The Thermal Agitated Phase Transitions on the Ti$_{32}$ Nanocluster: a Molecular Dynamics Simulation Study

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ABSTRACT
Molecular dynamics simulations were performed to investigate the stability with respect to increasing the simulated temperature from 300 to 2400 K of an isolated cluster composed of 32 titanium atoms. The interatomic interactions were modelled using Gupta potentials as implemented within the classical molecular dynamics simulation software DL_POLY. The radial distribution functions (RDF), diffusion coefficient, and density profiles were examined to study the structural changes as a function of temperature. It was found that the Ti$_{32}$ nanocluster exhibits temperature structural transition. The icosahedron and pentagonal bi-pyramid structures were found to be the most dominant building block fragments. Deformation of the nanocluster was also measured by diffusion coefficient, and it was found that the Ti$_{32}$ are mobile above the bulk melting point. The phase transitions from solid to liquid have been identified by a simple jump in the total energy curve, with the predicted melting temperature near the bulk melting point (1941.15 K). As expected, the RDF’s and density profile peaks decrease with increasing temperature.

KEYWORDS
Molecular dynamics, titanium cluster, radial distribution functions, diffusion coefficient, mean square displacement.

1. Introduction
Transition metal nanoclusters have attracted extensive investigation over the past decades due to their unique properties, which lie somewhere between those of bulk and single-particle species. They have many fascinating potential uses, including quantum computers or quantum dots, light-emitting diodes, chemical sensors and photochemical applications such as flat-panel displays.

Supported nanoclusters are also widely used in catalysis as a large percentage of a nanocluster’s metal atoms lie on the surface, and the configurations and electronic properties of surface atoms may differ substantially from those of the bulk. Moreover, the thermodynamics and other properties near the melting points of metallic nanoclusters are typically very different from those observed for corresponding bulk phases, thus also driving both theoretical and experimental interest in nanoclusters.

For many years, theoretical studies have been used to predict structural properties and reactivity of nanoclusters or nanoparticles, including the reduced heats of formation, surface premelting, size dependence of melting temperatures, and solid-liquid like phases. These predictions on the behaviour of the nanoclusters have also been confirmed using experiments. It was further reported that the melting point strongly depends on the cluster size. However, clusters of smaller sizes do not show pronounced melting temperatures. Moreover, classical molecular dynamics (MD) simulation was found to be both a reliable and a standard approach used to study the phase transition of the materials. The interest in applying this approach was to gain insight into the thermal stability and melting behaviour of clusters.

Employing MD, Wang et al. and Cleveland et al. investigated the melting behaviour of clusters and nanowires, focusing first on the melting temperature, thermal stability and mechanical properties during the melting process; secondly, on the structural evolutions and mechanical properties during heating; and thirdly on the variation of structural characteristics and size effects with temperature. Cleveland et al. reported a low temperature structural solid-solid transition, from the optimal structural motif to icosahedral structures, as a precursor to melting. Compared to the bulk phase, they predicted a lower melting temperature for nanoclusters. Moreover, a much earlier investigation of Borel reported that the melting temperature decreases with decreasing diameter of the nanoclusters. Similarly, Wang et al. found a structural transition within titanium nanowires below the melting point.

In addition to identifying the melting temperature of nanoclusters, some of the main findings include the broadening of the melting transition and the appearance of a characteristic S-shaped loop in the caloric curve. Other studies used the potential energy distribution of atoms in nanoclusters to explain many phenomena related to the phase transition of nanoclusters. Lee et al. found a new type of premelting mechanism in the Pd$_{34}$ nanocluster. However, Breaux et al. reported that Ga$_n$ nanoclusters (n = 17, 20, 30–50, 55) melt at temperatures ranging from 500–800 K and bulk Ga melting at a mere 303 K.

We have previously investigated the structural evolution of Ti$_n$ (n = 2–32) ground state nanoclusters and the evolution of their electronic structure. The ground state configurations were predicted using an evolutionary algorithm to find low energy local minima on the energy landscape defined by interatomic potentials. The atomic configurations were subsequently refined using an electronic structure approach.

The chosen global optimization was implemented within the
Knowledge Led Master Code (KLMC), which calls external codes GULP and FHI-aims in order to evaluate the energy and locally optimize the configurations.

This study focuses on the characteristics of ground-state configuration predicted for the Ti32 nanocluster using molecular dynamic simulation. Ti32 nanocluster is formed by four interpenetrating pentagonal fragments. It was also revealed that the 32 atom titanium nanocluster resembles a low-temperature hcp α-Ti. This structure was deduced from the predicted binding energy data as the cluster evolved towards the bulk system. In the next section, we outline the technique employed to simulate the melting behaviour of the Ti32 nanocluster. In section 3, we discuss the effect of temperature on the electronic and structural evolution of the 32-atom titanium nanocluster.

2. Methodology

The initial atomic configuration was taken from our previous study, where a genetic algorithm was employed to predict the ground state for Ti32. The energy landscape explored in our earlier work is defined by a combination of a Born-Mayer two-body and Embedded atom method (EAM) interatomic potentials. To properly simulate the thermodynamic properties of the Ti32 nanocluster, the EAM and the Born-Mayer interatomic potentials reported by Lazauskas et al. were incorporated together to express the total internal energy of pure metals in terms of Gupta potentials. Based on the second moment approximation of tight-binding theory, the Gupta potential and ion-ion interaction are described by an electronic band and a repulsive term. The total potential of system N atoms located at positions is expressed as follows:

\[ U = \sum_{i=1}^{N} \sum_{j>i} A \exp\left[-\frac{d_{ij}}{\sigma}\right] - \frac{1}{2} \sum_{i=1}^{N} \sum_{j>i} \sum_{k>i} Z_{ij} Z_{ik} \frac{d_{ij}}{\sigma_d} \exp\left[-\frac{d_{ij}}{\sigma}\right] \]

where the first term represents repulsive many-body and the second term represents the attractive many-body. In this approach, both terms are introduced in the exponential form, where d is the first-neighbour distance, \( \xi \) is an affective overlap integral between the electronic orbitals of the neighbouring atom, q and p control the decay of the exponential function related to bulk elastic constants. The MD simulations (heating/melting process) were performed in the NVT canonical ensemble. The nanocluster was confined in a cubic unit cell (at fixed lattice parameter, a = b = c = 50 Å) with periodic boundary conditions applied in the x, y, z directions implemented within DL_POLY software.

The temperature T was controlled by the Nose Hoover thermostat with a relaxation time of 0.001 ps. The time integration of the equation of motion was performed using the velocity Verlet leapfrog algorithm. The interatomic interactions were truncated at the cutoff radius of 4 Å.

One independent MD run was performed for 23 fixed temperatures, with 300 K as our lowest chosen temperature and 2400 K our highest. A run time of 300 ps was employed to equilibrate the cluster before collecting data for 600 ps.

3. Results and Discussion

3.1. Temperature Effect on the Ti32 Nanocluster

The minimum energy cluster for Ti32 is presented in Fig. 1. The snapshots of the thermally agitated Ti32 nanocluster are analyzed in detail to gain more insights regarding structural transition as a function of temperature (T). Note that the Ti32 nanocluster shows various geometrical configurations as the temperature is increased. The dominant configurations are a triangular bi-pyramid (Ti3), an octahedron (Ti6), a pentagonal bi-pyramid (Ti7), an icosahedron (Ti13), and interpenetrating icosahedra (Ti19), as shown in Fig. 1.

The temperature dependence of the equilibrium cluster structure for Ti32 is shown in Fig. 2 (see supplementary information). It was found that the configurational transitions involve distortion or displacement of atoms in the Ti32 nanocluster as the temperature increases. The distortion of the Ti32 nanocluster becomes more frequent from lower temperatures and increasingly severe with increasing temperature. The structural transients are shown in different colour coding as the structure of T32 nanocluster changes as a function of temperature.

The initial configuration starts as interpenetrating icosahedra, where one of the icosahedra is replaced with an icositetrahedra geometry. The transient at 300 K has two interpenetrating icosahedral units (maroon) with two pentagonal bi-pyramids (green and blue). As the temperature increases, the atomic displacement about the initial positions increases and leads to a change in the morphology of the nanocluster at 400 K to a Ti19 unit (red) interpenetrating with two pentagonal bi-pyramids, Ti7 (blue and lime-green), added on the sides of the Ti19. This change may be attributed to atoms in a solid that undergo vibrations about the equilibrium position, leading to distortions of crystal nanocluster. The transition of the nanocluster at 500 K is observed to have Ti32 (blue) polyhedron interpenetrating with icosahedron (gold), triangular bi-pyramid (violet) and an atom (red) connecting the triangular pyramidal and icosahedral units or nanoclusters. At 600 K, the nanocluster transitions to a Ti19 (gold) polyhedron interpenetrating with a Z13 Frank Casper polyhedron Ti14 (blue) and a triangular bi-pyramid (lim-green). The effect of thermal agitation at 700 K changes the Ti32 morphology into two interpenetrating Ti19 (gold and blue) polyhedra with a triangular unit connected to the Ti19 polyhedron described by the blue colour. At 800 K, the two Z12 Frank Kasper polyhedral Ti13 (green and blue) form the transient unit interconnected to pentagonal bi-pyramid (lime-green), triangular unit (violet) and an atom (red). The Ti13 nanocluster (maroon) was observed to coexist with four pentagonal bi-pyramids (blue, green, and gold) at 900 K. Two interpenetrating icosahedra (lime-green and blue) complemented by tetra-capped atoms (violet and maroon) on the sides are found to be the transient for 1000 K. The transition occurring at 1100 K leads to two icosahedra connected by dimers (black and lime-green).

