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**Electronic Supporting Information (ESI)**

For

# Effects of Mg-Zr codoping on the photoelectrochemical properties of $Ta_3N_5$ semiconductor: a theoretical insight

Submitted to ***Journal of Materials Chemistry A***

by

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**SI-1 Image charge correction**

In our calculations, the $Ta_3N_5$ supercell is a finite size cell and the charge states of some defects are very high, for example, the highest charge states of $V_N$ and $Zr_{int}$ are as high as +3 and +5, respectively. Therefore, the image charge correction proposed by Makov-Payne[S1] should be considered to ensure the reliability of our calculated results.

The image charge correction proposed by Makov and Payne is described in the below Eqn. (S1):

$$\Delta E = \frac{q^2\alpha}{2\varepsilon_0 V^{1/3}} + \frac{2\pi qQ}{2\varepsilon_0 V} + O(V^{-5/3}) \quad \text{(S1)}$$

The first and second terms in Eqn. (S1) are monopole and quadrupole corrections, respectively. The monopole and quadrupole corrections can be easily obtained by setting the 'IDIPOL' parameter in the VASP calculations. According to the VASP manual, the monopole correction can be applied for any arbitrary cell shape, while the quadrupole correction is only available for the cubic cell shape. Since the $Ta_3N_5$ supercell is not cubic (11.61×10.25×10.27 $Å^3$), only the monopole correction is adopted for the image charge correction in this study. However, our calculated results are still qualitatively correct because the quadrupole correction is typically ~30% of the monopole correction[s2]. Actually, the DFT study of TaON also only adopted the monopole correction for the image charge correction, which might be ascribed to the non-cubic cell shape of TaON.[s3]

What should be mentioned is that, during the VASP calculations, the dielectric constant is automatically set as unit 1. Then, the final correction energies must be scaled down by the real dielectric constant. In our previous theoretical work,[s4] according to the experimental work,[s5] we used 110 as the dielectric constant of bulk $Ta_3N_5$. However, due to the extrinsic microstructural features of $Ta_3N_5$, the 110 may be overestimated for the dielectric constant of $Ta_3N_5$. Then, according to another experimental work,[s6] we adopt 17 as the dielectric constant of $Ta_3N_5$ in the present study. Actually, we also used 110 as the dielectric constant of $Ta_3N_5$ to make a test calculation, the results showed that using 17 or 110 merely affected the absolute values of defect formation energies but did not affect the qualitative analysis.

**SI-2 Chemical potential calculations**

Since the chemical potential calculation details of Mg-O codoped $Ta_3N_5$ are the same as that of Zr-O coodoped $Ta_3N_5$, we simply use the Mg-O codoped $Ta_3N_5$ as an example to discuss the chemical potential calculation procedure. The chemical potentials of N, O, Mg and Ta are calculated by two steps:

First, we calculate the chemical potentials of N ($\Delta\mu_N$) and Ta ($\Delta\mu_{Ta}$). Under thermal equilibrium growth conditions, $Ta_3N_5$ should satisfy:

$$3\Delta\mu_{Ta} + 5\Delta\mu_N = E^f_{Ta_3N_5} = -9.39eV \quad \text{(S2)}$$

where $E^f_{Ta_3N_5}$ is the calculated formation energy of the undoped $Ta_3N_5$. Then, $\Delta\mu_N$ and $\Delta\mu_{Ta}$ under different growth conditions can be determined. Since only the N-rich growth condition is considered in this study, the $\Delta\mu_N = 0$ and $\Delta\mu_{Ta}$=-3.13 eV.

Second, on the basis of above $\Delta\mu_N$ and $\Delta\mu_{Ta}$, we calculate the chemical potentials of Mg ($\Delta\mu_{\mathrm{Mg}}$) and O ($\Delta\mu_O$). In the elements doped materials, precipitation of secondary phases should be avoided. For the Mg-O codoped $Ta_3N_5$, possible precipitation of secondary phases such as $Ta_2O_5$, TaON, MgO, $Mg_3N_2$, $MgTa_2O_6$, $Mg_4Ta_2O_9$, $MgTa_2N_{2.975}$, $N_2$ gas, $O_2$ gas, bulk Mg and bulk Ta must be avoided:

$$5\Delta\mu_O + 2\Delta\mu_{Ta} < E^f_{Ta2O5} = -18.59eV \quad \text{(S3)}$$

$$\Delta\mu_N + \Delta\mu_O + \Delta\mu_{Ta} < E^f_{TaON} = -6.26eV \quad \text{(S4)}$$

$$\Delta\mu_{\mathrm{Mg}} + \Delta\mu_O < E^f_{\mathrm{MgO}} = -5.92eV \quad \text{(S5)}$$

$$3\Delta\mu_{\mathrm{Mg}} + 2\Delta\mu_N < E^f_{Mg3N2} = -4.82eV \quad \text{(S6)}$$

$$\Delta\mu_{\mathrm{Mg}} + 2\Delta\mu_{Ta} + 6\Delta\mu_O < E^f_{MgTa2O6} = -27.24eV \quad \text{(S7)}$$

$$4\Delta\mu_{\mathrm{Mg}} + 2\Delta\mu_{Ta} + 9\Delta\mu_O < E^f_{Mg4Ta2O9} = -45.40eV \quad \text{(S8)}$$

$$\Delta\mu_{\mathrm{Mg}} + 2\Delta\mu_{Ta} + 2.975\Delta\mu_{\mathrm{N}} < E^f_{\mathrm{MgTa2N2.975}} = -8.26eV \quad \text{(S9)}$$

$$\Delta\mu_{\mathrm{N}} < 0, \Delta\mu_O < 0, \Delta\mu_{\mathrm{Mg}} < 0, \Delta\mu_{Ta} < 0 \quad \text{(S10)}$$

where $E_i^f$ ($i$= $Ta_2O_5$, TaON, MgO, $Mg_3N_2$, $MgTa_2O_6$, $Mg_4Ta_2O_9$, $MgTa_2N_{2.975}$) are formation energies of $i$, respectively. To avoid precipitation of all secondary phases, the inequations (S3)-(S10) must be simultaneously satisfied. In other words, the values of $\Delta\mu_{\mathrm{Mg}}$ and $\Delta\mu_O$ can only be selected in the shaded area of Fig S1a.

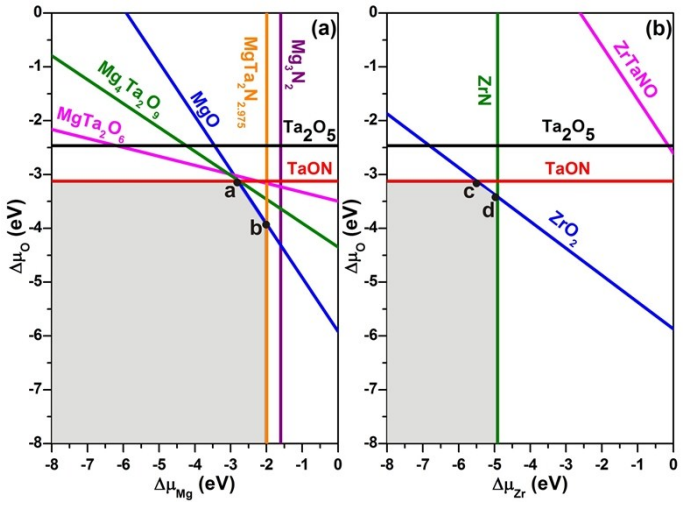


**Fig. S1** Chemical potentials of (a) Mg and O ($\Delta\mu_{\mathrm{Mg}}$ and $\Delta\mu_{\mathrm{O}}$) in the Mg-O codoped and (b) Zr and O ($\Delta\mu_{\mathrm{Zr}}$ and $\Delta\mu_{\mathrm{O}}$) in the Zr-O codoped $Ta_3N_5$ under the N-rich growth condition. The shaded areas in (a) and (b) are the accessible range of chemical potentials for equilibrium growth of the Mg-O codoped and Zr-O codoped $Ta_3N_5$, respectively. In (a) and (b), four critical chemical potentials are shown in black points a, b, c and d.

Theoretically, all points in the shaded regions of Fig. S1a can be safely selected. However, the points at doping limit, where the precipitations are avoided and simultaneously the dopants have the larger concentrations (*i.e.*, the smaller formation energies), are generally selected. These doping limit points are usually at the boundary of the shaded areas. For example, the points a and b in the Fig. S1a are the so-called doping limit points. Generally, selecting point a or b is sufficient for the formation energy calculations. In the present study, however, we do not select only one point but select the ranges from point a to b, which cover a wide range of chemical potentials. This is expected to ensure that our calculation results are more reliable and robust.

According to the above discussion, the $\Delta\mu_{Mg}$ in the range of -2.79 to -1.99 eV and the corresponding $\Delta\mu_{O}$ in the range of -3.12 to -3.92 eV are selected for the formation energy calculations. In Fig. 4a of the main text, the horizontal axis of defect formation energies of Mg-O codoped $Ta_3N_5$ is presented by the range of $\Delta\mu_{Mg}$. The $\Delta\mu_{Zr}$ and $\Delta\mu_{O}$ of the Zr-O codoped $Ta_3N_5$ can be obtained by the same procedure. The calculated accessible range of chemical potentials for Zr-O codoped $Ta_3N_5$ is shown in Fig. S1b. The $\Delta\mu_{Zr}$ is in the range of -5.50 to -4.91 eV and the corresponding $\Delta\mu_{O}$ is in the range of -3.12 to -3.42 eV.

In this study, besides the Mg-$O_N$/$V_N$ codoped and Zr-$O_N$/$V_N$ codoped models, the Mg-Zr-$O_N$/$V_N$ codoped models are also investigated. The below Fig. S2g-j show the four Mg-Zr-$O_N$/$V_N$ codoped models. When we calculate formation energies of these four models, we select point b and d in the Fig. S1, which correspond to the Mg-rich and Zr-rich doping limits, respectively. At the point b, the $\Delta\mu_{Mg}$ and $\Delta\mu_{O}$ are -1.99 and -3.92 eV, respectively. Then, based on the value of $\Delta\mu_{O}$, the $\Delta\mu_{Zr}$ (-4.91 eV) can be got from Fig. S1b. At the point d, the $\Delta\mu_{Zr}$ and $\Delta\mu_{O}$ are -4.91 and -4.32 eV, respectively. Then, based on the value of $\Delta\mu_{O}$, the $\Delta\mu_{Mg}$ (-2.50 eV) can be got from Fig. S1a.

