.285105705
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.581527829	0.663844109	0.191320360
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832068801	0.666492939	0.187535837
0.759343565	0.503110170	0.280363441
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.082937293	0.917113483	0.188203126
0.999228954	0.750726640	0.283519298
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.334570616	0.918198884	0.187591046
0.244858742	0.755434871	0.280432701
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003

0.582360268	0.913480937	0.189357594
0.498462588	0.756590903	0.285162926
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832612574	0.917055964	0.187486082
0.756576896	0.753635168	0.281950653
0.511489630	0.488777399	0.344589174
0.376823992	0.620852709	0.364345461
0.327405185	0.671358407	0.385265917

Ce@Ni-O_{top}

1.0

10.032299954	0.000000000	0.000000000
-5.0161499977	8.6882266544	0.000000000
0.000000000	0.000000000	21.1434993744

Ni	Ce	O
63	1	1

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.083663568	0.167080879	0.189813644
0.000466483	0.999495566	0.287390649
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.334717125	0.167670414	0.190198749
0.250257641	0.998180628	0.287109613
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.585377276	0.166974127	0.189743832
0.502383053	0.001027515	0.287276655

0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833947062	0.166129082	0.190843061
0.750548303	0.998175561	0.286442578
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.084065616	0.415512145	0.190109134
0.001405442	0.249027491	0.286370754
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335649431	0.417525232	0.193003654
0.247388616	0.243563756	0.285763353
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.583101690	0.417211026	0.192664981
0.498383135	0.243692189	0.285451949
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833506584	0.415084809	0.189719871
0.750174761	0.249830306	0.286604106
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.084242068	0.666140497	0.191188321
0.998861611	0.497577459	0.287177593
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334401429	0.665642798	0.190569758
0.246601313	0.500072002	0.287142128
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003

0.582722425	0.664656043	0.193023548
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832686484	0.665612221	0.190219596
0.756211877	0.501766443	0.285444617
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.084227934	0.916482091	0.190689251
0.001664787	0.749927580	0.287005514
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.334375978	0.916134536	0.191200033
0.250308067	0.749420702	0.288490951
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.584739208	0.916097105	0.190142810
0.499171942	0.753058970	0.287173390
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.833186090	0.916480660	0.189850390
0.756119072	0.752515197	0.285801381
0.501972198	0.497013688	0.353387058
0.501992464	0.496765673	0.453208596

Ce@Ni-O_{bridge}

1.0

10.032299954	0.000000000	0.000000000
-5.0161499977	8.6882266544	0.000000000
0.000000000	0.000000000	21.1434993744

Ni Ce O

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.083295666	0.167024031	0.187413722
0.999964178	0.999683738	0.284054160
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.333652109	0.167361945	0.187601864
0.249765620	0.999243200	0.283630162
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.585241854	0.166359290	0.186814055
0.501883507	0.001002070	0.282928556
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833758652	0.166090399	0.188212499
0.751199424	0.999549806	0.282856315
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.086308539	0.417014539	0.188857988
0.000393617	0.248862222	0.282889813
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335817993	0.417730659	0.190708205
0.247683600	0.241754889	0.282025546
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.581941366	0.417655826	0.189966887
0.497458696	0.241110399	0.280273855

0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.833447635	0.414775342	0.186838761
0.749671876	0.250128657	0.282724947
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.083202027	0.665774405	0.187919229
0.998665810	0.498170435	0.282841146
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.334177077	0.665810645	0.188524976
0.244507551	0.497245401	0.285938680
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582041085	0.664003968	0.190663978
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832188010	0.666052520	0.187577158
0.758051455	0.502008975	0.280417502
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083310127	0.916322172	0.188270584
0.999848604	0.749498904	0.283557385
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.334283113	0.916836441	0.187985063
0.246568710	0.753166914	0.282072484
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.582904875	0.913671911	0.188872129

0.502983928	0.755482554	0.285935968
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832953453	0.916593909	0.187482581
0.757397950	0.751566350	0.282076687
0.515162587	0.480999947	0.355228156
0.391797483	0.608761787	0.349788487

Ce@Ni-O_{hcp}

1.0

10.032299954	0.000000000	0.000000000
-5.0161499977	8.6882266544	0.000000000
0.000000000	0.000000000	21.1434993744

Ni	Ce	O
63	1	1

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.083419941	0.166969076	0.188239813
0.996975899	0.996815085	0.283028543
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.332443088	0.167938277	0.188840717
0.248977661	0.998653173	0.283028573
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.582783997	0.166565388	0.187387988
0.499584079	0.999760032	0.283773273
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001

0.832393110	0.166112989	0.188177854
0.746861577	0.996789932	0.283107758
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.083442748	0.416094661	0.188331053
0.991132736	0.245360598	0.282198846
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.333409607	0.416676074	0.189858541
0.244961232	0.242884710	0.285587996
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.580744803	0.417588055	0.190053314
0.499372184	0.246113971	0.282098293
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.832427919	0.414866745	0.186955065
0.746909857	0.249867067	0.283118397
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082736425	0.665984273	0.188051224
0.997268856	0.499752283	0.282967508
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.332373917	0.664310217	0.188870803
0.245723933	0.501942396	0.285696119
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.580835581	0.663071632	0.190051422
0.750000000	0.500000000	0.000000000

0.916480005	0.583260000	0.094250001
0.831865609	0.665912569	0.187509269
0.754712105	0.501209736	0.280774444
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.082781605	0.916597188	0.188035101
0.998987079	0.749271393	0.283567637
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333022296	0.916468680	0.188130602
0.248833060	0.750072360	0.283075303
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.582909524	0.916146398	0.187388152
0.499209464	0.753042221	0.282067001
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832426131	0.917496443	0.186933979
0.754496872	0.753152072	0.280822605
0.523144603	0.511097431	0.354999065
0.270591050	0.384820759	0.350462049

