

Contributions to Gemology

No.3 August 2004

THE CHALLENGE OF THE IDENTIFICATION OF A NEW GEMSTONE



CHEMISTRY AND CRYSTALLOGRAPHY (NEW BERYL-GROUP MINERAL)

MINERAL NAME: **PEZZOTTAITE**

CHEMICAL FORMULA:



CRYSTAL SYSTEM: **rhombohedral**

SPACE GROUP: **R3c**

$a = 15.946(2) \text{ \AA}$ $b = 15.946(2) \text{ \AA}$ $c = 27.803(8) \text{ \AA}$
($a, b, c = \text{unit-cell dimensions}$)

$\alpha = 90^\circ$ $\beta = 90^\circ$ $\gamma = 120^\circ$
($\alpha, \beta, \gamma = \text{angles of the unit-cell}$)

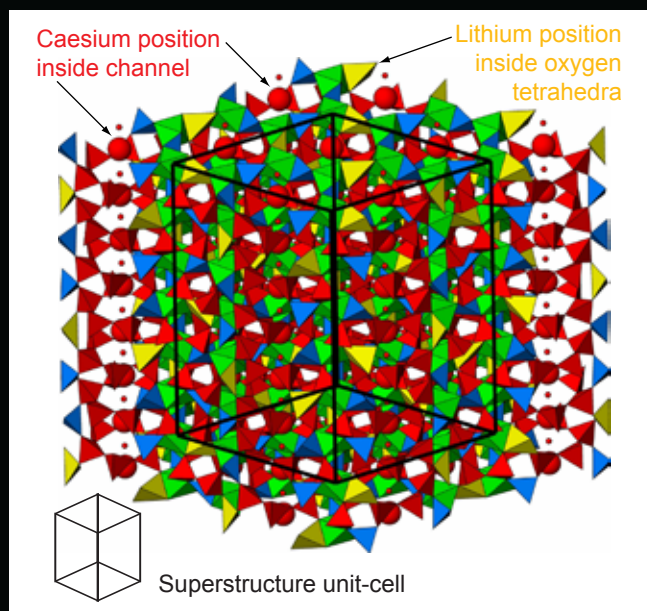
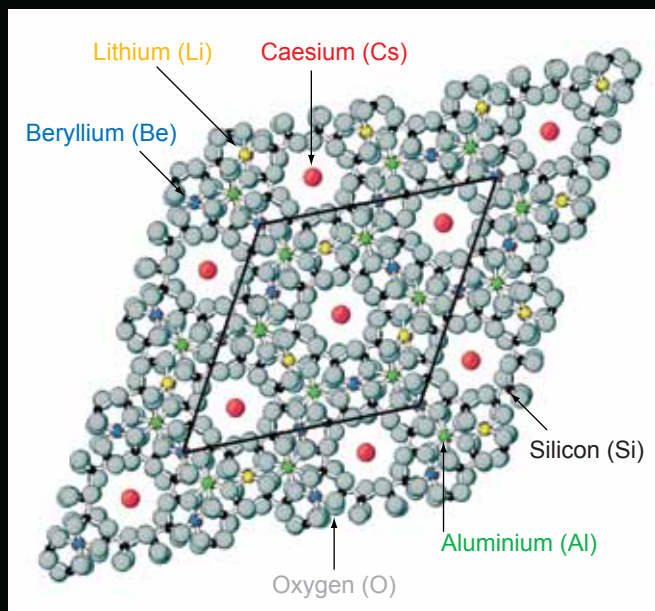
$V = 6122(2) \text{ \AA}^3$

($V = \text{Volume of unit cell, } \text{\AA} = \text{Angstrom, } 1\text{cm} = 100\,000\,000 \text{ \AA}$)

$Z = 18$

(Z is number of formula units per unit-cell)

NEW GEM MINERAL PEZZOTTAITE



ATOMIC ARRANGEMENTS

GRS

**GEMRESEARCH
SWISSLAB**



Editor

*Dr. A. Peretti, FGG, FGA, EurGeol
GRS Gemresearch Swisslab AG, P.O.Box 4028, 6002
Lucerne, Switzerland*

Adolf@Peretti.ch

Editorial Review Board

*Prof. Dr. B. Grobéty, Institute of Mineralogy and
Petrography, University of Fribourg, Fribourg,
Switzerland*

*Prof. Dr. J. Mullis, Institute of Mineralogy and
Petrography, University of Basel, Basel, Switzerland*

*Prof. Dr. W. Oberholzer, Institute of Mineralogy and
Petrology, Swiss Federal Institute of Technology
(ETH), Zurich, Switzerland.*

*Former Curator of the Mineralogical Museum (ETH
ZH).*

*Prof. Dr. K. Ramseyer, Institute for Geological Sciences,
University of Berne, Berne, Switzerland*

*Prof. Dr. D. Günther, Institute of Chemistry, Laboratory
for Inorganic Chemistry, ETH, Zurich, Switzerland*

This journal follows the rules of the Commission on
New Minerals and Mineral Names of the IMA in all
matters concerning mineral names and nomenclature.

Distributor

*GRS (Thailand) Co., LTD.
257/919 Silom Rd., JTC Building, Bangkok 10500,
Thailand.*

*Journal and Website Copyrighted by GRS
Gemresearch Swisslab AG, Lucerne, Switzerland*

*This report is published on-line at
www.gemresearch.ch*

Message From The Editor's Desk

About 4000 mineral species are known and about 20 to 30 new species are discovered each year. The majority of the new species occurs as very small crystals and is only detected with the help of very sophisticated optical and spectroscopic instrumentation available today. The discovery of a new mineral forming large crystal is thus exceptional. Such a rare and spectacular discovery of a new mineral with gem quality was made in Madagascar. "Pezzottaite", named after the Italian mineralogist Pezzotta, is a mineral belonging to the "beryl group". The appearance of this beryl-like mineral on diverse Mineral shows (Tucson) attracted various research groups worldwide and two groups identified almost simultaneously the material as a new mineral. The acceptance of a mineral as a new species requires the determination of a number of physical and chemical properties (optical character, hardness, chemical composition, crystal structure etc.). This "finger-print" has to be presented to the Commission on New Mineral and Mineral Names (CNMMN), a body of the International Mineralogical Association (IMA), which has to approve this new mineral and its name.

This special "new gem mineral edition" of Contribution to Gemology No.3 gives an inside into the details of the physical and chemical analyses that were undertaken for the identification of the new gem mineral "Pezzottaite" and the preparation of a successful IMA application.

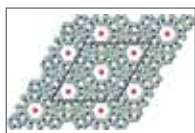


Adolf Peretti

What's inside?