**SI-3 The doping models**

In this study, we considered four Mg/Zr-$O_N$/$V_N$ models ($Zr_{Ta}$+$O_N$, 3$Zr_{Ta}$+$V_N$, $Mg_{Ta}$+$V_N$, $Mg_{Ta}$+3$O_N$), two interstitial doping models ($Zr_{int}$, $Mg_{int}$), and four Mg-Zr-$O_N$/$V_N$ codoped models ($Zr_{Ta}$+$O_N$+$Mg_{int}$, 3$Zr_{Ta}$+$V_N$+$Mg_{int}$, $Mg_{Ta}$+3$O_N$+$Zr_{int}$ and $Mg_{Ta}$+$V_N$+$Zr_{int}$). The atomic structures of these ten doping models are shown in below Fig. S2. The detailed information of these ten models can be found at the end of the ESI (in the format of CONTCAR).

As discussed in the main text, in $Ta_3N_5$, the Ta atom is coordinated with six neighboring N atoms, while N atoms are coordinated with 3 or 4 Ta atoms. Since both the experimental[s7] and theoretical[s8] investigations have proved that the 3-corridnated N atom is easily substituted by the O atom, the $O_N$ impurity in $Zr_{Ta}$+$O_N$ is then simulated by substitution of O atom for the 3-coordinated N atom. The $V_N$ in 3$Zr_{Ta}$+$V_N$ and $Mg_{Ta}$+$V_N$ are

also simulated by removing the 3-coordinated N atom. Note that, since the $V_N$ of $3Zr_{Ta}+V_N$ is coordinated with 3 Ta atoms, these 3 Ta atoms are simply substituted by Zr to simulate the $3Zr_{Ta}$.

The atomic structure of $Mg_{Ta}+3O_N$ should be paid more attention. Since the Ta atom is coordinated with six neighboring N atoms, the $3O_N$ of $Mg_{Ta}+3O_N$ can be simulated by several possible configurations. In this study, the atomic structure of $Mg_{Ta}+3O_N$ is constructed according to that of $Ba_{Ta}+3O_N$, which has been proved to be relatively more stable among various possible configurations in our previous theoretical work.[s9] Actually, the energy differences among different configurations of $3O_N$ are within 0.5 eV. Therefore, the selection of atomic structure of $Ba_{Ta}+3O_N$ may affect the quantitative results but not affect the qualitative analysis. The four Mg-Zr-$O_N$/$V_N$ codoped models in Fig. S2g-j are the simple combination of models in Fig. S2a-f. For example, the $Zr_{Ta}+O_N+Mg_{int}$ model is the combination of $Zr_{Ta}+O_N$ and $Mg_{int}$ models.

What should be mentioned is the doping rate in our study. In our study, the size of $Ta_3N_5$ supercell is a=11.61, b=10.25 and c=10.27 Å. There are 60N and 36Ta atoms in this supercell. On the basis of this supercell, the largest doping rate is about 11.1% ($3Zr_{Ta}+V_N+Mg_{int}$), which is smaller than the experimental doping rate of about 33%. However, using this supercell to simulate elements doping is reasonable based on the following three reasons:

Firstly, due to the periodic condition, the doped element actually has many neighboring images. To reflect the real doping effects, it is better to keep the nearly same neighboring image interactions along different directions.[s10] In other words, a cubic size of supercell is theoretically suitable for the elements doping study. The cell size of conventional $Ta_3N_5$ cell is a=3.87, b=10.25 and c=10.27 Å. Therefore, enlarging the lattice a three times larger is able to build a supercell which is very close to the cubic size. Actually, this supercell is also adopted in other DFT calculations of elements doped $Ta_3N_5$.[s11]

The second reason is that the near-cubic supercell is able to reduce error in the charged defects calculations. In our study, the defects such as $Mg_{Ta}$, $Zr_{Ta}$, $Mg_{int}$ and $Zr_{int}$ with different charge states are investigated. Then, the monopole-monopole and monopole-quadrupole interactions must be both considered to correct the charged defects.

Unfortunately, according to the VASP manual, a full correction is only possible for the cubic cell with the VASP. For the non-cubic cell, only the monopole-monopole interaction can be used to perform the correction. Since a near-cubic cell is able to reduce the proportion of monopole-quadrupole interaction in the full correction, our used near-cubic supercell of $Ta_3N_5$ is expected to improve the reliability of charge corrections. If we use a small cell of $Ta_3N_5$ to get closer to the experimental doping rate, the error of charge correction will be very large and our calculated results will be unreliable.

Thirdly, in the elements doping experiments, the final doping rates are generally not equal to the initial doping rates. Due to the preparation environment such as high temperature and high pressure, the doped elements may partially lose during the sample preparation. Furthermore, the doped elements are usually not completely doped into the expected sites of lattice but reacting with other elements and generate secondary phases. For example, in the Mg-Zr doped $Ta_3N_5$, the secondary phases such as MgO and $ZrO_2$ are observed. Therefore, the final doping rate of Mg-Zr is expected to be smaller than the initial doping rate of 33%.

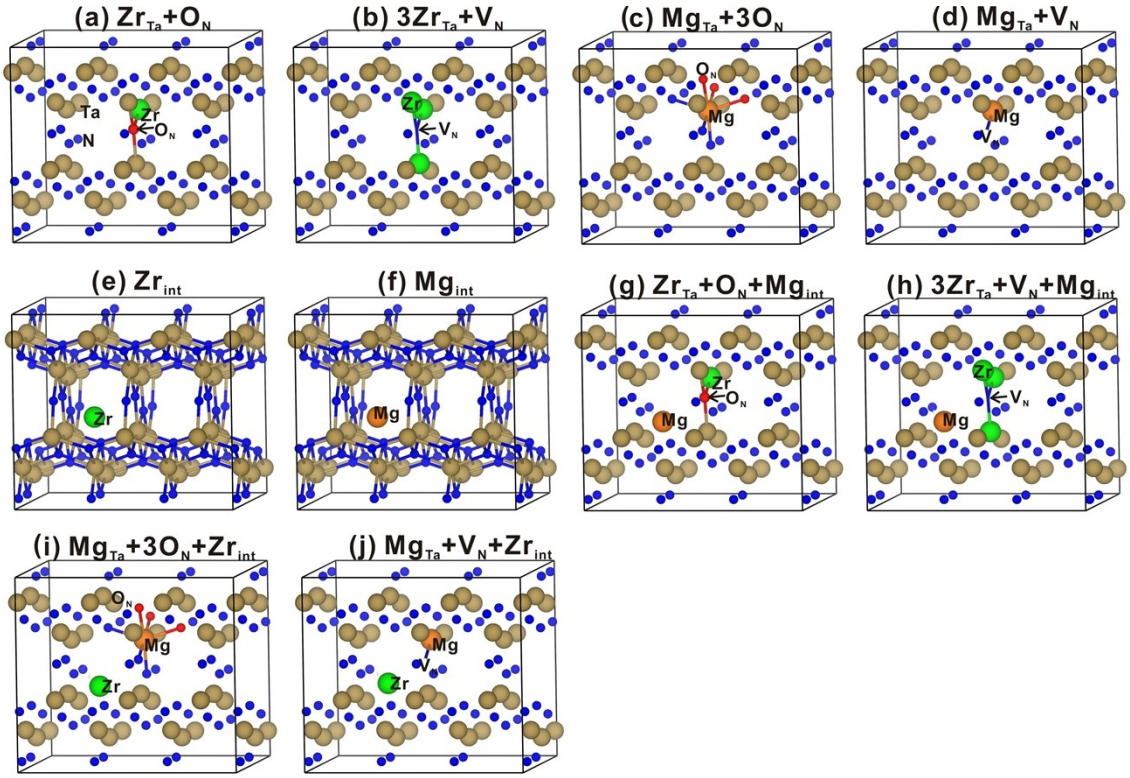


**Fig. S2** Atomic models of elements doped $Ta_3N_5$.

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## The CONTCARs of six doping models are listed below:

