

PRINGLEITE AND RUITENBERGITE, POLYMORPHS OF $\text{Ca}_9\text{B}_{26}\text{O}_{34}(\text{OH})_{24}\text{Cl}_4 \cdot 13\text{H}_2\text{O}$, TWO NEW MINERAL SPECIES FROM SUSSEX, NEW BRUNSWICK¹

ANDREW C. ROBERTS AND JOHN A.R. STIRLING

Geological Survey of Canada, 601 Booth Street, Ottawa, Ontario K1A 0E8

JOEL D. GRICE

Mineral Sciences Section, Canadian Museum of Nature, P.O. Box 3443, Station "D", Ottawa, Ontario K1P 6P4

PETER C. BURNS

Department of Geological Sciences, University of Manitoba, Winnipeg, Manitoba R3T 2N2

BRIAN V. ROULSTON AND JEFFREY D. CURTIS

Potash Company of America, P.O. Box 1489, Sussex, New Brunswick E0E 1P0

JOHN L. JAMBOR

CANMET, Energy, Mines & Resources Canada, 555 Booth Street, Ottawa, Ontario K1A 0G1

ABSTRACT

The new minerals pringleite and ruitenbergitte, polymorphs of idealized composition $\text{Ca}_9\text{B}_{26}\text{O}_{34}(\text{OH})_{24}\text{Cl}_4 \cdot 13\text{H}_2\text{O}$, are minor constituents of a single hand specimen collected from the Potash Company of America mine at Penobsquis, near Sussex, New Brunswick. Pringleite occurs sparingly as colorless to orange, platy, subhedral to anhedral cleaved masses up to 4 mm in size, associated with hilgardite-1A, halite, sylvite and traces of anhydrite, quartz and clays. Ruitenbergitte is present as a single anhedral 7×4 mm grain hosting numerous inclusions of hilgardite-1A. Pringleite is triclinic, space group $P1$, a 12.759(6), b 13.060(5), c 9.733(4) Å, α 102.14(4)°, β 102.03(3)°, γ 85.68(4)°, V 1550(1) Å³, $a:b:c$ 0.9769:1:0.7452, and $Z = 1$. The strongest seven lines of the X-ray powder-diffraction pattern [d in Å(N)(hkl)] are: 9.21(70)(110), 7.69(100)(11 $\bar{1}$), 5.74(60)(111,201), 4.63(40)(22 $\bar{1}$), 3.845(35)(222), 2.199(30b)(350,242,513,440) and 2.058(30)(152,602). Average results of electron-microprobe analyses, CaO 26.29, B₂O₃ 46.75, Cl 6.48, H₂O [21.94], sum 101.46, less O=Cl 1.46, total [100.00] wt.%, yield the empirical formula $\text{Ca}_{9.27}\text{B}_{26.56}\text{O}_{34.98}(\text{OH})_{24.64}\text{Cl}_{3.62} \cdot 11.76 \text{H}_2\text{O}$ on the basis of (O+Cl)=75. Water was confirmed and partitioned into (OH) and H₂O from bond-valence analysis in a separate crystal-structure determination. Pringleite is non-pleochroic, biaxial