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DOI: 10.1180/mgm.2025.10118

# The epidote-törnebohmite polysomatic series: structural relations and complexity

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*Running title*: Epidote-törnebohmite polysomatic series

## Abstract

The $ET_n$ homologous row of the epidote-törnebohmite polysomatic series is considered, which includes minerals of the epidote ($n$ = 0) and gatelite ($n$ = 1) supergroups and radekškodaite group ($n$ = 2). The crystal structures of members of the series are based upon the alternation of epidote ($E$) and törnebohmite ($T$) two-dimensional modules. The aristotype structure types of the members of the row crystallise in the $P2_1/m$ space group with the unit cell-parameters $a \sim 8.90$, $b \sim 5.65$, $c \sim (10.10 + 7.50n)$ Å, $\beta \sim 116.5^{o}$, $V \sim (455 + 338n)$ Å$^3$. The general formula for the members of the row can be expressed as $A_{2(n+1)}M_{n+3}[Si_2O_7][SiO_4]_{2n+1}X_{n+2}$ (X = O, OH, F). The structure model for the hypothetical $ET_3$ member of the series is constructed and the general formulae are derived for the calculation of the number of atoms per unit cell and the number and multiplicities of the atom sites for any value of $n$. The concept of $K$-sequence is introduced that is analogous to the concept of a Wyckoff sequence. The general formulae for the information-based complexity parameters are derived for the $ET_n$ homologous row of the epidote-törnebohmite polysomatic series with different parities of $n$. The present absence of the members of the series with $n > 2$ reflects the entropic restrictions on the polysomatic series that confirm the principle of maximal simplicity for modular inorganic structures.

**Keywords**: polysomatism; polysomatic series; crystal structure; chemical composition; epidote supergroup; gatelite supergroup; radekškodaite group; törnebohmite; structural complexity; information-based complexity parameters.

## Introduction

Polysomatism is an important concept in structural mineralogy and inorganic crystal chemistry that allows one to establish relations among different structure types (Thompson, 1970, 1978), correlate their chemical composition, structure and properties (Veblen, 1991; Ferraris, 1997), and predict new structure types (Merlino and Pasero, 1997; Collins *et al*., 2017; Ogawa and Walsh, 2025), etc. Whereas the term 'polysomatism' is due to Thompson (1978), the concept of modular construction of crystal structures and structural homology was recognised long before (see, *e.g*., Magnéli, 1953; Bragg and Claringbull, 1965). Ferraris *et al*. (2005) provided both conceptual and factual overviews of the concepts of modularity and polysomatism (note that the term 'polysome' is different from 'polymorph'; in contrast to polymorphs, different polysomes may have different chemical compositions). A number of recent works outline the usefulness of these approaches to the interpretation and description of both minerals and synthetic inorganic compounds (Cámara *et al*., 2021; Malcherek *et al*., 2021; Ciobanu *et al*., 2022; Rao *et al*., 2022; Yudintsev *et al*., 2022; Conconi *et al*., 2023; Hatert *et al*., 2023; Aksenov *et al*., 2023, 2024; Campo-Rodriguez *et al*., 2024; Tsuchiya *et al*., 2024).

This paper is devoted to the analysis of the epidote-törnebohmite polysomatic series. It was first proposed by Bonazzi *et al*. (2003) on the basis of their discovery of gatelite-(Ce), a mineral with a structure that can be described as an ordered alternation ($ET$) of epidote ($E$) and törnebohmite ($T$) two-dimensional modules. Further discoveries led Bonazzi *et al*. (2019) to the establishment of the gatelite supergroup that currently contains seven mineral species. In 2020, Kasatkin *et al*. discovered the natural $ETT$ (= $ET_2$) polysome of the epidote-törnebohmite polysomatic series and defined the radekškodaite group that now contains three members: radekškodaite-(Ce), radekškodaite-(La), and zilbermintsite-(La) (Kasatkin *et al*., 2020, 2024).

In addition to the interest from the crystal-chemical point of view, the minerals of the epidote-törnebohmite polysomatic series attract attention as a potential source of rare earth elements (*REE*) (Hentschel *et al*., 2020). For instance, allanite is mined as one of the *REE* ore minerals in the Nechalacho deposit (Northwest Territories, Canada) (Haque *et al*., 2014; see also: Xiao and Zhang, 2024). As the *REE* content of the epidote-törnebohmite polysomatic series increases from epidote to radekškodaite, further investigations are warranted to define the role of these minerals as *REE* concentrators in natural systems.

The aim of the present study is to derive the crystal-chemical formulae for the $ET_n$ row of the series ($n \geq 0$) and analyse the evolution of information-based structural complexity parameters with the increasing $n$ value. We shall demonstrate that for $n > 4$, the total information content of the crystal structure aristotypes is above 1000 bit per unit cell, which makes the corresponding polysomes unlikely to occur in nature as ordered crystals.