**(1) $Zr_{Ta}$+$O_N$**

```
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     0.0000000000000000     10.2498750964167993      0.0000000000000000
     0.0000000000000000      0.0000000000000000     10.2721500396728995
  N     O     Zr    Ta
 59     1     1     35
Direct
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```

| | | |
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**(2) $3Zr_{Ta}+V_N$**

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0.0000000000000000 0.0000000000000000 10.2721500396728995
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Direct
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0.0000000000000000 0.9537164214976670 0.3804429466161565
0.0000000000000000 0.6919846959470632 0.4226030541626571
0.1646568347405193 0.4524676597830677 0.3821010468918615
0.1660877071619424 0.1898921348408180 0.4271561473021634
0.0000000000000000 0.0483380616345528 0.8825730923948285
0.0000000000000000 0.3104117812354801 0.9318431973246035
0.1664353154081653 0.5473503565851985 0.8798318280440256
0.1647244217604609 0.8098031174566529 0.9278325393781799
0.0000000000000000 0.9545596503621070 0.1195500497269464
0.0000000000000000 0.6898924574311422 0.0716930135452927
0.1669417713486538 0.4530512874566028 0.1201005981671415
0.1666623960997597 0.1902132734551358 0.0769463751824375
0.0000000000000000 0.0470668004350969 0.6196935396456453
0.0000000000000000 0.3084361125865414 0.5758355090711191
0.1667084697720966 0.5482387683361551 0.6192000465404703
0.1656006238192518 0.8092155241887227 0.5714742096411811
0.3346778863079223 0.2414520070264743 0.2523399872048913
0.5000000000000000 0.7502522735414416 0.2347026005192703
0.3269016629261117 0.7701182606125769 0.7497309306567672
0.5000000000000000 0.2462898337858519 0.7613619242111156
0.3280327177357023 0.9529036498492047 0.3786821950049841
0.3265952672049295 0.6945795608697978 0.4194867244566041
0.5000000000000000 0.4486565490314121 0.3916607902181042
0.5000000000000000 0.1837339952254311 0.4302240497839591
0.3235692402307677 0.0473298873591261 0.8829968594735789
0.3321162002496081 0.3096786269295251 0.9287803390018183
0.5000000000000000 0.5404758579950126 0.8724451358813852
0.5000000000000000 0.8177690338174770 0.9288427701124959
0.3350544260477619 0.9553571161880683 0.1189574177486961
0.3328830598820076 0.6892960316491923 0.0698827910546882
0.5000000000000000 0.4550923195448391 0.1192938811200932
0.5000000000000000 0.1919391298180031 0.0741568954976444
0.3359880663501826 0.0432600594138393 0.6194063197676414

| | | |
|---|---|---|
| 0.3261234638117401 | 0.3062172257033779 | 0.5819059362001298 |
| 0.5000000000000000 | 0.7932753524254110 | 0.5660911384246674 |
| 0.6653221136920777 | 0.2414520070264743 | 0.2523399872048913 |
| 0.8354738582885943 | 0.7408154554798188 | 0.2449462343081521 |
| 0.6730983370738883 | 0.7701182606125769 | 0.7497309306567672 |
| 0.8358904013644590 | 0.2607092440574377 | 0.7555927039515424 |
| 0.6719672822642977 | 0.9529036498492047 | 0.3786821950049841 |
| 0.6734047327950705 | 0.6945795608697978 | 0.4194867244566041 |
| 0.8353431652594807 | 0.4524676597830677 | 0.3821010468918615 |
| 0.8339122928380576 | 0.1898921348408180 | 0.4271561473021634 |
| 0.6764307597692323 | 0.0473298873591261 | 0.8829968594735789 |
| 0.6678837997503919 | 0.3096786269295251 | 0.9287803390018183 |
| 0.8335646845918347 | 0.5473503565851985 | 0.8798318280440256 |
| 0.8352755782395391 | 0.8098031174566529 | 0.9278325393781799 |
| 0.6649455739522381 | 0.9553571161880683 | 0.1189574177486961 |
| 0.6671169401179924 | 0.6892960316491923 | 0.0698827910546882 |
| 0.8330582286513462 | 0.4530512874566028 | 0.1201005981671415 |
| 0.8333376039002403 | 0.1902132734551358 | 0.0769463751824375 |
| 0.6640119336498174 | 0.0432600594138393 | 0.6194063197676414 |
| 0.6738765361882599 | 0.3062172257033779 | 0.5819059362001298 |
| 0.8332915302279034 | 0.5482387683361551 | 0.6192000465404703 |
| 0.8343993761807482 | 0.8092155241887227 | 0.5714742096411811 |
| 0.5000000000000000 | 0.7070438545517206 | 0.7614170742457560 |
| 0.5000000000000000 | 0.6450130642622298 | 0.4086095289641705 |
| 0.5000000000000000 | 0.3395941828742011 | 0.5573556031383475 |
| 0.0000000000000000 | 0.8050170825357981 | 0.2473375125950596 |
| 0.1672161349385632 | 0.3038302938961976 | 0.2511023048148076 |
| 0.0000000000000000 | 0.1958365156232560 | 0.7524848968984017 |
| 0.1647982829951999 | 0.6980906437923906 | 0.7499990094463129 |
| 0.0000000000000000 | 0.8677575218859488 | 0.9405379234551390 |
| 0.1658250595684549 | 0.3668411531074156 | 0.9387503634036634 |
| 0.0000000000000000 | 0.1331548016809947 | 0.4393106497524215 |
| 0.1646857585779813 | 0.6341596072700924 | 0.4392280590420228 |
| 0.0000000000000000 | 0.8672776210726170 | 0.5601255323756007 |
| 0.1648158356942986 | 0.3665245360414602 | 0.5614555009722721 |
| 0.0000000000000000 | 0.1365948546154812 | 0.0628034760739524 |
| 0.1657719155002582 | 0.6326315395889210 | 0.0607693225847044 |
| 0.3275508178860775 | 0.8061215765500052 | 0.2448929975759313 |
| 0.5000000000000000 | 0.3103597251839076 | 0.2522449058742922 |
| 0.3299617694364585 | 0.1942222788064782 | 0.7531941190373388 |
| 0.3289787599288303 | 0.8675791017248429 | 0.9390723400746310 |
| 0.5000000000000000 | 0.3597730467291385 | 0.9367541941997359 |
| 0.3292990710474228 | 0.1286381703010022 | 0.4411817537835105 |
| 0.3332555592998432 | 0.8607419178698166 | 0.5602707057079854 |
| 0.3329757664188477 | 0.1367780057621530 | 0.0628974633190325 |
| 0.5000000000000000 | 0.6331924191266864 | 0.0570925898246273 |
| 0.6724491821139225 | 0.8061215765500052 | 0.2448929975759313 |
| 0.8327838650614368 | 0.3038302938961976 | 0.2511023048148076 |
| 0.6700382305635415 | 0.1942222788064782 | 0.7531941190373388 |
| 0.8352017170048001 | 0.6980906437923906 | 0.7499990094463129 |
| 0.6710212400711697 | 0.8675791017248429 | 0.9390723400746310 |
| 0.8341749404315451 | 0.3668411531074156 | 0.9387503634036634 |
| 0.6707009289525772 | 0.1286381703010022 | 0.4411817537835105 |
| 0.8353142414220187 | 0.6341596072700924 | 0.4392280590420228 |
| 0.6667444407001568 | 0.8607419178698166 | 0.5602707057079854 |
| 0.8351841643057014 | 0.3665245360414602 | 0.5614555009722721 |
| 0.6670242335811523 | 0.1367780057621530 | 0.0628974633190325 |
| 0.8342280844997418 | 0.6326315395889210 | 0.0607693225847044 |

**(3) $Mg_{Ta}+V_N$**

1.00000000000000

11.6112505410844999 0.0000000000000000 0.0000000000000000

0.0000000000000000 10.2498750964167993 0.0000000000000000

0.0000000000000000 0.0000000000000000 10.2721500396728995

N Mg Ta

59 1 35

Direct

| | | |
|---|---|---|
| 0.0000000000000000 | 0.2403954972972144 | 0.2514733960382287 |
| 0.1651157147151281 | 0.7391869411888194 | 0.2460967971506633 |
| 0.0000000000000000 | 0.7615211160131992 | 0.7497008367878379 |
| 0.1657455437000763 | 0.2599438656779824 | 0.7523031320502582 |
| 0.0000000000000000 | 0.9527923779519227 | 0.3807292272296010 |
| 0.0000000000000000 | 0.6935121541454734 | 0.4250894211641310 |
| 0.1681299365813729 | 0.4525503182468285 | 0.3815181320559020 |
| 0.1664407459845307 | 0.1886932988814962 | 0.4270265062968619 |
| 0.0000000000000000 | 0.0489435921489658 | 0.8821034608957987 |
| 0.0000000000000000 | 0.3100312337032918 | 0.9284732729678637 |
| 0.1663176742289707 | 0.5473305882508797 | 0.8808406514374454 |
| 0.1644636844137537 | 0.8115580285994284 | 0.9264155125803839 |
| 0.0000000000000000 | 0.9546657676483719 | 0.1201773652349090 |
| 0.0000000000000000 | 0.6903269118844264 | 0.0713641816774668 |
| 0.1660547863217872 | 0.4526013601025838 | 0.1196898747301915 |
| 0.1674709416109081 | 0.1909545688666938 | 0.0754738329816078 |
| 0.0000000000000000 | 0.0465161570009087 | 0.6192915941311199 |
| 0.0000000000000000 | 0.3098585103800033 | 0.5748410888366067 |
| 0.1644470050260907 | 0.5475612594101662 | 0.6196438204780961 |
| 0.1672241574156672 | 0.8096508434787921 | 0.5743170418669337 |
| 0.3361821693955704 | 0.2426602286323458 | 0.2516063648051343 |
| 0.5000000000000000 | 0.7426162207972311 | 0.2365620237161963 |
| 0.3307636282745321 | 0.7623929966963416 | 0.7534114778372540 |
| 0.5000000000000000 | 0.2534138520213958 | 0.7527944937876114 |
| 0.3320241564158124 | 0.9504339611675334 | 0.3788669035517671 |
| 0.3294099340766863 | 0.6948914029278939 | 0.4230269057681326 |
| 0.5000000000000000 | 0.4471203133882469 | 0.3958620864766402 |
| 0.5000000000000000 | 0.1826435199134266 | 0.4296743216680099 |
| 0.3279069170994120 | 0.0482628697631995 | 0.8826115783537389 |
