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CARBOBYSTRITE, $Na_8[Al_6Si_6O_{24}](CO_3)\bullet 4H_2O$, A NEW CANCRINITE-GROUP MINERAL SPECIES FROM THE KHIBINA ALKALINE MASSIF, KOLA PENINSULA, RUSSIA: DESCRIPTION AND CRYSTAL STRUCTURE

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Abstract

Carbobystrite, ideally $Na_8[Al_6Si_6O_{24}](CO_3)\bullet 4H_2O$, trigonal, *a* 12.6678(5), *c* 10.3401(4) Å, *V* 1437.0(2) Å^3, $c:a = 0.8162$, space group *P*31*c*, $Z = 2$, $R = 0.0271$ (for 4861 observed reflections collected with a four-circle X-ray diffractometer), is a new cancrinite-group mineral species from Mount Koashva, Khibina alkaline massif, Kola Peninsula, Russia. It formed in a pegmatitic environment. Associated minerals are: microcline, sodalite, megakalsilite, natrolite, pectolite, aegirine, natrite, nacaphite, vitusite-(Ce), fluorcaphite, belovite-(Ce), umbite, lemmleinite-K, lomonosovite, lovozerite, phlogopite, sphalerite and galena. The mineral was found in only one hand specimen of pegmatite as a corroded irregularly shaped grain about 3 mm across, intergrown with sodalite, megakalsilite and natrite. It is transparent, colorless with a white streak, a vitreous luster, and fluoresces pale yellow under ultraviolet light. Carbobystrite has a Mohs hardness of 6, is brittle with a conchoidal fracture, and has no cleavage. The calculated density is 2.366 g/cm^3. Carbobystrite is uniaxial negative, non-pleochroic, ω 1.500(2), ε 1.488 (2). The strongest six reflections in the X-ray powder-diffraction pattern [*d* in Å(I)(*hkl*)] are: 4.689(100)(012), 3.249(100)($\bar{1}$32, 122), 6.378(80) ($\bar{1}$20), 2.661(80)(041, 123, $\bar{1}$33), 3.867(70)($\bar{1}$31, 121), and 3.664(70)(030). An electron-microprobe analysis gives Na_2O 22.66, K_2O 1.75, SiO_2 35.74, Al_2O_3 30.42, CO_2 4.37, H_2O 6.26, sum 101.20 wt.%, with CO_2 and H_2O calculated from structural data. The empirical formula (based on O = 30.5 atoms per formula unit) is $(Na_{7.40}K_{0.38})_{\Sigma 7.78}(Al_{6.04}Si_{6.02})_{\Sigma 12.06}O_{24}(CO_3)\bullet 3.5H_2O$; the simplified formula is $Na_8[Al_6Si_6O_{24}](CO_3)\bullet 4H_2O$. The name *carbobystrite* denotes the compositional relation between the new mineral and bystrite, $(Na,K)_7Ca[Al_6Si_6O_{24}](S)_{1.5}\bullet H_2O$; they are related by the substitution $Na^+ + (CO_3)^{2-} + 2.5H_2O \rightarrow Ca^{2+} + (S^{2-})_{1.5}$. The framework of Si,Al–O tetrahedra can be described as an ABAC stacking sequence. In the crystal structure, there are two LOSOD cages, and two ε (cancrinite) cages per unit cell, giving a maximum of two (CO_3) groups and six H_2O groups for the LOSOD-type cages and two H_2O groups for the cancrinite cages, respectively. This is the first complex-sequence cancrinite-group mineral with (CO_3) groups in cages larger than the cancrinite cages. Carbobystrite suggests a new series of carbonate equivalents of all known complex sequences in the cancrinite group.

Keywords: carbobystrite, new mineral species, cancrinite group, electron-microprobe analysis, crystal structure, Khibina, Kola Peninsula, Russia.

Sommaire

Nous décrivons la carbobystrite, de composition idéale $Na_8[Al_6Si_6O_{24}](CO_3)\bullet 4H_2O$, trigonale, *a* 12.6678(5), *c* 10.3401(4) Å, *V* 1437.0(2) Å^3, $c:a = 0.8162$, groupe spatial *P*31*c*, $Z = 2$, $R = 0.0271$ (utilisant 4861 réflexions observées prélevées avec un diffractomètre à quatre cercles), nouvelle espèce minérale du groupe de la cancrinite provenant du mont Koashva, massif alcalin de Khibina, dans la péninsule de Kola, en Russie. Elle s'est formée dans un milieu pegmatitique. Lui sont associés: microcline, sodalite, mégakalsilite, natrolite, pectolite, aegyrine, natrite, nacaphite, vitusite-(Ce), fluorcaphite, belovite-(Ce), umbite, lemmleinite-K, lomonosovite, lovozerite, phlogopite, sphalérite et galène. Le minéral a été découvert dans un seul échantillon

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de pegmatite; il semble corrodé, et la forme du cristal d'environ 3 mm est xénomorphe, en intercroissance avec sodalite, mégakalsilite et natrite. Il est transparent, incolore avec une rayure blanche, un éclat vitreux, et avec une fluorescence jaune pâle en lumière ultraviolette. La carbobystrite possède une dureté de Mohs de 6; elle est cassante avec une fracture conchoïdale, et semble sans clivage. La densité calculée est 2.366 g/cm^3. La carbobystrite est uniaxe négative, non pléochroïque, ω 1.500(2), ε 1.488 (2). Les six réflections les plus intenses du spectre de diffraction X, méthode des poudres [*d* en Å(I)(*hkl*)] sont: 4.689(100)(012), 3.249(100)($\bar{1}$32, 122), 6.378(80)($\bar{1}$20), 2.661(80)(041, 123, $\bar{1}$33), 3.867(70)($\bar{1}$31, 121), et 3.664(70)(030). Une analyse avec une microsonde électronique a donné Na_2O 22.66, K_2O 1.75, SiO_2 35.74, Al_2O_3 30.42, CO_2 4.37, H_2O 6.26, pour une somme de 101.20% (poids), les teneurs en CO_2 et H_2O étant calculées à partir des données structurales. La formule empirique, fondée sur 30.5 atomes d'oxygène par unité formulaire), est $(Na_{7.40}K_{0.38})_{\Sigma 7.78}(Al_{6.04}Si_{6.02})_{\Sigma 12.06}O_{24}(CO_3)\bullet 3.5H_2O$; la formule simplifiée est $Na_8[Al_6Si_6O_{24}](CO_3)\bullet 4H_2O$. Le nom *carbobystrite* rappelle la relation compositionelle liant la carbobystrite à la bystrite, $(Na,K)_7Ca[Al_6Si_6O_{24}](S)_{1.5}\bullet H_2O$: $Na^+ + (CO_3)^{2-} + 2.5H_2O \rightarrow Ca^{2+} + (S^{2-})_{1.5}$. On peut décrire la charpente de tétraèdres Si,Al–O en termes d'une séquence d'empilement ABAC. Dans la structure, il y a deux cages de type LOSOD et deux cages ε de type cancrinite par maille élémentaire, ce qui donne un maximum de deux groupes (CO_3) et six groupes H_2O pour les cages de type LOSOD et deux groupes H_2O pour celles du type cancrinite, respectivement. Il s'agit du premier minéral du groupe de la cancrinite ayant une séquence complexe et des groupes (CO_3) dans des cages plus volumineuses que celles de la cancrinite. La carbobystrite serait représentative d'une nouvelle série d'équivalents carbonatés de toutes les séquences connues du groupe de la cancrinite.