Furthermore, for higher thermal agitation, these fragmenta tion patterns reveal the existence of a stable building block.
namely an icosahedron, or interpenetrating pentagonal bi-pyramid. At 1200, the coexistence of three-pentagonal bi-pyramid (blue, black and maroon) and triangular unit connecting all the penta-shaped units or nanoclusters with a dimer (lime-green) connecting the blue, maroon and black penta-shaped units. The transient observed for 1300 K comprises two icosahedral polyhedra (blue and lime-green) connected by six atoms. However, at 1400 K, the two interpenetrating icosahedra (blue and green) are found to coexist with a triangular bi-pyramid unit as well as a complementing dimer connecting the other fragments.

The structural transformation precursor at 1500 K is found to be two icosahedral fragments (lime-green and blue) connected by the hexagonal ring (violet, lime-green and black) or triangular bi-pyramid (violet) with an atom (black) connecting the icosahedra and triangular bi-pyramid. Furthermore, the structural transition for 1600 K, shown in Fig. 3 (see supplementary information), is noted to be two icosahedral isomers connected by triangular bi-pyramid shaped nanocluster (violet) and triangular unit (black). At 1700 K, two interpenetrating icosahedra (blue and violet) capped on top of one of the icosahedral configurations (lime-green) with an atom (black) was observed. The transient for 1800 K is found to be the icosahedron (maroon) bi-pentagonal bi-pyramid (blue and green) with tetra-coordinated capping atoms (black) completing the structure.

At 1900 K, the nanocluster transitions into three interpenetrat-
The most striking feature of these results is that the maximum in the total energy occurs at a temperature above the bulk melting point. In addition, there have been theoretical reports that small nanoclusters have elevated melting temperatures. Upon cooling, the cluster undergoes a liquid-solid transition. The nanocluster energies become lower from 600–300 K, 1000 K, 1400 K, 1900 K and 2000 K, suggesting the formation of a new stable configuration. There are cooling energies higher than heating energies observed at 800 K, 1500 K, 1700 K, 2100 K, 2200 K and 2300 K, respectively, suggesting the transition to less stable configurations. The solid-liquid and liquid-solid transition have similar energies at 700 K, 900 K, 1100–1300 K, 1600 K, 1800 K and 1941.15 K suggesting similar configurations. A weak hysteresis was observed at 2000 K, suggesting a phase change accompanied by the formation of new geometry. The melting-quenching cycle discloses that it is easier for the nanocluster to go from the solid-liquid phase than the liquid-solid phase, as observed from the total energy data.

In the case of the configuration energy in Fig. 4b, it is observed that at temperatures 300–700 K, the energy is constant, followed by a dip at 800 K, which results in a lower energy nanocluster compared to other temperatures. However, a sudden jump in the energy from 800–1000 K, is followed by the linear increase from 1000–1200 K. Furthermore, a stepwise increase in energies at temperatures from 1300–2300 K is observed, with an abrupt jump in the energy at 1941.15 K that is higher than other temperatures (1900 K and 2000 K). The abrupt jump may be attributed to the phase transition of the nanocluster from a solid phase to a liquid phase.

### 3.1.1. Heating and Cooling for Ti$_{32}$ Cluster

The melting transition of the cluster from a rigid or solid form in which atoms merely oscillate about the equilibrium structure to a liquid or fluid form characterized by atoms leaving their equilibrium basins and finding new ones with new equilibrium positions is spread over a range of temperatures from 300–2400 K. Figure 4a shows the energy varying smoothly with temperature up to 2000 K where it depicts a jump in the total energy closer to the melting temperature of bulk Ti. Thus, this behaviour may be ascribed to a solid-liquid phase transition that is in excellent agreement with the melting point of bulk Ti (1941.15 K). This positive deviation from linearity in the total energy may be attributed to the tendency of the nanocluster undergoing surface melting.

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### 3.1.2. The Diffusion Coefficient for Ti$_{32}$

Figure 5 shows the diffusivity, which was calculated from the mean square displacement at increasing temperature. The figure depicts no movement of atoms at temperatures lower than 1941.15 K, where the diffusivity reverts to zero. At 2000 K, the atoms appear to have a noticeable movement followed by a diffusivity jump at 2100 K, which might indicate the transition of the nanocluster from solid phase to liquid phase.

These observed transitions are justifiable since the melting temperature for Ti bulk is 1941.15 K which is closer to 2100 K. It is also noticed that as the cluster changes its shape, the diffusivity reverts to zero until the melting temperature is reached. This behaviour may be due to nanocluster transforming into a liquid phase and consequently resulting in surface melting. Similar behaviour was noted for Pd-Pt clusters. Their transition
temperature was observed to be in the temperature range 800–1200 K, corresponding to the surface melting stage. However, both Pd and Pt diffusion coefficients tended to increase with temperature whilst a decline is observed in this study. The decline behaviour might be due to differences in atomic sizes and the number of atoms in the cluster.

3.1.3. Radial Distribution Function and Density Profiles for the Ti32 Cluster

In Fig. 6a, the RDFs and the atomic distribution curves against temperature are shown. The 300 K peak shows that the nanocluster has a well-ordered structure.

However, as the temperature increases, the peaks become broader and decrease, indicating a phase change. The reduction in the probability of the peaks may be ascribed to nanocluster changing phases or fragments, which at some point will transition from a solid phase to a liquid phase at an elevated temperature near or above the melting point. This observation is in line with previous reports. The reduction in the sharpness of the peaks is indicative of the reduced crystallinity of the nanocluster, which results in the production of new configurations. Thus, representing the evolution of the nanocluster during heating.

In the case of the density profile plot (Fig. 6b), the atomic distribution of Ti32 nanocluster along the axis at different temperatures shows various trends. At lower temperatures, the distinct peaks indicate the solid-like features, where atoms have higher distribution at a certain distance from the centre. This plot depicts overlap of the peaks at 300 K and 800 K, suggesting that the nanocluster is still in its solid form. However, from 1400–1941.15 K, the peaks are observed to decrease and overlap, indicating minor thermally agitated changes in the system, i.e., the nanocluster is still in a solid phase.

Furthermore, it becomes easier to observe the changes along the Z (A) axis. As the temperature increases, the peaks become broader, decreasing the peak size due to uniformly distributed atoms in the liquid phase at elevated temperatures. Moreover, at 2000 K, which is beyond the bulk melting temperature, atomic distribution becomes extensively shorter, and the new peaks emerging allude to a liquid phase formation.

4. Summary and Conclusion

The molecular dynamics (MD) simulations were carried out to investigate the characteristics of the ground state configuration predicted for the Ti32 nanocluster. The thermal agitation shows the dominance of icosahedra, and pentagonal bipyramid geometries below 2000 K. As the temperature increases, the ordering of configurations or isomers changes are noticeable by a change in the morphology of the cluster at 400 K. We also observed a jump in the potential energy at 2000 K which is closer to the melting temperature of bulk Ti suggesting a transition from a solid phase to a liquid phase. The maxima in the potential energy occur at a temperature above bulk melting. However, upon cooling, the nanocluster is mostly solid below the melting temperature. We notice a weak hysteresis at 2000 K due to the structural changes as we cool the temperature.

As a consequence, the cooling transition occurs close to the melting temperature with the nanocluster, which is equivalent to the initial one. The diffusion coefficient results suggest no movement of atoms at temperatures below 1941.15 K; thus, the diffusivity reverts to zero. A noticeable vibration is observed above 2000 K, resulting in a jump in diffusivity at 2100 K. The RDFs shows the peaks decreasing with increasing temperature, and the density profiles reveal the melting temperature behaviour beyond bulk melting temperature, where atomic distribution becomes broader and shorter, and the new peaks emerging.

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![Figure 5](https://journals.sabinet.co.za/content/journal/chem/)

Figure 5  The diffusion coefficient for the Ti32 cluster showing phase changes at temperatures above the bulk Ti melting.

![Figure 6](https://journals.sabinet.co.za/content/journal/chem/)

Figure 6 (a) Radial distribution functions (RDF) and (b) the atomic distribution of Ti32 nanocluster along a Cartesian coordinate (z) at different temperatures.
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Supplementary Material
Supplementary information is provided in the online supple-
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1. Lattice geometry and ionic positions for Ti$_{32}$ at 300 K.

