

Supporting Information

Synergetic effect dependence on activated oxygen in the interface of NiO_x modified Pt nanoparticles for CO oxidation from first-principles

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1. Benchmarking calculation for calculation methods on NiO_x/Pt

Some benchmarking calculations has been done to show that our current computational methods are reasonably good in describing the CO oxidation process on NiO_x/Pt.

We calculated the CO adsorption energy and energy barrier of TS1 on Ni₅O₄/Pt₍₁₀₀₎ as an example with a higher cutoff energy of 500 eV. It is found the energy change is within 0.02 eV, which is negligible comparing with the adsorption energy and barrier. Moreover, a more dense KPOINTS with 5x5x1 mesh is also tested for comparison and the adsorption energy and barrier are converged. These results are listed in Table S1.

Table S1. Convergence test on CO adsorption energy and energy barrier of TS1 on Ni₅O₄/Pt(100).

	E _a (CO)	E _b (TS1)
Standard	-1.875	0.934
5x5x1 k-mesh	-1.878	0.934

D2 or D3 correction is essential in hydrogen bonding or large molecule adsorption systems which vdW interaction plays an important role. While for the small molecule CO and O₂, the calculated results shows that those corrected values are negligible to the strong chemical bonding (~2.0 eV for CO adsorption on Pt). The calculated CO adsorption energy and energy barrier of TS1 on NiO_x/Pt_{edge} with D3 correction are listed in Table S2. As can be seen, the corrected values are only increased by ~0.1 eV.

Table S2. The CO adsorption energy (E_a(CO))and the energy barrier of TS1 (E_b(TS1)) on NiO_x/Pt_{edge}.

	E _a (CO)	E _b (TS1)
Without D3 correction	-2.11	0.50
With D3 correction	-2.25	0.56

2. Supplementary Figures and Tables

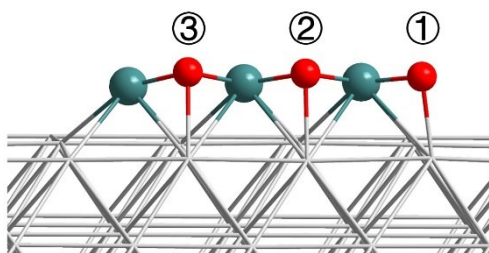


Figure S1. Structure of Ni₃O₃ atomic chain on Pt edge. The linear structure of Ni₃O₃

Table S3. E_{ov} of O labeled in Figure S1.

O atom label	E_{ov}/eV
①	1.09
②	1.49
③	2.02

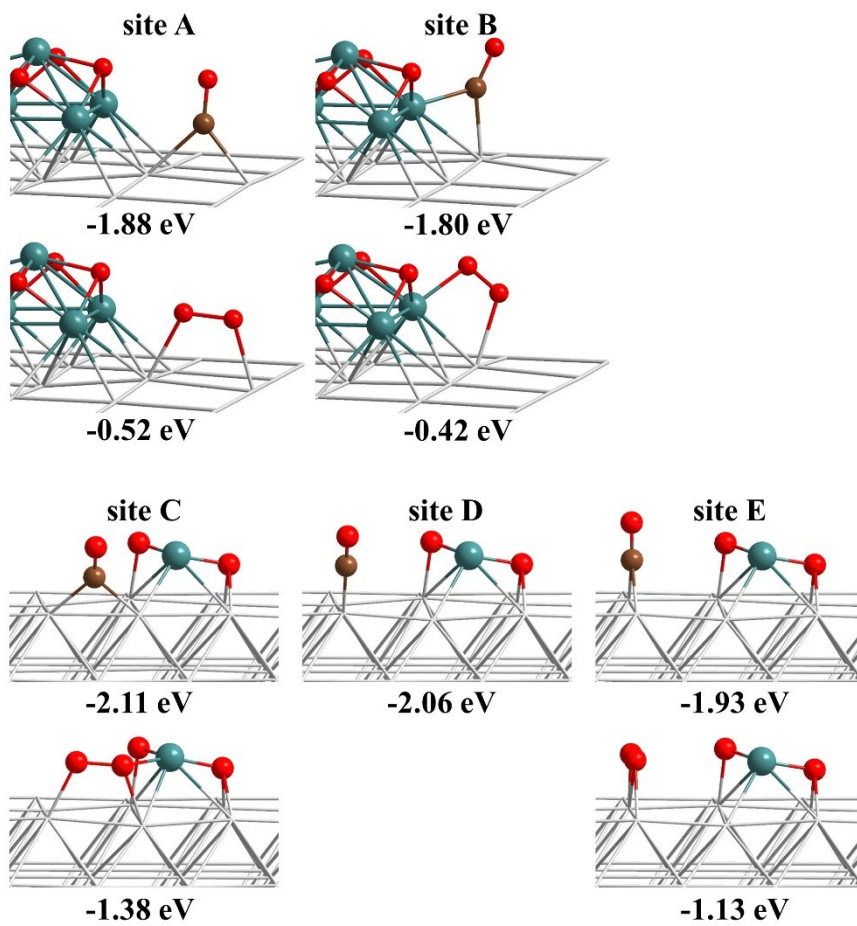


Figure S2. Atomic structures of CO and O₂ adsorption on sites of NiO_x/Pt.

Table S4. Pt-C and Pt-O bond lengths of CO and O₂ adsorption on clean Pt surface sites and NiO_x-Pt interfacial sites.

Adsorption sites		d(Pt-C)	d(Pt-O)
Pt(100)	Bridge	2.02	1.98
	Atop	1.84	-
Pt(211)	Edge-bridge	2.01	1.97
	Edge-atop	1.85	-
	Terrace-bridge	2.04, 2.01	1.98, 1.99
Facet	A	2.06, 1.99	2.05, 1.96
	B	1.94	2.01
Edge	C	2.02, 1.99	2.03, 1.98
	D	1.85	-
	E	2.04, 2.01	1.98, 1.99

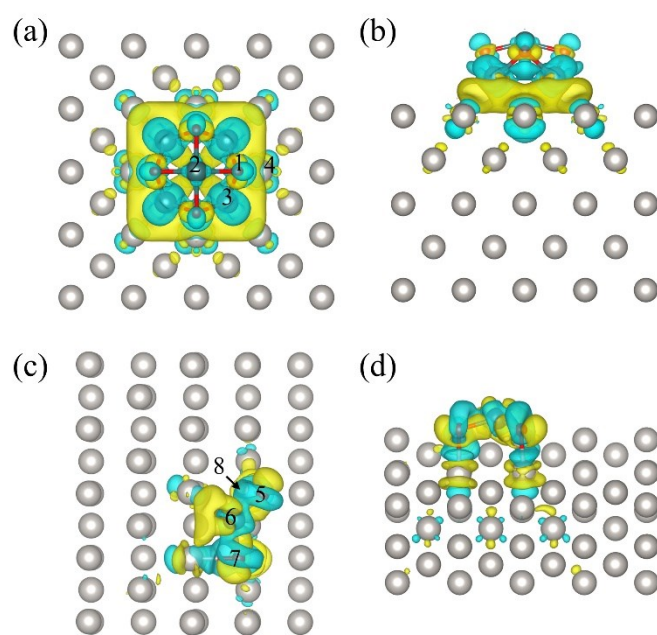


Figure S3. (a) and (b) Charge density difference of $\text{NiO}_x/\text{Pt}_{(100)}$ in top view and side view. (c) and (d) Charge density difference of $\text{NiO}_x/\text{Pt}_{\text{edge}}$ in top view and side view. Yellow (blue) isosurface represents charge accumulation (depletion). Bader charge analysis are applied to atoms 1-8 and the results are shown in Table S3.

Table S5. Element name and charge transfer of atoms 1-8 in Figure S3.

Label	Element	Charge transfer
1	O	$0.75e$
2	Ni	$-0.92e$
3	Ni	$-0.65e$
4	Pt	$0.16e$
5	O	$0.65e$
6	Ni	$-0.70e$
7	O	$0.70e$
8	Pt	$-0.31e$

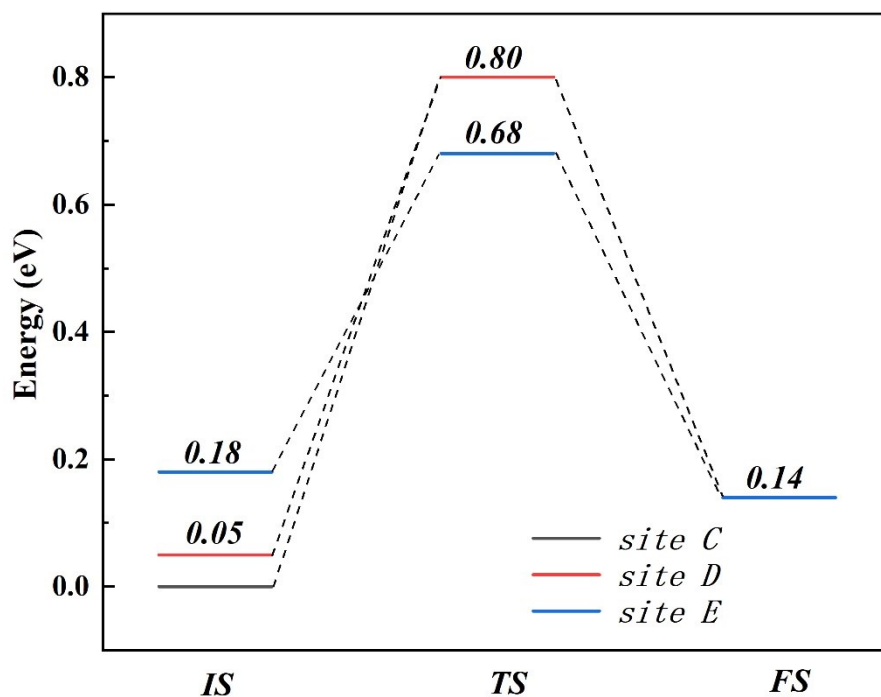


Figure S4. Energy profile of CO oxidation after CO adsorption at site C, site D and site E. The difference of E_a at various sites is small, and the transition state (TS) of CO oxidation at site E is lower in energy, therefore CO adsorption at site E is considered in the catalytic cycle of $\text{NiO}_x/\text{Pt}_{\text{edge}}$.