Ce@Ni-O_{fcc}

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O
63	1	1

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.082714520	0.167531088	0.187484130
0.999271214	0.000781816	0.283966213
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.333105534	0.168010473	0.187713936
0.249342546	0.001127384	0.283490449
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.584555268	0.167218447	0.186900422
0.501083434	0.003235544	0.282935262
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833070636	0.166974366	0.188166946
0.750213563	0.001058105	0.282800317
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.085328974	0.417420626	0.188807011
0.998947799	0.249702081	0.282809317
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003
0.335147142	0.418493271	0.190777078
0.246734664	0.244227141	0.282162964
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.581577122	0.418496370	0.189822212
0.496447325	0.244160429	0.280581981
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001

0.832786918	0.415445149	0.186922312
0.748171747	0.251830876	0.283016115
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.082866780	0.666230679	0.188069418
0.996879816	0.498970538	0.282982260
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333786249	0.666193128	0.188460931
0.242189080	0.498493373	0.285845160
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.581726193	0.664947629	0.190771505
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832009971	0.666963995	0.187750190
0.756017745	0.503603578	0.280616254
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.082874440	0.917035162	0.188171893
0.998838186	0.750693917	0.283508658
0.250000000	0.750000000	0.000000000
0.416740000	0.833220005	0.094250001
0.333778560	0.917109549	0.188037187
0.245573819	0.754372597	0.282424599
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.582674623	0.914697468	0.188768625
0.501456439	0.757923424	0.285831690
0.750000000	0.750000000	0.000000000

0.916480005	0.833220005	0.094250001
0.832524240	0.917345166	0.187469527
0.756072044	0.753598571	0.282210201
0.513758659	0.486921102	0.355390370
0.387978941	0.611906528	0.349835753

Ce@Ni-OH_{top}

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	1	1

Direct

0.000000000	0.000000000	0.000000000
0.166779995	0.083520003	0.094250001
0.082859308	0.167173341	0.187517345
0.999794602	0.000361790	0.283973813
0.250000000	0.000000000	0.000000000
0.416740000	0.083520003	0.094250001
0.333792835	0.167927653	0.188073039
0.250083625	0.000492928	0.283644527
0.500000000	0.000000000	0.000000000
0.666630030	0.083310001	0.093910001
0.584214211	0.167145386	0.187495172
0.500482261	0.000382603	0.283998877
0.750000000	0.000000000	0.000000000
0.916689992	0.083310001	0.093910001
0.833284795	0.166745678	0.188686863
0.749290764	0.998650789	0.283340603
0.000000000	0.250000000	0.000000000
0.167219996	0.333609998	0.094010003
0.082885161	0.415852576	0.187539861
0.001439154	0.250816196	0.283350497
0.250000000	0.250000000	0.000000000
0.416880012	0.333759993	0.094740003

0.335598737	0.417903095	0.190288052
0.247663230	0.246084481	0.282128334
0.500000000	0.250000000	0.000000000
0.666390002	0.333609998	0.094010003
0.581960917	0.417869866	0.190235838
0.497993261	0.245710716	0.281998992
0.750000000	0.250000000	0.000000000
0.916689992	0.333370000	0.093910001
0.832879663	0.415760726	0.187475920
0.749214828	0.250806481	0.283353299
0.000000000	0.500000000	0.000000000
0.166779995	0.583260000	0.094250001
0.083252832	0.666584730	0.188349143
0.999770999	0.499618441	0.284000903
0.250000000	0.500000000	0.000000000
0.416880012	0.583119988	0.094740003
0.333930641	0.666169405	0.188031077
0.247761503	0.502262235	0.282067686
0.500000000	0.500000000	0.000000000
0.666239977	0.583119988	0.094740003
0.582018018	0.664193571	0.190251604
0.750000000	0.500000000	0.000000000
0.916480005	0.583260000	0.094250001
0.832165658	0.666151762	0.187987119
0.754217982	0.501878142	0.281926066
0.000000000	0.750000000	0.000000000
0.166669995	0.833329976	0.094530001
0.083259098	0.916756034	0.188294172
0.999472857	0.749844193	0.283566236
0.250000000	0.750000000	0.000000000

0.416740000	0.833220005	0.094250001
0.333385974	0.916785061	0.188348576
0.249936596	0.750146151	0.283658743
0.500000000	0.750000000	0.000000000
0.666390002	0.832780004	0.094010003
0.584282517	0.917201579	0.187456787
0.498007774	0.752845705	0.281935394
0.750000000	0.750000000	0.000000000
0.916480005	0.833220005	0.094250001
0.832889378	0.917252302	0.187453568
0.754273236	0.752554476	0.281887174
0.502821743	0.501980662	0.360215187
0.522086382	0.513689101	0.461301714
0.543763459	0.526956618	0.506205082

Ni-Volmer-IS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	O	H
64	1	2

Direct

0.000000000	0.000000000	0.000000000
0.166966975	0.083481900	0.094098732
0.083841257	0.167214528	0.189160973
0.000023622	0.999908924	0.283802539
0.250000000	0.000000000	0.000000000
0.416802704	0.083385281	0.094117306
0.333527446	0.166508034	0.189204141

0.249876678	0.999269962	0.283665657
0.500000000	0.000000000	0.000000000
0.666765332	0.083373144	0.094243102
0.583771169	0.167167589	0.189368039
0.500377357	0.999833703	0.283900499
0.750000000	0.000000000	0.000000000
0.916769683	0.083359189	0.094184540
0.833691478	0.166780636	0.189313143
0.750500977	0.000055089	0.283665687
0.000000000	0.250000000	0.000000000
0.167537093	0.333773255	0.094466045
0.083947890	0.416368365	0.189246371
0.000582825	0.250114083	0.283660889
0.250000000	0.250000000	0.000000000
0.417030334	0.333565265	0.094442852
0.335441381	0.417564929	0.190665513
0.248533219	0.247872189	0.282991320
0.500000000	0.250000000	0.000000000
0.666416705	0.333663493	0.094574347
0.582812548	0.417383999	0.190848708
0.499818116	0.247783110	0.283286572
0.750000000	0.250000000	0.000000000
0.916728258	0.333298117	0.094242938
0.833123267	0.416456044	0.189367563
0.750641167	0.249795884	0.283615798
0.000000000	0.500000000	0.000000000
0.166899711	0.583367407	0.094132140
0.083583198	0.666665733	0.189432070
0.000335900	0.499860018	0.283897758
0.250000000	0.500000000	0.000000000