Format: XYZ file

|      |          |          |          |          |
|------|----------|----------|----------|----------|
| Ti   | -4.54666545 | 1.74008362 | 1.49626329 |
| Ti   | -4.74260780 | 0.83178665 | -0.94363262 |
| Ti   | -3.93857361 | 3.56455838 | -0.77847782 |
| Ti   | -3.44661830 | -0.58587495 | 0.96884685 |
| Ti   | -2.86438705 | 3.64574343 | 1.97224577 |
| Ti   | -1.86628293 | 1.17602400 | 2.45751194 |
| Ti   | -1.45731630 | 4.82527912 | -0.07961654 |
| Ti   | -2.22244554 | 1.73076495 | -0.13462636 |
| Ti   | -3.29633106 | 1.66934408 | -2.96571585 |
| Ti   | -2.70980713 | -0.88948005 | 1.64899221 |
| Ti   | -1.56272073 | 3.48356872 | -2.40635320 |
| Ti   | -0.18918204 | 3.31514708 | 2.01151072 |
| Ti   | -0.79635752 | -0.62136586 | 0.24574287 |
| Ti   | 1.23391571 | 5.14361754 | 0.55237043 |
| Ti   | 0.34551076 | 2.76665599 | -0.55571768 |
| Ti   | -0.96920349 | 1.91855838 | -4.6549581 |
| Ti   | 0.47842810 | 5.20014434 | -1.97460115 |
| Ti   | -0.66291296 | 0.83355581 | -2.20900978 |
| Ti   | 0.80102965 | 0.79761610 | 1.58925932 |
| Ti   | -1.78031608 | -0.57955159 | -4.12812922 |
| Ti   | -0.01979110 | -1.72291643 | -2.09862714 |
| Ti   | 1.19405491 | 2.60081483 | -3.06891562 |
| Ti   | 2.52784968 | 2.88427990 | 1.35294614 |
| Ti   | 1.70964301 | -1.77567569 | 0.17361538 |
| Ti   | 1.85758286 | 0.58270254 | -0.93360122 |
| Ti   | 2.87137486 | 3.73030728 | -1.34210858 |
| Ti   | 1.18976486 | 0.10448976 | -3.97688516 |
| Ti   | 2.64850135 | -1.60545951 | -2.48913107 |
| Ti   | 3.39159575 | 0.08627286 | 1.47896064 |
| Ti   | 3.62493641 | 1.13163737 | 2.86948315 |
| Ti   | 4.47836651 | 1.84410858 | 0.27256971 |
| Ti   | 4.38206540 | -0.75346386 | 0.72460533 |
2. Lattice geometry and ionic positions for Ti$_{32}$ at 400 K.

Format: XYZ file

|          | X         | Y         | Z         |
|----------|-----------|-----------|-----------|
| Ti       | -4.1503   | 0.8107    | 1.0792    |
| Ti       | -1.6649   | 0.7205    | 2.9265    |
| Ti       | -2.4545   | -1.6834   | 2.2228    |
| Ti       | -3.1692   | 2.7652    | -0.6104   |
| Ti       | -3.6148   | -1.6372   | -0.1875   |
| Ti       | -3.9741   | 0.5169    | -1.7934   |
| Ti       | -2.2801   | 2.9924    | 1.8861    |
| Ti       | -0.8851   | -2.3401   | -0.1283   |
| Ti       | -1.6766   | 0.3560    | 0.1507    |
| Ti       | -2.2801   | 2.9924    | 1.8861    |
| Ti       | -0.8851   | -2.3401   | -0.1283   |
| Ti       | -1.6766   | 0.3560    | 0.1507    |
| Ti       | -2.2801   | 2.9924    | 1.8861    |
| Ti       | -0.8851   | -2.3401   | -0.1283   |
| Ti       | -1.6766   | 0.3560    | 0.1507    |
| Ti       | -2.2801   | 2.9924    | 1.8861    |
| Ti       | -0.8851   | -2.3401   | -0.1283   |
| Ti       | -1.6766   | 0.3560    | 0.1507    |
| Ti       | -2.2801   | 2.9924    | 1.8861    |
| Ti       | -0.8851   | -2.3401   | -0.1283   |
| Ti       | -1.6766   | 0.3560    | 0.1507    |
| Ti       | -2.2801   | 2.9924    | 1.8861    |
| Ti       | -0.8851   | -2.3401   | -0.1283   |
| Ti       | -1.6766   | 0.3560    | 0.1507    |
| Ti       | -2.2801   | 2.9924    | 1.8861    |
| Ti       | -0.8851   | -2.3401   | -0.1283   |
| Ti       | -1.6766   | 0.3560    | 0.1507    |
| Ti       | -2.2801   | 2.9924    | 1.8861    |
| Ti       | -0.8851   | -2.3401   | -0.1283   |
| Ti       | -1.6766   | 0.3560    | 0.1507    |
| Ti       | -2.2801   | 2.9924    | 1.8861    |
| Ti       | -0.8851   | -2.3401   | -0.1283   |
| Ti       | -1.6766   | 0.3560    | 0.1507    |
| Ti       | -2.2801   | 2.9924    | 1.8861    |
| Ti       | -0.8851   | -2.3401   | -0.1283   |
| Ti       | -1.6766   | 0.3560    | 0.1507    |
| Ti       | -2.2801   | 2.9924    | 1.8861    |
| Ti       | -0.8851   | -2.3401   | -0.1283   |
| Ti       | -1.6766   | 0.3560    | 0.1507    |
| Ti       | -2.2801   | 2.9924    | 1.8861    |
| Ti       | -0.8851   | -2.3401   | -0.1283   |
| Ti       | -1.6766   | 0.3560    | 0.1507    |
| Ti       | -2.2801   | 2.9924    | 1.8861    |
| Ti       | -0.8851   | -2.3401   | -0.1283   |
| Ti       | -1.6766   | 0.3560    | 0.1507    |
| Ti       | -2.2801   | 2.9924    | 1.8861    |
| Ti       | -0.8851   | -2.3401   | -0.1283   |
| Ti       | -1.6766   | 0.3560    | 0.1507    |
3. Lattice geometry and ionic positions for Ti$_{32}$ at 500 K.

Format: XYZ file

|       |       |       |
|-------|-------|-------|
| Ti    | 0.431972 | -0.224854 | -3.542267 |
| Ti    | 2.897534 | -1.520845 | -2.343975 |
| Ti    | 2.658995 | 1.249110  | -3.112118 |
| Ti    | 0.226155 | -2.493015 | -2.013282 |
| Ti    | 0.655416 | 2.207507  | -4.868825 |
| Ti    | -1.980367 | 1.361883  | -3.933204 |
| Ti    | 4.297407 | 0.732940  | -1.027029 |
| Ti    | 1.357897 | -0.084555 | -0.795566 |
| Ti    | 3.550624 | -1.163240 | 0.602470  |
| Ti    | 1.742918 | -2.930926 | 0.066339  |
| Ti    | 2.783841 | 1.335689  | 1.312494  |
| Ti    | -0.983798 | 4.100081  | -3.633721 |
| Ti    | -1.477891 | 0.210078  | -1.208908 |
| Ti    | 1.858316 | 4.003276  | -3.230742 |
| Ti    | 0.268102 | 2.104423  | -2.213450 |
| Ti    | 0.944222 | 1.644117  | 3.196959  |
| Ti    | 2.545788 | 2.872452  | -0.766102 |
| Ti    | -0.026863 | 1.830855  | 0.530783  |
| Ti    | -3.686531 | 3.581806  | -3.216739 |
| Ti    | 1.134331 | -0.772075 | 1.864785  |
| Ti    | -0.765159 | -1.877976 | 0.433411  |
| Ti    | 0.993396 | 3.983696  | 1.632397  |
| Ti    | -2.501292 | 5.505766  | -1.813020 |
| Ti    | -4.109502 | 1.346860  | -1.678718 |
| Ti    | -2.021363 | 2.889233  | -1.408389 |
| Ti    | 0.256397 | 4.624318  | -1.110152 |
| Ti    | -1.358791 | 0.224656  | 2.236267  |
| Ti    | -3.377079 | -0.774116 | 0.318341  |
| Ti    | -4.390863 | 3.832885  | -0.657041 |
| Ti    | -1.406292 | 2.861327  | 2.785219  |
| Ti    | -1.820761 | 4.519904  | 0.820869  |
| Ti    | -3.033658 | 1.892015  | 0.816893  |
4. Lattice geometry and ionic positions for Ti$_32$ at 600 K.

Format: XYZ file

```
50.0000000000 0.0000000000 0.0000000000
0.0000000000 50.0000000000 0.0000000000
0.0000000000 0.0000000000 50.0000000000

Ti  4.29359883  1.41865620 -2.44312250
Ti  4.25121065 -0.11030434 -0.21956876
Ti  3.23051587  2.56783029  0.09783292
Ti  3.32596181 -1.21450902 -2.70886218
Ti  2.25411930  3.23122101 -2.58424074
Ti  2.06023180  0.92910484 -4.15700882
Ti  2.23913248  5.00285209 -0.56937434
Ti  1.93729541  0.75032928 -1.44484538
Ti  1.95515088  0.56996537  1.40502599
Ti  2.07215402 -1.78170234 -0.13497883
Ti  1.26716669  3.37942879  2.04186801
Ti -0.34490949  3.17257792 -4.43047323
Ti -0.58473629 -1.39753514  2.66585423
Ti -0.05253500  4.91451513 -2.08628202
Ti  0.36587451  2.77837526 -0.38478443
Ti -0.65138587  1.04470602  1.91664676
Ti -0.11385767  5.59165962  0.58398321
Ti -0.11506535 -0.15920164 -0.28211572
Ti -0.39679602  1.33649691 -2.67071054
Ti  0.11896375 -1.71340798  1.92969935
Ti -0.58409531 -2.78214534 -0.39017163
Ti -1.61182069  3.53770840  1.78850290
Ti -2.00457520  3.44850494  3.09735809
Ti -2.25097746 -1.08551531 -1.92162247
Ti -2.08857228  1.72666164 -0.54548517
Ti -2.39332938  4.45752146 -0.70682576
Ti -3.26463352  1.11225781  1.99551349
Ti -2.43689156 -1.16166572  0.86548435
Ti -3.30636616  1.01332173 -3.13614690
Ti -4.39204480  3.06181250  0.59126314
Ti -4.54774613  2.99201908 -1.98757706
Ti -4.40722865  0.44173393 -0.60443321
```

5
5. Lattice geometry and ionic positions for Ti$_{32}$ at 700 K.