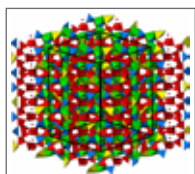
Identifying a new gem mineral 1
Analyzing the crystal structure 1



The superstructure: The difference between the two minerals "BERYL" and "PEZZOTTAITE" 2



Materials 3
The application to the Commission on New Minerals and Mineral Names (CNMMN IMA) 3



Rotating pezzottaite crystal model 4
BOX 1 Chemistry and crystallography 4



Pezzottaite rough, cut and in matrix 5



BOX 2 Origin and mineralogy 5



BOX 3 Physical and optical properties 6

Chemistry of pezzottaite



BOX 4A Electron microprobe analysis (EMPA) 7

BOX 4B Laser ablation mass spectroscopy analysis (LA-ICP-MS) 8

Crystallography of pezzottaite

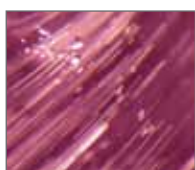


BOX 5A Single crystal X-ray diffraction analysis 9

X-ray powder diffraction analysis

BOX 5B Relations to other mineral species 10

BOX 6 Miscellaneous 10



Inclusion features, literature and acknowledgments 11



Appendix Pezzottaite gemstone examples 12

THE CHALLENGE OF THE IDENTIFICATION OF A NEW MINERAL SPECIES: EXAMPLE "PEZZOTTAITE"

Adolf Peretti (1), Thomas Armbruster (2), Detlef Günther (3), Bernard Grobéty (4),
Frank C. Hawthorne (5), Mark A. Cooper (5), William B. Simmons (6), Alexander U. Falster (6),
George R. Rossman (7), Brendan M. Laurs (8)

(1) GRS Gemresearch Swisslab AG, Hirschmattstr. 6, P.O. Box 4028, CH-6003 Lucerne, Switzerland

(2) Chem. Miner. Kristallogr., University of Berne, Freiestr. 3, CH-3012 Berne, Switzerland

(3) Laboratory of Inorganic Chemistry, ETH Hönggerberg, HCI, G113, CH-8093 Zurich, Switzerland

(4) Department of Geosciences, University of Fribourg, Pérolles, CH-1700 Fribourg, Switzerland

(5) Geological Sciences, University of Manitoba, Winnipeg, Manitoba, Canada R3T 2N2

(6) Geology & Geophysics, University of New Orleans, New Orleans, Louisiana, LA 70148, USA

(7) Division of Geological & Planetary Sciences, California Institute of Technology, Pasadena, CA 91125, USA

(8) Gemological Institute of America, Carlsbad, CA 92008, USA

(Authors (1)-(4) are referred in this article as the "Swiss research team" and authors

(5)-(8) are referred in this article as the "US-Canadian research team"

IDENTIFYING A NEW GEM MINERAL

In 2002, a new gem mineral of commercial importance was discovered. In accordance with the need for all new mineral discoveries to be scientifically characterized (see Nickel and Grice, 1998), the gemological community anxiously awaited the results of tests to positively identify the new mineral (Hawthorne et al., 2003, Hawthorne et al., submitted and Laurs et al., 2003). This period of analysis brought into play the question: Exactly what procedures are necessary for the positive characterization of a new mineral?

These principal steps of identification are illustrated in the following case study for identifying a new mineral of the beryl group - pezzottaite.

The identification of this new mineral provided two major challenges: first, the determination of the exact chemical composition, and secondly, the identification of its crystallographic structure (the geometrical arrangement of the atoms in three dimensions (see Box 1, Figs. P2 and P6). From special technique of analysis (Boxes 4 and 5A), the exact stoichiometric chemical formula, and the space group of this new mineral, have to be determined (Box 1). As soon as the mineral was characterized (Boxes 1-6), the differences between already existing minerals had also to be investigated (see Nickel and Grice, 1998 and Box 5B) and a decision had to be made regarding whether a new mineral had been found, and, if so, what would be its new name? (Hawthorne et al., 2003 and Box 6). In the case of pezzottaite, these analysis provided major challenges. As pezzottaite contains light elements - such as hydrogen, lithium, and beryllium, which cannot be directly analyzed by quantitative methods commonly used for mineral analysis such as electron microprobe (EMPA) or

XRF analysis - direct measurement by Laser Ablation Mass Spectroscopy was also used (see Box 4B and Fig. P16), as well as conventional methods used for chemical analysis (Box 4A). In addition to challenges in the analysis of chemical composition, determination of different atomic positions in the crystal structure was not trivial. A combination of various analytical techniques was necessary (Figs. P3 and P17) to finally elaborate the structural differences to beryl (Figs. P1 and P2 and Box 5B). It was discovered that the unit-cell of pezzottaite had unusually large dimensions, which is best described as a superstructure of conventional beryl (Figs. P1, P2 and P6). Also, the number of atoms necessary to define the crystal structure turned out to be unusually high in comparison with other beryl- group minerals (Boxes 1 and 5).

ANALYZING THE CRYSTAL STRUCTURE

The secrets of the nature of a new mineral are so small we cannot even identify them with the help of microscopic magnification. One way to explore this atomic world is with X-rays (Figs. P3 and P17).

X-rays have a very short wavelength (with dimensions similar to atoms), allowing them to penetrate and interact with atoms in a mineral structure. As atoms group together at very short distances, X-rays are diffracted when passing through a crystal and change their direction when they interact with them. Furthermore, diffracted X-rays interfere with each other, just like water waves emerging from two ships. The interaction between atoms and X-rays depends, among other factors, on the geometrical arrangement of the atoms and can be interpreted with X-ray diffraction diagrams, and computer calculations. A

THE SUPERSTRUCTURE: THE DIFFERENCE BETWEEN THE TWO MINERALS "BERYL" AND "PEZZOTTAITE"

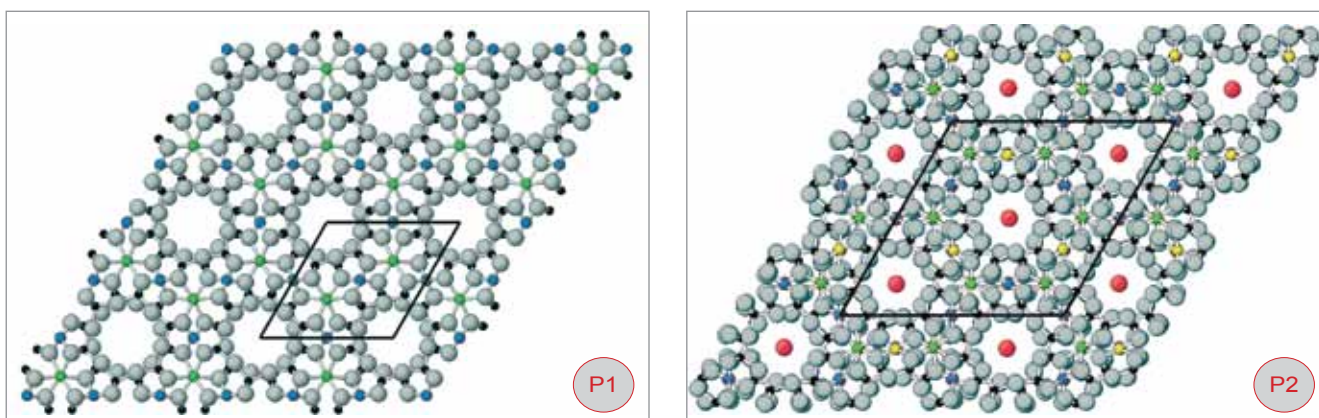


Fig. P1-2 Ball-and-stick models of beryl (Fig. P1) and pezzottaite (Fig. P2). A projection of the crystal structure in the direction of the c-axis is shown in order to explain some details of the ring systems in these two minerals. The size and position of the unit-cell (as seen perpendicular to the c-axis) is also shown. Green balls = aluminium cations (Al), blue = beryllium (Be), yellow = lithium (Li), red = caesium (Cs), grey = oxygen (O), black = silicon (Si). The structure of beryl is characterized by six-membered rings of SiO_4 tetrahedra alternating along the c-axis with twelve-membered rings composed of alternating BeO_4 and AlO_6 polyhedra. In the mineral pezzottaite, an arrangement of beryl-like rings is found, but there are two different types of twelve-membered rings: (1) Those identical to the corresponding rings in beryl, and (2) those assembled of LiO_4 , BeO_4 and AlO_6 polyhedra. To allow for the ordered (Be, Li) distribution in the structure of pezzottaite, the unit-cell had to be enlarged relative to beryl (compare P1 and P2). Both models are represented in hexagonal settings for better comparison. It must be remembered, however, that pezzottaite has a rhombohedral crystal lattice and beryl has a hexagonal lattice. In trigonal/rhombohedral symmetry, the highest symmetry element is a three-fold rotation axis, whereas in hexagonal symmetry a six-fold rotation axis is required.