positive, α 1.537(1), β 1.548(1), γ 1.570(1), $2V_{\text{meas}}$ 77(1)°, $2V_{\text{calc}}$ 71.4°. Indicatrix orientation is $X = c$, $Y : a = 40^\circ$ in γ acute, and $Z : b = 46^\circ$ in γ obtuse; strong dispersion, $r \ll v$. Individual crystals are subhedral to anhedral, platy to prismatic, do not exceed 2 mm in size, and have a good {110} cleavage. The color varies from colorless to very pale yellow, but may appear orange owing to underlying halite. The streak is white, and the mineral is brittle, nonfluorescent, vitreous in luster, translucent to transparent, with an even to slightly conchoidal fracture. Its hardness is estimated at 3–4. D_{meas} 2.22(1), D_{calc} 2.11 g/cm³ for the idealized composition. No crystal forms were observed. The mineral name honors Mr. Gordon J. Pringle for his contributions to Canadian mineralogy and to the study of minerals by electron-microprobe analysis. Ruitenbergitte is monoclinic, space group $P2_1$, a 19.88(1), b 9.715(4), c 17.551(9) Å, β 114.85(4)°, V 3077(3) Å³, $a:b:c$ 2.046:1:1.807, and $Z = 2$. The strongest ten lines of the X-ray powder-diffraction pattern [d in Å(N)(hkl)] are: 9.03(60)(200), 8.56(100)(110), 6.62(70)(210), 6.14(30b)(012,212), 5.12(30)(310), 3.786(30)(320), 3.493(30)(222), 2.890(30)(520,132,124), 2.134(30b)(418,440,318) and 2.037(30)(826). Average results of electron-microprobe analyses, CaO 26.33, B₂O₃ 46.72, Cl 6.28, H₂O [22.09], sum 101.42, less O=Cl 1.42, total [100.00] wt.%, yield the empirical formula $\text{Ca}_{9.27}\text{B}_{26.51}\text{O}_{34.97}(\text{OH})_{24.63}\text{Cl}_{3.50} \cdot 11.90\text{H}_2\text{O}$ on the basis of (O+Cl)=75. Water was confirmed and partitioned into (OH) and H₂O from bond-valence analysis in the crystal-structure determination. Ruitenbergitte is nonpleochroic, biaxial positive, α 1.542(1), β 1.545(1), γ 1.565(1), $2V_{\text{meas}}$ 47(1)°, $2V_{\text{calc}}$ 42.5°. Indicatrix orientation is $X = b$, $Y : a = 25^\circ$ in β obtuse, and $Z = c$. The physical properties of ruitenbergitte are identical to those of pringleite except for the good {100} cleavage. D_{calc} is 2.13 g/cm³ for the idealized composition. The mineral name honors Dr. Arie A. Ruitenbergt in recognition of his contributions to the mineral industry in the province of New Brunswick.