0.416903883	0.583263040	0.094420239
0.333610326	0.666777730	0.189194202
0.248734236	0.500325680	0.283086389
0.500000000	0.500000000	0.000000000
0.666480541	0.583062530	0.094458424
0.582729280	0.665019810	0.190662861
0.500481367	0.499629527	0.289492995
0.750000000	0.500000000	0.000000000
0.916703105	0.583246827	0.094103418
0.833660901	0.666700840	0.189187393
0.752309144	0.500447273	0.283200622
0.000000000	0.750000000	0.000000000
0.166773513	0.833331823	0.094435155
0.083695024	0.916597486	0.189351439
0.000774913	0.750208676	0.283647478
0.250000000	0.750000000	0.000000000
0.416853040	0.833340585	0.094109066
0.333492458	0.916582584	0.189432472
0.250356734	0.749857068	0.283715636
0.500000000	0.750000000	0.000000000
0.666352987	0.832543552	0.094503038
0.583956540	0.916445315	0.189264804
0.500196397	0.751586974	0.283125371
0.750000000	0.750000000	0.000000000
0.916660309	0.833163500	0.094100766
0.833265066	0.916599214	0.189140797
0.752237558	0.751522541	0.282945275
0.502147973	0.498415977	0.391016960
0.550018430	0.607171714	0.402812928
0.393738240	0.451927841	0.403205603

Ni-Volmer-TS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni O H

64 1 2

Direct

0.000000000	0.000000000	0.000000000
0.167130545	0.084153689	0.094077237
0.083455369	0.167776182	0.188929647
0.999743283	0.999762535	0.283724338
0.250000000	0.000000000	0.000000000
0.417416155	0.084038951	0.094195299
0.334980786	0.167621523	0.188911930
0.250443012	0.998699903	0.283580512
0.500000000	0.000000000	0.000000000
0.667213976	0.084555738	0.094263434
0.584370196	0.169073924	0.189756230
0.501222134	0.001836917	0.283672899
0.750000000	0.000000000	0.000000000
0.916560709	0.084025688	0.093932092
0.834634840	0.168772534	0.189159945
0.751571178	0.002238280	0.283455342
0.000000000	0.250000000	0.000000000
0.166418806	0.334119111	0.094687060
0.087536566	0.419746757	0.191448689
0.999185383	0.249068454	0.283294439
0.250000000	0.250000000	0.000000000

0.417106062	0.334284097	0.094217427
0.332552284	0.417515218	0.189973980
0.248949423	0.241683275	0.282447129
0.500000000	0.250000000	0.000000000
0.667361140	0.334529519	0.094834358
0.583166718	0.418920517	0.190340891
0.499764562	0.250517815	0.285041034
0.750000000	0.250000000	0.000000000
0.917718649	0.334737182	0.094371386
0.835094571	0.418588161	0.189544901
0.750550389	0.251263529	0.283628166
0.000000000	0.500000000	0.000000000
0.167124033	0.583826005	0.094588339
0.084719017	0.668487906	0.189495519
0.000405669	0.501059890	0.284099668
0.250000000	0.500000000	0.000000000
0.416676790	0.583889127	0.094388105
0.333889544	0.666689873	0.190421075
0.251094460	0.502692819	0.290003836
0.500000000	0.500000000	0.000000000
0.667075515	0.583737254	0.094187140
0.584392130	0.668098986	0.189010665
0.503513873	0.500810087	0.284538001
0.750000000	0.500000000	0.000000000
0.917357683	0.584048867	0.094163015
0.834352314	0.667921364	0.189177513
0.752416909	0.501575232	0.283595294
0.000000000	0.750000000	0.000000000
0.167332575	0.834192336	0.094370671
0.084632680	0.918024063	0.189353451

0.000572681	0.750755548	0.283711553
0.250000000	0.750000000	0.000000000
0.416774154	0.833370566	0.094132669
0.334843427	0.917549491	0.189238846
0.250676155	0.752147317	0.283591151
0.500000000	0.750000000	0.000000000
0.667162776	0.834278524	0.094022229
0.584533751	0.918369949	0.188791052
0.505325854	0.757249355	0.282180786
0.750000000	0.750000000	0.000000000
0.917074680	0.833992064	0.094110489
0.833981276	0.918119431	0.189140245
0.752134323	0.751848638	0.283143163
0.349882126	0.472524673	0.367867857
0.430969894	0.557244897	0.392648399
0.387985766	0.369745165	0.340794533

Ni-Volmer-FS

1.0

10.0322999954	0.000000000	0.000000000
-5.0161499977	8.6882266544	0.000000000
0.000000000	0.000000000	21.1434993744

Ni	O	H
64	1	2

Direct

0.000000000	0.000000000	0.000000000
0.166323796	0.083380356	0.094039097
0.083364472	0.167048678	0.189408526
0.998982012	0.999337673	0.283707619
0.250000000	0.000000000	0.000000000

0.416846335	0.083590508	0.094099671
0.333197922	0.166606531	0.189051911
0.248453811	0.997822225	0.283434898
0.500000000	0.000000000	0.000000000
0.666595995	0.083317608	0.094046213
0.582931101	0.167246208	0.189048469
0.500109196	0.001994407	0.283005506
0.750000000	0.000000000	0.000000000
0.916109622	0.083306111	0.094144367
0.832810163	0.166704431	0.188986152
0.751696348	0.002360794	0.283386171
0.000000000	0.250000000	0.000000000
0.166211203	0.333391249	0.094748311
0.085385948	0.417611331	0.190714806
0.997811019	0.248316094	0.283411801
0.250000000	0.250000000	0.000000000
0.416685462	0.333736002	0.094516382
0.332111388	0.416828811	0.190355599
0.246195570	0.243244857	0.284272373
0.500000000	0.250000000	0.000000000
0.666089296	0.333316684	0.094697155
0.580695331	0.417955220	0.191288158
0.500556529	0.246950075	0.284627199
0.750000000	0.250000000	0.000000000
0.916354239	0.333127201	0.094156533
0.832100689	0.416283429	0.188963175
0.749741137	0.249942586	0.283262730
0.000000000	0.500000000	0.000000000
0.166312397	0.582816541	0.094207063
0.082708292	0.666328490	0.188794255