(Traduit par la Rédaction)

Mots-clés: carbobystrite, nouvelle espèce minérale, groupe de la cancrinite, données de microsonde électronique, structure cristalline, Khibina, péninsule de Kola, Russie.

INTRODUCTION

In this paper, we describe a new cancrinite-group mineral discovered by the senior author in a highly mineralized pegmatite body on Mount Koashva in the Khibina alkaline massif, Kola Peninsula, Russia. A detailed study of the mineral, with documentation based on electron-microprobe and X-ray powder and single-crystal analyses, shows that it is structurally similar to bystrite, $(Na,K)_7Ca[Al_6Si_6O_{24}](S)_{1.5}\bullet H_2O$ (Sapozhnikov *et al.* 1991, Pobedimskaya *et al.* 1991) and chemically fairly similar to cancrisilite, $Na_7(Al_5Si_7O_{24})(CO_3)\bullet 3H_2O$ (Khomyakov *et al.* 1991a, 1991b). Given the crucial role of structure in the systematics of groups of complex minerals, it is appropriate to regard this mineral as the K-deficient (CO_3)–Na analogue of bystrite. The name *carbobystrite* denotes the compositional relation between carbobystrite and bystrite. The new mineral species and its name have been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA 2009–28). The holotype specimen of carbobystrite is deposited at the Fersman Mineralogical Museum, Russian Academy of Sciences, Moscow, Russia, catalogue #3836.

OCCURRENCE AND ASSOCIATED MINERALS

The Khibina alkaline massif in the Kola Peninsula offers examples of differentiated agpaitic complexes comparable to those at such famous mineral localities as Lovozero (Kola Peninsula), Ilímaussaq (South Greenland), and Mont Saint-Hilaire (Quebec, Canada). The majority of new minerals, as well as the new mineral in question, were identified in the context of detailed investigations of hyperagpaitic pegmatites, the extreme alkaline differentiates of nepheline-bearing syenitic magmas (Khomyakov 1995). Most of the pegmatite bodies of this type occur within the central arc of the Khibina massif, composed mainly of rischorrite and ijolite–urtite. Carbobystrite was found in a large body of hyperagpaitic pegmatite in ijolite–urtite, near its contact with apatite–nepheline rocks. The subvertically dipping pegmatite body, up to 5 m wide, was traced along the quarry wall for about 100 m. Where the body swells, it is seen to consist of an intensely mineralized core composed mainly of water-soluble sodium fluoride (villiaumite), sodium carbonates (natrite and thermonatrite), and sodium phosphate (natrophosphate), and a silicate rim of very large aegirine spherulites up to 1–1.5 m in diameter. Other minerals occurring mostly in the central zone of the body and at its contact with the aegirine-dominant rim are pectolite, microcline, sodalite and lomonosovite; less common phases are chkalovite, vitusite-(Ce) and REE,Sr-enriched fluorapatite, with sporadic megakalsilite (Khomyakov *et al.* 2002), natrolite, alkali amphibole, phlogopite (Ferraris *et al.* 2001), lamprophyllite, lovozerite, umbite, belovite-(Ce), fluorcaphite, nacaphite, nefedovite, bonshtedtite, sphalerite, galena and molybdenite. Lemmleinite-K pseudomorphs after lomonosovite also were observed. A very characteristic feature of this and similar bodies of pegmatite in the Mount Koashva area is the presence of abundant solid bitumen. So far, only one hand specimen of pegmatite containing approximately 30 mg of carbobystrite has been collected from the axial zone of the large pegmatite body. The mineral occurs as a corroded irregularly shaped grain about 3 mm across, intergrown with sodalite, megakalsilite and natrite. Judging from the mineral composition of the hand specimen, carbobystrite appears to have crystallized from residual peralkaline pegmatite-forming melt or solution.

PHYSICAL AND OPTICAL PROPERTIES

The main properties of carbobystrite are presented in Table 1, where they are compared to those of bystrite and cancrisilite. Carbobystrite is transparent, colorless, with a vitreous luster and a white streak. It fluoresces pale yellow under ultraviolet light in the range 240–400 nm. It is brittle, without cleavage, without parting, and it has a conchoidal fracture. It has a Mohs hardness of 6. Its density could not be measured directly because of the small amount of material available; the density calculated for the empirical formula is 2.366 g/cm^3. The mineral is uniaxial negative, ω 1.500(2), ε 1.488(2) (λ 589 nm), and non-pleochroic.

The infrared spectrum of carbobystrite (Fig. 1) was recorded an a two-beam spectrometer SPECORD 75 IR. The sample was prepared as a pellet of a carbobystrite + KBr, and a pellet of pure KBr was put under the reference beam. A digital version of two spectra is available from the Depository of Unpublished Data on the MAC website [document Carbobystrite CM48_291]. The spectrum is characterized by the following absorptions (cm^{-1}, s, m, w and sh equivalent to strong, medium and weak bands and shoulder, respectively): 3615 w, 3530 w, 1672 w, 1637 w, 1510 sh, 1491 s, 1412 s, 1100 sh, 1085 m, 1040 sh, 985 s, 970 sh, 945 sh, 746 w, 706 m, 687 s, 670 sh, 634 s, 616 sh, 562 w, 518 w, 485 s, 430 s, 420 sh and 400 w. The presence of H_2O in the structure is shown by bands at 3615–3530 and 1672–1637 cm^{-1}. The bands at 1510, 1491 and 1412 cm^{-1} indicate the presence of $(CO_3)^{2-}$ groups. The IR spectrum is very similar to that of cancrinite except for the relative frequency of the bands and the number of bands in the 1510–1400 cm^{-1} range, which are much more complex in cancrinite (Ballirano & Maras 2004, Della Ventura *et al.* 2009) owing to the disorder of the (CO_3) groups along the cancrinite channel.