Format: XYZ file

|        |          |          |          |
|--------|----------|----------|----------|
|        | 50.0000000000 | 0.0000000000 | 0.0000000000 |
|        | 0.0000000000 | 50.0000000000 | 0.0000000000 |
|        | 0.0000000000 | 0.0000000000 | 50.0000000000 |

| Ti     | 2.94256387 | 1.64989933 | 1.43067445 |
| Ti     | 1.99100525 | -0.80108794 | 2.50990522 |
| Ti     | 1.13739957 | 4.22237711 | 1.65562647 |
| Ti     | 1.27351528 | -2.67696880 | 0.6591985 |
| Ti     | 3.49051221 | 3.65609936 | -0.27777744 |
| Ti     | 1.84843300 | -1.44242403 | -2.00344207 |
| Ti     | 3.54863679 | -1.10329939 | 0.34483776 |
| Ti     | 1.15596676 | 0.02147128 | 0.19003386 |
| Ti     | 0.29660268 | 1.47842336 | 2.35024399 |
| Ti     | -0.65753648 | -1.15206630 | 1.86221756 |
| Ti     | 0.81393962 | 2.79464934 | -0.42054729 |
| Ti     | 2.39183002 | 0.41720303 | -3.80025914 |
| Ti     | -0.68025708 | 1.66139698 | -1.10902421 |
| Ti     | 3.11286234 | 1.08862291 | -1.23254045 |
| Ti     | 0.13866430 | 0.97291539 | -2.32230677 |
| Ti     | -2.62644125 | 0.73234310 | 2.45175281 |
| Ti     | 1.62811720 | 5.25752493 | -1.18024726 |
| Ti     | -1.34002912 | 0.76561992 | 0.12152141 |
| Ti     | -0.23311436 | -0.94957804 | -0.06145482 |
| Ti     | -3.14811501 | -1.11818834 | 0.37588329 |
| Ti     | -2.68239931 | 0.05171042 | -2.34133097 |
| Ti     | -1.69792149 | 3.15089396 | 1.34274860 |
| Ti     | 2.20605423 | 2.98359309 | 2.91648122 |
| Ti     | -1.97875015 | 1.95530405 | -4.08713711 |
| Ti     | -1.84074687 | 2.73253805 | -1.38849236 |
| Ti     | -0.93012841 | 5.1040268 | -0.49663162 |
| Ti     | -3.96184430 | 1.53726770 | 0.12351731 |
| Ti     | -4.36482209 | 2.38093427 | -2.50149547 |
| Ti     | -0.10348232 | 4.09118343 | -3.09008667 |
| Ti     | -3.69808332 | 4.25213183 | -0.27530976 |
| Ti     | -2.80397515 | 4.68185459 | -3.02578447 |
| Ti     | 0.43464433 | 1.97332006 | -4.84419536 |
6. Lattice geometry and ionic positions for Ti32 at 800 K.

Format: XYZ file

50.0000000000 0.0000000000 0.0000000000
0.0000000000 50.0000000000 0.0000000000
0.0000000000 0.0000000000 50.0000000000

| Ti   | x          | y          | z          |
|------|------------|------------|------------|
| -0.52136975 | -2.93398761 | -1.34305914 |
| -1.62217820 | -1.15158052 | -3.03788326 |
| 0.03637871  | -0.56328421 | -0.08950942 |
| 1.28103170  | -1.18327619 | -2.24720958 |
| -2.50878749 | -0.92734153 | -0.46435149 |
| 1.70403779  | -2.57576437 | 0.22551719  |
| -0.93482801 | -2.79235319 | 1.31224332  |
| -0.50066413 | 1.00204248  | -2.19697235 |
| -1.92657528 | 1.25404474  | -4.55023118 |
| 0.56656198  | 0.13733766  | -4.54868979 |
| -4.09669857 | 0.97238275  | 0.83880664  |
| 2.99784873  | 1.76436881  | 1.89163210  |
| 2.47499938  | 1.33086999  | -2.68809948 |
| 1.66983131  | -0.63472883 | 2.01952919  |
| 1.30546897  | 1.66252941  | -0.16221594 |
| -3.05255496 | 1.26194614  | -2.10072389 |
| -2.43222944 | 2.39201102  | 2.29702410  |
| -0.11551544 | 3.51635791  | -1.37697404 |
| 3.16410079  | -0.22357860 | -0.24889119 |
| -2.32739921 | 3.67524186  | -2.84797828 |
| 0.28146894  | 2.71426904  | -4.04986375 |
| -3.38372905 | 3.57618380  | -0.17688177 |
| 0.29190906  | 1.63228662  | 2.33244983  |
| 2.25022506  | 3.98218979  | -2.40401393 |
| -1.52400583 | 1.71508347  | 0.04040262  |
| -1.67769808 | -0.22224897 | 2.04212585  |
| -1.89994532 | 5.70940292  | -1.24485561 |
| -0.12040828 | 5.25267707  | -3.33916893 |
| 3.89635511  | 2.47964237  | -0.59949246 |
| -0.63811076 | 4.25537321  | 1.07523937  |
| 2.11516016  | 4.08209773  | 0.62009789  |
| 0.91042085  | 5.91307861  | -0.93402448 |
7. Lattice geometry and ionic positions for Ti\(_{32}\) at 900 K.

Format: XYZ file

|      |          |          |          |
|------|----------|----------|----------|
| Ti   | -3.2296327 | 0.60239816 | -1.40296004 |
| Ti   | -1.04883704 | 4.20218064 | 0.68227035 |
| Ti   | -1.84030362 | 0.48660635 | -3.64266440 |
| Ti   | 1.63142563 | 3.93566179 | 1.83143631 |
| Ti   | -3.28606210 | 2.80719242 | -3.12233180 |
| Ti   | -3.48210412 | 3.30667391 | -0.53368342 |
| Ti   | 0.15639020 | -1.87514308 | -3.42661313 |
| Ti   | -1.99012339 | 1.53539678 | 0.69403349 |
| Ti   | -3.26001328 | 3.15090480 | 2.39254881 |
| Ti   | -0.51051023 | 2.19884396 | 2.88105484 |
| Ti   | -4.56727418 | 0.80953351 | 1.21428263 |
| Ti   | -1.04379139 | 2.99134215 | -4.51765070 |
| Ti   | 0.75037985 | 1.94445231 | 0.36687243 |
| Ti   | 0.00118490 | -2.39364355 | -0.27401413 |
| Ti   | -0.38556957 | -0.04690457 | -1.32015894 |
| Ti   | -2.60916537 | 0.48172604 | 3.12404671 |
| Ti   | -2.05978383 | -1.89461569 | -1.93876591 |
| Ti   | 2.04885609 | 1.60303943 | -1.75046146 |
| Ti   | -1.41452278 | 4.88010930 | -2.22556448 |
| Ti   | 2.16179901 | 1.25318001 | 2.58230814 |
| Ti   | 3.48075161 | 2.51507952 | 0.41467994 |
| Ti   | -2.38980031 | -1.09498221 | 0.68996465 |
| Ti   | 0.70432320 | 0.79305477 | -3.97020842 |
| Ti   | 1.19872725 | 4.34400053 | -0.93448605 |
| Ti   | 0.86495946 | 2.42719587 | -1.73624700 |
| Ti   | 2.17727724 | -0.38756730 | 0.08264209 |
| Ti   | -0.11743893 | -0.28998539 | 1.75966624 |
| Ti   | 4.62302582 | 0.91900711 | -1.65037781 |
| Ti   | 1.24338778 | 3.46228236 | -3.54309950 |
| Ti   | 2.51459856 | -0.79026951 | -2.51250685 |
| Ti   | 3.28686672 | 1.47828883 | -4.00002807 |
| Ti   | 3.78432974 | 3.71823415 | -2.1700639 |
8. Lattice geometry and ionic positions for Ti$_{32}$ at 1000 K.