0.996716797	0.499476314	0.283325791
0.250000000	0.500000000	0.000000000
0.416521966	0.583197117	0.094380222
0.333053529	0.666128099	0.189662561
0.240020543	0.497622132	0.287015140
0.500000000	0.500000000	0.000000000
0.665958703	0.582750380	0.094407886
0.581321776	0.665112555	0.190350339
0.502702355	0.496734232	0.289585114
0.750000000	0.500000000	0.000000000
0.916137516	0.582972467	0.094042845
0.832236588	0.665933132	0.189005643
0.752087712	0.500514030	0.283504546
0.000000000	0.750000000	0.000000000
0.166380689	0.833242357	0.094080113
0.082938626	0.916538835	0.189248562
0.998959720	0.749665380	0.283471256
0.250000000	0.750000000	0.000000000
0.416747242	0.833211005	0.094266772
0.333115011	0.916686535	0.188833773
0.246095076	0.752808690	0.282362133
0.500000000	0.750000000	0.000000000
0.666091681	0.833291471	0.094688728
0.581878364	0.913971961	0.190472871
0.504243135	0.759763956	0.286345750
0.750000000	0.750000000	0.000000000
0.916336775	0.833136916	0.094108529
0.832283556	0.916248262	0.189201877
0.754331589	0.751602471	0.282683223
0.413448364	0.591047168	0.346618503

0.412228644	0.593760431	0.392639846
0.413467050	0.319681406	0.327599108

Ni-Heyrovsky-IS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	O	H
64	1	3

Direct

0.000000000	0.000000000	0.000000000
0.167282552	0.083709866	0.094094053
0.084069416	0.167464554	0.189026937
0.000977559	0.000909326	0.283453226
0.250000000	0.000000000	0.000000000
0.417271614	0.083835475	0.094018333
0.334380746	0.167270973	0.189132214
0.250817776	0.000125080	0.283450127
0.500000000	0.000000000	0.000000000
0.667066813	0.083611213	0.094193153
0.584483981	0.167957574	0.189367399
0.500943542	0.000356358	0.283783048
0.750000000	0.000000000	0.000000000
0.917065144	0.083705492	0.094032034
0.833988309	0.166997552	0.189197049
0.750949025	0.000677193	0.283416659
0.000000000	0.250000000	0.000000000
0.167830870	0.333890200	0.094469346
0.084052168	0.416758060	0.188936666

0.000952098	0.250573426	0.283482075
0.250000000	0.250000000	0.000000000
0.417462379	0.334016472	0.094563685
0.335835755	0.417988837	0.190674961
0.248888135	0.248097897	0.282718956
0.500000000	0.250000000	0.000000000
0.666753232	0.334192961	0.094767742
0.583001494	0.418033779	0.191469103
0.499650449	0.247330710	0.283507317
0.750000000	0.250000000	0.000000000
0.916986048	0.333395928	0.094039574
0.833717525	0.417277724	0.189330384
0.751083672	0.250324368	0.283373863
0.000000000	0.500000000	0.000000000
0.167239591	0.583649397	0.094057590
0.084383510	0.667414367	0.189277261
0.001180182	0.500132501	0.283479780
0.250000000	0.500000000	0.000000000
0.417420328	0.583460271	0.094521776
0.334410667	0.667434752	0.189010113
0.248871058	0.501029909	0.282524407
0.500000000	0.500000000	0.000000000
0.666717291	0.583352864	0.094809137
0.582967520	0.665302753	0.191221729
0.498095483	0.498952031	0.292840958
0.750000000	0.500000000	0.000000000
0.916920722	0.583454728	0.094105817
0.834532619	0.667298913	0.189254925
0.753697813	0.500258803	0.284549832
0.000000000	0.750000000	0.000000000

0.167251840	0.833671153	0.094296984
0.084376909	0.917221546	0.189244524
0.003639733	0.751812935	0.283520132
0.250000000	0.750000000	0.000000000
0.417284131	0.833550751	0.094005905
0.334699839	0.917415261	0.189197615
0.250955194	0.750626802	0.283514410
0.500000000	0.750000000	0.000000000
0.666860163	0.832705736	0.094721757
0.584626138	0.916867197	0.189231038
0.499723792	0.752396524	0.283264399
0.750000000	0.750000000	0.000000000
0.916929841	0.833509743	0.094126694
0.833587468	0.916434646	0.189349860
0.753240585	0.753169894	0.284597993
0.447859198	0.477027059	0.396943361
0.506471634	0.581736624	0.413688809
0.339493811	0.449421078	0.399777293
0.684740782	0.592398226	0.326682389

Ni-Heyrovsky-TS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	O	H
64	1	3

Direct

0.000000000	0.000000000	0.000000000
0.166386858	0.082607038	0.094035365

0.082574107	0.165042639	0.189195395
0.001538360	0.001109906	0.283720165
0.250000000	0.000000000	0.000000000
0.416416824	0.082881019	0.094061956
0.332714468	0.165752500	0.189135000
0.249960899	0.998850405	0.283438921
0.500000000	0.000000000	0.000000000
0.666392684	0.082904436	0.094289705
0.582874477	0.166405454	0.189362586
0.499301940	0.999201655	0.283687264
0.750000000	0.000000000	0.000000000
0.916417122	0.082624957	0.094070986
0.832908332	0.165077418	0.189077839
0.749511719	0.001176364	0.283308119
0.000000000	0.250000000	0.000000000
0.166472897	0.332350433	0.094442032
0.083376326	0.415140122	0.189161420
0.999316812	0.249161258	0.283396989
0.250000000	0.250000000	0.000000000
0.416389704	0.333085030	0.094409041
0.335293502	0.417191774	0.190506890
0.247890264	0.247651815	0.283109993
0.500000000	0.250000000	0.000000000
0.665861249	0.332944334	0.094324097
0.581704974	0.416765094	0.190341592
0.498974532	0.246626958	0.283432484
0.750000000	0.250000000	0.000000000
0.916356444	0.332906425	0.094392888
0.831867576	0.415864617	0.189209029
0.750039458	0.248439386	0.283368707