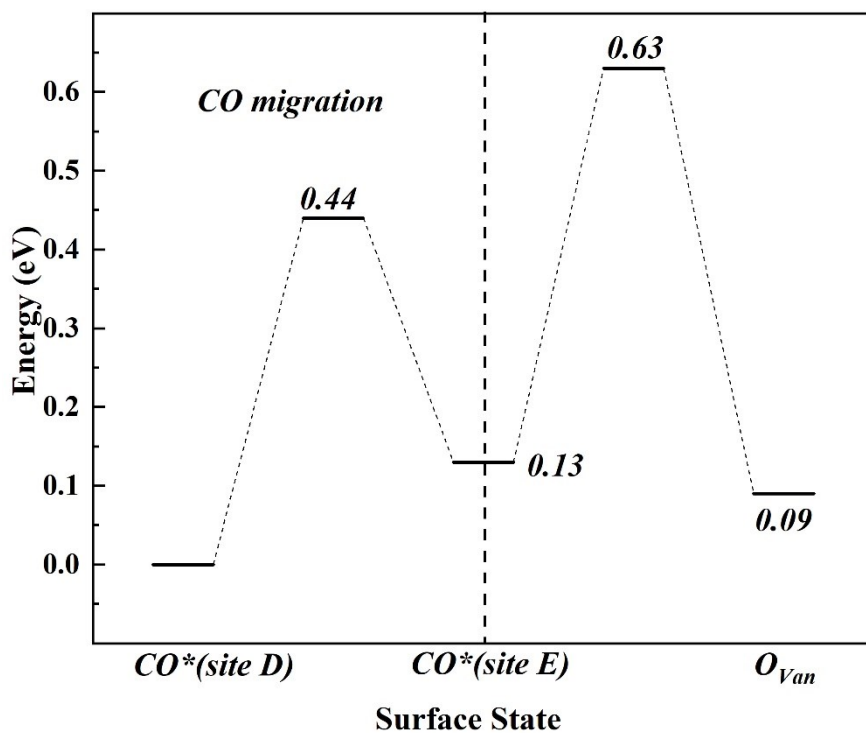


Figure S5. Energy profile of CO migration (at the left region) and the first CO₂ formation (at the right region). The barrier of CO₂ formation at site D is 0.75 eV according to Figure S4, therefore CO migration can occur prior to oxidation at site D.

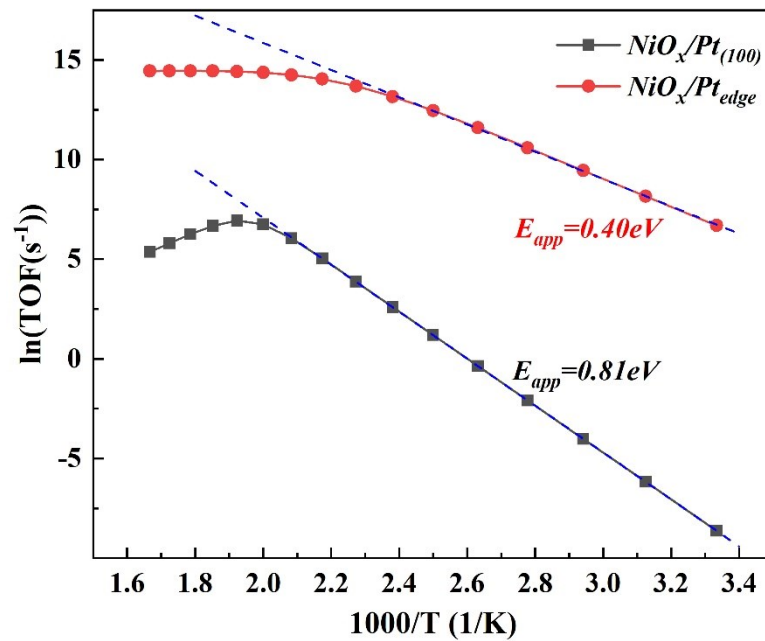


Figure S6. The apparent activation energy (E_{app}) of $\text{NiO}_x/\text{Pt}_{\text{edge}}$ and $\text{NiO}_x/\text{Pt}_{(100)}$.

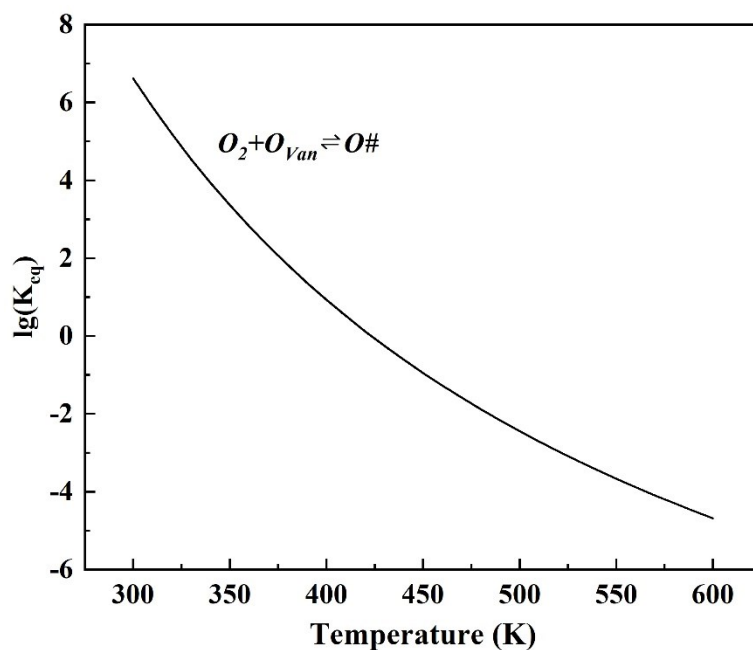


Figure S7. The equilibrium constant of O_2 adsorption on oxygen vacancy site of $NiO_x/Pt_{(100)}$ as function of temperature.

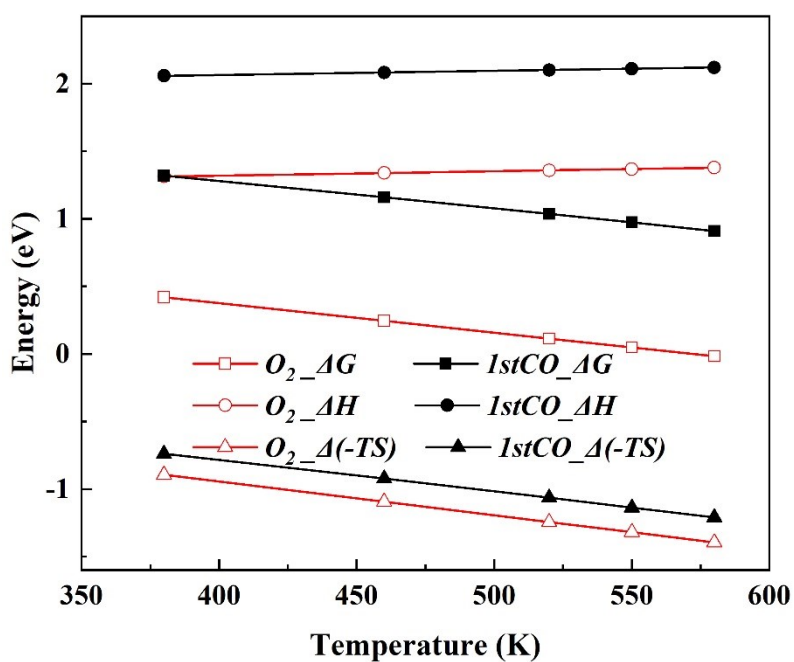


Figure S8. Variation of ΔG and its enthalpy and entropy terms (ΔH , $\Delta(-TS)$) for gas adsorption step on $NiO_x/Pt_{(100)}$. Red hollow symbol represents O_2 adsorption on vacancy site, black solid symbol represents the first CO adsorption.

3. Further validation on the results

3.1 The affection of Ni oxide stoichiometry on the results

As the oxygen vacancy formation energy (E_{ov}) is closely related to the CO oxidation activity, we have calculated the E_{ov} in a larger $Ni_{12}O_9$ cluster. The structure of optimized $Ni_{12}O_9/Pt_{(100)}$ and the E_{ov} is shown in Figure S9. The calculated E_{ov} (1.47 eV) is a little smaller than that on $Ni_5O_4/Pt_{(100)}$ (1.74 eV), which is still higher than that on NiO_x/Pt_{edge} (1.27 eV). The results shows that the stoichiometry would not change the main conclusion of the manuscript.

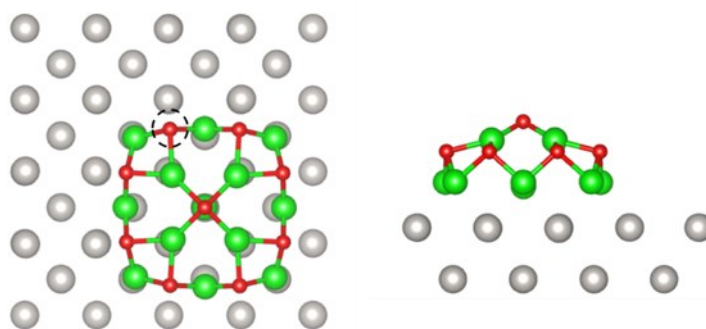


Figure S9. Top view (in the left) and side view (in the right) of $Ni_{12}O_9$ cluster on $Pt(100)$ surface. Pt, Ni, and O are represented by white, green, and red spheres, respectively. The circled oxygen in the top view is removed to evaluate the E_{ov} of $Ni_{12}O_9$.

3.2 The imaginary mode of TSs

We also calculate the vibrational frequencies and modes to make sure to find the correct transition state with only one imaginary frequency. The single imaginary frequencies of TS1, TS2 and TS3 on $Ni_5O_4/Pt(100)$ and NiO_2/Pt_{edge} are listed in Table S6 and those corresponding vibrational modes are shown in Figure S10.

Table S6. The imaginary frequency (in the unit of cm^{-1}) of TS1, TS2 and TS3 on $Ni_5O_4/Pt_{(100)}$ and NiO_2/Pt_{edge} .

