Trattnerite, $(Fe,Mg)_2(Mg,Fe)_3[Si_{12}O_{30}]$, a new mineral of the milarite group: mineral data and crystal structure

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Abstract: The new mineral trattnerite, $(Fe,Mg)_2(Mg,Fe)_3[Si_{12}O_{30}]$, a member of the milarite group, occurs in small cavities of a Si-rich xenolith at the haüyne-nephelinite quarry Stradner Kogel, eastern Styria, Austria. Trattnerite is hexagonal and forms hypidiomorphic, short prismatic to tabular crystals up to 1 mm. Associated minerals are sanidine, tridymite, quartz, hematite, ortho- and clinopyroxene and clinoamphibole. The colour is pleocroitic deep blue (ω) to yellowish-green (ϵ), the streak is white and the crystals have a vitreous luster. Optically, the mineral is uniaxial (-), $\omega = 1.589(1)$, $\epsilon = 1.586(1)$ at 589 nm. The cleavage parallel to (001) is good, poor parallel to (100), and the tenacity is brittle. Trattnerite is hexagonal, $P6/mcc$, with unit cell parameters $a = 10.050(1)$ Å, $c = 14.338(2)$ Å, $V = 1254.1(1)$ Å^3, $Z = 2$ and $D_{calc.} = 2.68$ g/cm^3. The strongest lines in the X-ray powder diffraction pattern (d_{obs} in Å, (hkl), I) are: 8.70, (100), 97; 7.17, (002), 100; 5.535, (102), 96; 5.026, (110), 61; 3.207, (211), 85. Two single-crystal structure refinements ($R(F) = 0.028$ and 0.025) of trattnerite yielded following site occupancies: the T1 tetrahedron of the double-ring unit is fully occupied by Si, the T2 tetrahedron and the A octahedron have a mixed (Mg,Fe) occupation with Fe predominantly in A and Mg in T2. The T2-O and A-O bond lengths indicate most of the iron to be in the trivalent state which is in accordance with the empirical formula: $^C(K_{0.07}Na_{0.01})_{0.08}{}^{A,T2}(Mg_{2.46}Fe^{3+}{}_{1.99}Fe^{2+}{}_{0.30}Mn_{0.08}Zn_{0.05}Al_{0.04}Ti_{0.01})_{4.93}{}^{T1}[Si_{12}O_{30}]$, obtained by a combination of electron microprobe data and LA-ICP-MS. The C-site located between consecutive double-ring units is occupied only by small amounts of K, the remaining 88-95 % being vacancies, which lead to increased C-O distances of 3.123 and 3.118 Å. Trattnerite could be described as an end member in the series merrihueite-trattnerite with the chemical substitution $Fe^{3+} + \square = Fe^{2+} + (K+Na)^+$.

Key-words: trattnerite, new mineral, milarite group, Mg-Fe-silicate, crystal structure, Stradner Kogel, Austria.

Introduction

Minerals of the milarite group are summarized in Hawthorne *et al.* (1991). The volcanic area of southeastern Styria and of Burgenland, Austria is known for the occurrence of minerals of the milarite group, namely roedderite, merrihueite, chayesite and osumilite (Postl *et al.*, 1992; Ettinger *et al.*, 1996).

The new mineral trattnerite was found by Mr. Walter Trattner in small cavities of a Si-rich xenolith in the haüyne-nephelinite quarry Stradner Kogel, about 5 km south of Bad Gleichenberg, Styria. X-ray powder diffraction data combined with chemical investigations indicated this mineral, which contains only very small amounts of Na and K, to be a new member of the milarite group (Postl *et al.,* 2000; Walter & Ettinger, 2001).

Both mineral and mineral name have been approved by the Commission on New Minerals and Mineral Names of the International Mineralogical Association (#2002-002). Type material is preserved in the Department of Mineralogy of the Landesmuseum Joanneum Graz (no. 82775-82779) and in the Department of Mineralogy of the Natural History Museum Vienna. The name is given in honour of Mr. Walter Trattner, a mineral collector with excellent knowledge of the mineralogy in the volcanic area of southeastern Styria and Burgenland.

