

Supplementary Information

Ni Cluster Nucleation and Growth on Anatase TiO₂(101) Surface: A Density Functional Theory Study

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Table S1. Atomic Bader Charges of Ni Atom and Surface Atoms for Clean Perfect TiO₂(101) Surface and Ni_{1,a}/TiO₂(101) Complexes.

	Ni	6cTi ¹	6cTi ²	5cTi ¹	5cTi ²	2cO ¹	2cO ²	3cO ¹	3cO ²
TiO ₂		1.94	1.94	1.92	1.92	-0.86	-0.86	-1.00	-1.03
Ni/TiO ₂	0.55	1.90	1.90	1.88	1.88	-0.97	-0.97	-1.03	-1.05

The sites of these atoms are labeled in Figure 2a .

Table S2. Atomic Bader Charges of Ni Atom and Surface Atoms for Clean Defective TiO₂(101) Surface and Ni_{1,A}/TiO₂(101) Complexes.

	Ni	Ti _{v-5c}	Ti _{v-4c}	6cTi	5cTi	3cO ^a	3cO ^b	2cO	3cO ^v
TiO ₂		1.86	1.83	1.93	1.90	-1.03	-1.05	-0.87	-1.00
Ni/TiO ₂	0.35	1.79	1.76	1.91	1.88	-1.07	-1.06	-0.95	-1.00

The sites of these atoms are labeled in Figure 3a .

Table S3. Atomic Bader Charges of Ni Atom and Surface Atoms for Clean Defective TiO₂(101) Surface and Ni_{1,B}/TiO₂(101) Complexes.

	Ni	Ti _{v-5c}	Ti _{v-4c}	3cO ^v	3cO ¹	3cO ²	3cO ³	3cO ⁴
TiO ₂		1.86	1.84	-1.01	-1.04	-1.06	-1.04	-1.06
Ni/TiO ₂	-0.29	1.77	1.71	-0.99	-1.02	-1.04	-1.02	-1.04

The sites of these atoms are labeled in Figure 3b .

1 The description of Ni_{1,b}, Ni_{1,c} and Ni_{1,d}

In the Ni_{1,b} configuration, the Ni adatom adsorbs at the 2cO–6cTi–2cO bridge site with the 2cO atom on the step edge, the 6cTi atom at the bottom of the step, and the 3cO atom on the lower terrace of the step. The Ni–2cO, Ni–6cTi and Ni–3cO bond lengths were 1.80, 2.32 and 1.82 Å, respectively. The Ni adatom existence elongates 2cO–6cTi and 3cO–6cTi bond lengths from 1.88 and 2.02 Å on the clean surface to 2.17 and 2.52 Å, respectively, weakening their interaction. By placing a Ni atom on top of either a 2cO or 5cTi atom shifts to the same final bridge site between 2cO and 5cTi atoms (namely 2cO–5cTi bridge site) after relaxation. The Ni_{1,d} structure, the least stable structure among three stable structures, has 1.81 eV

adsorption energy, the Ni–2cO and Ni–5cTi bond lengths are 1.75 and 2.40 Å. Ni adsorption at this site causes significant 2cO–5cTi bond elongation, from 1.84 Å on the clean surface to 2.00 Å.

2 The description of Ni_{1,B}

In Ni_{2,B} structure, the Ni atom adsorb in the vacancy site. The Ni–Ti_{v-5c} and Ni–Ti_{v-4c} bond lengths were 2.39 and 2.20 Å, respectively. The filling of the oxygen site by Ni adatom caused the two Ti atoms to move toward each other by 0.39 Å. Consequently, the Ti_{v-5c}–3cO^v–Ti_{v-4c} angle decreased from 126.23° of the clean defective surface to 101.93°, which is closer to that in the clean perfect surface (101.92°). This configuration's adsorption energy was 2.88 eV, which is even less than that of the Ni adatom on the bridge site of the two perfect surface 2cO atoms.

3 The description of Ni_{2,b}, Ni_{2,c} and Ni_{2,d}

Ni_{2,b} displays the second most stable adsorption, in which each of the individual Ni atoms bind at the 2cO–6cTi–3cO bridge site and the Ni–Ni bond is parallel to the [010] direction with Ni–Ni bond length maximally elongating (2.86 Å). Ni_{2,c} was built by adding the second Ni atom to the most stable single Ni adsorption (Ni_{1,a}). Allowing the structures to relax again, one Ni atom located at the 2cO bridge site, and another sites at the top of 3cO. The least stable was the Ni_{2,d} structure with two Ni atoms at the 2cO–5cTi bridge site and the Ni–Ni bond length was 2.33 Å.

4 The description of Ni_{2,B}, Ni_{2,C}

In the Ni_{2,B} configuration, the two Ni atoms symmetrically distributed two sides of the oxygen vacancy site and the Ni1-Ni2 bond axis was parallel with the [010] direction, with 2.34 Å bond length. The Ni_{2,B} adsorption energy on the surface was 3.72 eV, which is slightly less than that of Ni_{2,A} (3.81eV). Similar with Ni_{2,B}, in the most stable structure for Pd dimer adsorption on the defective surface, the two Pd atoms also prefer to symmetrically distribute at the oxygen vacancy site.³³ In the structure of Ni_{2,C}, the two Ni atoms occupy the oxygen vacancy site with Ni1 and Ni2 sitting almost atop of Ti_{v-5} and Ti_{v-4c} atoms, respectively, and the Ni–Ni bond axis perpendicular to the 2cO edge.

5 The description of Ni_{3,b}, Ni_{3,c}, Ni_{3,d}

Ni_{3,b} was also obtained by adding a third Ni adatom to the Ni_{2,b} structure. In the Ni_{3,b} configuration, the Ni₃ triangular plane was tilted to the left and laid almost parallel to the terrace. The Ni1–Ni2 bond length was 2.44 Å and those of Ni1–Ni3 and Ni2–Ni3 were both equal to 2.24 Å. The three Ni–Ni bonds were all shorter than those in Ni_{3,a} disclosing that the bonds strength was stronger than those of Ni_{3,a}. However, no direct interaction between the Ni3 atom and the TiO₂ surface led to slightly lower adsorption energy of 3.49 eV compared to 3.57 eV in Ni_{3,a}. Ni_{3,c}, the less stable configurations, was viewed as adding a third adatom to the Ni_{2,d} dimer with Ni1 and Ni2 atoms all absorbed at the 2cO–5cTi bridge sites. It also revealed a triangular plane parallel to the terrace. The Ni3 atom was located at the 2cO–6cTi–3cO bridge site with the distance of Ni1–Ni2, Ni1–Ni3, and Ni2–Ni3 equal to 2.22, 2.46, and 2.45 Å, respectively. In contrast to Ni_{3,a}, the Ni–Ni bonds parallel to the

2cO–2cO bond of Ni_{3,c} became shorter than the other two Ni–Ni bonds. Pd trimer kept its linear structure when absorbed on the perfect anatase TiO₂(101) surface.³³ The relaxed Ni trimer of Ni_{3,e}, however, was highly bent with the middle Ni2 atom and lifting by over 1 Å with respect to Ni1 and Ni2 atoms. Consequently, the linear structure was not stable and became a triangular plane with Ni1–Ni2 and Ni2–Ni3 bond length of 2.30 and 2.48 Å, respectively, and was almost perpendicular to the surface terrace. The adsorption energy was 3.18 eV, which is slightly lower than that of Ni_{3,c} (3.20 eV).

6 The description of Ni_{3,C} and Ni_{3,D}

In the Ni_{3,C} configuration, the Ni1–Ni2 bond axis was almost parallel to Ti_{v-5c}–Ti_{v-4c} direction, similar to that of Ni_{2,C}. The bond lengths of Ni1–Ni2, Ni1–Ni3 and Ni2–Ni3 were 2.27, 2.34 and 2.30 Å, respectively, and the distances between Ni1 and Ni2 were a little higher than that of 2.24 Å in Ni_{2,D} dimer. This structure was less stable than Ni_{3,A} and Ni_{3,B}, however, it was the most stable configuration for Pt₃ adsorption on the defective anatase TiO₂(101) surface.²⁷ The Ni_{3,D} was the least stable among the four adsorbed Ni₃ structures with initial linear Ni₃ adsorption on the defective surface. After relaxation on the defective surface, the Ni₃ was not able to keep its primary linear shape and was highly deformed with the middle Ni3 atom displaced by 0.99 Å to the left and slightly lifted with respect to the remaining two Ni atoms. The relaxation transformed the linear structure into the triangular configuration.

7 The description of Ni_{4,b} and Ni_{4,c}

In Ni_{4,b}, the initial 2D square structure of Ni₄ transformed into a distorted diamond-shape configuration after relaxation on the perfect surface. This structure might have also been seen as adding a Ni4 adatom on the top-right corner of the triangular Ni plane based on the Ni_{3,c}. Ni_{4,c} configuration was the least stable among these three structures, which was the result of relaxing initial structures constructed from adding a fourth atom on the top of triangle Ni ring based on the Ni_{3,a} configuration.

Table S1. Atomic Bader Charges of Ni Atom and Surface Atoms for Clean Perfect TiO₂(101) Surface and Ni_{1,a}/TiO₂(101) Complexes.

	Ni	6cTi ¹	6cTi ²	5cTi ¹	5cTi ²	2cO ¹	2cO ²	3cO ¹	3cO ²
TiO ₂		1.94	1.94	1.92	1.92	-0.86	-0.86	-1.00	-1.03
Ni/TiO ₂	0.55	1.90	1.90	1.88	1.88	-0.97	-0.97	-1.03	-1.05

The sites of these atoms are labeled in Figure 2a .

Table S2. Atomic Bader Charges of Ni Atom and Surface Atoms for Clean Defective TiO₂(101) Surface and Ni_{1,A}/TiO₂(101) Complexes.

	Ni	Ti _{v-5c}	Ti _{v-4c}	6cTi	5cTi	3cO ^a	3cO ^b	2cO	3cO ^v
TiO ₂		1.86	1.83	1.93	1.90	-1.03	-1.05	-0.87	-1.00
Ni/TiO ₂	0.35	1.79	1.76	1.91	1.88	-1.07	-1.06	-0.95	-1.00

The sites of these atoms are labeled in Figure 3a .

Table S3. Atomic Bader Charges of Ni Atom and Surface Atoms for Clean Defective TiO₂(101) Surface and Ni_{1,B}/TiO₂(101) Complexes.

	Ni	Ti _{v-5c}	Ti _{v-4c}	3cO ^v	3cO ¹	3cO ²	3cO ³	3cO ⁴
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TiO ₂	1.86	1.84	-1.01	-1.04	-1.06	-1.04	-1.06
Ni/TiO ₂	-0.29	1.77	1.71	-0.99	-1.02	-1.04	-1.02

The sites of these atoms are labeled in Figure 3b .

