



Article

Škachaite, $\text{CaCo}(\text{CO}_3)_2$, a new member of the dolomite group, from the Brod deposit near Příbram, Czech Republic

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Abstract

Škachaite (IMA2022–143) is a new mineral species discovered in samples from the hydrothermal vein B117, shaft No. 6 at the Brod deposit of the uranium and base-metal Příbram ore district, central Bohemia, Czech Republic. Škachaite is a Co-dominant member of the dolomite group and forms anhedral grains up to 50 μm in size and as 20–100 μm thick growth zones in škachaite–dolomite crystals as a part of carbonate (dolomite, calcite, siderite, spherocobaltite, ankerite, kutnohorite and minrecordite) gangue, associated with native silver, sulfides and arsenides. Škachaite is pale to bright pink with vitreous lustre. The Mohs hardness is ca. 3½–4, similar to other members of the dolomite group. The calculated density is 3.140 $\text{g}\cdot\text{cm}^{-3}$. Škachaite is optically uniaxial (–); the indices of refraction are $\omega = 1.741(3)$ and $\epsilon = 1.535(3)$. On the basis of electron-microprobe analyses, its empirical formula is $\text{Ca}_{1.00}(\text{Co}_{0.45}\text{Mg}_{0.38}\text{Ca}_{0.08}\text{Fe}_{0.05}\text{Mn}_{0.03}\text{Zn}_{0.01})_{\Sigma 1.00}(\text{CO}_3)_2$. The ideal formula is $\text{CaCo}(\text{CO}_3)_2$, which requires (in wt.%) CaO 25.60, CoO 34.21, CO_2 40.19, a total of 100.00. Škachaite is trigonal, $R\bar{3}$, with unit-cell parameters $a = 4.8177(18)$, $c = 16.093(7)$ Å, $V = 323.5(2)$ Å³ and $Z = 3$. The strongest reflections of the calculated powder X-ray diffraction pattern [d , Å, (I_{rel} , %) hkl] are: 3.704 (13) 10 $\bar{2}$; 2.896 (100) 104; 2.409 (15) 110; 2.019 (17) 202; 1.812 (19) 10 $\bar{8}$; and 1.792 (16) 11 $\bar{6}$. According to the single-crystal X-ray diffraction data ($R_1 = 0.0304$ for 94 reflections with $[I > 3\sigma(I)]$), the crystal structure of škachaite is isotypic with its Mg-analogue, dolomite. The Raman spectrum of škachaite, as well as the tentative assignment of observed bands, are given in this paper. The mineral is named in honour of Pavel Škacha, a Czech mineralogist and curator of the mineralogical collection of the Mining Museum Příbram, Czech Republic.

Keywords: škachaite; new mineral; carbonate; cobalt; dolomite group; crystal structure; Brod deposit; Příbram ore area; Czech Republic

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Introduction

During our long-term systematic mineralogical research on the Příbram ore area in the Czech Republic (Sejkora *et al.*, 2021, 2022; Škacha *et al.*, 2017, 2018, 2021; Dolníček *et al.*, 2023), we also focused attention on the study of the unique bonanza-type silver mineralisation of hydrothermal vein B117 of the Brod deposit. As part of this research, we identified a new species, a Co-dominant member of the dolomite group. In this paper, we report its description.

The new mineral is named škachaite in honour of Pavel Škacha (born 1981), a Czech mineralogist and curator of the mineralogical collection of the Mining Museum Příbram, Czech Republic. Pavel Škacha is the author of over sixty publications in the field of mineralogy and the history of mining, including the description of more than twelve new mineral species, especially from the Příbram ore area and from the Jáchymov ore district, Czech Republic. The new mineral and its name were

approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA2022–143, Sejkora *et al.*, 2023). Its mineral symbol, in accordance with Warr (2021), is Škác. The holotype material (polished section) of škachaite is deposited in the collections of the Department of Mineralogy and Petrology, National Museum in Prague, Cirkusová 1740, 193 00 Praha 9, Czech Republic, under the catalogue number P1P 52/2022. This polished section was taken from a large sample deposited in the same collection under catalogue number P1N 49.308. Another polished section (cotype) is deposited in the collection of the Mining Museum Příbram, Czech Republic (catalogue number 1/2024).

Occurrence and mineral description

Occurrence

Škachaite has been found in samples from the hydrothermal vein B117 between the 5th–6th level (depth 250–300 m below surface) of shaft No. 6 – Brod southeast of Příbram. In the period 1950–1991, this mine was one of the shafts open to the shallow parts of the Brod deposit, which belongs to the uranium and base-metal Příbram ore district, central Bohemia, Czech Republic (Komínek, 1995). The GPS coordinates for the occurrence of

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škáchaite are 49°40'5.094"N, 14°1'13.809"E. The uranium and base-metal Příbram ore district and the neighbouring Březové Hory ore district form the two main parts of the Příbram ore area.

The Příbram uranium and base-metal district represents the most significant accumulation of vein-type hydrothermal U ores in the Czech Republic. The hydrothermal U-mineralisation of late Variscan age is related to a 1–2 km wide and almost 25 km long zone formed by a strongly tectonised series of Upper Proterozoic sedimentary rocks along the contact with granitoids of the Devonian–Carboniferous Central Bohemian Plutonic Complex (Litochleb *et al.*, 2003). A complete list of over 320 minerals identified to date from this area is given on mindat.org at <http://www.mindat.org/loc-779.html>.