Occurrence

Trattnerite was found in a quarry (15°55'30''E, 46°50'20''N) close to the village Wilhelmsdorf, SSE of Bad Gleichenberg, eastern Styria (Austria). The quarry is situated SW of the Stradner Kogel, where a haüyne-nephelinite is a part of a plio-/pleistocene lava flow. The new mineral occurs in small cavities of a Si-rich xenolith. The fine-grained xenolith is hosted in a haüyne-nephelinite and consists mainly of sanidine, plagioclase and quartz. Further associated minerals are: tridymite, hematite, ortho- and clinopyroxene and clinoamphibole.

Physical and optical properties

Trattnerite forms hypidiomorphic, short prismatic to tabular and rarely long prismatic crystals up to 1 mm. The dominant

forms are {100}, {001}, {101} and {111} (Fig. 1). The colour varies between deep blue and yellowish-green corresponding to a strong pleochroism. The crystals are translucent with vitreous lustre and white streak. The mineral is brittle with a good cleavage parallel (001) and poor parallel (100). The Mohs hardness and the density could not be measured because of the small grain size. The calculated density is 2.68 g/cm^3 based on the empirical formula. Trattnerite is optically uniaxial (-) with $\omega = 1.589(1)$ and $\varepsilon = 1.586(1)$ (at 589 nm). The pleochroism is strong, ω: deep blue; ε: yellowish-green.

The infrared spectrum (Perkin-Elmer FT-IR spectrometer Paragon 500, KBr-pellet) of trattnerite shows two very strong bands at 1142 and 966 cm^{-1} with a shoulder at 991 cm^{-1}. Further bands are at 1383 (w), 790 (w), 630 (m), 576 (m), with shoulders at 494 and 466, 427 (w) and 366 cm^{-1}. Peaks in the range of 800-1100 cm^{-1} are generally assigned to Si-O stretching vibrations in chain and ring silicates (McMillan & Hofmeister, 1988). For the milarite-type mineral darapiosite (Ferraris *et al.*, 1999) a similar pattern compared to trattnerite is reported. In the spectras of both minerals no evidence of water was observed.

Chemical composition

The chemical characterisation has been performed using several methods. Microchemical analyses of crystals (*e.g.*, Fig. 2) from one xenolith were performed using an electron microprobe (Jeol JSM-6310, equipped with ED- and WD-spectrometer) operated at 15 kV / 5 nA specimen current on Al, and with a spot size of ~1.5 μm. Minerals have been used as standards (WD: jadeite, Na; ED: kaersutite, Mg, Ca, Ti, Fe; adularia, Al, Si, K; rhodonite, Mn; gahnite, Zn) and Phi-Rho-Z as data reduction. The mean element concentrations from 17 analyses, the range of values and the standard deviations for oxides along with the calculated formula normalized on Si = 12 and Fe^{2+}/Fe^{3+}-charge balance for 30 oxygens are listed in Table 1.

Li, Be and Ti were measured by LA-ICP-MS on a New Wave/Merchantek UP 213 nm laser ablation unit coupled to
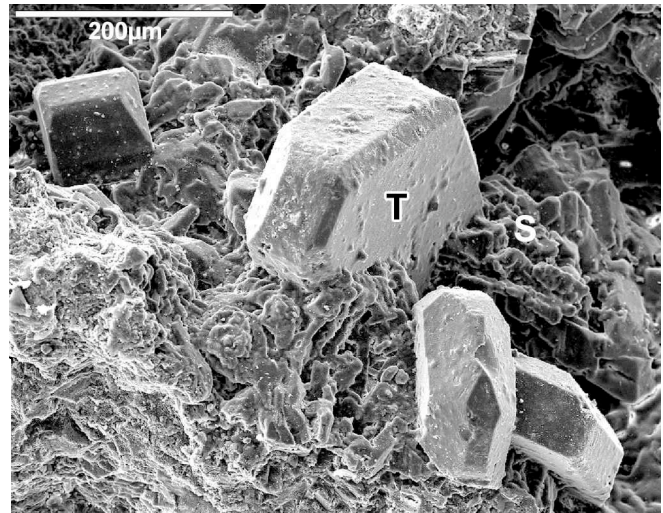