0.000000000	0.500000000	0.000000000
0.166469604	0.582680464	0.094234385
0.081998728	0.665003598	0.189305142
0.000042403	0.498639554	0.283603668
0.250000000	0.500000000	0.000000000
0.416644365	0.582559407	0.094510883
0.333333910	0.665703118	0.189052224
0.247731417	0.499072880	0.283009320
0.500000000	0.500000000	0.000000000
0.666300416	0.582909226	0.094759464
0.583732963	0.665096998	0.191716149
0.496826112	0.496669412	0.289733648
0.750000000	0.500000000	0.000000000
0.916032135	0.582839847	0.094021522
0.831940293	0.666526377	0.190452516
0.751748979	0.496199578	0.282726467
0.000000000	0.750000000	0.000000000
0.166153252	0.832356811	0.094342366
0.082670406	0.915171146	0.189305663
0.002736214	0.749640167	0.283415288
0.250000000	0.750000000	0.000000000
0.416496515	0.832753718	0.094039686
0.332468688	0.915267766	0.189234868
0.249353573	0.749145269	0.283431798
0.500000000	0.750000000	0.000000000
0.666297436	0.832231700	0.094803140
0.582979679	0.915036559	0.189288318
0.497398198	0.750746191	0.283004642
0.750000000	0.750000000	0.000000000
0.916066170	0.832604468	0.094489582

0.831409633	0.913609028	0.190331846
0.754468501	0.753277779	0.289581120
0.543458700	0.513461113	0.376337111
0.461301267	0.512764037	0.401467234
0.699328899	0.688785732	0.366077125
0.785106540	0.779153347	0.365105599

Ni-Heyrovsky-FS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	O	H
64	1	3

Direct

0.000000000	0.000000000	0.000000000
0.166706324	0.083615422	0.094347112
0.086325802	0.168115109	0.190864444
0.998302698	0.998474002	0.283545494
0.250000000	0.000000000	0.000000000
0.417154789	0.083598368	0.094334655
0.333951205	0.167146280	0.190010786
0.247260988	0.994352400	0.282780647
0.500000000	0.000000000	0.000000000
0.666780531	0.083376095	0.094202526
0.582406819	0.168437764	0.190833345
0.500468075	0.998556495	0.283510298
0.750000000	0.000000000	0.000000000
0.916701615	0.083405972	0.094211482
0.833417356	0.166648522	0.188991070

0.750506878	0.000601226	0.283398032
0.000000000	0.250000000	0.000000000
0.166638494	0.332876235	0.094728693
0.083654732	0.416408956	0.189224601
0.998335600	0.249940589	0.283474624
0.250000000	0.250000000	0.000000000
0.416704446	0.333221883	0.094345063
0.333813578	0.416190237	0.190010414
0.242057830	0.246090874	0.287037760
0.500000000	0.250000000	0.000000000
0.666580915	0.333050996	0.094756201
0.583172143	0.416364670	0.190056607
0.504365623	0.246369019	0.287051797
0.750000000	0.250000000	0.000000000
0.916710496	0.333132118	0.094167411
0.833511770	0.416685104	0.189150557
0.751945853	0.250023246	0.283444524
0.000000000	0.500000000	0.000000000
0.166895106	0.583436012	0.094133161
0.083846949	0.667222321	0.189443663
0.000142162	0.500104427	0.283892304
0.250000000	0.500000000	0.000000000
0.417057008	0.583404243	0.094322078
0.333881795	0.666861892	0.189097822
0.248238772	0.503712654	0.282763928
0.500000000	0.500000000	0.000000000
0.666667163	0.583525717	0.094328709
0.582055092	0.663880110	0.190718144
0.504498422	0.508676112	0.286963552
0.750000000	0.500000000	0.000000000

0.916772783	0.583324075	0.094086766
0.833483696	0.666934967	0.189040944
0.756047010	0.503830969	0.282786995
0.000000000	0.750000000	0.000000000
0.166810662	0.833383024	0.094226994
0.083452478	0.916729808	0.189094529
0.000452176	0.750264287	0.283691615
0.250000000	0.750000000	0.000000000
0.417031795	0.833382845	0.094134957
0.333841354	0.916979373	0.189103678
0.250401318	0.750229537	0.283646703
0.500000000	0.750000000	0.000000000
0.666783214	0.833298147	0.094429292
0.583922803	0.916665614	0.189055905
0.500766575	0.752121329	0.283446521
0.750000000	0.750000000	0.000000000
0.916646361	0.833420634	0.094105072
0.833218634	0.916640103	0.189028859
0.751805365	0.752157211	0.283352405
0.417273045	0.334038943	0.346226364
0.419482529	0.336098462	0.392272562
0.715414762	0.613074064	0.427367866
0.709578693	0.602609038	0.462758392

Ce@Ni-Volmer-IS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni Ce O H

63 1 1 2

Direct

0.000000000	0.000000000	0.000000000
0.166599289	0.083703019	0.094159380
0.082405850	0.167534903	0.188683122
0.998781204	0.999946237	0.284279644
0.250000000	0.000000000	0.000000000
0.416710079	0.083600268	0.094179541
0.333906651	0.168289080	0.189061403
0.248939589	0.998792887	0.283699661
0.500000000	0.000000000	0.000000000
0.666513920	0.083485208	0.093897477
0.584111750	0.167717174	0.188871995
0.500181079	0.000439105	0.284230232
0.750000000	0.000000000	0.000000000
0.916427672	0.083485238	0.093899384
0.832939744	0.166883379	0.189288884
0.749221325	0.999782979	0.283517331
0.000000000	0.250000000	0.000000000
0.167406231	0.334055394	0.093969546
0.082190543	0.415841490	0.188545346
0.999174953	0.250048637	0.283582419
0.250000000	0.250000000	0.000000000
0.416875660	0.333812952	0.094602488
0.334275872	0.417311132	0.190720305
0.245080158	0.244300172	0.282959640
0.500000000	0.250000000	0.000000000
0.666264236	0.333896577	0.093999334
0.582441986	0.417660952	0.190759987
0.497969121	0.246048003	0.283439457