	$Ni_5O_4/Pt_{(100)}$	NiO_2/Pt_{edge}

TS1	440	246
TS2	475	216
TS3	344	377

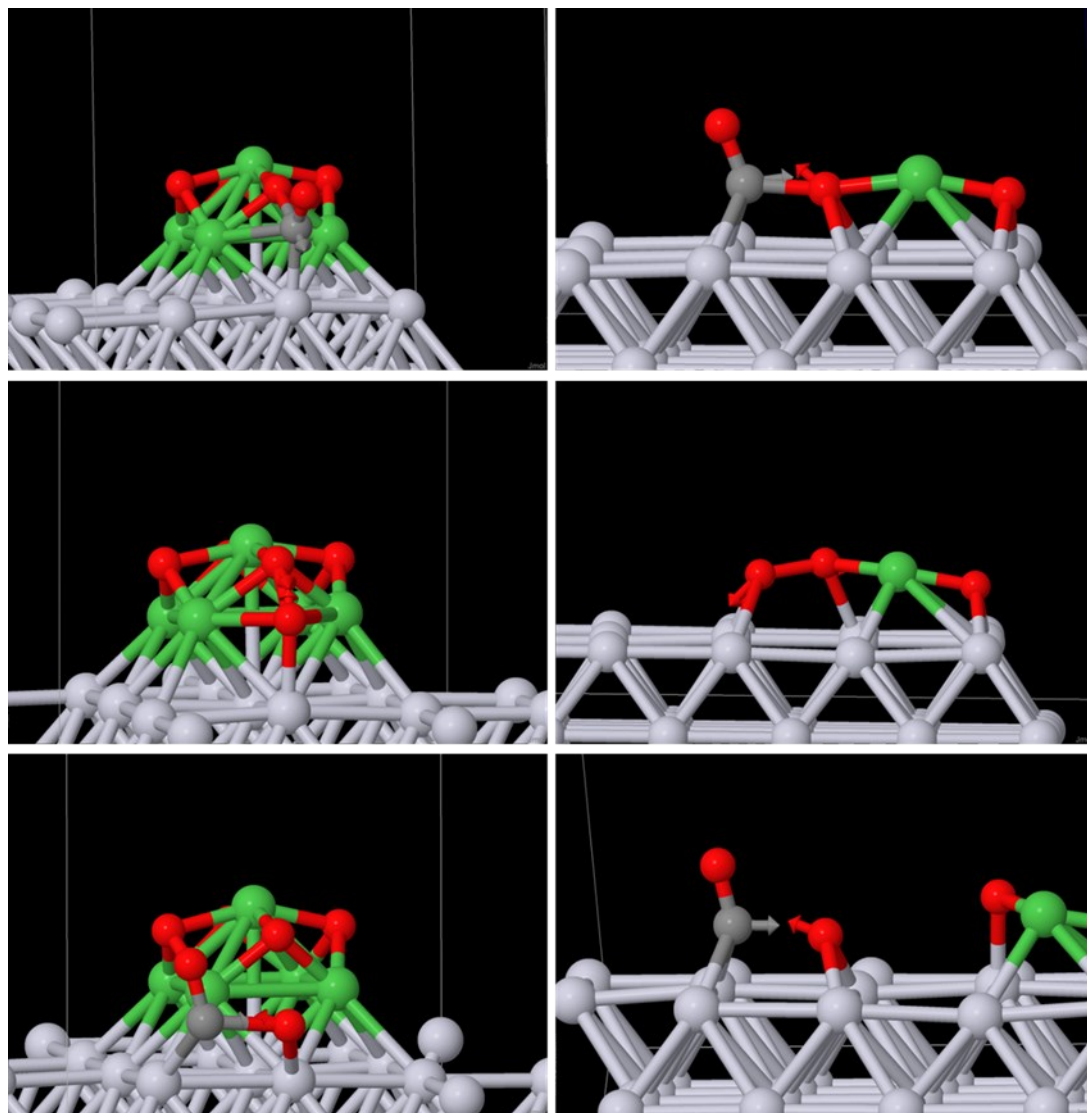


Figure S10. The direction of imaginary frequency of TS1-3 on Ni₅O₄/Pt₍₁₀₀₎ (the right region) and NiO₂/Pt_{edge} (the left region). Pt, Ni, O and C are represented by white, green, red and grey spheres, respectively.

4. The coordinates of optimized structures and TSs

NiO_x/Pt_{edge}

*

1.0

13.5928001404	0.0000000000	0.0000000000
0.0000000000	13.8731002808	0.0000000000
0.0000000000	0.0000000000	23.4076995850

Pt	Ni	O
80	1	2

Direct

0.166669995	0.000000000	0.000000000
0.333330005	0.000000000	0.136869997
0.000000000	0.000000000	0.068439998
0.158720002	0.001190000	0.209050000
0.333330005	0.100000001	0.034219999
0.000000000	0.100000001	0.171090007
0.166669995	0.100000001	0.102650002
0.323009998	0.100939997	0.242650002
0.666670024	0.000000000	0.000000000
0.832199991	0.999230027	0.146709993
0.488319993	0.997520030	0.270669997
0.500000000	0.000000000	0.068439998
0.663299978	0.997529984	0.206770003
0.833329976	0.100000001	0.034219999
0.500000000	0.100000001	0.171090007
0.666670024	0.100000001	0.102650002
0.166669995	0.200000003	0.000000000
0.333330005	0.200000003	0.136869997
0.000000000	0.200000003	0.068439998
0.159869999	0.199410006	0.209439993
0.333330005	0.300000012	0.034219999
0.000000000	0.300000012	0.171090007
0.166669995	0.300000012	0.102650002
0.320309997	0.298449993	0.242750004
0.666670024	0.200000003	0.000000000
0.835169971	0.199149996	0.144390002
0.484609991	0.197099999	0.276849985
0.500000000	0.200000003	0.068439998
0.671450019	0.197469994	0.205650002
0.833329976	0.300000012	0.034219999
0.500000000	0.300000012	0.171090007
0.666670024	0.300000012	0.102650002
0.166669995	0.400000006	0.000000000
0.333330005	0.400000006	0.136869997

0.000000000	0.400000006	0.068439998
0.158570006	0.400079995	0.208890006
0.333330005	0.500000000	0.034219999
0.000000000	0.500000000	0.171090007
0.166669995	0.500000000	0.102650002
0.318709999	0.501259983	0.242310002
0.666670024	0.400000006	0.000000000
0.835959971	0.400550008	0.142210007
0.479730010	0.404220015	0.270370007
0.500000000	0.400000006	0.068439998
0.681079984	0.405829996	0.208989993
0.833329976	0.500000000	0.034219999
0.500000000	0.500000000	0.171090007
0.666670024	0.500000000	0.102650002
0.166669995	0.600000024	0.000000000
0.333330005	0.600000024	0.136869997
0.000000000	0.600000024	0.068439998
0.158170000	0.601760030	0.208900005
0.333330005	0.699999988	0.034219999
0.000000000	0.699999988	0.171090007
0.166669995	0.699999988	0.102650002
0.320749998	0.701219976	0.242219999
0.666670024	0.600000024	0.000000000
0.832690001	0.600910008	0.146730006
0.487679988	0.601469994	0.270749986
0.500000000	0.600000024	0.068439998
0.663150012	0.602609992	0.206670001
0.833329976	0.699999988	0.034219999
0.500000000	0.699999988	0.171090007
0.666670024	0.699999988	0.102650002
0.166669995	0.800000012	0.000000000
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0.000000000	0.800000012	0.068439998
0.158859998	0.802510023	0.209309995
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0.166669995	0.899999976	0.102650002
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0.831929982	0.800019979	0.147349998
0.489230007	0.799579978	0.270920008
0.500000000	0.800000012	0.068439998
0.663169980	0.800159991	0.208079994
0.833329976	0.899999976	0.034219999

0.500000000	0.899999976	0.171090007
0.666670024	0.899999976	0.102650002
0.621720016	0.319000006	0.310959995
0.712320030	0.396079987	0.289990008
0.636219978	0.198109999	0.290300012

CO*

Pt	Ni	O	C
80	1	3	1

Direct

0.166669995	0.000000000	0.000000000
0.333330005	0.000000000	0.136869997
0.000000000	0.000000000	0.068439998
0.158720002	0.001190000	0.209050000
0.333330005	0.100000001	0.034219999
0.000000000	0.100000001	0.171090007
0.166669995	0.100000001	0.102650002
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0.666670024	0.000000000	0.000000000
0.832759976	0.999140024	0.146559998
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0.500000000	0.000000000	0.068439998
0.663439989	0.998250008	0.206499994
0.833329976	0.100000001	0.034219999
0.500000000	0.100000001	0.171090007
0.666670024	0.100000001	0.102650002
0.166669995	0.200000003	0.000000000
0.333330005	0.200000003	0.136869997
0.000000000	0.200000003	0.068439998
0.159869999	0.199410006	0.209439993
0.333330005	0.300000012	0.034219999
0.000000000	0.300000012	0.171090007
0.166669995	0.300000012	0.102650002
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0.500000000	0.200000003	0.068439998
0.671459973	0.196919993	0.205459997
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0.500000000	0.300000012	0.171090007
0.666670024	0.300000012	0.102650002
0.166669995	0.400000006	0.000000000
0.333330005	0.400000006	0.136869997

0.000000000	0.400000006	0.068439998
0.158570006	0.400079995	0.208890006
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0.666670024	0.500000000	0.102650002
0.166669995	0.600000024	0.000000000
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0.000000000	0.600000024	0.068439998
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0.333330005	0.699999988	0.034219999
0.000000000	0.699999988	0.171090007
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0.500000000	0.699999988	0.171090007
0.666670024	0.699999988	0.102650002
0.166669995	0.800000012	0.000000000
0.333330005	0.800000012	0.136869997
0.000000000	0.800000012	0.068439998
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0.833329976	0.899999976	0.034219999

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0.681580007	0.608240008	0.339540005
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TS1

Pt	Ni	O	C
80	1	3	1

Direct

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0.333330005	0.000000000	0.136869997
0.000000000	0.000000000	0.068439998
0.158720002	0.001190000	0.209050000
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0.000000000	0.100000001	0.171090007
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0.833329976	0.100000001	0.034219999
0.500000000	0.100000001	0.171090007
0.666670024	0.100000001	0.102650002
0.166669995	0.200000003	0.000000000
0.333330005	0.200000003	0.136869997
0.000000000	0.200000003	0.068439998
0.159869999	0.199410006	0.209439993
0.333330005	0.300000012	0.034219999
0.000000000	0.300000012	0.171090007
0.166669995	0.300000012	0.102650002
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0.666670024	0.200000003	0.000000000
0.835200012	0.199479997	0.144679993
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0.500000000	0.300000012	0.171090007
0.666670024	0.300000012	0.102650002

0.166669995	0.400000006	0.000000000
0.333330005	0.400000006	0.136869997
0.000000000	0.400000006	0.068439998
0.158570006	0.400079995	0.208890006
0.333330005	0.500000000	0.034219999
0.000000000	0.500000000	0.171090007
0.166669995	0.500000000	0.102650002
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0.487060010	0.403259993	0.273380011
0.500000000	0.400000006	0.068439998
0.673089981	0.398200005	0.205789998
0.833329976	0.500000000	0.034219999
0.500000000	0.500000000	0.171090007
0.666670024	0.500000000	0.102650002
0.166669995	0.600000024	0.000000000
0.333330005	0.600000024	0.136869997
0.000000000	0.600000024	0.068439998
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0.333330005	0.699999988	0.034219999
0.000000000	0.699999988	0.171090007
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0.500000000	0.600000024	0.068439998
0.667900026	0.600179970	0.208969995
0.833329976	0.699999988	0.034219999
0.500000000	0.699999988	0.171090007
0.666670024	0.699999988	0.102650002
0.166669995	0.800000012	0.000000000
0.333330005	0.800000012	0.136869997
0.000000000	0.800000012	0.068439998
0.158859998	0.802510023	0.209309995
0.333330005	0.899999976	0.034219999
0.000000000	0.899999976	0.171090007
0.166669995	0.899999976	0.102650002
0.320919991	0.899299979	0.242349997
0.666670024	0.800000012	0.000000000
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0.489840001	0.801599979	0.271250010
0.500000000	0.800000012	0.068439998

0.663789988	0.798969984	0.207369998
0.833329976	0.899999976	0.034219999
0.500000000	0.899999976	0.171090007
0.666670024	0.899999976	0.102650002
0.643869996	0.312550008	0.302500010
0.640910029	0.446559995	0.292109996
0.630389988	0.188759997	0.291839987
0.688160002	0.591229975	0.337029994
0.646459997	0.558830023	0.295870006

