The crystal structure of the new mineral species owensite, (Ba,Pb)$_6$(Cu,Fe,Ni)$_{25}$S$_{27}$, is cubic, with $a = 10.349(1)$ Å, space group $Pm3m$. Nine S atoms bond to each (Ba,Pb) atom. The unit cell contains a single (Cu,Fe,Ni) atom that is octahedrally coordinated by S; the other twenty-four (Cu,Fe,Ni) atoms are tetrahedrally coordinated. The structure is analogous to that of djerfisherite, $K_6Na(Fe,Ni,Cu)_{26}S_{26}Cl$, but it contains no monovalent ions. The K sites in djerfisherite are here occupied by (Ba,Pb) atoms; the Na site is occupied by one of the (Cu,Fe,Ni) atoms, whereas the Cl site is occupied by a S atom. The structure was solved and refined to an R index of 5.27% for MoKα data to $2\theta = 100^\circ$. The bond lengths and angles are all within the expected limits: Ba-S between 3.132(2) and 3.300(5) Å; (Cu,Fe)2S$_4$ between 2.302(3) and 2.356(2) Å [tetrahedral], or 2.501(5) Å [octahedral]. The Pb atom replaces the Ba atom within the S coordination cage, but is disordered and displaced from the Ba position as a result of the presence of the $6^{2}$ Pb electron pair. Four disordered Pb satellite positions exist, all 0.38 Å from the Ba position, and in a square with a side of 0.31 Å.

**Keywords:** owensite, barium copper-iron sulfide, structure refinement, atomic ratios, disordered lead, djerfisherite-group mineral.

**INTRODUCTION**

The new mineral species owensite, found in the Wellgreen deposit, Yukon Territory (Cabri et al. 1993), has been described in the previous paper (Laflamme et al. 1995). Interest in this mineral developed when it was realized that it promised to be a Ba transition-metal sulfide, as no Ba sulfide minerals have hitherto been described. It was expected from the chemistry and the X-ray powder-diffraction data that this mineral would have an argentopentlandite structure (Hall & Stewart 1973). However, electron-microprobe analyses on owensite grains indicated atomic proportions $[(\text{Ba}_{5.42}\text{Pb}_{0.56})_{25.39}\text{(Cu}_{12.6}\text{Fe}_{1.7}\text{Ni}_{0.14})_{224.71}\text{S}_{27.31}]$, based on 58 atoms, that are incompatible with the expected 9:8 metal:sulfur ratio. Given the observed proportions of Pb, Pb, Cu, Fe, Ni and S, it was not possible to account for the chemistry in terms of atomic sites within the known structural types. To this end, a structural determination was undertaken to elucidate the formula and to explain the determined chemical composition.

**EXPERIMENTAL**

An irregular fragment of owensite, dug out of a polished section and measuring <50 μm across, was
mounted on a CAD4 single-crystal diffractometer. This grain had been used previously to obtain the powder-diffraction data and to characterize the mineral by a single-crystal precession study. Unit-cell dimensions were refined from 45 unique reflections in the range $22.3 < 2\theta < 45.7^\circ$, using the NRCVAX routine TRUANG. This computer program measures and averages the angular positions for each of the four equivalent reflections ($hkl$ and $-h-k-l$ at $+2\theta$ and $-2\theta$). MoK$\alpha$ radiation was used throughout the data-collection procedure. The value of the $a$ parameter quoted here [10.349(1) Å] differs slightly from that quoted in the previous paper (Laflamme et al. 1995); the latter value (10.373 Å) was obtained from a refinement of X-ray powder-diffraction film data, uncorrected for film shrinkage. Four equivalent segments of diffraction data were collected in diffraction symmetry $3m$ (equivalent to eight segments in symmetry $m3m$, or one quarter of the sphere of reflection), to a limit of $2\theta = 100^\circ$. In view of the very small size of the crystal, slow scans (${1^\circ}$ in 20 min$^{-1}$) were used. Nevertheless, some reflections were still observed at the 20 limit of data collection, though most were unobserved, and the observed reflections were all weak. Empirical absorption-corrections were applied from correction curves obtained from $\psi$-sweeps for four reflections with widely differing $2\theta$ values. The intensities were measured at intervals of $5^\circ$ in $\psi$, and the corrected data were reduced in both diffraction symmetry $3m$ and $m3m$. With no systematic absences in the cubic system, the space group was identified as $Pm3m$ as $Pm3$, until it was realized that the very high angular correlations observed in the least-squares refinement symrnetry $3m$ (equivalent to eight segments in $m3$ and $m3m$) with no systematic absences in the cubic system, the space group was identified as $Pm3m$ or $P23$. 