| 0.3332606970457448 | 0.3117215864027401 | 0.9254817115146494 |
| 0.5000000000000000 | 0.5460284503223747 | 0.8566167041029686 |
| 0.5000000000000000 | 0.8181696512423358 | 0.9289353018708582 |
| 0.3343825593767633 | 0.9547282847580192 | 0.1208787001972595 |
| 0.3316518433010529 | 0.6901517502188810 | 0.0690495963841826 |
| 0.5000000000000000 | 0.4580372049639436 | 0.1119368406353232 |
| 0.5000000000000000 | 0.1949457246111663 | 0.0705749691566950 |
| 0.3344496172116251 | 0.0438868510275796 | 0.6182616661946980 |
| 0.3318026230815221 | 0.3128610407210388 | 0.5782794275220411 |
| 0.5000000000000000 | 0.7914364814660786 | 0.5798589406383101 |
| 0.6638178306044296 | 0.2426602286323458 | 0.2516063648051343 |
| 0.8348842852848719 | 0.7391869411888194 | 0.2460967971506633 |
| 0.6692363717254679 | 0.7623929966963416 | 0.7534114778372540 |
| 0.8342544562999237 | 0.2599438656779824 | 0.7523031320502582 |
| 0.6679758435841876 | 0.9504339611675334 | 0.3788669035517671 |
| 0.6705900659233137 | 0.6948914029278939 | 0.4230269057681326 |
| 0.8318700634186271 | 0.4525503182468285 | 0.3815181320559020 |
| 0.8335592540154693 | 0.1886932988814962 | 0.4270265062968619 |
| 0.6720930829005880 | 0.0482628697631995 | 0.8826115783537389 |
| 0.6667393029542552 | 0.3117215864027401 | 0.9254817115146494 |

0.8336823257710293 0.5473305882508797 0.8808406514374454
0.8355363155862463 0.8115580285994284 0.9264155125803839
0.6656174406232367 0.9547282847580192 0.1208787001972595
0.6683481566989471 0.6901517502188810 0.0690495963841826
0.8339452136782128 0.4526013601025838 0.1196898747301915
0.8325290583890919 0.1909545688666938 0.0754738329816078
0.6655503827883749 0.0438868510275796 0.6182616661946980
0.6681973769184779 0.3128610407210388 0.5782794275220411
0.8355529949739093 0.5475612594101662 0.6196438204780961
0.8327758425843328 0.8096508434787921 0.5743170418669337
0.5000000000000000 0.6423864585518260 0.4206089187283979
0.0000000000000000 0.8030174718444272 0.2497549587508274
0.1680304069065741 0.3041210261612051 0.2502347602142194
0.0000000000000000 0.1962412901029253 0.7499776082128164
0.1652252320737517 0.6972422899062565 0.7504050497918726
0.0000000000000000 0.8696800047313218 0.9414737372422479
0.1664269199037207 0.3661040960511244 0.9381799761924228
0.0000000000000000 0.1316696709605409 0.4394287542853021
0.1676584411063615 0.6345080869678767 0.4390070707081080
0.0000000000000000 0.8643458456066639 0.5612324959323658
0.1660213651928899 0.3675588894557791 0.5610782590332306
0.0000000000000000 0.1368907090850655 0.0631832833928812
0.1652405165005817 0.6325989545865056 0.0613719909367489
0.3315888768878210 0.7992893794879379 0.2509472396162522
0.5000000000000000 0.3184385069254461 0.2486061863636877
0.3315144733600306 0.1946021667757591 0.7518560604336386
0.5000000000000000 0.7138548560261810 0.7689271511475511
0.3265121657605832 0.8698579949338310 0.9433895464793309
0.5000000000000000 0.3669700828815508 0.9291327650946073
0.3276189185620382 0.1252476025411084 0.4410462889156292
0.3361064205613857 0.8561575692674310 0.5597503664152512
0.5000000000000000 0.3327521820736123 0.5432098328207999
0.3350531532729519 0.1363972902112494 0.0646298480321548
0.5000000000000000 0.6423684099793263 0.0661205896588086
0.6684111231121790 0.7992893794879379 0.2509472396162522
0.8319695930934259 0.3041210261612051 0.2502347602142194
0.6684855266399694 0.1946021667757591 0.7518560604336386
0.8347747679262483 0.6972422899062565 0.7504050497918726
0.6734878342394168 0.8698579949338310 0.9433895464793309
0.8335730800962793 0.3661040960511244 0.9381799761924228
0.6723810814379618 0.1252476025411084 0.4410462889156292
0.8323415588936385 0.6345080869678767 0.4390070707081080
0.6638935794386143 0.8561575692674310 0.5597503664152512
0.8339786348071101 0.3675588894557791 0.5610782590332306
0.6649468467270481 0.1363972902112494 0.0646298480321548
0.8347594834994183 0.6325989545865056 0.0613719909367489

**(4) $Mg_{Ta}+3O_N$**

1.00000000000000
11.6112505410844999 0.0000000000000000 0.0000000000000000
0.0000000000000000 10.2498750964167993 0.0000000000000000
0.0000000000000000 0.0000000000000000 10.2721500396728995
N O Mg Ta
57 3 1 35
Direct
0.0000869523737919 0.2387156309324681 0.2493978286145122
0.1649219914931663 0.7441169882278942 0.2491613398068466
0.9993042990591476 0.7602999274982096 0.7502151373793282

| | | |
|---|---|---|
| 0.1667891121340759 | 0.2607392325205282 | 0.7492129420202218 |
| 0.0005940274506102 | 0.9537027889322687 | 0.3812960445653957 |
| 0.9993693042232863 | 0.6894414964937639 | 0.4258267125118778 |
| 0.1733224844840038 | 0.4541145886003832 | 0.3803948306081324 |
| 0.1662326171669406 | 0.1927002115633414 | 0.4269165712261866 |
| 0.0011319550678408 | 0.0474123297042794 | 0.8802673073084577 |
| 0.0002634114379632 | 0.3107642188822197 | 0.9250074134239270 |
| 0.1722790934653986 | 0.5468287134968648 | 0.8808767458293403 |
| 0.1672053574511736 | 0.8091957419586677 | 0.9265670373900008 |
| 0.9980175945362930 | 0.9534620919508257 | 0.1183507987274339 |
| 0.9991492729630451 | 0.6907478498081900 | 0.0739470452114261 |
| 0.1604054363136385 | 0.4531923700065974 | 0.1189837959080435 |
| 0.1667556857349553 | 0.1908787216446015 | 0.0729357419787320 |
| 0.9976873521400336 | 0.0480993668840668 | 0.6193345930728213 |
| 0.9999315115950793 | 0.3103473080459196 | 0.5728066244260646 |
| 0.1625942416898098 | 0.5486430492404608 | 0.6188769456283296 |
| 0.1654134491429957 | 0.8141826582100506 | 0.5760278471039797 |
| 0.3328588548992286 | 0.2390556347337736 | 0.2487779599194369 |
| 0.3351690186459777 | 0.7593186177693880 | 0.7459783490885172 |
| 0.5001633501411504 | 0.2564101499791605 | 0.7520660867910394 |
| 0.3234217314738075 | 0.9539826858690290 | 0.3795588302406756 |
| 0.3322023490224240 | 0.6975112030266715 | 0.4266031143588549 |
| 0.5009385219848070 | 0.4438249095229239 | 0.3806482249322229 |
| 0.4997575173038484 | 0.1780941026474636 | 0.4240838403351361 |
| 0.3305502951246595 | 0.0458109919407406 | 0.8811424747891721 |
| 0.3329207344885106 | 0.3090305013388601 | 0.9256007687571568 |
| 0.4970811174796026 | 0.5452205836995461 | 0.8840424515993988 |
| 0.4994673677069699 | 0.8089847215987405 | 0.9302776886877666 |
| 0.3371456309181653 | 0.9519139109132766 | 0.1197383830560241 |
| 0.3338964955294514 | 0.6868543074597184 | 0.0810389819671116 |
| 0.5026612617723316 | 0.4509985097125835 | 0.1187601335961759 |
| 0.5003562639224342 | 0.1883451020352638 | 0.0695207934323889 |
| 0.3368939833973670 | 0.0458204441411212 | 0.6186146394070988 |
| 0.3339941016406698 | 0.3111195022101683 | 0.5746766702832602 |
| 0.5043656496964743 | 0.5472466902597120 | 0.6257223193895811 |
| 0.6676685996524867 | 0.2357652839228805 | 0.2494046416927276 |
| 0.8318703296744232 | 0.7431584295732918 | 0.2509655904204422 |
| 0.6645288672488618 | 0.7608385057091525 | 0.7485181310858664 |
| 0.8334588378612793 | 0.2629977278185791 | 0.7492029601945021 |
| 0.6634455087397839 | 0.9496430861186838 | 0.3841187312116787 |
| 0.8327312070966855 | 0.4537884790699067 | 0.3798902570554503 |
| 0.8339522744006871 | 0.1918063327917423 | 0.4259910920913228 |
| 0.6629791812790486 | 0.0463534460271475 | 0.8805247546611312 |
| 0.6674334140011453 | 0.3090656187310898 | 0.9259570027649744 |
| 0.8317667544649723 | 0.5472786594711394 | 0.8806084607956137 |
| 0.8322029106415556 | 0.8102313537514263 | 0.9253045929156158 |
| 0.6720209089776219 | 0.9531284879725064 | 0.1192410400329962 |
| 0.6654645066393314 | 0.6887333034122847 | 0.0770087754560151 |
| 0.8342472066524422 | 0.4533857923323836 | 0.1191664358816809 |
| 0.8338391240577110 | 0.1919014332752269 | 0.0719437058575565 |
| 0.6742489475214200 | 0.0467315179311001 | 0.6208610178417899 |
| 0.6660406158922214 | 0.3064766059351243 | 0.5723339701255057 |
| 0.8310408061271417 | 0.5478016123169382 | 0.6182097164233795 |
| 0.8322215590096178 | 0.8107976402158030 | 0.5729752824329566 |
| 0.5024863350271502 | 0.7466448784043322 | 0.2488199206679269 |
| 0.5015117781568321 | 0.8179881818335275 | 0.5743365736822099 |
| 0.6684685646501123 | 0.6921149812147362 | 0.4242717574558412 |
| 0.5020859395700441 | 0.6355029316203087 | 0.4355084388358321 |

0.9991118572327906 0.8053445417689176 0.2496153779170314
0.1677028035445005 0.3038131551665160 0.2502397598210493
0.0004071226591833 0.1982152927100813 0.7490106858555592
0.1675864552649813 0.6966675454331863 0.7517958036216115
0.9994669121969935 0.8663753491698571 0.9378907680300372
0.1674666906987667 0.3644741957275244 0.9394262205600796
0.0001542198270954 0.1359146635581041 0.4384069900754568