O_{Van}

Pt	Ni	O
80	1	1

Direct

0.166669995	0.000000000	0.000000000
0.333330005	0.000000000	0.136869997
0.000000000	0.000000000	0.068439998
0.158720002	0.001190000	0.209050000
0.333330005	0.100000001	0.034219999
0.000000000	0.100000001	0.171090007
0.166669995	0.100000001	0.102650002
0.323359996	0.101000004	0.242569998
0.666670024	0.000000000	0.000000000
0.832379997	0.999270022	0.146760002
0.488499999	0.997500002	0.270619988
0.500000000	0.000000000	0.068439998
0.663420022	0.996980011	0.206829995
0.833329976	0.100000001	0.034219999
0.500000000	0.100000001	0.171090007
0.666670024	0.100000001	0.102650002
0.166669995	0.200000003	0.000000000
0.333330005	0.200000003	0.136869997
0.000000000	0.200000003	0.068439998
0.159869999	0.199410006	0.209439993
0.333330005	0.300000012	0.034219999
0.000000000	0.300000012	0.171090007
0.166669995	0.300000012	0.102650002
0.322670013	0.298759997	0.242760003
0.666670024	0.200000003	0.000000000
0.835020006	0.199699998	0.144250005
0.485329986	0.197119996	0.275880009
0.500000000	0.200000003	0.068439998
0.674799979	0.194869995	0.207599998
0.833329976	0.300000012	0.034219999

0.500000000	0.300000012	0.171090007
0.666670024	0.300000012	0.102650002
0.166669995	0.400000006	0.000000000
0.333330005	0.400000006	0.136869997
0.000000000	0.400000006	0.068439998
0.158570006	0.400079995	0.208890006
0.333330005	0.500000000	0.034219999
0.000000000	0.500000000	0.171090007
0.166669995	0.500000000	0.102650002
0.320809990	0.500270009	0.242029995
0.666670024	0.400000006	0.000000000
0.833209991	0.400269985	0.146290004
0.485560000	0.404350013	0.270990014
0.500000000	0.400000006	0.068439998
0.666419983	0.402770013	0.206430003
0.833329976	0.500000000	0.034219999
0.500000000	0.500000000	0.171090007
0.666670024	0.500000000	0.102650002
0.166669995	0.600000024	0.000000000
0.333330005	0.600000024	0.136869997
0.000000000	0.600000024	0.068439998
0.158170000	0.601760030	0.208900005
0.333330005	0.699999988	0.034219999
0.000000000	0.699999988	0.171090007
0.166669995	0.699999988	0.102650002
0.321599990	0.700640023	0.242090002
0.666670024	0.600000024	0.000000000
0.832050025	0.600040019	0.147110000
0.488909990	0.601530015	0.270969987
0.500000000	0.600000024	0.068439998
0.663469970	0.600740016	0.207829997
0.833329976	0.699999988	0.034219999
0.500000000	0.699999988	0.171090007
0.666670024	0.699999988	0.102650002
0.166669995	0.800000012	0.000000000
0.333330005	0.800000012	0.136869997
0.000000000	0.800000012	0.068439998
0.158859998	0.802510023	0.209309995
0.333330005	0.899999976	0.034219999
0.000000000	0.899999976	0.171090007
0.166669995	0.899999976	0.102650002
0.321530014	0.900579989	0.242459998
0.666670024	0.800000012	0.000000000
0.832099974	0.799920022	0.147180006

0.489620000	0.799499989	0.270909995
0.500000000	0.800000012	0.068439998
0.663410008	0.799120009	0.207790002
0.833329976	0.899999976	0.034219999
0.500000000	0.899999976	0.171090007
0.666670024	0.899999976	0.102650002
0.640169978	0.325960010	0.301290005
0.635280013	0.201639995	0.291619986

O#

Pt	Ni	O
80	1	3

Direct

0.166669995	0.000000000	0.000000000
0.333330005	0.000000000	0.136869997
0.000000000	0.000000000	0.068439998
0.158720002	0.001190000	0.209050000
0.333330005	0.100000001	0.034219999
0.000000000	0.100000001	0.171090007
0.166669995	0.100000001	0.102650002
0.322910011	0.101039998	0.242430001
0.666670024	0.000000000	0.000000000
0.832000017	0.999530017	0.146709993
0.487879992	0.998420000	0.270649999
0.500000000	0.000000000	0.068439998
0.662670016	0.997950017	0.206939995
0.833329976	0.100000001	0.034219999
0.500000000	0.100000001	0.171090007
0.666670024	0.100000001	0.102650002
0.166669995	0.200000003	0.000000000
0.333330005	0.200000003	0.136869997
0.000000000	0.200000003	0.068439998
0.159869999	0.199410006	0.209439993
0.333330005	0.300000012	0.034219999
0.000000000	0.300000012	0.171090007
0.166669995	0.300000012	0.102650002
0.319860011	0.298709989	0.243080005
0.666670024	0.200000003	0.000000000
0.834050000	0.199120000	0.145730004
0.481350005	0.198220000	0.275990009
0.500000000	0.200000003	0.068439998
0.672089994	0.193269998	0.209700003
0.833329976	0.300000012	0.034219999
0.500000000	0.300000012	0.171090007

0.666670024	0.300000012	0.102650002
0.166669995	0.400000006	0.000000000
0.333330005	0.400000006	0.136869997
0.000000000	0.400000006	0.068439998
0.158570006	0.400079995	0.208890006
0.333330005	0.500000000	0.034219999
0.000000000	0.500000000	0.171090007
0.166669995	0.500000000	0.102650002
0.319429994	0.500020027	0.242090002
0.666670024	0.400000006	0.000000000
0.837360024	0.399980009	0.141530007
0.483170003	0.400720000	0.270550013
0.500000000	0.400000006	0.068439998
0.674950004	0.395529985	0.202509999
0.833329976	0.500000000	0.034219999
0.500000000	0.500000000	0.171090007
0.666670024	0.500000000	0.102650002
0.166669995	0.600000024	0.000000000
0.333330005	0.600000024	0.136869997
0.000000000	0.600000024	0.068439998
0.158170000	0.601760030	0.208900005
0.333330005	0.699999988	0.034219999
0.000000000	0.699999988	0.171090007
0.166669995	0.699999988	0.102650002
0.320069999	0.701089978	0.242139995
0.666670024	0.600000024	0.000000000
0.833039999	0.600870013	0.144859999
0.483929992	0.600790024	0.270779997
0.500000000	0.600000024	0.068439998
0.669459999	0.606209993	0.209869996
0.833329976	0.699999988	0.034219999
0.500000000	0.699999988	0.171090007
0.666670024	0.699999988	0.102650002
0.166669995	0.800000012	0.000000000
0.333330005	0.800000012	0.136869997
0.000000000	0.800000012	0.068439998
0.158859998	0.802510023	0.209309995
0.333330005	0.899999976	0.034219999
0.000000000	0.899999976	0.171090007
0.166669995	0.899999976	0.102650002
0.321159989	0.900820017	0.242530003
0.666670024	0.800000012	0.000000000
0.832759976	0.800710022	0.147060007
0.488660008	0.799790025	0.270790011

0.500000000	0.800000012	0.068439998
0.663500011	0.801810026	0.207509995
0.833329976	0.899999976	0.034219999
0.500000000	0.899999976	0.171090007
0.666670024	0.899999976	0.102650002
0.652610004	0.335990012	0.300269991
0.627669990	0.210170001	0.294140011
0.701529980	0.550090015	0.287129998
0.720120013	0.447829992	0.282359987

TS2

Pt Ni O
80 1 3

Direct

0.166669995	0.000000000	0.000000000
0.333330005	0.000000000	0.136869997
0.000000000	0.000000000	0.068439998
0.158720002	0.001190000	0.209050000
0.333330005	0.100000001	0.034219999
0.000000000	0.100000001	0.171090007
0.166669995	0.100000001	0.102650002
0.322809994	0.101109996	0.242510006
0.666670024	0.000000000	0.000000000
0.832390010	0.999419987	0.146469995
0.487819999	0.998399973	0.270570010
0.500000000	0.000000000	0.068439998
0.662959993	0.998399973	0.206609994
0.833329976	0.100000001	0.034219999
0.500000000	0.100000001	0.171090007
0.666670024	0.100000001	0.102650002
0.166669995	0.200000003	0.000000000
0.333330005	0.200000003	0.136869997
0.000000000	0.200000003	0.068439998
0.159869999	0.199410006	0.209439993
0.333330005	0.300000012	0.034219999
0.000000000	0.300000012	0.171090007
0.166669995	0.300000012	0.102650002
0.319770008	0.298779994	0.242880002
0.666670024	0.200000003	0.000000000
0.834720016	0.199159995	0.145050004
0.482919991	0.197310001	0.276309997
0.500000000	0.200000003	0.068439998
0.671899974	0.195319995	0.207760006
0.833329976	0.300000012	0.034219999

0.500000000	0.300000012	0.171090007
0.666670024	0.300000012	0.102650002
0.166669995	0.400000006	0.000000000
0.333330005	0.400000006	0.136869997
0.000000000	0.400000006	0.068439998
0.158570006	0.400079995	0.208890006
0.333330005	0.500000000	0.034219999
0.000000000	0.500000000	0.171090007
0.166669995	0.500000000	0.102650002
0.319889992	0.501519978	0.242359996
0.666670024	0.400000006	0.000000000
0.836860001	0.399949998	0.141739994
0.481169999	0.401140004	0.270260006
0.500000000	0.400000006	0.068439998
0.677540004	0.398900002	0.205090001
0.833329976	0.500000000	0.034219999
0.500000000	0.500000000	0.171090007
0.666670024	0.500000000	0.102650002
0.166669995	0.600000024	0.000000000
0.333330005	0.600000024	0.136869997
0.000000000	0.600000024	0.068439998
0.158170000	0.601760030	0.208900005
0.333330005	0.699999988	0.034219999
0.000000000	0.699999988	0.171090007
0.166669995	0.699999988	0.102650002
0.321159989	0.700469971	0.242459998
0.666670024	0.600000024	0.000000000
0.833980024	0.600830019	0.144700006
0.483850002	0.600880027	0.273079991
0.500000000	0.600000024	0.068439998
0.670690000	0.604910016	0.208409995
0.833329976	0.699999988	0.034219999
0.500000000	0.699999988	0.171090007
0.666670024	0.699999988	0.102650002
0.166669995	0.800000012	0.000000000
0.333330005	0.800000012	0.136869997
0.000000000	0.800000012	0.068439998
0.158859998	0.802510023	0.209309995
0.333330005	0.899999976	0.034219999
0.000000000	0.899999976	0.171090007
0.166669995	0.899999976	0.102650002
0.320829988	0.900629997	0.242440000
0.666670024	0.800000012	0.000000000
0.833000004	0.800599992	0.146599993

0.488180012	0.801100016	0.270529985
0.500000000	0.800000012	0.068439998
0.663659990	0.802150011	0.206780002
0.833329976	0.899999976	0.034219999
0.500000000	0.899999976	0.171090007
0.666670024	0.899999976	0.102650002
0.646399975	0.336239994	0.301560014
0.629880011	0.209800005	0.292890012
0.660529971	0.557269990	0.289590001
0.701370001	0.453999996	0.287919998