**Structure Determination and Refinement**

The structure was solved using direct methods initially in space group $Pm3$. It was being refined in this space group, until it was realized that the very high matrix correlations observed in the least-squares refinement were due to an additional mirror plane in the determined structure. Reassignment of the space group as $Pm3m$ yielded a model that refined to an acceptable residual with little difficulty. Scattering curves for neutral atoms (Cromer & Mann 1968) were used throughout the refinement. Population parameters were allowed to vary for the atoms in the metal sites (refined as Ba and Cu, respectively), with the population parameter of the S sites fixed at unity as a reference. With the proposed Ba site at about full occupancy and both Cu sites showing about 92% occupancy, weighted dual scattering factors were introduced. The scattering curve for the Ba site was adjusted to include the partial incorporation of Pb in that site, Ba:Pb = 0.9064:0.0936. Similarly, the Cu scattering curve was adjusted for the presence of Fe in the Cu:Fe proportion indicated by the microprobe results.

Unfortunately, in the currently used software for structure refinement, a maximum of only two atomic types can be assigned to a single site; Ni was therefore omitted. This is not likely to introduce any significant error, as the proportion of Ni is very small (<0.6% of the (Cu,Fe,Ni)), and the composite curve of Cu and Fe, in the proportions found in the microprobe analyses, is very close to the Ni curve. The structure refined using anisotropic thermal parameters to a residual $R$ of 6.2%. Of the 1209 unique reflections measured, 554 were observed with the criterion that $I_{obs} > 3\sigma(I_{obs})$. This residual is higher than one would like to see in a well-refined structure, but it was considered that this was an artifact of collecting the data on such a small crystal to the high 2$\theta$ limit of 100$^\circ$. Truncating the data to the more usual limit of $2\theta = 60^\circ$ improved the residual to 3.9%. Near the end of the refinement, the population parameters of all metal sites were allowed to vary in an attempt to check for incomplete occupancy of these sites in the structure. The resultant parameters did not differ significantly from unity for the (Cu,Fe) site [0.99(2)], and it must be concluded that all (Cu,Fe) sites are fully occupied. However, the Ba population parameter did decrease to less than the expected value. A difference synthesis calculated at this point in the refinement revealed small peaks distributed about the fourfold axis and about 0.5 Å from the Ba position. These were interpreted as being due to a disordered Pb atom, moved away from the Ba position by the interaction of the remaining Pb 6$s^2$ valence electrons with the anion coordinating sphere (see Moore et al. 1993, Szymański 1988). As the proportion of Ba:Pb is 0.9064:0.0936, and as the 0.0936 population parameter for Pb is now equally divided among the four disordered sites, its value is now only 0.0234 at each new site. Refinement of the position, of the occupancy and anisotropic thermal parameter of this very small peak (corresponding to 0.0234 × 82, or ~2 electrons) was strongly correlated, and very severe damping had to be used for the block-diagonal least-squares employed. The structure refined to $R = 5.2\%$ for all data and $R = 3.5\%$ for data below $2\theta = 60^\circ$. A difference synthesis did not reveal any peaks beyond 1 electron, and these were at high-symmetry positions, where cumulative errors in data tend to generate peaks. All crystallographic calculations were carried out using the NRCVAX system of programs (Gabe et al. 1989) on a 486-P.C. The crystal data on owensite are summarized in Table 1.