0.1690066205618095 0.6334632528857682 0.4401183122324142
0.9989468113980777 0.8684835142761855 0.5609297841645713
0.1680878233949628 0.3666154179803769 0.5615163116571793
0.0005814769921315 0.1342958443355187 0.0602939402634775
0.1664551913262073 0.6331471284493375 0.0597719934537650
0.3283735011425506 0.8008050397781332 0.2555292583886697
0.4994608371038964 0.3049803938218645 0.2566554367291332
0.3346323364879282 0.1949993724226928 0.7484528288058954
0.4994939203834434 0.6868062384485611 0.7498702436360603
0.3346327638376607 0.8670113059526656 0.9413882439559842
0.4993322364347392 0.3605783561016693 0.9403004293493566
0.3332604327364592 0.1327243012482313 0.4411454549820419
0.3295624792872545 0.8622965736333441 0.5583172428547201
0.4998672304461778 0.3745592597428882 0.5571439431252401
0.3345183063442647 0.1324241693936514 0.0628846925082556
0.4991487783800466 0.6297146133101066 0.0583606555921889
0.6700656844320747 0.8077983251561420 0.2457518378536676
0.8336824678257457 0.3029023389459908 0.2497540659457371
0.6656992774441264 0.1979087777922786 0.7491013279057555
0.8326800872069171 0.6965048938343514 0.7509709391706778
0.6642692875405345 0.8659234829090252 0.9369297727107337
0.8339549618140296 0.3648744307316534 0.9389277264379245
0.6654517402304236 0.1348623778938176 0.4363685726959687
0.8349777614767291 0.6325130756279478 0.4397490003515969
0.6693576931856597 0.8704026308496609 0.5644039473355917
0.8324517705094223 0.3651603106428851 0.5612009432022731
0.6663432978138246 0.1352844685941790 0.0595975414606613
0.8327955904249151 0.6328932187978040 0.0597620843945563

**(5) $Zr_{int}$**

1.00000000000000
11.6112505410844999 0.0000000000000000 0.0000000000000000
0.0000000000000000 10.2498750964167993 0.0000000000000000
0.0000000000000000 0.0000000000000000 10.2721500396728995
N Zr Ta
60 1 36
Direct
0.9996316422812868 0.2380217194916057 0.2500000000000000
0.1669460264475831 0.7365014624105015 0.2500000000000000
0.0010630623167032 0.7601068820978014 0.7500000000000000
0.1707377661000251 0.2676724054042907 0.7500000000000000
0.0002550648234916 0.9504798106691510 0.3803322754792902
0.0006220923055977 0.6898441900931758 0.4287381493909734
0.1626438972847168 0.4552744620945148 0.3776689777907194
0.1662762959738302 0.1919141047554689 0.4272230303386166
0.0025127094455470 0.0474013759650163 0.8814182207689996
0.9988846508529505 0.3121366209735612 0.9242798859152970
0.1862987884301148 0.5453511495670185 0.8787110805620912
0.1671847019978046 0.8082178414580525 0.9273550024033383
0.0002550648234916 0.9504798106691510 0.1196677245207098
0.0006220923055977 0.6898441900931758 0.0712618506090266

| | | |
|---|---|---|
| 0.1626438972847168 | 0.4552744620945148 | 0.1223310222092806 |
| 0.1662762959738302 | 0.1919141047554689 | 0.0727769696613834 |
| 0.0025127094455470 | 0.0474013759650163 | 0.6185817792310004 |
| 0.9988846508529505 | 0.3121366209735612 | 0.5757201140847030 |
| 0.1862987884301148 | 0.5453511495670185 | 0.6212889194379088 |
| 0.1671847019978046 | 0.8082178414580525 | 0.5726449975966617 |
| 0.3333339936215367 | 0.2424812775311835 | 0.2500000000000000 |
| 0.4997194003887842 | 0.7364967395879631 | 0.2500000000000000 |
| 0.3333335739821734 | 0.7738724095679359 | 0.7500000000000000 |
| 0.4959306372490673 | 0.2676678652875637 | 0.7500000000000000 |
| 0.3333344942892609 | 0.9560247258465395 | 0.3768312421342870 |
| 0.3333324503619579 | 0.6925487463224300 | 0.4247373559096204 |
| 0.5040251717796238 | 0.4552735280663285 | 0.3776713142882997 |
| 0.5003903568865908 | 0.1919151544229294 | 0.4272245353059603 |
| 0.3333336099728399 | 0.0444084595785128 | 0.8842098831056902 |
| 0.3333325686141393 | 0.3172494003873041 | 0.9235129351057196 |
| 0.4803615066939670 | 0.5453493945623364 | 0.8787101251857479 |
| 0.4994816883039164 | 0.8082142359495421 | 0.9273552397685947 |
| 0.3333344942892609 | 0.9560247258465395 | 0.1231687578657130 |
| 0.3333324503619579 | 0.6925487463224300 | 0.0752626440903796 |
| 0.5040251717796238 | 0.4552735280663285 | 0.1223286857117003 |
| 0.5003903568865908 | 0.1919151544229294 | 0.0727754646940397 |
| 0.3333336099728399 | 0.0444084595785128 | 0.6157901168943098 |
| 0.3333325686141393 | 0.3172494003873041 | 0.5764870648942804 |
| 0.4803615066939670 | 0.5453493945623364 | 0.6212898748142521 |
| 0.4994816883039164 | 0.8082142359495421 | 0.5726447602314053 |
| 0.6670336588130610 | 0.2380203382887416 | 0.2500000000000000 |
| 0.8333328707638330 | 0.7365812477818992 | 0.2500000000000000 |
| 0.6656029140267350 | 0.7601050077795009 | 0.7500000000000000 |
| 0.8333338838216520 | 0.2560801306040119 | 0.7500000000000000 |
| 0.6664089918602514 | 0.9504788622195832 | 0.3803319911600838 |
| 0.6660436949181374 | 0.6898432063417630 | 0.4287382803423654 |
| 0.8333328739037142 | 0.4524080707389757 | 0.3812080299275777 |
| 0.8333326034175030 | 0.1882120594929049 | 0.4268181108416726 |
| 0.6641545226531562 | 0.0474000434237638 | 0.8814184840003563 |
| 0.6677818997476734 | 0.3121371073128358 | 0.9242786570200749 |
| 0.8333337168917012 | 0.5481633466282290 | 0.8804249702375060 |
| 0.8333329799926190 | 0.8097832661457929 | 0.9267558521546349 |
| 0.6664089918602514 | 0.9504788622195832 | 0.1196680088399162 |
| 0.6660436949181374 | 0.6898432063417630 | 0.0712617196576346 |
| 0.8333328739037142 | 0.4524080707389757 | 0.1187919700724223 |
| 0.8333326034175030 | 0.1882120594929049 | 0.0731818891583274 |
| 0.6641545226531562 | 0.0474000434237638 | 0.6185815159996437 |
| 0.6677818997476734 | 0.3121371073128358 | 0.5757213429799251 |
| 0.8333337168917012 | 0.5481633466282290 | 0.6195750297624940 |
| 0.8333329799926190 | 0.8097832661457929 | 0.5732441478453651 |
| 0.3333268593640994 | 0.4589077019324819 | 0.7500000000000000 |
| 0.0003750099737019 | 0.7998555508371368 | 0.2500000000000000 |
| 0.1662044237108233 | 0.3013961025526726 | 0.2500000000000000 |
| 0.0010090286693014 | 0.1983289143609355 | 0.7500000000000000 |
| 0.1704806413800881 | 0.7023305255041734 | 0.7500000000000000 |
| 0.9999921592845453 | 0.8635188865046572 | 0.9362745194979638 |
| 0.1617720672667105 | 0.3618503830413786 | 0.9511856472193898 |
| 0.9981632597363799 | 0.1292388029489118 | 0.4381009657106461 |
| 0.1671250512647475 | 0.6362501230954294 | 0.4385099953956342 |
| 0.9999921592845453 | 0.8635188865046572 | 0.5637254805020362 |
| 0.1617720672667105 | 0.3618503830413786 | 0.5488143527806102 |
| 0.9981632597363799 | 0.1292388029489118 | 0.0618990342893539 |

0.1671250512647475 0.6362501230954294 0.0614900046043658
0.3333325360917314 0.8030594385667982 0.2500000000000000
0.5004627136633957 0.3013974735056522 0.2500000000000000
0.3333334609108647 0.1866797459183260 0.7500000000000000
0.4961858676587809 0.7023289923516955 0.7500000000000000
0.3333331637112238 0.8640026080717078 0.9431645369850159
0.5048939585098964 0.3618498763955103 0.9511821382797478
0.3333334595976822 0.1330967036816730 0.4416034263586042
0.4995398587130637 0.6362503389435545 0.4385091908783636
0.3333331637112238 0.8640026080717078 0.5568354630149841
0.5048939585098964 0.3618498763955103 0.5488178617202522
0.3333334595976822 0.1330967036816730 0.0583965736413958
0.4995398587130637 0.6362503389435545 0.0614908091216364
0.6662906965500994 0.7998541359383751 0.2500000000000000
0.8333328906585962 0.3021923353734337 0.2500000000000000
0.6656584779178445 0.1983271532480870 0.7500000000000000
0.8333334113282618 0.6984974164698912 0.7500000000000000
0.6666742993231409 0.8635176043876385 0.9362748658024245
0.8333332640800748 0.3687740280145633 0.9391795374992071
0.6685023025471466 0.1292378433214907 0.4381008693543080
0.8333330979536200 0.6355321529488620 0.4373225638650311
0.6666742993231409 0.8635176043876385 0.5637251341975755
0.8333332640800748 0.3687740280145633 0.5608204625007929
0.6685023025471466 0.1292378433214907 0.0618991306456920
0.8333330979536200 0.6355321529488620 0.0626774361349689

**(6) $Mg_{int}$**

1.00000000000000
11.6112505410844999 0.0000000000000000 0.0000000000000000
0.0000000000000000 10.2498750964167993 0.0000000000000000
0.0000000000000000 0.0000000000000000 10.2721500396728995
N Mg Ta
60 1 36
Direct
0.0006043972653202 0.2392422419552958 0.2500000000000000
0.1670053615798324 0.7348597172867031 0.2500000000000000
0.9982673687755437 0.7615579117635320 0.7500000000000000
0.1666115786338764 0.2568660289567717 0.7500000000000000
0.0011795970037412 0.9516243257203882 0.3799625409633975
0.0005065557047388 0.6897023851557833 0.4277384801553197
0.1622204100052613 0.4535347807038903 0.3814271313382207
