**Supporting Information**

# Energy Landscape and Crystal-to-Crystal Transition of Ternary Silicate $Mg_2SiO_4$

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## Part 1 Theoretical methods

### a. Stochastic Surface Walking (SSW) pathway sampling

The SSW algorithm[1] has an automated climbing mechanism to manipulate a structure configuration from a minimum to a high-energy configuration along one random mode direction. The method was initially developed for aperiodic systems, such as molecules and clusters[1a], and has been extended to periodic crystals[1][2]. The method inherits the idea of bias-potential driven constrained-Broyden-dimer (BP-CBD) method for TS location.[1c] In one particular SSW step, labeled as $i$, a modified PES $V_{m\text{-}to\text{-}n}$ ($n$ is the index of the bias potential, $n$=1,2$\cdots H$), as shown in Eq. 1, is utilized for moving from the current minimum, $\mathbf{R}_i^m$ to a high energy configuration $\mathbf{R}_i^H$ (the climbing), in which a series of bias Gaussian potential $v_n$ is added one by one consecutively along the direction $\mathbf{N}_i^n$.

$$V_{m-to-H} = V_{real} + \sum_{n=1}^{H} v_n = V_{real} + \sum_{n=1}^{H} w_n \times \exp\left[-\left((\mathbf{R}^t - \mathbf{R}_t^{n-1})\cdot \mathbf{N}_i^n\right)^2 \Big/ \left(2\times ds^2\right)\right] \qquad (1)$$

where $\mathbf{R}$ is the coordination vector of the structure and $V_{real}$ represents the unmodified PES; $\mathbf{R}_t^n$ are the $n^{th}$ local minima along the movement trajectory on the modified PES that is created after adding $n$ Gaussian functions. The Gaussian function is controlled by its height $w$ and its width $ds$, and is always added along one particular walking direction as defined by $\mathbf{N}^n$. Once the $\mathbf{R}_i^H$ is reached, all bias potential are removed and the local optimization is performed to quench the structure to a new minimum. The applications of SSW method can be found in our previous publications[2] (http://homepage.fudan.edu.cn/fdzpliu/publication/). The procedure is described below briefly.

**Pathway collection** In SSW pathway sampling, firstly, we start from one single phase (olivine $Mg_2SiO_4$ in this paper), and utilize the SSW method to explore all the likely phases nearby the phase. A structure selection module is utilized to decide whether to accept/refuse once a new minimum is reached. If the new phase different from the starting phase is identified by the SSW crystal method, we record/output the IS (i.e. olivine) and the FS (e.g. spinel) of the current SSW step. Then, the program will return back to the IS by rejecting the new minimum to continue the phase exploration; On the other hand, if the new minimum identified by SSW is still olivine, but with a permutation isomer with varied lattice, the program will accept the new isomeric phase and start the phase exploration from this phase. We repeat this procedure until a certain number of minima (>$10^5$ from first principles calculations) are explored, which produces a database including a large number of

IS/FS pairs (>200 pairs).

**Pathway screening** Secondly, we use Euclidian distance between IS/FS pairs as an important quantity to screen out the candidate pathways from the database. For the crystal systems, we need to utilize a generalized coordinate {$\boldsymbol{L}$, $\boldsymbol{q'}$} to define the structure, including both the lattice $\boldsymbol{L}$ and the atom degrees of freedom $\boldsymbol{q'}$, as defined in the following equations.

$$\boldsymbol{G} = \boldsymbol{L}^{\mathrm{T}}\boldsymbol{L} \quad (2)$$

$$\boldsymbol{G}_r = (\mathbf{G_{IS}} + \mathbf{G_{FS}})/2 \quad (3)$$

$$\boldsymbol{S} = \mathbf{G_r}^{1/2} \quad (4)$$

$$\boldsymbol{q}' = \boldsymbol{S}\boldsymbol{q} \quad (5)$$

where $\boldsymbol{L}$ is the lattice vector in real distance units, e.g., in Å, $\boldsymbol{G}$ is a rotational invariant matrix, S is scaling matrix, which is defined as the square root of the metric tensor $\boldsymbol{G}_\mathbf{r}$. The fractional coordinate $\boldsymbol{q}$ can then be transformed to a new set of scaled coordinate, $\boldsymbol{q,'}$ which is compatible with the lattice length. Then we can use the generalized coordinate {$\boldsymbol{L}$, $\boldsymbol{q}$'} to calculate the Euclidian distance between IS/FS pairs. According to our previous studies of phase transition on various materials, it have shown that the lowest energy pathway usually has the shortest Euclidian distance between IS/FS pairs, indicating a good structure match between IS and FS is a general requirement for low energy pathways.[2] Thus here we use Euclidian distance between IS and FS as an important quantity to screen out the low energy pathways from the large number of IS/FS pairs.