Keywords: pringleite, ruitenbergitte, hydrated calcium borate hydroxide chloride, Potash Company of America mine, Sussex, New Brunswick, X-ray diffraction data, electron-microprobe data, optical data, new mineral species, polymorphs.

¹ Geological Survey of Canada contribution number 17992.

SOMMAIRE

Les nouvelles espèces minérales pringléite et ruitenbergitte, polymorphes de la composition idéale $\text{Ca}_9\text{B}_{26}\text{O}_{34}(\text{OH})_{24}\text{Cl}_4 \cdot 13\text{H}_2\text{O}$, sont des constituants mineurs d'un seul échantillon prélevé à la mine de la Potash Company of America à Penobscus, près de Sussex, au Nouveau-Brunswick. La pringléite, éparse, se présente en amas incolores ou orangés, en plaquettes sub-idiomorphes à xénomorphes jusqu'à 4 mm de large, en association avec hilgardite-1A, halite, sylvite, et des traces d'anhydrite, quartz et argiles. Nous avons trouvé un seul grain de ruitenbergitte, xénomorphe, 7×4 mm, contenant plusieurs inclusions de hilgardite-1A. La pringléite est triclinique, groupe spatial $P1$, a 12.759(6), b 13.060(5), c 9.733(4) Å, α 102.14(4)°, β 102.03(3)°, γ 85.68(4)°, V 1550(1) Å³, $a:b:c$ 0.9769:1:0.7452, et $Z = 1$. Les sept raies les plus intenses du cliché de diffraction X [d en Å(hkl)] sont: 9.21(70)(110), 7.69(100)(111), 5.74(60)(111,201), 4.63(40)(221), 3.845(35)(222), 2.199(30b)(350,242,513,440) et 2.058(30)(152,602). Les analyses à la microsonde électronique ont donné, en moyenne, CaO 26.29, B₂O₃ 46.75, Cl 6.48, H₂O [21.94], somme 101.46, moins O = Cl 1.46, total [100.00]% par poids, ce qui mène à la formule empirique $\text{Ca}_{9.27}\text{B}_{26.56}\text{O}_{34.98}(\text{OH})_{24.64}\text{Cl}_{3.62} \cdot 11.76\text{H}_2\text{O}$ [(O + Cl) = 75]. La présence de l'eau a été confirmée; la répartition en (OH) et en H₂O vient des résultats d'une analyse des valences de liaisons suite à la détermination de la structure cristalline. La pringléite est non pléochroïque, biaxe positive, α 1.537(1), β 1.548(1), γ 1.570(1), $2V_{\text{mes}}$ 77(1)°, $2V_{\text{calc}}$ 71.4°. L'orientation de l'indicatrice est $X = c$, $Y:a = 40^\circ$ dans l'angle γ aigu, et $Z:b = 46^\circ$ dans l'angle γ obtus. Il y a une forte dispersion, $r \ll v$. Les cristaux individuels sont sub-idiomorphes à xénomorphes, en plaquettes ou en prismes inférieurs à 2 mm, ayant un bon clivage {110}. Les cristaux sont incolores ou jaune très pâle, mais ils peuvent paraître orangés à cause de la halite sous-jacente. La rayure est blanche, et le minéral est cassant, non fluorescent, à éclat vitreux, transparent à translucide, avec une cassure égale ou légèrement conchoïdale. La dureté serait entre 3 et 4. La densité mesurée est de 2.22(1), et calculée, 2.11 pour la composition idéale. Il n'y a aucune forme cristalline identifiable. Le nom choisi honore Gordon J. Pringle pour ses contributions à la minéralogie au Canada, et surtout ses études par microsonde électronique. La ruitenbergitte est monoclinique, groupe spatial $P2_1$, a 19.88(1), b 9.715(4), c 17.551(9) Å, β 114.85(4)°, V 3077(3) Å³, $a:b:c$ 2.046:1:1.807, et $Z = 2$. Les dix raies les plus intenses du cliché de diffraction X [d en Å(hkl)] sont: 9.03(60)(200), 8.56(100)(110), 6.62(70)(210), 6.14(30b)(012,212), 5.12(30)(310), 3.786(30)(320), 3.493(30)(222), 2.890(30)(520,132,124), 2.134(30b)(418,440,318) et 2.037(30)(826). Les analyses à la microsonde électronique ont donné, en moyenne, CaO 26.33, B₂O₃ 46.72, Cl 6.28, H₂O [22.09], somme 101.42, moins O = Cl 1.42, total [100.00]% par poids, ce qui mène à la formule empirique $\text{Ca}_{9.27}\text{B}_{26.51}\text{O}_{34.97}(\text{OH})_{24.63}\text{Cl}_{3.50} \cdot 11.90\text{H}_2\text{O}$ [(O + Cl) = 75]. La présence de l'eau a été confirmée; la répartition en (OH) et en H₂O vient des résultats d'une analyse des valences de liaisons suite à la détermination de la structure cristalline. La ruitenbergitte est non pléochroïque, biaxe positive, α 1.542(1), β 1.545(1), γ 1.565(1), $2V_{\text{mes}}$ 47(1)°, $2V_{\text{calc}}$ 42.5°. L'orientation de l'indicatrice est $X = b$, $Y:a = 25^\circ$ dans l'angle β obtus, et $Z = c$. Les propriétés physiques de la ruitenbergitte sont identiques à celles de la pringléite, sauf pour le bon clivage {100}. La densité calculée est 2.13 pour la composition idéale. Le nom choisi honore Arie A. Ruitenbergitte pour ses contributions à l'industrie minière du Nouveau-Brunswick.

(Traduit par la Rédaction)

Mots-clés: pringléite, ruitenbergitte, borate hydraté de calcium à hydroxyle et chlorure, mine de la Potash Company of America, Sussex, Nouveau-Brunswick, données de diffraction X, données par microsonde électronique, données optiques, nouvelles espèces minérales, polymorphes.