8 Lattice Vectors and Fractional Coordinates of the Optimized Ni_n/TiO₂ (n = 1–6) systems

Ni_{1,a}:

1.0000000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 48 1

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0865026104509098	0.6590079936929742	0.2889281633715610	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2529620023847438	0.1587489356289860	0.2889100867751889	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F

0.2533896406781663	0.8868947246142479	0.2495586083138259	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0863819912698342	0.3877436573990286	0.2495404914424105	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4217287921746239	0.6602483088026706	0.2890437504328950	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5864115657202841	0.1575246646341222	0.2895707272620237	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5865804341871873	0.8894808200479080	0.2468231351127876	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4192929518046238	0.3844889459215721	0.2462914011941921	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7513490429232117	0.6603408426974287	0.2890900806913878	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9198433645579082	0.1586823760519510	0.2889132166513392	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9198454027994303	0.8868868586894496	0.2494932925881757	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7536055025523207	0.3845189189545354	0.2463320871857772	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0865700386830756	0.8472634571779353	0.2490786883249234	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2526345194870537	0.3477193566054735	0.2490541250375864	T	T	T
0.2538927389019409	0.0700343411232163	0.2009470833289340	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F

0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0862828769096440	0.5698066453941852	0.2009611783719191	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0863629450221270	0.2103039605317101	0.3018445302328270	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2538525884877305	0.7101907987137563	0.3022061379550939	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2536551755462781	0.9968742955509589	0.3343479153467346	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0864353831901084	0.4970356415605889	0.3344785675388502	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4193111730053681	0.8476446124325602	0.2479614421034143	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5864749293554431	0.3418440389675412	0.2418971386374285	T	T	T
0.5865957539715708	0.0716846959719173	0.2001630323407912	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4196493666219979	0.5702214318522889	0.2012373256524103	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4201011939145316	0.2122747686417239	0.3025202990580034	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5865655789872024	0.7227783590027462	0.3028774954526716	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5864347820265022	0.9965319193656152	0.3338453198305341	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F

0.4210211024405086	0.4946076233233014	0.3383525047125938	T	T	T
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7538531518675432	0.8475895110768012	0.2478756222988900	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9201452911326966	0.3479003967988306	0.2491445484038583	T	T	T
0.9192797978724675	0.0700600690068203	0.2009008817431982	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7536636899313444	0.5701784404673913	0.2013117335380226	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7528115527933644	0.2123182099261375	0.3025969162962912	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9192338720764401	0.7102946494595849	0.3023201556435461	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9194795709631998	0.9968657050289110	0.3343183255776835	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7511597895132662	0.4947649064824741	0.3384015643032439	T	T	T
0.5860308130285825	0.4811567609405257	0.3320545873001500	T	T	T

N_{i,b}:

1.0000000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 48 1

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0858539990174214	0.6587783769697519	0.2882958429480121	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2521230591999161	0.1558595294963361	0.2912295157817089	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2512593564483976	0.8871161933298931	0.2488152821114028	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0880413860417045	0.3864788482057138	0.2492537583056162	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4199303994182319	0.6656467743182221	0.2914996394779876	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5875491632376307	0.1558995621662106	0.2912174309791909	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5886400743962327	0.8871295587455936	0.2488531713635622	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4198192635600525	0.3983616183230573	0.2429685928386902	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7540626576839948	0.6588779413491581	0.2883267344521585	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9197531108229677	0.1599058761166390	0.2884147746448985	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9200397383149207	0.8880066299954916	0.2491428123878135	T	T	T

0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7517614689451920	0.3866335810604888	0.2492869775971446	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0850070074076353	0.8458238248698268	0.2458074488599561	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2560532807479141	0.3450791744423916	0.2483121058699657	T	T	T
0.2589562276138057	0.0705834013415977	0.2015208304688603	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0865745717824276	0.5691386341255902	0.2005497469831337	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0861405513938762	0.2117607441185610	0.3022330584686384	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2510267246208159	0.7126154242046185	0.3014903593803205	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2409902881554316	0.9925527704884196	0.3344675457981483	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0889856827254155	0.4965343575685693	0.3338136218602358	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4199366666900206	0.8516068040916035	0.2517699094424447	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5836803587395180	0.3452273479294731	0.2484534962255026	T	T	T
0.5809026656142710	0.0705677180034362	0.2015295381068882	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F

0.4198540611316832	0.5730944711594440	0.2019435868021734	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4198574344767099	0.1877598021197164	0.3172835082807480	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5888381951947257	0.7125451429784614	0.3015055497639701	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5987518974071246	0.9925840422243691	0.3344833542550426	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.4197034068175359	0.5131128004647657	0.3448690142192567	T	T	T
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7549140472022473	0.8458697952353681	0.2458871054792448	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9198664635754423	0.3487422285316534	0.2490345795529204	T	T	T
0.9198671846327661	0.0705549267175220	0.2005568616283373	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7533146138328836	0.5691560696778990	0.2005814683445211	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7535575523674148	0.2118049005975639	0.3022662181020143	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9199825822974621	0.7113491616076899	0.3029649979848352	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9199639265027224	0.9975928374785413	0.3338753427268752	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7510605960558187	0.4966202031837127	0.3338580279805470	T	T	T

0.4195126806538643 0.3416624399661136 0.3689089475993808 T T T

Ni_{1,c}:

1.0000000000000000

11.3280000686999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 10.2098999023000001 0.0000000000000000

0.0000000000000000 0.0000000000000000 17.8448009491000015

Ti O Ni

24 48 1

Direct

0.0865600030000024 0.5369399790000031 0.0900399980000017 F F F

0.0856569378427633 0.6584052658243764 0.2882438873380548 T T T

0.2532300060000026 0.0369400009999978 0.0900399980000017 F F F

0.2537681999191498 0.1588494202493326 0.2881799041923156 T T T

0.2532300060000026 0.7527499790000007 0.0408900010000011 F F F

0.2516823574386350 0.8873945005077003 0.2489453828403272 T T T

0.0865600030000024 0.2527500090000032 0.0408900010000011 F F F

0.0867902679187792 0.3865283645678531 0.2491807522863118 T T T

0.4198899869999977 0.5369399790000031 0.0900399980000017 F F F

0.4197272032466599 0.6653710255077285 0.2906594700582265 T T T

0.5865600110000031 0.0369400009999978 0.0900399980000017 F F F

0.5858685235035481 0.1587984786842025 0.2881621767099445 T T T

0.5865600110000031 0.7527499790000007 0.0408900010000011 F F F

0.5882710306101139 0.8873098682553250 0.2488208016778277 T T T

0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4197611329375635	0.3891949783887537	0.2469749512921779	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7543457629457926	0.6586396422851054	0.2880876090486922	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9197602795773958	0.1593397149710734	0.2885651160529498	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9200901207088334	0.8882610095461269	0.2494455750274680	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7527753216745581	0.3866421523373931	0.2492353951273680	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0859203124938736	0.8479904113271841	0.2479194631799559	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2523817789629756	0.3465254359019678	0.2485673731738585	T	T	T
0.2528663923083155	0.0695202775121420	0.2004499013204841	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0854192386695516	0.5693122996137636	0.2005419243592801	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0863726418304485	0.2106547864764493	0.3020369293088099	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2511195517565653	0.7114521539635834	0.3010580768916870	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2522659323895390	0.9962662251686170	0.3338559380007070	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F

0.0868678960683208	0.4968995769443065	0.3341576915113968	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4198900725484272	0.8466651040908678	0.2493064589957041	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5872280328086655	0.3465709474336742	0.2486071339881960	T	T	T
0.5869292705384163	0.0695980432182078	0.2004023083738052	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4198847077649351	0.5667652953438351	0.2023188721978185	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4198433446028687	0.2081831237832850	0.3006563433460299	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5888909253467810	0.7115914905712706	0.3006911812606884	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5875635323799284	0.9961679512808818	0.3337960028769493	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.4196195630198673	0.4861551724717620	0.3370879698158151	T	T	T
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7541550313348507	0.8481897754198114	0.2479370097907456	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9197713704681069	0.3470606190977349	0.2488460856175356	T	T	T
0.9198154955342779	0.0699373955182977	0.2007638313844191	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7546365573400313	0.5692884876056210	0.2005055103266443	T	T	T

0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7532396592681884	0.2106833992269429	0.3021108554845883	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9199894268619323	0.7116859706788665	0.3023526783855343	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9199806138809971	0.9971511145775082	0.3343093843747684	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7525052460974042	0.4971531032632932	0.3341761252975823	T	T	T
0.4281488379688768	0.5848927317792950	0.4170181580886897	T	T	T

Ni_{1,A}:

1.00000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 47 1

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0864589120058146	0.6579787204410297	0.2903100194186995	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2513935979813861	0.1590113844636441	0.2906830016478049	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2488466394010727	0.8916885053893934	0.2467105130772159	T	T	T

0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0868577702255847	0.3890643156108058	0.2477504542563526	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4138334509883796	0.6740864486856643	0.2833030105829391	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5847577868283985	0.1578768375379695	0.2921596181155081	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5880417286976252	0.8936183164821481	0.2457619705687100	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4162467794123580	0.3783800079392698	0.2368104438274208	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7583504174620945	0.6624393647857486	0.2882446849853074	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9197991020938971	0.1578687491848558	0.2894067917106827	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9206370502310530	0.8890088492458240	0.2469392176966989	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7591895141145126	0.3855646255639620	0.2450558814426791	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0866736883534428	0.8486464745082645	0.2481858042456191	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2541707398018103	0.3568611781082063	0.2584073404303737	T	T	T
0.2517190691917577	0.0721013518651662	0.2012771387471803	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F

0.0887085419276897	0.5712946534753296	0.2014272509605555	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0853087326698807	0.2119638755377387	0.3001547237578540	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2535918378689647	0.7107921807620843	0.3066700513734419	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2534580520734675	-0.0033912980707662	0.3342461688387701	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0822603912478353	0.4982459601225769	0.3351559167718132	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4211129322745424	0.8450628859310567	0.2432201383852713	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5816451872159925	0.3570402028076283	0.2632336692985057	T	T	T
0.5864783257874938	0.0714653279009169	0.2019608852205339	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4030425886460115	0.5674193180216173	0.2018121151233390	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4178989563144925	0.2106026149163414	0.2995779053701763	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5815298596952996	0.7017196939563318	0.3119172227541344	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5832915063140841	-0.0039452712097456	0.3350339211846627	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F

0.7504095133109833	0.8462752234118426	0.2496401480713273	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9201468793561539	0.3515496963908282	0.2496364723663716	T	T	T
0.9195630368953898	0.0702902109391220	0.2007865694637959	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7594008759212297	0.5726365964103776	0.2003482970052832	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7523801127866444	0.2122383969900811	0.2983357921702594	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9207627493721738	0.7119390482633382	0.3019813848447312	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9191305392246879	-0.0032685284544131	0.3338927819946619	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7507201167911322	0.4977242309934015	0.3355683709845939	T	T	T
0.5764819128479682	0.5164424088923060	0.3148195106929126	T	T	T

Ni_{1,B}:

1.0000000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 47 1

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0862887399042992	0.6610685542420809	0.2880398164663036	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2518662040303665	0.1600538912738748	0.2891270971853530	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2526809829871863	0.8889914205273162	0.2495745699173311	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0860953755023595	0.3893013594008666	0.2495692069654026	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4200086855907627	0.6645993732141200	0.2871344675307434	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5880754546550810	0.1599709907052082	0.2891375964192164	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5876201456292249	0.8888920925544529	0.2495457605157797	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4199065271681960	0.3816997181931720	0.2445841310897748	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7540332471690783	0.6611013436350531	0.2880344100665025	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9198526373620014	0.1601977942315963	0.2886081067744403	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9201873731883781	0.8894062820435653	0.2493680405679424	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7536472144616210	0.3893136979974978	0.2495566482166877	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F