**Description of the Structure of Owensite**

There are four unique S sites. These are: S1 at the origin [0,0,0], (multiplicity 1); S2 at [x,½,0], (multiplicity 12); S3 at [½,½,z], (multiplicity 6); S4 at [x,x,x] (multiplicity 8). There are thus 27 S atoms within the unit cell. The (Cu,Fe,Ni) atom is found at the [½,½,½]
TABLE 1. CRYSTAL DATA FOR OWENSITE

Owensite, simplified formula: \((\text{Ba,Pb})_6(\text{Cu,Fe,Ni})_{25}\)S_{27},
Electron-microprobe formula, based on 58 atoms:
\((\text{Ba}_{1.48}\text{Pb}_{0.52})_6\text{Cu}_{15.75}\text{Fe}_{15.17}\text{Ni}_{14.79}\)S_{27.97}.

Symmetry: cubic, \(a = 10.349(1)\) Å, \(\text{Pm}3\text{m} (\#221)\), \(Z = 1\).

Systematic absences: none

Space-group choices: \(\text{Pm}3\text{m}, \text{Pn}3\text{m}, \text{Pn}3\text{m}, \text{or Pn}23\).

Source: Wellgreen Cu-Ni-Pt-Pd deposit, Yukon Territory (Cabri et al. 1993).

Density: \(D_{\text{calc}} = 4.83\ \text{Mg m}^{-3}\) for stoichiometric formula,
4.78 Mg m\(^{-3}\) for empirical formula derived from electron-microprobe data; \(D_{\text{calc}}\) not determined.

Absorption: \(\mu(\text{MoK}α) = 180.4\ \text{cm}^{-1}\).

Intensity data: 4 unique segments collected in
diffraction symmetry \(\text{I}m\) (equivalent to 8 segments in \(\text{Pn}3\text{m}\)) to a limit of 2θ = 100°
using \(\text{MoK}α\) radiation. Averaged to yield
1209 unique reflections measured, 554 with
\(I_{\text{rel}} > 3\sigma(I_{\text{rel}}).

Refinement: full-matrix least-squares to \(R = 5.2\%\),
block-diagonal in final cycles to refine
disordered Pb position.

Laflemane et al. (1993).

Discussion of the coordination polyhedra around the
Ba and Cu atoms follows. For Ba, the coordination is
position (multiplicity 1) and at \([x,y,z]\) (multiplicity 24)
for a total of 25 (Cu,Fe,Ni) atoms in the unit cell.
The Ba atom is found at a six-fold site at \([0,0,z]\), and the Pb
atom is within the same S cage, but is displaced from
the Ba position toward the origin and away from
the fourfold axis. It is positionally disordered,
and statistically distributed in a site at \([x,x,z]\) with 24-fold
multiplicity and located 0.380(12) Å from the Ba atom.
This results in the formula \((\text{Ba,Pb})_6(\text{Cu,Fe,Ni})_{25}\)S_{27},
with \(Z = 1\).

Discussion of the coordination polyhedra around the
Ba and Cu atoms follows. For Ba, the coordination is
position (multiplicity 1) and at \([x,y,z]\) (multiplicity 24)
for a total of 25 (Cu,Fe,Ni) atoms in the unit cell.
The Ba atom is found at a six-fold site at \([0,0,z]\), and the Pb
atom is within the same S cage, but is displaced from
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the fourfold axis. It is positionally disordered,
and statistically distributed in a site at \([x,x,z]\) with 24-fold
multiplicity and located 0.380(12) Å from the Ba atom.
This results in the formula \((\text{Ba,Pb})_6(\text{Cu,Fe,Ni})_{25}\)S_{27},
with \(Z = 1\).

Discussion of the coordination polyhedra around the
Ba and Cu atoms follows. For Ba, the coordination is

illustrated in Figure 1. With S1 at the origin and Ba
along each axis, there is a fourfold axis through these
two atoms. There are four S2 atoms at \([3.239(3)\ \text{Å}]\)
and four S4 atoms at \([3.302(3)\ \text{Å}]\) arranged in a somewhat
distorted square antiprism. S1 is the ninth coordinating
sulfur atom at 3.148(2) Å. A tridecahedron (13 faces)
with nine vertices is thus formed around Ba. This poly-

![Fig. 1. Coordination of (Ba,Pb). S1 is at the origin, with a
fourfold axis through S1 and Ba (larger circle at center).
Pb is displaced from the Ba position and disordered over
the four sites close to the axis (small circles near Ba).
S4 lies along the body-diagonal of the cell, whereas S2 is
in the plane of two axes. A square antiprism is thus formed
from the four S2 and four S4, whereas S1 occupies an
axial position above the antiprism. Each S4–S1–S4
triangular face is face-shared to form a cruciform
assembly around the origin.