The holotype polished section of the new mineral was taken from a museum specimen (National Museum Prague, catalogue number P1N 49.308) with dimensions 45 × 42 × 13 cm, which represents the complete profile through a 22 cm thick symmetrical vein filling, also including surrounding rock (Fig. 1). This unique sample of bonanza-type silver mineralisation contains abundant elongated native silver aggregates up to 6 cm in length in gangue formed by various types of carbonates: calcite, siderite, spherocobaltite, ankerite, kutnohorite, minrecordite and members of the dolomite–škáchaite series. Other associated minerals are safflorite, löllingite, cobaltpentlandite, Co-analogue of heazlewoodite, siegenite, carrollite, mckinstryite, jalpaite, chalcocite, tetrahedrite-(Zn), argentotetrahedrite-(Fe), not yet approved 'argentotennantite-(Fe)' (IMA2023-126 under voting), hematite, sphalerite, galena, chalcopyrite, pyrite and hisingerite (Litochleb *et al.*, 2002). Škáchaite is of low-temperature hydrothermal origin.

Physical and optical properties

Škáchaite occurs as anhedral grains up to 50 µm in size and growth zones in škáchaite–dolomite zoned crystals (Fig. 2) with thickness up to 100 µm but usually only 5–20 µm. Škáchaite is pale to bright pink in colour; tiny fragments are translucent. The mineral has a white streak and vitreous lustre. It does not

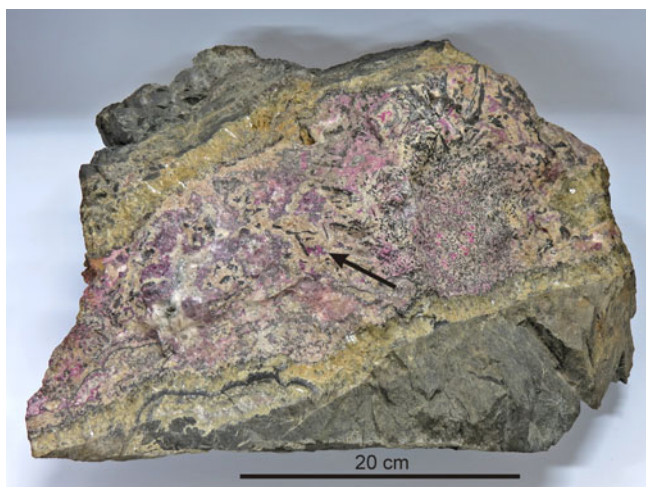


Figure 1. Overall photo of symmetrical vein filling with abundant elongated native silver aggregates up to 6 cm in length in gangue formed by various types of carbonates – calcite, siderite, spherocobaltite, ankerite, kutnohorite, minrecordite and members of the dolomite–škáchaite series (catalogue number P1N 49.308, mineralogical collection of the National Museum Prague); vein B117, Brod deposit, the uranium and base-metal Příbram ore district (Czech Republic). The holotype of škáchaite was taken from a central part of the sample with bright pink carbonate aggregates.

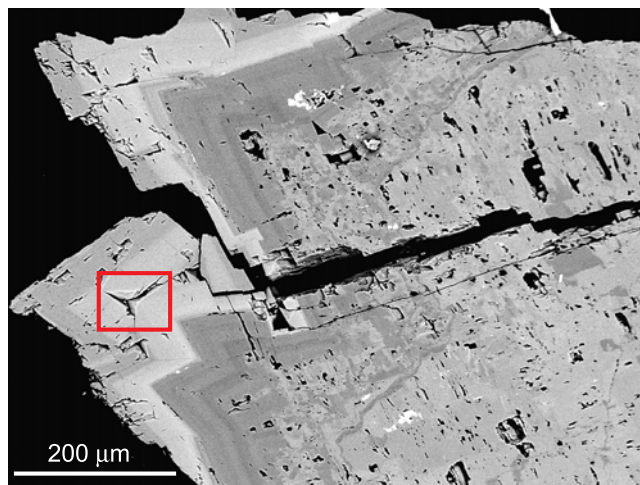


Figure 2. Back-scattered electron image of holotype material (P1P 52/2022) – zoned škáchaite-dolomite crystals. Škáchaite zones are white, whereas dolomite (with variable Mg/Co/Fe ratios) is grey. The red box indicates the area used for the single-crystal X-ray diffraction study.

fluoresce under either short- or long-wave ultraviolet light. The mineral is brittle, cleavage on {10 $\bar{1}$ 1} is perfect; the Mohs hardness cannot be measured due to the small size of škáchaite grains and may be close to 3½–4, similar to other members of the dolomite group. The density could not be measured directly because of the small amount of available material. The calculated density is 3.140 g/cm³ based on the empirical formula and unit-cell volume from single-crystal data.

In thin section, škáchaite is pink with a distinct rhombohedral cleavage. It is optically uniaxial (–), with $\omega = 1.741(3)$ and $\epsilon = 1.535(3)$ (measured at 589 nm). Škáchaite is not pleochroic and has hints of undulatory extinction. The Gladstone–Dale compatibility index, $1 - (K_p/K_c)$, is –0.050 for the empirical formula and unit-cell parameters from single-crystal data, indicating good compatibility (Mandarino, 1981).

Chemical composition

Chemical analyses were performed using a Cameca SX100 electron microprobe operating in wavelength-dispersive mode (15 kV, 10 nA and 3 µm beam size). The following standards and X-ray lines were used to minimise line overlaps: Co (CoK α), diopside (MgK α), hematite (FeK α), rhodonite (MnK α), wollastonite (CaK α) and ZnO (ZnK α). Peak counting times were 20 s for all elements and 10 s for each background. Contents of other measured elements (Al, Ba, Cu, Na, Ni, P, Pb, Si and Sr) were always below detection limits. Matrix correction using the PAP algorithm (Pouchou and Pichoir, 1985) was applied to the data (measured oxides and calculated amount of CO₂ resting to analytical sum of 100 wt.%). Carbonate content could not be analysed directly because of the minute amount of material available; it was confirmed by Raman spectroscopy and single-crystal structure study and calculated by stoichiometry based on the ideal content of two CO₃ groups in the crystal structure of dolomite-group minerals.