CHEMICAL COMPOSITION

The chemical analysis (Table 2) was done with a Cameca SX–100 electron microprobe (wavelength-dispersion mode, 15 kV, 10 nA, 20 µm beam diameter). The following standards (X-ray lines and analyzing crystals) were used: albite (Na$K\alpha$ on LTAP), andalusite (Al$K\alpha$ on TAP), diopside (Si$K\alpha$ on TAP and Ca$K\alpha$ on LPET), orthoclase (K$K\alpha$ on LPET), $SrTiO_3$ (Sr$L\alpha$ on LPET), barite (S$K\alpha$ in LPET and Ba$L\alpha$ on LPET), olivine (Mg$K\alpha$ on TAP), fayalite (Fe$K\alpha$ on LLiF), spessartine (Mn$K\alpha$ on LLiF), riebeckite (F$K\alpha$ in LTAP), and tugtupite (Cl$K\alpha$ in LPET). In addition to the tabulated data, the mineral contains minor amounts (0.005–0.02 wt%) of SrO, BaO, MgO, FeO, MnO, SO_3 and F; CaO and Cl were sought but not detected. Neither H_2O nor CO_2 was determined directly because of insufficient material. We calculated the amount of H_2O and CO_2 by stoichiometry from the results of the crystal-structure analysis. The presence of H_2O and CO_2 was confirmed by infrared spectroscopy (see previous section). The empirical formula (based on 30.5 anions) is $(Na_{7.40}K_{0.38})_{\Sigma 7.78}(Al_{6.04}Si_{6.02})_{\Sigma 12.06}O_{24}(CO_3)\bullet 3.5H_{2.01}O$. The simplified formula is $Na_8[Al_6Si_6O_{24}](CO_3)\bullet 4H_2O$, which requires

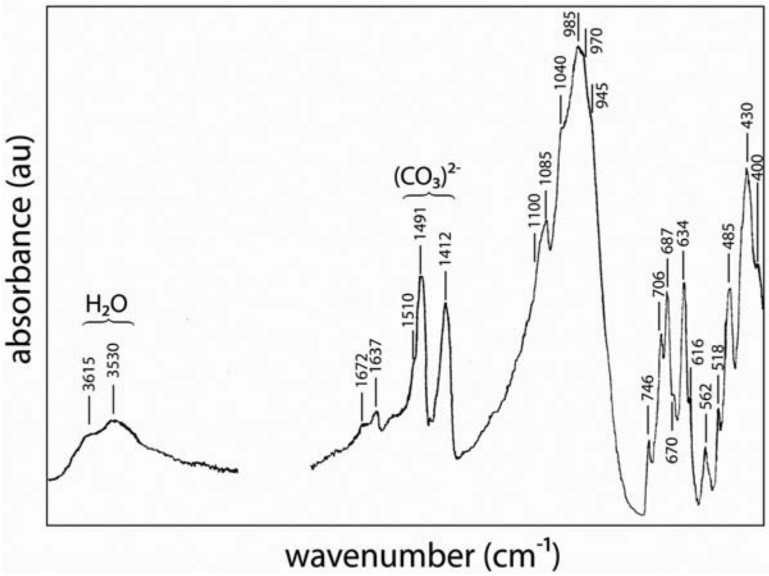

FIG. 1. Infrared spectrum of carbobystrite (N.V. Chukanov, analyst).

TABLE 1. COMPARISON OF CARBOBYSTRITE, BYSTRITE AND CANCRISILITE

	Carbobystrite*	Bystrite**	Cancrisilite***
Formula	$Na_8[Al_6Si_6O_{24}](CO_3)\cdot4H_2O$	$(Na,K)_7Ca[Al_6Si_6]O_{24}S_{1.5}\cdot H_2O$	$Na_7[Al_5Si_7O_{24}](CO_3)\cdot3H_2O$
System	Trigonal	Trigonal	Hexagonal
Space group	*P*31*c*	*P*31*c*	$P6_3mc$
a (Å)	12.6678(5)	12.855	12.575
c	10.3401(1)	10.700	5.105
V (Å^3)	1437.0(2)	1531.8	699.1
Z	2	2	1
D_{meas} (g/cm^3)	2.37	2.45	2.40
Strongest XRD lines [*d* in Å (I)(*hkl*)]	4.689(100)(012)	3.720(100)(300)	3.22(100)(211)
	3.249(100)(122+)	3.313(90)(212)	3.65(90)(300)
	6.378(80)($\bar{1}$20)	3.919(80)(211)	6.30(70)(110)
	2.661(80)(041+)	4.824(70)(102)	4.61(50)(101)
	3.867(70)(121+)	2.676(70)(004)	2.722(50)(400)
	3.664(70)(030)	2.471(35)(114)	2.597(20)(311)
	2.117(60)(034+)	3.396(25)(103)	2.402(20)(401)
	2.399(50)(114+)	2.784(25)(400)	2.097(20)(330)
Optical char.	Uniaxial negative	Uniaxial positive	Uniaxial negative
ω	1.500	1.584	1.509
ε	1.488	1.660	1.490
Pleochroism	None	Deep yellow to colorless	None
Color	Colorless	Deep yellow	Lilac

* This work; ** Sapozhnikov *et al.* (1991), Pobedimskaya *et al.* (1991); *** Khomyakov *et al.* (1991a,b).

TABLE 2. CHEMICAL COMPOSITION AND CHEMICAL FORMULA* OF CARBOBYSTRITE

oxide	wt.%	range		*apfu*
Na_2O	22.66	22.21 – 23.05	Na	7.40
K_2O	1.75	1.68 – 1.81	K	0.38
SiO_2	35.74	35.33 – 36.00	Si	6.02
Al_2O_3	30.42	29.97 – 30.84	Al	6.04
CO_2**	4.37		C	1.00
H_2O**	6.26		H	2.01
Total	101.20		Σ	22.85

* calculated on the basis of 30.5 O atoms; ** calculated from structure refinement.

