1   **Revision I**

2   **Revision of the symmetry and the crystal structure of čejkaite, Na$_4$(UO$_2$)(CO$_3$)$_3$$^\$$**

3

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8

9   **ABSTRACT**

10   The crystal structure of čejkaite, Na$_4$(UO$_2$)(CO$_3$)$_3$, from the type locality, was

11 determined for the first time by single-crystal X-ray diffraction. In contrast to the previously

12 reported pseudohexagonal triclinic symmetry, the current data indicate čejkaite is monoclinic,

13 triply twinned, space group *Cc*. Refined unit cell parameters are *a* = 9.2919(8) Å, *b* =

14 16.0991(11) Å, *c* = 6.4436(3) Å, β = 91.404(5)°, and *V* = 963.62(12) Å^3. The monoclinic unit

15 cell is also supported by the good fit to the powder diffraction data. The structure of čejkaite

16 consists of uranyl tricarbonate clusters, forming sheets sub-parallel to (001) by sharing edges

17 with (NaΦ) polyhedra. Sheets are interconnected through the uranyl O atoms and columns of

18 (Na1Φ) polyhedra that share their trigonal faces. All Na atoms in the structure are [6]–

19 coordinated. The structure refinement yielded R_{obs} = 0.0424 for 1687 observed reflections

20 [I_{obs} > 3σ(*I*)] and 0.0538 for all 2016 unique reflections. Refinement and bond-valence

21 analysis of the structure confirmed the previously proposed formula Na$_4$(UO$_2$)(CO$_3$)$_3$, *Z* = 4.

22

23 $^\$$ Dedicated with best wishes to Jiří Čejka, D.Sc. (born September 2, 1929 in Roudnice nad

24 Labem) on the occasion of his 83rd birthday.

25

26 **Keywords:** čejkaite, uranyl carbonate, symmetry, crystal structure, single-crystal, twinning,
27 X-ray diffraction

28

29 **INTRODUCTION**

30 Čejkaite was described as a new mineral from Jáchymov, Western Bohemia, Czech

31 Republic by Ondruš et al. (2003) in honor of Jiří Čejka, for his contribution to science,

32 especially to the knowledge of uranium minerals and their spectroscopy. Ondruš et al. (2003)

33 used a Rietveld refinement to propose that it is triclinic, P–1 or $P1$, with the unit cell $a =$

34 9.291(2), b = 9.292(2), c = 12.895(2) Å, α = 90.73(2), β = 90.82(2), γ = 120.00(1)°, V =

35 963.7(4) Å^3, and formula $Na_4(UO_2)(CO_3)_3$, Z = 4. The lack of natural sample prompted

36 Ondruš et al. (2003) to use Rietveld analysis of a synthetic powder sample. They also

37 prepared trigonal $Na(UO_2)(CO_3)_3$ by a hydrothermal recrystallization and refined its crystal

38 structure (Císařová et al. 2001). Based on the Rietveld refinement for the synthetic powder,

39 Ondruš et al. (2003) described the structure of čejkaite as very similar to that of the trigonal

40 analogue (Císařová et al. 2001; Li et al. 2001), with refined triclinic unit cell parameters only

41 slightly deviating from hexagonal symmetry (see above). Catalano and Brown (2004)

42 provided information on bond-lengths in the uranium coordination polyhedron in čejkaite

43 obtained by analysis of its EXAFS spectrum. Subsequently, Čejka et al. (2010) reported

44 Raman spectra for čejkaite and its trigonal synthetic analogue. Čejkaite, although rare in

45 Nature, has been found at several localities worldwide. In addition to the type locality –

46 Jáchymov, it has been found in Rožná, Western Moravia, Czech Republic (Sejkora et al.

47 2008), in Mina Euréka, Pyrenees, Spain (Abella and Viñals 2009; Castillo et al. 2009) and

48 from localities in Hungary and U.S.A. (see for details MinDat homepage, www.mindat.org).

49 Čejkaite was also found in sediments at Hanford site where it results from uranium

50 contamination (Deutsch et al. 2004; Krupka et al. 2006), and the trigonal analogue occurs as

51 the weathering product on the surface of the Chernobyl lava (Burakov et al. 1999).

52 Here we present the structure of čejkaite determined for the first time from single-

53   crystal X-ray diffraction data that was collected for a twinned microcrystal, and re-

54   determination of its symmetry.

55

56   EXPERIMENTAL METHODS

57   *Occurrence*

58   The čejkaite sample used in this study originates from the Rovnost mine

59   (50º22'18.421''N, 12º53'32.83''E), Jáchymov, Western Bohemia, Czech Republic. The same

60   specimen was studied previously in the course of the reinvestigation of grimselite by Plášil et

61   al. (2012). The sample (approximately $10 \times 5 \times 3.5$ cm) of mostly quartz dolomitic vein is

62   covered by Fe and Mn oxyhydroxides, which are X-ray amorphous. Rich aggregates

63   composed of translucent light to grass green grimselite crystals (up to ~2 mm long) are partly

64   covered by tiny prismatic (up to 0.4 mm long) čejkaite crystals. Čejkaite also forms rich

65   crystalline aggregates of greenish color, covering areas of a few cm^2 (Fig. 1).