## General crystallography of the epidote-törnebohmite series

### *Homologous rows*

Figure 1 shows the crystal structures of allanite-(Ce) and törnebohmite-(Ce) as end members of the series with indications of the $E$ and $T$ modules, respectively. Table 1 contains the modular description of the representative members of the polysomatic series. It should be noted that the existing members of the series (Table 1) represent only one possible homologous row, namely, one that includes addition of $T$ modules to the initial $E$ module. This homologous row can be described by the general formula $ET_n$. Other homologous rows can be theoretically foreseen, such as $EET_n$, $EETET_n$, and $EETEET_n$. As only the $ET_n$ members of the series have been observed in nature so far, only this homologous row is considered here.

### *Aristotype structures*

Each member of the polysomatic series can be characterised by its aristotype structure, which is defined here as a structure type with maximal possible symmetry. For instance, the crystal structure of perbøeite-(Ce) is an aristotype for the *ET* member, whereas that of gatelite-(Ce) is not, since the latter is a 2×1×1 superstructure with regard to its aristotype; its *a* parameter is doubled (Table 1). By analogy, the experimentally determined crystal structure of törnebohmite-(Ce) does not correspond to its aristotype, owing to its 1×1×2 superstructure. Table 2 contains full information about the aristotype structure model of törnebohmite-(Ce). The aristotype structures of all members of the $ET_n$ homologous row of the epidote-törnebohmite polysomatic series belong to the $P2_1/m$ space-group-type. Their chemical formulae and approximate unit-cell parameters are listed in Table 3 as dependent upon the *n* value (i.e., the number of törnebohmite modules in a polysome). Figures 2a and b shows crystal structures of perbøeite-(Ce) and radekškodaite-(Ce) as aristotype structures for the *ET* and $ET_2$ members of the polysomatic series, respectively.

### *K-sequences*

The concept of *K*-sequence is a generalisation of the concept of Wyckoff sequence that reflects the diversity and numbers of Wyckoff sites occupied in a particular crystal structure (Hornfeck, 2022). Usually, the Wyckoff sequence contains the space-group number followed by a sequence of Wyckoff letters corresponding to the sites occupied by atoms in a particular crystal structure. In cases of more than one site of particular Wyckoff type, the number of such sites is indicated by a superscript. The following example is taken from Hornfeck (2022). The unit cell of the crystal structure of $RbAg_4I_5$ (space group $P4_132$ (no. 213)) contains 80 atoms distributed over six Wyckoff sites (crystallographic orbits) of four different types: two 24*e* (*x*, *y*, *z*), one 12*d* (1/8, *y*, *y* + ¼), two 8*c* (*x*, *x*, *x*), and one 4*a* (3/8, 3/8, 3/8). The total Wyckoff sequence is 213 $e^2\ d\ c^2\ a$. The *K*-sequence is a sequence of multiplicities of the occupied Wyckoff sites with the number of sites with the same multiplicities written in a subscript. For the crystal structure of $RbAg_4I_5$, the *K*-sequence is simply $24^2 12^1 8^2 4^1$. The *K*-sequence does not distinguish between different Wyckoff sites with the same multiplicity. For instance, the crystal structure of allanite-(Ce) (Hoshino *et al*., 2005) contains one 2*a* (0, 0, 0), one 2*c* (0, 0, ½), thirteen 2*e* (*x*, ¼, *z*), and three 4*f* (*x*, *y*, *z*) sites. The Wyckoff sequence is $11\ f^3\ e^{13}\ c\ a$, whereas the *K*-sequence is $4^3 2^{15}$.

Table 4 contains *K*-sequences for the representative members of the epidote-törnebohmite polysomatic series listed in Table 1 classified according to the atom types (A, M, Si, O, X) as well as *K*-sequences for the total crystal structures. The detailed analysis of the dependencies of the *K*-sequences upon the *n* value for the known members of the $ET_n$ homologous row allows one to derive general formulae, which are different for even and odd *n*. The corresponding formulae are $4^{(5n+7)/2} 2^{9n+14}$ and $4^{(5n+6)/2} 2^{9n+15}$ for even and odd *n* values, respectively. The number *v* of atoms in the unit cell is expressed by the same formula, irrespective of the parity of *n*: $v = 14(2n + 3)$. In contrast, the numbers *k* of occupied Wyckoff sites (crystallographic orbits) are also dependent on the parity of *n* and are equal to $(23n + 35)/2$ and $(23n + 36)/2$ for odd and even *n*, respectively. It should be emphasised, however, that the formulae obtained (see also Table 3) are for the aristotype structures of the respective polysomes. In reality, structure types may be different for the same aristotype, owing to the formation of superstructures, as is the case for gatelite-(Ce) that has the 2×1×1 superstructure relative to its aristotype (as a consequence, the space-group type changes from $P2_1/m$ to $P2_1/c$).