Format: XYZ file

```
50.0000000000 0.0000000000 0.0000000000
0.0000000000 50.0000000000 0.0000000000
0.0000000000 0.0000000000 50.0000000000

Ti  0.71983952  1.54236427 -4.33744936
Ti  3.04082485 -0.43410389 -1.05150172
Ti  1.12219514 -2.46730775 -0.24143506
Ti  2.57989018  3.31090161 -4.01335977
Ti -1.60442292  2.86940159 -4.59238115
Ti -0.01976401  5.44788204 -0.68691106
Ti  0.74507634  1.00711282  2.20329608
Ti  1.70955732  1.78555077 -1.97491140
Ti -0.97653286 -1.91871064 -1.90814120
Ti  3.58784265  2.80126782  2.27453060
Ti  0.97876500 -0.78357510 -2.96088287
Ti  4.26007668  2.24465001 -1.99362096
Ti -1.48213106  0.24785127 -3.56006427
Ti  0.45548462 -0.04312178  2.0329608
Ti -3.39271051  2.05353022 -3.05803191
Ti -3.91697168  0.18980307 -3.6060671
Ti  3.26951151  0.53150142 -3.76520628
Ti -1.65986930  1.44648807  0.79057499
Ti  2.56149189  4.24092203 -1.23596715
Ti  0.42878918 -1.73735168  2.2891122
Ti -1.85952457  0.28482548  3.06704141
Ti -1.63741926 -1.22923504  0.69958493
Ti  3.18339835  1.92435005  0.42280213
Ti -3.75911370  2.66044463 -0.57926630
Ti -0.91689248  2.29807767  1.78320148
Ti  0.39439738  4.50847049 -3.16355104
Ti -0.96601102  3.02977444  2.93389238
Ti -2.29782611  4.63884834 -2.28708503
Ti -3.10366386  0.02645222 -1.10219431
Ti -2.05289735  4.24546053  0.66485012
Ti  0.74911502  3.11696319  0.44206530
Ti  2.69828111 -0.76621482  1.52617291
```
9. Lattice geometry and ionic positions for Ti$_{32}$ at 1100 K.

Format: XYZ file

| X           | Y           | Z           |
|-------------|-------------|-------------|
| 50.0000000000 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 50.0000000000 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 50.0000000000 |

| Ti  | -1.10116610 | 2.51277279  | -3.09873473 |
| Ti  | -0.71768472 | -0.06902173 | -3.14657944 |
| Ti  | -2.75171575 | -0.91827436 | -1.09506641 |
| Ti  | 1.35340181  | 1.32677274  | -4.20827225 |
| Ti  | 3.54822441  | 3.3229705   | -4.55566754 |
| Ti  | -1.07901968 | 0.89299191  | 3.68701495  |
| Ti  | 3.58704658  | 1.50692572  | -1.99954380 |
| Ti  | -2.73663077 | 3.62179580  | -1.23758972 |
| Ti  | -3.43600701 | 1.21683142  | -2.57894897 |
| Ti  | -2.04115954 | 2.64850008  | 1.53282095  |
| Ti  | -1.42536518 | -2.67411746 | 1.04170785  |
| Ti  | -0.66635778 | 5.10925197  | -2.75206240 |
| Ti  | -4.23438170 | 1.24115361  | 0.07928708  |
| Ti  | 2.67789668  | 3.24414445  | -0.08857145 |
| Ti  | 1.61494237  | 3.60038252  | -2.59660965 |
| Ti  | -2.24930555 | -1.45080805 | 3.60741074  |
| Ti  | 0.03981925  | -0.89450330 | -0.65701925 |
| Ti  | -4.00322185 | 0.85133094  | 2.77664902  |
| Ti  | -2.04289442 | -0.05804546 | 1.28410017  |
| Ti  | 2.04483285  | -2.47479569 | 0.40448154  |
| Ti  | 1.82346792  | 5.75245436  | -1.03079216 |
| Ti  | 0.48859664  | 1.44358002  | 1.48230585  |
| Ti  | 2.06513443  | -0.86243721 | -2.37753511 |
| Ti  | -0.16666897 | 3.75639200  | -0.42957167 |
| Ti  | 1.00255808  | 1.48316247  | -1.41603751 |
| Ti  | 2.12052925  | 5.73668983  | -3.94765070 |
| Ti  | -4.13293113 | -1.53165196 | 1.29047307  |
| Ti  | 2.54824756  | 0.19034793  | 0.16611722  |
| Ti  | 4.08558071  | 4.64983554  | -2.28884249 |
| Ti  | 0.33044392  | -1.26092030 | 2.17262547  |
| Ti  | -1.54373405 | 1.33626205  | -0.82816981 |
| Ti  | 0.66062250  | 3.82397369  | -5.14775071 |
10. Lattice geometry and ionic positions for Ti$_{32}$ at 1200 K.

Format: XYZ file

| Ti      | x     | y     | z     |
|---------|-------|-------|-------|
| -3.2494521 | -2.29358213 | 0.18457825 |
| -0.07733300 | 4.30548945 | -3.40084304 |
| -1.32328876 | 2.05756170 | 1.73866155 |
| -0.72899120 | 0.80254119 | -1.87506096 |
| 0.75059424 | 1.34458696 | 0.22127903 |
| -1.18996287 | -1.77154529 | -1.94420488 |
| -2.41889544 | 2.44336569 | -3.37010598 |
| 3.79253372 | 0.87152226 | -3.60060572 |
| -4.19504149 | 0.18364144 | 0.94903729 |
| -2.69833438 | -1.35595344 | 2.64519023 |
| -0.60339485 | 3.29565492 | -0.96397467 |
| -1.45516907 | -0.15145359 | -4.17916099 |
| 2.64879154 | 3.56721322 | -3.99337839 |
| 3.17556464 | 0.11421514 | -1.04233542 |
| -2.31562991 | 4.52187230 | 0.91797809 |
| 1.30129129 | -0.46286039 | -3.22026086 |
| -2.98436291 | 2.26670182 | -0.43739274 |
| -1.65302524 | -0.20353860 | 0.38538538 |
| 0.32140246 | 4.33926089 | 1.20665127 |
| -0.62801968 | -2.81786109 | 1.28740325 |
| 1.75477273 | 4.60130562 | -1.30801220 |
| -3.38855983 | 0.18031895 | -1.86976740 |
| 1.65224765 | 2.08968402 | -2.1749931 |
| -0.67513007 | 5.90648495 | -0.89349989 |
| 2.70268603 | 0.11443077 | 1.62094006 |
| 1.38611890 | 2.31261115 | 2.74287463 |
| 0.08879315 | -0.33751845 | 2.43426578 |
| 0.95119183 | -1.29325621 | -0.38517678 |
| 0.54034805 | 1.87482876 | -4.47165403 |
| -2.80304919 | 4.79755528 | -1.82183287 |
| 2.88540303 | 2.78869267 | 0.49152020 |
| 4.09949457 | 2.98130343 | -1.82702076 |
11. Lattice geometry and ionic positions for Ti$_{32}$ at 1300 K.

Format: XYZ file

```
50.0000000000  0.0000000000  0.0000000000
0.0000000000  50.0000000000  0.0000000000
0.0000000000  0.0000000000  50.0000000000

Ti    -2.14023985     2.35584763    -3.16680627
Ti     1.42132756    -0.60227100     1.53601269
Ti    -2.94429809    -2.30919996     0.99966712
Ti    -2.39214659     1.56865126     3.74201568
Ti    -0.57721432    -0.96212111    -0.17328831
Ti    -4.01279510     2.12691615    -0.69527723
Ti     1.05363918     1.39807770    -0.42276145
Ti     2.69431733     3.74616808    -1.05711377
Ti     4.58104829     1.70081752     2.27413665
Ti    -0.17889041     0.51127668    -2.75788683
Ti     2.08716807    -0.82900202    -1.58209540
Ti    -2.80997609    -0.11008548    -1.73499433
Ti     0.31734266     3.33716690     2.42055346
Ti    -1.38486355     2.09956798    -0.65266394
Ti     0.59091760     2.36830974    -4.68893797
Ti     0.07274551     1.45912254     2.15263610
Ti    -3.77868975    -0.88424633     3.06867354
Ti    -1.99454242     4.57400742    -1.51709890
Ti     2.47121438     2.68502166     1.69399889
Ti     4.43936799     0.07826240    -3.06296060
Ti     0.74816154     4.61863866    -4.10247913
Ti     4.71786262     2.58959858    -2.70162117
Ti     2.35075410     1.62506415    -2.93309854
Ti     3.58098495     2.30750835    -5.22153180
Ti     1.93800104    -0.42817406    -4.65389219
Ti     3.82740011     1.23525397    -0.45358763
Ti     0.18683103     3.88626630     0.45535281
Ti    -2.23323927     3.26421770     1.85672834
Ti    -2.49009812     0.56584639     1.09616741
Ti    -1.05298897    -0.96332773     2.73554369
Ti     2.27936433     4.42697025    -4.05796225
```
12. Lattice geometry and ionic positions for Ti$_3$2 at 1400 K.