66

67   *Single-crystal XRD*

68   A crystal of čejkaite with dimensions $0.17 \times 0.02 \times 0.02$ mm was selected for the

69   single-crystal diffraction experiment. We used an Oxford Diffraction Gemini single-crystal

70   diffractometer equipped with the Atlas CCD detector and graphite-monochromatized MoKα

71   radiation from a classical sealed X-ray tube, collimated with fiber optics. The diffraction

72   pattern revealed multiple twins, as best resolved along $c*$ (see Supplementary file), and split

73   reflections also along $b*$ (see Supplementary file). Three twin components are bounded by

74   the operation of rotation, which can be described by two matrices given in Table 1. Čejkaite

75   was found to be monoclinic, space group Cc, with unit cell parameters $a = 9.2919(8)$ Å, $b =$

76    $16.0991(11)$ Å, $c = 6.4436(3)$ Å, $\beta = 91.404(5)°$, and $V = 963.62(12)$ Å^3, $Z = 4$. The unit cell

77   was refined by a least-squares algorithm within the CrysAlis Pro Package (Agilent

78   Technologies 2011) from 3248 reflections between 3.16 and 29.43°θ. A total of 14213

79   reflections for all three twin-domains was collected.

80   Data reduction was performed for three twin domains described by the twin matrices.

81   Data were corrected for background, Lorentz and polarization effects, and an analytical

82   correction for absorption was applied (Clark and Reid 1995) with corresponding R_{int} = 0.0878

83   for the strongest twin domain. There were 2016 unique and 1687 observed [I_{obs} > 3σ(I)]

84   reflections for that twin domain.

85   The structure was solved by the charge-flipping algorithm of the Superflip program

86   (Palatinus and Chapuis 2007) and subsequently refined using the JANA2006 software

87   (Petříček et al. 2006). Details of the data collection and structure refinement are listed in

88   Table 1. The solution provided a structure model, which refined to $R_{1\ (obs)}$ = 0.0425, $R_{1\ (all)}$ =

89   0.0538 and $wR_{2\ (all)}$ = 0.0526 with a GOF$_{all}$ = 1.51. The U and Na displacement parameters

90   were refined anisotropically, with the remaining atoms treated with isotopic displacement

91   parameters. All sites were fully occupied. Final atomic coordinates and displacement

92   parameters are given in Table 2, selected bond distances in Table 3 and bond-valence analysis

93   is listed in Table 4.

94

95   *Powder diffraction*

96   In order to support the selected monoclinic unit cell and space group, powder

97   diffraction data for čejkaite were acquired, since powder diffraction is not affected by

98   twinning. Powder data were collected from a flat sample in Bragg-Brentano geometry using a

99   PANalytical Empyrean powder diffractometer equipped with a Cu X-ray tube and PIXcel^{3D}

100   solid-state detector. The powder pattern was measured from 6° to 80° 2θ with a step size

101   0.013° 2θ and a counting time 40s per step (details of the measurement: CuK$_{α1,2}$, Ni beta

102   filter, incident 1/4° fixed divergence slit, 0.02 rad incident and diffracted Soller slits). Prior to

103   this measurement the diffractometer was calibrated against a LaB_6 standard with the same

104   settings. Data were processed by the Jana2006 software (Petříček et al. 2006) utilizing LeBail

105   decomposition of the diffraction pattern (variables: background, shift, *FWHM* function, unit

106   cell parameters, asymmetry by divergence) (Fig. 2). Data were corrected for serial

107   correlations after Bérar and Lelann (1991). The fit resulted in residuals $R_p = 0.0269$, $R_{wp} =$

108   0.0383 (with GOF = 1.66). Refined unit cell parameters for the LeBail fit are $a = 9.2944(4)$

109   Å, $b = 16.0967(7)$ Å, $c = 6.4356(3)$ Å, $\beta = 91.410(5)°$ with $V = 962.53(4)$ Å^3.

110   Since diffraction data for čejkaite with *hkl* indices based on previous descriptions are

111   available, we provide here new diffraction data indexed according to the monoclinic unit cell

112   (Table 5). Single-peak fitting procedure was done by Xfit software (Cheary and Coelho 1992;

113   1998a,b; Cheary et al. 2004) utilizing a split PearsonVII shape function. Unit cell parameters

114   were refined by a non-linear least-squares algorithm in the Unitcell program (Holland and

115   Redfern 1997), giving: $a = 9.294(1)$ Å, $b = 16.105(4)$ Å, $c = 6.442(1)$ Å, $\beta = 91.40(2)°$ with V

116     $= 963.9(4)$ Å^3.

117

118   **CRYSTAL STRUCTURE OF ČEJKAITE**

119   We present here the structure of čejkaite in the non-centrosymmetric monoclinic space

120   group *Cc*. The output from the Superflip program (Palatinus and Chapuis 2007) indicated

121   *C2/c* symmetry from the distribution of electron density (F_o). The program Superflip may

122   encounter some problems when used for structure solution from data affected by twinning.