On the basis of atom coordinates for the $ET_n$ members of the series with $n = 0$, 1, and 2, the structure model for the hypothetic $ET_3$ polysome with $n = 3$ was constructed (see Table 5 for crystallographic parameters and Fig. 2c for the structure diagram).

## Information-based analysis of structural complexity

The evolution of structural complexity with the changing *n* value in the $ET_n$ homologous row of the series was investigated using information-based measures first proposed in Krivovichev (2012, 2013) and developed in Krivovichev *et al*. (2022).

For a crystal structure having *v* atoms per reduced unit cell split into *k* crystallographic orbits with multiplicities ($m_1$, $m_2$, …., $m_k$), the amounts of structural Shannon information per atom ($I_\mathrm{G}$; in bit/atom) and per unit cell ($I_\mathrm{G,total}$; in bit/cell) are calculated according to the following equations:

$$I_G = -\sum_{\mathrm{i}=1}^{\mathrm{k}} \mathrm{p}_i \log_2 p_i \qquad \text{(bit/atom)} \qquad (1),$$

$$I_{G,total} = v \times {}^{\mathrm{str}}I_G = -v \times \sum_{\mathrm{i}=1}^{\mathrm{k}} \mathrm{p}_i \log_2 p_i \qquad \text{(bit/cell)} \qquad (2),$$

where $p_i$ is the random choice probability for an atom from the *i*th crystallographic orbit, that is:

$$p_i = m_i / v \qquad (3).$$

The structural complexity parameters for the representative members of the series listed in Table 1 are given in Table 4. The analytical expression of the *K*-sequences given in Table 3 (note their dependence on the parity of *n*) allows for the derivation of formulae for the calculation of structural complexity parameters using *n* as the only variable. The formulae are given in Table 3, whereas Fig. 3 shows the behavior of both $I_G$ and $I_{G,total}$ values with increasing *n*. The dependence is almost linear for the total amount of structural information amount exceeding the level of 1000 bit/cell for $n = 5$. At this value, the structure belongs to the very complex class (Krivovichev, 2013, 2014), though there are no principal obstacles for its formation either in nature or experiment. However, possible natural occurrences of such structures would be very rare, since even the radekškodaite-group members are considered as rare mineral species, presently known from one world locality only (Molchalin Log, South Urals, Russia) (Kasatkin *et al*., 2020, 2024).

## Conclusions

As has been pointed out elsewhere (Krivovichev, 2013, 2014; Krivovichev *et al*., 2022), modularity (or polysomatism) is one of the most important complexity-generating mechanisms in the realm of mineral and synthetic inorganic structures. In the complexity analysis of polysomatic series, it is important to look at the complexity of aristotype structures (maximal-symmetry realisations of polysomes). The example of the epidote-törnebohmite polysomatic series considered here demonstrates that aristotype structures of the end members of the series (epidote and törnebohmite) are relatively simple (172.477 and 98.606 bit/cell, respectively). The simplest combination of the $E$ and $T$ modules is that of $E$:$T$ = 1 realised in the crystal structures of gatelite-supergroup minerals with the aristotype structure model more complex than those of the end members (335.050 bit/cell). The addition of $T$ modules results in the increasing structural complexity; the structures with $n > 2$ are presently unknown as minerals or synthetic compounds. It is likely that the higher members of the series can be found at the contacts between grains of lower members. It is of interest that mineral diversity generally correlates with the increasing trend of complexity in the polysomatic series: the epidote supergroup contains at present at least thirty-six mineral species, whereas the gatelite supergroup has seven, and the radekškodaite group only three. This further confirms the principle of maximal simplicity for modular inorganic crystal structures proposed in Krivovichev (2021): structures with minimal information dominate over other structures with the same building principles. This principle has entropic origins and reflects the tendency of inorganic nature to form structures of high entropy.

Finally, it should be pointed out that temperature-driven phase transitions can be expected for those members of the series that form superstructures relative to their aristotypes (e.g., törnebohmite and gatelite-(Ce)) with the space-group change from $P2_1/c$ to $P2_1/m$ with twofold unit-cell volume contraction.

## Acknowledgements

This manuscript is a contribution to the 80th anniversary celebration of Professor Edward Grew. I am grateful to Robert F. Martin, Luca Bindi and two anonymous referees for the constructive remarks on the manuscript. This research was supported by the Russian Science Foundation, grant number 24-17-00083, https://rscf.ru/project/24-17-00083/ (accessed on 6 May 2025).