The chemical composition (mean of eleven analyses) of the škáchaite grain used for the single-crystal study (holotype polished section) is given in Table 1. Individual point analyses (Supplementary Table S1) show a Co-dominant character

Table 1. Chemical composition (in wt.%) of škáchaite

Element	Mean	Range	S.D.
CaO	29.59	28.78–30.28	0.42
FeO	1.61	1.27–2.09	0.23
MgO	7.55	6.83–8.14	0.41
CoO	16.32	15.17–17.56	0.69
MnO	1.19	0.89–1.54	0.19
ZnO	0.23	0.00–0.42	0.12
CO ₂ *	42.90	42.21–43.34	0.34
Total	99.39		

* CO₂ content was calculated on the basis of two CO₃ groups present in the crystal structure of dolomite-group minerals.

S.D. – standard deviation

(0.41–0.49 apfu) with Mg (0.35–0.41 apfu) and minor Fe (0.04–0.06 apfu), Mn (0.03–0.05 apfu) and Zn (up to 0.01 apfu). On the basis of Σ cations = 2 atoms per formula unit (apfu), the average empirical formula is Ca_{1.00}(Co_{0.45}Mg_{0.38}Ca_{0.08}Fe_{0.05}Mn_{0.03}Zn_{0.01})_{Σ1.00}(CO₃)₂. The ideal formula is CaCo(CO₃)₂, which requires (in wt.%) CaO 25.60, CoO 34.21, CO₂ 40.19, a total 100.00.

Škáchaite was also determined in another 26 polished sections (taken from the same museum sample) usually in thin (units to tens μm) zones in škáchaite–dolomite grains. In the chemical analyses (Supplementary Table S2), the predominant Co (0.35–0.59 apfu) is accompanied by Mg (0.17–0.44 apfu), Fe (0.03–0.31 apfu), Mn (0.01–0.12 apfu) and minor Ni and Zn up to 0.06 and 0.03 apfu, respectively.

Raman spectroscopy

The Raman spectra of škáchaite were collected in the range 50–4000 cm⁻¹ using a DXR dispersive Raman Spectrometer (Thermo Scientific) mounted on a confocal Olympus microscope. The Raman signal was excited by an unpolarised red 633 nm He–Ne gas laser and detected by a CCD detector. The experimental parameters were: 100× objective, 10 s exposure time, 100 exposures, 50 μm pinhole spectrograph aperture and 8 mW laser power level. The eventual thermal damage of the measured points was excluded by visual inspection of the excited surface after measurement, observation of possible decay of spectral features at the start of excitation and checking for thermal downshift of Raman lines. The instrument was set up by a software-controlled calibration procedure using multiple neon emission lines (wavelength calibration), multiple polystyrene Raman bands (laser frequency calibration) and standardised white-light sources (intensity calibration). Spectral manipulations were performed using *Omnic 9* software (Thermo Scientific).

The Raman spectrum of škáchaite is given in Fig. 3. The main bands observed are (in wavenumbers): 1748, 1437, 1094, 723, 294 and 173 cm⁻¹. The experimental spectrum of škáchaite agrees very well with published Raman spectra of dolomite (e.g. Gillet *et al.*, 1993; Perrin *et al.*, 2016). The strong band at 1094 cm⁻¹ is attributed to the symmetric stretching vibration (ν_1) and the band at 1437 cm⁻¹ to the asymmetric stretching vibration (ν_3) of (CO₃)²⁻ groups. A band at 723 cm⁻¹ is assigned to the in-plane bending vibration (ν_4). The out-of-plane bending vibration (ν_2) is inactive in the Raman spectrum, while its overtone (2 ν_2) is observed at 1748 cm⁻¹. The bands below 300 cm⁻¹ (294 and 173 cm⁻¹) are attributed to lattice modes.

X-ray diffraction data

Single-crystal X-ray studies were carried out on a thin growth zone retrieved from a larger fragment identified by wavelength-

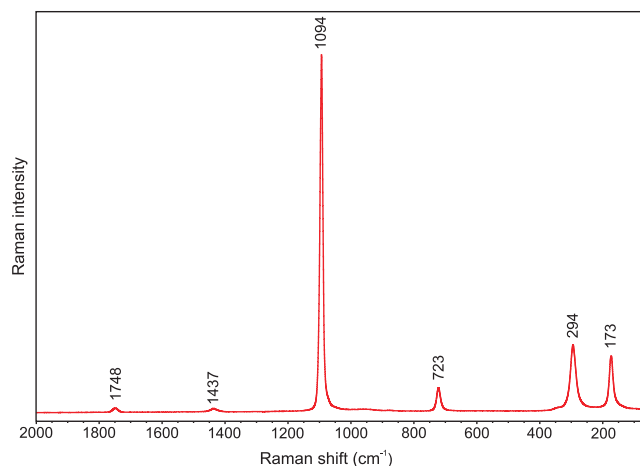


Figure 3. Raman spectrum of škáchaite.

dispersive spectroscopy (WDS), which was selected to be tested on a Rigaku SuperNova single-crystal diffractometer equipped with the Atlas S2 CCD detector (microfocused MoK α radiation). The approximate dimensions of the fragment are 0.06 × 0.01 × 0.01 mm and the diffraction experiment yielded the following data: trigonal space group $R\bar{3}$ (no. 148), $a = 4.8177(18)$, $c = 16.093(7)$ Å, $V = 323.5(2)$ Å³ and $Z = 3$. The $c:a$ ratio calculated from unit cell parameters is 3.3404. The intensity data for škáchaite were processed using the Rigaku *CrysAlis* package, including applying an empirical multi-scan absorption correction (Rigaku, 2019). The structure was solved using the intrinsic phasing algorithm of the *SHELXT* program (Sheldrick, 2015). Refinement proceeded by full-matrix least-squares on F^2 using *Jana2020* (Petříček *et al.*, 2023). A reverse–obverse twinning (Table 2) was taken into account during the refinement in *Jana* (see Petříček *et al.*, 2016). The anisotropic structural model converged to $R_1 = 0.0304$ for 94 reflections with $F_o > 3\sigma(F_o)$ for 20 refined parameters, including site-occupancy refinement for Mg/Co. The final refinement returned site occupancies of Co_{0.503} and Mg_{0.497}; the corresponding site scattering 19.5 e^- is in line with those obtained from the WDS (20.7 e^-). Details of data collection and refinement are given in Table 2. Fractional atomic coordinates and equivalent isotropic displacement parameters are reported in Table 3 and selected bond-distances and polyhedral volumes in Table 4. Anisotropic displacement parameters are reported in the crystallographic information file (cif) deposited with the Principal Editor of *Mineralogical Magazine* and available as Supplementary material (see below).