Na_2O 24.06, Al_2O_3 29.69, SiO_2 34.99, CO_2 4.27, H_2O 6.99, for a total of 100.00 wt%. Carbobystrite decomposes readily in 50% HCl and HNO_3. A Gladstone–Dale calculation gives a compatibility index of 0.010, which is rated as superior (Mandarino 1981), indicating excellent agreement between the physical and chemical data.

X-Ray Crystallography

Powder-diffraction data for carbobystrite were collected using a Debye–Scherrer camera 114.6 mm in diameter with a Gandolfi attachment (Table 3). Reflections were indexed using a simulated powder pattern obtained from observed intensity data from the single-crystal X-ray-diffraction experiment. Unit-cell parameters obtained from the refinement of the X-ray powder data are as follows: *a* 12.692(3), *c* 10.365(4) Å, *V* 1446.0(7) Å^3. Carbobystrite is trigonal, space group *P*31*c*, *Z* = 2. The *c*:*a* ratio calculated from the unit-cell parameters is 0.816.

Crystal Structure

Data collection and crystal-structure refinement

A single crystal of carbobystrite was mounted on a Bruker AXS diffractometer with an APEX CCD 1K detector, Mo*K*α radiation and a crystal-to-detector distance of 4 cm. The intensities of 34937 reflections were extracted with the Saint V6.45A (® Bruker AXS) software package to 74° 2θ using frames collected at 5 s per 0.2° frame. The refined unit-cell parameters (Table 1) were obtained from 8082 reflections with $I > 10\sigma I$. An empirical absorption correction (Sadabs, Sheldrick 1998) was applied, and the data were merged to 4893 unique reflections, yielding $R_{(int)}$ = 2.6%. The structure was solved by direct methods in the space group *P*31*c* using Sir2004 (Burla *et al.* 2005) giving a partial model, mainly of framework cations and anions. On the basis of the similarity of lattice parameters and space group to those of bystrite, weighted full-matrix least-squares refinement on F_o^2 (Shelxl-97; Sheldrick 2008) was done using the coordinates of the framework atoms in bystrite (Pobedimskaya *et al.* 1991). The extra-framework anions were successively found in difference-Fourier maps. Two *Na* sites of bystrite, *Na*(1) and *Na*(3), merged into a single site, *Na*(3), in carbobystrite, close to the position of the *Na*(3) site in bystrite. The extra-framework (CO_3) and two (H_2O) groups were located within the cages. All atoms were refined with anisotropic displacement parameters using neutral scattering factors from the International Tables for X-ray Crystallography (1992). Site occupancies were fixed for all framework cation and anion sites, and refined for all extra-framework sites. After convergence, the site occupancies of the *Na*(1), *Na*(2) and *C* sites were fixed at full occupancy. The observed agreement-factor was slightly high ($R1$ = 6.1 % for 4861 reflections with $F_o > 4\sigma F$), even after testing using the Flack parameter, leading us to suspect that merohedral twinning is present, as it commonly is the case in minerals of the cancrinite group. The PLATON/TWINROTMAT software (Spek 2008) indicated the possible presence of a twin operation consisting of a two-fold rotation about (110) with twin the matrix (010/100/00$\bar{1}$). After applying this matrix, the agreement factor decreased to 2.7% for 4861 reflections with $F_o > 4\sigma F$.

Details of data collection and structure refinement are given in Table 4, final atom parameters and refined site-scattering values are given in Table 5, anisotropic displacement parameters are reported in Table 6, and selected interatomic distances in Table 7. Bond-valence values are given in Table 8. Observed and calculated structure-factors are available from the Depository of Unpublished Data on the MAC website [document Carbobystrite CM48_291].

TABLE 3. X-RAY POWDER-DIFFRACTION DATA FOR CARBOBYSTRITE

$I_{est.}$	d_{meas} (Å)	d_{calc} (Å)	h k l	$I_{est.}$	d_{meas} (Å)	d_{calc} (Å)	h k l
30	7.551	7.541	0 1 1	10	2.026	2.024	0 5 2
80	6.378	6.346	1 1 0	10	1.970	1.970	1 4 3
10	5.178	5.183	0 0 2			1.970	$\bar{1}$ 5 3
100	4.689	4.688	0 1 2	10	1.935	1.939	$\bar{1}$ 6 1
<5	4.167	4.154	1 2 0			1.939	1 5 1
10	4.007	4.014	$\bar{1}$ 2 2			1.940	0 2 5
		4.014	1 1 2	<5	1.884	1.885	0 4 4
70	3.867	3.856	$\bar{1}$ 3 1	10	1.849	1.845	1 5 2
		3.856	1 2 1			1.845	$\bar{1}$ 6 2
70	3.664	3.664	0 3 0	20	1.806	1.807	3 4 0
10	3.455	3.454	0 3 1			1.807	$\bar{2}$ 5 4
20	3.286	3.296	0 1 3			1.807	2 3 4
100	3.249	3.242	$\bar{1}$ 3 2			1.804	0 6 1
		3.242	1 2 2			1.804	0 3 5
<5	3.049	3.049	$\bar{1}$ 4 0	<5	1.780	1.780	$\bar{3}$ 7 1
10	2.925	2.925	1 3 1			1.780	3 4 1
		2.925	$\bar{1}$ 4 1			1.780	$\bar{2}$ 6 3
20	2.750	2.748	0 4 0			1.780	2 4 3
80	2.661	2.656	0 4 1	20	1.759	1.760	$\bar{2}$ 7 0
		2.656	1 2 3			1.760	1 4 4
		2.656	$\bar{1}$ 3 3			1.760	$\bar{1}$ 5 4
30	2.597	2.591	0 0 4	<5	1.732	1.735	2 5 1
40	2.521	2.522	0 1 4			1.735	$\bar{2}$ 7 1
		2.514	0 3 3	10	1.709	1.706	$\bar{3}$ 7 2
40	2.430	2.428	0 4 2			1.706	3 4 2
50	2.399	2.399	1 4 0			1.707	0 1 6
		2.399	1 1 4	30	1.653	1.655	0 4 5
		2.399	$\bar{1}$ 2 4	10	1.595	1.595	1 6 2
40	2.271	2.267	2 3 2			1.595	$\bar{1}$ 7 2
		2.267	$\bar{2}$ 5 2			1.595	1 2 6
20	2.151	2.150	0 5 1			1.595	$\bar{1}$ 3 6
		2.151	0 4 3	10	1.592	1.587	**4 4 0
60	2.117	2.115	3 3 0	<5	1.551	1.552	3 5 1
		2.116	0 3 4			1.552	$\bar{3}$ 8 1
10	2.033	2.037	$\bar{2}$ 5 3				
		2.037	2 3 3				

* Ni-filtered Cu radiation, λ = 1.54178 Å; the strongest eight lines are shown in bold. Intensities are estimated visually; not corrected for shrinkage, and no internal standard was used. **: line omitted from unit-cell refinement because of poor agreement on 2θ error (a check excluded the possibility of being due to K-feldspar). Indexed on *a* 12.692(3), *c* 10.365(4) Å, γ 120.0°, *V* 1446.0(7) Å^3.