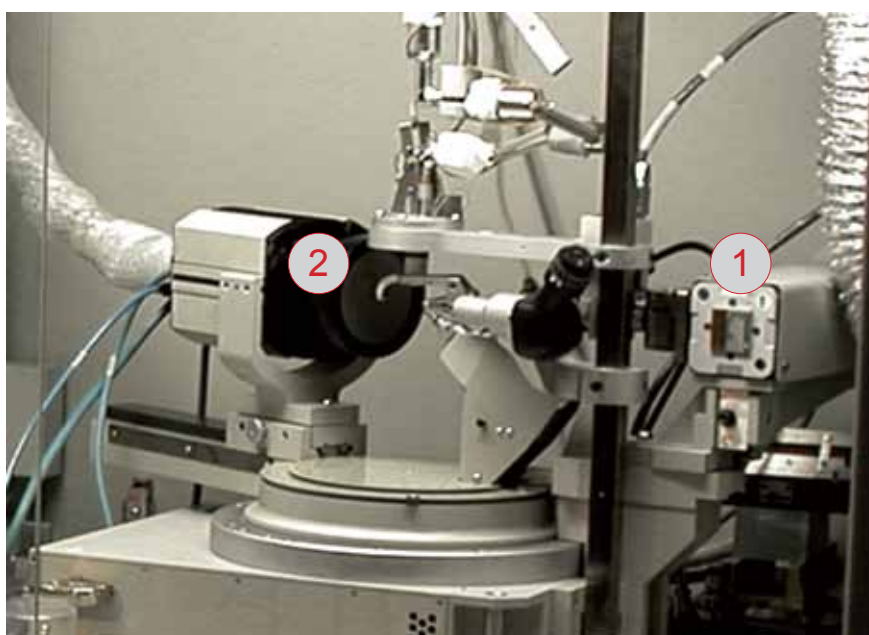


Fig. P3 Single crystal X-ray diffractometer

One of the instruments used for the analysis of the crystal structure of the new mineral pezzottaite. Critical parts of the instrument include an X-ray generator (1), a multichannel X-ray detector (2), and utilizing the latest computer software for visualization and analyzing signals (not shown). X-ray can be used to compute the geometrical arrangement of atoms (Figs. P1,2 and P6) in a mineral. The result leads to the determination of crystal structure details (Box 5A).

diffraction pattern of a single crystal consists of symmetrically arranged spots, where the spot separation determines the periodicity of the lattice (unit-cell dimensions) and the arrangement of the spots provides clues to the symmetry of the structure.

Finally, the unit-cell and the space group can be determined (Boxes 1 and 5A). This is a crystallographic code that identifies the crystallographic nature of a mineral.

MATERIALS

The new gem material was first introduced to the international mineralogical community at the Tucson show in February 2003, where it was recognized as a mineral of unusual gemological properties not referenced in world literature (see Laurs et al., 2003). For details on materials tested, see Hawthorne et al. (submitted) and Laurs et al. (2003). Three of the totally tested samples are officially registered reference materials (Box 6). They are deposited in the USA, Canada and in Switzerland.

The samples analyzed by the Swiss team are shown in Figs. P4-P5, P7-8, P12-13 and Box 7. Three samples were investigated by chemical and crystallographic investigation. These include 0.5cm-sized samples obtained from the large mother piece (Fig. P5). One of the small fragments entered the collection as a type locality specimen (Box 6).

THE APPLICATION TO THE COMMISSION ON NEW MINERALS AND MINERAL NAMES

The Swiss research group (authors 1-4) filed an application to the Commission on New Minerals and Mineral Names of the International Mineralogical Association (CNMMN, <http://www.geo.vu.nl/users/ima-cnmmn/>), stating that they had characterized a new mineral. The chairman of CNMMN informed the Swiss team that he had just received a proposal for the same mineral from a different research group (US-Canadian, authors 5-8). He further stated that both proposals were complementary to each other. An agreement was established that both groups' information and data should be merged and a new joint proposal should be submitted. Subsequently, CNMMN members decided unanimously that the new mineral should be accepted with the name 'pezzottaite'.

Box 1 to 6 summarized original data of the merged IMA application submitted by:

Hawthorne F.C., Cooper M.A., Peretti A., Simmons W.B., Armbruster T., Rossman G.R., Günther D., Laurs B.M., Grobety B. (2003)

Check-list for new mineral proposals: Pezzottaite. Proposal submitted to the International Mineralogical Association, 8 pp. Application No. 2003-022.

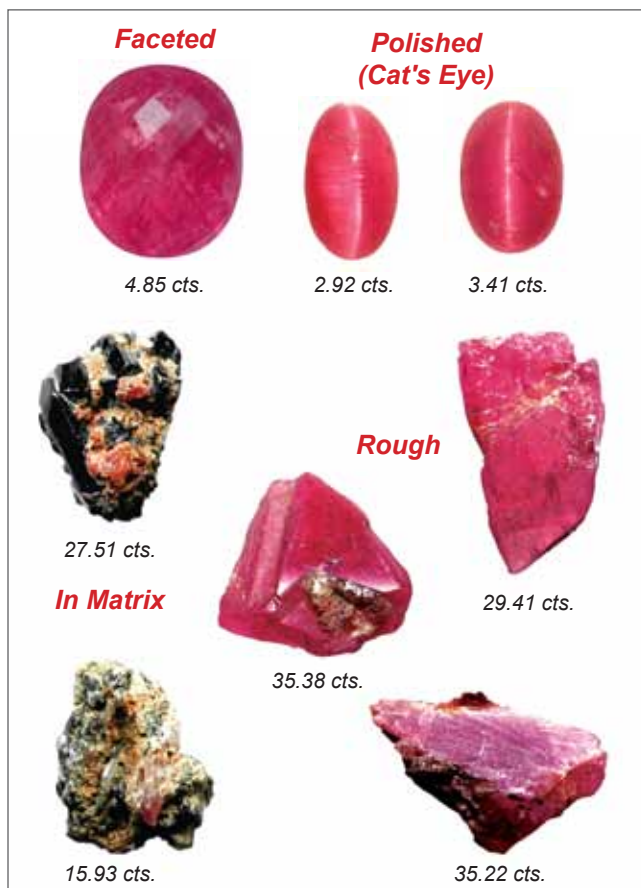


Fig. P4 A reference set of pezzottaite including a faceted sample of 4.85 ct, 2 pezzottaite cat's eyes, 2 tabular rough crystals (35.38ct, 29.41ct), 1 large crystal fragment with matrix (35.22 ct), 2 tabular pezzottaite crystals with host rock, and one with tourmaline intergrowth (27.51 ct). On public display at the Natural History Museum of the University of Fribourg (Switzerland), GRS collection.



Fig. P5 Pezzottaite tabular crystal of 29.41ct and a broken part of it (lower right), which served as the sample used for the Swiss team's detailed chemical and crystallographic investigations. The lower right piece parted in 3 different fragments which are currently at the University of Berne (see Box 6), the University of Fribourg, and the SFIT (Switzerland). The remaining motherpiece of 29.41 ct is in the GRS collection.