123   Further, the refinement indicated that the symmetry operators for *C2/c* are applicable only for

124   the heavy atoms. Space group *Cc* provided an acceptable refinement for the light atoms and

125   generated reasonable positions of the CO_3 groups. Pseudo-hexagonal symmetry of the *hk0*

126   reciprocal lattice of čejkaite, reported from SAED by Ondruš et al. (2003), was also

127   encountered in the current data and we concluded that this pseudo-symmetry is due to the

128   positions of U atoms in the structure only. The contribution of the U atom in the structure is

129   displayed in Fig. 3a, giving a pseudohexagonal pattern where viewed along c*. The light

130   atoms are inconsistent with the pseudo-hexagonality as shown by the difference in the

131   intensities of reflections Fig. 3b. The choice of the unit cell by Ondruš et al. (2003)

132   apparently overlooked centering of the cell, which not unexpected for powder data. However,

133   the triclinic symmetry of čejkaite reported by Ondruš et al. (2003), as derived from the

134   Rietveld refinement (see the unit cell parameters), may have been questioned had higher

135   symmetry been sought (a comparison of the current unit cell choice and the unit cell of

136   Ondruš et al. (2003) is provided also on the Figure deposited as supplementary file). The

137   monoclinic space group was confirmed by powder diffraction, showing very good match

138   between calculated and observed diffractions. The diffraction peaks observed are consistent

139   with the proposed monoclinic unit cell (Fig. 2).

140   According to the single-crystal diffraction data, there is one symmetrically unique U

141   atom, three non-equivalent C atoms, four Na atoms and eleven O atoms in the asymmetric

142   unit of the čejkaite structure. The uranium atom is strongly bonded to two O atoms forming a

143   nearly linear uranyl ion $(UO_2)^{2+}$, with <O10–U–O11> angle 172.4(3)°. The bond-lengths

144   obtained from the refinement (Table 3) are higher than the value given by Burns et al. (1997),

145   1.80 Å, as the most common for [8]–coordinated U atom. However, we are convinced that

146   obtained value arises from the quality of data, affected by some unresolved twinning features.

147   The uranyl ion is further coordinated by six O atoms, arranged in the equatorial apices of

148   hegaxonal bipyramids. The three edges of the bipyramid are shared with planar CO_3^{2-} groups,

149   forming the basic structural motif, a characteristic uranyl tricarbonate cluster,

150     $[(UO_2)(CO_3)_3]^{4-}$ (Fig. 4). This cluster has been found in chemically related, however not

151   isotypic, minerals such as agricolaite, $K_4[(UO_2)(CO_3)_3]$, $C2/c$ (Skála et al. 2011) and

152   grimselite, $K_3Na[(UO_2)(CO_3)_3]$, $P–62/c$ (Li and Burns 2001; Plášil et al. 2012). Uranyl

153 tricarbonate clusters are oriented with their equatorial planes perpendicular to [001]. All Na$^+$

154 cations in the čejkaite structure are [6]–coordinated by O atoms. The coordination polyhedron

155 around Na1 atoms is a strongly distorted (Na1Φ_6) octahedron, sharing its trigonal faces with

156 two other (Na1Φ) octahedra, and thus forming irregular columns along [001]. Polyhedra

157 (Na2Φ), (Na3Φ) and (Na4Φ) share common edges, forming a triplet, with composition

158 Na$_3$O$_{16}$ (Fig. 5). These triplets are also linked with (Na1Φ) polyhedra by sharing apices, and

159 due to this linkage a complex uranyl–carbonate–(NaΦ) sheet extends sub-parallel to (001) in

160 čejkaite. These sheets are then interconnected through the O$_{Ur}$ atoms, in common edge of the

161 triplets, and by irregular columns of (Na1Φ) polyhedra. Structure refinement and bond-

162 valence analysis (Table 4) confirmed the formula proposed for čejkaite by Ondruš et al.

163 (2003), Na$_4$(UO$_2$)(CO$_3$)$_3$, $Z = 4$.

164

165   **ACKNOWLEDGEMENTS**

175

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250

251   **Caption to Figures**

252   Figure 1. Aggregates of long prismatic čejkaite crystals on a limonite matrix. FOV 5 mm
253   (photo P. Škácha).

254

255   Figure 2. LeBail decomposition of the diffraction data of čejkaite, performed for the
256   monoclinic space group *Cc*. All observed diffraction peaks are described by the model except
257   one, which belongs to an admixture of quartz (indicated on the difference profile).

258

259   Figure 3. Reciprocal space reconstruction of the *hk0* layer based on I_{calc}, **a)** where only U
260   atoms are included in the calculation, showing apparent pseudohexagonal symmetry, **b)**
261   where only the "light" atoms (all except uranium) are included in the calculation, showing the
262   violation of pseudohexagonal symmetry. The reciprocal unit-cell is displayed with a* red and
263   b* green.