![Fig. 2. The (Ba,Pb)–S polyhedra, comprising the units shown in Figure 1
without the Pb face-sharing to form a cruciform assembly at each
origin and between adjacent origins. The unit-cell
edge is indicated. These polyhedra extend along
and fill the space close to each of the three axes.]
hedron is repeated in each of the positive and negative axial directions, with the S2 atoms midway along the axes being shared between adjacent polyhedra (Fig. 2). The edges of the cell are thus fully defined, and the space between adjacent origins is filled with these Ba-S polyhedra.

Cu1 is at the center of the unit cell, and is surrounded by six S3 atoms (at \( \frac{1}{2}, \frac{1}{2}, z \)) at a distance of 2.499(5) Å in perfect octahedral coordination. Cu2 is in a somewhat distorted tetrahedral coordination, with an S2 at 2.357(2) Å, a second S2 at 2.358(3) Å, an S3 at 2.347(4) Å and an S4 at 2.304(3) Å. One angle (S3-Cu-S4) is opened up to 127.1°; the remainder are between 105.1° and 106.3°.

The coordination of the S atoms is as follows: S1, at the origin, is in perfect octahedral coordination by Ba atoms at 3.148(2) Å. S2 is bonded to two Ba atoms and four Cu atoms in a distorted triangular prism (Fig. 3). The distances to Ba are 3.239(3) Å and to Cu are 2.357(2) Å. S3 is bonded to four Cu2 atoms [2.347(3) Å] at the base of a square pyramid, with Cu1 [2.499(5) Å] at the apex (Fig. 4). S4 has three Cu2 atoms [2.302(3) Å] adjacent to each other and three Ba atoms [3.304(3) Å] adjacent to each other. A distorted octahedron is thus formed with Cu and Ba atoms always trans to each other across the S4 atoms.

It is clear that the Ba coordination polyhedra account for the space between adjacent origins, that the Cu1 octahedron occupies the center of the cell, and that the rest of the space within the unit cell is filled with tetrahedrally coordinated Cu2 atoms.

The refined atomic parameters are listed in Table 2. These parameters can be related to those published for djerfisherite (Dmitrieva et al. 1979) by transforming the origin to the center of the cell. Bond lengths and

**Fig. 4.** The square pyramid coordination of S3. A fourfold axis passes through Cu1 (at the apex) and S3.

**Table 2.** Atomic Parameters with Standard Deviations

<table>
<thead>
<tr>
<th>Atomic Parameters ( x,y,z ) and ( Ba )</th>
</tr>
</thead>
<tbody>
<tr>
<td>E.S.D.'s refer to the last digit printed.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Atom site occ.</th>
<th>( x )</th>
<th>( y )</th>
<th>( z )</th>
<th>( r_{\text{ave}}(\AA) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>S1</td>
<td>1a</td>
<td>1.0</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>S2</td>
<td>12a</td>
<td>1.0</td>
<td>0.1</td>
<td>0.0</td>
</tr>
<tr>
<td>S3</td>
<td>6f</td>
<td>1.0</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>S4</td>
<td>8g</td>
<td>1.0</td>
<td>0.2170(30)</td>
<td>0.21703</td>
</tr>
<tr>
<td>Ba</td>
<td>6e</td>
<td>0.3064</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Pb</td>
<td>24m</td>
<td>0.0334</td>
<td>0.0149</td>
<td>0.0149</td>
</tr>
<tr>
<td>Cu1</td>
<td>1b</td>
<td>0.5237</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Cu2</td>
<td>24n</td>
<td>0.5277</td>
<td>0.5</td>
<td>0.45</td>
</tr>
</tbody>
</table>

* \( \{(Pb+Ba) = 1.00\}; \ # \ (Fe = 0.4763) |

Table of \( u(i,j) \) values x 1000. E.S.D.'s refer to the last digit printed.

