PHASE TRANSITIONS

Ferroelectricity and Pressure-Induced Phase Transitions in HgTiO$_3$

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Abstract—Using ab initio density functional theory, the ground state of mercury titanate is determined and phase transitions occurring in it at pressures $P \leq 210$ kbar are analyzed. It is shown that the $R3c$ structure experimentally observed in HgTiO$_3$ is metastable at $P = 0$. The ground state structure at $T = 0$ varies according to the scheme $R3c \rightarrow R3 \rightarrow Phnn$ with increasing pressure in agreement with available experimental data. It is shown that the appearance of ferroelectricity in HgTiO$_3$ at $P = 0$ is associated with an unstable soft mode. Some properties of crystals in the $R3c$ phase are calculated, in particular, the band gap in the GW approximation ($E_g = 2.43$ eV), which is in better agreement with experimental data than the value obtained in the LDA approximation (1.49 eV). An analysis of the thermodynamic stability explains why the synthesis of mercury titanate is possible only at high pressures.

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There are only a few studies of mercury titanate HgTiO$_3$ that indicate its interesting, but contradictory ferroelectric properties. Mercury titanate can be synthesized under a pressure of 60–65 kbar [1, 2]. These crystals have a rhombohedrally distorted perovskite structure. Observation of the second harmonic generation in HgTiO$_3$ at 300 K [1] enabled one to propose that the space group of the crystal is $R3c$; however, because of a limited accuracy, the atomic coordinates were determined only for the centrosymmetric $R3c$ structure. Subsequent studies of dielectric properties of mercury titanate [2, 3] did not detect pronounced dielectric anomalies: a wide strongly asymmetric peak with a maximum near 220 K and with an appreciable hysteresis in the cooling–heating cycle as well as a weak narrow peak near 515 K were observed on the temperature dependence. At 300 K, no dielectric hysteresis loops were appeared up to fields of $10^6$ V/m [2, 3]. Scanning calorimetry detected weak anomalies in the 420–480 K temperature range [2, 3]; however, these temperatures differed from the temperatures of peaks in the dielectric constant. Furthermore, X-ray studies under hydrostatic pressure [2, 3] detected non-monotonic behavior of the $d_{02a}$ interplanar distance and the $(104)-(110)$ doublet splitting at a pressure of ~20 kbar, which were explained by the rhombohedral-to-cubic phase transition. The electronic structure of the rhombohedral and cubic modifications of HgTiO$_3$ was studied in [4]; it was shown that the rhombohedral phase is a semiconductor and the cubic phase is a metal.

To resolve the contradictions concerning the ferroelectric properties of HgTiO$_3$ and to obtain new data on this compound, in this paper, ab initio calculations of physical properties of mercury titanate were performed.

The calculations were carried out within the density functional theory by analogy with the previous study [5]. The pseudopotentials for Ti and O atoms used in the calculations were taken from that study, the scalar–relativistic pseudopotential for the Hg atom was constructed according to the RRKJ scheme [6] using the OPIUM program for the configuration Hg$^{2+}$ (5d$^{10}$6s$^2$6p$^6$) with the following parameters: $r_s = 1.78$, $r_p = 2.0$, $r_d = 1.78$, $q_s = 7.37$, $q_p = 7.07$, $q_d = 7.37$ a.u. (for the notation of parameters, see [5]). The plane-wave energy cut-off used in the calculations was 30 Ha (816 eV). Integration over the Brillouin zone was performed on the $8 \times 8 \times 8$ Monkhorst–Pack mesh. To test the quality of the mercury pseudopotential, the calculations were carried out for two polymorphs of HgO with orthorhombic and rhombohedral structures. The former one (the montroydite mineral) had a slightly lower total energy. The calculated lattice parameters of these phases ($a = 3.4663$ Å, $b = 6.6253$ Å, $c = 5.3013$ Å, and $a = 3.5092$ Å, $c = 8.5417$ Å, respectively) were in reasonable agreement with experimental data [7] ($a = 3.5215$ Å, $b = 6.6074$ Å, $c = 5.5254$ Å; $a = 3.577$ Å, $c = 8.681$ Å). The phonon spectra were calculated using the scheme similar to that used in [5].