Format: XYZ file

| Ti     | 2.04567109 | 4.62404136 | -3.1556015  
| Ti    | -2.40844808 | 3.29059112 | 2.08218676  
| Ti    | 2.09245054 | -0.19806638 | -0.83537513  
| Ti    | 3.48389637 | 1.41570666 | 0.36648480  
| Ti    | -0.29029794 | 3.99438662 | 0.99568104  
| Ti    | -0.72897762 | -0.59267823 | 0.1965627  
| Ti    | 4.34674700 | 0.50361935 | 0.91311690  
| Ti    | -0.03637733 | -1.70052218 | -2.39049032  
| Ti    | 1.21340792 | 1.81217523 | -0.02549767  
| Ti    | 3.59602071 | 2.56851869 | -4.19208774  
| Ti    | -1.48249586 | 0.57998585 | 2.43675874  
| Ti    | -3.33479074 | -0.88521241 | 0.91311690  
| Ti    | 2.10891804 | 4.21256991 | -0.09146371  
| Ti    | -2.53665409 | 2.46309045 | -2.59487170  
| Ti    | 0.85259401 | -2.83232676 | 0.15706875  
| Ti    | -0.06880155 | 3.42120501 | -1.64550189  
| Ti    | 0.40910331 | 5.96735000 | 1.35169931  
| Ti    | 1.18908076 | -0.80305628 | 1.92616220  
| Ti    | 0.85333906 | 2.46589692 | -4.25285244  
| Ti    | -1.25622731 | -2.36452617 | 1.99391252  
| Ti    | -4.37916909 | 3.41471410 | -0.11663065  
| Ti    | -2.51240571 | -0.60174441 | -1.92219830  
| Ti    | -0.02027526 | 0.82694033 | -1.92898266  
| Ti    | -1.16253269 | 4.74592676 | -3.59169569  
| Ti    | -4.64602356 | 0.19328833 | -0.73321852  
| Ti    | 2.21469557 | 2.14363092 | -1.91000775  
| Ti    | 4.55212176 | 3.33067882 | -1.83494234  
| Ti    | -2.10914616 | 4.94203233 | -0.69212737  
| Ti    | -1.82964299 | -2.89699792 | -0.66564214  
| Ti    | -4.14683293 | 1.30189180 | 2.00996883  
| Ti    | 0.89025912 | 1.61874725 | 0.63748068  

13. Lattice geometry and ionic positions for Ti$_32$ at 1500 K.

Format: XYZ file

```
50.0000000000  0.0000000000  0.0000000000
0.0000000000  50.0000000000  0.0000000000
0.0000000000  0.0000000000  50.0000000000

Ti  -2.27607051  6.65628630  -1.28894540
Ti  -0.77314793  2.36553055  -2.25649551
Ti   2.62750668 -0.04405092  -2.21442525
Ti   2.78911408 -0.14272941   2.49583016
Ti  -2.27341289  4.64548915  -3.38156794
Ti   0.40917868  0.26122250  -3.73035839
Ti   2.64269200  1.54525732  -4.33059998
Ti  -0.98542374 -1.44790425   0.45441938
Ti  -2.01945058  2.21833258  -4.52285249
Ti   4.30066655 -0.75343502   0.08475329
Ti   1.77036986  2.73037575  -2.18868869
Ti  -2.17780346  3.96984985  -0.66164957
Ti   2.79324119  1.51004990   0.02001613
Ti   0.62600922 -1.92656843   2.64431148
Ti   0.07866114  0.92427587   2.08116704
Ti   0.61833892 -3.71470312   0.49223052
Ti  -0.76567399  5.72624371   0.96667314
Ti   2.99212083 -2.71618869  1.67517354
Ti   0.37884589  0.48732877  -0.96866767
Ti  -2.07450993  1.09208116   0.43768859
Ti  -3.45245964  2.17159969  -2.33030325
Ti  -4.48131561  2.73152040   0.25298750
Ti   1.59895467 -1.07438406   0.26456475
Ti   0.54511265  3.24261517  -4.66619758
Ti   0.22445026  4.96006417  -1.59954121
Ti   4.61406916  5.12448543  -1.34456859
Ti   0.58548779 -1.94272393  -2.04601630
Ti   3.04795974 -2.78920354  -1.10311445
Ti  -1.50880588  3.19217231   1.93710954
Ti   0.43264195  2.99646357   0.14568052
Ti  -3.50154541  5.13700465   1.17594463
Ti  -1.89456264 -0.06308408  -2.45057982
```
14. Lattice geometry and ionic positions for Ti$_{32}$ at 1600 K.

Format: XYZ file

50.0000000000  0.0000000000  0.0000000000
0.0000000000  50.0000000000  0.0000000000
0.0000000000  0.0000000000  50.0000000000

Ti  0.30872785  1.00205901 -2.88841271
Ti  1.83909784  3.60631425 -2.8526974
Ti  1.46656123  5.46391534 -4.55647656
Ti -4.84107354 -1.29559858  0.99390362
Ti  2.87834848  1.02533874 -3.58600189
Ti -0.22997627 -2.24750394  0.65568809
Ti -2.00600360  1.55788314 -1.65227896
Ti -2.13502920  4.19107727 -0.89532443
Ti -2.53763026 -2.09169785  2.52386785
Ti -2.95093293 -2.63220603 -0.20763687
Ti -0.69465556  0.13098653  2.57552367
Ti  3.67754685  3.79829772 -4.65503064
Ti  1.86029749 -0.65960796  1.38907288
Ti -0.23295166  4.73367034  0.82800667
Ti -4.07436183 -0.61689407 -1.7260354
Ti  0.23193959 -2.45713714  3.12772480
Ti  0.16167873  2.94338678 -0.95900597
Ti -3.59541206  0.67185517  2.89407043
Ti -2.51115356 -0.12585386  0.59816419
Ti -1.51432958 -0.98463235 -2.16529019
Ti -0.00282363  0.25274394 -0.26710425
Ti  3.49406590  5.71412176 -2.67124202
Ti  1.16128460  2.14911072  1.47625720
Ti  2.40807628  1.39798452 -0.93230355
Ti  1.62428190 -1.22656348 -1.81486538
Ti  0.81639692  5.55278350 -1.54634072
Ti  4.36471193  2.99500704 -2.09848570
Ti -0.92709359  3.64342098 -3.32652825
Ti  2.68282192  4.02553335 -0.13119246
Ti -4.39448233  1.62343190  0.02315511
Ti  1.01051063  2.53720679 -5.14708851
Ti -1.67533783  2.39483983  1.03775796
15. Lattice geometry and ionic positions for Ti$_{32}$ at 1700 K.

Format: XYZ file

50.0000000000 0.0000000000 0.0000000000
0.0000000000 50.0000000000 0.0000000000
0.0000000000 0.0000000000 50.0000000000

Ti  0.22133977   -0.46486036   -0.72720512
Ti  -1.74521920   -0.02421044   -2.57399156
Ti   0.40280781    2.05916173   -1.72866598
Ti  -1.60990075    3.45091807    0.36491517
Ti   1.90263550    5.83619006   -2.83691113
Ti  -4.23346553    2.39485182    1.04698770
Ti  -2.19537762   -0.48948949    4.21224424
Ti   0.51467777    4.61482181   -2.75779588
Ti   -3.83458426   -0.43991883    1.91337835
Ti   3.78023634    1.26504708   -3.44173300
Ti  -2.87532947    2.49386939   -2.11635472
Ti   2.65780406    6.56504713   -5.19781430
Ti   1.26514033    0.31466156   -3.17902568
Ti  -2.29013202    1.56103163    2.77238578
Ti  -0.00096650   -1.88731603    3.85910006
Ti  -0.72208352    2.24333437   -4.38185628
Ti   0.49127297    0.61908565    3.65284991
Ti   1.10431613    4.16135524   -0.48479022
Ti   3.53266769    3.80136523   -1.41868736
Ti   2.27038150    1.50878062   -1.01240538
Ti   2.17397574    2.02291499   -5.47304573
Ti   2.09426103    0.83965505    0.06146648
Ti   1.09960270    4.48755655   -5.32777808
Ti  -2.22117927   -2.79681969    2.77132924
Ti  -0.94338177   -0.64538336    1.79851911
Ti   0.38293672    1.74021798    0.98485340
Ti   0.00899209   -2.85499666    1.10517572
Ti  -4.20520854   -0.10537530   -1.50199562
Ti   3.77328740    4.35060027   -4.40934920
Ti   1.69496070   -0.65074958    1.39466655
Ti   1.71475175    3.00237578   -3.06594067
Ti  -2.52262558   -1.90044891   -0.25854770

16
16. Lattice geometry and ionic positions for Ti$_32$ at 1800 K.

Format: XYZ file

|        |        |        |        |
|--------|--------|--------|--------|
|        | 50.0000000000 | 0.0000000000 | 0.0000000000 |
|        | 0.0000000000 | 50.0000000000 | 0.0000000000 |
|        | 0.0000000000 | 0.0000000000 | 50.0000000000 |

|        | 3.80323296 | 3.43989446 | -2.99144545 |
| Ti     | 0.43508932 | -0.59007861 | 1.24348692 |
| Ti     | 2.94941260 | 0.35577585 | -3.44172976 |
| Ti     | -0.73331889 | 4.19733040 | -0.43960134 |
| Ti     | -5.42603798 | 3.42025731 | -0.31415477 |
| Ti     | -1.71728822 | 2.93464468 | -2.84670036 |
| Ti     | 2.00100553 | -0.00467876 | -0.92238140 |
| Ti     | 1.19946771 | 2.50489047 | -2.60549732 |
| Ti     | -0.35935678 | 1.60950263 | -0.75603711 |
| Ti     | 1.63368206 | 1.79672296 | 1.46217997 |
| Ti     | 4.57631291 | -1.24669168 | -0.68841687 |
| Ti     | -4.99759445 | 0.75907862 | -0.84565606 |
| Ti     | 5.22280111 | 1.11975346 | -2.39425007 |
| Ti     | -3.23944617 | 5.00183917 | -0.91771869 |
| Ti     | -0.25442503 | -1.51208708 | -1.13920281 |
| Ti     | 2.18918217 | -1.97824970 | -2.55957539 |
| Ti     | 2.09199989 | -2.56199088 | 0.27365922 |
| Ti     | -7.14603396 | 2.09431467 | -1.75578955 |
| Ti     | -6.95125131 | 1.51049630 | 0.73788772 |
| Ti     | -2.90511317 | 3.97782094 | 1.65310714 |
| Ti     | 5.93249452 | 3.43158216 | -1.42070830 |
| Ti     | 2.01481984 | 4.39311171 | -1.07249773 |
| Ti     | 3.34113123 | -0.12621799 | 1.35881181 |
| Ti     | -4.32527943 | 2.87870296 | -2.55756641 |
| Ti     | -2.96767245 | 2.32796426 | -0.37655521 |
| Ti     | 5.93720409 | 1.29328756 | 0.13853134 |
| Ti     | -4.13885826 | 1.58081325 | 1.68304848 |
| Ti     | -2.51367419 | -0.15775585 | 0.12953541 |
| Ti     | 3.58761427 | 2.22717563 | -0.64072884 |
| Ti     | -2.51042070 | 0.25688678 | -2.55477413 |
| Ti     | 0.18177715 | 0.10903920 | -3.26578627 |
| Ti     | -1.24835562 | 2.03013850 | 1.87050394 |
17. Lattice geometry and ionic positions for Ti$_{32}$ at 1900 K.