ROTATING PEZZOTTAITE CRYSTAL MODEL

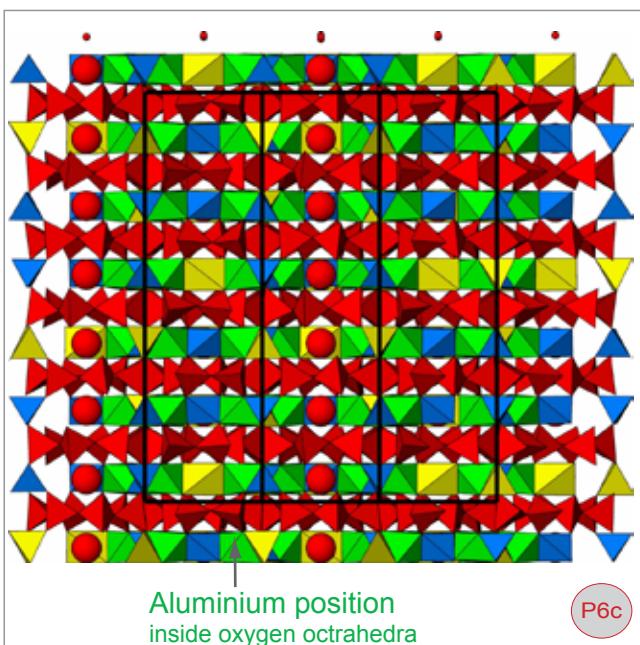
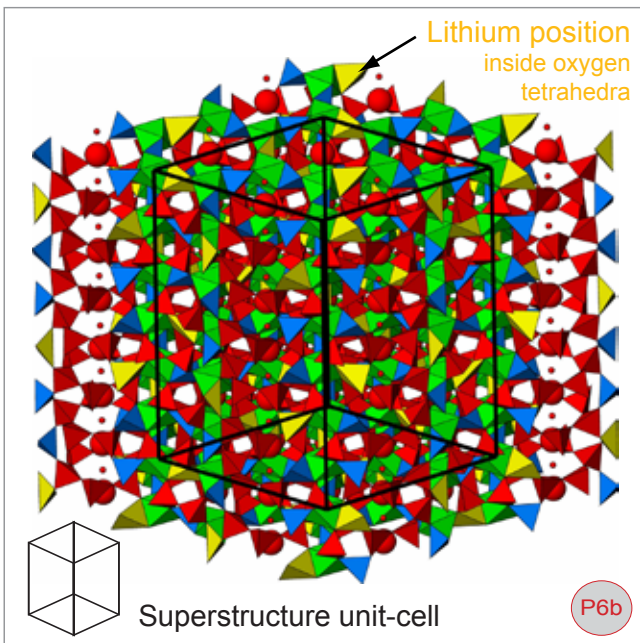
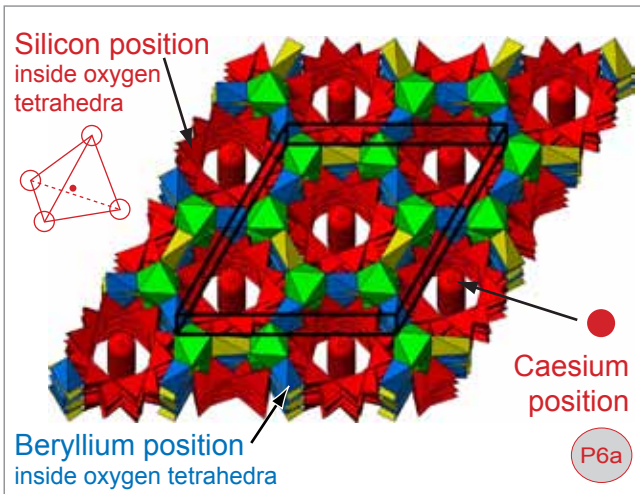


Fig.P6a-c
NEW RHOMBOHEDRAL SUPERSTRUCTURE OF PEZZOTTAITE.

Crystal structure model with oxygen polyhedra surrounding a cat ion in the centre. **Yellow oxygen tetrahedra: containing lithium (Li), blue tetrahedra with beryllium (Be), red tetrahedra with silicon (Si), green octahedra with aluminium (Al), and red spheres indicating caesium (Cs) positions.** Solid outlines mark the superstructure cell. Substitutions in tetrahedral and octahedral positions by other elements such as Ti, Ca, Mn, Fe, Na, K, Rb and Sc see Laurs et al. (2003) and Box 4B.

Rotating the crystal model of pezzottaite (P6a-c) shows the arrangement of caesium (Cs) in the direction of the c-axis within the channels. The Cs atoms are surrounded by six-membered rings involving Si, and 2 different types of twelve-membered rings. One ring is composed of Be and Al and the second composed of Be, Al and Li. With further rotation of the unit-cell, the complexity of the pezzottaite crystal structure becomes more clearly visible and the third dimension of the complicated crystal structure is more exposed (Fig. P6b). In a view perpendicular to the c-axis (Fig. P6c), the arrangement of Cs in the channels in the direction of the c-axis become visible. In the case of beryl, channels may be partially occupied by H₂O, while in pezzottaite, the corresponding position is mainly occupied by Cs.

BOX 1
CHEMISTRY AND CRYSTALLOGRAPHY
(IMA Application)

MINERAL NAME: **PEZZOTTAITE**

CHEMICAL FORMULA:



CRYSTAL SYSTEM: **rhombohedral**

SPACE GROUP: **R3c**

a = 15.946(2) Å b = 15.946(2) Å c = 27.803(8) Å
(a, b, c = unit-cell dimensions)

α = 90° β = 90° γ = 120°
(α, β, γ = angles of the unit-cell)

V = 6122(2) Å³

(V = Volume of unit-cell, Å = in Angstrom, 10⁻⁸ cm = 1Å)

Z = 18

(Z is number of formula units per unit-cell)

PEZZOTTAITE ROUGH, CUT AND IN MATRIX



Fig. P7 A rough pezzottaite crystal of over 80ct and its final product after cutting reveals a gem quality cabochon of 59.98ct. Rough and cut stone courtesy of MJ3 Inc. (NY, USA), cut by G.E.O. LTD (Bangkok, Thailand).

Fig. P8 Mineral specimen of pezzottaite in matrix. Length of pezzottaite 10 mm. Collection GRS.

BOX 2 ORIGIN AND MINERALOGY (IMA)

ORIGIN

The mine deposit is located in central Madagascar, about 140 km southwest of Antsirabe (Coordinates 20° 44.78' S and 46° 04.45' E and at an elevation of 920m (3020 feet). The route to the mine leads to Ambatofinandrahana and passes through Amborompotsy and Mandrosonoro.

ASSOCIATED MINERALS

Boron-bearing minerals: tourmaline, danburite.
Lithium-bearing minerals: lepidolite and spodumene (kunzite)
Other silicates or oxides: quartz, K-feldspar (amazonite), albite (cleveandite)

OCCURRENCE OF PEZZOTTAITE

Pezzottaite occurs in a miarolitic cavity in a mixed-feature granitic pegmatite (such pegmatites are fairly common in this region (Pezzotta 2001)). Pezzottaite crystallized from fluids in the cavity over a relatively large time-span forms both relatively early and late-stage crystals, the latter having (in some cases) Cs-enriched margins.