0.0860932206498138	0.8500872271365829	0.2478074824853554	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2519410874254588	0.3488446784167333	0.2502276754226163	T	T	T
0.2530872019980510	0.0720437555005834	0.2008930191325118	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0857024324828177	0.5707624311731029	0.2004739497067341	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0860004910858242	0.2122958312026295	0.3025097588840177	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2515273586523555	0.7134896930428555	0.3010115424602247	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2516406604097853	-0.0016425805785515	0.3346787194753296	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0863771014756389	0.4994974622814561	0.3341998893638787	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4200409815172219	0.8532994891382419	0.2494961917840965	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5879372945505514	0.3487476915055553	0.2501750044371402	T	T	T
0.5871011643178350	0.0720311363776095	0.2008801062950741	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4197034477295031	0.5654714613424359	0.2023496907039069	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4199740601847356	0.2132200694617876	0.3039280733885207	T	T	T

0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5886274248143344	0.7133754518502382	0.3007745367670129	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5885130958354859	-0.0017276092928371	0.3346701908957292	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7541344151788394	0.8500989015059907	0.2478452759196954	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9198846566887230	0.3488339326684592	0.2490191523182849	T	T	T
0.9198245768737938	0.0713694369883807	0.2006347675126404	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7547985496048237	0.5707337560883343	0.2004813390558554	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7538687311148188	0.2123291185039521	0.3026741746382868	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9201356294989048	0.7136448859924955	0.3022313625578019	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9201529843207699	-0.0013774913462978	0.3343665375677859	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7533200576472526	0.4995311601097950	0.3342048706020391	T	T	T
0.4208947127441885	0.4928044072178588	0.3631802054889580	T	T	T

Ni_{2,a}:

1.0000000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 48 2

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0848035471786238	0.6576700603855449	0.2888871418001923	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2516588768188709	0.1558374476063943	0.2908153424615837	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2513806522573903	0.8866251283671864	0.2490252908042807	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0882694241053279	0.3860434653050898	0.2493314044545100	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4196813926602300	0.6677453014012361	0.2919446715946176	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5872424539665765	0.1553194324876774	0.2922776545604638	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5899698689399764	0.8893560243547680	0.2467507551737637	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4239240755163199	0.3955231872631721	0.2420560827452000	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7510521145099667	0.6597928986173812	0.2891588879982006	T	T	T

0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9197021170972447	0.1596748387091320	0.2883891401023907	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9205519018427943	0.8868461660123528	0.2495235822340420	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7507885434189027	0.3833708241748144	0.2477122082056563	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0856526504714103	0.8441193783873884	0.2460264188709830	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2576737548445575	0.3455255116913561	0.2508128607315884	T	T	T
0.2585172672090498	0.0697416722875491	0.2014718835611590	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0870075548816802	0.5683762701442286	0.2008418221909630	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0863244181670105	0.2106621436153172	0.3021402813478979	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2521990905646244	0.7104495306333698	0.3028354705918993	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2418290078466323	0.9919630435162268	0.3343980909568748	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0880821030493968	0.4954605617431456	0.3342182084460174	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4193003653682410	0.8495269209685750	0.2505285627781086	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F

0.5838238811130195	0.3331607526022940	0.2381716216202823	T	T	T
0.5797453910185081	0.0697990615181119	0.2013444749040852	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4193735492494804	0.5718898159933058	0.2031881089808330	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4193037655813375	0.1869908267179958	0.3171373056516522	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5871734477081667	0.7230089704056941	0.3038495714097917	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.6000476922210508	0.9922632596976528	0.3341955325976785	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.4289854005361570	0.5144311132476078	0.3522051059708479	T	T	T
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7556270987046911	0.8444971295075941	0.2451768202885671	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9205072357105905	0.3475466754357344	0.2487270638031987	T	T	T
0.9196120530217410	0.0699379764484025	0.2005721207810986	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7497088503472851	0.5686036141896094	0.2014940994030159	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7534830679297805	0.2118678047677849	0.3031903864597296	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9199973527000367	0.7100832886660133	0.3033885540959704	T	T	T

0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9202305788545876	-0.0031484901233377	0.3338207976039569	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7581746890543216	0.4911023608629829	0.3383676636262668	T	T	T
0.5957290382751820	0.4983683963180895	0.3422093411231600	T	T	T
0.4278118007752840	0.3378988177720845	0.3707611174505291	T	T	T

Ni_{2,b}:

1.00000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 48 2

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0865784684125972	0.6593756622293339	0.2883774111305830	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2526518103802549	0.1572949270352534	0.2900338462969510	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2518301766520994	0.8871001074712891	0.2491797565608058	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0869483419975271	0.3869836235841063	0.2500468422339670	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F

0.4204717006326500	0.6644223900851794	0.2903045367238376	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5868583315836305	0.1540710753877920	0.2956314238595499	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5866022412549634	0.8894442677349913	0.2473244180076174	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4230251242936051	0.3950193357200664	0.2436363722736283	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7530750699762577	0.6645526952119362	0.2903718248525357	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9207403322209757	0.1574338565080046	0.2901585505236418	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9212877561359634	0.8874084130455174	0.2492584365383670	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7509405462444073	0.3952271408967138	0.2437297257588815	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0865593341525053	0.8437833095661733	0.2443641722991919	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2570312860207802	0.3480032535572982	0.2518318202140666	T	T	T
0.2586674633306969	0.0708769749206346	0.2010832544170546	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0865833783279498	0.5680449463615095	0.2008386739269519	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0867284937899287	0.2112655222588423	0.3012829191946081	T	T	T

0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2518701903524280	0.7115078776991912	0.3029366662533292	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2432786038526777	0.9938228165762518	0.3341998665881287	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0868044067677530	0.4963303684309208	0.3341882641214206	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4185262780745911	0.8497136061295161	0.2491801689122428	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5869030390799240	0.3418891673976350	0.2401637207627245	T	T	T
0.5871761658065788	0.0702476635868194	0.2021863077851529	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4181297574540222	0.5705501438099723	0.2016404645424148	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4190275036707080	0.1946419840007391	0.3152941709241660	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5867166217614206	0.7142864534011165	0.2994680691977379	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5863359488671949	0.9889000578649498	0.3357613603912878	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.4335030843518922	0.5110506134105122	0.3434483862693199	T	T	T
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7548321317316170	0.8498413326153896	0.2493078313471626	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F

0.9166048642267079	0.3480445301300997	0.2519876486744110	T	T	T
0.9145760624513549	0.0709336539380955	0.2011970137961017	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7557419264158677	0.5707129914638686	0.2017220335518743	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7545676790615844	0.1947834309471806	0.3156881119672534	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9214499420282009	0.7116798586243918	0.3031736052353171	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9300918060961990	0.9939638907582700	0.3343204397513347	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7403011507973525	0.5112189429120438	0.3435609949727539	T	T	T
0.4586410320528400	0.3412479925163495	0.3704595328525150	T	T	T
0.7145294793803365	0.3415525222018642	0.3705931967432156	T	T	T

Ni_{2,c}:

1.0000000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 48 2

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0873818492373814	0.6572772910537549	0.2892450768839250	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2514992063510503	0.1562062167837023	0.2897674164734470	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2534309875215692	0.8865217250500992	0.2471970200683000	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0856613301518345	0.3867387947037508	0.2480372423648811	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4180046038609486	0.6598907721390999	0.2910822787164262	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5854875521628462	0.1563683581162622	0.2911614647599646	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5866981536760127	0.8916567844024220	0.2436797722541206	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4146139520848949	0.3825348623891074	0.2440538339732278	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7586122765461245	0.6615811787230023	0.2890967345341540	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9194586244558592	0.1573191482107809	0.2900161460241250	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9209105793778036	0.8882687229944748	0.2469772433167565	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7549057042666940	0.3835833229263265	0.2444638954663966	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F

0.0865217112769196	0.8462428801713286	0.2490924255828910	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2509482399961159	0.3453863486220832	0.2468440820877702	T	T	T
0.2521662038968337	0.0688199084878551	0.2010693245576509	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0855001050490081	0.5699762433947310	0.2009291587073043	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0852650029514108	0.2103735186462339	0.3022283056905875	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2537881308230559	0.7085507585051612	0.3021128992480006	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2540663657969416	0.9944168176355332	0.3339918170314244	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0872900826206190	0.4955131552093309	0.3341139021690823	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4205990477294471	0.8444541658477082	0.2478248445526087	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5852501449369953	0.3481698670191001	0.2487074325341541	T	T	T
0.5866670268994151	0.0727391107864960	0.2007273985218942	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4244918390004617	0.5684765321389960	0.2023802571015695	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4184767301603952	0.2097328494177988	0.3008364141013881	T	T	T

0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5903532338894331	0.7272365765841076	0.3067397599260455	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5864950466489146	0.9963729644939104	0.3344658572809341	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.4121723735898162	0.4872569746839500	0.3374752662992336	T	T	T
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7539119793175716	0.8451684092377379	0.2464720861008863	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9189492377674178	0.3488506160775270	0.2490701413326458	T	T	T
0.9199434864394583	0.0699416098841450	0.2011140795580781	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7556168602635963	0.5694913487468384	0.2018128710607485	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7524944093536047	0.2117543463704466	0.3015204273485490	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9199672644882984	0.7093755017558798	0.3036383724760304	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9184487963683402	0.9956010804578801	0.3341051756303776	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7440090266081433	0.4939754175831800	0.3375432449435152	T	T	T
0.5658951824485640	0.6661014847654723	0.4027509414680027	T	T	T
0.5776500016185816	0.4727208218033895	0.3373255563548478	T	T	T

Ni_{2,A}:

1.00000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 47 2

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0826062245358526	0.6628191076709702	0.2882805461308661	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2527253116563821	0.1569885040756202	0.2905282704264828	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2511751443275000	0.8893729526672789	0.2464461684998587	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0846264053530434	0.3871628999646988	0.2452659356454441	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4153061177620617	0.6650194780908903	0.2874064905920743	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5890234366359854	0.1564701608704693	0.2894201118520499	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5863638813190515	0.8864723069724205	0.2480221502043056	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4241886902506993	0.3794203746668514	0.2411407579107901	T	T	T

0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7523400053777041	0.6606263118904945	0.2886871331016560	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9204179291129932	0.1590462613167576	0.2897043566340340	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9185473878774787	0.8897232792509480	0.2478635869600264	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7544631694739915	0.3894807135847863	0.2487725400807007	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0842203596878354	0.8485516483730232	0.2469871026017603	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2533189690997151	0.3513336456641376	0.2486471207288410	T	T	T
0.2512326094866595	0.0733331197801706	0.2006537119313964	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0805125781086151	0.5706162206789543	0.2010051510073129	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0868107271128801	0.2141915250841979	0.3017266820972734	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2491934350035052	0.7190376612127645	0.3014575993127989	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2512210759852484	-0.0032221897453716	0.3343846726001279	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0996019749304008	0.5006771826228013	0.3371942894547811	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F

0.4188476667699561	0.8504552204493773	0.2485180825090828	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5885882373279884	0.3502690549645837	0.2526660256618702	T	T	T
0.5887301282703469	0.0705633429641763	0.2007704796635487	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4226553773617694	0.5656155220754213	0.2022608775425873	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4209313921424626	0.2094995350274766	0.2993156474831432	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5862799788679869	0.7115880791136965	0.3015485802775707	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5870824387026543	-0.0042774733580347	0.3344147490245376	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7532555478328093	0.8482094031953674	0.2481537972196922	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9203151483200868	0.3516988998326868	0.2506595788904695	T	T	T
0.9199624064205560	0.0716657367576682	0.2010031984575184	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7550613499665407	0.5706262651795758	0.2009513579505134	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7547750139862117	0.2119298862682213	0.3017357026410574	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F