Format: XYZ file

\[ \begin{array}{llll}
50.0000000000 & 0.0000000000 & 0.0000000000 \\
0.0000000000 & 50.0000000000 & 0.0000000000 \\
0.0000000000 & 0.0000000000 & 50.0000000000 \\
\end{array} \]

| Ti          | X         | Y         | Z         |
|-------------|-----------|-----------|-----------|
| 0.31940411  | -1.26185027 | 3.79255998 |
| 0.52279901  | 5.01553086  | -3.77210969 |
| 1.63617818  | 0.65671031  | -2.02507403 |
| 0.10582176  | 1.32113433  | 2.34922812 |
| -3.88375337 | -0.92604003 | 1.51674784 |
| 3.12599004  | 3.59144295  | -2.48367111 |
| 0.40506843  | -3.47539018 | 2.02474321 |
| -1.35665267 | -5.25872611 | 2.83294983 |
| 1.94689670  | 2.65220195  | 0.06951864 |
| -0.94644603 | 0.86898715  | -3.11976303 |
| 1.32369540  | 5.16586425  | -0.71173470 |
| -0.99479268 | 5.62064040  | -1.44063627 |
| -0.38663507 | 1.00544283  | -0.33243292 |
| 0.19926370  | 4.41522237  | -6.30241665 |
| -1.35631103 | 3.24733604  | -4.13977687 |
| 2.70098311  | 4.52246986  | -5.30979803 |
| 0.62258105  | 7.57249518  | -2.66002737 |
| -2.42181658 | 2.50702975  | -0.99120268 |
| 1.51680477  | 2.13723001  | -4.35798508 |
| -0.45377311 | 3.60328382  | 0.80425807 |
| 0.39561720  | -3.34121875 | -0.60371879 |
| -2.24127934 | -0.22080007 | 3.81106599 |
| 0.33060140  | 3.14784315  | -2.13219358 |
| -2.09200710 | -3.37781526 | 0.77625279 |
| 3.09515633  | 6.31797442  | -3.18654826 |
| 1.31220207  | 6.99741731  | -5.02947650 |
| -2.11520680 | -2.98718575 | 3.79530282 |
| -2.71508054 | -0.38124638 | -0.78549647 |
| -2.5661306  | 1.28703727  | 1.40069191 |
| -1.27516962 | -1.01138456 | 1.54574797 |
| 1.40261780  | -1.04281452 | 0.55144576 |
| -0.49334332 | -1.29554895 | -1.84247278 |
18. Lattice geometry and ionic positions for Ti$_{32}$ at 1941.15 K.

Format: XYZ file

|      |        |        |        |
|------|--------|--------|--------|
| Ti   | 1.90087119 | -3.67982871 | 2.41172697 |
| Ti   | -2.39211734 | 4.79787051  | -0.62959978 |
| Ti   | -3.54429929 | 5.96273005  | -2.93407354 |
| Ti   | -0.95932292 | -2.82419881 | 3.13734947 |
| Ti   | -1.06604402 | 2.14895515  | -4.12152407 |
| Ti   | -2.59059968 | 4.44332694  | -5.04715162 |
| Ti   | -2.70939754 | 1.97790121  | 0.15774545 |
| Ti   | -1.62437783 | 7.00712537  | -4.51950326 |
| Ti   | -3.24340234 | 2.95909168  | -2.79588507 |
| Ti   | -0.60540023 | 2.73158875  | 1.51820155 |
| Ti   | -0.00128007 | -1.51101873 | -1.41756381 |
| Ti   | 1.67537456  | 3.67208717  | -2.83107986 |
| Ti   | -0.11623609 | 0.63175884  | -0.16047466 |
| Ti   | -2.07031082 | 0.49533857  | -2.00046463 |
| Ti   | 1.22520538  | -1.09793284 | 3.96489061 |
| Ti   | 3.28728463  | -1.37799488 | 2.03065386 |
| Ti   | 2.02868320  | 2.31924380  | -0.35267567 |
| Ti   | -2.10171142 | -1.41183030 | 0.11876167 |
| Ti   | 1.79849754  | 1.02392995  | 1.87496697 |
| Ti   | 1.95750171  | -3.16354304 | -0.38924321 |
| Ti   | 0.87308308  | 6.26858284  | -3.49319314 |
| Ti   | -1.18027018 | 4.81698017  | -3.10622409 |
| Ti   | 2.36348418  | -0.57545222 | -0.66290283 |
| Ti   | 4.41479519  | -3.60903960 | 0.84418521 |
| Ti   | -0.71969426 | 2.69876400  | -1.62567284 |
| Ti   | -0.57049752 | -3.52925068 | 0.25258439 |
| Ti   | -1.30570078 | 7.04042023  | -1.56921553 |
| Ti   | 0.89982383  | 0.87669402  | -2.74198967 |
| Ti   | -1.27613074 | -0.04364784 | 2.43234712 |
| Ti   | 0.41302347  | 4.26868815  | -5.04843186 |
| Ti   | 0.59490786  | -1.51091515 | 1.38779340 |
| Ti   | 0.30735800  | 5.26684877  | -0.64038941 |
19. Lattice geometry and ionic positions for Ti$_{32}$ at 2000 K.

Format: XYZ file

```
50.0000000000 0.0000000000 0.0000000000
0.0000000000 50.0000000000 0.0000000000
0.0000000000 0.0000000000 50.0000000000

Ti  1.52050722  -1.20109972  1.29003469
Ti  5.07163847   1.68205488  -0.82041216
Ti  1.95364933  -2.68916844  -2.82071077
Ti  2.56187883  -1.00074438  -1.56408223
Ti  2.76310454   1.18109195   0.40542348
Ti  3.15236748  -0.76694933  -1.45920741
Ti  1.20713192   4.62394776  -3.02637820
Ti  4.77525292   1.22962567  -2.17496589
Ti  2.51362359   2.38729886  -1.85116159
Ti  1.33653318  -0.72532225   0.65090468
Ti  -0.07441413   3.28850250  -1.04358302
Ti  0.76047534   0.45188978  -0.94323912
Ti  2.80616046   2.88683200  -3.22109629
Ti  1.58609225   5.22651431  -0.48115169
Ti  1.68432818   3.39738282   1.24940603
Ti  -5.30117412   0.42098659   2.38061779
Ti  -4.26730427  -0.58637454   0.25190925
Ti  2.36151331   3.05654525  -4.50851012
Ti  -3.59650415   2.08602767   1.12943190
Ti  3.72570586   4.91423702  -2.81837209
Ti  -3.91020164  -2.12431772   2.37437055
Ti  3.95251478   3.61158862  -0.93455380
Ti  -2.48398255   0.23370783   2.56976025
Ti  0.02670070  1.51439641   1.62473880
Ti  0.20235002  1.59717891  -3.31763916
Ti  -5.98811980   1.72689721   0.09201773
Ti  0.49693339  -2.08973919  -0.74971287
Ti  -1.81846406   4.12385479   0.72763746
Ti  2.50973815   0.40943792  -3.91208567
Ti  4.25225808   4.14520353  -0.29417846
Ti  4.83626817   2.63665623  -3.37787666
Ti  2.03537898  1.42513044  -1.19932181
```
20. Lattice geometry and ionic positions for Ti$_{32}$ at 2100 K.