Powder X-ray diffraction data could not be collected due to the paucity of available material. The experimental pseudo-Gandolfi scan was attempted to be collected, but the observed intensities were extremely weak. This is most probably due to the small volume of diffracting material (see the crystal dimensions). Consequently, powder X-ray diffraction data, given in Table 5, were calculated using the software *PowderCell 2.3* (Kraus and Nolze, 1996) and based on the structural model given in Tables 2 and 3.

Crystal structure of škáchaite

The crystal structure of škáchaite is proven (as expected) to be isotypic with dolomite. The study of Perchiazzi *et al.* (2018) based on samples from the Tenke–Fungurume district, Democratic Republic of Congo, documented the then maximum Co

Table 2. Crystal data and refinement details for škáchaite.

Crystal data	
Formula derived from refinement	Ca(Co _{0.503} Mg _{0.497})(CO ₃) ₂
Unit cell parameters	
<i>a</i> (Å)	4.8177(18)
<i>c</i> (Å)	16.093(7)
<i>V</i> (Å ³)	323.5(2)
<i>Z</i>	3
Space group	<i>R</i> $\bar{3}$
<i>D</i> _{calc} (g cm ⁻³)	3.108
Data collection	
Temperature (K)	296
Wavelength	MoK α , 0.71073 Å
Crystal dimensions (mm)	0.061 × 0.014 × 0.013
Collection mode	ω scans to fill an Ewald sphere
Frame width, counting time	1.0, 400 s
Limiting θ angles; completeness to θ_{\max}	3.80–28.30°; 0.71
Limiting Miller indices	–2 < <i>h</i> < 5, –4 < <i>k</i> < 3, –17 < <i>l</i> < 16
No. of reflections	167
No. of independent reflections	127
No. of observed reflections (criterion)	94 [<i>I</i> > 3 σ (<i>I</i>)]
Absorption correction (mm ⁻¹), method	3.35, multi-scan
<i>T</i> _{min} / <i>T</i> _{max}	0.884/1
<i>R</i> _{int}	0.015
<i>F</i> ₀₀₀	298
Refinement	
Refinement	by <i>Jana2020</i> on <i>F</i> ²
Parameters, constraints, restraints	20, 2, 0
<i>R</i> ₁ , <i>wR</i> ₂ (obs)	0.0304, 0.0375
<i>R</i> ₁ , <i>wR</i> ₂ (all)	0.0418, 0.0437
GOF (obs, all)	0.98, 1.01
Weighting scheme, weights	$\sigma, 1/(\sigma^2(I) + 0.000004I^2)$
$\Delta\rho_{\min}, \Delta\rho_{\max}$ (e Å ⁻³)	–0.32, 0.29
Twin fractions 1, 2, 3	0.637(17)/0.031(12)/0.332(12)
Twin matrices 1/2	$\begin{pmatrix} 1 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

substitution for Mg in dolomite corresponding to the formula Ca(Mg_{0.70}Co_{0.30})(CO₃)₂ (crystal named CD6). The crystal fragment (Fig. 2) investigated in the current study yielded the composition Ca(Co_{0.503}Mg_{0.497})(CO₃)₂ (and further WDS analyses have proven even more Co for some of the points measured – up to 0.59 apfu). A comparison of selected polyhedral measures and interatomic distances is given in Tables 4, 6 and 7. With the

Table 3. Atom coordinates, equivalent atomic displacement parameters (in Å²) and site-occupancies for škáchaite.

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}	Site occupancy	BVS*
A (Ca)	0	0	0	0.0126(7)	Ca _{1.00}	1.91
B (Co,Mg)	0	0	½	0.0115(7)	Co _{0.503(10)} Mg _{0.497(10)}	1.96
C	0	0	0.2431(5)	0.0133(18)	C _{1.00}	4.06
O	0.2496 (7)	–0.0304 (8)	0.2442(2)	0.0169(14)	O _{1.00}	2.33

* BVS – sum of the bond valences (in valence units) incident upon the atomic site

Table 4. Bond-distances (in Å) and polyhedral volumes (in Å³) for škáchaite in comparison with selected members of the dolomite–škáchaite series.

	Reference	A*–O (×6)	B*–O (×6)	<i>V</i> _A (Å ³)	<i>V</i> _B (Å ³)
škáchaite	This paper	2.376(3)	2.107(5)	17.82(1)	12.46(1)
CD6	Perchiazzi et al. (2018)	2.3765(9)	2.0970(9)	17.85(1)	12.29(1)
CD1	Perchiazzi et al. (2018)	2.3821(6)	2.0836(6)	17.98(1)	12.05(1)
sphercobaltite	Pertlik (1986)		2.110(1)		12.51(1)

Note: CD1 0.00 apfu Co, CD6 0.30 apfu Co.

*General formula AB(CO₃)₂, where A = Ca and B = Co and Mg.