264

265   Figure 4. Cluster of polyhedra around the U atom in the structure of čejkaite, coordinated by
266   eight O atoms to form a hexagonal uranyl bipyramid that shares three edges with C1, C2 and
267   C3 carbonate groups and the remaining three edges with Na2 and Na3 polyhedra. Na1

268   polyhedra share their trigonal faces (parallel to the plane of the sketch) and form columns
269   extending in the [001] direction.
270
271   Figure Supplementary. Reciprocal space view of single-crystal data of čejkaite; along a) c*,
272   showing all three twin domains, b) b*, with splitting of reflections contributed from the
273   second twin domain reflections, c) c*, where the comparison of pseudohexagonal unit cell
274   given by Ondruš et al. (2003), in thin lines, and currently obtained unit cell settings
275   (centered), in thicker lines. The reciprocal unit cell is displayed with a* red, b* green and c*
276   blue.
277

Čejkaite, LeBail refinement
(for *Cc* space group)

Quartz, $d_{011} = 3.34$ Å

a)   b)

3

4
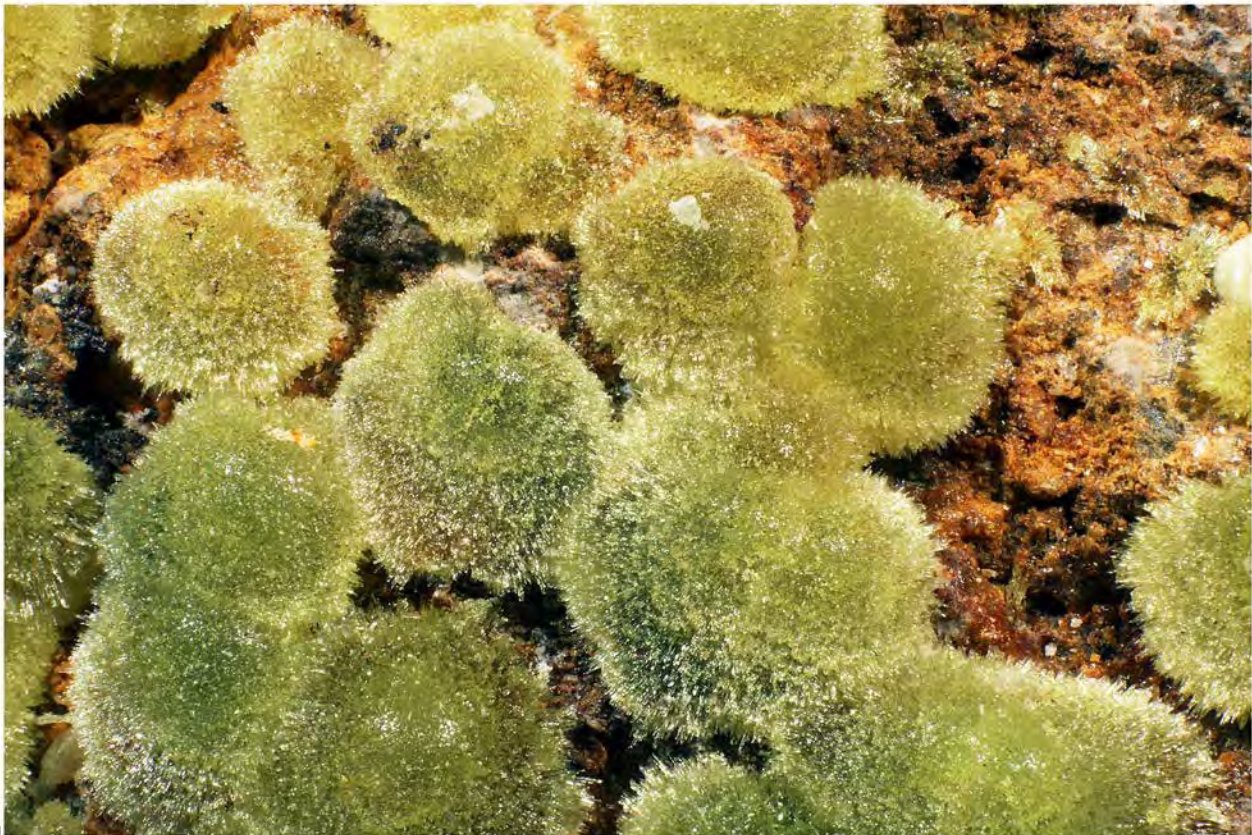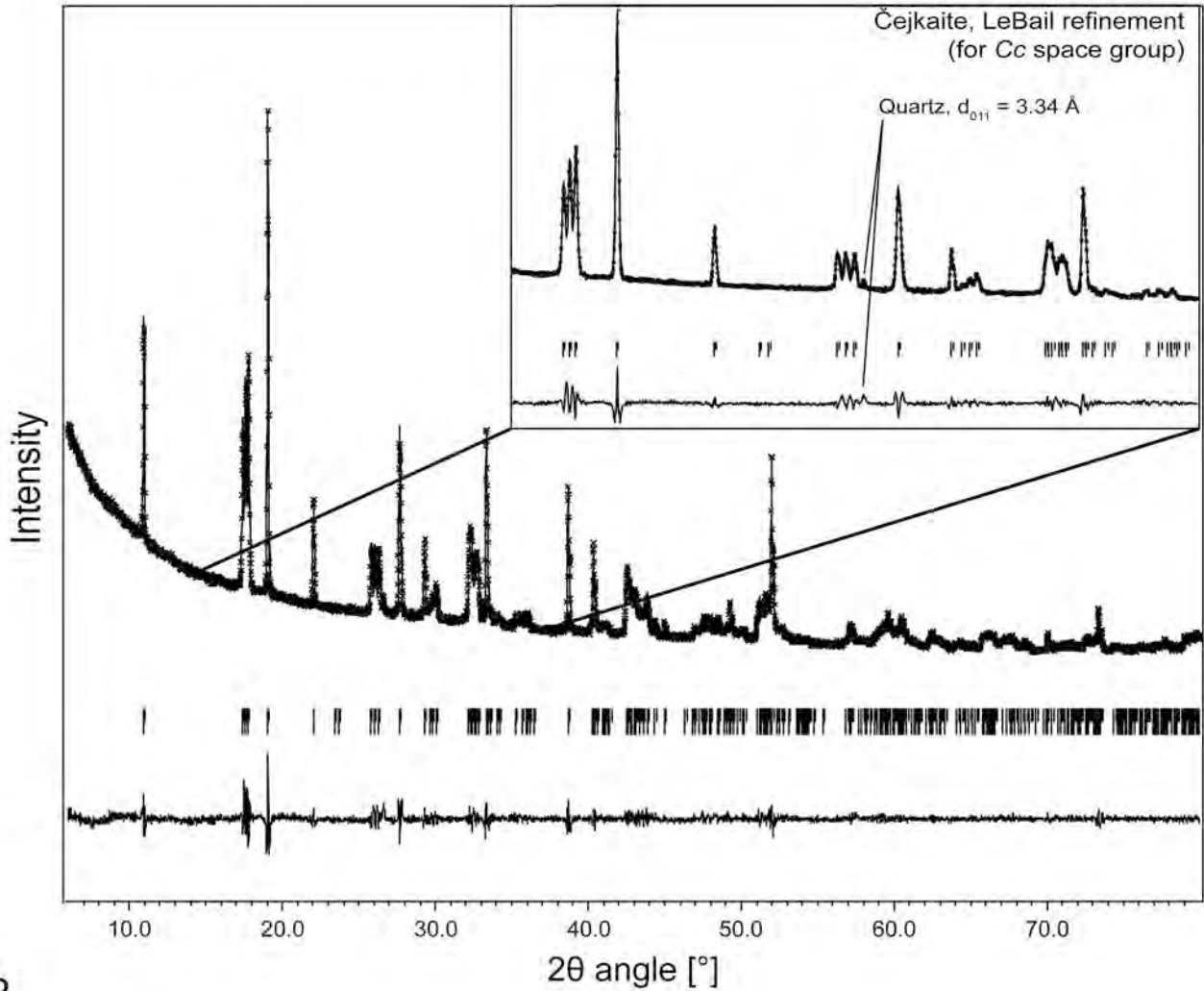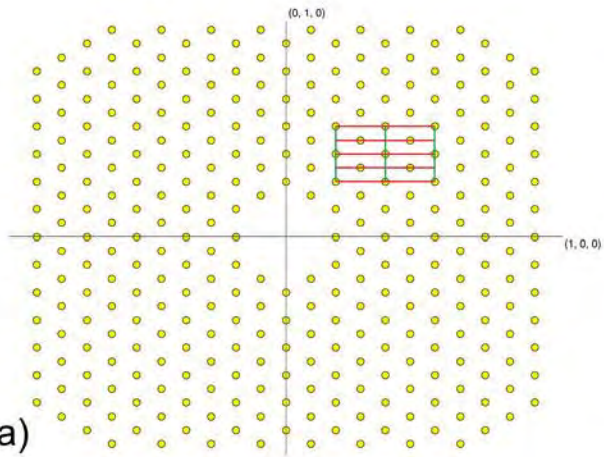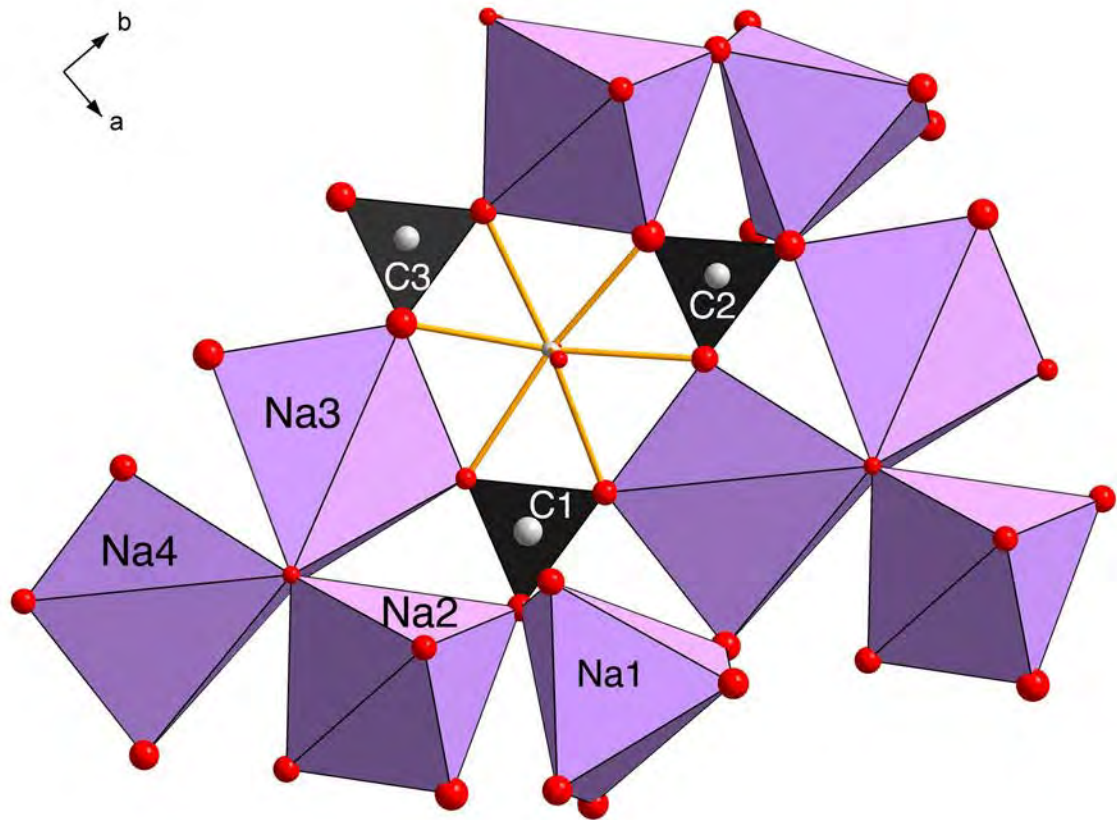
Tables