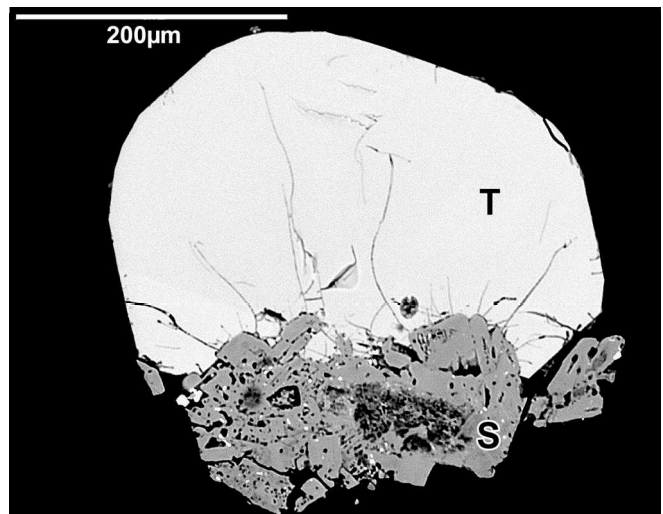Fig. 1. Trattnerite (T) on sanidine (S) from Stradner Kogel, Styria; SE-image.

Fig. 2. Chemically homogeneous trattnerite (T) on sanidine (S) from Stradner Kogel, Styria; polished thin section, BSE-image.
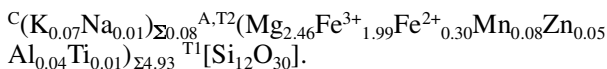
a quadrupole HP Agilent 4500 mass spectrometer. A homogenized laser beam with a flat top profile and spot size of 60 μm was operated at 5 Hz repetition rate, argon was used as carrier gas at ~ 1.3 l/min flow, and data were acquired in time-resolved mode. Every 960 ms the intensity of 13 selected isotopes were evaluated, ablation time being typically 30 s followed by 30 s of background measurement with the laser turned off. On a polished thin section which has also been previously used for the microprobe analyses a total of five spots, each with five repetitions were measured at manually selected integration intervals, and the gross signal was corrected for background using the preablation signal. Using SRM NIST 612 and BCR-2 glass as external standards and Mg as internal standard, the following results were obtained: Li: 240 ± 71 ppm; Be: 17 ± 6 ppm; Ti: 468 ± 135 ppm (= 0.06-0.10 wt.% TiO$_2$, which is in agreement with the microprobe data). No H$_2$O-content could be detected by IR-spectroscopy.

Table 1. Chemical analysis and formula of trattnerite.

Trattnerite Stradner Kogel				Si=12; O=30	
		analyses	(n=17)		apfu
oxide	mean	range	stdev.	Si	12.00
SiO$_2$	70.80	70.37 – 71.08	0.4	Ti	0.01
TiO$_2$	0.07	0.06 – 0.10	<0.1	Al	0.04
Al$_2$O$_3$	0.21	0.09 – 0.29	0.1	Fe^{3+}	1.99
Fe$_2$O$_3$	17.93	17.39 – 18.35	0.5	Fe^{2+}	0.30
MnO	0.56	0.48 – 0.63	0.1	Mn	0.08
MgO	9.75	9.37 – 10.28	0.5	Mg	2.46
ZnO	0.36	0.27 – 0.47	0.1	Zn	0.05
CaO	0.02	0.00 – 0.04	<0.1	Ca	0.00
Na$_2$O	0.03	0.02 – 0.04	<0.1	Na	0.01
K$_2$O	0.33	0.22 – 0.47	0.1	K	0.07
Σ	100.06	recalculated		Σ A+T	16.93
		Fe$_2$O$_3$	15.60	Σ C	0.08
		FeO	2.12	Σcat.	17.01

Table 2. X-ray powder diffraction data for trattnerite.