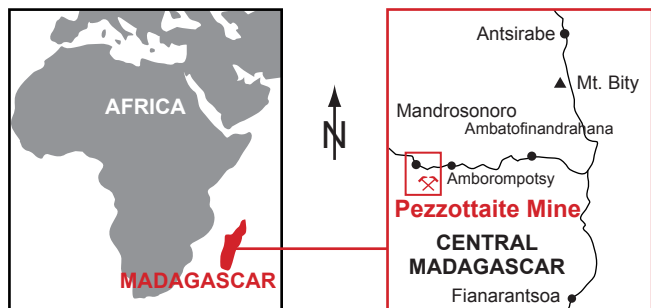


Fig. P9 The position of the Pezzottaite mine within Central Madagascar



Fig. P10 Occurrence of pezzottaite in Li, Be, B and Cs-bearing pegmatites. The pockets containing pezzottaite are excavated in small shafts and tunnels. (Picture P10 and P11 as of spring 2003, courtesy of MJ3 Inc., New York)



Fig. P11 The mining camp and a view of the topography next to the mining site where the new gem mineral pezzottaite was found.

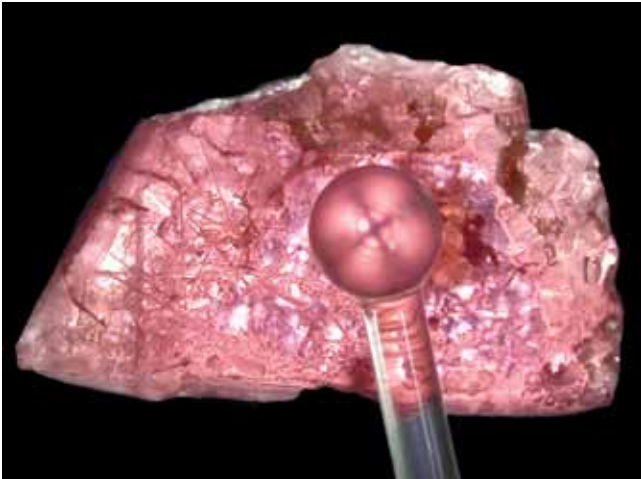


Fig. P12 Natural cat's eye pezzottaite

Cutting of pezzottaite as a cabochon intersecting the direction of the growth tubes produces a so-called cat's eye effect (see white line produced by a directed light source perpendicular to the direction of the c-axis).

Fig. P13 Pezzottaite rough of 29.41ct (see also Fig. P5) is shown as seen through crossed polarizers. A projection sphere is introduced to show the uniaxial property of "pezzottaite" (Cross pattern if viewed in the direction of the c-axis).

BOX 3 PHYSICAL AND OPTICAL PROPERTIES (IMA)

APPEARANCE AND PHYSICAL PROPERTIES

Pezzottaite occurs as usually isolated crystals that range in color from whitish pink to a deep raspberry red. There are three distinct types of crystals: (1) Irregularly-shaped flat masses (up to 8 cm in diameter) that fill cavities between cleveandite, quartz and tourmaline; (2) subhedral-to-euhedral hexagonal tabular crystals (up to 7 cm in diameter); (3) small (< 0.5 cm in diameter) euhedral flat-to-elongated crystals attached to faces of large tourmaline crystals.

COLOUR (megascopic) raspberry pink to red

Moderate dichroism is present:

orange-pink (red);
purplish pink (red) to purple

STREAK colorless to white

LUSTRE vitreous

TRANSPARENT to TRANSLUCENT

FLUORESCENCE inert to long- and short-wave
UV radiation

HARDNESS: Mohs': 8

RADIOACTIVITY: None

CLEAVAGE {001} imperfect

PARTING none observed

TENACITY brittle

FRACTURE irregular and conchoidal

DENSITY (meas.) 3.09 - 3.11 g/cm³

DENSITY (calc.) 3.06 g/cm³ (using unit-cell)

OPTICAL PROPERTIES

WAVELENGTH = Na light

UNIAXIAL (B) ω 1.615-1.619, ϵ 1.607-1.610

BIREFRINGENCE 0.008 - 0.009 (negative)

PLEOCHROISM strong (ϵ) orange pink (red) to
(ω) purple

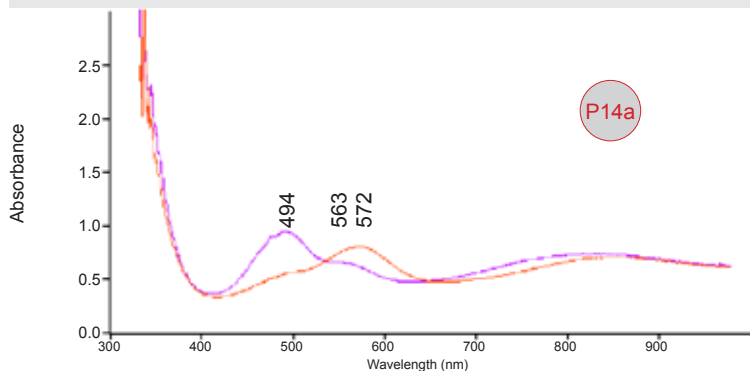


Fig. P14a: Polarized UV-VIS-NIR spectra on a 6 mm thick slice of pezzottaite which was used for chemical and crystal structure analysis. Note: Absorption bands at 494 and 563 (polarized perpendicular to the c-axis) and 572 nm (polarized parallel to the c-axis).



Fig. P14b: Pleochroism of pezzottaite with orange-red to purple is shown which is distinctively different from other minerals of the beryl group, such as pink beryl "morganite" (see Laurs et al., 2003).

BOX 4A EMPA ELECTRON MICROPROBE ANALYSIS (IMA Application)



Fig.P15 Example of an Electron Microprobe. University of New Orleans, USA (A.U. Falster).

Explanation of method. The method is used to analyze the chemical composition. For analytical purposes, the analyzed mineral must be coated with an electron-conducting layer and positioned in a highly evacuated vacuum chamber (1). The mineral is bombarded by electrons, which have previously been produced and accelerated in an electron gun (2). The different atoms in the mineral react to the impacting electrons by creating signals. These signals include X-rays,

which can be detected by various kinds of detectors, such as WDS (3). From the responding signals, the chemical composition can be determined, providing standard materials (materials of known composition or "Probe Standards") are analyzed for comparison. Light elements such as beryllium or lithium are determined by other methods.

ELECTRON MICROPROBE WDS 20 kV 10 nA beam: 5 Fm

NOTE: H₂O was determined by LOI and a value of 1.72 wt.% was obtained. However, the crystals are riddled with tubules that are occupied by a fluid; the paragenesis (granitic pegmatite) indicates that the fluid will be an aqueous fluid which will therefore result in an anomalously high value of H₂O. The crystal-structure refinement gives the total scattering within the channel, and this value minus the scattering from the channel constituents determined by EMPA gives the amount of (H₂O) in the channel: ~0.1 apfu, 0.28 wt.% H₂O. Li by ICP.

ANALYTICAL RESULTS: Number of analyses: 8

Constituent	Wt.%	Range	Standard Deviation	Probe Standard
SiO ₂	56.52	55.8 - 57.2	0.59	Spessartine
Al ₂ O ₃	15.60	14.9 - 17.0	0.65	Spessartine
Sc ₂ O ₃	0.03	0.02 - 0.04	0.01	Thortveitite
FeO	0.01	0.00 - 0.02	0.01	Clinopyroxene
MnO	0.09	0.07 - 0.11	0.02	Rhodonite
Na ₂ O	0.52	0.41 - 0.61	0.06	Clinopyroxene
K ₂ O	0.15	0.13 - 0.19	0.03	Adulina
Rb ₂ O	0.76	0.70 - 0.80	0.03	Synthetic Rb-leucite
Cs ₂ O	13.57	13.39 - 13.72	0.11	Pollucite
Li ₂ O	2.16	-	-	
BeO	8.05*	-	-	
Total	97.46			

* The BeO content was calculated from the relation Be = 3 - Li.