**Lowest energy pathway determination** Thirdly, we utilize the variable-cell double-ended surface walking (DESW) method[3-4] to establish the pseudopathway connecting IS to FS for all IS/FS pairs. The approximate barrier is obtained according to DESW pseudopathway, where the maximum energy point along the pathway is generally a good estimate for the true TS. It might be mentioned that at this stage, we generally examined thoroughly all the pathways we identified. Basically, even before we locate exactly the TS, we can have the following important information, including the approximate barrier, the pattern of lattice and atom movement from IS to FS, the habit plane and the OR for the pathways, From these, we can safely rule out the similar pathways and focus on the selected, distinct and low energy pathways. Next, the candidate lowest energy pathways are selected to locate exactly the "true" TS by using DESW TS-search method.[4] By sorting the barrier calculated, the energy difference between the TS and the IS, the lowest energy pathways can be

finally obtained. All the lowest energy pathways will be further confirmed by extrapolating TS towards IS and FS and the phonon frequency calculations.

### b. Classical force field potential calculations

In order to ensure a proper sampling of all low energy structures and pathways, we also tested to utilize the classical force field potential [5] in SSW global structure search and pathway sampling, in both 28-atom and 56-atom supercells. This potential [5] has been utilized to calculate a number of $Mg_2SiO_4$ phases, which show a good agreement with the experimental data. More than $10^7$ minima on PES have been visited and more than $10^3$ IS/FS pairs were collected. We found that the lowest energy pathway from the classic potential is the same as the DFT obtained pathway in both 28-atom and 56-atom supercells.

### c. Phonon and free energy calculation (also see Part 3-4)

The phonon frequencies of the crystals were determined using the finite displacement method[6,7], employing the PHONOPY package [8]. In these calculations, the size of the system was increased to (2×2×2) supercell (168-atom supercell) and the K-point utilized is (1×2×2) Monkhorst-Pack mesh. With a displacement of ±0.01 Å on nonequivalent atoms, a set of displaced supercells was generated and the forces of these supercells were calculated using plane-wave DFT package, VASP program. These forces were carried back to the PHONOPY to calculate the phonon dispersion curves. Helmholtz free energy (F), entropy of vibration ($S_{vib}$), and zero-point energy (ZPE) at finite temperature can be obtained from phonon spectra based on quasiharmonic approximation. At a given temperature the lowest value of the free energy determines the stable phase. The free energy of the crystal is a sum of the ground state energy and the free energy contribution from the lattice vibrations. The first term is directly obtained from DFT calculation, i.e. at T=0 K. The second one is temperature dependent and in the harmonic approximation it is calculated from the phonon density of states using the following equation,

$$F_{\text{harm}} = \mathrm{r}k_B T \int_0^{\infty} g(\varpi) \ln[2\sinh(\frac{\hbar\varpi}{2k_B T})] d\varpi$$

where r is the number of degree of freedom in a primitive unit cell, ω denotes the phonon frequency, g(ω) denotes the density of phonon states (DOS), ħ is the Planck constant, and $k_B$ is the Boltzmann constant. In this approach the thermal expansion of crystal is neglected.

## Part 2 DFT optimized lattice constants for $Mg_2SiO_4$ crystals

Table S1. Lattice parameters for $Mg_2SiO_4$ polymorphs from DFT calculations at 15 GPa. For all the phases, the α and β angles of lattice are always $90^o$.