0.9190698158985739	0.7119718271339854	0.3036346089487834	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9200966782045067	-0.0022110836777004	0.3343669747123642	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7491841736123634	0.4991477200262924	0.3349922059291729	T	T	T
0.2719845915468787	0.4700276999091989	0.3343592031080276	T	T	T
0.4633239342451898	0.5021389730970217	0.3682411672712022	T	T	T

Ni₂B:

1.00000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 47 2

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0847662611617042	0.6624145530366983	0.2888727983422629	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2517846970007217	0.1565557722332210	0.2890936804871870	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2523791801204948	0.8879538104874656	0.2471382662623636	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0857240233860217	0.3893751703933629	0.2476416353012972	T	T	T

0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4194254018607498	0.6641944826789291	0.2865346467978500	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5879979769740760	0.1561948773764358	0.2890868622438756	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5869313174519559	0.8876023281965033	0.2471040510771302	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4204317236778887	0.3795311559093724	0.2409250207719138	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7546174175774021	0.6622560342282271	0.2888034372195442	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9197427704501600	0.1598159755917010	0.2895920282187139	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9196952371401208	0.8902224773938469	0.2483038875547671	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7535771717404910	0.3892958691710739	0.2476063181613268	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0845234509758125	0.8482794803244263	0.2473672031986232	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2524377102633504	0.3546645023833761	0.2573778176845154	T	T	T
0.2489690947769513	0.0729153571140659	0.1999189140757630	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0790910685709821	0.5702083347001848	0.2014587976364804	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F

0.0853479143903147	0.2131784754880376	0.3002144213661816	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2510084952399656	0.7179455143852220	0.3005591961630868	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2511235620386030	-0.0032191697290473	0.3340953896488165	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.1094354967668573	0.5037485191014301	0.3367471923784382	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4196373672422209	0.8523117705521359	0.2478586471949814	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5877476196009326	0.3530437203999289	0.2559687154845537	T	T	T
0.5905344963983477	0.0724988390740727	0.1999344694363330	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4196941545997051	0.5681491561801728	0.2000442687856594	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4199629197179416	0.2049206053606469	0.2954888227069015	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5882556230289139	0.7175016115443377	0.3002872637963255	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5882499332468382	-0.0037300799215944	0.3340491679678469	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7549487240412548	0.8481769593637144	0.2473949295327866	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F

0.9197747637662215	0.3585614685970269	0.2573999612016767	T	T	T
0.9196276011268966	0.0721888107548810	0.2009326067081940	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7607690507347667	0.5701430205444210	0.2014110547349785	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7543206593538690	0.2130783707940520	0.3005959616183553	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9197220233349727	0.7111247263301267	0.3051337828698631	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9198470875075659	-0.0011116923531985	0.3345474247874029	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7292115710690712	0.5035208705320997	0.3364423110159185	T	T	T
0.3150839452227041	0.4818564537500514	0.3434905439872461	T	T	T
0.5213905748571609	0.4847805866818496	0.3444904340681164	T	T	T

Ni₂C:

1.0000000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 47 2

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0852530216287333	0.6602162863947129	0.2878393630251127	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2518457693814029	0.1599259089726595	0.2911983663043932	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2507581044368965	0.8893773369295936	0.2494427040987162	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0867852431861927	0.3881644805395918	0.2488871024954441	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4202595825058970	0.6705061940221179	0.2940358604916699	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5879627986178564	0.1600397311244743	0.2911886642822313	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5888946467274581	0.8895485289235057	0.2494542245249670	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4197259285717976	0.3850959726428086	0.2393722232274950	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7543672306971615	0.6600883095510585	0.2880252247392281	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9198351190026760	0.1602910932283444	0.2888407299039477	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9197538364878722	0.8898942556270454	0.2491158317773276	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7530547560197847	0.3882454051738180	0.2488485644661405	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F

0.0853227953375344	0.8507413126997504	0.2467935440253278	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2519014979369464	0.3452816968651153	0.2473363039349593	T	T	T
0.2586206130258180	0.0724999666074718	0.2019292766707764	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0849893664482476	0.5700836931612958	0.2001169743864478	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0865218136742884	0.2116285134804017	0.3030343841207672	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2488955828490754	0.7138721336377293	0.3004249413952299	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2481256565982495	-0.0029005832367372	0.3352638460526770	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0871097934225482	0.4986790136140691	0.3336395770335488	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4198872829571018	0.8513645273835128	0.2535250745988967	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5877843179854391	0.3456873930180601	0.2475618987889506	T	T	T
0.5810434593687049	0.0724589923219831	0.2019271772757820	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4196831121044964	0.5641171154151139	0.2075693061769958	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4200507595885065	0.2174810027201836	0.3150724613669905	T	T	T

0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5906437551005848	0.7135412802009440	0.3006015177166664	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5917226850704497	-0.0028312941092729	0.3352414021509660	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7541550839924693	0.8504915001974747	0.2468321837652737	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9199080017337044	0.3476938429310614	0.2489382923305176	T	T	T
0.9197754244348560	0.0717639498313457	0.2006498156863732	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7546490252424528	0.5701194389774337	0.2002018020858348	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7532643829737555	0.2116831272049539	0.3029638906636438	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9197948733330951	0.7140137391472307	0.3022630399974535	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9197317775427114	-0.0015260388632311	0.3344174543187676	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7528437558335169	0.4985355131229107	0.3337007999544417	T	T	T
0.4201663015954573	0.3956945899715867	0.3609840150007100	T	T	T
0.4107174558815378	0.5978291213039628	0.4095629920789940	T	T	T

Ni_{3,a}:

1.00000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 48 3

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0866115895516150	0.6605570591703462	0.2884120399757739	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2500942609611717	0.1600453496536302	0.2887897623445084	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2521780413170391	0.8896610709559163	0.2489462744314866	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0867823595831907	0.3903301365651241	0.2491751621783260	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4186489410157420	0.6662412089358942	0.2884505256714799	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5870918753337397	0.1610276120677593	0.3004517368310404	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5868091380034297	0.8986155285871346	0.2464059042934488	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4244332370391168	0.3878051963169269	0.2455534015207469	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F

0.7547852710641090	0.6665538093655659	0.2882835790147089	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9240632025101327	0.1599344093102255	0.2887793518402102	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9216535196228962	0.8896777105332584	0.2489603853406329	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7494654676875865	0.3879464825983642	0.2456646284665536	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0868733040925016	0.8474341808234853	0.2461384212110525	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2554248275944349	0.3511776673454969	0.2506934704667051	T	T	T
0.2542785007785902	0.0712490101205146	0.2005159495736235	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0866096143052645	0.5705707103483508	0.2005688092486775	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0870175950286879	0.2157435440686053	0.3035349767287027	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2521376197914397	0.7123088135853638	0.3018751176269900	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2468917026658511	0.9968651168726247	0.3338891402748516	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0865770959150027	0.4991110758043475	0.3343442987994374	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4194764704191268	0.8490625436661486	0.2496327369707037	T	T	T

0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5869611299378478	0.3323049012445526	0.2331578154438097	T	T	T
0.5866329731351607	0.0675803391723433	0.2026556743771991	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4197600453407427	0.5681556005542461	0.2026953296463328	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4148545380563221	0.2039048268217385	0.3075562893874282	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5868218579376904	0.7105910466822246	0.3043312030870277	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5868102041037671	0.9916658210196845	0.3366911746161363	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.4215951515673488	0.5076926288852373	0.3480811479772906	T	T	T
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7542173964821487	0.8492533531727062	0.2495560608492991	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9185722327667909	0.3509279545478143	0.2504694064237331	T	T	T
0.9198139345444281	0.0712692710883812	0.2004892954141255	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7539733513591065	0.5682248699292931	0.2026267020345496	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7593168992661391	0.2038477311613670	0.3075676198537374	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F

0.9214310054982184	0.7126462115080475	0.3020223958609641	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9269980140318086	0.9968308934503856	0.3339230914034304	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7528423138230483	0.5077291437996588	0.3478323888752317	T	T	T
0.5872295771123521	0.5345166795365454	0.3512956392500490	T	T	T
0.4770981344489215	0.3313074094473630	0.3736427169249417	T	T	T
0.6974144517718255	0.3314549460277766	0.3737038863330031	T	T	T

Ni_{3,b}:

1.0000000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 48 3

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0862403589117341	0.6593212167251221	0.2891176084041654	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2498784370495144	0.1576900699503616	0.2881510486110699	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2535754937670350	0.8852124930284211	0.2495323117186579	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F

0.0862997785427329	0.3890873255870447	0.2491098976295254	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4214792042601978	0.6578363131594713	0.2897023910945171	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5865496617136225	0.1584148419944685	0.3014224898222450	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5862335914939147	0.8922653642535893	0.2475582191505102	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4207629135938086	0.3865480743757564	0.2438411684880916	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7511789849966897	0.6579837318480430	0.2898057625524106	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9229738593051400	0.1575404168371213	0.2883247632329762	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9190601915550188	0.8852704219135226	0.2496381362755168	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7520775983620868	0.3866720574046508	0.2439293196350718	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0862805771529808	0.8457326222337263	0.2482355063949639	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2531150896424898	0.3483495380001150	0.2488955518659318	T	T	T
0.2532243018524477	0.0686289302238668	0.2004777979893265	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0861405466682167	0.5698265224722512	0.2009827432259995	T	T	T

0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0863852985274511	0.2119677504762032	0.3027662584683876	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2530660121238587	0.7095473731880315	0.3028853158075171	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2515116134585242	0.9953795990749279	0.3339127250575113	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0862012069902354	0.4967333373218979	0.3344748062251593	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4197195079100787	0.8440785614161064	0.2494607657297175	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5864844916642835	0.3418426555681032	0.2416836118115498	T	T	T
0.5865736353159858	0.0670793265338080	0.2040480289371234	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4188419343758969	0.5689724818989186	0.2009991542996639	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4150398428690413	0.2101650905086767	0.3039937308422217	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5863073468435339	0.7079403499863376	0.3025228130950002	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5862676997491462	0.9889099071943942	0.3376114890517526	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.4266118370476336	0.4952533263383053	0.3380864654700783	T	T	T
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F

0.7529661322910411	0.8440524261175093	0.2494624268553539	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9196425161368529	0.3482981378739433	0.2489319662212803	T	T	T
0.9196616950488206	0.0686150548940108	0.2005756749108223	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7543427734066769	0.5690092789404404	0.2010822280660232	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7579654620610544	0.2104291340079002	0.3044131123437786	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9195607500959905	0.7097224977609590	0.3031835082499559	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9209565161774139	0.9953117174360966	0.3340826695153293	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7458725483576920	0.4953511979631627	0.3381272782530199	T	T	T
0.5858861462235414	0.1935711878907127	0.4504663656718023	T	T	T
0.4782045019770420	0.3343455625009124	0.3818977498900357	T	T	T
0.6939029379004724	0.3346161508330346	0.3821984379448152	T	T	T

Ni_{3,c}:

1.0000000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 48 3

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0873585855809512	0.6595447510948866	0.2882367585750230	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2540603151230703	0.1608501292114976	0.2891538338588675	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2514015105866614	0.8918272421487410	0.2489417760867741	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0874296226583962	0.3874629639735849	0.2491326832906858	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4146975691018291	0.6669332734088397	0.2887408475305571	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5872013490686211	0.1559504993928141	0.2915403565139734	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5873253977695682	0.8893008773796175	0.2418875610909056	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4204313844248055	0.3895643473267434	0.2500795407498269	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7601454824458074	0.6669163934452892	0.2888882387603970	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9201040619152534	0.1609409369038264	0.2891554045281370	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9231586903908561	0.8919359934410581	0.2490590682981219	T	T	T

0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7543169871703763	0.3897458506496763	0.2500084817463259	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0872681792209184	0.8483611212718608	0.2455911159847075	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2538012770117757	0.3471812409641523	0.2488646926739319	T	T	T
0.2538227446922961	0.0714823577207500	0.2008353571881498	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0870330897145052	0.5701807791574188	0.2004792355144179	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0872309610333942	0.2130141216858564	0.3027301914937829	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2506791981527296	0.7150099528734114	0.3034165163951317	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2499602607126873	-0.0014245512797570	0.3345550351151129	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0878059950014896	0.4979250762312339	0.3339606920444362	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4176155048548706	0.8514888440744500	0.2481449157724381	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5872859985679828	0.3456634975480619	0.2546401415331823	T	T	T
0.5870670380077285	0.0734849028574655	0.2010304013333966	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F

0.4171411683713992	0.5650206350908574	0.2021352606614772	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4205056653498060	0.2078782398588961	0.3035907945358667	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5874053509353547	0.7073297632497172	0.2810175194406029	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5873472914986171	0.9880316230996383	0.3377631286216487	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.4126324883396247	0.4926702293149772	0.3385456819189199	T	T	T
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7570574361511810	0.8515092814633795	0.2482967214929917	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9207130221232269	0.3473904324128087	0.2490092652876756	T	T	T
0.9202290183311648	0.0715832977608789	0.2008584888244681	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7576861976475915	0.5651967687625180	0.2021053434891741	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7539788931251955	0.2079100259399404	0.3035512412498694	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9240859690048607	0.7149935089287811	0.3035756577926957	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9247413194744271	-0.0012711413024130	0.3345786606895762	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7619077352554566	0.4926697073388647	0.3385329140382294	T	T	T

0.5872460515709463	0.8059115056996193	0.3782140328925498	T	T	T
0.4890532790868581	0.5985221026219211	0.4094419248509844	T	T	T
0.6851917676653297	0.5983730459305634	0.4093904202862368	T	T	T

Ni_{3,d}:

1.00000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 48 3

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0805048386114484	0.6669391254641293	0.2871491580836877	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2537884283059347	0.1594427762020922	0.2888421100063023	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2527720820046895	0.8902857690863538	0.2472975860231214	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0860244450127613	0.3880424145961663	0.2485393388979992	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4216900038102134	0.6650982263186613	0.2931152592665923	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5872012170326605	0.1597316731579217	0.2888296385164617	T	T	T

0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5867244482675273	0.8918973608344896	0.2469859432802937	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4212687800834358	0.3840397666333344	0.2432073570654789	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7549034789819850	0.6648051714830929	0.2878500411076099	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9200663360239700	0.1609962664281341	0.2890965097358332	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9182832420626404	0.8919400524000277	0.2479807122028412	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7537181830262015	0.3869304379382791	0.2472274281559522	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0852965655953522	0.8496382683012051	0.2461403478999966	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2545203247314313	0.3502237033088766	0.2515454132986799	T	T	T
0.2537486533423854	0.0703919441073626	0.2004643110656350	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0881729455210198	0.5697286450959925	0.2013475079274631	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0866772342816832	0.2113455931206004	0.3012972592358110	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2530661655965303	0.7188658476977487	0.3064026152005970	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F

0.2530781847089019	0.9977275709693078	0.3338395998302421	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0796932572047540	0.4930623325609975	0.3376776605976403	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4202005267435196	0.8445133431044071	0.2474359004213812	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5877438814015108	0.3441327046212569	0.2450676133766856	T	T	T
0.5873004768055493	0.0700262782764791	0.2003941951838298	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4190659325450459	0.5675639833919437	0.2049388768654852	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4205981591668855	0.2064933334559010	0.2988882606511623	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5893692459874519	0.7235608887261599	0.3088512340576250	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5877701798731697	0.9982509808012509	0.3339204862852390	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.4447702008958468	0.4698510324126688	0.3418744187649017	T	T	T
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7535429503923273	0.8495475308801956	0.2446152828329441	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9200262802448679	0.3500233291885899	0.2488602818524125	T	T	T
0.9193815681100406	0.0723850873784417	0.2006484157988768	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F

0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7516644937205521	0.5706676245056791	0.2010120349960191	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7538889453010955	0.2125299020801616	0.3022794077972984	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9177391137817149	0.7164585506284011	0.3049239243277274	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9189719719396496	-0.0010252994367993	0.3340582668995460	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7491913982487312	0.4931390607184442	0.3362928864673168	T	T	T
0.2237253213704826	0.5682760017048075	0.3645522090083393	T	T	T
0.4026019050308974	0.5530076494790692	0.4252059432196548	T	T	T
0.5936898071054815	0.5588909791235760	0.3580786314112296	T	T	T

Ni_{3,A}:

1.0000000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 47 3

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0841361807653990	0.6631938403547981	0.2884269510107254	T	T	T

0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2523932506611918	0.1559926436223300	0.2895384601949388	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2511554780254937	0.8875614884866686	0.2464948774522945	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0836505423789499	0.3913507057621641	0.2494879740769975	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4203166979348189	0.6676266515390850	0.2909066740981069	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5871212746397014	0.1551590474222035	0.2897656792044924	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5871744103305491	0.8883762712291036	0.2453991884723031	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4200189306383457	0.3811402205299262	0.2379431592627020	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7550006707121246	0.6636958736760228	0.2879317634305809	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9189982840107387	0.1602970331011161	0.2891470953885449	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9192042448783027	0.8915026840786597	0.2475846260163398	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7542267604005459	0.3891909359088580	0.2457571459114416	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0840170107238745	0.8504284885856087	0.2471441048377361	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F

0.2550580816445125	0.3610322455279473	0.2679970592526459	T	T	T
0.2504540724233462	0.0732550298096424	0.1999886592512767	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0826843985036769	0.5707721422533101	0.2011286558737456	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0851065333425672	0.2128130451374878	0.2977449767984855	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2492356037404257	0.7158346490022987	0.2996315692831503	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2505193838307530	-0.0034797459877456	0.3342547957493044	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0919639832522186	0.5035078458763103	0.3365033099106014	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4189801786916568	0.8500562692825597	0.2490317208074492	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5858043199835994	0.3537767814779310	0.2550457975838713	T	T	T
0.5901793185917505	0.0733283995385656	0.1997619137696868	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4195139769861395	0.5653260532355252	0.2029604867640907	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4201516484988191	0.2033125648566838	0.2943649537767091	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5898667318826427	0.7194240402161517	0.2979867420534271	T	T	T

0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5882810388430433	-0.0045433361335166	0.3339565160230425	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7547135350827686	0.8495510704193330	0.2464124730343018	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9186403050024697	0.3589655122025172	0.2557720760069963	T	T	T
0.9182593280920660	0.0729755795707699	0.2005753979452884	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7612161037273906	0.5704839461937854	0.2009351980731928	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7533063697336607	0.2149381208792172	0.3001352017764284	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9185613747776542	0.7138284196262434	0.3043578867701784	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9190780358942393	0.0002061926269801	0.3343984286525048	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7270234191725293	0.5039776116413964	0.3362608047920426	T	T	T
0.3282029774378598	0.4655879404832182	0.3486187341414144	T	T	T
0.5453483087322798	0.4687492251102774	0.3417783101499723	T	T	T
0.4390449529292342	0.6044696561464089	0.4176296282242674	T	T	T

Ni_{3,B}:

1.00000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 47 3

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0829794834672602	0.6586003225056501	0.2889493051818878	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2519515400388097	0.1564461383606899	0.2917187470700515	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2487937741486722	0.8906414040812887	0.2475481419283267	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0909080822924688	0.3847583908928882	0.2463665126800089	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4192129878693581	0.6789048178018523	0.2842052208940040	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5874102038475251	0.1563637682271625	0.2916733959131945	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5905050011476274	0.8903823422355832	0.2477010842631864	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4196232973682693	0.3952857874159400	0.2424314481653377	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7561052922469367	0.6583605369933410	0.2891009172215795	T	T	T

0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9198115738808289	0.1619193079262650	0.2897293273925622	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9196175181058613	0.8910697087191847	0.2481713560319554	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7487193757529341	0.3847864249855570	0.2465314670005600	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0832071059079300	0.8421055625611354	0.2468358257007043	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2561127429390249	0.3377418579803683	0.2430948328630626	T	T	T
0.2552094483253037	0.0695266943993320	0.2018890261296429	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0774162292739756	0.5683134481141958	0.2016794636099152	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0864259646089275	0.2133959356721861	0.3027193611103751	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2503647553657286	0.7148529776375638	0.3044295062240135	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2405941410223784	-0.0069159225900842	0.3347183027087291	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.1217688583003059	0.4977287058493179	0.3342544765501798	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4196241575881817	0.8594485540878503	0.2489799094681036	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F

0.5832848109141017	0.3381869264280591	0.2435799417668897	T	T	T
0.5840821243866026	0.0693896378222884	0.2019236244505606	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4195138332326935	0.5705239803643418	0.2008741683311616	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4196789066394601	0.1928765235870374	0.3165186508019141	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5885946096962492	0.7141111937346609	0.3044616815582988	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5985699484162984	-0.0069939450769678	0.3347541307715243	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7560936487744914	0.8421566446816939	0.2469590140772124	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9198257584634901	0.3551662782891759	0.2554389820090538	T	T	T
0.9199013536632592	0.0714620195545193	0.2014342448079319	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7615501631714700	0.5683726258118937	0.2017300047301066	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7530822213797872	0.2130811864022439	0.3025367427352151	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9197062744729375	0.7048986660375981	0.3074223239180186	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F

0.9196633847466875	-0.0013791350502029	0.3340293269494147	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7190536645627456	0.4974241249824965	0.3344219146792247	T	T	T
0.4191226489688070	0.3504925191434503	0.3703160376592408	T	T	T
0.5279656659859578	0.5384684977099853	0.3575532075102807	T	T	T
0.3094668713639556	0.5378058730787197	0.3574583410713214	T	T	T

Ni₃C:

1.00000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 47 3

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0860062836046764	0.6594562426025677	0.2888962326987626	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2521419552141296	0.1597054769439984	0.2909718107092845	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2506974106741444	0.8901250633189527	0.2485530834014756	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0874804956214452	0.3882996099739605	0.2478019430917534	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F

0.4191544269486108	0.6724054697847779	0.2927844613573028	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5884032652015873	0.1587234985618622	0.2922976154777956	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5891543536663015	0.8913309936104351	0.2471022706772592	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4222280208219670	0.3849520124662891	0.2378855633728661	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7575071558089170	0.6623513738656291	0.2877945496967004	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9197466945903587	0.1604742608775485	0.2893377559536590	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9205946127119038	0.8908824922432792	0.2478138691280787	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7520428676694998	0.3856435603635449	0.2452037372173813	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0859495230159122	0.8493329113095742	0.2473535737674872	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2552864098821738	0.3481266402803359	0.2503319141418144	T	T	T
0.2593740371446561	0.0725732041365662	0.2019368035140857	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0867740884095203	0.5707223144530720	0.2007233113387640	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0870273652851388	0.2114644393284586	0.3008132527745174	T	T	T