EMPIRICAL FORMULA (Cs_{0.62} Rb_{0.05} K_{0.02} Na_{0.11})_{S=0.80} (Be_{2.07} Li_{0.93})_{S=3} (Al_{1.97} Mn_{0.01})_{S=1.98} Si_{6.05} O₁₈

BASIS OF CALCULATION 18 O-atoms

SIMPLIFIED FORMULA (Cs,□) (Be,Li)₃ Al₂ Si₆ O₁₈

BOX 4B LA-ICP-MS CHEMICAL ANALYSIS (IMA Application)

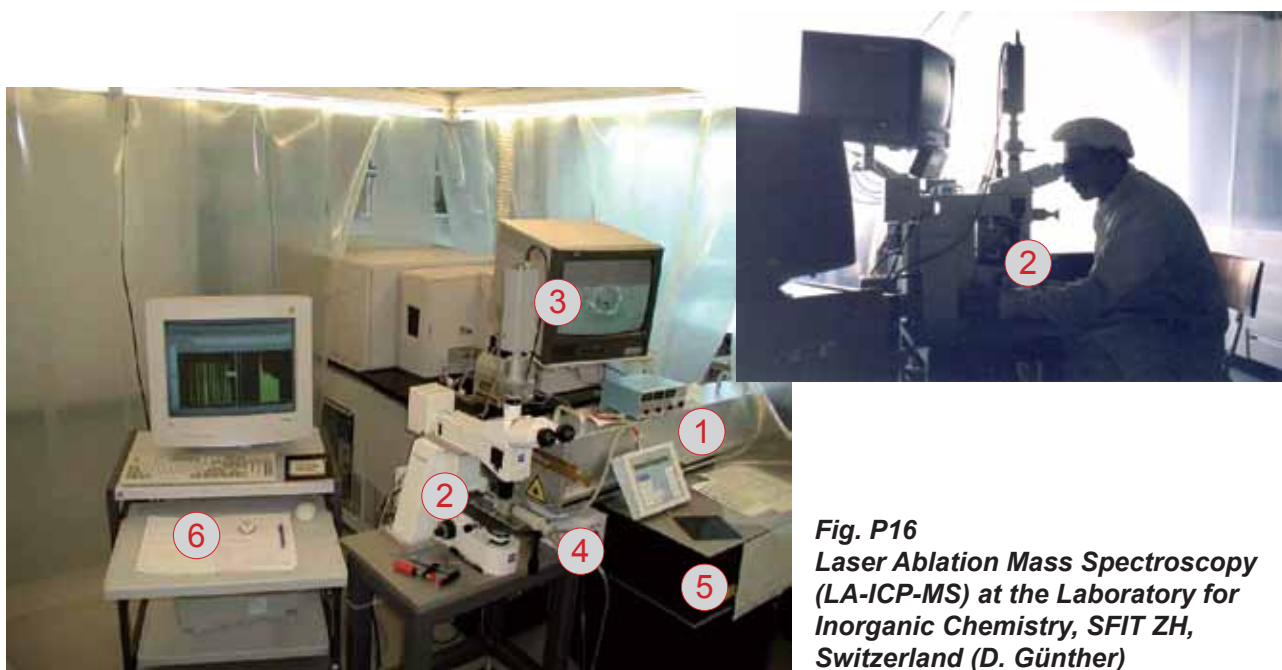


Fig. P16
Laser Ablation Mass Spectrometry (LA-ICP-MS) at the Laboratory for Inorganic Chemistry, SFIT ZH, Switzerland (D. Günther)

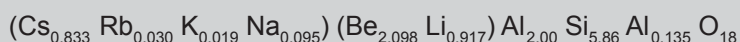
Explanation of method

The laser ablation technique (LA) uses a 193 nm excimer laser (1) which is focused onto the sample surface via microscope lenses (2). The laser is ablating (carrying away) the material (crater diameter 4 to 80 microns) (3). The mobilized material is suspended in a carrier gas (4) and transported via transport tube into an Inductively Coupled Plasma Mass Spectrometer (ICP-MS) (5). The material/elements (except those that cannot be ionized, such as gases and fluorine) are vaporized, atomized and ionized within the ICP. The created ions are then transferred to the mass spectrometer and separated by their mass divided by charge (5). The detector allows measuring major, minor and trace elements within a single analysis. Very light elements, such as boron, lithium or beryllium, can be detected, along with a large series of other elements at concentrations of less than 1 ppm. The quantification at low concentrations is possible by LA-ICP-MS due to a matrix-independent calibration, e.g. glass standard was used for quantification of pezzottaite including special computer analysis and specific software (6). The use of complementary solid-analysis methods (such as EMPA and XRF) for comparison and validation purposes (e.g. for quantitative measurement of silicon and aluminium) must be applied (see Box 4A).

LA-ICP mass-spectrometry ANALYTICAL RESULTS

Constituent	Wt. %
SiO ₂	54.58
Al ₂ O ₃	16.88
Sc ₂ O ₃	n.d.
FeO	0.02
MnO	0.02
Na ₂ O	0.46
K ₂ O	0.14
CaO	0.22
Rb ₂ O	0.44
Cs ₂ O	18.23
Li ₂ O	2.12
BeO	8.14
Total	101.26

EMPIRICAL FORMULA



IONS PER 18 OXYGENS, ANHYDROUS BASIS

Si	5.860	Be	2.098
Ti	0.001	Li	0.917
Al	0.139	ΣBe+Li	3.016
Σtetrahedral	6.000	Al	1.996
Na	0.095	Ca*	0.025
K	0.019	Sc	nd
Rb	0.030	Mn	0.002
Cs	0.833	Fe2+	0.001
Σchannel	0.977	Σoctahedral	2.024

* Ca is assumed present at the octahedral site, but it may occur elsewhere in the pezzottaite structure. n.d. = not determined

BOX 5A CRYSTALLOGRAPHIC ANALYSIS (IMA)

SINGLE-CRYSTAL STUDY

METHOD 4-circle
 CRYSTAL SYSTEM rhombohedral (hexagonal setting)
 SPACE GROUP R3c
 CELL PARAMETERS a 15.946(2) Å α 90°
 b 15.946(2) Å β 90°
 c 27.803(8) Å γ 120°
 V 6122(2) Å³ Z = 18

POWDER DATA CuKα

Diffractometer
 CELL PARAMETERS REFINED FROM POWDER DATA
 CRYSTAL SYSTEM rhombohedral (hexagonal setting)
 SPACE GROUP R3c
 a 15.973(4) Å α 90°
 b 15.973(4) Å β 90°
 c 27.850(11) Å γ 120°
 V 6153(3) Å³ Z = 18

See Table 1 for X-ray Powder-Diffraction Data

CRYSTAL STRUCTURE R = 2.9%
 MORPHOLOGY
 HABIT tabular
 FORMS {001} dominant, {100}, {110}
 TWINNING none observed
 c:a 1 : 1.7436
 (from unit-cell parameters)

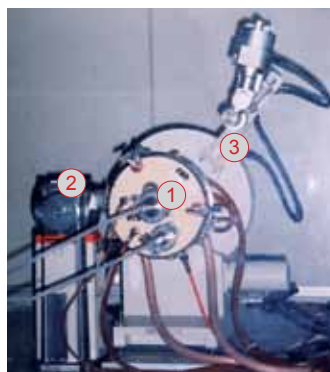


Fig. P17
X-ray diffraction analysis.