<table>
<thead>
<tr>
<th>( u_{11} )</th>
<th>( u_{22} )</th>
<th>( u_{33} )</th>
<th>( u_{12} )</th>
<th>( u_{13} )</th>
<th>( u_{23} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>S1</td>
<td>1.39(21)</td>
<td>1.39</td>
<td>1.39</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>S2</td>
<td>1.30(14)</td>
<td>1.47(14)</td>
<td>1.33(13)</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>S3</td>
<td>1.50(12)</td>
<td>1.50</td>
<td>1.02(19)</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>S4</td>
<td>1.60(7)</td>
<td>1.60</td>
<td>1.60</td>
<td>0.23(09)</td>
<td>0.23</td>
</tr>
<tr>
<td>Ba</td>
<td>1.54(3)</td>
<td>1.54</td>
<td>1.20(5)</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Cu1</td>
<td>1.60(12)</td>
<td>1.60</td>
<td>1.60</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Cu2</td>
<td>1.67(3)</td>
<td>1.61</td>
<td>2.17(6)</td>
<td>-0.16(5)</td>
<td>0.04(4)</td>
</tr>
<tr>
<td>Pb</td>
<td>U(iso)</td>
<td>1.52(42)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Anisotropic Temperature Factors are of the form: \( 2\pi^{2}\left(h^2a^2*++&h^2b^2*+a^2+b^2*a^2+b^2\right) \)
angles are given in Table 3. The observed structure-factors \((10 \times F_0)\) with standard deviations and calculated \((10 \times F_0)\) structure-factors are given in Table 4, which is available at a nominal charge from the Depository of Unpublished Data, CISTI, National Research Council of Canada, Ottawa, Ontario K1A 0L4.

<table>
<thead>
<tr>
<th>3. Coordination of (S^2) - triangle pyramid.</th>
</tr>
</thead>
<tbody>
<tr>
<td>(S^3 = Cu_2)</td>
</tr>
<tr>
<td>(S^3 = Cu_2, j, h, k)</td>
</tr>
</tbody>
</table>

**TABLE 3. BOND LENGTHS (Å) AND ANGLES (°) FOR OWENSITE**

1. Coordination of \(S^1\) - Regular octahedron. \(S^1 = 3.483(15)\) All angles 90 or 180

2. Coordination of \(S^2\) - Distorted triangular prism. \(S^2 = Ba(\tilde{g}, \tilde{F})\) \(2 \times 3.239(3)\)

3. Coordination of \(S^3\) - \(S^4\) - square pyramid. \(S^3 = Cu_2\) \(1 \times 2.499(8)\) (apical bond)

4. Coordination of \(S^4\) - triangular antiprism, or distorted octahedron. \(S^4 = Cu_2, j, h, k\) \(4 \times 2.347(3)\) (square base)