O*

Pt	Ni	O
80	1	3

Direct

0.166669995	0.000000000	0.000000000
0.333330005	0.000000000	0.136869997
0.000000000	0.000000000	0.068439998
0.158720002	0.001190000	0.209050000
0.333330005	0.100000001	0.034219999
0.000000000	0.100000001	0.171090007
0.166669995	0.100000001	0.102650002
0.322710007	0.101180002	0.242599994
0.666670024	0.000000000	0.000000000
0.832780004	0.999319971	0.146239996
0.487760007	0.998390019	0.270489991
0.500000000	0.000000000	0.068439998
0.663250029	0.998839974	0.206290007
0.833329976	0.100000001	0.034219999
0.500000000	0.100000001	0.171090007
0.666670024	0.100000001	0.102650002
0.166669995	0.200000003	0.000000000
0.333330005	0.200000003	0.136869997
0.000000000	0.200000003	0.068439998
0.159869999	0.199410006	0.209439993
0.333330005	0.300000012	0.034219999
0.000000000	0.300000012	0.171090007
0.166669995	0.300000012	0.102650002
0.319680005	0.298850000	0.242689997
0.666670024	0.200000003	0.000000000
0.835399985	0.199210003	0.144370005
0.484479994	0.196410000	0.276639998
0.500000000	0.200000003	0.068439998
0.671700001	0.197359994	0.205809996

0.833329976	0.300000012	0.034219999
0.500000000	0.300000012	0.171090007
0.666670024	0.300000012	0.102650002
0.166669995	0.400000006	0.000000000
0.333330005	0.400000006	0.136869997
0.000000000	0.400000006	0.068439998
0.158570006	0.400079995	0.208890006
0.333330005	0.500000000	0.034219999
0.000000000	0.500000000	0.171090007
0.166669995	0.500000000	0.102650002
0.320360005	0.503019989	0.242630005
0.666670024	0.400000006	0.000000000
0.836369991	0.399910003	0.141949996
0.479180008	0.401560009	0.269980013
0.500000000	0.400000006	0.068439998
0.680130005	0.402269989	0.207670003
0.833329976	0.500000000	0.034219999
0.500000000	0.500000000	0.171090007
0.666670024	0.500000000	0.102650002
0.166669995	0.600000024	0.000000000
0.333330005	0.600000024	0.136869997
0.000000000	0.600000024	0.068439998
0.158170000	0.601760030	0.208900005
0.333330005	0.699999988	0.034219999
0.000000000	0.699999988	0.171090007
0.166669995	0.699999988	0.102650002
0.322250009	0.699859977	0.242780000
0.666670024	0.600000024	0.000000000
0.834919989	0.600790024	0.144539997
0.483770013	0.600969970	0.275389999
0.500000000	0.600000024	0.068439998
0.671920002	0.603609979	0.206949994
0.833329976	0.699999988	0.034219999
0.500000000	0.699999988	0.171090007
0.666670024	0.699999988	0.102650002
0.166669995	0.800000012	0.000000000
0.333330005	0.800000012	0.136869997
0.000000000	0.800000012	0.068439998
0.158859998	0.802510023	0.209309995
0.333330005	0.899999976	0.034219999
0.000000000	0.899999976	0.171090007
0.166669995	0.899999976	0.102650002
0.320490003	0.900430024	0.242359996
0.666670024	0.800000012	0.000000000

0.833230019	0.800490022	0.146139994
0.487699986	0.802399993	0.270260006
0.500000000	0.800000012	0.068439998
0.663810015	0.802489996	0.206049994
0.833329976	0.899999976	0.034219999
0.500000000	0.899999976	0.171090007
0.666670024	0.899999976	0.102650002
0.621829987	0.318190008	0.311800003
0.636520028	0.197579995	0.290410012
0.626089990	0.604279995	0.286190003
0.712419987	0.393029988	0.288370013

CO~O*

Pt	Ni	O	C
80	1	4	1

Direct

0.166669995	0.000000000	0.000000000
0.333330005	0.000000000	0.136869997
0.000000000	0.000000000	0.068439998
0.158720002	0.001190000	0.209050000
0.333330005	0.100000001	0.034219999
0.000000000	0.100000001	0.171090007
0.166669995	0.100000001	0.102650002
0.322340012	0.100539997	0.242520005
0.666670024	0.000000000	0.000000000
0.832769990	0.999260008	0.146589994
0.487480015	0.000320000	0.270449996
0.500000000	0.000000000	0.068439998
0.663309991	0.999700010	0.205789998
0.833329976	0.100000001	0.034219999
0.500000000	0.100000001	0.171090007
0.666670024	0.100000001	0.102650002
0.166669995	0.200000003	0.000000000
0.333330005	0.200000003	0.136869997
0.000000000	0.200000003	0.068439998
0.159869999	0.199410006	0.209439993
0.333330005	0.300000012	0.034219999
0.000000000	0.300000012	0.171090007
0.166669995	0.300000012	0.102650002
0.319270015	0.298619986	0.242630005
0.666670024	0.200000003	0.000000000
0.835640013	0.199000001	0.144400001
0.483539999	0.197369993	0.276870012
0.500000000	0.200000003	0.068439998

0.671570003	0.197469994	0.205870003
0.833329976	0.300000012	0.034219999
0.500000000	0.300000012	0.171090007
0.666670024	0.300000012	0.102650002
0.166669995	0.400000006	0.000000000
0.333330005	0.400000006	0.136869997
0.000000000	0.400000006	0.068439998
0.158570006	0.400079995	0.208890006
0.333330005	0.500000000	0.034219999
0.000000000	0.500000000	0.171090007
0.166669995	0.500000000	0.102650002
0.319770008	0.503570020	0.242599994
0.666670024	0.400000006	0.000000000
0.836780012	0.400119990	0.141800001
0.478210002	0.401179999	0.270139992
0.500000000	0.400000006	0.068439998
0.681119978	0.400959998	0.207719997
0.833329976	0.500000000	0.034219999
0.500000000	0.500000000	0.171090007
0.666670024	0.500000000	0.102650002
0.166669995	0.600000024	0.000000000
0.333330005	0.600000024	0.136869997
0.000000000	0.600000024	0.068439998
0.158170000	0.601760030	0.208900005
0.333330005	0.699999988	0.034219999
0.000000000	0.699999988	0.171090007
0.166669995	0.699999988	0.102650002
0.323659986	0.700869977	0.242599994
0.666670024	0.600000024	0.000000000
0.834850013	0.600839972	0.144749999
0.482919991	0.599529982	0.275389999
0.500000000	0.600000024	0.068439998
0.671060026	0.601490021	0.206279993
0.833329976	0.699999988	0.034219999
0.500000000	0.699999988	0.171090007
0.666670024	0.699999988	0.102650002
0.166669995	0.800000012	0.000000000
0.333330005	0.800000012	0.136869997
0.000000000	0.800000012	0.068439998
0.158859998	0.802510023	0.209309995
0.333330005	0.899999976	0.034219999
0.000000000	0.899999976	0.171090007
0.166669995	0.899999976	0.102650002
0.322149992	0.899739981	0.242369995

0.666670024	0.800000012	0.000000000
0.831979990	0.800570011	0.146640003
0.493880004	0.802370012	0.272859991
0.500000000	0.800000012	0.068439998
0.671800017	0.802309990	0.211870000
0.833329976	0.899999976	0.034219999
0.500000000	0.899999976	0.171090007
0.666670024	0.899999976	0.102650002
0.621450007	0.318349987	0.311830014
0.635559976	0.197699994	0.290399998
0.625389993	0.597700000	0.285569996
0.712559998	0.392630011	0.288509995
0.682359993	0.808279991	0.339430004
0.639479995	0.805899978	0.295599997

TS3

Pt	Ni	O	C
80	1	4	1

Direct

0.166669995	0.000000000	0.000000000
0.333330005	0.000000000	0.136869997
0.000000000	0.000000000	0.068439998
0.158720002	0.001190000	0.209050000
0.333330005	0.100000001	0.034219999
0.000000000	0.100000001	0.171090007
0.166669995	0.100000001	0.102650002
0.322340012	0.100539997	0.242520005
0.666670024	0.000000000	0.000000000
0.832769990	0.999260008	0.146589994
0.487480015	0.000320000	0.270449996
0.500000000	0.000000000	0.068439998
0.663309991	0.999700010	0.205789998
0.833329976	0.100000001	0.034219999
0.500000000	0.100000001	0.171090007
0.666670024	0.100000001	0.102650002
0.166669995	0.200000003	0.000000000
0.333330005	0.200000003	0.136869997
0.000000000	0.200000003	0.068439998
0.159869999	0.199410006	0.209439993
0.333330005	0.300000012	0.034219999
0.000000000	0.300000012	0.171090007
0.166669995	0.300000012	0.102650002
0.319270015	0.298619986	0.242630005
0.666670024	0.200000003	0.000000000

0.835640013	0.199000001	0.144400001
0.483539999	0.197369993	0.276870012
0.500000000	0.200000003	0.068439998
0.671570003	0.197469994	0.205870003
0.833329976	0.300000012	0.034219999
0.500000000	0.300000012	0.171090007
0.666670024	0.300000012	0.102650002
0.166669995	0.400000006	0.000000000
0.333330005	0.400000006	0.136869997
0.000000000	0.400000006	0.068439998
0.158570006	0.400079995	0.208890006
0.333330005	0.500000000	0.034219999
0.000000000	0.500000000	0.171090007
0.166669995	0.500000000	0.102650002
0.319770008	0.503570020	0.242599994
0.666670024	0.400000006	0.000000000
0.836780012	0.400119990	0.141800001
0.478210002	0.401179999	0.270139992
0.500000000	0.400000006	0.068439998
0.681119978	0.400959998	0.207719997
0.833329976	0.500000000	0.034219999
0.500000000	0.500000000	0.171090007
0.666670024	0.500000000	0.102650002
0.166669995	0.600000024	0.000000000
0.333330005	0.600000024	0.136869997
0.000000000	0.600000024	0.068439998
0.158170000	0.601760030	0.208900005
0.333330005	0.699999988	0.034219999
0.000000000	0.699999988	0.171090007
0.166669995	0.699999988	0.102650002
0.323659986	0.700869977	0.242599994
0.666670024	0.600000024	0.000000000
0.834850013	0.600839972	0.144749999
0.482919991	0.599529982	0.275389999
0.500000000	0.600000024	0.068439998
0.671060026	0.601490021	0.206279993
0.833329976	0.699999988	0.034219999
0.500000000	0.699999988	0.171090007
0.666670024	0.699999988	0.102650002
0.166669995	0.800000012	0.000000000
0.333330005	0.800000012	0.136869997
0.000000000	0.800000012	0.068439998
0.158859998	0.802510023	0.209309995
0.333330005	0.899999976	0.034219999

0.000000000	0.899999976	0.171090007
0.166669995	0.899999976	0.102650002
0.322149992	0.899739981	0.242369995
0.666670024	0.800000012	0.000000000
0.831979990	0.800570011	0.146640003
0.493880004	0.802370012	0.272859991
0.500000000	0.800000012	0.068439998
0.671800017	0.802309990	0.211870000
0.833329976	0.899999976	0.034219999
0.500000000	0.899999976	0.171090007
0.666670024	0.899999976	0.102650002
0.621450007	0.318349987	0.311830014
0.635559976	0.197699994	0.290399998
0.712559998	0.392630011	0.288509995
0.637849987	0.631690025	0.293709993
0.678089976	0.812640011	0.335539997
0.641460001	0.773039997	0.295850009

NiO_x/Pt₍₁₀₀₎

*

1.0

11.0985002518	0.0000000000	0.0000000000
0.0000000000	11.0985002518	0.0000000000
0.0000000000	0.0000000000	25.8477993011