0.1674874568254623 0.1914274092319772 0.4277119035547514
0.9995108840003155 0.0467137343422976 0.8818291896161270
0.9995348006317641 0.3113501812808011 0.9251746877682052
0.1832005155413299 0.5462636133891294 0.8774798568077244
0.1660606270561686 0.8079309815400606 0.9265977159057641
0.0011795970037412 0.9516243257203882 0.1200374590366025
0.0005065557047388 0.6897023851557833 0.0722615198446803
0.1622204100052613 0.4535347807038903 0.1185728686617793
0.1674874568254623 0.1914274092319772 0.0722880964452486
0.9995108840003155 0.0467137343422976 0.6181708103838730
0.9995348006317641 0.3113501812808011 0.5748253122317948
0.1832005155413299 0.5462636133891294 0.6225201431922756
0.1660606270561686 0.8079309815400606 0.5734022840942359
0.3333330524040434 0.2408307767521265 0.2500000000000000
0.4996608463043941 0.7348593092552349 0.2500000000000000
0.3333330040917630 0.7590940296175432 0.7500000000000000
0.5000537982797724 0.2568654713293341 0.7500000000000000

| | | |
|---|---|---|
| 0.3333331747885424 | 0.9521266352167004 | 0.3793388217129703 |
| 0.3333329805038758 | 0.6922104743201558 | 0.4267447712022587 |
| 0.5044455438762725 | 0.4535349774002242 | 0.3814270031822815 |
| 0.4991785250994454 | 0.1914273739789891 | 0.4277120608820155 |
| 0.3333326828514203 | 0.0451712284388890 | 0.8830900585735932 |
| 0.3333328423384287 | 0.3162901168605643 | 0.9182280147513140 |
| 0.4834646738400252 | 0.5462636015076541 | 0.8774797744291192 |
| 0.5006053782018967 | 0.8079310876183570 | 0.9265974956779530 |
| 0.3333331747885424 | 0.9521266352167004 | 0.1206611782870297 |
| 0.3333329805038758 | 0.6922104743201558 | 0.0732552287977413 |
| 0.5044455438762725 | 0.4535349774002242 | 0.1185729968177185 |
| 0.4991785250994454 | 0.1914273739789891 | 0.0722879391179845 |
| 0.3333326828514203 | 0.0451712284388890 | 0.6169099414264068 |
| 0.3333328423384287 | 0.3162901168605643 | 0.5817719852486860 |
| 0.4834646738400252 | 0.5462636015076541 | 0.6225202255708808 |
| 0.5006053782018967 | 0.8079310876183570 | 0.5734025043220470 |
| 0.6660615712936604 | 0.2392425254214245 | 0.2500000000000000 |
| 0.8333331478427652 | 0.7384196615406111 | 0.2500000000000000 |
| 0.6683985513411699 | 0.7615576772901775 | 0.7500000000000000 |
| 0.8333327907776109 | 0.2597562533634843 | 0.7500000000000000 |
| 0.6654864982502389 | 0.9516242301688820 | 0.3799625005251599 |
| 0.6661595475107092 | 0.6897022948615827 | 0.4277385970879664 |
| 0.8333330987826315 | 0.4523235428165080 | 0.3809610252172178 |
| 0.8333329648637857 | 0.1886214910974218 | 0.4257518842584602 |
| 0.6671557411097098 | 0.0467136928969936 | 0.8818291889621150 |
| 0.6671308707372887 | 0.3113504349482454 | 0.9251744734443079 |
| 0.8333330802278809 | 0.5478392044558902 | 0.8808109347066946 |
| 0.8333329757482417 | 0.8087168621172438 | 0.9283477181817830 |
| 0.6654864982502389 | 0.9516242301688820 | 0.1200374994748401 |
| 0.6661595475107092 | 0.6897022948615827 | 0.0722614029120336 |
| 0.8333330987826315 | 0.4523235428165080 | 0.1190389747827822 |
| 0.8333329648637857 | 0.1886214910974218 | 0.0742481157415398 |
| 0.6671557411097098 | 0.0467136928969936 | 0.6181708110378850 |
| 0.6671308707372887 | 0.3113504349482454 | 0.5748255265556921 |
| 0.8333330802278809 | 0.5478392044558902 | 0.6191890652933054 |
| 0.8333329757482417 | 0.8087168621172438 | 0.5716522818182170 |
| 0.3333334134424391 | 0.4954415680162114 | 0.7500000000000000 |
| 0.9999872446319102 | 0.8004783601516934 | 0.2500000000000000 |
| 0.1660688240736548 | 0.3037630635186233 | 0.2500000000000000 |
| 0.9995754101408636 | 0.1962779779758392 | 0.7500000000000000 |
| 0.1633361678731973 | 0.7042273908766461 | 0.7500000000000000 |
| 0.9986130397226489 | 0.8647375811528946 | 0.9390842707422351 |
| 0.1647207100912951 | 0.3639247405202326 | 0.9423293893675364 |
| 0.9995588070967969 | 0.1317360481728187 | 0.4386919506579758 |
| 0.1668125070012678 | 0.6359386918865937 | 0.4378740507216321 |
| 0.9986130397226489 | 0.8647375811528946 | 0.5609157292577649 |
| 0.1647207100912951 | 0.3639247405202326 | 0.5576706106324636 |
| 0.9995588070967969 | 0.1317360481728187 | 0.0613080493420242 |
| 0.1668125070012678 | 0.6359386918865937 | 0.0621259492783679 |
| 0.3333332942735083 | 0.7997986030473569 | 0.2500000000000000 |
| 0.5005973179234218 | 0.3037630788150523 | 0.2500000000000000 |
| 0.3333328227931531 | 0.1898281988336805 | 0.7500000000000000 |
| 0.5033297293855910 | 0.7042272624158343 | 0.7500000000000000 |
| 0.3333330581893748 | 0.8619613817021872 | 0.9395168903914737 |
| 0.5019450758941204 | 0.3639245208416213 | 0.9423297445201584 |
| 0.3333329866336570 | 0.1304918852283379 | 0.4377019403132678 |
| 0.4998534143193325 | 0.6359387712824329 | 0.4378743254768267 |
| 0.3333330581893748 | 0.8619613817021872 | 0.5604831096085263 |

0.5019450758941204 0.3639245208416213 0.5576702554798416
0.3333329866336570 0.1304918852283379 0.0622980596867322
0.4998534143193325 0.6359387712824329 0.0621256745231733
0.6666788899378773 0.8004779629009349 0.2500000000000000
0.8333329997643446 0.3023366545841952 0.2500000000000000
0.6670903700204391 0.1962780087337492 0.7500000000000000
0.8333330531681327 0.6972655531645628 0.7500000000000000
0.6680530573281587 0.8647374191438928 0.9390842547768088
0.8333329122717998 0.3675592626237503 0.9391327842524433
0.6671073415815343 0.1317357600968023 0.4386920702382895
0.8333331585960480 0.6347916340639159 0.4372898393642402
0.6680530573281587 0.8647374191438928 0.5609157452231912
0.8333329122717998 0.3675592626237503 0.5608672157475567
0.6671073415815343 0.1317357600968023 0.0613079297617105
0.8333331585960480 0.6347916340639159 0.0627101606357598

**(7) $Zr_{Ta}+O_N+Mg_{int}$**

1.00000000000000
11.6112505410844999 0.0000000000000000 0.0000000000000000
0.0000000000000000 10.2498750964167993 0.0000000000000000
0.0000000000000000 0.0000000000000000 10.2721500396728995
N O Mg Zr Ta
59 1 1 1 35
Direct
0.0003824203494786 0.2343102241618857 0.2503554000355481
0.1659341801836735 0.7316594274195929 0.2478249381786850
0.9983178942918067 0.7642641954515735 0.7509063066604265
0.1662294020494665 0.2616784742679828 0.7502800945756227
0.0013333819329918 0.9529146330101880 0.3790251042941413
0.0007701824668127 0.6924445150769084 0.4278888281096340
0.1622605912132176 0.4536327019021765 0.3796344227223964
0.1670554298338071 0.1932793707977837 0.4296523772830529
0.9991809946840432 0.0474815301226727 0.8807536516264955
0.9995269423307115 0.3098498215603229 0.9260328365219033
0.1833026131200418 0.5455386211192917 0.8768661108938878
0.1658098157560140 0.8091852968354348 0.9258329742439817
0.0015585398497866 0.9530930520013520 0.1206013994689308
0.0007582339469566 0.6903308080246349 0.0694888924299266
0.1618037329614218 0.4530136228729747 0.1202480334442951
0.1673889912967964 0.1933960437217027 0.0709760798442578
0.9993667554253790 0.0472320716084893 0.6193731209620869
0.9995255332837379 0.3102879538414803 0.5744366177263351
0.1829457361602230 0.5464265057622671 0.6224158506998958
0.1656928667634777 0.8090024036781749 0.5761548789089677
0.3336908526133318 0.2353974452473217 0.2505418401019562
0.4993969774217867 0.7386884944961303 0.2439188145350367
0.3330611940273716 0.7595826370269829 0.7509636457910366
0.5001065778689945 0.2580771075230169 0.7510740399588580
0.3328058587584685 0.9538293367865119 0.3783117440940288
0.3284264807335982 0.6986985370943649 0.4256666255927817
0.5081014944184671 0.4435410488020058 0.3831956981419221
0.4990354864271906 0.1896654347085153 0.4327496640209570
0.3320986985308368 0.0455356425967953 0.8820879465943406
0.3332557549048560 0.3151853752782709 0.9190412108033115
0.4847868495297753 0.5455601348287736 0.8755785777767218
0.5005624852525871 0.8098658221610617 0.9252239862321017
0.3321563806665165 0.9541732650075667 0.1205372160160644
0.3331347586932658 0.6927545675799601 0.0710652878088774

| | | |
|---|---|---|
| 0.5031507922212635 | 0.4527329485997567 | 0.1197591770247638 |
| 0.4993638356394455 | 0.1925262849579824 | 0.0691826653996049 |
| 0.3321928074616775 | 0.0450689096724737 | 0.6181933667159502 |
| 0.3325401788535334 | 0.3162519526502784 | 0.5826584861915236 |
| 0.5005273728713694 | 0.8065821753002982 | 0.5788874990955453 |
| 0.6660243269896770 | 0.2323384696808789 | 0.2504508097588630 |
| 0.8349708522973928 | 0.7352681080562130 | 0.2477017763216292 |
| 0.6686556054376129 | 0.7615384840185175 | 0.7509969987655518 |
| 0.8336944827802378 | 0.2638077595777260 | 0.7501809796839856 |
| 0.6658901421077786 | 0.9530550556798245 | 0.3784177078628711 |