INTRODUCTION

Pringléite and ruitenbergitte, polymorphs of idealized formula $\text{Ca}_9\text{B}_{26}\text{O}_{34}(\text{OH})_{24}\text{Cl}_4 \cdot 13\text{H}_2\text{O}$, are two new mineral species from an evaporite deposit near Sussex, New Brunswick. Pringléite was initially noted by one of the authors (JARS) in a program of quantitative electron-microprobe analyses of polished thin and thick sections prepared from borate-rich specimens collected from the Potash Company of America mine (also known as the PCA mine). The analyses indicated that the mineral is a calcium borate chloride; X-ray powder patterns of grains subsequently extracted from a polished thick section failed to produce a match with any inorganic compound listed in the ICDD Powder Diffraction File. It was during this initial phase of the mineralogical study of pringléite that ruitenbergitte was discovered by the first author. Routine X-ray powder diffraction of supposed "pringléite" grains in a polished thick section uncovered another calcium borate chloride, chemically identical to pringléite, but with a

distinctly different X-ray powder pattern. A full mineralogical investigation of both phases was initiated, and the resultant data are reported herein. It should be noted that, although quantitative electron-microprobe analyses clearly indicated the chemical identity of the two species, it was not until the crystal-structure studies of both minerals had been completed that it was proven that the two minerals are polymorphs.

Pringléite (pronounced PRINGLAIT) is named for Gordon J. Pringle, mineralogist at the Geological Survey of Canada, Ottawa, Ontario. Mr. Pringle, a native of New Brunswick, has made important contributions both to Canadian mineralogy and to the study of minerals by electron-microprobe analysis.

Ruitenbergitte (pronounced RÜ.TĚ.N.BÖRGAIT) is named for Dr. Arie A. Ruitenbergitte, geologist at the Geological Surveys Branch, New Brunswick Department of Natural Resources, Sussex, New Brunswick. Dr. Ruitenbergitte has made many significant contributions to the mineral industry in the province of New Brunswick.

Both new minerals and their names were approved by the Commission on New Minerals and Mineral Names, I.M.A. Holotype material for both minerals, consisting of one $5.5 \times 4.5 \times 2$ cm hand specimen, two polished thick sections, a polished thin section and one vial of loose material, are housed in the Systematic Reference Series of the National Mineral Collection of Canada (NMCC) at the Geological Survey of Canada, Ottawa, Ontario, under catalogue number 66920. Additional parts of the holotype for pringleite, consisting of the crystals used for a study of its optical properties and the crystal-structure analysis, as well as a $5 \times 2 \times 1$ cm specimen and 1 g of loose material, are housed in the Display Series of the NMCC at the Canadian Museum of Nature, Ottawa, Ontario, under catalogue number 82047.

OCCURRENCE AND ASSOCIATED MINERALS

The general geology of the Sussex, New Brunswick evaporite deposits is described by Roulston & Waugh (1981). The deposits are of Mississippian age and occur in the Windsor Group of the Moncton sub-basin, a part of the northeasterly trending Fundy epigeosyncline. Roulston & Waugh (1981) described a suite of borate minerals that occur in the separate, but closely related, Penobsquis and Salt Springs deposits. Most of the borate minerals reported by them occur in the Middle Halite member of the evaporite sequence and include the following: boracite, colemanite, danburite, hilgardite, howlite, hydroboracite, priceite, szaibelyite, ulexite, veatchite and volkovskite. The discovery of borate mineral assemblages at Sussex, New Brunswick, has generated considerable interest within the mineralogical community; to date, it has resulted in a detailed study of the mineralogy of hilgardite-4M (Rachlin *et al.* 1986), a redefinition of volkovskite (Mandarino *et al.* 1990) and the description of the new mineral trembathite (Burns *et al.* 1992).

Pringleite, megascopically visible as brightly reflecting cleaved surfaces, and ruitenbergitte are minor constituents in the holotype hand specimen, which is composed principally of halite and hilgardite-1A, with minor sylvite and traces of anhydrite, quartz and clays. The sample was collected from a middle ore salt horse at the 1900-3 East tailings ramp, 184 Section, Potash Company of America mine, located at Penobsquis, near Sussex, New Brunswick, at latitude $45^{\circ}45'N$ and longitude $65^{\circ}15'W$. Stratigraphically, the sample is from the Potash Member of the Cassidy Lake Formation.

Ruitenbergitte seems to be much less common than the associated pringleite and has only been found as a single grain in a polished thick section. Both new minerals are considered to have been derived from the evaporitic sequence and are probably primary phases that have been recrystallized.