The calculated phonon spectrum of HgTiO$_3$ with a cubic perovskite structure (space group $Pm3m$) is shown in Fig. 1. One can see that two types of instabil-
ity simultaneously appear in mercury titanate: the stronger one associated with deformation and rotation of octahedra, which is not accompanied with the appearance of dipole moments (the \(\Gamma_{25} - X_3 - M_3\),  \(\Gamma_{15} - R_{25} - M_3\) branch), and the ferroelectric (antiferroelectric at the Brillouin zone boundary) one (the \(\Gamma_{15} - X_3 - M_3\) - \(\Gamma_{15}\) branch). The absence of \(\text{LO} - \text{TO}\) mode splitting at the \(\Gamma\) point is explained by the metallic character of the band structure of cubic HgTiO\(_3\).

To determine the ground state structure, energies of different distorted phases which arise from the cubic perovskite structure during condensation of the above determined unstable modes were calculated taking into account their degeneracy (Table 1). Among these phases, the \(R3\) one has the lowest energy. It is formed from the cubic structure by antiphase rotations of octahedra about all three fourfold axes as a result of condensation of the triply degenerate \(R_{25}\) mode at the Brillouin zone boundary (the \(a' a' a'\) Glazer tilt system). The energy of this phase is even lower than that of the \(Pbnm\) phase, in contrast to other titanates of Group II elements [5]. We note that as the structure becomes more distorted, the overlap of the energy bands disappears, and all phases with energies below 300 meV are semiconductors.

The ferroelectric instability of the parent cubic structure of HgTiO\(_3\) is also retained in the \(R\overline{3}c\) phase. Calculations show that unstable modes of symmetry \(A_{2u}\) and \(E_u\) with frequencies 135 cm\(^{-1}\) and 211 cm\(^{-1}\) are observed in the phonon spectrum of this phase at the \(\Gamma\) point. Among the corresponding ferroelectrically distorted phases, the \(R3c\) phase has the lowest energy. The fact that this phase corresponds to the ground state is proved by that all phonon frequencies at the Brillouin zone center and at high-symmetry points \(A, D,\) and \(Z\) at its boundary are positive, and the elastic moduli matrix is positive-definite (see below). The calculated lattice parameters and atomic coordinates in the \(R\overline{3}c\) and \(R3c\) structures are given in Table 2.

It is seen that they are in good agreement with experimental data [1]. The calculated interatomic distances for the \(R\overline{3}c\) phase and average calculated distances for the \(R3c\) phase are also in good agreement with interatomic distances obtained from X-ray diffraction studies (Table 3).

In addition to the phases derivative of the cubic perovskite structure, the possible formation of other phases should be considered, in particular, the ilmenite structure characteristic of titanates of Group II elements, i.e., MgTiO\(_3\), ZnTiO\(_3\), and CdTiO\(_3\) [7]. Calculations showed that the ilmenite structure (space group \(R\overline{3}\)) has the lowest energy at normal pressure (\(P = 0\)) among the considered phases (Table 1). The fact that the \(R\overline{3}c\) or \(R3c\) phases are observed in X-ray experiment enables to suppose that these phases are metastable. Their metastability is obviously associated with the significant difference between \(R3c\) (\(R\overline{3}c\)) and \(R3\) structures in both the lattice parameter and the rhombohedral angle (see Table 2). Therefore, the phase transition between them is the first-order transition for which a wide metastability region is character-

![Fig. 1. Phonon spectrum of HgTiO\(_3\) in the cubic \(Pm3m\) phase. Labels near the curves indicate the symmetry of unstable modes. The absence of \(\text{LO} - \text{TO}\) splitting at the \(\Gamma\) point is associated with metallic conductivity of the phase.](image)