Table 5. Calculated powder X-ray diffraction data for škáchaite.*

<i>l</i> _{calc}	<i>d</i> _{calc}	<i>h k l</i>	<i>l</i> _{calc}	<i>d</i> _{calc}	<i>h k l</i>
2	5.364	0 0 3	3	1.569	2 1 1
13	3.704	1 0 2	4	1.548	1 2 2
100	2.896	1 0 4	8	1.548	2 1 2
2	2.682	0 0 6	1	1.501	1 0 10
15	2.409	1 1 0	4	1.468	2 1 4
11	2.197	1 1 3	5	1.468	1 2 4
10	2.197	1 1 3	4	1.448	2 0 8
17	2.019	2 0 2	1	1.436	1 1 9
7	1.852	2 0 4	2	1.436	1 1 9
19	1.812	1 0 8	1	1.416	2 1 5
10	1.792	1 1 6	9	1.391	3 0 0
16	1.792	1 1 6	4	1.341	0 0 12

*Intensity and *d*_{hkl} (in Å) were calculated using the software *PowderCell2.3* (Kraus and Nolze, 1996) and based on the structural model given in Tables 2 and 3. Only reflections with *l*_{calc} > 1 are listed. The six strongest reflections are given in bold.

increasing Co-content in the dolomite-group minerals, both the unit cell parameters increase as well, with substantial increments in *a* as well as in *c* parameters (Figs 4 and 5). As has been already pointed out and discussed by Perchiazzi et al. (2018) the AO₆ octahedron is always larger than the corresponding BO₆ octahedron. Increasing the Co content, the B–O bond length (2.107(5) Å for škáchaite) and BO₆ polyhedral volume (12.46(1) Å³ for škáchaite) both increase, whereas the opposite behaviour is apparent for the AO₆ polyhedron (Table 4). Perchiazzi et al. (2018) also pointed out that with increasing Co content, the AO₆ and BO₆ octahedra behave distinctly: the AO₆ octahedron shrinks anisotropically through the shortening of its basal edges, leading to a meagre increase of the *a* cell parameter. The BO₆ octahedron instead expands, stretching both its ‘basal’ and ‘lateral’ edges (Table 6). The explanation for the anisotropic expansion of unit cell parameters of all ‘Co-dolomites’ (including škáchaite) known to date, is caused by the anisotropic variation of AO₆ and BO₆ polyhedral volumes, coupled with the presence of rigid CO₃ groups lying in the (0001) plane (Perchiazzi et al., 2018).

Discussion

Cobalt mineralogy is dominated by S and As bearing minerals, both of primary or supergene origin (Hazen et al., 2017).

Table 6. ‘Basal’- and ‘lateral’-edge dimensions (in Å) of AO₆ (Ca) and BO₆ (Co/Mg) polyhedra in selected members of the dolomite–škáchaite series.

	Reference	AO ₆ lateral	AO ₆ basal	BO ₆ lateral	BO ₆ basal
Škáchaite	This paper	3.438(6)	3.280(5)	3.018(6)	2.940(8)
CD6 *	Perchiazzi <i>et al.</i> (2018)	3.4331(13)	3.2871(13)	3.0055(11)	2.9250(14)
CD1 *	Perchiazzi <i>et al.</i> (2018)	3.4372(10)	3.2990(8)	2.9886(10)	2.9040(10)

*Note: CD1 0.00 apfu Co, CD6 0.30 apfu Co.

Table 7. Geometry of the CO₃ groups in selected members of the dolomite–škáchaite series.

	Reference	C–O (×3)	aplanarity
Škáchaite	This paper	1.282(5)	0.017(1)
CD6 *	Perchiazzi <i>et al.</i> (2018)	1.284(1)	0.016(2)
CD1 *	Perchiazzi <i>et al.</i> (2018)	1.284(1)	0.010(1)

*Note: CD1 0.00 apfu Co, CD6 0.30 apfu Co.

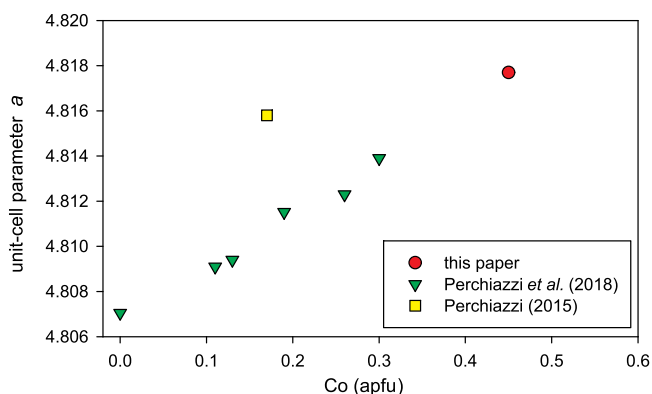


Figure 4. The correlation of unit-cell parameter *a* (in Å) and Co contents (apfu); note: composition published by Perchiazzi (2015) is based on EDS data, only (see remarks in the text).

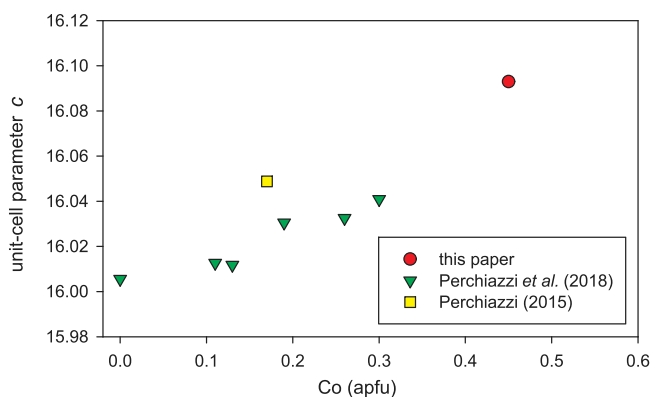


Figure 5. The correlation of unit-cell parameter *c* (in Å) and Co contents (apfu); note: composition published by Perchiazzi (2015) is based on EDS data, only (see remarks in text).