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Table 1

Representative members of the epidote-törnebohmite polysomatic series

| Mineral name | Chemical formula | Modular composition | Space group | *a*, Å | *b*, Å | *c*, Å | *β*, deg | *V*, Å$^3$ | Ref. |
|---|---|---|---|---|---|---|---|---|---|
| allanite-(Ce) | $(CaCe)(Al_2Fe^{2+})[Si_2O_7][SiO_4]O(OH)$ | *E* | $P2_1/m$ (11) | 8.905 | 5.761 | 10.123 | 114.78 | 471.5 | 1 |
| perbøeite-(Ce) | $(CaCe_3)(Al_3Fe^{2+})[Si_2O_7][SiO_4]_3O(OH)_2$ | *ET* | $P2_1/m$ (11) | 8.894 | 5.619 | 17.755 | 116.95 | 794.8 | 2 |
| gatelite-(Ce) | $(Ca,Ce)_4(Al,Mg,Fe)_4[Si_2O_7][SiO_4]_3(O,F,OH)_3$ | *ET* | $P2_1/c$ (14) | 17.770 | 5.651 | 17.458 | 116.18 | 1573.3 | 3 |
| radekškodaite-(Ce) | $(CaLa_5)(Fe^{2+}Al_4)[Si_2O_7][SiO_4]_5O(OH)_3$ | $ET_2$ | $P2_1/m$ (11) | 8.960 | 5.727 | 25.113 | 116.63 | 1152.0 | 4 |
| törnebohmite-(Ce) | $Ce_2Al[SiO_4]_2(OH)$ | *T* | $P2_1/c$ (14) | 7.383 | 5.673 | 16.937 | 112.04 | 657.5 | 5 |
| törnebohmite-(Ce)* | $Ce_2Al[SiO_4]_2(OH)$ | *T* | $P2_1/m$ (11) | 7.383 | 5.673 | 8.964 | 112.04 | 328.8 | 5 |

* aristotype structure model

References: (1) Hoshino *et al*. (2005); (2) Bonazzi *et al*. (2014); (3) Bonazzi *et al*. (2003); (4) Kasatkin *et al*. (2020); (5) Shen and Moore (1982).

Table 2

Aristotype structure model for törnebohmite-(Ce)

| Atom | Site | *x* | *y* | *z* |
|---|---|---|---|---|
| Törnebohmite-(Ce) aristotype<br>$P2_1/m$ (11), $a = 7.383$, $b = 5.673$, $c = 8.964$ Å, $\beta = 112.04^{\circ}$ | | | | |
| Al | 2*d* | ½ | 0 | ½ |
| Si1 | 2*e* | 0.529 | ¼ | 0.419 |
| Si2 | 2*e* | 0.931 | ¼ | 0.338 |
| O1 | 2*e* | 0.382 | ¼ | 0.933 |
| O2 | 2*e* | 0.749 | ¼ | 0.969 |
| O3 | 4*f* | 0.508 | 0.012 | 0.720 |
| O4 | 2*e* | 0.041 | ¼ | 0.548 |
| O5 | 2*e* | 0.694 | ¼ | 0.553 |

| | | | | |
|---|---|---|---|---|
| O6 | 4*f* | 0.999 | 0.476 | 0.789 |
| OH | 2*e* | 0.324 | ¼ | 0.429 |
| Ce1 | 2*e* | 0.813 | ¾ | 0.456 |
| Ce2 | 2*e* | 0.219 | ¾ | 0.370 |

Table 3
Crystallographic parameters and formulae for the calculation of information-based complexity parameters for the aristotype structures of the $ET_n$ row of the epidote-törnebohmite polysomatic series

| $n$ | odd | even |
|---|---|---|
| Chemical formula | $A_{2(n+1)}M_{n+3}[Si_2O_7][SiO_4]_{2n+1}X_{n+2}$ (X = O, OH, F) | |
| Space group | $P2_1/m$ (11) | |
| $a$ [Å] | ~ 8.90 | |
| $b$ [Å] | ~ 5.65 | |
| $c$ [Å] | ~ (10.10 + 7.50$n$) | |
| $\beta$ [deg] | ~ 116.5 | |
| $V$ [Å$^3$] | ~ (455 + 338$n$) | |
| $k$ [orbits] | $(23n + 35)/2$ | $(23n + 36)/2$ |
| $v$ [atoms] | $14(2n + 3)$ | |
| $K$-sequence | $4^{(5n+7)/2}2^{9n+14}$ | $4^{(5n+6)/2}2^{9n+15}$ |
| $I_G$ [bit/atom] | $\log_2[7(2n+3)] – (5n+7)/[7(2n+3)]$ | $\log_2[7(2n+3)] – (5n+6)/[7(2n+3)]$ |
| $I_{G,total}$ [bit/cell] | $14(2n+3)\log_2[7(2n+3)] – 2(5n+7)$ | $14(2n+3)\log_2[7(2n+3)] – 2(5n+6)$ |