| Structure | Calculated | | | | | Experimental[9-11]* | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | a(Å) | b(Å) | c(Å) | γ($^o$) | V(Å$^3$) | a(Å) | b(Å) | c(Å) | γ($^o$) | V(Å$^3$) |
| ol(Z=4) | 4.69 | 9.87 | 5.84 | 90 | 270.56 | 4.75 | 10.19 | 5.98 | 90 | 289.53 |
| sp(Z=8) | 7.95 | 7.95 | 7.95 | 90 | 502.72 | 8.07 | 8.07 | 8.07 | 90 | 526.7 |
| wad(Z=8) | 5.58 | 11.21 | 7.95 | 90 | 496.91 | 5.70 | 11.46 | 8.26 | 90 | 539.26 |
| OI(Z=4) | 5.35 | 8.32 | 6.05 | 90 | 269.33 | | | | | |
| OII(Z=8) | 5.86 | 16.14 | 5.48 | 90 | 518.32 | | | | | |
| MI(Z=8) | 9.69 | 14.63 | 5.72 | 139.5 | 527.18 | | | | | |

* data taken in ambient pressure condition.

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## Part 3 Phonon spectra

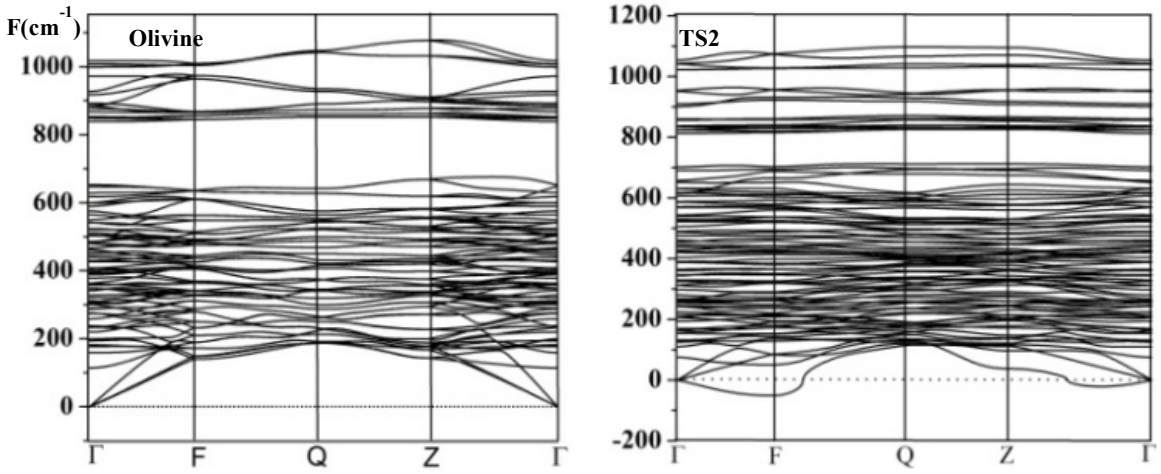


**FIG. S1.** Calculated phonon dispersion curves for olivine and TS2 (see Figure 2b). The high-symmetry points of the Brillouin zone are denoted as Γ(0,0,0), F(0,0.5,0), Q(0,0.5,0.5) and Z(0,0,0.5). The TS2 has the largest negative frequency at F point, indicating a strong coupling between lattice deformation and atom movement, which is consistent with its shear-related phase transition (see Figure 2c in text).

## Part 4 Pressure and temperature effects on olivine-spinel solid phase transition

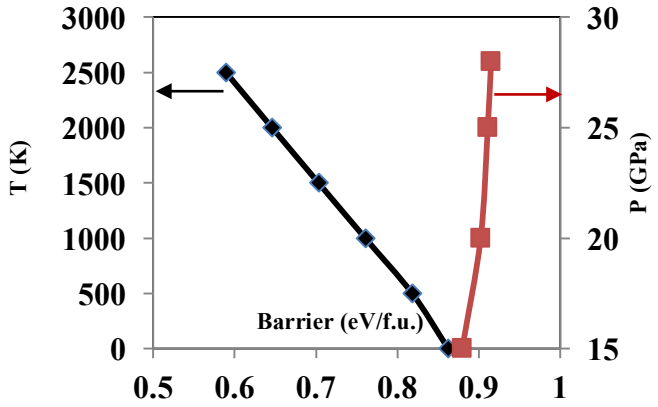


**FIG. S2.** The overall barrier (TS1 with respect to olivine) for olivine-to-spinel solid phase transition at different temperatures and pressures.

For the pressure effect on reaction, we have computed the reaction at different pressure conditions. The barrier for the reaction increases slightly, within ~0.1 eV/f.u. from the pressure 15 GPa to 25 GPa, indicating the reaction is not sensitive to the external pressure. This is in fact consistent with the fact that the olivine to OI reaction, the rate-controlling step, has very small overall volume change.