Explanation of method. The method is used to investigate the crystal structure (atomic positions and geometry). A small crystal fragment of usually 0.1 mm size is investigated by exposing the mineral to X-rays (single crystal analysis see also fig. P3). Instead of using a single crystal, a small sample is ground into a powder. This powder is mounted in such a way that the target consists of many extremely small crystal fragments which are oriented in random fashion (1). A monochromatic X-ray beam (e.g. CuKα) is focused on the sample (2). The interaction of the X-rays with the numerous randomly oriented particles yields an X-ray powder-diffraction pattern. These interference signals are collected at different diffraction angles by using an X-ray sensitive detector (3). The signals can be used to obtain information about the unit-cell parameters and to collect characteristic 'fingerprints' for each mineral structure (d-values, hkl). The relative intensity of the X-ray signal (0-100) as well as the d-values are listed in reference manuals for identification purposes (such as below).

TABLE 1. X-RAY POWDER-DIFFRACTION DATA FOR PEZZOTTAITE

Intensity	d measured	d calculated	h	k	l	Intensity	d measured	d calculated	h	k	l
4	4.642	4.643	0	0	6	3	1.834	1.834	-4	8	6
10	4.611	4.617	0	3	0	6	1.801	1.801	-2	7	9
2	4.013	4.010	-1	2	6	12	1.749	1.749	-3	6	12
2	3.993	3.993	-2	4	0	12	1.743	1.743	-3	9	0
100	3.271	3.272	0	3	6	10	1.713	1.713	-3	9	3
41	3.027	3.028	-2	4	6	9	1.704	1.704	-1	8	6
29	3.019	3.019	-1	5	0	14	1.636	1.635	0	6	12
52	2.871	2.872	-1	5	3	6	1.632	1.632	-3	9	6
9	2.662	2.662	-3	6	0	2	1.581	1.582	-1	5	15
6	2.321	2.321	0	0	12	3	1.577	1.577	-1	8	9
6	2.309	2.309	-3	6	6	2	1.547	1.547	0	0	18
4	2.305	2.305	0	6	0	11	1.518	1.519	-3	9	9
12	2.229	2.229	-1	2	12	1	1.514	1.514	-4	8	12
14	2.215	2.215	-2	7	0	4	1.509	1.509	-2	10	0
6	2.155	2.155	-2	7	3	2	1.490	1.490	-8	10	3
9	2.065	2.065	0	6	6	7	1.467	1.467	0	3	18
2	1.999	1.999	-2	7	6	6	1.459	1.459	0	9	6
5	1.840	1.840	-1	5	12	2	1.443	1.443	-2	4	18

BOX 5B RELATIONS TO OTHER MINERAL SPECIES (IMA)

RELATIONSHIP TO OTHER SPECIES

Pezzottaite is related to the beryl group (see table 2), but differs in having a superstructure involving ordering of Be and Li in tetrahedral coordination (see Fig. P1, P2 and P6).

TABLE 2. THE MINERALS OF THE BERYL GROUP: (2a) $\text{Be}_3\text{Al}_2\text{Si}_6\text{O}_{18}(\text{H}_2\text{O})_{<1}$

	Beryl ¹	Bazzite ²	Stoppaniite ³	Indialite ⁴	Pezzottaite ⁵
a (Å)	9.210	9.521	9.397	9.800	15.946
c (Å)	9.194	9.165	9.202	9.345	27.803
V (Å ³)	675.4	719.5	703.7	777.3	6122
ε	1.577	1.602	1.619	1.532	1.608
ω	1.580	1.622	1.625	1.537	1.616
D (g/cm ³)	2.66	2.77	2.79	2.51	3.06
Z	2	2	2	2	18
2a	-	-	-	-	[Cs]
Be	Be ₃	Be ₃	Be ₃	Al ₂ Si	[Be ₂ Li]
Al	Al ₂	Sc ₂	Fe ³⁺ ₂	Mg ₂	[Al ₂]

¹ Aurisicchio et al. (1988); ² Armbruster et al. (1995); ³ Della Ventura et al. (2000), Ferraris et al. (1998);⁴ Meagher & Gibbs (1977); ⁵ Hawthorne et al.(submitted).

End-member formulae

Beryl:	<input type="checkbox"/>	Be ₃	Al ₂	Si ₆	O ₁₈
Bazzite:	<input type="checkbox"/>	Be ₃	Sc ₂	Si ₆	O ₁₈
Stoppaniite:	<input type="checkbox"/>	Be ₃	Fe ³⁺ ₂	Si ₆	O ₁₈
Indialite	<input type="checkbox"/>	(Al ₂ Si)	Mg ₂	(Al ₂ Si ₄)	O ₁₈
Pezzottaite:	Cs	Be₂Li	Al₂	Si₆	O₁₈

Armbruster T., Libowitzky E., Diamond L., Auernhammer M., Bauerhansl P., Hoffmann C., Irran E., Kurka A., Rosenstingl H. (1995) Crystal chemistry and optics of bazzite from Furkabasistunnel (Switzerland). *Mineralogy and Petrology*, Vol. 52, pp. 113-126.

Aurisicchio, C., Fioravanti, G., Grubessi, O. & Zanazzi, P.F. (1988): Reappraisal of the crystal chemistry of beryl. *American Mineralogist* 73, 826-837.

Della Ventura G., Rossi P., Parodi G.C., Mottana A., Raudsepp M., Prencipe M. (2000) Stoppaniite, (Fe,Al,Mg)₄(Be₆Si₁₂O₃₆)*(H₂O)₂(Na,□), a new mineral of the beryl group from Latium (Italy). *European Journal of Mineralogy*, Vol.12, pp.121-127.

Ferraris, G., Prencipe, M. & Rossi, P. (1998): Stoppaniite, a new member of the beryl group: crystal structure and crystal-chemical implications. *European Journal of Mineralogy*, Vol.10, pp.491-496.

Hawthorne F.C., Cooper M.A., Simmons W.B., Falster A.U., Laurs B.M., Armbruster T., Rossman G.R., Peretti A., Günther D., Grobety B. : Pezzottaite, Cs(Be₂Li)Al₂Si₆O₁₈, a spectacular new mineral related to the beryl group, from Madagascar. *Mineralogical Record*. Submitted.

Meagher, E.P. & Gibbs, G.V. (1977): The polymorphism of cordierite: II. The crystal structure of indialite. *Canadian Mineralogist*, Vol.15, pp.43-49.

BOX 6 MISCELLANEOUS (IMA)

NAME

Named after Federico Pezzotta, Museo Civico, Milano, Italy; born 1967. Dr. Pezzotta has played a major role in characterizing the granitic pegmatites of Madagascar and their constituent minerals. He has made major contributions to our knowledge of the paragenesis of tourmaline-group minerals, particularly in Elba, Italy.

Pezzotta, F., Ed. (2001) Madagascar, a Mineral and Gemstone Paradise. Extralapis English, No. 1. Lapis International LLC, East Hampton, 100pp.