Škáchaite is only the second anhydrous Co carbonate mineral to be defined after spherocobaltite; four other known Co carbonates: comblainite, kaznakhtite, kolwezite and perchiazziite, contain hydroxyl groups or water.

Cobalt-containing dolomites have been described from several occurrences in the Central African Copperbelt (Deliens and Piret,

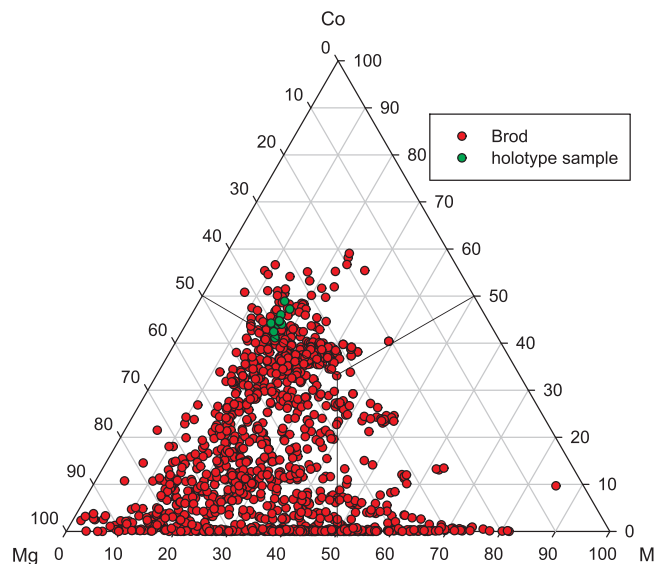


Figure 6. Chemical composition of dolomite-group minerals (~1400 point analyses) from the hydrothermal vein B117 of the Brod deposit (unpublished data of authors) in the Mg–Co–M graph (M = Fe + Mn + Zn + Cu + Ni).

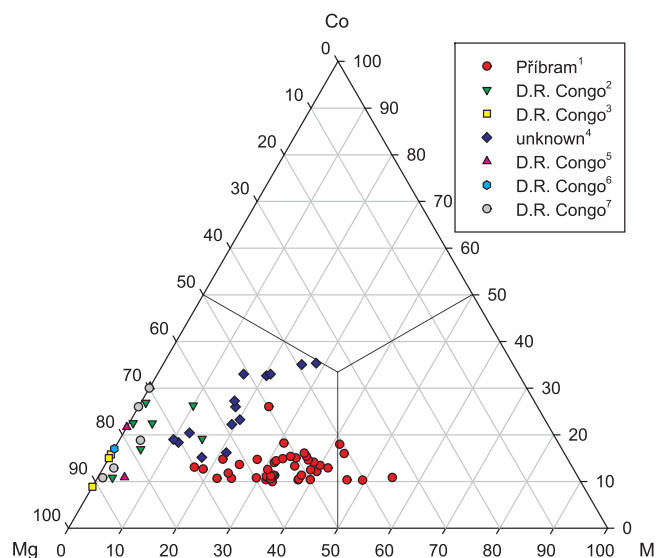


Figure 7. Chemical composition of Co-containing (with Co > 0.1 apfu) dolomite-group minerals in the Mg–Co–M graph (M = Fe + Mn + Zn + Cu + Ni); Příbram¹ – samples from other occurrences in the Příbram uranium district (unpublished data of authors), D.R. Congo² – samples from the Democratic Republic of Congo (unpublished data of authors), D.R. Congo³ – published data (Douglass, 1992, 1999); unknown⁴ – published data for unknown locality (Minceva-Stefanova, 1997); D.R. Congo⁵ – published data (Barton *et al.*, 2014); D.R. Congo⁶ – published data (Perchiazzi, 2015); D.R. Congo⁷ – published data (Perchiazzi *et al.*, 2018).

Table 8. Comparison of škáchaite and other Ca-dominant members of the dolomite group.

Mineral	Škáchaite	Dolomite	Kutnohorite	Ankerite	Minrecordite
Reference	This paper	Perchiazzi <i>et al.</i> (2018)	Peacor <i>et al.</i> (1987)	Reeder and Dollase (1989)	Garavelli <i>et al.</i> (1982)
Colour	pink	white	pink	white	white
Ideal formula	CaCo(CO ₃) ₂	CaMg(CO ₃) ₂	CaMn(CO ₃) ₂	Ca(Fe ²⁺ ,Mg)(CO ₃) ₂	CaZn(CO ₃) ₂
B _{emp} *	Co _{0.45} Mg _{0.38} Ca _{0.08} Fe _{0.05} Mn _{0.03} Zn _{0.01}	Mg _{1.00} Fe _{0.01}	Mn _{0.73} Ca _{0.27}	Fe _{0.68} Mg _{0.27} Mn _{0.05}	Zn _{0.92} Mg _{0.07} Fe _{0.03}
Space group	R $\bar{3}$	R $\bar{3}$	R $\bar{3}$	R $\bar{3}$	R $\bar{3}$
a (Å)	4.8177(18)	4.80705(9)	4.894(1)	4.8312(2)	4.8183(4)
c (Å)	16.093(7)	16.0056(4)	16.50(1)	16.1663(3)	16.0295(10)
V (Å ³)	323.5(2)	320.31(1)	342.3(3)	326.77(3)	322.28

*Note: B_{emp} – empirical occupation of BO₆ polyhedra.