hkl	d_{obs}	d_{calc}	I_{obs}	I_{calc}
100	8.7	8.7	97 *	46
002	7.17	7.17	100 *	48
102	5.535	5.534	96	74
110	5.026	5.025	61	53
200	4.352	4.352	53	43
112	4.116	4.115	37	41
202	3.721	3.720	30	33
004	3.585	3.585	31	28
104	3.315	3.315	31	34
211	3.207	3.206	85	100
212	2.990	2.990	32	38
114	2.918	2.918	33	47
204	2.767	2.767	38	52
213	2.710	2.710	11	11
220	2.5121	2.5126	19	28
214	2.4238	2.4237	10	9
311	2.3806	2.3804	3	4
222	2.3711	2.3712	4	7
312	2.2880	2.2877	3	3
313	2.1548	2.1547	8	12
402	2.0823	2.0822	4	5
224	2.0577	2.0574	2	3
314	2.0026	2.0023	18	27
320	1.9968	1.9968	14	12
216	1.9337	1.9334	4	4
411	1.8826	1.8828	11	17
315	1.8465	1.8467	9	17
008	1.7921	1.7923	7	12
500	1.7409	1.7407	3	4
226	1.7315	1.7316	15	29
511	1.5540	1.5540	6	10
326	1.5322	1.5323	4	4
334	1.5176	1.5175	4	8
228	1.4591	1.4591	8	16

d in Å, * preferred orientation caused by cleavage,
I_{calc} calculated from structure refinement of tr1

The empirical formula for trattnerite is:

$^C(K_{0.07}Na_{0.01})_{\Sigma 0.08}\,^{A,T2}(Mg_{2.46}Fe^{3+}_{1.99}Fe^{2+}_{0.30}Mn_{0.08}Zn_{0.05}Al_{0.04}Ti_{0.01})_{\Sigma 4.93}\,^{T1}[Si_{12}O_{30}]$.

The Mg- and Fe-distribution on the T2 and A sites could not be determined before the structure refinement.
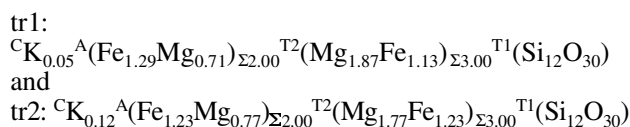
X-ray experiments and structure refinement

Powder diffraction data for trattnerite (Table 2) were obtained using a D5000 diffractometer (Bruker AXS, twin-Goebel mirrors, CuK_α). From one sample two hexagonal trattnerite crystals (0.16 x 0.16 x 0.07 mm (tr1) and 0.25 x 0.15 x 0.10 mm (tr2)) were used for collecting single-crystal X-ray diffraction data at 100 K. For tr1 intensity data were collected up to $\theta = 26°$ in ω-scan mode with a STOE diffractometer using graphite-monochromatized MoK_α X-radiation. Cell dimensions were refined from $h00$ and $00l$ reflections yielding $a = 10.050(1)$ and $c = 14.338(2)$ Å, $V =$

1254.1(1) Å^3. A total of 3237 reflections were measured with $-12 \le h \le 11$, $-11 \le k \le 12$ and $-2 \le l \le 17$. Those with hhl, $h0l$ and $00l$ with $l = 2n+1$ were systematically absent and indicated $P6/mcc$ or $P6cc$ as possible space groups. Reflections with $I < 2\sigma(I)$ were rejected leaving 428 unique data. Data reduction included background and Lorentz-polarisation correction, and no absorption correction for tr1 was applied. Tr2 was investigated on a Bruker AXS SMART APEX single-crystal diffractometer using graphite-monochromatized MoK_α X-radiation. Cell parameters with $a = 10.065(1)$, $c = 14.341(2)$ Å, $V = 1258.2(1)$ Å^3 were obtained from least-squares refinement and are in good agreement with results from powder diffraction data. A total of 9682 reflections were measured with $-12 \le h \le 12$, $-12 \le k \le 12$ and $-17 \le l \le 17$ ($\theta_{max} = 26.4°$). Systematic absences and intensity statistics indicated the same possible two space groups as found for tr1. Data reduction included background, Lorentz-polarisation correction, and an empirical absorption correction (SADABS, Bruker/Siemens area detector absorption correction) with $R(int) = 0.084$ before and $R(int) = 0.038$ after parameter refinement. Reflections with $I < 2\sigma(I)$ were excluded leaving 449 unique data. The $1/\sigma^2(F_o^2)$ weighted structure refinements for tr1 and tr2 were carried out in space group $P6/mcc$ (in accordance with chayesite and merrihueite) with SHELXL-97 (Sheldrick, 1997) using neutral atom scattering factors and corrections for anomalous dispersion. No extinction corrections were applied. Atomic coordinates for MAS-osumilite (Winter *et al.*, 1995) were used as starting parameters for tr1 and tr2. Si was assigned to the T1-site, Mg and Fe (Fe = Fe + Mn + Zn) according to the chemical analysis to the T2- and A-sites. Refinement of positional, displacement parameters and site occupancies resulted in difference-Fourier maps for both crystals which showed small positive peaks at the C-site; the B-sites were found to be empty. The final refinement with K and vacancies on the C-site gave for tr1: $R(F) = 0.028$ for 350 $F_o > 4\sigma(F_o)$ and w$R(F^2) = 0.052$ for 428 data and for tr2: $R(F) = 0.025$ for 447 $F_o > 4\sigma(F_o)$ and w$R(F^2) = 0.060$ for 449 data. Final difference-Fourier maps for both crystals did not exhibit peaks higher than ± 0.30 e/Å^3 (tr1) and ± 0.35 e/Å^3 (tr2). A list of observed and calculated structure factors can be obtained from F. Walter.