0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2499767801361063	0.7145005677307369	0.3044810190117958	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2491881095433036	0.9973983912308754	0.3351614741252490	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0890311365659728	0.4979694009512342	0.3341691448014366	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4205513739326782	0.8499132274679001	0.2514087986272092	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5871683359312665	0.3397682710341590	0.2416901650557657	T	T	T
0.5820066192401329	0.0708195686739546	0.2022903054678620	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4174909503853628	0.5647947396173515	0.2076954346288811	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4214408910301016	0.2166489031375576	0.3152383781559115	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5922320154178204	0.7173745432823223	0.3054779527219815	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5926681589230095	0.9961338381069846	0.3350845817618630	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7551221868440894	0.8480037610664428	0.2460146309422476	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9191452029003859	0.3517342821474790	0.2512086124344282	T	T	T

0.9191758197174489	0.0723067311116080	0.2008853042317892	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7578533505958494	0.5700529293437570	0.2009010551930902	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7530259997614980	0.2130067399256211	0.3028389921569057	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9201374624592144	0.7120568820752162	0.3038540101880665	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9198651859926654	0.9988541082811777	0.3341852881085480	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7343889494322902	0.4966267677385728	0.3351999130047881	T	T	T
0.5716939607015326	0.5493954413737753	0.3626648290581411	T	T	T
0.3864155801352717	0.5880510140325119	0.4109766097898553	T	T	T
0.4274808868751231	0.3851205881859960	0.3662764691228416	T	T	T

Ni_{3,D}:

1.0000000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 47 3

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0841986985106777	0.6659027288190174	0.2874217086977813	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2519476340397648	0.1585367276559324	0.2904505519160803	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2530222772223319	0.8909967068433760	0.2475829162109165	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0857074952872876	0.3877069185220836	0.2488363640445045	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4199071542543699	0.6667194172182243	0.2894734118936145	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5876168696642521	0.1585045870586735	0.2904314568298368	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5867880337304701	0.8909355848013778	0.2475697366404738	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4197668662299502	0.3798643154427111	0.2434738356648876	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7557166148434368	0.6659451630888596	0.2873473753844332	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9197490834250180	0.1600681415894555	0.2892002763518965	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9198955881613312	0.8903320807230209	0.2482567284340222	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7538072293333623	0.3877164776750973	0.2487932295638582	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F

0.0863561212834492	0.8496578897619366	0.2459485105159171	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2529297962747314	0.3443514608460446	0.2478700250017999	T	T	T
0.2540458883315942	0.0703089121676274	0.2013779736958610	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0886947711856660	0.5699171694161232	0.2012067750889057	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0861987525184996	0.2112559938911044	0.3028835986747263	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2542145206654843	0.7200513444236646	0.3089139403679976	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2527524469580421	-0.0031265818193474	0.3348874857278202	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0809352325239703	0.4934853219486711	0.3374610381648974	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4198798680139412	0.8478534717535058	0.2458200652889559	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5866186947837227	0.3443296591331198	0.2478654062664712	T	T	T
0.5856581556414667	0.0702774099669306	0.2013773713473817	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4197680904393719	0.5665912835521054	0.2048378335871448	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4198124336511836	0.2110122969565437	0.3049396521180719	T	T	T

0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5856462640284510	0.7200855987069271	0.3088639080777709	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5869026057775667	-0.0031418725761528	0.3348818484383895	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7534446248459667	0.8497068373122650	0.2458891922189118	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9198244173692541	0.3483833609762513	0.2485999769213441	T	T	T
0.9198514249121533	0.0719764453695831	0.2007296043202920	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7510398265865003	0.5699399273689444	0.2011377139488847	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7533438342700244	0.2112820373668705	0.3028743279875163	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9198767025599952	0.7158071082946366	0.3038110349269507	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9197836327487371	-0.0021214419088638	0.3340890236586691	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7589659267596208	0.4934651213551144	0.3373424778722111	T	T	T
0.2360289882324620	0.5543695799525412	0.3548265506946391	T	T	T
0.4199607785721741	0.4548642977087249	0.3670564805290932	T	T	T
0.6038397498233412	0.5540806631803270	0.3545359168406692	T	T	T

Ni_{4,a}:

1.0000000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 48 4

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0866743624036688	0.6591652344980203	0.2880702923300071	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2540734125484762	0.1606976581537975	0.2891482316795898	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2507170175715717	0.8916224137905155	0.2489631329249353	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0867514634728235	0.3870323580494986	0.2491824818924280	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4138438794881581	0.6666580129532832	0.2882678804070065	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5867061853617327	0.1532212686508266	0.2922792218160532	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5865616104528009	0.8881248661111225	0.2419943666809207	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4208472027170523	0.3890557986910853	0.2497469310744198	T	T	T

0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7594041461027039	0.6666792894592349	0.2882695188858102	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9194361089442371	0.1608202584909636	0.2890535999859716	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9225277496029857	0.8915788506216890	0.2490651201917542	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7525967620641584	0.3890848869746541	0.2498672498049211	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0866490172170676	0.8478426302407057	0.2455711648264082	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2539101012560979	0.3476401064038042	0.2496253823902644	T	T	T
0.2539343883890369	0.0714653948570659	0.2008150453885063	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0867387977232650	0.5698687573038321	0.2003703585093823	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0867160383061455	0.2126318427089243	0.3021329188454401	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2499377479509702	0.7141981777551233	0.3033430179590359	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2489465298420327	0.9985417935905618	0.3345587262585014	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0866113055423470	0.4975120520089244	0.3339126852117071	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F

0.4165142040447249	0.8510624138304810	0.2482835954476781	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5866956458121666	0.3440936041664501	0.2527838385518415	T	T	T
0.5864868427633609	0.0724158404152299	0.2013210812363039	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4138149497305426	0.5643325132043712	0.2018826293806130	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4202332879150670	0.2076960578505458	0.3039066771962814	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5866022538166911	0.7043188845459958	0.2783817959484077	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5865370795252931	0.9866288412744750	0.3389038454311318	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.4181002323940240	0.4939472736424148	0.3384311068243233	T	T	T
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7568063801493198	0.8512065621354953	0.2484181236592028	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9195348922452589	0.3478719610787778	0.2496964882157187	T	T	T
0.9197543893490653	0.0714695356187652	0.2007637956542556	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7594771358281055	0.5643765499031013	0.2019025534431566	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7531821113219667	0.2077033922667177	0.3037874653474378	T	T	T

0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9233446404368119	0.7142118372187598	0.3033259752554769	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9242369266501684	0.9986731572347028	0.3345722150893479	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7554937270985629	0.4942314906975435	0.3385066943512904	T	T	T
0.6872797775776726	0.5963645531759223	0.4130260393548894	T	T	T
0.4854382968246767	0.5962708773961484	0.4130909453868610	T	T	T
0.5860324974152227	0.7268249896592407	0.4958895969517914	T	T	T
0.5863126605432845	0.8019714476529546	0.3745129812550512	T	T	T

Ni_{4,b}:

1.00000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 48 4

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0851338324138526	0.6604178228199783	0.2870730265282795	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2547414206099756	0.1606976164369762	0.2904061112461623	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F

0.2474938023207247	0.8897825941987079	0.2429862227891204	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0883315969625212	0.3887685276692171	0.2496112032874965	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4235670969332768	0.6696708231061449	0.2834788852702153	T	T	T
0.5865600110000031	0.036940009999978	0.0900399980000017	F	F	F
0.5882446262083328	0.1627531202709277	0.2897314487911241	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5905513050964037	0.8913404702516982	0.2439322221245746	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4201894497738438	0.3936152052201085	0.2522225002058137	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7532270227724988	0.6719575321096026	0.2833107361832082	T	T	T
0.9198899869999977	0.036940009999978	0.0900399980000017	F	F	F
0.9205829729869436	0.1643355741594845	0.2892382799828326	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9217770578671776	0.8955606912938853	0.2504710880642526	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7539418445857355	0.3939674073444820	0.2517417043289683	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0861946553847440	0.8568479096302954	0.2492097780358276	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2540751412269164	0.3457120758184103	0.2514117464906198	T	T	T
0.2491086999744014	0.0726001518239468	0.2013485063444055	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F

0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0838678074915792	0.5696991521469139	0.2001051758470781	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0883745838913953	0.2123049754614878	0.3039896847628442	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2501020683132220	0.7133067975301726	0.2917261721017161	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2637538198948704	-0.0028826710500128	0.3387067814422083	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0899664766267429	0.5011111853229318	0.3341962227403093	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4190490189973116	0.8644778409202928	0.2555063054066590	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5875414068552507	0.3510369305802232	0.2526045507481082	T	T	T
0.5867142801847028	0.0733149337073106	0.2010783698783359	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4056793610035848	0.5604312611431165	0.1997234195380922	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4214333298833686	0.2102084267883751	0.3041989716390289	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5875732275358339	0.6996422235341088	0.2557081430555239	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5963998343964093	0.0014714480678086	0.3403293408644760	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F

0.4195657464713325	0.5025287332822328	0.3380752433074372	T	T	T
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7562008796921742	0.8594948063197730	0.2500691388861992	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9221477605288930	0.3512895578237133	0.2521403251302566	T	T	T
0.9211814476819149	0.0744661466736596	0.2010817785125854	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7703261482343252	0.5631830264762120	0.2007266366582396	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7550535784928228	0.2141822084642666	0.3033602311810952	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9214873483867854	0.7177011472318807	0.2999062525875273	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9216457178814705	0.0023882758691207	0.3356969027039707	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7496498521539798	0.5038818656578073	0.3387449519952688	T	T	T
0.3872280622966263	0.8747948117880111	0.3689938384789180	T	T	T
0.4715377631418393	0.6482696320793648	0.4061166496193291	T	T	T
0.6695927033541141	0.6232464364275582	0.4014483809068284	T	T	T
0.5855820082083767	0.8416492793656949	0.3926372162261049	T	T	T

Ni_{4,c}:

1.00000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 48 4

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0861806605135813	0.6579320064631550	0.2888821556612240	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2497414339036048	0.1564885558957924	0.2894096325688876	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2523490063011710	0.8862416412786983	0.2479079410135234	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0864297878036963	0.3877017174634599	0.2477155457030906	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4177870482459661	0.6608993780571260	0.2893111746973230	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5865641343431492	0.1571408251689624	0.3012064064799216	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5861634118292309	0.8956627893690758	0.2454729292405249	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4200189758641170	0.3846247481383905	0.2432114723933592	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7547152545950140	0.6608602640166642	0.2892980277086781	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F

0.9230932025796790	0.1566703647446464	0.2893584114103200	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9200401377026628	0.8863142141507925	0.2480162736051705	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7527699313629908	0.3846967126558770	0.2431872526188543	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0861890288146948	0.8468603669470169	0.2474991752529238	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2538926847447043	0.3469352291363927	0.2488066379115036	T	T	T
0.2545876132915132	0.0695635984375255	0.2008462687181806	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0859751030242792	0.5695010930374826	0.2006848707297042	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0863903675515238	0.2112513964352068	0.3027609649660696	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2519811217896230	0.7105210536143574	0.3016021617823594	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2503099073562801	0.9939454677956879	0.3338836545622850	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0864467439216799	0.4959912010255651	0.3338240759244406	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4209345148669083	0.8440714354191179	0.2494455060561686	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5864580074638471	0.3392124136287237	0.2409440213186216	T	T	T