Pt Ni O

80 5 4

Direct

0.0000000000	0.0000000000	0.0000000000
0.0000000000	0.0000000000	0.151810005
0.999961972	0.000135000	0.307092994
0.125000000	0.125000000	0.075900003
0.125542998	0.125700995	0.230226994
0.250000000	0.000000000	0.000000000
0.250000000	0.000000000	0.151810005
0.248777002	0.000421000	0.307220012
0.375000000	0.125000000	0.075900003
0.374985009	0.125712007	0.230462000
0.500000000	0.000000000	0.000000000
0.500000000	0.000000000	0.151810005
0.499922007	0.000408000	0.307327986
0.625000000	0.125000000	0.075900003
0.624966979	0.125729993	0.230453998
0.750000000	0.000000000	0.000000000
0.750000000	0.000000000	0.151810005
0.751101971	0.000556000	0.307209998
0.875000000	0.125000000	0.075900003
0.874418020	0.125758007	0.230241001
0.000000000	0.250000000	0.000000000
0.000000000	0.250000000	0.151810005
0.999998987	0.249001995	0.307222009
0.125000000	0.375000000	0.075900003
0.125413999	0.375124007	0.230456993
0.250000000	0.250000000	0.000000000
0.250000000	0.250000000	0.151810005
0.247171000	0.247611001	0.309731007
0.375000000	0.375000000	0.075900003
0.374096006	0.374231994	0.230134994
0.500000000	0.250000000	0.000000000
0.500000000	0.250000000	0.151810005
0.500033975	0.243773997	0.309307992
0.625000000	0.375000000	0.075900003
0.625917971	0.374267012	0.230140001

0.750000000	0.250000000	0.000000000
0.750000000	0.250000000	0.151810005
0.752793014	0.247750998	0.309733987
0.875000000	0.375000000	0.075900003
0.874522984	0.375169009	0.230467007
0.000000000	0.500000000	0.000000000
0.000000000	0.500000000	0.151810005
0.999882996	0.500223994	0.307330012
0.125000000	0.625000000	0.075900003
0.125363007	0.625102997	0.230418995
0.250000000	0.500000000	0.000000000
0.250000000	0.500000000	0.151810005
0.243233994	0.500401974	0.309246004
0.375000000	0.625000000	0.075900003
0.374027014	0.626048028	0.230113000
0.500000000	0.500000000	0.000000000
0.500000000	0.500000000	0.151810005
0.499994993	0.500418007	0.303557992
0.625000000	0.625000000	0.075900003
0.625898004	0.626073003	0.230105996
0.750000000	0.500000000	0.000000000
0.750000000	0.500000000	0.151810005
0.756657004	0.500568986	0.309267014
0.875000000	0.625000000	0.075900003
0.874504030	0.625153005	0.230416998
0.000000000	0.750000000	0.000000000
0.000000000	0.750000000	0.151810005
0.999849975	0.751323998	0.307209998
0.125000000	0.875000000	0.075900003
0.125476003	0.874602973	0.230230004
0.250000000	0.750000000	0.000000000
0.250000000	0.750000000	0.151810005
0.246975005	0.753289998	0.309688002
0.375000000	0.875000000	0.075900003
0.374949992	0.874805987	0.230413005
0.500000000	0.750000000	0.000000000
0.500000000	0.750000000	0.151810005
0.499927998	0.757115006	0.309213996
0.625000000	0.875000000	0.075900003
0.624942005	0.874864995	0.230416000
0.750000000	0.750000000	0.000000000
0.750000000	0.750000000	0.151810005
0.752668977	0.753461003	0.309680998
0.875000000	0.875000000	0.075900003

0.874396980	0.874646008	0.230228007
0.499855995	0.501043975	0.430947989
0.625793993	0.374846995	0.372842997
0.374173999	0.626568973	0.372662008
0.374105006	0.374794990	0.372792006
0.625881016	0.626522005	0.372759998
0.499906987	0.336149007	0.419512004
0.664669991	0.500867009	0.419416994
0.335054994	0.500874996	0.419333011
0.499980986	0.665814996	0.419362009

CO*

Pt	Ni	O	C
80	5	5	1

Direct

0.000000000	0.000000000	0.000000000
0.000000000	0.000000000	0.151810005
0.000639000	0.000682000	0.306309015
0.125000000	0.125000000	0.075900003
0.126117006	0.126543999	0.229567006
0.250000000	0.000000000	0.000000000
0.250000000	0.000000000	0.151810005
0.249592006	0.001340000	0.306270003
0.375000000	0.125000000	0.075900003
0.375851989	0.126497000	0.230176002
0.500000000	0.000000000	0.000000000
0.500000000	0.000000000	0.151810005
0.500617981	0.001029000	0.306493998
0.625000000	0.125000000	0.075900003
0.625056982	0.127000004	0.230203003
0.750000000	0.000000000	0.000000000
0.750000000	0.000000000	0.151810005
0.751392007	0.001212000	0.306695998
0.875000000	0.125000000	0.075900003
0.874228001	0.126745000	0.229917005
0.000000000	0.250000000	0.000000000
0.000000000	0.250000000	0.151810005
0.001021000	0.247447997	0.306133002
0.125000000	0.375000000	0.075900003
0.125770003	0.376421005	0.230413005
0.250000000	0.250000000	0.000000000
0.250000000	0.250000000	0.151810005
0.248673007	0.248379007	0.308975011
0.375000000	0.375000000	0.075900003

0.376910001	0.374556005	0.229845002
0.500000000	0.250000000	0.000000000
0.500000000	0.250000000	0.151810005
0.500569999	0.244681999	0.309767008
0.625000000	0.375000000	0.075900003
0.628875017	0.375809014	0.230829999
0.750000000	0.250000000	0.000000000
0.750000000	0.250000000	0.151810005
0.751244009	0.247654006	0.309818000
0.875000000	0.375000000	0.075900003
0.875245988	0.376836985	0.231328994
0.000000000	0.500000000	0.000000000
0.000000000	0.500000000	0.151810005
0.010733000	0.500576973	0.311668009
0.125000000	0.625000000	0.075900003
0.125551999	0.624590993	0.230376005
0.250000000	0.500000000	0.000000000
0.250000000	0.500000000	0.151810005
0.249936000	0.501390994	0.307597995
0.375000000	0.625000000	0.075900003
0.376837999	0.626295984	0.229756996
0.500000000	0.500000000	0.000000000
0.500000000	0.500000000	0.151810005
0.504956007	0.501147985	0.304208010
0.625000000	0.625000000	0.075900003
0.629124999	0.625042975	0.230817005
0.750000000	0.500000000	0.000000000
0.750000000	0.500000000	0.151810005
0.761891007	0.501205981	0.316354990
0.875000000	0.625000000	0.075900003
0.875370979	0.623924017	0.231277004
0.000000000	0.750000000	0.000000000
0.000000000	0.750000000	0.151810005
0.000889000	0.753924012	0.306089014
0.125000000	0.875000000	0.075900003
0.126093000	0.874692023	0.229494005
0.250000000	0.750000000	0.000000000
0.250000000	0.750000000	0.151810005
0.248392999	0.754482985	0.308654994
0.375000000	0.875000000	0.075900003
0.375791997	0.874834001	0.229981005
0.500000000	0.750000000	0.000000000
0.500000000	0.750000000	0.151810005
0.500663996	0.757817984	0.309220999

0.625000000	0.875000000	0.075900003
0.625252008	0.874378026	0.230022997
0.750000000	0.750000000	0.000000000
0.750000000	0.750000000	0.151810005
0.751730025	0.754905999	0.309529990
0.875000000	0.875000000	0.075900003
0.874332011	0.874412000	0.229819998
0.491539001	0.503618002	0.432763010
0.621174991	0.375330001	0.375674993
0.372803003	0.628230989	0.372258008
0.372837991	0.376439989	0.372763991
0.621710002	0.629815996	0.375187010
0.493896991	0.338301986	0.421344012
0.654855013	0.503293991	0.422733009
0.328310996	0.503102005	0.418482006
0.494042009	0.668657005	0.420542002
0.904444993	0.497604012	0.416296005
0.898357987	0.499195993	0.370779991

TS1

Pt	Ni	O	C
80	5	5	1

Direct

0.000000000	0.000000000	0.000000000
0.000000000	0.000000000	0.151810005
0.000639674	0.000681190	0.306309253
0.125000000	0.125000000	0.075900003
0.126118183	0.126542270	0.229567856
0.250000000	0.000000000	0.000000000
0.250000000	0.000000000	0.151810005
0.249591306	0.001340175	0.306269705
0.375000000	0.125000000	0.075900003
0.375851154	0.126497895	0.230177671
0.500000000	0.000000000	0.000000000
0.500000000	0.000000000	0.151810005
0.500618994	0.001029378	0.306492746
0.625000000	0.125000000	0.075900003
0.625057936	0.126999766	0.230202019
0.750000000	0.000000000	0.000000000
0.750000000	0.000000000	0.151810005
0.751391292	0.001211002	0.306697398
0.874999940	0.125000000	0.075900003
0.874228895	0.126746625	0.229917854
0.000000000	0.250000000	0.000000000

0.000000000	0.250000000	0.151810005
0.001020918	0.247448534	0.306132108
0.125000000	0.375000000	0.075900003
0.125770316	0.376420528	0.230412111
0.250000000	0.250000000	0.000000000
0.250000000	0.250000000	0.151810005
0.248671800	0.248379096	0.308976978
0.375000000	0.375000000	0.075900003
0.376910150	0.374557227	0.229843140
0.500000000	0.250000000	0.000000000
0.500000000	0.250000000	0.151810005
0.500569940	0.244681507	0.309768230
0.625000000	0.375000000	0.075900003
0.628873289	0.375809461	0.230830014
0.750000000	0.250000000	0.000000000
0.750000000	0.250000000	0.151810005
0.751242638	0.247652784	0.309818834
0.874999940	0.375000000	0.075900003
0.875247121	0.376838207	0.231329262
0.000000000	0.500000000	0.000000000
0.000000000	0.500000000	0.151810005
0.010732180	0.500577807	0.311668843
0.125000000	0.625000000	0.075900003
0.125551224	0.624590874	0.230377406
0.250000000	0.500000000	0.000000000
0.250000000	0.500000000	0.151810005
0.249937519	0.501390755	0.307598650
0.375000000	0.625000000	0.075900003
0.376838982	0.626297712	0.229758024
0.500000000	0.500000000	0.000000000
0.500000000	0.500000000	0.151810005
0.504957438	0.501148820	0.304208457
0.625000000	0.625000000	0.075900003
0.629123211	0.625041664	0.230817765
0.750000000	0.500000000	0.000000000
0.750000000	0.500000000	0.151810005
0.761890769	0.501207590	0.316356719
0.874999940	0.625000000	0.075900003
0.875370502	0.623922348	0.231278330
0.000000000	0.750000000	0.000000000
0.000000000	0.750000000	0.151810005
0.000889162	0.753922760	0.306089550
0.125000000	0.874999940	0.075900003
0.126091823	0.874691486	0.229492858