0.750000060	0.250000000	0.000000000
0.916469812	0.333465278	0.093810126
0.832476139	0.416191936	0.188790724
0.749210179	0.250230968	0.283466339
0.000000000	0.500000000	0.000000000
0.166794047	0.583562732	0.094178975
0.083269835	0.667043447	0.189474702
0.999045074	0.499485970	0.284317464
0.250000000	0.500000000	0.000000000
0.417048573	0.583349347	0.094677046
0.334080279	0.666279972	0.189004317
0.244697809	0.501175642	0.282730550
0.500000000	0.500000000	0.000000000
0.666244149	0.583400488	0.094665974
0.582422316	0.665568590	0.190918177
0.750000060	0.500000000	0.000000000
0.916587532	0.583519459	0.094187781
0.831619799	0.666215956	0.189185500
0.753809333	0.501467407	0.283365577
0.000000000	0.750000000	0.000000000
0.166762084	0.833728671	0.094642043
0.082973585	0.917295694	0.189538360
0.000087099	0.750431418	0.283749729
0.249999985	0.750000000	0.000000000
0.416806549	0.833546102	0.094150975
0.333617389	0.917143345	0.189515799
0.248772219	0.750753105	0.283761173
0.500000000	0.750000000	0.000000000
0.666251302	0.832948804	0.094103090
0.584061444	0.917208731	0.188915104

0.497490466	0.752396345	0.283517599
0.750000000	0.750000000	0.000000000
0.916522980	0.833462059	0.094203673
0.832296669	0.917059422	0.188952193
0.753435493	0.752789080	0.283527672
0.495289743	0.498559415	0.324522346
0.337732077	0.444848686	0.429842532
0.245344520	0.439048558	0.410721302
0.299901098	0.350742936	0.454653025

Ce@Ni-Volmer-TS

1.0

10.032299954	0.000000000	0.000000000
-5.0161499977	8.6882266544	0.000000000
0.000000000	0.000000000	21.1434993744

Ni	Ce	O	H
63	1	1	2

Direct

0.000000000	0.000000000	0.000000000
0.166624382	0.082573012	0.094115801
0.082745202	0.165411189	0.188800320
0.999381661	0.998455763	0.284209728
0.250000000	0.000000000	0.000000000
0.416507304	0.082402214	0.094058283
0.333554149	0.166582048	0.189230427
0.249294996	0.997743309	0.283541411
0.500000000	0.000000000	0.000000000
0.666706979	0.082483165	0.093986943
0.583457053	0.165282726	0.188865334
0.500006676	0.999074101	0.284285009

0.750000000	0.000000000	0.000000000
0.916585445	0.082789376	0.093891352
0.833268583	0.165204331	0.189644173
0.748740911	0.997414708	0.283603340
0.000000000	0.250000000	0.000000000
0.167687699	0.332989961	0.094359301
0.083145522	0.413998306	0.189173058
0.998569965	0.247527927	0.284148932
0.250000000	0.250000000	0.000000000
0.416915148	0.332961202	0.094882332
0.335919142	0.416246653	0.191715866
0.243600145	0.243260950	0.283861369
0.500000000	0.250000000	0.000000000
0.666248620	0.332503825	0.093941770
0.583538771	0.416029066	0.190971747
0.497752249	0.245188847	0.282941818
0.750000060	0.250000000	0.000000000
0.916941226	0.332408071	0.093853153
0.832720339	0.413386852	0.188560233
0.749261081	0.248313308	0.283478528
0.000000000	0.500000000	0.000000000
0.166720048	0.582403660	0.094212122
0.082517721	0.663895607	0.189613834
0.000238740	0.497785628	0.284295410
0.250000000	0.500000000	0.000000000
0.416782498	0.582140505	0.094915494
0.333206058	0.663320422	0.189673111
0.245747060	0.496036440	0.284678757
0.500000000	0.500000000	0.000000000
0.666062891	0.582220018	0.094691403

0.582845271	0.664039314	0.191090956
0.750000060	0.500000000	0.000000000
0.916445017	0.582500815	0.094062336
0.832061768	0.664695561	0.189041555
0.757235110	0.499604404	0.283111989
0.000000000	0.750000000	0.000000000
0.166298300	0.832216442	0.094654180
0.082841277	0.915020466	0.189523727
0.001850755	0.749398291	0.283788532
0.249999985	0.750000000	0.000000000
0.416421860	0.832360744	0.094216168
0.332874984	0.914602697	0.189606428
0.249424741	0.748040497	0.283687115
0.500000000	0.750000000	0.000000000
0.666016221	0.831701577	0.093958259
0.583559692	0.914954603	0.189033836
0.497267276	0.750362635	0.283326507
0.750000000	0.750000000	0.000000000
0.916416109	0.832653880	0.094097070
0.832340062	0.915916443	0.188663065
0.756351531	0.752900481	0.283139855
0.513919652	0.506044030	0.330172718
0.327776432	0.384695768	0.406364352
0.243898004	0.355668008	0.350883275
0.280985802	0.282769024	0.425710559