**Table 1.** Energy and volume per formula unit in different distorted phases of HgTiO\(_3\) at \(P = 0\)

| Unstable mode | Space group | Energy, meV | Cell volume, Å\(^3\) |
|---------------|-------------|-------------|---------------------|
| \(X_3\)       | \(P4_g/mmc\) | -88         | 57.275              |
| \(\Gamma_{15}\) | \(R3m\)     | -94         | 58.923              |
| \(\Gamma_{15}\) | \(R4mm\)    | -122        | 59.444              |
| \(\Gamma_{25}\) | \(P4m2\)    | -139        | 57.088              |
| \(\Gamma_{15}, \Gamma_{25}\) | \(Amm2\) | -151        | 59.749              |
| \(X_4\)       | \(Pmna\)    | -202        | 57.916              |
| \(\Gamma_{25}\) | \(Cmcm\)    | -306        | 57.867              |
| \(R_{25}\)    | \(R32\)     | -467        | 56.956              |
| \(M_{3}\)     | \(I4/mcm\)  | -778        | 56.188              |
| \(R_{25} + M_{3}\) | \(P4/mnb\) | -809        | 56.195              |
| \(R_{25} + R_{25}\) | \(Pbnm\) | -936        | \textbf{55.853}      |
| \(R_{25}\)    | \(Imma\)    | -940        | 56.099              |
| \(R_{25}\)    | \(R\overline{3}c\) | -974        | 56.336              |
| \(A_{2u}\)    | \(R3c\)     | -982        | 56.632              |
| \(R\overline{3}\) |             | \textbf{-1059} | 60.140              |

Note: The energy of the cubic phase is taken as the energy reference. The phase with the lowest specific energy and the phase with the lowest specific volume are denoted by bold font.

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istic. The fact that namely the metastable $R3c$ ($R\bar{3}c$) phase appears during the synthesis can be caused by that HgTiO$_3$ is synthesized at a pressure of 60–65 kbar at which (as shown below) the $R\bar{3}c$ phase is the most stable. The energy of two more possible hexagonal HgTiO$_3$ phases with the two-layer BaNiO$_3$ structure and the six-layer hexagonal BaTiO$_3$ structure (the space group of both is $P6_3/mmc$) is higher than the energy of the $Pm\bar{3}m$ phase by 269 and 73 meV, respectively.

We discuss now the ferroelectric properties and the nature of the ferroelectric phase transition in HgTiO$_3$. Since the change in the Hg–O bond lengths during phase transition to the ferroelectric phase does not exceed 0.1 Å, and the energy difference of the $R3c$ and $R\bar{3}c$ phases is only 8.1 meV, it is unlikely that the Curie temperature in HgTiO$_3$ will exceed 300 K. Therefore, it is in better agreement with a temperature of 220 K at which the dielectric constant maximum was experimentally observed. The absence of the dielectric hysteresis loops at 300 K also supports this interpretation. Therefore, in what follows, being oriented on experiments performed at 300 K, we will focus on the properties of the $R\bar{3}c$ phase. The fact that the authors of [1] observed a signal of the second harmonic at room temperature can be associated with the sample defectness which is discussed in what follows.

An analysis of the eigenvector of the $A_{2u}$ ferroelectric mode in the $R\bar{3}c$ phase shows that the displacements of Hg atoms in this mode is smaller than that of Ti atoms by a factor of 22. This means that collective displacements of the titanium atoms with respect to the oxygen ones are responsible for the ferroelectric phase transition, rather than the mercury atom jumps between wells of the two-well potential. The effective Born charges of the mercury atoms also indicate their weak ferroelectric activity: they are $Z_{\text{Hg}} = 3.20$ and $Z_{\text{Ti}} = 2.42$ and differ slightly from the nominal ionic charge.

The calculated static dielectric constant at 0 K in the $R\bar{3}c$ phase is almost isotropic ($\varepsilon_{xx} = 97$, $\varepsilon_{zz} = 101$);

**Table 2.** Lattice parameters and atomic coordinates in the mercury titanate phases with space groups $R3c$, $R\bar{3}c$, and $R\bar{3}$ at $P = 0$ and the space group $Pbnm$ at 141 kbar

| Phase   | $a$, Å  | $\alpha$, deg | Atom     | Position | $x$     | $y$     | $z$     |
|---------|---------|---------------|----------|----------|---------|---------|---------|
| $R3c$   | 5.4984  | 58.4093       | Hg       | $2a$     | 0.24904 | 0.224904| 0.24904 |
|         |         |               | Ti       | $2a$     | -0.00333| -0.00333| -0.00333|
| $R\bar{3}c$ | 5.4881  | 58.4252       | Hg       | $2a$     | 0.25000 | 0.25000 | 0.25000 |
|         |         |               | Ti       | $2b$     | 0.00000 | 0.00000 | 0.00000 |
| $R\bar{3}c$ (exp.)* | 5.4959  | 58.59        | Hg       | $2a$     | 0.25     | 0.25     | 0.25    |
|         |         |               | Ti       | $2b$     | 0.0      | 0        | 0       |
| $R\bar{3}$ | 5.8304  | 53.9320       | Hg       | $2c$     | 0.36869 | 0.36869 | 0.36869 |
|         |         |               | Ti       | $2c$     | 0.84974 | 0.84974 | 0.84974 |
| $Pbnm$  | 5.2678(a) | –             | Hg       | $4c$     | -0.00445| 0.03190 | 0.25000 |
|         | 5.2983(b) |             | Ti       | $4b$     | 0.50000 | 0.00000 | 0.00000 |
|         | 7.5501(c) |             | O        | $4c$     | 0.08502 | 0.47264 | 0.25000 |