OPTICAL PROPERTIES

Optical measurements for both minerals were made with a spindle stage using Na gel-filtered light (λ 589.9 nm). Pringleite is biaxial positive, α 1.537(1), β 1.548(1), γ 1.570(1); $2V_{\text{meas}}$ 77(1) $^{\circ}$, $2V_{\text{calc}}$ 71.4 $^{\circ}$. There is no pleochroism, but there is strong dispersion, $r \ll v$. The orientation of the indicatrix is $X = c$, $Y : a = 40^{\circ}$ in γ acute, and $Z : b = 46^{\circ}$ in γ obtuse. Twinning is rare, but simple twinning was observed in polished thin section. Ruitenbergitte is nonpleochroic, biaxial positive, α 1.542(1), β 1.545(1), γ 1.565(1); $2V_{\text{meas}}$ 47(1) $^{\circ}$, $2V_{\text{calc}}$ 42.5 $^{\circ}$. The quality of the dispersion is unknown, as we were unable to obtain a centered optic axis figure. The orientation of the indicatrix is $X = b$, $Y : a = 25^{\circ}$ in β obtuse, and $Z = c$. Both minerals are colorless in transmitted light, and their characteristic medium polish, frosted appearance, and a distinctive blue-grey color distinguish them from associated hilgardite-1A and halite in reflected light.

PHYSICAL PROPERTIES

In hand specimen, pringleite has been observed as colorless to orange, platy, subhedral to anhedral, brightly reflecting cleaved aggregates up to 4 mm in size, in and around rosettes of white opaque hilgardite-1A, and also associated with dull orange massive halite. The presence of hilgardite-1A has been confirmed by crystal-structure analysis, results of which will be published later. A thin section study shows that the cleavage planes of pringleite are, in turn, the host for numerous small inclusions of hilgardite-1A. Individual crystals of pringleite, up to 2 mm in size, are platy to prismatic and are subhedral to anhedral. They are brittle, possess a good {110} cleavage, and have an even to slightly conchoidal fracture. Crystal forms were not sufficiently developed to be measured by optical goniometer. The color varies from colorless to very pale yellow, but may appear to be orange in hand specimen owing to underlying masses of halite. The streak of pringleite is white, its luster is vitreous, aggregates are translucent, and individual crystals are transparent; it is nonfluorescent under both long- and short-wave ultraviolet light. A SEM back-scatter photomicrograph of several pringleite grains in polished thick section is presented in Figure 1. The mineral is easily scratched by a needle; the hardness is estimated to be between 3 and 4. The measured density, determined by heavy liquid methods using petroleum-ether-diluted bromoform, is 2.22(1) g/cm 3 . Two of the grains, dug out of a polished thick section and used for the determination of density, were confirmed to be pringleite by means of Gandolfi X-ray powder camera study. The measured density is about 5% higher than the calculated density of 2.11 g/cm 3 ; this is ascribed to a small amount of admixed hilgardite-1A, which has a calculated density of 2.67 g/cm 3 , but

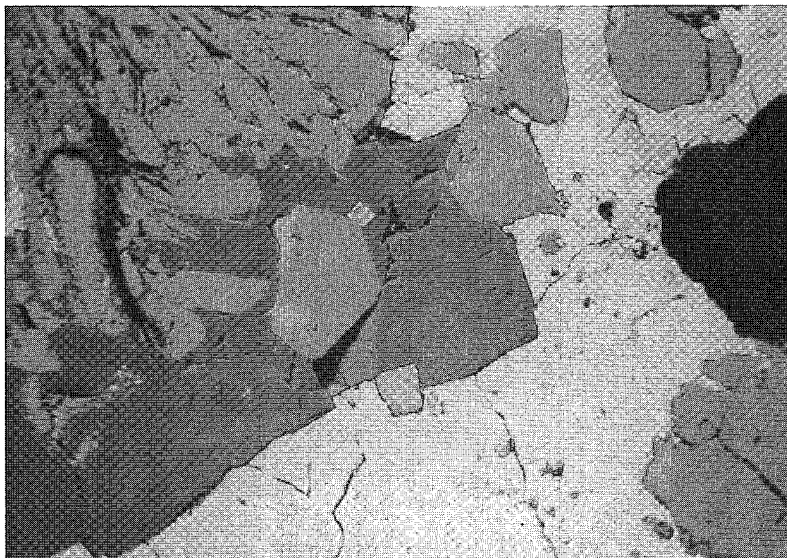


FIG. 1. SEM back-scatter photomicrograph of a polished thick section containing pringleite (dark grey), hilgardite-1A (medium grey) and halite (white). Field of view is approximately 2 mm.