| 0.6714012027681807 | 0.6963818465139141 | 0.4259162375624837 |
| 0.8331605311595142 | 0.4523760536236920 | 0.3795789916044155 |
| 0.8335428438427742 | 0.1907860401693564 | 0.4288046367499194 |
| 0.6689521899889966 | 0.0465948183117138 | 0.8805334220867356 |
| 0.6674003617661520 | 0.3096842762935303 | 0.9256780167659495 |
| 0.8338976978593052 | 0.5466808643690975 | 0.8801166456894394 |
| 0.8336363906452928 | 0.8092327503789465 | 0.9276180817335213 |
| 0.6665235465894005 | 0.9530280610098104 | 0.1200009736601288 |
| 0.6663424724742986 | 0.6893189051340131 | 0.0703654383959940 |
| 0.8334309721507464 | 0.4518048987139980 | 0.1206004624297088 |
| 0.8334553246242499 | 0.1909599115682198 | 0.0720573436368153 |
| 0.6680108293585242 | 0.0461164177673416 | 0.6194176707921865 |
| 0.6678374981132453 | 0.3108715187139964 | 0.5759863046502183 |
| 0.8344540376400789 | 0.5476079338560478 | 0.6192886719276871 |
| 0.8337468610329390 | 0.8094165082523825 | 0.5745326663925808 |
| 0.4765765099306140 | 0.5407978701960947 | 0.6261615183270015 |
| 0.3322025073665497 | 0.4926832920221194 | 0.7490300842939652 |
| 0.4998099206225463 | 0.6369968784846656 | 0.4333701308177010 |
| 0.0002370372207256 | 0.8014959116789706 | 0.2483973846804637 |
| 0.1664243416755638 | 0.3019168983926006 | 0.2502442860753241 |
| 0.9994911833610344 | 0.1965804275151134 | 0.7500479514605720 |
| 0.1629637901806554 | 0.7036749004463148 | 0.7505975334370434 |
| 0.9986757155586645 | 0.8675992718799291 | 0.9410375586394831 |
| 0.1644615381672659 | 0.3634572827556911 | 0.9429421323330536 |
| 0.9995121910802593 | 0.1333393027072900 | 0.4391491885509974 |
| 0.1659347160395820 | 0.6348215418926096 | 0.4393567299342912 |
| 0.9986685526126102 | 0.8672497365547447 | 0.5587356829143724 |
| 0.1641965689924464 | 0.3641014074901598 | 0.5564739539681314 |
| 0.9996039816300530 | 0.1343376461202893 | 0.0610032058011140 |
| 0.1665925778291912 | 0.6333204302569915 | 0.0609224900303281 |
| 0.3315994943885064 | 0.8016646025531308 | 0.2487483507668055 |
| 0.5007130996173297 | 0.3010963803943646 | 0.2503099560892333 |
| 0.3326660094113965 | 0.1897668657297654 | 0.7502568844751141 |
| 0.5033932266306096 | 0.7049550525555781 | 0.7573825497507842 |
| 0.3316290051869000 | 0.8651221267265159 | 0.9420237593252914 |
| 0.5021812978230936 | 0.3621375096428612 | 0.9425464822011032 |
| 0.3316554429359467 | 0.1309370285324349 | 0.4400382267759108 |
| 0.3334506760442145 | 0.8624739010670395 | 0.5583158919376127 |
| 0.5024317084663050 | 0.3539526636987445 | 0.5525812524643243 |
| 0.3331667651927265 | 0.1335999683957479 | 0.0609647132144171 |
| 0.4999412444862872 | 0.6338701658127202 | 0.0624039560177027 |
| 0.6685414177651755 | 0.8012255878688909 | 0.2486506629088679 |
| 0.8331010808269999 | 0.3008683326492332 | 0.2504484780457016 |
| 0.6678665799748660 | 0.1954169636054078 | 0.7507110841803268 |
| 0.8339904947876421 | 0.6964148197335559 | 0.7505148571300198 |
| 0.6695353883332822 | 0.8676554190672814 | 0.9414814307446276 |
| 0.8336093066644890 | 0.3662548610286869 | 0.9400575474198837 |
| 0.6685643245232760 | 0.1315351631120601 | 0.4404005038990152 |

0.8346432848105704 0.6338662203226070 0.4390058868427102
0.6676887849861690 0.8647175275458656 0.5580668038762649
0.8337660257649131 0.3669826977583503 0.5597923874783881
0.6674077821842658 0.1342405089430519 0.0612374344690145
0.8338391769753721 0.6323257607532256 0.0609618217265211

**(8) $3Zr_{Ta}+V_N+Mg_{int}$**

1.00000000000000
11.6112505410844999 0.0000000000000000 0.0000000000000000
0.0000000000000000 10.2498750964167993 0.0000000000000000
0.0000000000000000 0.0000000000000000 10.2721500396728995
N Mg Zr Ta
59 1 3 33
Direct
0.0011578612880291 0.2342891112293988 0.2509611855520119
0.1650806692266374 0.7326000940408702 0.2466060138633412
0.9979654747663406 0.7683020181191634 0.7504850748068206
0.1639626007546294 0.2623326895485388 0.7541363261782102
0.0027410092718807 0.9539138759289733 0.3787900522350653
0.0000503922651718 0.6923372562692953 0.4250610972326776
0.1619155650871708 0.4545875289346673 0.3801493181077537
0.1684327028788948 0.1949174529936269 0.4300531828283975
0.9988416684407874 0.0467364379204385 0.8817575289291874
0.9991350592846406 0.3084408599615445 0.9303344961758758
0.1822427044034994 0.5448886607935214 0.8768679570004182
0.1647490263942175 0.8066270964915098 0.9278406128438653
0.0013746103732858 0.9530707039636104 0.1211540099846708
0.0001963536381489 0.6897445926738843 0.0716701852824898
0.1609685523416281 0.4533122610194367 0.1209875066319445
0.1671095608109045 0.1927884445913247 0.0735810666944282
0.9989398009019200 0.0468262572503948 0.6201644639330275
0.9993419349868986 0.3075139867695412 0.5750110585186535
0.1764443448741022 0.5479145084063483 0.6229974449528936
0.1642563397204854 0.8087734371163895 0.5734265637190870
0.3331722546173434 0.2379473071255632 0.2500430696323290
0.4986772758604333 0.7407145627879393 0.2396151880419740
0.3281426413679101 0.7702813537757329 0.7489654489823737
0.5015119596597440 0.2467587440960799 0.7579728893538927
0.3319161433269890 0.9550146337485464 0.3762733030224313
0.3262580023984316 0.7002486608150732 0.4238888235366159
0.5003522503870479 0.4481418841488840 0.3801396529710330
0.4995644446180594 0.1884179867546246 0.4304787725706411
0.3301918574590044 0.0440758673738794 0.8822853380302372
0.3320146330642277 0.3114783633750385 0.9222662984795950
0.4770672941849608 0.5368690081817624 0.8724578790894918
0.5002832297032238 0.8095496587973638 0.9306592825059444
0.3300559597346694 0.9536741259347205 0.1201121362987019
0.3321318379743874 0.6902674550498271 0.0716518388012863
0.5082919061070034 0.4523303360615774 0.1178946198262540
0.4992994520189188 0.1885038795231135 0.0714498390532919
0.3314094072168272 0.0468247673868106 0.6167048543547766
0.3286632972785152 0.3234424940106090 0.5940464205440209
0.5001570723128258 0.8083371430261407 0.5684979997761718
0.6670859423499049 0.2350840203017714 0.2511086295532950
0.8347290279878952 0.7360230646232009 0.2464691924827064
0.6735851079642204 0.7720606197995975 0.7494731548471633
0.8358060456474503 0.2663237544136505 0.7537323003285354
0.6665173145904947 0.9536661294987197 0.3770663269972663

0.6719002575200850 0.6950194959441847 0.4223065555660547
0.8350931814881950 0.4520424681862144 0.3806594705341715
0.8349337635151204 0.1893932372622057 0.4264201697060822
0.6718634737507732 0.0455931696100755 0.8819040716209757
0.6681722955045767 0.3082123225434097 0.9276797242058554
0.8331309553785518 0.5465923612052909 0.8793181116170633
0.8343073995948015 0.8071573585251103 0.9294879291619312
0.6677440372521649 0.9527276975282686 0.1201606946783960
0.6661107239602866 0.6879942427324071 0.0706809370920814
0.8339305970251454 0.4523753270164519 0.1211483821879401
0.8336197056938558 0.1903480934377964 0.0749700958862188
0.6706274368459771 0.0439666815294321 0.6197036635190397
0.6741065126946527 0.3031511434058752 0.5779368835165991
0.8336391511434097 0.5478568113212404 0.6199994327002908
0.8346049510417044 0.8075261957229107 0.5710945208438840
0.3254680855827961 0.4897829955234879 0.7514094271780111
0.5041089486604083 0.7015112573423831 0.7499335373527808
0.4983986918444159 0.6391444321132203 0.4265378352046315
0.5034662740322512 0.3583671229254681 0.5619242159106055
0.9997219951767709 0.8018166477950898 0.2482631767215917
0.1669468648876684 0.3034515261411139 0.2510344554679443
0.9999060673510829 0.1960638704965245 0.7517723106680648
0.1622724814398108 0.7056273223777081 0.7497327995139728
0.9987034176856476 0.8667034237412310 0.9421481816804163
0.1637388323155109 0.3621112699138647 0.9443269483824223
0.0005700345583014 0.1335916133192930 0.4404669321205149
0.1650878168393160 0.6355314667154788 0.4396860832867140
0.9983550298113694 0.8680315984663184 0.5573985547832239
0.1630648164312846 0.3652284754874204 0.5566108136373473
0.9993634234171301 0.1337574501854354 0.0613891650383375
0.1660491455873870 0.6325624081447279 0.0594372380541668
0.3304841081360332 0.8031703216669914 0.2466184712274572
0.5009473736701573 0.3054454449003670 0.2556329836219116
0.3331580761129507 0.1895167293557835 0.7512260084260234
0.3330921715554560 0.8635557309713626 0.9398384443757246
0.5021526096631962 0.3593155277293174 0.9443023000601095
0.3337806885727139 0.1297448824554611 0.4375287824833609
0.3334899271729659 0.8630173745487535 0.5590519844345151
0.3336139342362466 0.1323071993004267 0.0600678042894796
0.4990153915910999 0.6321085816468375 0.0566668260000989
0.6682143039468059 0.8023283291072766 0.2473614118597547