For the temperature effect, we have computed the free energy of the solid phase transition by correcting DFT enthalpy with the calculated phonon entropy contributions. We found that the barrier decreases rapidly with the increase of temperature, which is consistent with the fact that the reaction can only occur at high temperatures, e.g. 1500 $^{o}$C.

## Part 5 The XYZ Cartesian coordinates for key states in reaction pathway

| **Olivine** | a= 9.8729 b= 5.8387 c= 4.6936 | α=90 $^{o}$ β=90 $^{o}$ γ=90$^{o}$ | |
|---|---|---|---|
| | X | Y | Z |
| O | 1.6356 | 0.1669 | 1.2740 |
| O | 0.9039 | 1.4597 | 3.6087 |
| O | 1.6356 | 2.7525 | 1.2740 |
| O | 9.3096 | 1.4597 | 1.2973 |
| O | 8.2374 | 5.6719 | 3.4197 |
| O | 8.2374 | 3.0863 | 3.4197 |
| O | 8.9691 | 4.3791 | 1.0850 |
| O | 0.5635 | 4.3791 | 3.3964 |
| O | 6.5721 | 0.1669 | 1.0730 |
| O | 6.5721 | 2.7525 | 1.0730 |
| O | 4.3731 | 1.4597 | 1.0498 |
| O | 5.8404 | 1.4597 | 3.4319 |
| O | 3.3010 | 5.6719 | 3.6208 |
| O | 3.3010 | 3.0863 | 3.6208 |
| O | 4.0327 | 4.3791 | 1.2620 |
| O | 5.4999 | 4.3791 | 3.6442 |
| Mg | 0.0001 | 0.0001 | 0.0000 |
| Mg | 4.9365 | 0.0001 | 2.3470 |
| Mg | 0.0001 | 2.9194 | 0.0000 |
| Mg | 4.9365 | 2.9194 | 2.3470 |
| Mg | 2.7190 | 1.4597 | 4.6414 |
| Mg | 2.2176 | 4.3791 | 2.2946 |
| Mg | 7.1541 | 4.3791 | 0.0524 |
| Mg | 7.6554 | 1.4597 | 2.3992 |
| Si | 0.9359 | 1.4597 | 2.0004 |
| Si | 8.9371 | 4.3791 | 2.6932 |
| Si | 5.8724 | 1.4597 | 0.3466 |
| Si | 4.0007 | 4.3791 | 4.3473 |

| **TS1** | a= 8.669 b= 6.0277 c= 5.1306 | α=89.92 $^{o}$ β=90.01 $^{o}$ γ=90$^{o}$ | |
|---|---|---|---|
| | X | Y | Z |
| O | 2.054192 | 0.347215 | 1.664616 |
| O | 0.472654 | 1.528923 | 3.780222 |
| O | 2.421235 | 2.811911 | 2.569857 |
| O | 8.795328 | 1.815579 | 1.299721 |
| O | 6.594557 | 5.81979 | 2.498576 |
| O | 6.968981 | 3.358945 | 3.412125 |
| O | 8.558746 | 4.538375 | 1.30604 |
| O | 0.216966 | 4.83775 | 3.785042 |
| O | 6.757296 | 0.282384 | -0.06629 |
| O | 6.387114 | 2.745518 | 0.842574 |
| O | 4.461778 | 1.275301 | 1.205803 |

| | | | |
|---|---|---|---|
| O | 4.804739 | 1.569238 | 3.856029 |
| O | 2.63344 | 5.765195 | 4.225178 |
| O | 2.260762 | 3.303977 | 5.13554 |
| O | 4.223926 | 4.58095 | 1.200168 |
| O | 4.552748 | 4.288715 | 3.852227 |
| Mg | 0.118604 | 0.157852 | 0.100631 |
| Mg | 4.560208 | -0.07983 | 2.654226 |
| Mg | 0.228496 | 3.17096 | -0.14868 |
| Mg | 4.451324 | 2.933732 | 2.404356 |
| Mg | 2.916903 | 1.441142 | 5.104885 |
| Mg | 1.755702 | 4.673069 | 2.54772 |
| Mg | 6.091721 | 4.448999 | -0.03861 |
| Mg | 7.251628 | 1.6549 | 2.5319 |
| Si | 1.341925 | 1.628351 | 2.39029 |
| Si | 7.677081 | 4.641316 | 2.688099 |
| Si | 5.676559 | 1.46484 | 0.114859 |
| Si | 3.342898 | 4.483123 | 4.948108 |