Results

Final atomic and displacement parameters are given in Table 3. Selected interatomic distances and bond angles are summarized in Table 4. The refinement of two trattnerite crystals (tr1 and tr2) yielded the following structural formulae:

tr1:
$^CK_{0.05}\,^A(Fe_{1.29}Mg_{0.71})_{\Sigma 2.00}\,^{T2}(Mg_{1.87}Fe_{1.13})_{\Sigma 3.00}\,^{T1}(Si_{12}O_{30})$
and
tr2: $^CK_{0.12}\,^A(Fe_{1.23}Mg_{0.77})_{\Sigma 2.00}\,^{T2}(Mg_{1.77}Fe_{1.23})_{\Sigma 3.00}\,^{T1}(Si_{12}O_{30})$

with the refined Fe$_{tot}$/Mg ratios 0.94 for tr1 and 0.97 for tr2 (Fe$_{tot}$ = Fe + Mn + Zn). In order to obtain a charge-balanced formula there must be 1.95 apfu Fe^{3+} in tr1 and 1.88 apfu Fe^{3+} in tr2 which is in good agreement with Fe^{3+} = 1.99 apfu in the empirical formula.

Table 3. Fractional coordinates, displacement parameters and site occupancies for trattnerite (sample tr1 and tr2).

Site	Population	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
	Sample tr1									
T1	Si	0.1184(1)	0.3554(1)	0.1085(1)	0.0092(5)	0.0105(5)	0.0082(4)	0.0050(4)	-0.0002(4)	-0.0008(4)
T2	$Mg_{0.62}Fe_{0.38(1)}$	1/2	1/2	1/4	0.0185(7)	0.0185(7)	0.0102(8)	0.0153(7)	0	0
A	$Fe_{0.65}Mg_{0.35(1)}$	1/2	2/3	1/4	0.0079(5)	0.0079(5)	0.0071(7)	0.0040(3)	0	0
C	$K_{0.05(1)}$	0	0	1/4	0.02(1)*					
O1	O	0.1345(4)	0.4019(4)	0	0.021(2)	0.018(2)	0.012(2)	0.008(2)	0	0
O2	O	0.2277(3)	0.2848(3)	0.1318(2)	0.017(1)	0.021(1)	0.022(1)	0.014(1)	0.001(1)	0.001(1)
O3	O	0.1588(2)	0.5004(2)	0.1739(1)	0.014(1)	0.014(1)	0.013(1)	0.0072(9)	-0.0011(8)	-0.0034(9)
	Sample tr2									
T1	Si	0.11856(7)	0.35553(7)	0.10866(4)	0.0101(4)	0.0108(4)	0.0071(4)	0.0052(3)	-0.0000(2)	-0.0005(2)
T2	$Mg_{0.59}Fe_{0.41(1)}$	1/2	1/2	1/4	0.0145(5)	0.0145(5)	0.0081(5)	0.0104(5)	0	0
A	$Fe_{0.62}Mg_{0.38(1)}$	1/2	2/3	1/4	0.0075(4)	0.0075(4)	0.0065(5)	0.0038(2)	0	0
C	$K_{0.12(1)}$	0	0	1/4	0.019(6)	0.019(6)	0.015(8)	0.009(3)	0	0
O1	O	0.1339(3)	0.4009(3)	0	0.016(1)	0.015(1)	0.010(1)	0.007(1)	0	0
O2	O	0.2273(2)	0.2842(2)	0.1323(1)	0.0163(9)	0.0170(9)	0.0155(9)	0.0105(7)	0.0007(7)	0.0002(7)
O3	O	0.1595(2)	0.5012(2)	0.1737(1)	0.0139(8)	0.0133(8)	0.0104(8)	0.0077(7)	-0.0015(6)	-0.0025(6)