Ce@Ni-Volmer-FS

1.0

10.0322999954	0.000000000	0.000000000
-5.0161499977	8.6882266544	0.000000000

	0.0000000000	0.0000000000	21.1434993744
Ni	Ce	O	H
63	1	1	2
Direct			
	0.0000000000	0.0000000000	0.0000000000
	0.166613296	0.084109135	0.094189078
	0.086515978	0.168856278	0.190829262
	0.996832728	0.996303618	0.283622652
	0.250000000	0.000000000	0.000000000
	0.416870892	0.083880864	0.094247408
	0.333101183	0.168229461	0.190117419
	0.244841948	0.991485476	0.281566173
	0.500000000	0.000000000	0.000000000
	0.666523695	0.084621802	0.094014972
	0.580880582	0.168413877	0.190747172
	0.499275863	0.997255445	0.283635885
	0.750000000	0.000000000	0.000000000
	0.917627037	0.084906645	0.094261140
	0.833130181	0.167684570	0.189014465
	0.748764873	0.999298215	0.283113092
	0.000000000	0.250000000	0.000000000
	0.167638078	0.333748996	0.094728604
	0.082180604	0.415799499	0.188633725
	0.995807946	0.248132333	0.284393400
	0.250000000	0.250000000	0.000000000
	0.416858017	0.333960772	0.095284075
	0.335532486	0.418160975	0.192154408
	0.242540151	0.242134675	0.288337916
	0.500000000	0.250000000	0.000000000
	0.665683568	0.333697319	0.094692506

0.581264913	0.417916000	0.192229807
0.499650657	0.241848171	0.286370277
0.750000060	0.250000000	0.000000000
0.916349351	0.333349526	0.093755886
0.831867754	0.415471047	0.188693568
0.750057697	0.249151811	0.283331335
0.000000000	0.500000000	0.000000000
0.166467100	0.583355725	0.093969159
0.082414441	0.665982246	0.189201891
0.997447312	0.500001669	0.283886820
0.250000000	0.500000000	0.000000000
0.416464180	0.582928300	0.094588220
0.332394093	0.664534569	0.188909531
0.244629398	0.501603842	0.284782320
0.500000000	0.500000000	0.000000000
0.665637136	0.582692921	0.094538495
0.582819343	0.666727483	0.189850107
0.750000060	0.500000000	0.000000000
0.916198492	0.583183348	0.093994029
0.831243396	0.665496826	0.188696265
0.754507661	0.501716018	0.283055216
0.000000000	0.750000000	0.000000000
0.166345328	0.833359778	0.094267435
0.081595816	0.916523576	0.188541189
0.999899030	0.749148846	0.283658743
0.249999985	0.750000000	0.000000000
0.416806847	0.833318949	0.093926527
0.333186418	0.915989518	0.188647717
0.247740448	0.749297678	0.283503920
0.500000000	0.750000000	0.000000000

0.666501522	0.834173679	0.093523547
0.583983779	0.917881370	0.188148424
0.495946378	0.752996504	0.282221258
0.750000000	0.750000000	0.000000000
0.915828645	0.833240151	0.093915731
0.832638741	0.918694377	0.188040182
0.756166160	0.754899323	0.282255560
0.515220821	0.527658939	0.326886535
0.399887085	0.277866244	0.362656295
0.162199944	0.338946670	0.327165753
0.356035501	0.191846535	0.392242134

Ce@Ni-Heyrovsky-IS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	1	3

Direct

0.000000000	0.000000000	0.000000000
0.166897669	0.083495118	0.094144322
0.082672112	0.166902721	0.188639224
0.998659015	0.998205781	0.283970743
0.250000000	0.000000000	0.000000000
0.416723490	0.083367415	0.094241306
0.333335251	0.168168262	0.189568400
0.249188572	0.998199284	0.283642620
0.500000000	0.000000000	0.000000000
0.666323900	0.083003253	0.093958385

0.583779335	0.167011201	0.189004496
0.500332117	0.999935150	0.284195542
0.750000000	0.000000000	0.000000000
0.916492879	0.083315536	0.093811534
0.833397686	0.166525751	0.189349383
0.749079525	0.999114037	0.283432126
0.000000000	0.250000000	0.000000000
0.167466775	0.333676189	0.094120905
0.082742371	0.415439218	0.188723266
0.997407138	0.248547584	0.284509420
0.250000000	0.250000000	0.000000000
0.416924477	0.333471417	0.094729617
0.334967822	0.417292386	0.190719858
0.245953456	0.243925348	0.284692794
0.500000000	0.250000000	0.000000000
0.666314721	0.333297968	0.094049767
0.582806230	0.416902184	0.190757796
0.497927457	0.245867908	0.283615649
0.750000060	0.250000000	0.000000000
0.916541457	0.332852751	0.093815036
0.832916617	0.415271431	0.188659146
0.749145508	0.249743193	0.283391565
0.000000000	0.500000000	0.000000000
0.166859940	0.583238423	0.094180644
0.083187588	0.666172504	0.189433917
0.998864770	0.500424564	0.283996135
0.250000000	0.500000000	0.000000000
0.416866392	0.583258808	0.094780661
0.333300829	0.664780557	0.189680874
0.245617837	0.501158714	0.284861952

0.500000000	0.500000000	0.000000000
0.666194260	0.582974970	0.094663158
0.582696199	0.665260613	0.190779969
0.750000060	0.500000000	0.000000000
0.916551292	0.583159387	0.094092466
0.831697583	0.665655851	0.189057484
0.754952312	0.501002908	0.283378005
0.000000000	0.750000000	0.000000000
0.166683525	0.833338439	0.094630994
0.083018057	0.916925609	0.189366162
0.001335102	0.750563860	0.283747375
0.249999985	0.750000000	0.000000000
0.416594207	0.833227813	0.094264090
0.333340883	0.916519523	0.189513370
0.249315023	0.750626564	0.283744782
0.500000000	0.750000000	0.000000000
0.666105986	0.832610607	0.094068870
0.583674669	0.916321874	0.189061806
0.497724652	0.751449466	0.283640504
0.750000000	0.750000000	0.000000000
0.916521609	0.833250105	0.094128989
0.832543075	0.917092025	0.188637897
0.754952848	0.753686905	0.283283889
0.504760563	0.502498686	0.324184388
0.389274925	0.469845265	0.438615531
0.307299972	0.495200396	0.434145033
0.340480119	0.368517131	0.458498180
0.168681487	0.333903879	0.326967448