* Coordinates were recalculated for the rhombohedral setting.

**Table 3.** Interatomic distances in the HgTiO$_3$ phases with space groups $R3c$ and $R\bar{3}c$

| Atom pair | Distance, Å | $R3c$ | $R\bar{3}c$ | Ref. [1] | Number of bonds |
|-----------|-------------|-------|--------------|----------|-----------------|
| Hg–O      | 2.198       | 2.195 | 2.20(4)      | 3        | 3 + 3           |
| Hg–O      | 2.698, 2.888| 2.786 | 2.77(4)      | 3 + 3    | 3 + 3           |
| Hg–O      | 3.172       | 3.162 | –            | 3        |                 |
| Ti–O      | 1.906, 2.064| 1.977 | 1.96(4)      | 3 + 3    |                 |
in the $R\bar{3}$ phase, the dielectric constant is notably lower ($\varepsilon_{xx} = 28$, $\varepsilon_{zz} = 27$). For comparison, the maximum dielectric constant experimentally observed at 220 K is ~800 [2, 3]. The calculated spontaneous polarization in the $R3c$ phase appears unexpectedly high, $P_s = 0.37 \text{ C/m}^2$. This is probably a result of the large effective charge of the $A_{2u}$ mode in the paraelec-

We consider now some other physical properties of HgTiO$_3$ at $P = 0$. The calculations of the electronic structure performed in this work confirmed the data of [4] that the $R3\bar{c}$ phase is a direct-gap semiconductor with the band extrema located at the $\Gamma$ point. The band gap of mercury titanate at $P = 0$ is $E_g^{\text{LDA}} = 1.49$ eV, its pressure coefficient is $dE_g^{\text{LDA}}/dP = +0.44$ meV/kbar. The value of $E_g$ obtained in the LDA approximation agrees with the value of 1.6 eV found in the GGA approximation using the FP-LAPW method [4]. However, both results disagree with the experimental fact that HgTiO$_3$ crystals are light yellow [1]. It is well known that the density functional theory always underestimates the band gap because of its limitations with respect to the calculation of the excited states energy. One of the approaches that yield the $E_g$ values in good agreement with experiment is based on the consideration of many-body effects (electron correlations, dynamic screening, local field effects) within the GW approximation [8]. The calculations performed in this work within this approximation yielded $E_g^{\text{GW}} = 2.43$ eV in the $R3c$ phase, which agrees much better with the sample color reported in [1] than the band gap in the LDA approximation.

The elastic moduli tensor in the $R3\bar{c}$ phase is presented by seven independent components: $C_{11} = C_{22} = 347.2 \text{ GPa}$, $C_{33} = 260.3 \text{ GPa}$, $C_{12} = 178.5 \text{ GPa}$, $C_{13} = C_{23} = 149.9 \text{ GPa}$, $C_{44} = C_{55} = 76.3 \text{ GPa}$, $C_{66} = 84.8 \text{ GPa}$, and $C_{14} = -C_{44} = C_{56} = 18.3 \text{ GPa}$. The bulk elastic modulus calculated from them is $B = 205.8 \text{ GPa}$; it slightly differs from the value of 178 GPa obtained in [4] ignoring the relaxation of internal degrees of freedom.