Table 4
*K*-sequences and information-based complexity parameters* for some members of the epidote-törnebohmite polysomatic series

| Mineral name | MC** | *n* | Space group | *K*-sequences | | | | | Complexity parameters | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | A | M | Si | O+X | total | $k$ [orbits] | $v$ [atoms] | $I_G$ [bit/atom] | $I_{G,total}$ [bit/cell] |
| allanite-(Ce) | *E* | 0 | $P2_1/m$ | $2^2$ | $2^3$ | $2^3$ | $4^3 2^7$ | $4^3 2^{15}$ | 18 | 42 | 4.107 | 172.477 |
| perbøeite-(Ce) | *ET* | 1 | $P2_1/m$ | $2^4$ | $4^1 2^2$ | $2^5$ | $4^5 2^{12}$ | $4^6 2^{23}$ | 29 | 70 | 4.786 | 335.050 |
| gatelite-(Ce) | *ET* | 1 | $P2_1/c$ | $4^4$ | $4^4$ | $4^5$ | $4^{22}$ | $4^{35}$ | 35 | 140 | 5.129 | 718.100 |
| radekškodaite-(Ce) | $ET_2$ | 2 | $P2_1/m$ | $2^6$ | $4^1 2^3$ | $2^7$ | $4^7 2^{17}$ | $4^8 2^{33}$ | 41 | 98 | 5.288 | 518.242 |
| hypothetic | $ET_3$ | 3 | $P2_1/m$ | $2^8$ | $4^2 2^2$ | $2^9$ | $4^9 2^{22}$ | $4^{11} 2^{41}$ | 52 | 126 | 5.628 | 709.137 |
| general (*n* = even) | $ET_n$ | *n* | $P2_1/m$ | $2^{2(n+1)}$ | $4^{n/2} 2^3$ | $2^{2n+3}$ | $4^{2n+3} 2^{5n+7}$ | $4^{(5n+6)/2} 2^{9n+15}$ | $(23n+36)/2$ | $14(2n+3)$ | see Table 3 | |
| general (*n* = odd) | $ET_n$ | *n* | $P2_1/m$ | | $4^{(n+1)/2} 2^2$ | | | $4^{(5n+7)/2} 2^{9n+14}$ | $(23n+35)/2$ | | | |
| törnebohmite-(Ce) | *T* | - | $P2_1/c$ | $4^2$ | $4^1$ | $4^2$ | $4^9$ | $4^{14}$ | 14 | 56 | 3.807 | 213.212 |
| törnebohmite-(Ce)*** | *T* | - | $P2_1/m$ | $2^2$ | $2^1$ | $2^2$ | $4^2 2^5$ | $4^2 2^{10}$ | 12 | 28 | 3.522 | 98.606 |

* without contributions from H atoms

** modular composition

*** aristotype structure model

Table 5

Atom coordinates* for the aristotype $A_8M_6[Si_2O_7][SiO_4]_7X_5$ structure of the hypothetic $ET_3$ member of the epidote-törnebohmite polysomatic series

| Atom | Site | $x$ | $y$ | $z$ | Atom | Site | $x$ | $y$ | $z$ |
|---|---|---|---|---|---|---|---|---|---|
| M1 | 2*a* | 0 | ½ | 0 | O6 | 4*f* | 0.2384 | 0.4930 | 0.0100 |
| M2 | 2*e* | 0.3124 | ¾ | 0.0670 | O7 | 2*e* | 0.3740 | ¼ | 0.9665 |
| M3 | 4*f* | 0.0280 | 0.4995 | 0.1600 | O8 | 2*e* | 0.4848 | ¼ | 0.2090 |
| M4 | 4*f* | 0 | ½ | 0.3850 | O9 | 2*e* | 0.0559 | ¼ | 0.3530 |
| A1 | 2*e* | 0.7710 | ¼ | 0.0494 | O10 | 2*e* | 0.9676 | ¾ | 0.1910 |
| A2 | 2*e* | 0.2294 | ¾ | 0.7210 | O11 | 2*e* | 0.0944 | ¼ | 0.1320 |
| A3 | 2*e* | 0.5923 | ¼ | 0.3620 | O12 | 4*f* | 0.3041 | 0.4748 | 0.3420 |
| A4 | 2*e* | 0.4306 | ¾ | 0.1820 | O13 | 4*f* | 0.8140 | 0.5129 | 0.1090 |
| A5 | 2*e* | 0.6161 | ¼ | 0.1360 | O14 | 4*f* | 0.3271 | 0.4784 | 0.1140 |
| A6 | 2*e* | 0.2470 | ¾ | 0.2770 | O15 | 4*f* | 0.7842 | 0.5123 | 0.3340 |
| A7 | 2*e* | 0.7530 | ¼ | 0.4930 | O16 | 4*f* | 0.7138 | 0.5231 | 0.2000 |
| A8 | 2*e* | 0.4080 | ¾ | 0.4080 | O17 | 2*e* | 0.0541 | ¼ | 0.0480 |
| Si1 | 2*e* | 0.2014 | ¼ | 0.1020 | O18 | 4*f* | 0.2419 | 0.4883 | 0.2130 |
| Si2 | 2*e* | 0.3556 | ¼ | 0.2290 | O19 | 2*e* | 0.5174 | ¼ | 0.0560 |
| Si3 | 2*e* | 0.7027 | ¾ | 0.0890 | O20 | 2*e* | 0.5534 | ¾ | 0.1030 |
| Si4 | 2*e* | 0.8393 | ¾ | 0.2160 | O21 | 2*e* | 0.4520 | ¼ | 0.2830 |
| Si5 | 2*e* | 0.6719 | ¾ | 0.3150 | O22 | 2*e* | 0.5360 | ¾ | 0.3340 |
| Si6 | 2*e* | 0.1828 | ¼ | 0.3280 | O23 | 2*e* | 0.0600 | ¼ | 0.2750 |
| Si7 | 2*e* | 0.3412 | ¼ | 0.0120 | O24 | 2*e* | 0.9590 | ¾ | 0.2690 |
| Si8 | 2*e* | 0.3280 | ¼ | 0.4550 | O25 | 4*f* | 0.2158 | 0.0123 | 0.4364 |
| Si9 | 2*e* | 0.8172 | ¾ | 0.4419 | O26 | 2*e* | 0.4130 | ¼ | 0.5096 |
| O1 | 2*e* | 0.9256 | ¼ | 0.4070 | O27 | 2*e* | 0.4640 | ¼ | 0.4356 |
| O2 | 2*e* | 0.1068 | ¾ | 0.1380 | O28 | 2*e* | 0.9440 | ¾ | 0.4165 |
| O3 | 2*e* | 0.9504 | ¼ | 0.1830 | O29 | 4*f* | 0.6960 | 0.9748 | 0.4279 |
| O4 | 2*e* | 0.0639 | ¾ | 0.0420 | O30 | 2*e* | 0.9400 | ¾ | 0.4951 |
| O5 | 2*e* | 0.5870 | ¾ | 0.2600 | O31 | 2*e* | 0.0744 | ¾ | 0.3630 |