0.5864331623529349	0.0681632497558661	0.2038401025253604	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4220809656294613	0.5678854679116732	0.2020030789312051	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4154504732612935	0.2083187639837766	0.3073457803419447	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5862535235296263	0.7029709229814380	0.3091029582141717	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5863270062321183	0.9892893874508550	0.3367730122716414	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.4135654731044999	0.4963080586902029	0.3405515986497667	T	T	T
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7515485388499078	0.8439836705216194	0.2494790648780795	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9189713105360173	0.3471701841007681	0.2488595959881945	T	T	T
0.9183854852353951	0.0696748864794823	0.2008209048028993	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7508239500264741	0.5678752051186526	0.2019868101837261	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7574613114581153	0.2088349113604144	0.3076146861974735	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9204230348173253	0.7105494921836535	0.3017036325464560	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F

0.9220340787332449	0.9941520792723432	0.3338843656071858	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7583437515648964	0.4965082852856853	0.3406383055763920	T	T	T
0.6917107202593912	0.3248180852885511	0.3835158926281002	T	T	T
0.4807432300833808	0.3234525184107144	0.3833188311927504	T	T	T
0.5853366217529293	0.4109483252572656	0.4795540298880728	T	T	T
0.5853425907554576	0.5343513224498276	0.3650410043053869	T	T	T

Ni_{5,a}:

1.00000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 48 5

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0894572687141093	0.6604274829826342	0.2900965744110958	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2534264880124779	0.1598056468115263	0.2903599372153707	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2542411903118288	0.8919602027236988	0.2475216903736659	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0866310130177873	0.3881656960782008	0.2500443024732035	T	T	T

0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4194485246165099	0.6625197837623998	0.2908575384691797	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5860189285673327	0.1548304181420920	0.2912671124744460	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5860948202446783	0.8887433311872875	0.2406584300079171	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4186015457793338	0.3870268228397898	0.2452126619322887	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7610953612535875	0.6681657853062803	0.2882973843556408	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9193447456716768	0.1613478637319076	0.2893998680418380	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9247491445611156	0.8917874741702230	0.2487864193859088	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7505904304592153	0.3912095159500779	0.2529012404466292	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0897708361765058	0.8464924130391092	0.2458474579359148	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2517744013364093	0.3437376717985471	0.2483531566069208	T	T	T
0.2510461542951815	0.0702816783943198	0.2017983041073079	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0913191273867934	0.5708650194162250	0.2017643859502201	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F

0.0862652023928702	0.2119816989551269	0.3036288171222010	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2521647271563943	0.7227605742919559	0.3156460706624046	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2576372961219321	-0.0031269490401204	0.3363801341205469	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0898463453142451	0.4978059430299115	0.3351181443258098	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4168407299031583	0.8468455160903624	0.2426983676226461	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5867530253033051	0.3453989253034561	0.2518133937648351	T	T	T
0.5884881506446292	0.0729974327436018	0.2005512430702885	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4084905265131670	0.5636772961098090	0.2006353675488480	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4199365146904364	0.2070056058166884	0.3017260153860502	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5881617778267133	0.7034041983240802	0.2770788376919794	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5821394814666003	-0.0112262870962828	0.3374588632118536	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.4140973275586091	0.4847679050175928	0.3352618376538100	T	T	T
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7579836770527241	0.8521810352026963	0.2498231968206016	T	T	T

0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9188936991242250	0.3503889454408434	0.2525938787336076	T	T	T
0.9203700985632780	0.0719975965133458	0.2010201521845394	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7625396935011154	0.5643562695402270	0.2031777590020158	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7526449298718916	0.2094681808287345	0.3049152587902064	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9257332738588434	0.7135783984723404	0.3037370734867891	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9258886863868400	-0.0013612612347245	0.3344864010843122	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7451610432983781	0.5023139316020147	0.3419516723206332	T	T	T
0.5299731290511162	0.7455819599828820	0.4911641305604792	T	T	T
0.5741968701314182	0.8057393627849050	0.3714453330887580	T	T	T
0.4626498614398203	0.5827231456870506	0.4158706759064649	T	T	T
0.6637099481148205	0.6044581420119743	0.4134609599223650	T	T	T
0.3598900333619294	0.7786735575308814	0.4027950819981010	T	T	T

Ni_{6,a}:

1.0000000000000000

11.3280000686999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 10.2098999023000001 0.0000000000000000

0.0000000000000000 0.0000000000000000 17.8448009491000015

Ti O Ni

24 48 6

Direct

0.0865600030000024	0.2966000139999991	0.0900399980000017	F	F	F
0.0867642551901621	0.4197282251765940	0.2885333529670294	T	T	T
0.2532300060000026	0.7965999839999967	0.0900399980000017	F	F	F
0.2553098865283464	0.9178144429165572	0.2916776987012365	T	T	T
0.2532300060000026	0.5124099849999979	0.0408900010000011	F	F	F
0.2526581867104474	0.6495618642834088	0.2442322433202728	T	T	T
0.0865600030000024	0.0124100000000027	0.0408900010000011	F	F	F
0.0877485745187446	0.1469259144695545	0.2505566316147552	T	T	T
0.4198899869999977	0.2966000139999991	0.0900399980000017	F	F	F
0.4231385961588595	0.4297521528457748	0.2868999299536672	T	T	T
0.5865600110000031	0.7965999839999967	0.0900399980000017	F	F	F
0.5860884500999036	0.9200320336477038	0.2886467722881161	T	T	T
0.5865600110000031	0.5124099849999979	0.0408900010000011	F	F	F
0.5867463127222285	0.6477346373809074	0.2421861159138827	T	T	T
0.4198899869999977	0.0124100000000027	0.0408900010000011	F	F	F
0.4192966525914578	0.1530292563922224	0.2507131826497762	T	T	T
0.7532299760000001	0.2966000139999991	0.0900399980000017	F	F	F
0.7564113586602206	0.4271796642940883	0.2881559512903523	T	T	T
0.9198899869999977	0.7965999839999967	0.0900399980000017	F	F	F
0.9195381214426955	0.9209050567466426	0.2896784329928670	T	T	T
0.9198899869999977	0.5124099849999979	0.0408900010000011	F	F	F

0.9224841632423665	0.6515331377249388	0.2491977081783193	T	T	T
0.7532299760000001	0.0124100000000027	0.0408900010000011	F	F	F
0.7524967727834454	0.1503744454216365	0.2488889300166050	T	T	T
0.0865600030000024	0.4761500059999975	0.0491500010000010	F	F	F
0.0877673626073714	0.6108118946467040	0.2475791624915590	T	T	T
0.2533174582587672	0.1036331931373736	0.2519884379821316	T	T	T
0.2532300060000026	0.9761499760000021	0.0491500010000010	F	F	F
0.2532300060000026	0.6919599770000033	0.0000000000000000	F	F	F
0.2498866804228632	0.8310096601767057	0.2022697129663238	T	T	T
0.0865600030000024	0.1919600069999987	0.0000000000000000	F	F	F
0.0887750145442181	0.3292111143170047	0.2011204659103787	T	T	T
0.0865600030000024	0.8328599929999996	0.0817899999999980	F	F	F
0.0875207873352526	0.9693033229786475	0.3044611745168533	T	T	T
0.2532300060000026	0.3328599929999996	0.0817899999999980	F	F	F
0.2509519845578815	0.4780756402832445	0.3052274473356524	T	T	T
0.2532300060000026	0.6170499919999983	0.1309400049999994	F	F	F
0.2669675706679200	0.7524286238664146	0.3389705922660294	T	T	T
0.0865600030000024	0.1170499999999990	0.1309400049999994	F	F	F
0.0884771891351838	0.2582854312691080	0.3348372502710990	T	T	T
0.4198899869999977	0.4761500059999975	0.0491500010000010	F	F	F
0.4184791599935080	0.6101684469074115	0.2392547161266964	T	T	T
0.5860595979227193	0.1067072398061856	0.2497763843055859	T	T	T
0.5865600110000031	0.9761499760000021	0.0491500010000010	F	F	F
0.5865600110000031	0.6919599770000033	0.0000000000000000	F	F	F
0.5892474415211173	0.8320050074731647	0.1999323284836320	T	T	T

0.4198899869999977	0.1919600069999987	0.0000000000000000	F	F	F
0.4051846783831925	0.3225579179729766	0.2007901341662930	T	T	T
0.4198899869999977	0.8328599929999996	0.0817899999999980	F	F	F
0.4202008357485671	0.9702936603963710	0.3039807131633567	T	T	T
0.5865600110000031	0.3328599929999996	0.0817899999999980	F	F	F
0.5894997758591893	0.4587069853943210	0.2696795044794587	T	T	T
0.5865600110000031	0.6170499919999983	0.1309400049999994	F	F	F
0.5791141737692855	0.7552653095505140	0.3363226054396711	T	T	T
0.4198899869999977	0.1170499999999990	0.1309400049999994	F	F	F
0.4233183917860830	0.2584939842496268	0.3386052768836686	T	T	T
0.7532299760000001	0.4761500059999975	0.0491500010000010	F	F	F
0.7562677597136581	0.6130787704349747	0.2500023638751879	T	T	T
0.9208263731735850	0.1081951562083794	0.2521389897795616	T	T	T
0.9198899869999977	0.9761499760000021	0.0491500010000010	F	F	F
0.9198899869999977	0.6919599770000033	0.0000000000000000	F	F	F
0.9215943608039301	0.8315692511122649	0.2014297662473264	T	T	T
0.7532299760000001	0.1919600069999987	0.0000000000000000	F	F	F
0.7688638668438594	0.3242257704492270	0.2016868901183943	T	T	T
0.7532299760000001	0.8328599929999996	0.0817899999999980	F	F	F
0.7530505408109991	0.9700552935288614	0.3031826337879442	T	T	T
0.9198899869999977	0.3328599929999996	0.0817899999999980	F	F	F
0.9234791504668447	0.4747075890892101	0.3030855479365424	T	T	T
0.9198899869999977	0.6170499919999983	0.1309400049999994	F	F	F
0.9195828835972246	0.7579517682568818	0.3359019245807760	T	T	T
0.7532299760000001	0.1170499999999990	0.1309400049999994	F	F	F

0.7428724844764589	0.2559166377831038	0.3377218761307534	T	T	T
0.5813374433786924	0.4911887643253173	0.5011085370482729	T	T	T
0.4604353480703281	0.3865027980791642	0.4138031879332520	T	T	T
0.5508485001725920	0.6043341511919654	0.3905161660567636	T	T	T
0.3437270930128812	0.5943144161869572	0.3849657607751423	T	T	T
0.6753090672857938	0.3589865464189138	0.4126855893016615	T	T	T
0.7422554250185277	0.5661137494348242	0.4366004421722002	T	T	T

Ni_{4,A}:

1.00000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 47 4

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0840424638793958	0.6599878580347170	0.2881432439684494	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2528468300822124	0.1577538687766846	0.2916823082419316	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2517851815124045	0.8889075481179289	0.2471868414086718	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0881085114804991	0.3829543041897981	0.2445298946186462	T	T	T