TABLE 1. Summary of data collection conditions and refinement parameters for čejkaite.

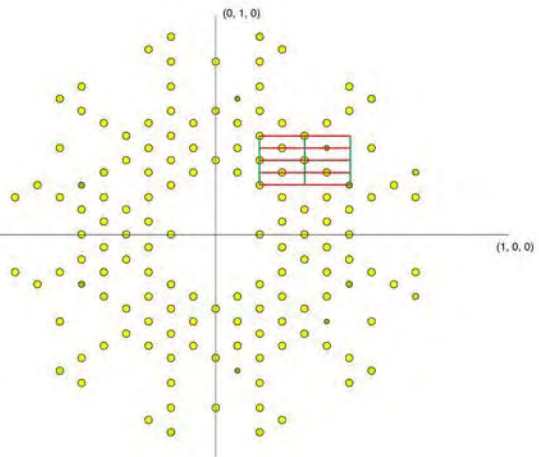| Crystal data	
Structural formula	$Na_4(UO_2)(CO_3)_3$
Space group	*Cc*
Unit-cell parameters	
a (Å)	9.2919(8)
b (Å)	16.0991(11)
c (Å)	6.4436(3)
β (°)	91.404(5)
V (Å^3)	963.62(12)
Z	4
Calculated density (g/cm^3)	3.74
μ (mm^{-1}), correction type	17.00, analytical
T_{min}/T_{max}	0.346/0.755
Crystal size (mm)	0.17×0.02×0.02
Data collection	
Radiation, wavelength (Å)	Mo*K*α, 0.71073
θ range for data collection (°)	3.16 – 29.43
h, *k*, *l* ranges	-11<*h*<12, -20<*k*<22, -8<*l*<8
Axis, frame width (°), time per frame (s)	ω, 0.9, 60
Total reflections collected	14123
Unique reflections	2016
Unique observed reflections [$I_{obs}>3\sigma(I)$]	1687
Data completeness to θ$_{max}$ (%), R_{int}	99.80, 0.0878
Structure refinement by JANA2006	
Refinement method	Full-matrix least-squares on *F*
No. parameters, constraints, restraints	103, 3, 2
Weighting details	σ, w = 1/(σ^2(*I*) + 0.004I^2)
R_1, wR_2 for [$I_{obs}>3\sigma(I)$]	0.0424, 0.0507
R_1, wR_2 for all data	0.0537, 0.0528
Goodness-of-fit (S) on F_{obs}/on F_{all}	1.51/1.43
Largest diff. peak and hole (e/Å^3)	4.28, -2.14
Twin fractions	0.40(5)/0.32(4)/0.28(4)
Twin matrices Tw$_{1,2}$; Tw$_{1,3}$	$\begin{pmatrix} -0.5 & -0.5 & 0 \\ 1.5 & -0.5 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \begin{pmatrix} 0.5 & 0.5 & 0 \\ 1.5 & -0.5 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

TABLE 2. Atomic coordinates, site occupancies and atomic displacement parameters (in Å^2) for čejkaite.