it was not detected in the Gandolfi X-ray films. Twinning was not observed megascopically or in the X-ray single-crystal investigation, but simple twinning was observed in polished thin section, although it is very rare.

Ruitenbergitte has been found only in one polished thick section, where it occurs as a single 7×4 mm anhedral grain, associated with hilgardite-1A, halite and pringleite. This grain is also the host to numerous 0.5-mm inclusions of hilgardite-1A. Ruitenbergitte is megascopically indistinguishable from pringleite and was accidentally encountered during preliminary X-ray powder-diffraction studies of supposed "pringleite" grains. As far as we can determine, the physical properties of ruitenbergitte match those listed above for pringleite. The only exception is the cleavage, which is $\{100\}$, good. A measured specific gravity was unobtainable due to a dearth of pure inclusion-free material. In summary, the two polymorphs are physically and chemically identical and can be reliably distinguished only by detailed optical, X-ray powder or X-ray single-crystal study.

CHEMISTRY

Several grains of pringleite and the single grain of ruitenbergitte were chemically analyzed with a Cameca SX-50 electron microprobe utilizing an operating voltage of 10 kV, a 20 nA beam current, a 20- μ m spot

size, a counting time of 20 seconds per element and the PAP correction program (Pouchou & Pichou 1984). The following standards were employed for both minerals: wollastonite (Ca), priceite (B) and halite (Cl). An on-line overlap-correction procedure developed at the GSC was used to correct for the overlap of Cl on B. An energy-dispersion spectrum indicated the absence of elements with atomic number greater than 9 other than those reported here; Mg, Mn, Fe and F were specifically sought, but not found. A dearth of pure inclusion-free material prevented the chemical determination of H_2O for either phase; it was calculated by difference. Quantitative values for both H_2O and (OH) were determined from bond-valence calculations derived from the crystal-structure analyses of both minerals (Grice *et al.* 1994). The simplified formula for both pringleite and ruitenbergitte, based on their crystal structures, is $Ca_9B_{26}O_{34}(OH)_{24}Cl_4 \cdot 13H_2O$, which requires: CaO 25.62, B_2O_3 45.93, Cl 7.20, H_2O 22.87, sum 101.62, less O=Cl 1.62, total 100.00 wt.%. Both minerals are insoluble in cold H_2O and dilute HCl.

The average of five electron-microprobe analyses for pringleite gave CaO 26.29(11), B_2O_3 46.75(23), Cl 6.48(29), H_2O [21.94], sum 101.46, less O=Cl 1.46, total [100.00] wt.%. With (O+Cl)=75, the empirical formula is $Ca_{9.27}B_{26.56}O_{34.98}(OH)_{24.64}Cl_{3.62} \cdot 11.76 H_2O$. The average result of two electron-microprobe analyses for ruitenbergitte gave CaO 26.33(8), B_2O_3

46.72(21), Cl 6.28(3), H₂O [22.09], sum 101.42, less O=Cl 1.42, total [100.00] wt.%. With (O+Cl)=75, the empirical formula is Ca_{9.27}B_{26.51}O_{34.97}(OH)_{24.63}Cl_{3.50}·11.90 H₂O.