* $P2_1/m$, $a = 8.9702$, $b = 5.7044$, $c = 32.600$ Å, $\beta = 116.766^{\circ}$.

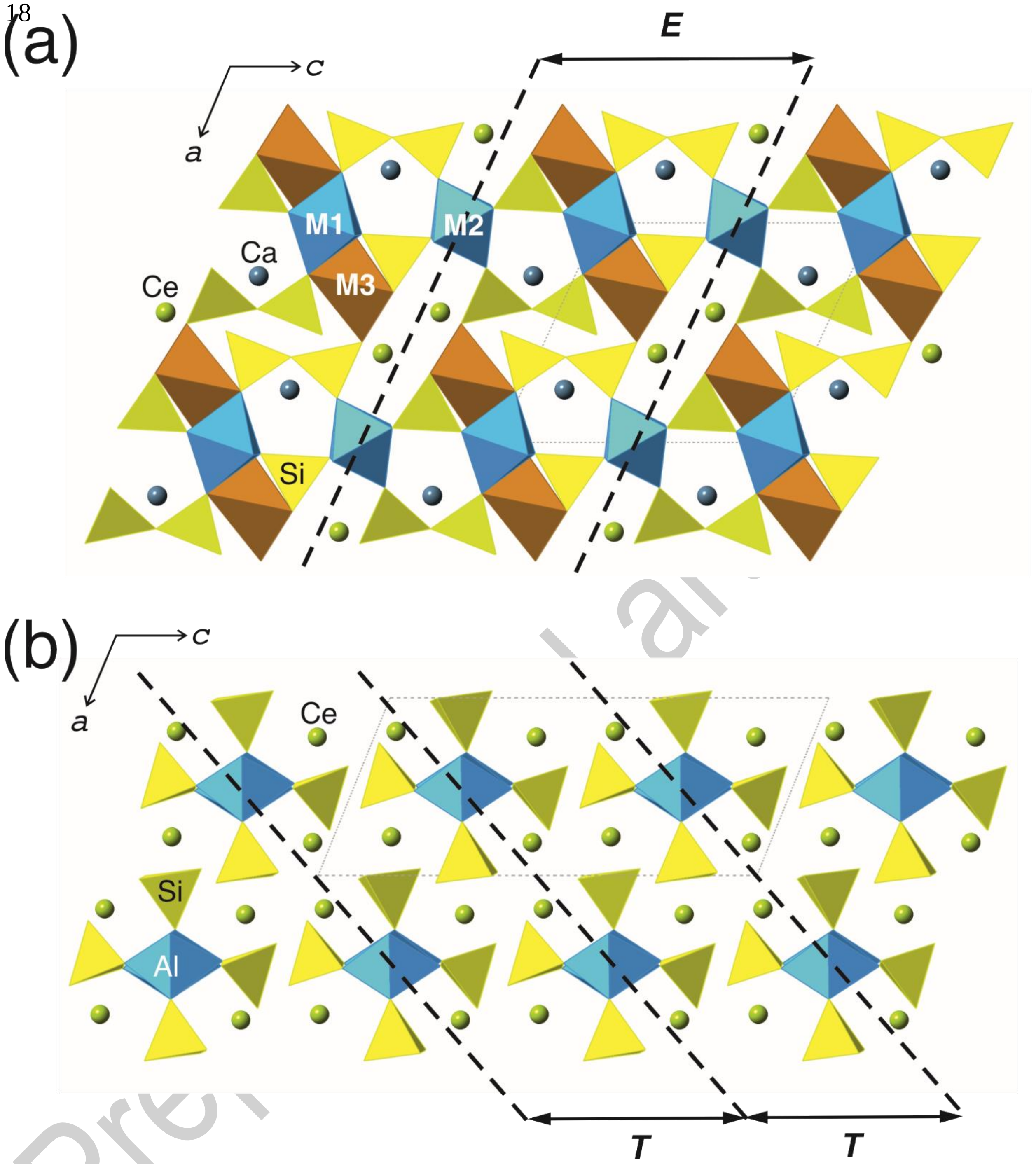

**Fig. 1**. The crystal structures of allanite-(Ce) (a) and törnebohmite-(Ce) (b) projected along the *b* axes with the indication of the *E* and *T* modules by the dashed lines, respectively. Legend: $M^{3+}O_6$ octahedra = light-blue; $M^{2+}O_6$ octahedra = brown; $SiO_4$ tetrahedra = yellow; Ce and Ca (A) atoms are shown as yellow and blue balls, respectively.