To interpret future experiments on infrared (IR) reflection and Raman scattering, the phonon frequencies calculated at the $\Gamma$ point for $R3c$, $R\bar{3}$ phases at normal pressure and the $Pbnm$ phase at 147 kbar, given in Table 4, can be useful. In the low-temperature $R3c$ phase, the $A_1$ and $E$ modes are active in both IR and Raman spectra. In the $R\bar{3}$ phase, the $A_u$ and $E_u$ modes

| Structure $R3c$ | Structure $Pbnm$ |
|----------------|------------------|
| mode | $\nu$, cm$^{-1}$ | mode | $\nu$, cm$^{-1}$ | mode | $\nu$, cm$^{-1}$ | mode | $\nu$, cm$^{-1}$ |
| $A_1$ | 78 | $E$ | 81 | $A_g$ | 68 | $B_{1g}$ | 439 | $B_{1u}$ | 530 |
| 181 | 121 | 144 | 782 | 86 | $B_{2u}$ | 38 |
| 379 | 139 | 277 | 104 | 141 |
| 476 | 165 | 476 | 165 | 277 | 104 | 141 |
| $A_2$ | 62 | 274 | 417 | 266 | 190 | 431 |
| 347 | 312 | 462 | 450 | 345 | 355 | 443 | 559 | 542 | 356 |
| 417 | 495 | $A_u$ | 65 | 819 | 431 |
| 753 | 515 | 74 | 118 | 496 |
| $A_3$ | 73 | $E_g$ | 94 | $A_g$ | 141 | $B_{1g}$ | 439 | $B_{1u}$ | 530 |
| 204 | 189 | 303 | 539 | 114 | $B_{2u}$ | 38 |
| 306 | 311 | 375 | 732 | 165 |
| 440 | 442 | 498 | $B_{1u}$ | 38 | 246 |
| 651 | 565 | $B_{3g}$ | 118 | 496 |
| 133 | 148 | $B_{1g}$ | 539 | 84 | 301 |
| 348 | 256 | 103 | 243 | 403 |
| 477 | 371 | 139 | 387 | 448 |
| 647 | 452 | 350 | 475 | 547 |
are IR active; the $A_g$ and $E_g$ modes are Raman active. In the high-pressure $Pbnm$ phase, the $B_{1u}$, $B_{2u}$, and $B_{3u}$ modes are IR-active; the $A_u$, $B_{1g}$, $B_{2g}$, and $B_{3g}$ modes are active in Raman spectra.

To discuss the experimental data [2, 3] on the effect of the hydrostatic pressure on the HgTiO$_3$ structure, we calculated the properties of mercury titanate under pressure. At a nonzero pressure, the phase which is characterized by the lowest enthalpy $H = E_{\text{tot}} + PV$, rather than by the lowest total energy $E_{\text{tot}}$, is thermodynamically stable at $T = 0$. To compare phases with different number of molecules in the unit cell, we use the specific total energy and the specific unit cell volume defined per one formula unit. Calculations show that as the pressure changes, the relative contribution of the $PV$ term to the change in $H$ is ~95% in the crystals under study. Therefore, the phases with the lowest specific volume should become the most stable as the pressure increases. As follows from Table 1, the $Pbnm$ phase has the smallest volume at $P = 0$ among the considered phases; then, in order of increasing the specific volume, the phases are arranged as follows: $Imma$, $I4/mcm$, $P4/mmb$, $R3\bar{c}$, $R3c$. The largest unit cell volume is characteristic of the ilmenite $R3$ phase, whose total energy at $P = 0$ is the lowest. This enables to expect that the sequence of stable phases will vary with increasing pressure as follows: $R3 \rightarrow R3c \rightarrow Pbnm$. In addition, the suppression of ferroelectricity (the $R3c \rightarrow R3\bar{c}$ phase transition) should be observed with increasing pressure.

The differences between enthalpies of the phases under consideration and the enthalpy of the $R3\bar{c}$ phase as a function of pressure are shown in Fig. 2. It is seen that the $R3 \rightarrow R3c$ and the $R3\bar{c} \rightarrow Pbnm$ phase transitions occur in HgTiO$_3$ at $P = 38$ and 141 kbar, respectively. Since the specific volume of the unit cell changes stepwise (by 6 and 0.71%, respectively) at both phase transitions, they should be of the first order. The $Imma$ phase, whose enthalpy at $P = 0$ is lower than that of the $Pbnm$ phase, becomes energetically less favorable with increasing pressure, and can be excluded from the consideration. The similar behavior, when the stable $R3$ phase transformed to the pressure-stabilized $Pbnm$ phase under high temperatures and pressures and then relaxed from the latter phase to the metastable $R3\bar{c}$ phase as pressure was released, was also observed in MnTiO$_3$ [9], FeTiO$_3$ [10], and ZnGeO$_3$ [11]. Ferroelectric LiTaO$_3$ also exhibits the $R3c \rightarrow Pbnm$ phase transition at high pressures [12].