0.250000000	0.750000000	0.000000000
0.250000000	0.750000000	0.151810005
0.248391792	0.754481912	0.308653027
0.375000000	0.874999940	0.075900003
0.375791252	0.874832332	0.229980364
0.500000000	0.750000000	0.000000000
0.500000000	0.750000000	0.151810005
0.500662565	0.757818878	0.309220314
0.625000000	0.874999940	0.075900003
0.625251472	0.874378800	0.230022043
0.750000000	0.750000000	0.000000000
0.750000000	0.750000000	0.151810005
0.751730025	0.754907131	0.309530020
0.874999940	0.874999940	0.075900003
0.874330997	0.874411523	0.229819834
0.493158162	0.502281010	0.436954349
0.614347875	0.373306990	0.376053542
0.374388784	0.625965536	0.374300480
0.374411851	0.377752662	0.374605358
0.614610732	0.630335987	0.375681847
0.493854016	0.339479029	0.421630800
0.667208672	0.502243698	0.419967771
0.333308071	0.502157331	0.418657184
0.493947297	0.664833069	0.421168327
0.888669431	0.497685492	0.420336932
0.810292423	0.499439329	0.388880253

O_{Van}

Pt	Ni	O
80	5	3

Direct

0.000000000	0.000000000	0.000000000
0.000000000	0.000000000	0.151810005
0.000037000	0.000302000	0.306468010
0.125000000	0.125000000	0.075900003
0.124929003	0.125875995	0.229822993
0.250000000	0.000000000	0.000000000
0.250000000	0.000000000	0.151810005
0.249011993	0.000397000	0.306544006
0.375000000	0.125000000	0.075900003
0.374695003	0.126294002	0.230204999
0.500000000	0.000000000	0.000000000
0.500000000	0.000000000	0.151810005
0.500461996	0.000440000	0.306661010

0.625000000	0.125000000	0.075900003
0.624974012	0.125810996	0.229872003
0.750000000	0.000000000	0.000000000
0.750000000	0.000000000	0.151810005
0.750681996	0.000523000	0.306713998
0.875000000	0.125000000	0.075900003
0.874481022	0.125927001	0.229884997
0.000000000	0.250000000	0.000000000
0.000000000	0.250000000	0.151810005
0.998902023	0.249387994	0.306962013
0.125000000	0.375000000	0.075900003
0.125304997	0.375645012	0.230529994
0.250000000	0.250000000	0.000000000
0.250000000	0.250000000	0.151810005
0.246234000	0.248772994	0.308620989
0.375000000	0.375000000	0.075900003
0.374244988	0.375840992	0.230524004
0.500000000	0.250000000	0.000000000
0.500000000	0.250000000	0.151810005
0.495721996	0.242887005	0.308266997
0.625000000	0.375000000	0.075900003
0.625391006	0.375155002	0.230472997
0.750000000	0.250000000	0.000000000
0.750000000	0.250000000	0.151810005
0.750500977	0.249152005	0.308272988
0.875000000	0.375000000	0.075900003
0.873914003	0.375972986	0.230676994
0.000000000	0.500000000	0.000000000
0.000000000	0.500000000	0.151810005
0.999253988	0.500221014	0.307386011
0.125000000	0.625000000	0.075900003
0.125193998	0.624722004	0.230517998
0.250000000	0.500000000	0.000000000
0.250000000	0.500000000	0.151810005
0.244632006	0.500376999	0.310274005
0.375000000	0.625000000	0.075900003
0.374170989	0.624638975	0.230497003
0.500000000	0.500000000	0.000000000
0.500000000	0.500000000	0.151810005
0.500721991	0.500299990	0.305698007
0.625000000	0.625000000	0.075900003
0.625334024	0.625395000	0.230465993
0.750000000	0.500000000	0.000000000
0.750000000	0.500000000	0.151810005

0.754778981	0.500461996	0.312171996
0.875000000	0.625000000	0.075900003
0.873809993	0.624446988	0.230682999
0.000000000	0.750000000	0.000000000
0.000000000	0.750000000	0.151810005
0.998749018	0.751089990	0.306979001
0.125000000	0.875000000	0.075900003
0.124812998	0.874516010	0.229830995
0.250000000	0.750000000	0.000000000
0.250000000	0.750000000	0.151810005
0.246052995	0.752004027	0.308564007
0.375000000	0.875000000	0.075900003
0.374612004	0.874292016	0.230168000
0.500000000	0.750000000	0.000000000
0.500000000	0.750000000	0.151810005
0.495570987	0.757875979	0.308187991
0.625000000	0.875000000	0.075900003
0.624956012	0.874734998	0.229890004
0.750000000	0.750000000	0.000000000
0.750000000	0.750000000	0.151810005
0.750442982	0.751869023	0.308259010
0.875000000	0.875000000	0.075900003
0.874432027	0.874503016	0.229885995
0.504033983	0.500658989	0.431968004
0.617909014	0.369635999	0.371297002
0.374523014	0.627596974	0.375126988
0.374318004	0.373432994	0.375337988
0.617944002	0.631101012	0.371239007
0.507107973	0.340113997	0.419544011
0.341145992	0.500639975	0.418219000
0.506986976	0.661171973	0.419402003

O#

Pt	Ni	O
80	5	5

Direct

0.000000000	0.000000000	0.000000000
0.000000000	0.000000000	0.151810005
0.000186000	0.000148000	0.306425005
0.125000000	0.125000000	0.075900003
0.125993997	0.125552997	0.230047002
0.250000000	0.000000000	0.000000000
0.250000000	0.000000000	0.151810005
0.249469995	0.000150000	0.306946009

0.375000000	0.125000000	0.075900003
0.375752985	0.125762999	0.230653003
0.500000000	0.000000000	0.000000000
0.500000000	0.000000000	0.151810005
0.500226021	0.000147000	0.307233006
0.625000000	0.125000000	0.075900003
0.624741971	0.125622004	0.230508000
0.750000000	0.000000000	0.000000000
0.750000000	0.000000000	0.151810005
0.750833988	0.000194000	0.306820989
0.875000000	0.125000000	0.075900003
0.874633014	0.125562996	0.229968995
0.000000000	0.250000000	0.000000000
0.000000000	0.250000000	0.151810005
0.000484000	0.249422997	0.306692004
0.125000000	0.375000000	0.075900003
0.125798002	0.375156999	0.230267003
0.250000000	0.250000000	0.000000000
0.250000000	0.250000000	0.151810005
0.250196993	0.249693006	0.308481008
0.375000000	0.375000000	0.075900003
0.374807000	0.374444991	0.230114996
0.500000000	0.250000000	0.000000000
0.500000000	0.250000000	0.151810005
0.501518011	0.246758997	0.310784012
0.625000000	0.375000000	0.075900003
0.625263989	0.374222994	0.229929000
0.750000000	0.250000000	0.000000000
0.750000000	0.250000000	0.151810005
0.751151025	0.249590993	0.308443993
0.875000000	0.375000000	0.075900003
0.874702990	0.375086010	0.230214998
0.000000000	0.500000000	0.000000000
0.000000000	0.500000000	0.151810005
0.000212000	0.500077009	0.306869000
0.125000000	0.625000000	0.075900003
0.125735000	0.624935985	0.230261996
0.250000000	0.500000000	0.000000000
0.250000000	0.500000000	0.151810005
0.246097997	0.500078976	0.309222013
0.375000000	0.625000000	0.075900003
0.374716997	0.625648022	0.230092004
0.500000000	0.500000000	0.000000000
0.500000000	0.500000000	0.151810005

0.500298023	0.500136018	0.304477990
0.625000000	0.625000000	0.075900003
0.625225008	0.625904024	0.229902998
0.750000000	0.500000000	0.000000000
0.750000000	0.500000000	0.151810005
0.753727973	0.500217974	0.308277011
0.875000000	0.625000000	0.075900003
0.874702990	0.625091016	0.230195001
0.000000000	0.750000000	0.000000000
0.000000000	0.750000000	0.151810005
0.000372000	0.750764012	0.306683987
0.125000000	0.875000000	0.075900003
0.125933006	0.874596000	0.230031997
0.250000000	0.750000000	0.000000000
0.250000000	0.750000000	0.151810005
0.249981999	0.750606000	0.308434010
0.375000000	0.875000000	0.075900003
0.375634998	0.874485016	0.230597004
0.500000000	0.750000000	0.000000000
0.500000000	0.750000000	0.151810005
0.501224995	0.753642023	0.310595006
0.625000000	0.875000000	0.075900003
0.624671996	0.874635994	0.230452001
0.750000000	0.750000000	0.000000000
0.750000000	0.750000000	0.151810005
0.751039982	0.750835001	0.308353990
0.875000000	0.875000000	0.075900003
0.874601007	0.874660015	0.229968995
0.485141993	0.500850976	0.449672997
0.622626007	0.380145997	0.376450002
0.377328992	0.621698976	0.375842005
0.377606988	0.378704011	0.376004010
0.622389019	0.621168971	0.376233995
0.498571992	0.346596986	0.421555996
0.332374007	0.500365019	0.420336992
0.498100013	0.654829025	0.421328008
0.643163979	0.501416028	0.468461990
0.694746017	0.501137972	0.418518007

TS2

Pt	Ni	O
80	5	5

Direct

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

0.000000000	0.000000000	0.151810005
0.000027000	0.000036000	0.306243986
0.125000000	0.125000000	0.075900003
0.125900999	0.125635996	0.229703993
0.250000000	0.000000000	0.000000000
0.250000000	0.000000000	0.151810005
0.249321997	0.000001000	0.306977987
0.375000000	0.125000000	0.075900003
0.375364006	0.125804007	0.230345994
0.500000000	0.000000000	0.000000000
0.500000000	0.000000000	0.151810005
0.499886990	0.999774992	0.307045996
0.625000000	0.125000000	0.075900003
0.624382019	0.125833005	0.230142996
0.750000000	0.000000000	0.000000000
0.750000000	0.000000000	0.151810005
0.750352979	0.999686003	0.307011008
0.875000000	0.125000000	0.075900003
0.874280989	0.125727996	0.229796007
0.000000000	0.250000000	0.000000000
0.000000000	0.250000000	0.151810005
0.999189019	0.248576000	0.307188004
0.125000000	0.375000000	0.075900003
0.124968000	0.375492990	0.230684996
0.250000000	0.250000000	0.000000000
0.250000000	0.250000000	0.151810005
0.247713998	0.247943997	0.308302999
0.375000000	0.375000000	0.075900003
0.375030011	0.374455988	0.229995996
0.500000000	0.250000000	0.000000000
0.500000000	0.250000000	0.151810005
0.500138998	0.246459007	0.310571015
0.625000000	0.375000000	0.075900003
0.626047015	0.375037998	0.230561003
0.750000000	0.250000000	0.000000000
0.750000000	0.250000000	0.151810005
0.749768019	0.245838001	0.308366001
0.875000000	0.375000000	0.075900003
0.874616027	0.375515014	0.230495006
0.000000000	0.500000000	0.000000000
0.000000000	0.500000000	0.151810005
0.003114000	0.500050008	0.307175010
0.125000000	0.625000000	0.075900003
0.124921001	0.624688029	0.230685994