TABLE 1. X-RAY POWDER DATA FOR PRINGLEITE

est.	dÅmeas.	dÅcalc.	hkl	est.	dÅmeas.	dÅcalc.	hkl
20	12.71	12.76	010				
		9.33	001			2.477	422
70	9.21	9.07	110	10	2.472	2.476	332
		8.37	011			2.473	152
5	8.34	8.30	101	5	2.449	2.449	423
100	7.69	7.69	111			2.449	511
		6.40	111			2.432	114
10	6.38	6.39	111	10	2.428	2.425	512
5	6.24	6.24	200	5	2.387	2.384	402
5	5.87	5.84	021	20	2.364	2.364	441
		5.74	111	5	2.344	2.346	024
60	5.74	5.73	201	5	2.344	2.341	204
5	5.01	5.00	121	10	2.315	2.316	442
20	4.78	4.77	201	5	2.299	2.299	313
40	4.63	4.63	221	20	2.364	2.279	223
5	4.52	4.53	220	5	2.274	2.268	440
		4.40	121			2.255	114
10	4.40	4.39	220	10	2.253	2.253	114
5	4.26	4.25	030			2.252	352
		4.18	022	5	2.227	2.227	532
20b	4.17	4.15	202			2.208	350
		4.14	131	30b	2.199	2.198	242
		4.07	130			2.197	513
20b	4.07	4.06	311	10	2.171	2.194	440
10	3.96	3.99	130			2.170	334
10	3.90	3.91	310	20	2.137	2.137	441
35	3.845	3.846	222	10	2.117	2.135	441
5	3.746	3.737	112			2.117	114
20	3.687	3.686	221			2.102	261
20	3.551	3.546	132	15	2.097	2.100	531
5	3.498	3.500	312			2.100	062
		3.451	022			2.100	424
10	3.430	3.432	320	10	2.073	2.074	404
		3.425	202			2.072	441
5	3.290	3.302	231	30	2.058	2.064	152
		3.295	322			2.056	602
20	3.196	3.202	312	25	2.031	2.033	043
5	2.993	2.994	223	5	2.011	2.032	512
10	2.918	2.918	042			2.012	403
		2.879	240			1.998	243
5b	2.872	2.867	402	15b	1.987	1.989	061
5	2.841	2.845	133			1.984	442
25	2.799	2.803	240	5	1.957	1.981	423
5	2.749	2.751	241			1.957	154
5	2.715	2.739	132	10	1.944	1.946	063
25	2.660	2.662	331			1.944	263
10	2.623	2.623	241	10b	1.918	1.930	225
5	2.588	2.590	421			1.923	444
15	2.562	2.586	203			1.921	262
		2.564	333			1.913	623
5	2.532	2.535	223			1.911	503
		2.532	511	15b	1.892	1.902	314
5	2.498	2.500	242			1.901	352
		2.499	151	10	1.860	1.891	622
				5	1.836	1.889	261
						1.858	621
						1.836	172
						1.825	334
				20b	1.820	1.814	550
						1.809	153

114.6 mm Gandolfi camera; Co radiation, Fe filter (λ CoK α 1.79021 Å) pattern run at CANMET by Mr. Paul Carrière. Intensities estimated visually; b = broad line not corrected for shrinkage and no internal standard used indexed on a 12.759, b 13.060, c 9.733 Å, α 102.14°, β 102.03°, γ 85.68°

Calculations using the Gladstone–Dale relationship and using constants reported by Mandarino (1981) yield $1-(K_p/K_c) = -0.046$ for pringleite and -0.042 for ruitenbergitte. These values indicate good compatibility between the physical and chemical data (Mandarino 1981).

X-RAY CRYSTALLOGRAPHY

Both minerals were examined by precession single-crystal methods employing Zr-filtered Mo radiation. Pringleite is triclinic, with permissible space-groups $P1(1)$ or $\bar{P}1(2)$ (diffraction aspect P^*). The correct space-group is $P1$ on the basis of the crystal-structure determination (Grice *et al.* 1994). The refined unit-cell parameters, a 12.759(6), b 13.060(5), c 9.733(4) Å, α 102.14(4)°, β 102.03(3)°, γ 85.68(4)°, V 1550(1) Å³, $a:b:c$ 0.9769:1.07452, are based on 23 uncorrected X-ray powder lines between 3.845 and 1.836 Å for which unambiguous indexing was possible. This cell can be related to a C -centered pseudomonoclinic cell with unit-cell parameters a 18.90, b 17.51, c 9.73 Å, β 107° by the transformation [110/ $\bar{1}$ 10/001]. A fully indexed Gandolfi powder pattern is presented in Table 1. All indexed reflections were checked on single-crystal precession films and were also confirmed by examination of powder-pattern intensities calculated using the refined crystal-structure parameters.