Atom	x	y	z	U_{eq}	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
U	0.43392(8)	0.33354(4)	0.32192(7)	0.01095(16)	0.0090(3)	0.0080(3)	0.0159(3)	-0.0001(4)	0.0020(2)	-0.0014(4)
Na1	0.437(3)	-0.0026(12)	0.073(3)	0.025(2)	0.026(4)	0.024(4)	0.025(2)	0.001(3)	0.005(2)	-0.003(3)
Na2	0.6545(10)	0.3473(5)	-0.1412(12)	0.022(2)	0.020(5)	0.012(4)	0.034(4)	0.002(3)	0.000(3)	-0.003(3)
Na3	0.3456(10)	0.2161(5)	-0.1967(14)	0.029(3)	0.012(4)	0.019(5)	0.056(4)	0.010(4)	0.002(4)	0.005(4)
Na4	0.3039(10)	0.4363(5)	0.7959(13)	0.026(3)	0.006(4)	0.019(4)	0.052(5)	-0.003(3)	0.003(3)	-0.002(3)
C1	0.634(2)	0.130(2)	-0.161(3)	0.019(4)						
C2	1.023(3)	0.337(1)	-0.160(3)	0.017(4)						
C3	0.643(2)	0.535(2)	-0.205(3)	0.023(4)						
O1	0.236(2)	0.573(1)	0.872(2)	0.026(3)						
O2	0.896(2)	0.311(1)	-0.137(2)	0.030(3)						
O3	0.508(2)	0.1081(10)	-0.153(2)	0.024(3)						
O4	1.064(2)	0.4098(9)	-0.160(2)	0.026(3)						
O5	0.178(2)	0.1163(9)	-0.240(2)	0.018(3)						
O6	0.682(2)	0.2049(9)	-0.165(2)	0.019(3)						
O7	0.507(2)	0.5217(8)	0.823(2)	0.013(2)						
O8	0.733(2)	0.4806(9)	-0.211(2)	0.020(3)						
O9	0.116(2)	0.2748(10)	-0.193(2)	0.020(3)						
O10	0.455(2)	0.334(1)	0.607(2)	0.010(2)*						
O11	0.438(2)	0.332(1)	0.030(2)	0.010(2)*						

U_{eq} is defined as a third of the trace of the orthogonalized U_{ij} tensor; the anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$. * atoms were constrained to have same U_{eq}

TABLE 3. Selected interatomic distances and polyhedral geometry for čejkaite.

U1–O1[i]	2.402(17)	C1–O1[vii]	1.34(3)	C3–O5[ix]	1.37(3)
U1–O2[ii]	2.377(17)	C1–O3	1.22(3)	C3–O7[viii]	1.30(3)
U1–O5[iv]	2.447(15)	C1–O6	1.29(3)	C3–O8	1.21(3)
U1–O6[ii]	2.421(15)	<C1–O>	1.28	<C3–O>	1.29
U1–O7[i]	2.426(13)				
U1–O9[iv]	2.434(15)	C2–O2	1.27(3)		
U1–O10	1.841(11)	C2–O4	1.23(2)		
U1–O11	1.885(11)	C2–O9[ix]	1.35(3)		
<U–O$_{Ur}$>	1.86	<C2–O>	1.28		
<U–O$_{Eq}$>	2.42				
Na1–O3		2.40(3)	Na2–O2		2.31(2)
Na1–O3[v]		2.52(2)	Na2–O5[iv]		2.656(15)
Na1–O4[ii]		2.55(3)	Na2–O6		2.313(17)
Na1–O4[vi]		2.39(3)	Na2–O8		2.313(17)
Na1–O8[ii]		2.41(3)	Na2–O10[viii]		2.443(18)
Na1–O8[vi]		2.62(3)	Na2–O11		2.33(2)
<Na1–O>		2.48	<Na2–O>		2.39
Na3–O2[iv]		2.918(17)	Na4–O1		2.340(19)
Na3–O3		2.314(18)	Na4–O1[iii]		2.794(16)
Na3–O5		2.251(17)	Na4–O4[xii]		2.292(19)
Na3–O9		2.333(18)	Na4–O7		2.335(16)
Na3–O10[viii]		2.506(19)	Na4–O10		2.507(19)
Na3–O11		2.501(19)	Na4–O11[xiii]		2.561(19)
<Na3–O>		2.47	<Na4–O>		2.47

Symmetry codes: (i) x, −y+1, z−1/2; (ii) x−1/2, −y+1/2, z+1/2; (iii) x, −y+1, z+1/2; (iv) x+1/2, −y+1/2, z+1/2; (v) x, −y, z+1/2; (vi) x−1/2, y−1/2, z; (vii) x−1/2, y+1/2, z+1; (viii) x, y, z−1; (ix) x+1, y, z; (x) x+1/2, −y+1/2, z−1/2; (xi) x+1/2, y+1/2, z; (xii) x+1, y, z−1; (xiii) x, y, z+1; (xiv) x−1/2, y−1/2, z−1; (xv) x−1/2, −y+1/2, z−1/2.

TABLE 4 Bond-valence analysis for čejkaite.