The present calculations enable to propose a new interpretation of the phase transition observed in X-ray experiments at hydrostatic pressure [2, 3]. The energy of the cubic $Pm3m$ phase, which was attributed to the high-pressure phase in [2, 3], is higher than that of the $R3\bar{c}$ phase by almost 1 eV, and the specific cell volume of this phase exceeds that of the $R3\bar{c}$ phase (Table 1). This means that the sufficiently large difference between the enthalpies of these phases will only increase with increasing pressure. Therefore, the $Pm3m$ phase cannot be considered as a high-pressure phase. According to our calculations, the rhombohedron angle in the $R3\bar{c}$ phase increases with a rate of 0.0054°/kbar with increasing pressure; therefore, at $P = 20$ kbar the structure should remain strongly distorted, and the relative decrease in the interplane distance should be $P/3B \approx 0.32\%$, which is several times smaller than that observed at the phase transition. However, if we admit that the pressures in [2, 3] were determined with an error (according to our estimates, they are underestimated by a factor of 5–7) and take the relative change in the interplane distance $d_{024}$ as a measure of pressure, the agreement between the present calculations and the experimental data becomes satisfactory. For example, at the $R3\bar{c} \rightarrow Pbnm$ transition point (141 kbar), the calculated decrease in the $d_{024}$ interplane distance in comparison with the case of $P = 0$ is 2.0%, whereas the experimental value is 2.3%, and the calculated jump of the average interplane distance$^2$ at the phase transition point (0.054%) is close to the experimental value of ~0.05%.

1 The $d_{024}$ value at $P = 0$, shown in Fig. 3 of [2], does not correspond to the lattice parameters given in the paper for this pressure (disagreement is ~5%).

2 During the $R3\bar{c} \rightarrow Pbnm$ phase transition, the peak (012) splits into two components with indices (110) and (002).
The lattice parameters and atomic coordinates in the \( Pbnm \) structure at 141 kbar are given in Table 2. The calculated X-ray diffraction patterns of \( R\bar{3}c \) and \( Pbnm \) phases at 141 kbar are shown in Fig. 3. The calculated X-ray diffraction pattern of the \( Pbnm \) phase is indeed similar to the experimental X-ray diffraction pattern of the high-pressure phase \([2, 3]\). During the transition to the orthorhombic phase, the (012) line broadens, since a pair of closely spaced reflections (002) and (110) appears in the orthorhombic phase. The new line (021) appearing in the orthorhombic phase is easily seen in the X-ray diffraction patterns recorded as the pressure is released. A notable disagreement between the experimental and calculated X-ray diffraction patterns is the absence of the (111) line in the X-ray diffraction pattern of the high-pressure phase. It is possible that this disagreement results from an incompleteness of the structural transformation. Therefore, to confirm the interpretation proposed in this paper, additional studies of HgTiO\(_3\) under pressure are required.

As noted above, the contradiction between the absence of dielectric hysteresis loops in HgTiO\(_3\) at 300 K and the observation of the second harmonic generation signal can be caused by the existence of defects. Indeed, according to the data of \([1]\), the samples rapidly darkened upon exposure to light. The absence of a sharp peak in the dielectric constant can also be caused by defects. This propensity of HgTiO\(_3\) for the defect formation is confirmed by simple ab initio calculations of its thermodynamics: at \( P = 0 \), the enthalpy of the \( R\bar{3}c \) phase of mercury titanate is higher than the sum of enthalpies of orthorhombic HgO and rutile TiO\(_2\) by 150 meV (per formula unit). This means that mercury titanate is thermodynamically unstable with respect to its decomposition into starting components. However, since the specific volume of the HgTiO\(_3\) unit cell is noticeably smaller than the sum of specific volumes of HgO and TiO\(_2\), the stability of HgTiO\(_3\) increases with increasing pressure. For example, at a pressure of 58.8 kbar, the HgTiO\(_3\) enthalpy appears lower than the sum of enthalpies of orthorhombic HgO and rutile TiO\(_2\) by 75 meV. This explains why the synthesis of mercury titanate is possible only under high-pressure conditions.

The calculations presented in this paper were performed on the laboratory computer cluster (16 cores).

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