**OI** a= 8.6691 b= 6.0277 c= 5.1306 α=89.92 $^{o}$ β=90.01 $^{o}$ γ=89.99$^{o}$

| | X | Y | Z |
|---|---|---|---|
| O | 2.185546 | 0.219973 | 2.6537 |
| O | 0.184335 | 1.51964 | 3.937029 |
| O | 2.186981 | 2.817279 | 2.658261 |
| O | 8.532827 | 1.520273 | 1.394246 |
| O | 6.14733 | 5.855306 | 2.691456 |
| O | 6.150726 | 3.258043 | 2.694229 |
| O | 8.151586 | 4.559136 | 1.413182 |
| O | -0.19816 | 4.559318 | 3.955954 |
| O | 6.356638 | 0.22302 | 0.016763 |
| O | 6.353074 | 2.820755 | 0.019562 |
| O | 4.365213 | 1.51889 | 1.280981 |
| O | 4.353534 | 1.51908 | 4.087434 |
| O | 1.981586 | 5.858249 | 5.328305 |
| O | 1.980168 | 3.26048 | 5.332802 |
| O | 3.982157 | 4.558494 | 1.26202 |
| O | 3.97064 | 4.557855 | 4.068541 |
| Mg | 0.001472 | 0.000334 | 0.000624 |
| Mg | 4.167345 | -0.00042 | 2.674715 |
| Mg | -0.00226 | 3.039501 | 0.00049 |
| Mg | 4.169024 | 3.038707 | 2.674611 |
| Mg | 2.76732 | 1.521011 | 5.378921 |
| Mg | 1.400512 | 4.556928 | 2.705172 |
| Mg | 5.568556 | 4.561239 | -0.02908 |
| Mg | 6.934722 | 1.51742 | 2.646696 |
| Si | 1.243161 | 1.519147 | 2.671932 |
| Si | 7.092093 | 4.557758 | 2.67777 |
| Si | 5.412238 | 1.52066 | 0.002968 |

| | | | |
|---|---|---|---|
| Si | 2.923563 | 4.558909 | 5.346457 |

| **OI** | a=5.3578 b= 8.3350 c=6.0807 | α=89.96 ° | β=89.99 ° | γ=90.00° |
|---|---|---|---|---|
| | X | Y | Z | |
| O | 2.693502 | 2.283802 | 0.26745 | |
| O | 0.014875 | 2.082762 | 5.909718 | |
| O | 2.700869 | 6.248439 | 3.310797 | |
| O | 0.022049 | 6.453385 | 2.866406 | |
| O | 2.697709 | 6.25022 | 5.910069 | |
| O | 0.018542 | 6.451449 | 0.267043 | |
| O | 2.6906 | 2.285837 | 2.866738 | |
| O | 0.0116 | 2.080945 | 3.310389 | |
| O | 3.9634 | 0.287839 | 1.56929 | |
| O | 1.2881 | 4.457514 | 1.568039 | |
| O | 1.2848 | 4.07861 | 4.608103 | |
| O | 3.9674 | 8.243999 | 4.609348 | |
| O | 1.4224 | 8.244509 | 4.608421 | |
| O | 4.0976 | 4.07483 | 4.608855 | |
| O | 4.1010 | 4.457368 | 1.56878 | |
| O | 1.4185 | 0.291793 | 1.568338 | |
| Mg | 0.0132 | 0.097974 | 0.048402 | |
| Mg | 2.6920 | 4.265326 | 0.04787 | |
| Mg | 0.0134 | 0.099691 | 3.088682 | |
| Mg | 2.6922 | 4.267231 | 3.088175 | |
| Mg | 0.0159 | 2.866331 | 1.569152 | |
| Mg | 2.6957 | 1.500268 | 4.60769 | |
| Mg | 0.0065 | 5.66781 | 4.607348 | |
| Mg | 2.6850 | 7.033658 | 1.569563 | |
| Si | 2.6926 | 1.342744 | 1.567796 | |
| Si | 0.0140 | 3.023966 | 4.60941 | |
| Si | 2.6944 | 7.191409 | 4.609875 | |
| Si | 0.0153 | 5.510312 | 1.567427 | |