	U	Na1	Na2	Na3	Na4	C1	C2	C3	∑BV
O1	0.51				0.30	1.14			1.95
O2	0.53		0.25	0.05			1.38		2.21
O3		0.34		0.25		1.58			2.17
O4		0.34			0.27		1.54		2.15
O5	0.47		0.10	0.30				1.06	1.93
O6	0.49		0.25			1.31			2.05
O7	0.49				0.24			1.28	2.01
O8		0.30	0.25					1.63	2.18
O9	0.48			0.24			1.11		1.83
O10	1.50		0.18	0.15	0.15				1.98
O11	1.38		0.24	0.15	0.13				1.89
∑BV	5.84	0.98	1.27	1.14	1.09	4.03	4.03	3.97	

Notes: Values are expressed in valence units (vu). Na–O, bond strengths from Brown and Altermatt (1985); C–O bond strengths from Brese and O'Keeffe (1991); U^{6+}–O bond strengths ($r_0 = 2.051$, $b = 0.519$) from Burns et al. (1997).

Table 5 Powder diffraction data for čejkaite.

I_{rel}	d_{obs}	d_{calc}	h	k	l	I_{rel}	d_{obs}	d_{calc}	h	k	l
42	8.058	8.052	0	2	0	7	2.0631	2.0632	1	1	3
		8.047	1	1	0			2.0618	0	6	2
31	5.084	5.081	-1	1	1	3	2.0394	2.0397	3	3	2
41	5.029	5.029	0	2	1	3	2.0132	2.0131	0	8	0
47	4.971	4.977	1	1	1			2.0117	4	4	0
100	4.647	4.648	1	3	0	5	1.9088	1.9109	-2	2	3
		4.646	2	0	0			1.9087	4	4	1
22	4.025	4.026	0	4	0	4	1.8952	1.8957	-2	6	2
		4.023	2	2	0			1.8942	0	4	3
13	3.450	3.446	-2	2	1	4	1.8780	1.8774	2	2	3
13	3.415	3.414	0	4	1	4	1.8724	1.8735	2	6	2
13	3.380	3.380	2	2	1			1.8470	2	8	0
35	3.220	3.220	0	0	2	8	1.8469	1.8466	3	7	0
		3.043	1	5	0			1.8459	5	1	0
16	3.042	3.042	2	4	0	2	1.8299	1.8300	1	7	2
		3.041	3	1	0	2	1.8176	1.8195	3	5	2
2	3.009	3.012	-1	1	2	4	1.7873	1.7861	-5	1	1
4	2.9908	2.9897	0	2	2	7	1.7819	1.7824	-3	7	1
7	2.9687	2.9678	1	1	2	5	1.7776	1.7740	-3	1	3
15	2.7781	2.7761	-3	1	1	9	1.7703	1.7708	2	8	1
20	2.7714	2.7685	-2	4	1	4	1.7689	1.7683	3	7	1
19	2.7616	2.7603	-1	5	1			1.7675	-2	4	3
12	2.7419	2.7429	1	5	1	4	1.7619	1.7631	5	1	1
13	2.7326	2.7338	2	4	1			1.7571	1	9	0
43	2.6839	2.6841	0	6	0	39	1.7565	1.7562	4	6	0
22	2.6792	2.6823	3	3	0			1.7559	5	3	0
3	2.6656	2.6623	-1	3	2	3	1.7483	1.7475	1	5	3
2	2.6314	2.6317	1	3	2	3	1.7401	1.7408	2	4	3
1	2.6163	2.6165	2	0	2	3	1.7342	1.7342	3	1	3
2	2.5441	2.5406	-2	2	2	1	1.7078	1.7070	0	8	2
3	2.5155	2.5147	0	4	2	1	1.6912	1.6901	4	4	2
3	2.4873	2.4883	2	2	2	4	1.6106	1.6099	0	0	4
30	2.3241	2.3238	2	6	0			1.6105	0	10	0
		2.3228	4	0	0	4	1.5627	1.5657	-4	2	3
19	2.2327	2.2331	1	7	0	4	1.5552	1.5570	-5	3	2
		2.2322	3	5	0	7	1.5493	1.5492	3	9	0
		2.2316	4	2	0			1.5485	6	0	0
2	2.2172	2.2208	-1	5	2	6	1.5289	1.5299	4	6	2
2	2.2018	2.2028	1	5	2			1.5292	4	2	3
2	2.1909	2.1938	2	4	2	3	1.4865	1.4881	-6	2	1
14	2.1224	2.1244	-4	2	1			1.4861	-4	8	1
		2.1212	-3	5	1			1.4462	1	11	0
11	2.1136	2.1140	-1	7	1	2	1.4458	1.4454	5	7	0
9	2.1059	2.1060	1	7	1			1.4452	6	4	0
9	2.0978	2.0977	3	5	1	3	1.4172	1.4173	-6	4	1
5	2.0819	2.0851	-1	1	3			1.4168	-5	1	3
		2.0830	-3	3	2	3	1.3819	1.3806	-5	7	1
5	2.0754	2.0741	0	2	3						