RESULTS

The observed stacking sequence for the framework of carbobystrite is ABAC. Following the Zhdanov notation (Zhdanov 1945, Patterson & Kasper 1959), the observed basic partition is |(2)|(2)|, which corresponds to the space group $P6_3/mmc$. However, this space group is not compatible with Si,Al order in the tetrahedra of the aluminosilicate framework, which is usual for other complex-stacking-sequence minerals of the cancrinite group (Bonaccorsi & Merlino 2005). Results of the EMP analysis provide the ratio Si : Al = 1 : 1; thus, in accordance with Loewenstein's rule and with all previous refinements of the structure of minerals of the cancrinite–sodalite group, a long-range order of Si and Al is expected. Therefore, the symmetry must be lowered to $P\bar{6}2c$ or $P31c$. The structure of carbobystrite is also very similar to that of synthetic "Losod", $Na_6[Al_6Si_6O_{24}]$•$9H_2O$, described in space group $P6_3/mmc$ by Sieber & Meier (1974). "Losod" was successively described in space group $P6_3mc$ by Schicker (1988), although Baur (1991) proposed that order of Al and Si would probably lead to space group $P\bar{6}2c$ or $P31c$. Carbobystrite is also isostructural with synthetic $Na_8(Al_6Ge_6O_{24})(CO_3)$•$3H_2O$ (Sokolov *et al.* 1978) (ICSD 20177) in space group $P31c$. In the synthetic aluminogermanate $Na_8(Al_6Ge_6O_{24})(CO_3)$•$3H_2O$, Al and Ge are ordered at the tetrahedral sites of the

TABLE 4. MISCELLANEOUS STRUCTURE-REFINEMENT DATA FOR CARBOBYSTRITE

Temperature (K)	298(2)
Wavelength (Å)	0.71073
$D_{calc.}$ (g/cm^3)	2.366
Absorption coefficient (mm^{-1})	0.766
$F_{(000)}$	1004.5
Crystal size (mm)	0.56 × 0.30 × 0.20
θ range for data collection (°)	1.97 to 37.00.
Index ranges	$-21 \le h \le 21$, $-21 \le k \le 21$, $-17 \le l \le 17$
Reflections collected	34937
Independent reflections	4893
R_{int} (%)	2.59
Completeness to theta = 37.00° (%)	100
Absorption correction	Semi-empirical from equivalents (SADABS)
Max. and min. transmission	0.8618 and 0.759
Refinement method	Full-matrix least-squares on F_o^2
Data / restraints / parameters	4893 / 1 / 181
Goodness-of-fit on F_o^2	1.079
Final R indices [$I > 2\sigma(I)$]	$R1$ = 2.71, wR2 = 7.28
R indices (all data)	$R1$ = 2.72, wR2 = 7.29
Absolute structure parameter	0.17(11)
Largest diff. peak and hole (e.Å^{-3})	1.237 and –0.761

TABLE 5. COORDINATES AND EQUIVALENT ISOTROPIC DISPLACEMENT PARAMETERS (Å^2) OF ATOMS IN CARBOBYSTRITE

	carbobystrite					bystrite**
Atom	Site occupancy	*x*/*a*	*y*/*b*	*z*/*c*	U_{eq}*	Atom: site occupancy
Na(1)	1Na	0	0	-0.0505(2)	0.030(1)	Ca: 0.94Ca + 0.06 □
Na(2)	1Na	0.0941(1)	0.5484(1)	0.0646(1)	0.021(1)	Na(2): 0.6Na + 0.2K + 0.2 □
Na(3)	0.977(3) Na	0.3822(1)	0.1920(1)	0.7808(1)	0.024(1)	Na(3): 0.45Na + 0.15K Na(1): 0.30Na + 0.10K
Na(4)	0.63(3) Na	2/3	1/3	0.1343(9)	0.033(2)	Na(4): 0.75Na + 0.25K
K(4)	0.36(3) K	2/3	1/3	0.1216(6)	0.020(1)	
Si(1)	1Si	0.2510(1)	0.2517(1)	0.0190(1)	0.007(1)	Si,Al(1): 0.51Si + 0.49Al
Al(1)	1Al	0.6745(1)	0.0872(1)	0.2702(1)	0.008(1)	Si,Al(2): 0.51Si + 0.49Al
Si(2)	1Si	0.0805(1)	0.4192(1)	0.7688(1)	0.008(1)	Si,Al(3): 0.51Si + 0.49Al
Al(2)	1Al	0.2550(1)	-0.0007(1)	0.0182(1)	0.008(1)	Si,Al(4): 0.51Si + 0.49Al
O(1)	1O	0.3773(1)	0.0305(1)	0.4153(1)	0.013(1)	
O(2)	1O	0.2684(1)	0.1388(1)	-0.0249(1)	0.013(1)	
O(3)	1O	0.7081(1)	-0.0014(1)	0.1674(1)	0.013(1)	
O(4)	1O	0.6641(1)	0.0317(1)	0.4273(2)	0.014(1)	
O(5)	1O	0.2096(1)	0.1084(1)	0.5037(1)	0.014(1)	
O(6)	1O	0.0597(1)	0.5304(1)	0.7264(1)	0.012(1)	
O(7)	1O	0.2235(1)	0.4648(1)	0.7558(1)	0.016(1)	
O(8)	1O	0.0027(1)	0.3072(1)	0.1744(1)	0.012(1)	
C	1C	1/3	2/3	0.1588(3)	0.018(1)	
O(9)	1O	0.4481(2)	0.7248(3)	0.1465(3)	0.055(1)	
O(10)	0.35(1)O	0.7979(7)	0.4424(8)	-0.0759(12)	0.057(4)	
O(11)	0.47(2)O	0.5594(7)	0.2052(7)	-0.0716(11)	0.065(3)	
O(12)	0.34(1)O	0.0230(20)	-0.0207(17)	-0.2717(7)	0.063(4)	Cl,O(9): 0.48Cl + 0.48O

* $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor. ** Note that in the crystal structure of bystrite, the Na(3) and Na(1) atoms are separated by a short distance, 1.2 Å.