| **TS2** | a=5.2262 b= 8.9506 c=5.9282 | α=77.63 ° | β=90 ° | γ=90.00° |
|---|---|---|---|---|
| | X | Y | Z | |
| O | 2.986841 | 2.617615 | 0.547304 | |
| O | 0.372946 | 3.469314 | 5.379637 | |
| O | 2.805048 | 7.732638 | 4.069565 | |
| O | 0.193528 | 7.305079 | 1.855115 | |
| O | 2.720826 | 8.437442 | 6.612332 | |
| O | 0.107143 | 6.598692 | -0.68748 | |
| O | 2.468055 | 2.982854 | 3.044631 | |
| O | -0.14494 | 3.104117 | 2.882105 | |
| O | 3.767615 | 0.670359 | 2.13947 | |
| O | 1.181495 | 4.839168 | 0.974285 | |
| O | 1.1536 | 5.416332 | 3.78736 | |
| O | 3.793622 | 10.199 | 4.952078 | |

| | | | |
|---|---|---|---|
| O | 1.341811 | 9.989995 | 4.888801 |
| O | 3.862258 | 5.180145 | 4.022375 |
| O | 3.955803 | 5.047298 | 1.039648 |
| O | 1.250302 | 0.906776 | 1.905096 |
| Mg | -0.11171 | 0.102899 | 0.61929 |
| Mg | 2.501382 | 4.714581 | -0.48185 |
| Mg | -0.0706 | 1.247936 | 3.494557 |
| Mg | 2.54093 | 4.83888 | 2.433226 |
| Mg | -0.27127 | 3.339162 | 1.007623 |
| Mg | 2.340456 | 2.748338 | 4.919049 |
| Mg | -0.49385 | 6.910799 | 3.626177 |
| Mg | 2.119813 | 8.126287 | 2.297183 |
| Si | 2.623417 | 1.842819 | 1.937633 |
| Si | 0.009322 | 4.24404 | 3.989322 |
| Si | 2.652554 | 9.008492 | 5.129268 |
| Si | 0.039725 | 6.028987 | 0.795993 |

| **OII** | a= 5.4864 b=8.6083 | c=5.8744 | α=69.98 $^{o}$ β=89.99 $^{o}$ γ=89.99$^{o}$ |
|---|---|---|---|
| | X | Y | Z |
| O | 2.687740936 | 2.321382 | 0.231478 |
| O | -0.055385823 | 4.228258 | 5.375832 |
| O | 2.860070936 | 8.06667 | 4.238715 |
| O | 0.116817517 | 7.090734 | 1.368259 |
| O | 2.860562 | 9.045581 | 6.91151 |
| O | 0.117160436 | 6.111139 | -1.3045 |
| O | 2.583621665 | 3.187665 | 2.543865 |
| O | -0.159366366 | 3.360935 | 3.063593 |
| O | 4.190100642 | 0.951777 | 2.094398 |
| O | 1.438235779 | 4.881844 | 0.656603 |
| O | 1.447070715 | 5.596912 | 3.512624 |
| O | 4.181595764 | 10.27567 | 4.950517 |
| O | 1.647320627 | 10.38703 | 4.89939 |
| O | 4.201517101 | 5.65516 | 3.513155 |
| O | 4.39032437 | 4.770312 | 0.707697 |
| O | 1.458362834 | 0.893479 | 2.093763 |
| Mg | 0.153904183 | 0.404506 | 0.62252 |
| Mg | 2.897050319 | 4.134455 | -0.5353 |
| Mg | 0.157157606 | 1.456742 | 3.558925 |
| Mg | 2.900250327 | 5.090885 | 2.048277 |
| Mg | 0.44753146 | 3.338472 | 1.277886 |
| Mg | 3.190663784 | 3.211215 | 4.329364 |
| Mg | -1.263978434 | 7.608916 | 2.79457 |
| Mg | 1.47927054 | 7.547536 | 2.812236 |
| Si | 2.817089531 | 1.785302 | 1.749994 |
| Si | 0.073991157 | 4.763526 | 3.857159 |
| Si | 2.857566316 | 9.350304 | 5.284334 |
| Si | 0.114138954 | 5.807079 | 0.322777 |