* = U_{iso}, standard deviations are in parentheses

The T1 tetrahedron

The mean T1-O distances 1.610 and 1.613 Å for tr1 and tr2 respectively, suggest a preferred occupancy of the T1 site by Si. Microprobe analyses (Table 1) gave an average SiO_2 content of 70.8 wt.% normalized to 12 Si for the T1 site of the structural formula.

The T2 tetrahedron

The refinement of T2 site occupancies, microprobe analyses and the mean T2-O distances, 1.932 Å (tr1) and 1.938 Å (tr2), indicate T2 to be occupied by both Mg and Fe. The O3-T2-O3 angles testify an extremely distorted tetrahedron (O3-T2-O3 = 88.3° to 131.8°). Only Mg on the T2 site is reported from merrihueite (T2-O = 1.955 Å, Khan *et al.*, 1972). In members of the roedderite-chayesite series T2 is occupied by Mg and small amounts of Fe^{3+}, leading to T2-O distances between 1.932 and 1.941 Å (Alietti *et al.*, 1994). For trattnerite the site occupancy refinements of T2 yield high Fe concentrations of 38 % (tr1) and 41 % (tr2). From these refinements and the T2-O bond lengths, we suggest that T2 is dominantly occupied by Mg but also hosts large amounts of Fe^{3+}. For osumilite the size of the T2-tetrahedron seems not to be affected by the size of the adjacent A-octahedron (Armbruster & Oberhänsli, 1988).

The A octahedron

The A-O distance is 2.032 Å (tr1) and 2.029 Å (tr2). From site occupancy refinement both crystals show a mixed Mg/Fe occupation on the A sites with Fe being dominant (65 % Fe (tr1) and 62 % Fe (tr2)). The A-O distance in trattnerite is too short for an osumilite-type MgO_6 octahedron with Mg-O = 2.118 Å in osumilite from Antarctica (Armbruster & Oberhänsli, 1988) and 2.104 Å in merrihueite (Khan *et al.*,

1972). In the roedderite-chayesite series the A site is occupied by Mg and small amounts of Fe^{3+} with A-O bond lengths of 2.079 to 2.087 Å, indicating the iron to be in the trivalent state (Alietti *et al.*, 1994). From the chemical analyses of trattnerite there are no significant amounts of small cations, which could shorten the A-O distance to 2.03 Å. This bond length therefore suggests iron on the A site of trattnerite to be Fe^{3+}. The short A-O distance in trattnerite causes also a shortening of the *a* axis (*a* = 10.050 Å and 10.065 Å in tr1 and tr2 respectively, compared with *a* = 10.118 to 10.135 Å in roedderite-chayesite, Alietti *et al.*, 1994). The strong positive correlation between the size of the cation on A and the length of the *a* axis was reported for osumilites by Armbruster & Oberhänsli (1988).

The cage position C

The very small contents of Na, K and Ca, measured by EPMA are striking (K = 0.05-0.1 apfu, Na and Ca near detection limits). The site occupancy refinement of C resulted in an occupation of 5 % K (tr1) and 12 % K (tr2) with 95 % and 88 % vacancies on C which is in good agreement with the content of K (0.07 apfu, Table 1) in the empirical formula of trattnerite. The C-O distances, 3.123 Å (tr1) and 3.118 Å (tr2), are longer than in the fully occupied C site of osumilite-type minerals (*e.g.*, roedderite-chayesite C-O = 3.062 to 3.067 Å, Alietti *et al.*, 1994).

The other possible atomic sites for cations of the milarite-type structure, especially the B-site, which could be occupied by Na, were found to be completely empty.