TABLE 6. ANISOTROPIC DISPLACEMENT PARAMETERS* (Å^2) OF ATOMS IN CARBOBYSTRITE

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Na(1)	0.021(1)	0.021(1)	0.047(1)	0.000	0.000	0.011(1)
Na(2)	0.021(1)	0.021(1)	0.020(1)	0.001(1)	0.002(1)	0.010(1)
Na(3)	0.035(1)	0.022(1)	0.019(1)	0.004(1)	0.008(1)	0.018(1)
K(4)	0.024(2)	0.024(2)	0.050(4)	0.000	0.000	0.012(1)
Na(4)	0.021(1)	0.021(1)	0.019(1)	0.000	0.000	0.010(1)
Si(1)	0.008(1)	0.007(1)	0.007(1)	0.000(1)	0.000(1)	0.004(1)
Al(1)	0.008(1)	0.009(1)	0.008(1)	0.000(1)	0.000(1)	0.005(1)
Si(2)	0.009(1)	0.007(1)	0.007(1)	0.000(1)	0.000(1)	0.004(1)
Al(2)	0.008(1)	0.007(1)	0.008(1)	-0.001(1)	0.000(1)	0.004(1)
O(1)	0.011(1)	0.019(1)	0.008(1)	0.002(1)	0.002(1)	0.007(1)
O(2)	0.016(1)	0.010(1)	0.015(1)	0.000(1)	0.001(1)	0.008(1)
O(3)	0.017(1)	0.016(1)	0.010(1)	-0.001(1)	0.001(1)	0.010(1)
O(4)	0.018(1)	0.020(1)	0.010(1)	0.002(1)	-0.001(1)	0.014(1)
O(5)	0.017(1)	0.009(1)	0.018(1)	-0.004(1)	-0.005(1)	0.008(1)
O(6)	0.017(1)	0.009(1)	0.012(1)	0.000(1)	-0.001(1)	0.009(1)
O(7)	0.011(1)	0.017(1)	0.023(1)	0.000(1)	0.000(1)	0.008(1)
O(8)	0.014(1)	0.016(1)	0.009(1)	-0.003(1)	0.000(1)	0.009(1)
C	0.014(1)	0.014(1)	0.024(1)	0.000	0.000	0.007(1)
O(9)	0.017(1)	0.025(1)	0.121(2)	-0.006(2)	-0.014(1)	0.009(1)
O(10)	0.035(4)	0.039(5)	0.076(8)	-0.003(4)	-0.028(4)	0.003(3)
O(11)	0.047(4)	0.044(4)	0.087(6)	0.017(4)	0.017(4)	0.010(3)
O(12)	0.091(13)	0.060(7)	0.038(3)	-0.016(5)	-0.009(6)	0.036(4)

* The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12}]$.

framework. Although compared to carbobystrite, the aluminogermanate has another site for an H_2O group, the H_2O groups within the LOSOD-type cage are not disordered in two positions: all the refined sites for H_2O groups show low occupancy (up to a total of 1.64 *pfu*). Carbobystrite has a higher content of H_2O (up to 3.5 *pfu* from refinement).

Description of the structure

From the observed bond-distances in the tetrahedra of the framework, it is evident that Si and Al are fully ordered in the framework of the carbobystrite structure: <Si(1,2)–O> = 1.618–1.619 Å; <Al(1,2)–O> = 1.740–1.743 Å (Table 7). For bystrite, Pobedimskaya *et al.* (1991) reported disorder of Si and Al, and <Si,Al(1,2,3,4)–O> in the range 1.661–1.679 Å. Rastsvetaeva *et al.* (2007) reported Si,Al disorder in cancrisilite; <Si,Al(1,2,3,4)–O> in the range 1.655–1.684 Å; however, in this case, it occurs as a consequence of the Si : Al ratio in this mineral (which also has a different topology, ABAB). Sokolov *et al.* (1978) described the Al,Ge order in synthetic $Na_8(Al_6Ge_6O_{24})(CO_3)•3H_2O$: <Al(1,2)–O> = 1.697–1.773; <Ge(1,2)–O> = 1.716–1.781 Å, although in this case, the order is resolved owing to the difference in scattering power of Al and Ge. The presence of Be,P order has also been reported

TABLE 7. SELECTED INTERATOMIC DISTANCES (Å) AND ANGLES (°) IN CARBOBYSTRITE

Na(1)–O(2) ×3	2.957(1)	Si(1)–O(2)	1.619(2)
Na(1)–O(5) ×3	2.367(1)	Si(1)–O(3)	1.616(2)
Na(1)–O(12)	2.337(7)	Si(1)–O(4)	1.622(2)
Na(1)–O(12)	2.922(7)	Si(1)–O(5)	1.615(2)
$^{[VIII]}$< Na(1)–O>	2.654	< Si(1)–O>	1.618
Na(2)–O(1)	2.446(2)	Al(1)–O(3)	1.745(1)
Na(2)–O(4)	2.439(2)	Al(1)–O(4)	1.748(2)
Na(2)–O(6)	2.376(1)	Al(1)–O(6)	1.739(2)
Na(2)–O(8)	2.903(2)	Al(1)–O(7)	1.727(2)
Na(2)–O(9)	2.410(3)	<Al(1)O>	1.740
Na(2)–O(9)	2.443(3)		
$^{[VI]}$<Na(2)–O>	2.503	Si(2)–O(1)	1.625(1)
		Si(2)–O(6)	1.618(2)
Na(3)–O(1)	2.969(2)	Si(2)–O(7)	1.609(2)
Na(3)–O(2)	2.366(1)	Si(2)–O(8)	1.626(1)
Na(3)–O(3)	2.381(2)	<Si(2)–O>	1.619
Na(3)–O(4)	2.982(2)		
Na(3)–O(8)	2.363(2)	Al(2)–O(1)	1.751(2)
Na(3)–O(9)	2.323(2)	Al(2)–O(2)	1.746(2)
Na(3)–O(10)*	2.612(11)	Al(2)–O(5)	1.738(2)
Na(3)–O(11)*	2.650(11)	Al(2)–O(8)	1.737(2)
$^{[VII]}$<Na(3)–O>$^{[O(10)]}$	2.571	< Al(2)–O>	1.743
$^{[VII]}$<Na(3)–O>$^{[O(11)]}$	2.576		
		C–O(9) ×3	1.265(2)
Na(4)–O(7) ×3	2.549(5)		
Na(4)–O(10) ×3	2.664(13)	O(10)…O(9)	3.03(1)
Na(4)–O(11) ×3	2.609(14)	O(10)…O(4)	2.89(1)
$^{[VI]}$<Na(4)–O>$^{[O(10)]}$	2.607	O(4)–O(10)–O(9)	99.5(4)
$^{[VI]}$<Na(4)–O>$^{[O(11)]}$	2.579		
		O(11)…O(9)	3.07(1)
K(4)–O(7) ×3	2.616(4)	O(11)…O(1)	2.85(1)
K(4)–O(10) ×3	2.559(13)	O(1)–O(11)–O(9)	96.4(3)
K(4)–O(11) ×3	2.504(12)		
$^{[VI]}$<K(4)–O>$^{[O(10)]}$	2.588	O(12)…O(3)	3.35(3)
$^{[VI]}$<K(4)–O>$^{[O(11)]}$	2.560	O(12)…O(8)	3.51(3)
		O(12)…O(5)	3.14(3)
		O(12)…O(5)	3.13(3)
		O(5)–O(12)–O(3)	47.5(4)
		O(5)–O(12)–O(8)	50.4(4)