| **TS3** | a= 5.4535 | b=9.5899 | c=5.728 | α=60.77 $^{o}$ β=89.99 $^{o}$ γ=90.00$^{o}$ |
|---|---|---|---|---|
| | X | | Y | Z |
| O | 2.71533 | | 1.988453 | -0.51737 |
| O | 5.4424 | | 5.605695 | 5.550066 |
| O | 2.878898 | | 9.259869 | 3.850425 |
| O | 0.151953 | | 7.925554 | 1.184152 |
| O | 2.875248 | | 7.875526 | 1.224252 |
| O | 0.148576 | | 9.310107 | 3.810377 |
| O | 2.608205 | | 3.276045 | 1.625071 |
| O | 5.335462 | | 4.319471 | 3.407414 |
| O | 4.141059 | | 0.872037 | 1.554523 |
| O | 1.498065 | | 5.601985 | 0.904384 |
| O | 1.414262 | | 6.724415 | 3.480201 |
| O | 4.22557 | | 11.58371 | 4.130524 |
| O | 1.680827 | | 11.7264 | 4.028426 |
| O | 4.2465 | | 6.812909 | 3.467513 |
| O | 4.406655 | | 5.458842 | 1.005751 |
| O | 1.520001 | | 0.782891 | 1.566534 |
| Mg | 0.20778 | | 0.319632 | 0.137247 |
| Mg | 2.933968 | | 7.278267 | 4.896318 |
| Mg | 0.183078 | | 1.464243 | 2.844761 |
| Mg | 2.908731 | | 6.13169 | 2.190046 |
| Mg | 0.631496 | | 4.114746 | 1.678293 |
| Mg | 3.35816 | | 3.479262 | 3.354429 |
| Mg | 4.228523 | | 8.629549 | 2.495656 |
| Mg | 1.501666 | | 8.55666 | 2.538437 |
| Si | 2.793472 | | 1.69827 | 1.059026 |
| Si | 0.06654 | | 5.8973 | 3.973885 |
| Si | 2.871435 | | 10.72827 | 4.581135 |
| Si | 0.143916 | | 6.457203 | 0.453553 |

| **Spinel** | a= 5.6233 | b=9.7373 | c=5.6225 | α=54.73 $^{o}$ β=89.99 $^{o}$ γ=89.99$^{o}$ |
|---|---|---|---|---|
| | X | | Y | Z |
| O | 2.81171 | | 1.62277 | -1.08045 |
| O | 5.62340 | | 6.49240 | 5.67111 |
| O | 2.81173 | | 9.80114 | 3.46519 |
| O | 0.00005 | | 8.05143 | 1.12541 |
| O | 2.81173 | | 8.11474 | 1.08049 |
| O | 0.00005 | | 9.73774 | 3.51015 |
| O | 2.81172 | | 3.18278 | 1.12539 |
| O | 5.62339 | | 4.93246 | 3.46521 |
| O | 4.16265 | | 0.84349 | 1.12520 |
| O | 1.35101 | | 5.71220 | 1.12520 |
| O | 1.35099 | | 7.27171 | 3.46548 |
| O | 4.16271 | | 12.14038 | 3.46546 |
| O | 1.46080 | | 12.14037 | 3.46545 |

| | | | |
|---|---|---|---|
| O | 4.27244 | 7.27171 | 3.46547 |
| O | 4.27244 | 5.71220 | 1.12519 |
| O | 1.46077 | 0.84348 | 1.12520 |
| Mg | 0.00004 | 0.00010 | 0.00000 |
| Mg | 2.81173 | 8.11524 | 4.59058 |
| Mg | 0.00005 | 1.62319 | 2.29540 |
| Mg | 2.81175 | 6.49198 | 2.29537 |
| Mg | 1.40589 | 4.05763 | 2.29528 |
| Mg | 4.21755 | 4.05762 | 2.29528 |
| Mg | 4.21755 | 8.92622 | 2.29532 |
| Mg | 1.40590 | 8.92621 | 2.29531 |
| Si | 2.81172 | 1.62307 | 0.57387 |
| Si | 0.00006 | 6.49211 | 4.01681 |
| Si | 2.81173 | 11.36080 | 4.01676 |
| Si | 0.00004 | 6.49176 | 0.57386 |