Format: XYZ file

|        | x             | y             | z             |
|--------|---------------|---------------|---------------|
| Ti     | 1.95425996    | -1.53934485   | -3.02270161   |
| Ti     | 2.57417095    | -0.08209874   | 1.77648621    |
| Ti     | 3.82709799    | -2.58466259   | 1.00696054    |
| Ti     | 3.19742165    | 2.61187919    | 1.47361879    |
| Ti     | 2.67725159    | -1.02006122   | -0.75812675   |
| Ti     | 3.82929286    | 1.52861162    | -1.15980446   |
| Ti     | -5.71347681   | 3.61371395    | -0.50089199   |
| Ti     | -3.15014219   | 5.13866118    | -4.31790786   |
| Ti     | 0.98343653    | -3.33791890   | -0.91824886   |
| Ti     | 2.47557826    | 4.46770602    | -0.73375590   |
| Ti     | -3.66868094   | 1.72944332    | -0.41897863   |
| Ti     | 0.11530629    | 0.80805752    | -2.43333153   |
| Ti     | -4.72361156   | 2.59625259    | -2.76029466   |
| Ti     | -5.08957555   | 2.46195384    | 2.00101959    |
| Ti     | -2.72422776   | -0.89928723   | -0.43670694   |
| Ti     | -4.86831920   | 5.10765046    | -2.72367391   |
| Ti     | 5.10095858    | -1.88481794   | -1.58203642   |
| Ti     | 4.78750893    | -0.17319935   | 0.51581081    |
| Ti     | 3.30075257    | -3.72024680   | -2.07583569   |
| Ti     | 1.22537736    | 3.23330697    | -2.56977840   |
| Ti     | 1.34997264    | 1.69746665    | -0.33253240   |
| Ti     | 0.00326769    | -0.72491868   | -0.00395349   |
| Ti     | -1.77445290   | 5.80100981    | -2.24995052   |
| Ti     | 1.01008046    | 4.23474656    | 1.82130138    |
| Ti     | 0.02751895    | 4.55092281    | -0.50711478   |
| Ti     | -2.60681233   | 0.41669784    | -2.73139827   |
| Ti     | -0.70971740   | -1.85607670   | -2.35680874   |
| Ti     | -3.29262761   | 4.81370642    | -0.40169263   |
| Ti     | -1.89890276   | 3.07456353    | -2.76894133   |
| Ti     | -1.16012491   | 1.99573667    | -0.53264641   |
| Ti     | -1.52439478   | 3.55713790    | 1.68136009    |
| Ti     | 0.12891417    | 1.45637652    | 2.06453291    |
21. Lattice geometry and ionic positions for Ti$_{32}$ at 2200 K.

Format: XYZ file

|        |        |        |        |        |        |
|--------|--------|--------|--------|--------|--------|
| 50.0000000000 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 50.0000000000 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 50.0000000000 |

| Ti  | 15.17694595 | 12.28030204 | 19.00113839 |
| Ti  | 10.77186367 | 10.56844640 | 17.00039658 |
| Ti  | 12.89548441 | 18.17038072 | 17.32182090 |
| Ti  | 13.29415259 | 12.63758982 | 12.82071943 |
| Ti  | 10.72873037 | 15.61971545 | 21.73165821 |
| Ti  | 13.36112496 | 11.54356370 | 20.95030571 |
| Ti  | 13.38686866 | 10.90352685 | 15.10949775 |
| Ti  | 10.52964675 | 14.56581889 | 18.99195819 |
| Ti  | 10.59200921 | 12.96203331 | 21.72465883 |
| Ti  | 13.13048546 | 15.59108689 | 15.49300724 |
| Ti  | 11.54264356 | 13.46516966 | 14.61001668 |
| Ti  | 10.88876732 | 15.83568318 | 14.22602440 |
| Ti  | 13.20414299 | 16.84968728 | 20.75505680 |
| Ti  | 12.07646406 | 8.96058682  | 18.60327225 |
| Ti  | 13.06360646 | 11.07355997 | 17.69427972 |
| Ti  | 10.86110999 | 17.65529660 | 19.93145772 |
| Ti  | 14.73305741 | 14.76223041 | 17.36542519 |
| Ti  | 10.29742311 | 16.08693749 | 16.94815194 |
| Ti  | 12.58393286 | 13.43396822 | 16.92914512 |
| Ti  | 12.69309953 | 15.86239656 | 18.10596107 |
| Ti  | 10.62733455 | 18.28810246 | 15.14779057 |
| Ti  | 15.11401361 | 17.08579630 | 16.38056171 |
| Ti  | 15.71183833 | 13.05265749 | 22.04647383 |
| Ti  | 14.86206862 | 13.13196803 | 14.90911480 |
| Ti  | 15.53298375 | 15.47133300 | 19.94413075 |
| Ti  | 7.47873195  | 16.17665500 | 17.47533531 |
| Ti  | 11.22255950 | 12.02944573 | 19.19218746 |
| Ti  | 9.29470503  | 13.18882494 | 16.37121206 |
| Ti  | 13.43484789 | 14.11105021 | 20.00376312 |
| Ti  | 13.71473619 | 14.78645366 | 22.61011876 |
| Ti  | 11.63450633 | 9.81043922  | 21.12729384 |
| Ti  | 11.22325966 | 11.11273407 | 13.52209179 |
22. Lattice geometry and ionic positions for Ti32 at 2300 K.

Format: XYZ file

50.0000000000  0.0000000000  0.0000000000
0.0000000000  50.0000000000  0.0000000000
0.0000000000  0.0000000000  50.0000000000

| Ti      |   X      |   Y      |   Z      |
|---------|----------|----------|----------|
| -2.88206330 | 1.23859922 | -1.19661742 |
| -0.90052964 | -1.91380674 | 1.67057149  |
| 2.48103754  | 3.00074503  | -2.29227809 |
| 0.60252428  | 4.46840189  | -4.09339670 |
| -1.56085627 | -1.86236224 | -0.90736412 |
| -0.31645468 | 2.30874574  | -2.14859575 |
| 1.32743799  | -2.39674467 | 0.12550111  |
| -2.50430851 | 4.82515309  | 1.93925428  |
| -1.13032845 | 0.28825237  | -3.89133345 |
| -0.97283151 | 2.72539701  | -5.02560675 |
| -1.61116796 | 4.58721296  | -2.55485691 |
| 0.56773460  | 4.92960788  | 1.48548482  |
| 3.42959771  | -0.08882420 | -3.10289029 |
| -1.28299391 | 3.20811228  | 0.11966189  |
| 0.92407239  | -1.77059411 | -4.41172018 |
| 0.63413029  | 4.95326081  | -1.38681681 |
| -2.24684362 | 0.73884205  | 2.02539621  |
| 1.50344596  | 1.37772645  | -4.10526342 |
| -3.86848022 | 4.17786339  | -1.11348511 |
| 2.06443211  | 1.91744854  | 3.53992198  |
| -4.03149240 | 2.55426421  | 1.11219141  |
| 2.74029695  | -0.15248290 | 2.22297901  |
| 1.36535737  | 2.79739627  | 0.52102374  |
| 0.25287198  | -0.17555557 | 3.71226856  |
| 2.99914145  | -2.54801853 | -1.98694930 |
| 0.61384140  | -0.39385775 | -2.18779135 |
| 2.61501209  | 0.35965190  | -0.72151042 |
| 0.03931858  | -3.59356287 | -2.55143877 |
| 0.17496046  | 0.11840275  | 0.71594807  |
| -0.50473126 | 2.74611323  | 2.61575668  |
| -3.15093734 | 2.55478593  | -3.70073128 |
| -1.70809333 | 6.09308935  | -0.38333499 |
23. Lattice geometry and ionic positions for Ti$_{32}$ at 2400 K.

**Format: XYZ file**

|     | X          | Y          | Z          |
|-----|------------|------------|------------|
| Ti  | -20.89617835 | 14.26363588 | -21.28528833 |
| Ti  | -13.27304327 |  8.90971657  | -19.35799602 |
| Ti  | -18.99122224 | 14.49472705  | -18.46473089 |
| Ti  | -20.85738323 | 13.45212287  | -23.77369397 |
| Ti  | -19.56448613 | 12.03043406  | -17.33927863 |
| Ti  | -19.19194791 | 12.31211883  | -20.08080634 |
| Ti  | -19.27483409 | 14.16431413  | -15.47524033 |
| Ti  | -14.87828027 | 11.21300929  | -17.31115377 |
| Ti  | -17.29771800 | 10.16658595  | -21.47863410 |
| Ti  | -16.01228387 | 14.39541866  | -19.36399669 |
| Ti  | -21.90314167 | 12.93153566  | -18.71165935 |
| Ti  | -17.28983380 | 16.30241771  | -17.35038004 |
| Ti  | -13.51572443 | 10.69842611  | -21.42862407 |
| Ti  | -15.72318109 | 12.31513733  | -22.21781654 |
| Ti  | -18.41869620 | 14.69665817  | -21.22319757 |
| Ti  | -14.48670484 | 15.73898669  | -15.79938808 |
| Ti  | -17.90806777 | 16.79206961  | -19.60847566 |
| Ti  | -14.99898818 |  8.68406769  | -21.1085687 |
| Ti  | -14.75569359 |  6.60251189  | -19.61434294 |
| Ti  | -18.81247255 | 12.36103947  | -22.72178891 |
| Ti  | -16.09815233 |  9.14575238  | -19.04135546 |
| Ti  | -22.17277824 | 11.64158103  | -22.55883961 |
| Ti  | -16.48532225 | 11.87635667  | -19.57961291 |
| Ti  | -14.84651297 | 17.09976598  | -18.09152058 |
| Ti  | -16.60851169 | 13.53688234  | -16.46031017 |
| Ti  | -13.88774897 | 14.01560831  | -17.52778676 |
| Ti  | -12.90644284 |  7.25200457  | -21.85427411 |
| Ti  | -17.66755965 |  7.54840945  | -20.83623678 |
| Ti  | -21.00869177 | 16.27026029  | -19.14888527 |
| Ti  | -21.49559567 | 14.64813122  | -17.06336590 |
| Ti  | -13.78254926 | 12.20178613  | -19.17745017 |
| Ti  | -19.59694117 |  9.31106757  | -20.90132607 |