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	1	3

Direct

0.000000000	0.000000000	0.000000000
0.167779446	0.083578698	0.094068274
0.085471064	0.167977720	0.188828304
0.001339674	0.999997377	0.284203112
0.250000000	0.000000000	0.000000000
0.417796791	0.083307609	0.094373062
0.335745186	0.167984143	0.188973203
0.250986010	0.997894526	0.283681273
0.500000000	0.000000000	0.000000000
0.667817712	0.083054870	0.093955755
0.587019503	0.167222202	0.188728139
0.502846122	0.999527931	0.284212023
0.750000000	0.000000000	0.000000000
0.917891085	0.083676971	0.093789279
0.835877895	0.167196780	0.189252451
0.751531124	0.999585748	0.283262670
0.000000000	0.250000000	0.000000000
0.168724671	0.334202498	0.094592050
0.086846009	0.417015880	0.190063253
0.000000000	0.247952983	0.283375442
0.250000000	0.250000000	0.000000000
0.417898446	0.334051013	0.094686709
0.337238878	0.418315291	0.193001211

0.248432308	0.241089210	0.282768220
0.500000000	0.250000000	0.000000000
0.668224573	0.333748698	0.094095528
0.585036039	0.416437715	0.190720767
0.499781758	0.242785484	0.282834500
0.750000060	0.250000000	0.000000000
0.918336928	0.333425999	0.093763322
0.836626112	0.416092128	0.188725576
0.751361430	0.249446690	0.283453852
0.000000000	0.500000000	0.000000000
0.167937279	0.583300769	0.094648942
0.085427970	0.666549385	0.189643994
0.000820398	0.499581605	0.284376889
0.250000000	0.500000000	0.000000000
0.417502850	0.582773566	0.095329925
0.334602118	0.663599968	0.190803051
0.247195914	0.498524219	0.290023476
0.500000000	0.500000000	0.000000000
0.666998148	0.582803428	0.094665460
0.584719300	0.664737344	0.191157967
0.750000060	0.500000000	0.000000000
0.917795122	0.583493829	0.094035760
0.833811224	0.665834486	0.189025462
0.758496642	0.501225948	0.282872170
0.000000000	0.750000000	0.000000000
0.167823285	0.833462059	0.094593734
0.085172154	0.916808844	0.189496204
0.003413238	0.751156747	0.283811182
0.249999985	0.750000000	0.000000000
0.417332798	0.832655191	0.094103634

0.335827410	0.916134834	0.189636469
0.251863331	0.751365244	0.283670515
0.500000000	0.750000000	0.000000000
0.667112112	0.832175255	0.093900651
0.585627079	0.916022897	0.188710153
0.502435684	0.753531694	0.282796860
0.750000000	0.750000000	0.000000000
0.917652905	0.833307326	0.094007842
0.834870756	0.917503834	0.188388765
0.758875012	0.755207360	0.282985300
0.514226198	0.501047254	0.329924047
0.389533192	0.486534029	0.420083642
0.280095041	0.485766917	0.378645033
0.335698903	0.441975176	0.459537297
0.183963209	0.476005763	0.358680069

Ce@Ni-Heyrovsky-FS

1.0

10.0322999954	0.0000000000	0.0000000000
-5.0161499977	8.6882266544	0.0000000000
0.0000000000	0.0000000000	21.1434993744

Ni	Ce	O	H
63	1	1	3

Direct

0.000000000	0.000000000	0.000000000
0.166504487	0.083485223	0.094046965
0.082570709	0.167398185	0.188618481
0.999078274	0.999867618	0.284195423
0.250000000	0.000000000	0.000000000
0.416396827	0.083489701	0.094079554

0.333342254	0.168127775	0.189060390
0.248867124	0.999036014	0.283552796
0.500000000	0.000000000	0.000000000
0.666511893	0.083494052	0.093837321
0.583575130	0.167298585	0.188668266
0.499988973	0.999997437	0.284098595
0.750000000	0.000000000	0.000000000
0.916413963	0.083575711	0.093800500
0.832600892	0.166653886	0.189233258
0.748810887	0.998981714	0.283356398
0.000000000	0.250000000	0.000000000
0.167789549	0.334136516	0.094375357
0.083673112	0.416141480	0.189321250
0.998069286	0.248301029	0.283042550
0.250000000	0.250000000	0.000000000
0.416482598	0.334255040	0.094993748
0.334528565	0.418104142	0.192573488
0.244811878	0.243565708	0.282987505
0.500000000	0.250000000	0.000000000
0.665894687	0.333965629	0.094102480
0.581882477	0.417427629	0.191388011
0.496737897	0.244546786	0.282873839
0.750000060	0.250000000	0.000000000
0.917007267	0.333542854	0.093953975
0.832030654	0.415267557	0.188484162
0.748531878	0.249984369	0.283315331
0.000000000	0.500000000	0.000000000
0.166753605	0.583314657	0.094221637
0.082863502	0.666515172	0.189329714
0.996803641	0.499360412	0.283342749

0.250000000	0.500000000	0.000000000
0.416655451	0.582900167	0.095095128
0.333193690	0.665155947	0.189929754
0.243779793	0.501474619	0.286216766
0.500000000	0.500000000	0.000000000
0.665892959	0.583165944	0.094752185
0.582438350	0.665329754	0.191379398
0.750000060	0.500000000	0.000000000
0.916383624	0.583434105	0.094039619
0.831671715	0.666039944	0.189051822
0.753774762	0.501569450	0.282746106
0.000000000	0.750000000	0.000000000
0.166517690	0.833335638	0.094479494
0.082650051	0.916856050	0.189371258
0.999842048	0.750385880	0.283667296
0.249999985	0.750000000	0.000000000
0.416274905	0.832710624	0.094198026
0.333180189	0.916841388	0.189275190
0.248510137	0.751784682	0.283336967
0.500000000	0.750000000	0.000000000
0.665768802	0.832244575	0.094046563
0.583690286	0.916864574	0.188609898
0.498154908	0.753027797	0.282953918
0.750000000	0.750000000	0.000000000
0.916401625	0.833354414	0.094054960
0.832213223	0.917102337	0.188633665
0.754601479	0.753317058	0.282944471
0.504032075	0.499756366	0.338402808
0.501152396	0.486037999	0.436146438
0.236224279	0.526944578	0.399956882

0.494144320

0.464821160

0.481206834

0.189888686

0.450801641

0.381306678

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