0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4201366778101610	0.6672541250108933	0.2962769439040409	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5868676707254418	0.1578212221203359	0.2916213611641560	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5880923061932382	0.8889536550231977	0.2471516420060816	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4198355036536746	0.3863245529832294	0.2388222673470952	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7559701808238334	0.6600205577169491	0.2880622676925995	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9198238884146804	0.1594801690407492	0.2897057421593491	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9198977779534868	0.8899705786043524	0.2479984198038994	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7516910354484836	0.3829309255190612	0.2444696221714880	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0849387588403854	0.8469605678067972	0.2470769314165092	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2546318530297451	0.3384167283059983	0.2415891169575373	T	T	T
0.2595988044063157	0.0697809124392769	0.2020490843855753	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0840451431574585	0.5688297688678788	0.2009549473260432	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F

0.0875185602231232	0.2107843892460637	0.3016858530384925	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2485922908630805	0.7146596048980720	0.3041479042630164	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2498335410281812	-0.0052458307830422	0.3346697060883003	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0988924859163067	0.4926257078360177	0.3354692815353311	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4199510470771025	0.8445151105612808	0.2518477376703773	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5851502688531751	0.3384977172340941	0.2416027305484006	T	T	T
0.5801833321915136	0.0698207593939101	0.2019892229419628	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4199831387249020	0.5656711902752973	0.2077379985046308	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4198739640091937	0.2173753481487870	0.3165760497806511	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5914560717480337	0.7148675883307813	0.3040644054710193	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5900301466691305	-0.0051380003238738	0.3346479930450753	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7549392538645606	0.8469159987484004	0.2469505401628745	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F

0.9198802574043432	0.3502198235206204	0.2507254429058489	T	T	T
0.9199569021801184	0.0712528732613068	0.2012359142379980	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7559184505769795	0.5688770441022482	0.2008886406284120	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7522223438893521	0.2108703011487168	0.3016983323947385	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9199104148172160	0.7097698620945696	0.3045372653937746	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9198002669911983	-0.0021058822784200	0.3344888072473204	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7408931275872624	0.4926383593369574	0.3353811921719250	T	T	T
0.5774048664029038	0.5278000999684054	0.3580253924720626	T	T	T
0.4197733326369335	0.3804518583907133	0.3724743179082041	T	T	T
0.4197731324584371	0.5851894880425634	0.4293941383462563	T	T	T
0.2623795071233699	0.5281647990941715	0.3578578762307258	T	T	T

Ni_{5,A}:

1.0000000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0854817062912051	0.6632081423136644	0.2882750322858721	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2476103729492893	0.1546648005159986	0.2956329459434357	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2522858130854757	0.8894395799284337	0.2462062458320151	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0813864957259036	0.3883733122693768	0.2446552786158652	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4193665425299600	0.6649577601494792	0.2927151875581175	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5919089347581800	0.1533676681942579	0.2918522231032172	T	T	T
0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5871039848626767	0.8868941840784328	0.2457334217469972	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4181856951439272	0.3809562997561331	0.2387148186774249	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7555173448289659	0.6626790143656971	0.2877070972663337	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9189214669891185	0.1579750564494479	0.2902980845415342	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9197154747401345	0.8895961292662664	0.2472287574542348	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F

0.7537989524412912	0.3872934713272426	0.2446403180639980	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0852227443171313	0.8477032865399782	0.2465585742735585	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2508554148496074	0.3513823057084426	0.2487371924858871	T	T	T
0.2534664182767342	0.0721155338057030	0.2027545578119142	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0845149838674290	0.5706149206586977	0.2008431213595317	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0829290932364466	0.2132207965483300	0.3018485807461521	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2503735840004617	0.7147209293599476	0.3013144958242203	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F
0.2460700127604084	-0.0071436093809853	0.3362978377412700	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.0870983031257052	0.4995318434819732	0.3369618130675731	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4190915024388362	0.8493736386100805	0.2513056673580580	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5883111404355837	0.3460570795118034	0.2454661131862709	T	T	T
0.5882537745889250	0.0713885991581029	0.2007550320797310	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4145283422403712	0.5633179686950377	0.2059276915830666	T	T	T

0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4217016379980107	0.1989267209856221	0.3001531875548420	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5889780558803537	0.7150849122951913	0.2973036065591886	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5930199427288425	-0.0077705465025719	0.3345043798035247	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7551251522288670	0.8478627374688968	0.2463860425009410	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9183163022187194	0.3509063209037908	0.2489917122431199	T	T	T
0.9185268077173623	0.0715440108894033	0.2010078682726705	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F
0.7603814192912057	0.5698194647746232	0.2006033505647701	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7550559223948199	0.2150733345778312	0.3040050909927824	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9199456490647203	0.7120646437972671	0.3037062092849095	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9196925921339750	-0.0033410469983942	0.3343831142223984	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7365508355914522	0.5015847543940390	0.3364826719657248	T	T	T
0.4146929569838627	0.5424004767562388	0.4065679318299161	T	T	T
0.2481216415236086	0.4390982298078751	0.3472907705284706	T	T	T

0.4107038964778303	0.3153039610292151	0.3836666572247361	T	T	T
0.5658530477171946	0.4579725946054117	0.3352265062627792	T	T	T
0.2895832166030885	0.4037903280191178	0.4724949578311981	T	T	T

Ni_{6,A}:

1.00000000000000

11.3280000686999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.2098999023000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8448009491000015

Ti O Ni

24 47 6

Direct

0.0865600030000024	0.5369399790000031	0.0900399980000017	F	F	F
0.0839704449023716	0.6632087821105362	0.2894927393669878	T	T	T
0.2532300060000026	0.0369400009999978	0.0900399980000017	F	F	F
0.2470207283701021	0.1557636150736175	0.2938341215094158	T	T	T
0.2532300060000026	0.7527499790000007	0.0408900010000011	F	F	F
0.2499537524854619	0.8931889708721924	0.2446982332858673	T	T	T
0.0865600030000024	0.2527500090000032	0.0408900010000011	F	F	F
0.0840618913689148	0.3888220756054428	0.2441219658792397	T	T	T
0.4198899869999977	0.5369399790000031	0.0900399980000017	F	F	F
0.4208244249557814	0.6764293856646526	0.2894937491232624	T	T	T
0.5865600110000031	0.0369400009999978	0.0900399980000017	F	F	F
0.5936408371942896	0.1557576155323501	0.2938357530924528	T	T	T

0.5865600110000031	0.7527499790000007	0.0408900010000011	F	F	F
0.5917130504062384	0.8932854696212417	0.2444886272626528	T	T	T
0.4198899869999977	0.2527500090000032	0.0408900010000011	F	F	F
0.4204025815417745	0.3803659598654411	0.2388095469692227	T	T	T
0.7532299760000001	0.5369399790000031	0.0900399980000017	F	F	F
0.7578843271965728	0.6633713487091208	0.2894918327378171	T	T	T
0.9198899869999977	0.0369400009999978	0.0900399980000017	F	F	F
0.9202316950690419	0.1590625583100872	0.2905415736791132	T	T	T
0.9198899869999977	0.7527499790000007	0.0408900010000011	F	F	F
0.9208683588092615	0.8913310937657003	0.2459853534180345	T	T	T
0.7532299760000001	0.2527500090000032	0.0408900010000011	F	F	F
0.7565688752738449	0.3889575073217458	0.2441234880808905	T	T	T
0.0865600030000024	0.7164899710000014	0.0491500010000010	F	F	F
0.0852460030702377	0.8460470454948549	0.2443387018427558	T	T	T
0.2532300060000026	0.2164900000000003	0.0491500010000010	F	F	F
0.2519520934145086	0.3508477095957073	0.2501727928032536	T	T	T
0.2458002292415084	0.0709314453220302	0.2013138380412472	T	T	T
0.2532300060000026	0.9322999720000027	0.0000000000000000	F	F	F
0.0865600030000024	0.4323000010000015	0.0000000000000000	F	F	F
0.0837630215083686	0.5714959475185895	0.2014762711281425	T	T	T
0.0865600030000024	0.0732000020000001	0.0817899999999980	F	F	F
0.0827288542642873	0.2162773954640247	0.3031129305656832	T	T	T
0.2532300060000026	0.5731999870000024	0.0817899999999980	F	F	F
0.2477764482365331	0.7249512767671168	0.3087985233780741	T	T	T
0.2532300060000026	0.8573899869999977	0.1309400049999994	F	F	F

0.2461576064569914	-0.0055123651190317	0.3356799834887201	T	T	T
0.0865600030000024	0.3573899869999977	0.1309400049999994	F	F	F
0.1011432171142233	0.4999922427470551	0.3371511452110076	T	T	T
0.4198899869999977	0.7164899710000014	0.0491500010000010	F	F	F
0.4206644255884253	0.8506968364375902	0.2477880438919474	T	T	T
0.5865600110000031	0.2164900000000003	0.0491500010000010	F	F	F
0.5887218505986206	0.3510530791554333	0.2499667700358562	T	T	T
0.5948109410607173	0.0711123808236346	0.2012662093858649	T	T	T
0.5865600110000031	0.9322999720000027	0.0000000000000000	F	F	F
0.4198899869999977	0.4323000010000015	0.0000000000000000	F	F	F
0.4204420365307354	0.5624091189542944	0.2065809024550415	T	T	T
0.4198899869999977	0.0732000020000001	0.0817899999999980	F	F	F
0.4202550819388058	0.1862156687039863	0.2874330433899304	T	T	T
0.5865600110000031	0.5731999870000024	0.0817899999999980	F	F	F
0.5938551834103613	0.7254243712935555	0.3086079998735193	T	T	T
0.5865600110000031	0.8573899869999977	0.1309400049999994	F	F	F
0.5955129550613401	-0.0054657422395409	0.3355651173857778	T	T	T
0.4198899869999977	0.3573899869999977	0.1309400049999994	F	F	F
0.7532299760000001	0.7164899710000014	0.0491500010000010	F	F	F
0.7563452130681196	0.8462833326233020	0.2441244908239198	T	T	T
0.9198899869999977	0.2164900000000003	0.0491500010000010	F	F	F
0.9202993419475251	0.3553118938587643	0.2495438031150705	T	T	T
0.9204060468105241	0.0723705094259431	0.2009877547014398	T	T	T
0.9198899869999977	0.9322999720000027	0.0000000000000000	F	F	F
0.7532299760000001	0.4323000010000015	0.0000000000000000	F	F	F

0.7568747814240265	0.5715978914911937	0.2014429843342058	T	T	T
0.7532299760000001	0.0732000020000001	0.0817899999999980	F	F	F
0.7578178343494323	0.2164336958348777	0.3030316240141754	T	T	T
0.9198899869999977	0.5731999870000024	0.0817899999999980	F	F	F
0.9207983280813126	0.7123047422089008	0.3057929005629886	T	T	T
0.9198899869999977	0.8573899869999977	0.1309400049999994	F	F	F
0.9205220342965341	-0.0029278543257352	0.3338720913565205	T	T	T
0.7532299760000001	0.3573899869999977	0.1309400049999994	F	F	F
0.7406607096772960	0.5000775168650929	0.3371444007795897	T	T	T
0.2673249355654141	0.4431951813356815	0.3475248836493968	T	T	T
0.5257253798888594	0.6470097382572630	0.3995754317646570	T	T	T
0.4221354685779956	0.4713394465385768	0.4496742668268751	T	T	T
0.3171865529489853	0.6464450462027700	0.3998940668243040	T	T	T
0.5746841183980040	0.4430872751618116	0.3474463505179048	T	T	T
0.4210684362426818	0.2950842746388944	0.3720308713300904	T	T	T