5. Coordination of \(Ba\) - distorted square antiprism with ninth atom at apex. \(Ba = S1\) \(1 \times 3.483(15)\)

6. Coordination of \(Cu^1\) - regular octahedron. \(Cu^1 = S3, (-b, d, a, t, u)\) \(2.499(5)\)

7. Coordination of \(Cu^2\) - distorted tetrahedron. \(Cu^2 = Cu_2 - S2^\prime\) 105.1(1)

**Discussion**

From its powder-diffraction pattern and from its proportions of heavy-metal, transition-metal and sulfur atoms as obtained from electron-microprobe analyses, owensite was initially considered a derivative of the argentopentlandite structure, \(AgFe_6S_8\) (Hall & Stewart 1973). Indeed, stoichiometrically owensite is close to argentopentlandite; the metal/sulfur ratio in owensite is 31/27 (1.148), and in argentopentlandite it is 9/8 (1.125). Owensite is the first example of a Ba-containing sulfide mineral. The total absence of monovalent cations and of Cl made the relationship to djerfisherite unclear, until it was kindly pointed out to the author by two (anonymous) members of the Committee on New Minerals and Mineral Names, IMA, during the name approval process. When the structure had been solved, and the relationship of owensite to djerfisherite was understood, specimens of owensite were probed again, to determine the absolute level of possible CI presence. At the detection limit of the microprobe (Laflamme et al. 1995), the possible limit for CI is less than 0.012 atom/formula unit. Structurally, CI can play no part in owensite. The difference between the two structural types is that owensite and djerfisherite have space group \(Pm\bar{3}m\), whereas argentopentlandite is \(Fm\bar{3}m\); the cell edges for the three are similar: owensite, 10.373(1) Å (this work); djerfisherite 10.465(1) Å (Dmitrieva et al. 1978); argentopentlandite 10.521(3) Å (Hall & Stewart 1973). The development of the owensite structure from that of argentopentlandite can be rationalized as follows: in argentopentlandite, where the Ag atom occupies one of the octahedrally coordinated metal sites of the reference structure of pentlandite, the Ag–S distance is only 2.676 Å. In owensite, the presence of the much larger (Ba,Pb) atom demands a larger hole, and this results in an increased coordination number from six to nine. The S atoms in the structure are required to surround this large Ba atom, and fewer are thus available for octahedral coordination throughout the cell. Only the unique \(Cu^1\) atom retains an octahedral coordination at the center of the...
The distorted octahedral coordination around S4, showing three barium atoms (larger circles) and three Cu2 atoms (smaller circles). Each copper is trans to a barium atom.

The distortion that occurs as Pb replaces Ba in the large heavy-metal site has been discussed at some length by Moore et al. (1993) and has been observed in many lead salts and minerals, where the coordination sphere of anions around the Pb atom is asymmetrical. The effect is to displace the 6σ electron density (which is about the size of an O2− anion) away from the smaller bond-pair densities. Moore et al. (1993) proposed that this effect is electrostatic in origin. A pear-shaped orbital results, and the greater part of the electron density is moved away from the position where, in the present case, the Ba atom is located within the same S cage. The refined atomic position of Pb is on the (x,x,z) mirror plane and around the four-fold axis. This results in four possible atomic sites, in a square of 0.307(30) Å, with the Pb site being 0.380(12) Å from the Ba site. Only one of the Pb sites can be occupied in any given sulfur cage at any given time, and only if Pb has replaced Ba within that cage. There is thus no point in discussing at length all Ba–Pb distances and angles, as these cannot exist in reality.

The residual $R$, achieved before invoking disorder (6.2%), was somewhat higher in the present refinement than one would like to see in a well-refined structure. However, it was considered originally that this was an artifact of collecting the data out to $2\theta = 100^\circ$ on such a small crystal. The large number of weak reflections observed at high diffraction-angles from this very small crystal results in an artificial raising of the agreement factor to above what should be expected. When refinement was restricted to data below $2\theta = 60^\circ$, the $R$ value converged to about 3.9%. With the structural model involving Pb disorder away from the Ba position, the residual for all data dropped to 5.2%, with the data below $2\theta = 60^\circ$ giving an $R$ of 3.5%. The improvement in the refinement using the disordered model is very significant The process of averaging the eight segments of intensity data in symmetry $m3m$ gives rise to an agreement factor of about 3% between equivalent segments, and this is usually a good barometer of the possible degree of refinement and the ultimate $R$ value that can be obtained with a well-refined, nondisordered structure. Thus, in the present case, the refinement achieved for the final disordered model is not significantly greater than the expected 3% for the observed data to a $2\theta$ of 60°.

Conclusions

Djerfisherite-group minerals have been considered to have a chemical composition in which Cl is essential (1 Cl per formula unit), monovalent ions are present (6 K and 1 Na), and the proportion of the transition metal has been reported as less than stoichiometric (Clarke et al. 1994). Owensite obeys none of these conditions. It has large divalent (Ba,Pb) atoms replacing K, a (Cu,Fe,Ni) atom replacing Na, and a S atom replacing Cl, and its (Cu,Fe,Ni) sites are fully occupied. Other than that, it is isostructural with djerfisherite and with the T1 equivalent, thalfenisite. These structures should be considered as a group, with the crystal symmetry, rather than the chemistry, being the common factor.

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his suggested improvements and his invaluable comments on the question of disorder in the Pb position caused by the lone pair of electrons.

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