0.250000000	0.500000000	0.000000000
0.250000000	0.500000000	0.151810005
0.247061998	0.499992013	0.308308989
0.375000000	0.625000000	0.075900003
0.374956995	0.625733972	0.229975998
0.500000000	0.500000000	0.000000000
0.500000000	0.500000000	0.151810005
0.502686977	0.500456989	0.306528986
0.625000000	0.625000000	0.075900003
0.626039028	0.625162005	0.230568007
0.750000000	0.500000000	0.000000000
0.750000000	0.500000000	0.151810005
0.757290006	0.498286992	0.313663989
0.875000000	0.625000000	0.075900003
0.874624014	0.624684989	0.230477005
0.000000000	0.750000000	0.000000000
0.000000000	0.750000000	0.151810005
0.999104977	0.751537025	0.307135999
0.125000000	0.875000000	0.075900003
0.125852004	0.874566972	0.229695007
0.250000000	0.750000000	0.000000000
0.250000000	0.750000000	0.151810005
0.248015001	0.751987994	0.308275014
0.375000000	0.875000000	0.075900003
0.375272006	0.874499977	0.230306998
0.500000000	0.750000000	0.000000000
0.500000000	0.750000000	0.151810005
0.500512004	0.753306985	0.310609013
0.625000000	0.875000000	0.075900003
0.624357998	0.874439001	0.230120003
0.750000000	0.750000000	0.000000000
0.750000000	0.750000000	0.151810005
0.749459028	0.752960980	0.308326989
0.875000000	0.875000000	0.075900003
0.874261022	0.874511003	0.229789004
0.487017989	0.498800993	0.434022993
0.616155028	0.366851002	0.382243007
0.368256003	0.625164986	0.374819994
0.366959989	0.374675006	0.374830991
0.620419979	0.634181023	0.384705991
0.486948013	0.334601998	0.421543986
0.326344013	0.499918997	0.418985009
0.486541003	0.664116025	0.422078013
0.665625989	0.502750993	0.428104997

	0.787436008	0.494769990	0.388718992
O*			
Pt	Ni	O	
80	5	5	
Direct			
	0.000000000	0.000000000	0.000000000
	0.000000000	0.000000000	0.151810005
	0.999737024	0.000150000	0.306098998
	0.125000000	0.125000000	0.075900003
	0.125808001	0.125719994	0.229359999
	0.250000000	0.000000000	0.000000000
	0.250000000	0.000000000	0.151810005
	0.249050006	0.000388000	0.306311011
	0.375000000	0.125000000	0.075900003
	0.374976009	0.125845999	0.230039001
	0.500000000	0.000000000	0.000000000
	0.500000000	0.000000000	0.151810005
	0.499862999	0.000342000	0.306620002
	0.625000000	0.125000000	0.075900003
	0.624022007	0.126044005	0.229778007
	0.750000000	0.000000000	0.000000000
	0.750000000	0.000000000	0.151810005
	0.750140011	0.000380000	0.306457013
	0.875000000	0.125000000	0.075900003
	0.873929024	0.125893995	0.229624003
	0.000000000	0.250000000	0.000000000
	0.000000000	0.250000000	0.151810005
	0.999779999	0.245233998	0.306223005
	0.125000000	0.375000000	0.075900003
	0.124139003	0.375829011	0.231103003
	0.250000000	0.250000000	0.000000000
	0.250000000	0.250000000	0.151810005
	0.248980999	0.248132005	0.308642000
	0.375000000	0.375000000	0.075900003
	0.375254005	0.374466002	0.229877993
	0.500000000	0.250000000	0.000000000
	0.500000000	0.250000000	0.151810005
	0.498793006	0.245128006	0.309673011
	0.625000000	0.375000000	0.075900003
	0.626830995	0.375851989	0.231191993
	0.750000000	0.250000000	0.000000000
	0.750000000	0.250000000	0.151810005
	0.748292029	0.246484995	0.308362007

0.875000000	0.375000000	0.075900003
0.874529004	0.375945002	0.230774999
0.000000000	0.500000000	0.000000000
0.000000000	0.500000000	0.151810005
0.012625000	0.500177026	0.310341001
0.125000000	0.625000000	0.075900003
0.124107003	0.624440014	0.231110007
0.250000000	0.500000000	0.000000000
0.250000000	0.500000000	0.151810005
0.250055999	0.500276029	0.308458000
0.375000000	0.625000000	0.075900003
0.375196993	0.625819981	0.229861006
0.500000000	0.500000000	0.000000000
0.500000000	0.500000000	0.151810005
0.499105990	0.500265002	0.305711001
0.625000000	0.625000000	0.075900003
0.626854002	0.624419987	0.231232002
0.750000000	0.500000000	0.000000000
0.750000000	0.500000000	0.151810005
0.750586987	0.500455976	0.313145995
0.875000000	0.625000000	0.075900003
0.874544978	0.624278009	0.230758995
0.000000000	0.750000000	0.000000000
0.000000000	0.750000000	0.151810005
0.999710023	0.755010009	0.306241989
0.125000000	0.875000000	0.075900003
0.125771001	0.874538004	0.229358003
0.250000000	0.750000000	0.000000000
0.250000000	0.750000000	0.151810005
0.248833001	0.752550006	0.308613002
0.375000000	0.875000000	0.075900003
0.374909997	0.874516010	0.230018005
0.500000000	0.750000000	0.000000000
0.500000000	0.750000000	0.151810005
0.498705000	0.755634010	0.309592009
0.625000000	0.875000000	0.075900003
0.624045014	0.874240994	0.229788005
0.750000000	0.750000000	0.000000000
0.750000000	0.750000000	0.151810005
0.748365998	0.754173994	0.308385015
0.875000000	0.875000000	0.075900003
0.873921990	0.874361992	0.229609996
0.491569012	0.500921011	0.437873006
0.617138028	0.376785010	0.377400994

0.371771008	0.624777973	0.375752985
0.371722013	0.376358986	0.375932992
0.617093980	0.624614000	0.377319008
0.493146986	0.337586999	0.421591014
0.329946011	0.500757992	0.419853985
0.493039995	0.664106011	0.421431005
0.653647006	0.500846982	0.422569007
0.888016999	0.499669999	0.361728013

CO~O*

Pt	Ni	O	C
80	5	6	1

Direct

0.000000000	0.000000000	0.000000000
0.000000000	0.000000000	0.151810005
0.000311000	0.998495996	0.305575997
0.125000000	0.125000000	0.075900003
0.125808001	0.125719994	0.229359999
0.250000000	0.000000000	0.000000000
0.250000000	0.000000000	0.151810005
0.249557003	0.000125000	0.306497991
0.375000000	0.125000000	0.075900003
0.374976009	0.125845999	0.230039001
0.500000000	0.000000000	0.000000000
0.500000000	0.000000000	0.151810005
0.499577999	0.000413000	0.306791991
0.625000000	0.125000000	0.075900003
0.624022007	0.126044005	0.229778007
0.750000000	0.000000000	0.000000000
0.750000000	0.000000000	0.151810005
0.749504030	0.998467028	0.306066006
0.875000000	0.125000000	0.075900003
0.873929024	0.125893995	0.229624003
0.000000000	0.250000000	0.000000000
0.000000000	0.250000000	0.151810005
0.003011000	0.245528996	0.311096996
0.125000000	0.375000000	0.075900003
0.124139003	0.375829011	0.231103003
0.250000000	0.250000000	0.000000000
0.250000000	0.250000000	0.151810005
0.249766007	0.248142004	0.308306992
0.375000000	0.375000000	0.075900003
0.375254005	0.374466002	0.229877993
0.500000000	0.250000000	0.000000000

0.500000000	0.250000000	0.151810005
0.500684023	0.245767996	0.309345990
0.625000000	0.375000000	0.075900003
0.626830995	0.375851989	0.231191993
0.750000000	0.250000000	0.000000000
0.750000000	0.250000000	0.151810005
0.749001980	0.246111006	0.313937992
0.875000000	0.375000000	0.075900003
0.874529004	0.375945002	0.230774999
0.000000000	0.500000000	0.000000000
0.000000000	0.500000000	0.151810005
0.011787000	0.501809001	0.310061991
0.125000000	0.625000000	0.075900003
0.124107003	0.624440014	0.231110007
0.250000000	0.500000000	0.000000000
0.250000000	0.500000000	0.151810005
0.249597996	0.500159025	0.308326006
0.375000000	0.625000000	0.075900003
0.375196993	0.625819981	0.229861006
0.500000000	0.500000000	0.000000000
0.500000000	0.500000000	0.151810005
0.498569012	0.500302970	0.305765986
0.625000000	0.625000000	0.075900003
0.626854002	0.624419987	0.231232002
0.750000000	0.500000000	0.000000000
0.750000000	0.500000000	0.151810005
0.748296976	0.502771974	0.312480003
0.875000000	0.625000000	0.075900003
0.874544978	0.624278009	0.230758995
0.000000000	0.750000000	0.000000000
0.000000000	0.750000000	0.151810005
0.999900997	0.754818022	0.306225985
0.125000000	0.875000000	0.075900003
0.125771001	0.874538004	0.229358003
0.250000000	0.750000000	0.000000000
0.250000000	0.750000000	0.151810005
0.248941004	0.752493024	0.308396012
0.375000000	0.875000000	0.075900003
0.374909997	0.874516010	0.230018005
0.500000000	0.750000000	0.000000000
0.500000000	0.750000000	0.151810005
0.498587012	0.755666971	0.309547007
0.625000000	0.875000000	0.075900003
0.624045014	0.874240994	0.229788005

0.750000000	0.750000000	0.000000000
0.750000000	0.750000000	0.151810005
0.747987986	0.754307985	0.308456004
0.875000000	0.875000000	0.075900003
0.873921990	0.874361992	0.229609996
0.488846987	0.502319992	0.438484013
0.614188015	0.378385007	0.378390014
0.370810986	0.625124991	0.375553995
0.370703995	0.377047002	0.375966996
0.615225971	0.625446022	0.377748013
0.490449995	0.339121014	0.422360986
0.327731013	0.501577020	0.419636995
0.490788996	0.665062010	0.421602994
0.651072025	0.502363026	0.423272997
0.885767996	0.505021989	0.361032993
0.883467019	0.230693996	0.414032012
0.880236030	0.237222001	0.368490010

TS3

Pt	Ni	O	C
80	5	6	1

Direct

0.000000000	0.000000000	0.000000000
0.000000000	0.000000000	0.151810005
0.000311000	0.998495996	0.305575997
0.125000000	0.125000000	0.075900003
0.125808001	0.125719994	0.229359999
0.250000000	0.000000000	0.000000000
0.250000000	0.000000000	0.151810005
0.249557003	0.000125000	0.306497991
0.375000000	0.125000000	0.075900003
0.374976009	0.125845999	0.230039001
0.500000000	0.000000000	0.000000000
0.500000000	0.000000000	0.151810005
0.499577999	0.000413000	0.306791991
0.625000000	0.125000000	0.075900003
0.624022007	0.126044005	0.229778007
0.750000000	0.000000000	0.000000000
0.750000000	0.000000000	0.151810005
0.749504030	0.998467028	0.306066006
0.875000000	0.125000000	0.075900003
0.873929024	0.125893995	0.229624003
0.000000000	0.250000000	0.000000000
0.000000000	0.250000000	0.151810005

0.003011000	0.245528996	0.311096996
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0.250000000	0.250000000	0.151810005
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0.750000000	0.250000000	0.151810005
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0.875000000	0.375000000	0.075900003
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0.885477006	0.456330001	0.362250000
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