TYPE MATERIAL

Smithsonian Institution

Canadian Museum of Nature, PO Box 3443, Station D, Ottawa, Ontario, Canada

Natural History Museum Bern, Bern, Switzerland

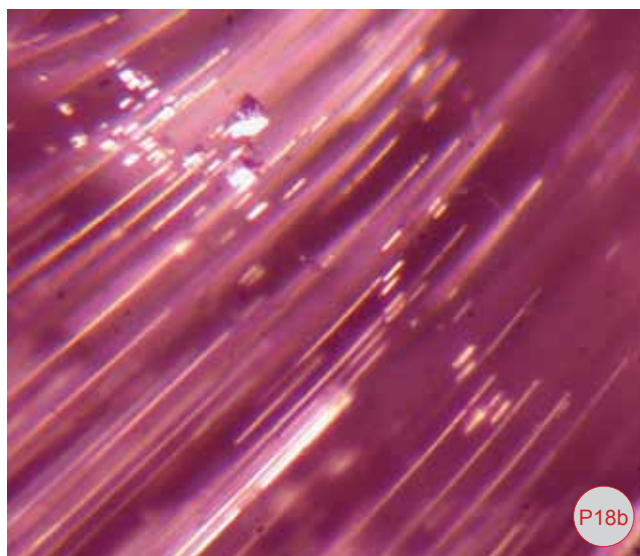
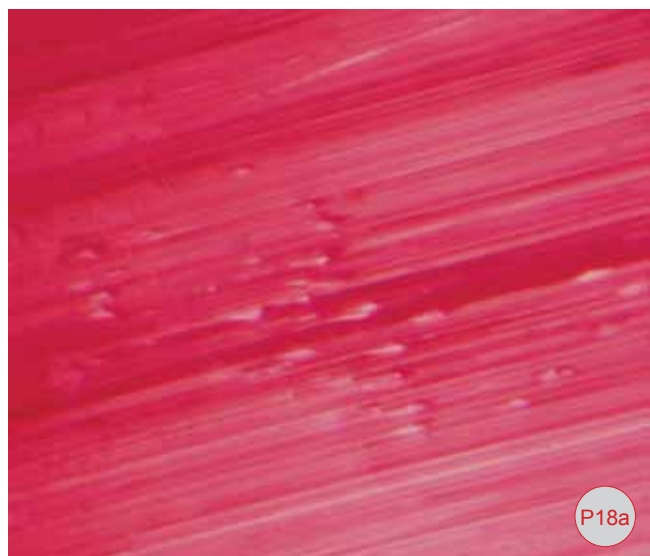


Fig. P18a/b Microfeatures observed in pezzottaite. Negative crystal in connection with growth tubes (P18a) and growth tubes of various length parallel to the c-axis (P18b). Images taken at 40-60x microscopic magnification (microphotographs A. Peretti).

About the authors

Dr. Peretti is Director of the GRS Gemresearch Swisslab Ltd., Lucerne, Switzerland
Adolf@Peretti.ch

Dr. Armbruster is Professor of Mineralogical Crystallography at the University of Berne, Switzerland
thomas.armbruster@krist.unibe.ch

Dr. Günther is Professor for Trace Elements and Microanalysis at the Laboratory for Inorganic Chemistry, ETH Zurich, Switzerland
guenther@inorg.chem.ethz.ch

Dr. Grobéty is Professor of Mineralogy at the University of Fribourg, Switzerland
Bernard.Grobety@unifr.ch

Dr. Hawthorne is Professor of Mineralogy and Mr. Cooper Laboratory technician, at the University of Manitoba, Winnipeg, Canada
frank_hawthorne@umanitoba.ca
mark_cooper@umanitoba.ca

Dr. Simmons is Professor of Mineralogy and University Research Professor and Mr. Falster is Senior Research Technologist, at the University of New Orleans, Louisiana, USA
wsimmons@uno.edu
afalster@uno.edu

Dr. Rossman is Professor of Mineralogy at the California Institute of Technology, Pasadena, USA
grr@gps.caltech.edu

Mr. Laurs is Editor of Gems & Gemology at GIA in Carlsbad, California, USA
blaurs@gia.edu

Acknowledgements

The authors are grateful to all research scientists of different Institutions for their contributions and to the experts of the IMA Commission. Special thanks to gem dealers who supported this research with samples. The senior author would like to thank Steve Jaquith and Marc Jobin MJ3 Inc. (NY, USA), G.E.O. International Co., LTD (Bangkok, Thailand) and Papas Gem Co., LTD for supply of samples. This report was prepared with the help of Anong Imaging (Bangkok), Mr. Sumet Tanthadilok, IMAGIMAX Animation & Design Studio (Bangkok, Thailand) and Mr. Saleem Michael.

BOX 7 PEZZOTTAITE GEMSTONE EXAMPLES



Natural Pezzottaite
 Weight: 59.98 ct
 Dimensions: 26.38 x 18.75 x 14.32 mm
 Cut: Cabochon/sugar loaf
 Shape: Rectangular cushion
 Color: Pinkish-red



Natural Cat's Eye Pezzottaite
 Weight: 8.85 ct
 Dimensions: 13.65 x 8.3 x 9.05 mm
 Cut: Cabochon/partially polished
 Shape: Oval
 Color: Pinkish-red



Natural Cat's Eye Pezzottaite
 Weight: 5.74 ct
 Dimensions: 14.07 x 8.41 x 5.64 mm
 Cut: Cabochon
 Shape: Oval
 Color: Pinkish-red



Natural Pezzottaite
 Weight: 10.07 ct
 Dimensions: 13 x 12.4 x 8.96 mm
 Cut: Faceted/step
 Shape: Cushion
 Color: Pink
 RI: 1.61-1.620
 SG: 3.11



Natural Pezzottaite
 Weight: 5.27 ct
 Dimensions: 11.39 x 8.68 x 6.82 mm
 Cut: Faceted/step
 Shape: Cushion
 Color: Pink
 RI: 1.61-1.20
 SG: 3.11



Natural Cat's Eye Pezzottaite
 Weight: 4.16 ct
 Dimensions: 8.92 x 8.31 x 6.9 mm
 Cut: Cabochon/partially polished
 Shape: Oval
 Color: Pink
 RI Spot: 1.62
 SG: 3.09



Natural Pezzottaite Rough Crystal
 Weight: 4.36 ct
 Length: 10.4 mm



Natural Pezzottaite Rough Crystal
 Weight: 9.33 ct
 Length: 16.5 mm



Natural Pezzottaite Rough Crystal
 Weight: 7.25 ct
 Length: 13.0 mm

Selected Literature

Brendan M. Laurs, William B. (Skip) Simmons, George R. Rossman, Elizabeth P. Quinn, Shane F. McClure, Adolf Peretti, Thomas Armbruster, Frank C. Hawthorne, Alexander U. Falster, Detlef Günther, Mark A. Cooper, and Bernard Grobóty (2003): PEZZOTTAITE FROM AMBATOVITA, MADAGASCAR: A NEW GEM MINERAL. *Gems&Gemology*, Vol 39, No. 4, pp. 284-301..

Hawthorne F.C., Cooper M.A., Peretti A., Simmons W.B., Armbruster T., Rossman G.R., Günther D., Laurs B.M., Grobóty B. (2003) Check-list for new mineral proposals: Pezzottaite. Proposal submitted to

the International Mineralogical Association, 8 pp.

Hawthorne F.C., Cooper M.A., Simmons W.B., Falster A.U., Laurs B.M., Armbruster T., Rossman G.R., Peretti A., Günther D., Grobóty B.: Pezzottaite, Cs(Be₂Li)Al₂Si₆O₁₈, a spectacular new mineral related to the beryl group, from Madagascar. *Mineralogical Record*. Submitted.

Nickel E.H. and Grice J.D. (1998): The IMA Commission on New Mineral Names: Procedures and Guidelines on Mineral Nomenclature, *Canadian Mineralogist*, Vol. 36, pp. 3-16.



Copyright by GRS Gemresearch Swissslab AG, P.O.Box 4028, 6002 Lucerne, Switzerland
www.gemresearch.ch