Conclusions

The new mineral trattnerite is a member of the milarite-group. It is decisively different from all other minerals of this group by the strong dominance of vacancies on the C

Table 4. Selected interatomic distances (Å) and bond angles (°) for trattnerite crystals tr1 and tr2.

	Mult.	tr1	tr2
T1-O1	1	1.608 (1)	1.609 (1)
T1-O2	1	1.612 (2)	1.617 (2)
T1-O2	1	1.615 (2)	1.618 (2)
T1-O3	1	1.606 (2)	1.608 (2)
<T1-O>		1.610	1.613
O1-O2	1	2.634 (3)	2.640 (2)
O1-O2	1	2.641 (3)	2.643 (2)
O1-O3	1	2.648 (2)	2.652 (2)
O2-O2	1	2.623 (2)	2.622 (2)
O2-O3	1	2.576 (3)	2.587 (2)
O2-O3	1	2.653 (3)	2.660 (2)
O1-T1-O2	1	109.7 (1)	109.8 (1)
O1-T1-O2	1	110.0 (1)	109.9 (1)
O1-T1-O3	1	111.0 (1)	111.0 (1)
O2-T1-O2	1	108.7 (2)	108.2 (1)
O2-T1-O3	1	111.0 (1)	111.2 (1)
O2-T1-O3	1	106.3 (1)	106.6 (1)
T2-O3	4	1.932 (2)	1.938 (2)
O3-O3	2	2.699 (4)	2.700 (3)
O3-O3	2	3.189 (4)	3.200 (3)
O3-O3	2	3.523 (4)	3.538 (3)
O3-T2-O3	2	88.6 (1)	88.3 (1)
O3-T2-O3	2	111.2 (1)	111.3 (1)
O3-T2-O3	2	131.5 (1)	131.8 (1)
A-O3	6	2.032 (2)	2.029 (2)
O3-O3	3	2.699 (4)	2.700 (3)
O3-O3	3	2.852 (4)	2.854 (3)
O3-O3	6	2.968 (4)	2.960 (3)
O3-A-O3	3	83.3 (1)	83.4 (1)
O3-A-O3	3	89.2 (1)	89.4 (1)
O3-A-O3	6	93.9 (1)	93.7 (1)
C-O2	12	3.123 (2)	3.118 (2)
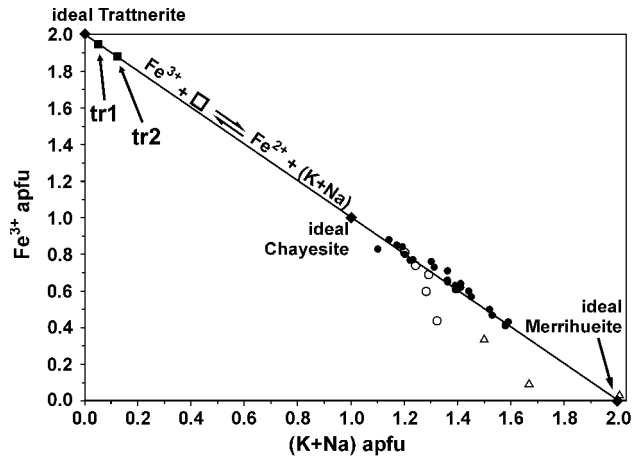
Fig. 4. The plot of calculated Fe^{3+} vs. (Na+K) shows the positions of the two refined trattnerite crystals and the relation to merrihueite and chayesite (modified after Alietti et al., 1994).