Ruitenbergitte is monoclinic, with permissible space-groups $P2_1(4)$ and $P2_1/m(11)$ (diffraction aspect $P2_1/m^*$). The correct space-group is $P2_1$ on the basis of the crystal-structure determination (Grice *et al.* 1994). The refined unit-cell parameters, a 19.88(1), b 9.715(4), c 17.551(9) Å, β 114.85(4)°, V 3077(3) Å³, $a:b:c$ 2.046:1:1.807, are based on 22 uncorrected X-ray powder lines between 4.087 and 1.886 Å for which unambiguous indexing was possible. A fully indexed Gandolfi powder pattern is presented in Table 2. All indexed reflections were checked by the two methods described above for pringleite. As indicated earlier, the triclinic pringleite has a pseudomonoclinic C -centered cell. This forms the substructure for the monoclinic cell of ruitenbergitte. The two polymorphs are related by the transformation matrix [101/ $\bar{1}$ 01/010] (*i.e.*, triclinic to monoclinic).

The powder data for both minerals are unique and bear no resemblance to each other nor to any other inorganic phase listed in the Powder Diffraction File. With $Z = 1$, the calculated density for pringleite with the simplified formula is 2.11 g/cm³. With $Z = 2$, the calculated density for ruitenbergitte with the same simplified formula is 2.13 g/cm³.

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TABLE 2 X-RAY POWDER DATA FOR RUITENBERGITE

Test.	d _{meas.}	d _{calc.}	hkl	Test.	d _{meas.}	d _{calc.}
20	15.4	15.6	101	10	2.518	2.517
60	9.03	9.02	200	25	2.493	2.491
100	8.56	8.55	110	5	2.470	2.475
5	6.87	6.90	211	5	2.438	2.438
70	6.62	6.61	210	20	2.402	2.397
3	6.38	6.36	102			2.345
		6.16	012	10	2.345	2.341
30b	6.14	6.09	212	5	2.283	2.277
5	5.33	5.32	112	5	2.264	2.262
10	5.23	5.24	312	10	2.245	2.243
30	5.12	5.11	310	5	2.219	2.215
5	4.86	4.86	020			2.197
		4.69	120	25	2.197	2.197
5	4.66	4.66	013	15	2.173	2.172
		4.65	021			2.139
10	4.47	4.46	212	30b	2.134	2.139
20	4.39	4.38	312			2.130
10	4.27	4.28	220	10	2.099	2.099
30	4.09	4.09	410			2.078
5	3.99	3.98	004	25	2.075	2.073
10	3.909	3.909	404			2.063
30	3.786	3.779	320	5	2.058	2.053
30	3.493	3.489	222	30	2.037	2.039
5	3.447	3.452	322			2.011
10	3.379	3.383	510	5	2.009	2.004
5	3.262	3.256	224	25	1.984	1.983
		3.194	324	10	1.970	1.969
10	3.182	3.187	130	5	1.954	1.956
		3.171	131	5	1.941	1.943
5	3.104	3.109	304			1.932
5	3.044	3.048	230	10	1.929	1.931
3	2.958	2.961	314	15	1.909	1.909
		2.897	520			1.890
30	2.890	2.886	132	10	1.886	1.885
		2.884	124			
		2.851	330			
10	2.844	2.843	324			
20	2.802	2.801	106			
		2.766	422			
15	2.765	2.763	306			
10	2.696	2.692	116			
		2.658	316			
10	2.655	2.651	714			
25	2.631	2.631	430			
15	2.563	2.561	016			

- 114.6 mm GandoIfi camera; Co radiation, Fe filter ($\lambda_{\text{CoK}\alpha}$ 1.79021 Å)
 - pattern run at CANMET by Mr. Paul Carrière
 - intensities estimated visually; b = broad line
 - not corrected for shrinkage and no internal standard used
 - indexed on a 19.88, b 9.715, c 17.551 Å, β 114.85°

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