1980; Fay and Barton, 2012; Van Langendonck *et al.*, 2013). Their chemical composition was studied by energy-dispersive spectroscopy (EDS) analyses (Douglass 1992, 1999; Gauthier and Deliens, 1999), which found Co contents in the B site not exceeding 0.11–0.18 apfu. Sweeney *et al.* (1986) state that samples from Konkola Basin in Zambia have up to 0.08 apfu Co. Minceva-Stefanova (1997) reported data from electron microprobe analysis performed on strongly zoned Co-rich dolomite crystals from an unknown locality with Co contents up to 0.35 apfu. A crystallographic study of cobalt-rich dolomite from Kolwezi (Democratic Republic of Congo) was performed by Perchiazzi (2015), who reported its chemical data with 0.17 apfu Co based on EDS data, only. A complete genetic, geochemical and mineralogical study of Co-rich carbonates from the Tenke–Fungurume District, Democratic Republic of Congo, was published by Barton *et al.* (2014), with a maximum observed Co content of 0.30 apfu; the same material was used for single-crystal structural studies (Perchiazzi *et al.*, 2018).

The observed Co contents in the samples from the Brod deposit (Fig. 6) are significantly higher than those published so far (Fig. 7). We found thin (tens μm) zones with contents up to 0.59 apfu Co. The grain extracted for single-crystal X-ray diffraction shows 0.41–0.49 apfu Co contents; cobalt always prevails over Mg (Fig. 6).

The Figs 4 and 5 show that the unit cell parameters of Co-rich dolomites and škáchaite expand with increasing Co content; the discrepancy of a sample from Kolwezi (Perchiazzi, 2015) could be explained by the Mg/Co ratio only being measured by EDS; by the presence of a fine undetected chemical zoning; by unrecognised contamination by mineral inclusion(s) in the analysed volume; or by an error introduced by twinning on the unit cell determination (Perchiazzi *et al.*, 2018).

Conclusion

Škáchaite is a new Ca-Co dominant member of the dolomite group (Table 8) together with ankerite (Ca–Fe), dolomite (Ca–Mg), kutnohorite (Ca–Mn), minrecordite (Ca–Zn) and norsethite (Ba–Mg); Strunz Class 5.AB.10. It does not correspond to any valid or invalid unnamed mineral (Smith and Nickel, 2007).

Škáchaite discovery and its comparison with previously known Co-containing dolomites confirm the fundamental role played by the investigation of natural mineral assemblages to reveal the possibilities of contents of elements such as Co in the crystal structure of dolomite-group minerals. In the past, it has been reported “Cobalt does not form a stable dolomite-structured carbonate, either with other transition metal ions or with Ca²⁺” (Reeder, 1983; Barton *et al.*, 2014) and Co-dominant dolomite has so far

not been obtained in synthetic runs (e.g. Goldsmith and Northrop, 1965; Rosenberg and Foit, 1979).

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Competing interests. The authors declare none.

References

- Barton I.F., Yang H. and Barton M.D. (2014) The mineralogy, geochemistry, and metallurgy of cobalt in the rhombohedral carbonates. *The Canadian Mineralogist*, **52**, 653–670.
- Deliens M. and Piret P. (1980) La kolwesite, un hydrocarbonate de cuivre et de cobalt analogue a la glaukosphaerite et a la rosasite. *Bulletin de Mineralogie*, **103**, 179–184.
- Dolníček Z., Ulmanová J., Sejkora J., Knížek F. and Škácha P. (2023) Mineralogy and genesis of the Pb–Zn–Sb–Ag vein H32A in the Příbram uranium and base-metal district, Bohemian Massif, Czech Republic. *Ore Geology Reviews*, **162**, 105695.
- Douglass D.L. (1992) Cobaltoan Calcite = Cobaltoan Dolomite. *Mineralogical Record*, **23**, 445–446.
- Douglass D.L. (1999) Cobaltoan calcites and dolomites from Katanga. *Mineralogical Record*, **30**, 269–273.
- Fay I. and Barton M.D. (2012) Alteration and ore distribution in the Proterozoic Mines Series, Tenke–Fungurume Cu–Co district, Democratic Republic of Congo. *Mineralium Deposita*, **47**, 501–519.
- Garavelli C.G., Vurro F. and Fioravanti G.C. (1982) Minrecordite a new mineral from Tsumeb. *The Mineralogical Record*, **13**, 131–136.
- Gauthier G. and Deliens M. (1999) Cobalt minerals of the Katanga Crescent, Congo. *Mineralogical Record*, **30**, 255–267.
- Gillet P., Biellmann C., Reynard B. and McMillan P. (1993) Raman spectroscopic studies of carbonates Part I: High-pressure and high-temperature behaviour of calcite, magnesite, dolomite and aragonite. *Physics and Chemistry of Minerals*, **20**, 1–18.
- Goldsmith J.R. and Northrop D.A. (1965) Subsolidus phase relations in the systems CaCO₃–MgCO₃–CoCO₃ and CaCO₃–MgCO₃–NiCO₃. *The Journal of Geology*, **73**, 817–829.
- Hazen R.M., Hystad G., Golden J.J., Hummer D.R., Liu C., Downs R.T., Morrison S.M., Ralph J. and Grew E.S. (2017) Cobalt mineral ecology. *American Mineralogist*, **102**, 108–116.
- Kominek J. (1995) *Geology of the wide surroundings and of the deposit, part I and II. Final report on the uranium district Příbram*. MS DIAMO, Příbram, 418 p. [in Czech].