* mutually exclusive for O(10) and O(11) involving bond distances.

for synthetic Li$_8$(HPO$_4$)(BePO$_4$)$_6$•H$_2$O (space group *P*31*c*, Z = 2, isostructural with carbobystrite): <Be(1,2)–O> = 1.610–1.632 Å; <P(1,2)–O> = 1.523–1.539 Å (Harrison *et al.* 1993). Interestingly, this compound has an (HPO$_4$) group coordinated by Li atoms within the LOSOD cage.

The framework of carbobystrite has two types of cages: cancrinite cages (ε, also known as [$4^6 6^5$] following the IUPAC recommendations of McCusker *et al.* 2001) and LOSOD cages [$4^6 6^{11}$]. The ε and LOSOD cages are assembled into two different chains, (ε–ε–ε …) and (LOSOD–LOSOD–LOSOD…), along [001]: chains of ε cages occur at (0,0,*z*); chains of LOSOD cages, at ($^2/_3$,$^1/_3$,*z*) (Fig. 2).

The ε cages: The ε cages host H$_2$O groups at the O(12) site. These (H$_2$O) groups coordinate Na atoms at the *Na*(1) sites, which are placed off the plane of the top and lower windows formed by the 6-membered rings perpendicular to [001]. Bond-valence values indicate an (H$_2$O) group (Table 8). The O(12) site is slightly off-axis, with a mutual exclusion of O(12)–O(12), at a distance of 0.84(2) Å, and has therefore a maximal occupancy of 1/3. The anion occurs alternatively at one of three possible positions in the ε cages along [001]. The cation at the *Na*(1) site is [4]-coordinated if we consider short distances (<2.4 Å; see Table 7) and [8]-coordinated if we consider distances up to 3 Å (Table 7). In carbobystrite, the *Na*(1) site is occupied by 1 *apfu* of Na. The corresponding site in bystrite is occupied by Ca (and there is named the *Ca* site, see Table 5).

We did not find H positions in the difference-Fourier map because of the low occupancy expected (1/3). As a result of a comparison with the geometry in cancrinite

TABLE 8. BOND-VALENCE TABLE (*vu*)* FOR CARBOBYSTRITE

atom	Si(1)	Al(1)	Si(2)	Al(2)	Na(1)	Na(2)	Na(3)	Na(4)	K(4)	C	Σ
O(1)			1.014	0.755		0.168	0.051				1.988
O(2)	1.031			0.765	$0.053^{\times3}\downarrow$		0.201				2.050
O(3)	1.040	0.767					0.195				2.001
O(4)	1.022	0.761				0.171	0.050				2.003
O(5)	1.043			0.781	$0.201^{\times3}\downarrow$						2.024
O(6)		0.779	1.034			0.197					2.010
O(7)		0.804	1.060					$0.114^{\times3}\downarrow$	$0.228^{\times3}\downarrow$		1.978† 2.092‡
O(8)			1.011	0.783		0.059	0.203				2.056
O(9)						0.182 0.169	0.222			$1.420^{\times3}\downarrow$	1.994
O(10)							0.115	$0.130^{\times3}\downarrow$	$0.180^{\times3}\downarrow$		0.245† 0.295‡
O(11)							0.106	$0.147^{\times3}\downarrow$	$0.201^{\times3}\downarrow$		0.253† 0.307‡
O(12)					0.215 0.057						0.272
Total	4.136	3.11	4.119	3.083	1.033	0.946	1.143	0.732$^{[O10]}$ 0.784$^{[O11]}$	1.224$^{[O10]}$ 1.289$^{[O11]}$	4.261	

* Bond-valence parameters from Brown (1981); † sum excluding K(4); ‡ sum excluding Na(4).

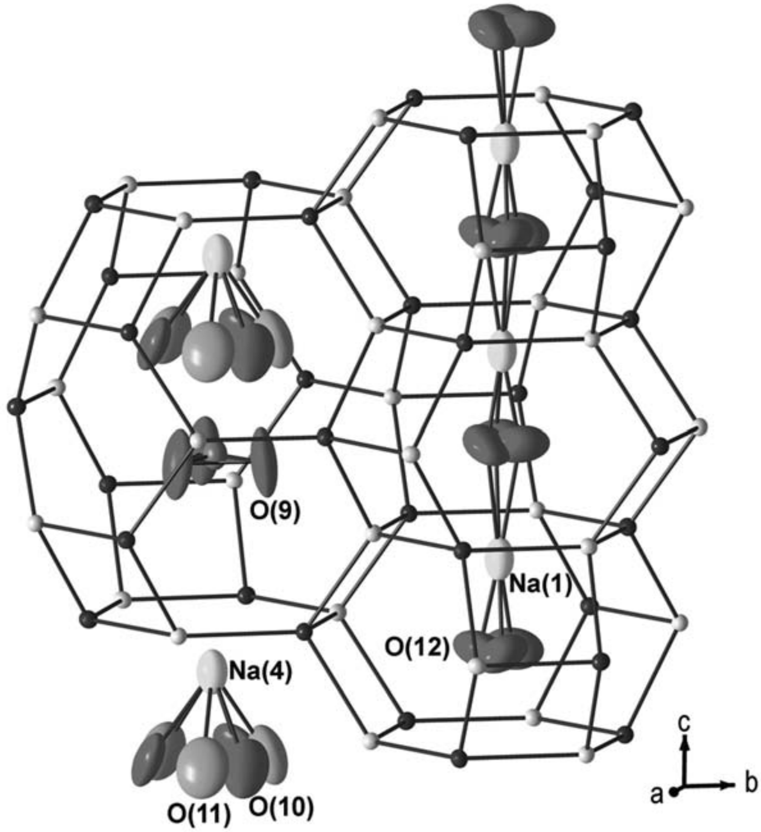

FIG. 2. Sketch of the cages in the carbobystrite structure showing the position of CO_3 and H_2O groups. Small, light grey spheres: Si, small, dark grey spheres: Al. The three equivalent positions for O(12) are mutually exclusive. Atoms O(10) and O(11) are mutually exclusive. The Na(2) and Na(3) are not reported in order to simplify the plot.