0.8333979931743495 0.3017003389107815 0.2508759845789910
0.6696559142657349 0.1936749293467467 0.7508460966097427
0.8340443536733382 0.6983746159533173 0.7500340384308478
0.6686509237515545 0.8659251001365892 0.9400566627676781
0.8332674949841573 0.3665144683244744 0.9402833167146061
0.6688706956749573 0.1313660439155941 0.4413878458994471
0.8339527637730598 0.6333032546761773 0.4394729701529943
0.6677365290882232 0.8641639643492331 0.5566532923578148
0.8345912606700624 0.3668890513741622 0.5609366152259603
0.6670834168481489 0.1325937636706755 0.0613751225822645
0.8333031063372714 0.6318567759017031 0.0600603052117388

**(9) $Mg_{Ta}+3O_N+Zr_{int}$**

1.00000000000000

| | | |
|---|---|---|
| 11.6112505410844999 | 0.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 10.2498750964167993 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 10.2721500396728995 |

N O Mg Zr Ta
57 3 1 1 35
Direct
0.9997392921040800 0.2326696364319667 0.2499578109282968
0.1644844545105926 0.7409786240493361 0.2495924103316962
-0.0000475286218009 0.7634798728396157 0.7483667749752893
0.1712007382791713 0.2719635206391605 0.7492169140168584
0.9986773132791684 0.9529895914233013 0.3802558726018871
-0.0001849605506754 0.6884736893738793 0.4275654940487587
0.1644979825165768 0.4553318216868767 0.3761373101531629
0.1667610430798785 0.1931961231204478 0.4286888947172879
0.0032394312899997 0.0468503164367434 0.8793413570653607
0.9995103567480216 0.3096038816782202 0.9247523982397986
0.1823063204072806 0.5465166091375624 0.8795228369748982
0.1676813642002705 0.8075966476744091 0.9287447949655393
0.9978021516758949 0.9518625783090152 0.1190955275593375
0.9991681069088121 0.6896796000338908 0.0738224232874643
0.1591981633917088 0.4549680568442291 0.1240997411914177
0.1667152566858534 0.1923790628869335 0.0727430067515285
0.0017297326274622 0.0480440378810919 0.6202025773091165
0.9991074708519180 0.3109007922548191 0.5747692615430626
0.1814472718728108 0.5470332898667624 0.6216631516765996
0.1664259674342346 0.8129223273409741 0.5711104791219180
0.3338916112555319 0.2379547424927446 0.2498820218977242
0.3364425437579866 0.7765207447873522 0.7452985860209450
0.4990522590084939 0.2632659494437730 0.7548410509557399
0.3296947708079522 0.9572777391887479 0.3763832198600093
0.3316356870345723 0.6967251352196290 0.4240150261460594
0.5094310757465581 0.4473241758913539 0.3766516442946750
0.5005912424035307 0.1875964729509020 0.4303312316281498
0.3324092353679820 0.0437584583263548 0.8822710909520842
0.3323151248958928 0.3168640784421618 0.9230105250973517
0.4768150460026064 0.5444222145783308 0.8813465982054743
0.4993501225852979 0.8049595365531818 0.9297397564521267
0.3357532878875318 0.9548246425050594 0.1222928661767771
0.3339837613140433 0.6890992156081300 0.0821597257091896
0.5106854767074634 0.4529801874482232 0.1214252315238236
0.5005792739137068 0.1908599791989979 0.0699777902133974
0.3374358864927323 0.0435431274922109 0.6175618491154088
0.3343598161700321 0.3184667128784323 0.5778648136803103
0.4802717187411975 0.5424313072753739 0.6305796306200647
0.6676641714698360 0.2285309914788146 0.2499179759762272
0.8313308895402872 0.7380587407600299 0.2515194951878363
0.6637703726079488 0.7627037504543736 0.7469610288181420
0.8342409007349604 0.2617055210938042 0.7494750600054441
0.6630416225463347 0.9498226247558559 0.3818040648142726
0.8328872229828046 0.4523137096475947 0.3791824923765295
0.8335103224194584 0.1917951738228422 0.4293016309973833
0.6634573430867846 0.0451438440907489 0.8799451363173452
0.6690888310897337 0.3089834277513052 0.9252287809957739
0.8325109791518422 0.5472945284496479 0.8792477689128247
0.8323372255177868 0.8078194599714413 0.9263630854010065
0.6700807112616995 0.9513448982882391 0.1199238952131692
0.6646123100966974 0.6887911064448844 0.0751865579649751
0.8333010057915974 0.4519870718854096 0.1197428744192678
0.8337709526199303 0.1908565163220359 0.0706928293988567
0.6685572915175109 0.0451104042124704 0.6213284677060932
0.6672681608227093 0.3074432469649238 0.5752124193901180

0.8315482281731265 0.5479287813575542 0.6188784382070056
0.8318450783901861 0.8100843233659267 0.5700762815219831
0.5021550933772240 0.7421120958819231 0.2481806185792979
0.5021088091660274 0.8073876952091281 0.5680139582777135
0.6679665735246374 0.6906542890939226 0.4251372958658359
0.5002316783516969 0.6360623754845171 0.4357832103563183
0.3286111031337723 0.4623712846875915 0.7503672544685681
0.9980093968916092 0.8038168590051648 0.2498378904958233
0.1675135036470838 0.3002412852758053 0.2507687748700270
0.0021582060893290 0.1999068242885478 0.7495531859079216
0.1717045171575541 0.7045785190940564 0.7507707558040437
0.9994039805400513 0.8652043574252815 0.9374004738914318
0.1625739585795074 0.3623634575415258 0.9523231858062260
0.9986983385832273 0.1336710989598649 0.4388420866129478
0.1693401550935031 0.6346308729488863 0.4409788484076444
0.9989406426877281 0.8680003436491742 0.5614456082923918
0.1630800941208683 0.3628304737411707 0.5487867751818465
0.9989562012324430 0.1317420899379119 0.0598095222115220
0.1659636444297610 0.6347036813669859 0.0602328077013642
0.3277230155238178 0.8018748954687023 0.2548688787148663
0.5012963279495873 0.3023356519094577 0.2552299459781844
0.3357654692029526 0.1887753603783255 0.7499912563929918
0.4962484871119057 0.6960680123245681 0.7496685052221314
0.3344067371491183 0.8662578137297645 0.9448870565084816
0.5047917725325184 0.3571261324320545 0.9507865004094959
0.3343267800878323 0.1343885824824698 0.4437461072551701
0.3303516712816381 0.8636810014295655 0.5538672942530327
0.5043056718435088 0.3699470934432521 0.5467994430486428
0.3338907737060404 0.1330241599920173 0.0588481327115536
0.4978386813369321 0.6304406792332590 0.0572362908137417
0.6692907247295177 0.8051272295071653 0.2457327877479750
0.8335761770062912 0.3002642960060669 0.2498225791315493
0.6655906092652583 0.1974917813081046 0.7498114666046467
0.8328740466495107 0.6981644178064977 0.7501066289119873
0.6652979316354091 0.8637981658244851 0.9371645333036029
0.8341936022622706 0.3662363827218104 0.9396435346320942
0.6671103352613138 0.1331795698304167 0.4378681983285697
0.8353106113859703 0.6317870673131699 0.4399086296935716
0.6693183797988048 0.8685022275955099 0.5618849675303245
0.8325492939382076 0.3657901803321896 0.5605927403135045
0.6683786252971071 0.1320662972858124 0.0591766545354955
0.8324668843015273 0.6324227778806812 0.0588556355945859

**(10) $Mg_{Ta}+V_N+Zr_{int}$**

1.00000000000000

11.6112505410844999 0.0000000000000000 0.0000000000000000
0.0000000000000000 10.2498750964167993 0.0000000000000000
0.0000000000000000 0.0000000000000000 10.2721500396728995

N Mg Zr Ta
59 1 1 35

Direct
0.9987560573017664 0.2334597012235226 0.2502850239478331
0.1646906831774469 0.7330998458335118 0.2469284482012023
0.0008429418651945 0.7633984753049053 0.7497380211961946
0.1704935599125204 0.2703989621125790 0.7506241850145799
0.9994097576007395 0.9518380669568290 0.3790900625159358
0.0004937960671544 0.6936267089621317 0.4278613260628793
0.1596461710202731 0.4545897373298651 0.3768626915246013

| | | |
|---|---|---|
| 0.1654286950620861 | 0.1913483581774671 | 0.4267002196795728 |
| 0.0016812198924780 | 0.0482460764960700 | 0.8804862982345796 |
| 0.9990090136828649 | 0.3095813482668553 | 0.9256362585270457 |
| 0.1828542746396246 | 0.5460710764093717 | 0.8781116055391743 |
| 0.1659799568128888 | 0.8096761384712651 | 0.9267194557886995 |
| 0.9996702905309286 | 0.9523509349289586 | 0.1201642808812023 |
| 0.0005231926980201 | 0.6911003914200248 | 0.0691785444387012 |
| 0.1607265972280603 | 0.4547018751146406 | 0.1223950588032777 |
| 0.1661502167015733 | 0.1933370640244474 | 0.0729071280981675 |
| 0.0023306297538829 | 0.0464891181052833 | 0.6201087862564749 |
| 0.9988971495434279 | 0.3090457139669207 | 0.5750954230999822 |
| 0.1839565851046434 | 0.5448212423854227 | 0.6212626003447926 |
| 0.1673566407678420 | 0.8082507495229491 | 0.5734652290059479 |
| 0.3338159717563958 | 0.2419434771556904 | 0.2505713994347843 |
| 0.4999424481809786 | 0.7436609197322813 | 0.2373620860129898 |
| 0.3314437894394072 | 0.7768020595194760 | 0.7526203373863323 |
| 0.4951954721112473 | 0.2755641635809776 | 0.7511871122356368 |
| 0.3307834214689765 | 0.9546865047819001 | 0.3778540703631048 |
| 0.3296521380246506 | 0.6947123640885958 | 0.4217465252922424 |
| 0.5050812278548494 | 0.4505126741493168 | 0.3878453776990605 |
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