- Kraus W. and Nolze G. (1996) POWDER CELL – a program for the representation and manipulation of crystal structures and calculation of the resulting X-ray powder patterns. *Journal of Applied Crystallography*, **29**, 301–303.
- Litochleb J., Sejkora J. and Šrein V. (2002) Mineralogy of silver mineralization from Brod near Příbram (the Příbram uranium - polymetallic district, central Bohemia, Czech Republic). *Bulletin mineralogicko-petrologického oddělení Národního muzea v Praze*, **10**, 221–234 [in Czech].
- Litochleb J., Černý P., Litochlebová E., Sejkora J. and Šreinová B. (2003) The deposits and occurrences of mineral raw materials in the Střední Brdy Mts. and the Brdy piedmont area (Central Bohemia). *Bulletin mineralogicko-petrologického oddělení Národního muzea v Praze*, **11**, 57–86 [in Czech].
- Mandarino J.A. (1981) The Gladstone-Dale relationship: Part IV. The compatibility concept and its application. *The Canadian Mineralogist*, **19**, 441–450.
- Minceva-Stefanova J. (1997) First finding of high miscibility in the system $\text{CaMg}(\text{CO}_3)_2$ – $\text{CaCo}(\text{CO}_3)_2$ in nature. *Geochemistry, Mineralogy and Petrology*, **32**, 5–16.
- Peacor D.R., Essene E.J. and Gaines A.M. (1987) Petrologic and crystal-chemical implications of cation order-disorder in kutnahorite ($\text{CaMn}(\text{CO}_3)_2$). *American Mineralogist*, **72**, 319–328.
- Perchiazzi N. (2015) Crystal structure study of a cobaltoan dolomite from Kolwezi, Democratic Republic of Congo. *Acta Crystallographica*, **E71**, i3–i3.
- Perchiazzi N., Barton I. F. and Vignola P. (2018) Incorporation of Co in the dolomite structure: coupled EPMA and single crystal structural studies of Co-rich dolomite from the Tenke-Fungurume district, Democratic Republic of Congo. *The Canadian Mineralogist*, **56**, 151–158.
- Perrin J., Vielzeuf D., Laporte D., Ricolleau A., Rossman G.R. and Floquet N. (2016) Raman characterization of synthetic magnesian calcites. *American Mineralogist*, **101**, 2525–2538.
- Pertlik F. (1986) Structures of hydrothermally synthesized cobalt(II) carbonate and nickel(II) carbonate. *Acta Crystallographica*, **C42**, 4–5.
- Petříček V., Dušek M. and Plášil J. (2016) Crystallographic computing system Jana2006: solution and refinement of twinned structures. *Zeitschrift für Kristallographie*, **231**, 583–599.
- Petříček V., Palatinus L., Plášil J. and Dušek M. (2023) Jana2020 – a new version of the crystallographic computing system Jana. *Zeitschrift für Kristallographie*, **238**, 271–282.
- Pouchou J.L. and Pichoir F. (1985) “PAP” (ρZ) procedure for improved quantitative microanalysis. Pp. 104–106 in: *Microbeam Analysis* (J.T. Armstrong, editor). San Francisco Press, San Francisco.
- Reeder R.J. (1983) Crystal chemistry of the rhombohedral carbonates. Pp. 1–47 in: *Carbonates: Mineralogy and Chemistry* (R.J. Reeder, editor). Reviews in Mineralogy and Geochemistry, 11. Mineralogical Society of America, Washington DC.
- Reeder R.J. and Dollase W.A. (1989) Structural variation in the dolomite-ankerite solid-solution series: An X-ray, Mössbauer, and TEM study. *American Mineralogist*, **74**, 1159–1167.
- Rigaku (2019) *CrysAlis CCD and CrysAlis RED*. Rigaku- Oxford Diffraction Ltd, Yarnton, Oxfordshire, UK.
- Rosenberg P.E. and Foit Jr F.F. (1979). The stability of transition metal dolomites in carbonate systems: a discussion. *Geochimica et Cosmochimica Acta*, **43**, 951–955.
- Sejkora J., Škácha P., Plášil J., Dolníček Z. and Ulmanová J. (2021) Hrabákite, $\text{Ni}_9\text{PbSbS}_8$, a new member of the hauchecornite group from Příbram, Czech Republic. *Mineralogical Magazine*, **85**, 189–196.
- Sejkora J., Dolníček Z., Zachariáš J., Ulmanová J., Šrein V. and Škácha P. (2022) Mineralogical and fluid inclusion evidence for reworking of Au (-Bi) mineralization by Ag-Sb-base metal-rich fluids from the Bytíz deposit, Příbram uranium and base-metal ore district, Czech Republic. *Minerals*, **12**, 1539.
- Sejkora J., Plášil J., Dolníček Z. and Škoda R. (2023) Škáchaite, IMA 2022-143. CNMNC Newsletter 72; *Mineralogical Magazine*, **87**, <https://doi.org/10.1180/mgm.2023.21>.
- Sheldrick G.M. (2015) Crystal structure refinement with SHELXL. *Acta Crystallographica*, **C71**, 3–8.
- Škácha P., Sejkora J. and Plášil J. (2017) Selenide mineralization in the Příbram uranium and base-metal district (Czech Republic). *Minerals*, **7**, 91.
- Škácha P., Sejkora J. and Plášil J. (2018) Bytízite, a new Cu-Sb selenide from Příbram, Czech Republic. *Mineralogical Magazine*, **82**, 199–209.
- Škácha P., Sejkora J., Plášil J., Dolníček Z. and Ulmanová J. (2021) Grimmitite, NiCo_2S_4 , a new thiospinel from Příbram, Czech Republic. *European Journal of Mineralogy*, **33**, 175–187.
- Smith D.G.W. and Nickel E.H. (2007) A system for codification for unnamed minerals: report of the Subcommittee for Unnamed Minerals of the IMA Commission on New Minerals, Nomenclature and Classification. *The Canadian Mineralogist*, **45**, 983–1055.
- Sweeney M., Turner P. and Vaughan D.J. (1986) Stable isotope and geochemical studies of the role of early diagenesis in ore formation, Konkola Basin, Zambian Copper Belt. *Economic Geology*, **81**, 1838–1852.
- Van Langendonck S., Muchez P., Dewaele S., Kalubi A. J. and Cailteux J.A. (2013) Petrographic and mineralogical study of the sediment-hosted Cu-Co ore deposit at Kambove West in the central part of the Katanga Copperbelt (DRC). *Geologica Belgica*, **16**, 91–104.
- Warr L.N. (2021) IMA-CNMNC approved mineral symbols. *Mineralogical Magazine*, **85**, 291–320.