site (5-12% K) and an empty B site. The C site is located between consecutive double-rings built by the T1-tetrahedron (Fig. 3). The missing cation on C induces an elongation of the C-O2 distance as compared with minerals of the chayesite-roedderite series. Only the synthetic MAS osumilite with a completely vacant C site (Winter et al., 1995) has a longer C-O2 distance (3.179 Å) than trattnerite. The reported distortion of the T1 tetrahedron in the double ring of the MAS osumilite (T1-O between 1.600 and 1.680 Å) caused by the increased C-O2 distance (Winter et al., 1995), could not be found in the trattnerite structure: T1-O = 1.606-1.615 Å (tr1) and 1.608-1.619 Å (tr2). In trattnerite T1-O3 is the shortest of the four T1-O bonds with 1.606 Å (tr1) and 1.608 Å (tr2), reflecting the attempt to counteract the under-
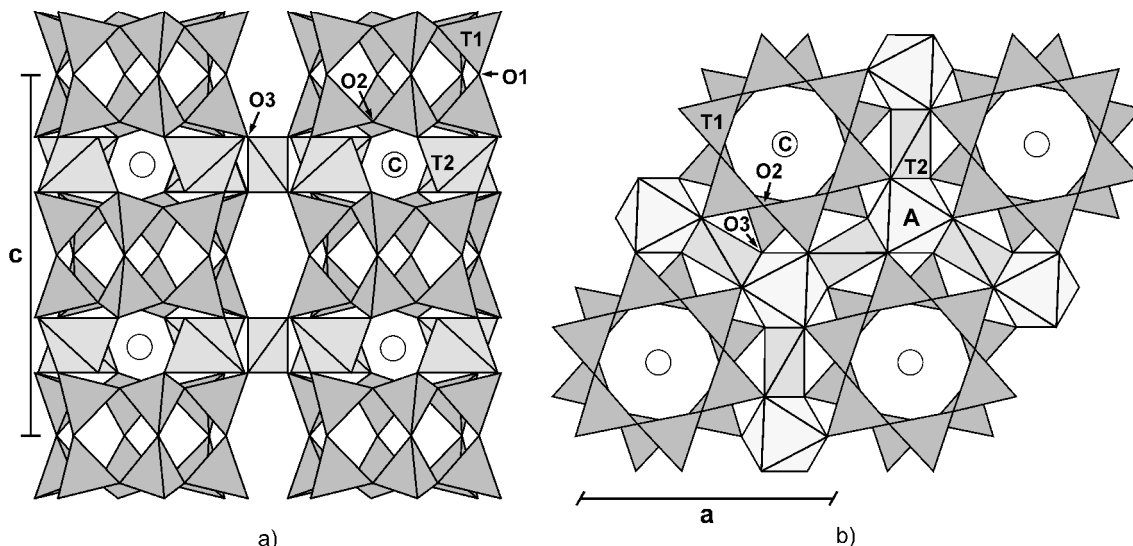
Fig. 3. Projections of the structure of trattnerite: a) along [-1 1 0]; the A-octahedron has been omitted for clarity. b) along [0 0 1]; the location of the almost empty C-site is marked with a circle.

bonding of O3 caused by the lower bond-valence sums of the cations on T2 and A. Winter *et al.* (1995) found average O1-T1-O2 angles in double-ring silicates with underbonded O3 to vary between 109.2° and 110.2°. This is also confirmed by the O1-T1-O2 angles in trattnerite with 109.7° (tr1) and 109.8° (tr2). Trattnerite plots below the line characteristic for ideal tetrahedra in Fig. 2 of Winter *et al.* (1995), common to all double-ring silicates with only Si on T1. These authors also report that O2-T1-O2 angles of natural double-ring silicates are within a narrow range between 102.4° and 105.0° (*e.g.*, in roedderite-chayesite 104.4-104.6°, Alietti *et al.*, 1994). In MAS osumilite the largest angle for O2-T1-O2 = 110.9° was observed. Winter *et al.* (1995) conclude that a narrow O2-T1-O2 angle compensates for an energetically favoured C-O distance, and that the angle increases if the C site is empty.

Trattnerite could be described as an end member of the milarite-group with a probable solid-solution series merrihueite-trattnerite (Fig. 4). The characteristic chemical substitution is $Fe^{3+} + \square = Fe^{2+} + (K+Na)^+$, which was also described for the roedderite-chayesite series (Alietti *et al.*, 1994). In trattnerite the oxidation of iron is nearly complete (in the empirical formula $Fe^{3+}/(Fe^{3+}+Fe^{2+}) = 0.87$) thus Na and K are missing or only present in very small amounts although sanidine coexists with this new mineral. The ideal formula for trattnerite is $^{A}(Fe,Mg)_2 {}^{T2}(Mg,Fe)_3 {}^{T1}[Si_{12}O_{30}]$, with $Fe^{3+} = 2.0$.

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