from a recent single-crystal neutron-diffraction structure (Della Ventura *et al.* 2009), we expect the H atoms to lie slightly off the plane of the O(12) sites, forming weak bifurcated hydrogen bonds with the O(5) anion of the six-membered rings [O(12)…O(5) = 3.13(1) Å] and either O(3) or O(8) anions of the middle 12-membered ring with [O(12)…O(3) = 3.35(1) Å] or [O(12)…O(8) = 3.51(1) Å], respectively.

LOSOD cages: Within the LOSOD cages, H_2O groups at the O(10) and O(11) sites coordinate Na atoms at the *Na*(2), *Na*(3) and *Na*(4) sites. Bond-valence values for both sites are compatible with an (H_2O) group (Table 8). These are two mutually excluding positions, O(10) and O(11) [O(10)–O(11) = 1.10 Å], and thus these sites have a maximum possible occupancy of 0.5. The LOSOD cage also hosts a (CO_3) group, and the observed C–O(9) × 3 distances [1.265(2) Å] are similar to those in cancrinite (see Della Ventura *et al.* 2009, and references therein). As observed by Ballirano & Maras (2004) and later confirmed by Della Ventura *et al.* (2009) in cancrinite, the O(9) and C atoms in carbobystrite are not strictly coplanar as z C ≠ z O(9) (Table 5). However, the displacement parameters are highly anisotropic along the [001] direction for the O(9) site, thus affecting accuracy of the determination of atom positions. This situation was also observed for (CO_3) groups in cancrinite, as previously reported (Grundy & Hassan 1982, Ballirano & Maras 2004, Della Ventura *et al.* 2009), although in their data, the *C* site also has elongate ellipsoids along [001]; in carbobystrite, the thermal motion of the C atom is more isotropic. In addition, in cancrinite, the (CO_3) groups show static disorder (Grundy & Hassan 1982). This does not occur in carbobystrite, where the O(9) anion of the (CO_3) group coordinates Na atoms at the *Na*(2) and *Na*(3) sites (Table 7), which are occupied exclusively by Na (Table 5). The anisotropy of the thermal motion of the O(9) atom might therefore be due to a possible weak hydrogen bond from H_2O groups at the O(10) and O(11) sites [O(9)…O(10) = 3.028; O(9)…O(11) = 3.068 Å]. The other hydrogen bond will be with the O(4) and O(1) anions [O(10)…O(4) = 2.888 Å, O(4)–O(10)–O(9) = 99.5°; O(11)…O(1) = 2.854 Å, O(1)–O(11)–O(9) = 96.4°]. The presence of different hydrogen bonding may explain the two main bands in the IR spectrum at 1491 and 1412 cm^{-1}.

The (H_2O) groups at the O(10) and O(11) sites alternatively coordinate the *Na*(4) site, which is the only site occupied by both Na and K. We observe static disorder at that site as a consequence of the Na–K substitution and therefore in our model, the *Na*(4) site splits into the *Na*(4) and *K*(4) sites (Table 7). Chemical analysis gives a K content of 0.38 *apfu* (Table 2), which is in perfect agreement with the refined scattering refined at the K(4) site, 0.36 *apfu*. However, the bond lengths reported in Table 7 are still rather short for K. We hypothesize that K(4) is occupied by K.

Carbobystrite has two LOSOD cages and two ε cages per unit cell, giving a maximum of 2 (CO_3) groups and 6 H_2O groups for the LOSOD-type cages and 2 H_2O groups for the cancrinite cages, *i.e.*, 2 (CO_3) + 8 H_2O per unit cell.

RELATION TO OTHER SPECIES

Carbobystrite, ideally $Na_8[Al_6Si_6O_{24}](CO_3)\bullet 4H_2O$, is a K-deficient ($CO_3$)–Na analogue of bystrite, ideally $(Na,K)_7Ca(Al_6Si_6)O_{24}S_{1.5}\bullet H_2O$. Carbobystrite is chemically related to bystrite by the substitution $Na^+ + (CO_3)^{2-} + 2.5H_2O \rightarrow Ca^{2+} + (S^{2-})_{1.5}$. In general, carbobystrite is topologically isostructural with bystrite (Sapozhnikov *et al.* 1991, Pobedimskaya *et al.* 1991). Carbobystrite and bystrite differ in several structural details: (1) in the LOSOD cages of carbobystrite and bystrite, (CO_3) + H_2O groups and S atoms occur, respectively; (2) carbobystrite shows complete order of Si and Al in the tetrahedra of the framework, whereas Si,Al disorder occurs in bystrite; (3) in carbobystrite, Na is dominant at the special site (0,0,0) and is bonded to an (H_2O) group located within the cancrinite cages; in bystrite, Ca is the dominant species at the special site (0,0,0), and is bonded to Cl anions and (or) (H_2O) groups.

The LOSOD cage also occurs in other complex cancrinite-group minerals such as liottite (Ballirano *et al.* 1996), franzinite (Ballirano *et al.* 2000), tounkite (Rozenberg *et al.* 2004), sacrofanite (Ballirano & Bonaccorsi 2005), biachellaite (Rastsvetaeva & Chukanov 2008) and fantappièite (Cámara *et al.* 2010), where the cage can host two sulfate groups surrounded by (Na,Ca) cations and separated by groups of three cations in equatorial positions. Carbobystrite is the first complex-sequence cancrinite-group mineral with (CO_3) groups in LOSOD cages; (CO_3) groups are known to occur in LOSOD cages of synthetic compounds or in the 12-membered ring (12mR) channel parallel to [001] in cancrinite and cancrisilite. Therefore, this new end-member suggests a new series of carbonate equivalents of all known complex sequences.

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