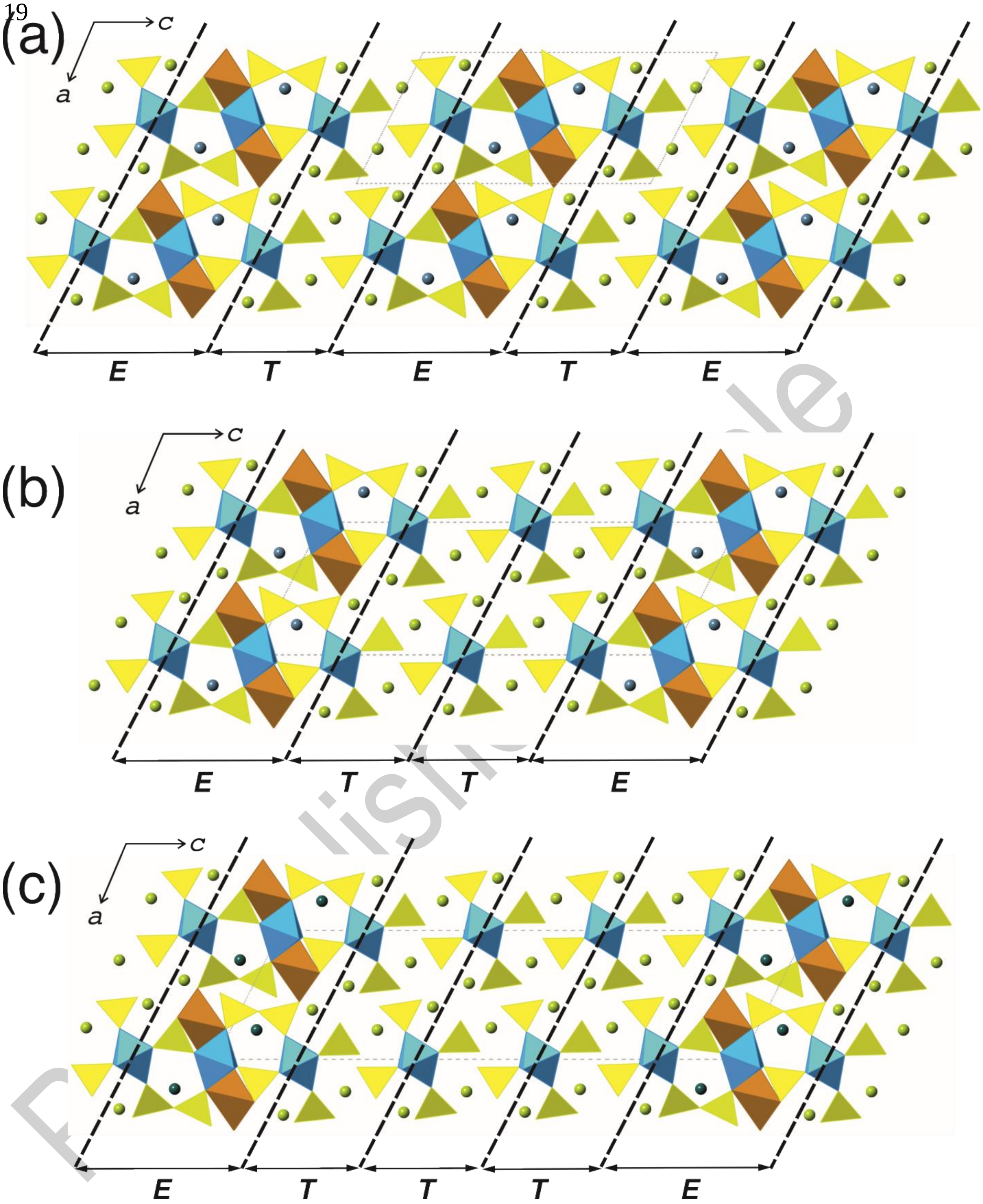

**Fig. 2**. The crystal structures of perbøeite-(Ce) (a), radekškodaite-(Ce) (b), and hypothetic $ET_3$ members of the epidote-törnebohmite polysomatic series (c) projected along the *b* axes with the indication of the *E* and *T* modules by the dashed lines. Legend as in Fig. 1.

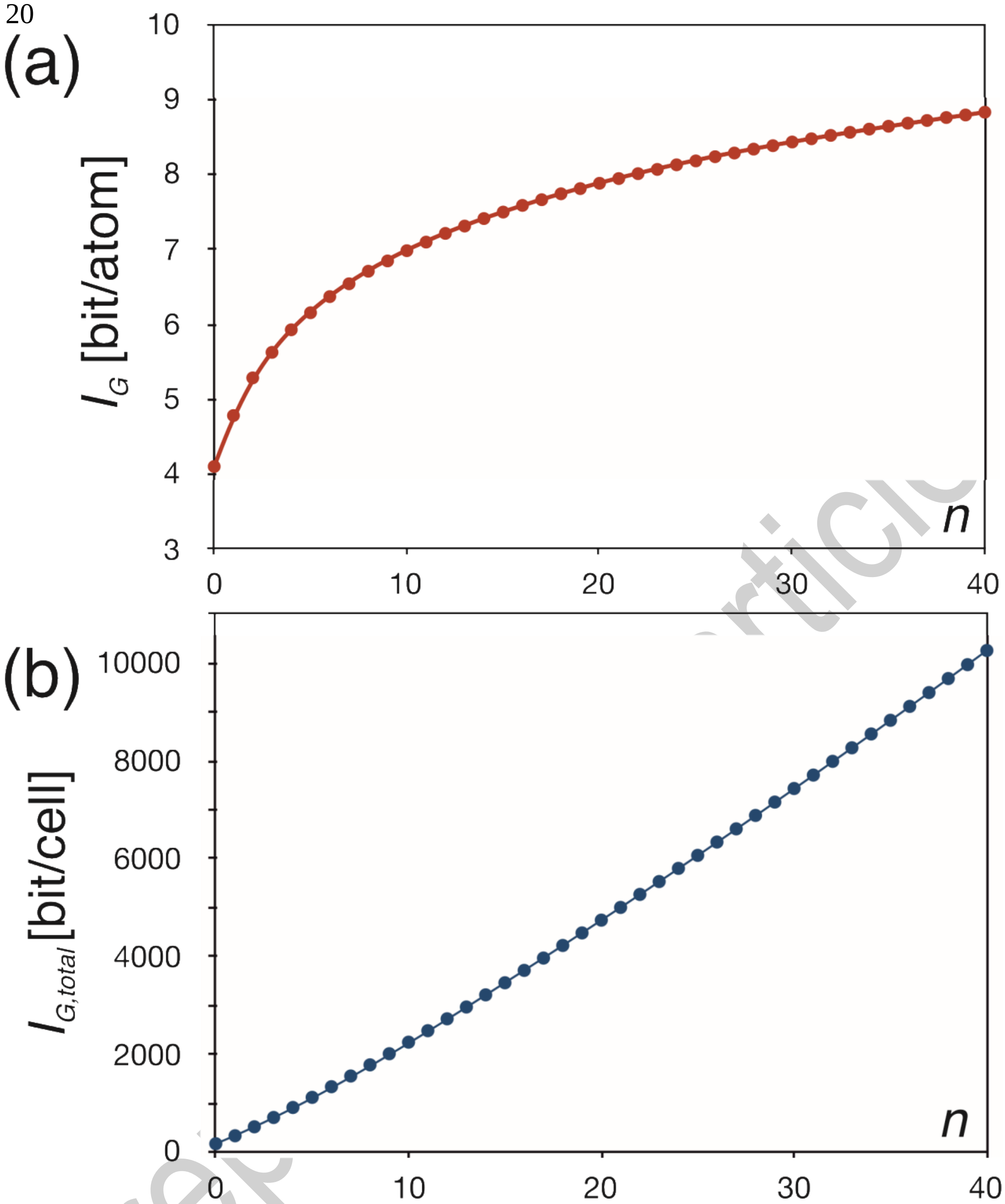

**Fig. 3**. The dependence of the atomic (a) and total (b) information contents *versus* *n* value for the $ET_n$ homologous row of the epidote-törnebohmite polysomatic series.