

1 **Revision 1**

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3 **Finchite, Sr(UO₂)₂(V₂O₈)·5H₂O, a new uranyl sorovanadate with the francevillite anion**
4 **topology**

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28 **ABSTRACT**

29 Finchite (IMA2017-052), Sr(UO₂)₂(V₂O₈)·5H₂O, is the first uranium mineral known to contain
30 essential Sr. The new mineral occurs as yellow-green blades up to ~10 μm in length in surface
31 outcrops of the calcrete-type uranium deposit at Sulfur Springs Draw, Martin County, Texas,
32 USA. Crystals of finchite were subsequently discovered underground in the Pandora mine, La
33 Sal, San Juan County, Utah, USA, as diamond-shaped golden-yellow crystals reaching up to
34 1 mm. The crystal structure of finchite from both localities was determined using single crystal
35 X-ray diffraction and is orthorhombic, *Pcan*, with $a = 10.363(6)$ Å, $b = 8.498(5)$ Å, $c =$
36 $16.250(9)$ Å, $V = 1431.0(13)$ Å³, $Z = 4$ ($R_1 = 0.0555$) from Sulfur Springs Draw; and $a =$

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37 10.3898(16), $b = 8.5326(14)$, $c = 16.3765(3)$ Å, $V = 1451.8(4)$ Å³, $Z = 4$ ($R_1 = 0.0600$) from the
38 Pandora mine. Electron-probe microanalysis provided the empirical formula
39 $(\text{Sr}_{0.88}\text{K}_{0.17}\text{Ca}_{0.10}\text{Mg}_{0.07}\text{Al}_{0.03}\text{Fe}_{0.02})\Sigma_{1.20}(\text{UO}_2)_2(\text{V}_{2.08}\text{O}_8) \cdot 5\text{H}_2\text{O}$ for crystals from Sulfur Springs
40 Draw, and $(\text{Sr}_{0.50}\text{Ca}_{0.28}\text{Ba}_{0.22}\text{K}_{0.05})\Sigma_{0.94}(\text{U}_{0.99}\text{O}_2)_2(\text{V}_{2.01}\text{O}_8) \cdot 5\text{H}_2\text{O}$ for crystals from the Pandora
41 mine, based on 17 O atoms per formula unit. The structure of finchite contains uranyl vanadate
42 sheets based upon the francevillite topology. Finchite is a possible immobilization species for
43 both uranium and the dangerous radionuclide ⁹⁰Sr because of the relative insolubility of uranyl
44 vanadate minerals in water.

45 INTRODUCTION

46 Uranyl vanadate minerals are ubiquitous where uranium and vanadium ore has oxidized due to
47 their limited aqueous solubility over a range of geochemical conditions (Barton 1958; Weeks
48 1961; Tokunaga 2012; Plášil 2014) and are important in limiting the environmental mobility of
49 the UO_2^{2+} uranyl ion (Avasarala et al. 2017). Several uranyl vanadate minerals contain sheets
50 with the francevillite anion topology, which is compatible with interstitial cations of varying
51 size, coordination, and ionic charge (Cesbron and Morin 1968; Krivovichev et al. 2013), leading
52 to extensive solid solution between species (Spano et al. 2017a). Finchite, a newly recognized
53 uranyl vanadate mineral species described herein, possesses the francevillite anion topology and
54 represents a Sr-bearing end-member of the francevillite–curienite solid solution series (Spano
55 et al. 2017b).

56 The name *finchite* honors American uranium geologist Warren I. Finch (1924–2014). Mr.
57 Finch worked at the U.S. Geological Survey (USGS) as a uranium resource specialist for
58 50 years, and the new mineral was discovered as part of a continuation of the exploration
59 program that he devoted his life to promoting. Mr. Finch received his bachelor's of science

60 degree in geological engineering from the South Dakota School of Mines and Geology in 1948
61 and his master's of science degree in geology from the University of California, Berkeley, in
62 1954. He pursued additional graduate study at the Colorado School of Mines from 1958 to 1959.
63 Mr. Finch first joined the USGS in 1948 as a field assistant and spent his entire 50-year
64 professional career at that institution, advancing to the rank of senior scientist. He was awarded
65 the Meritorious (1981) and Distinguished (1994) Service Awards from the Department of the
66 Interior and served as the first chief of the Uranium and Thorium Resources Branch from 1973 to
67 1979. In 1974, he began a decades-long association with the International Atomic Energy
68 Agency, serving as U.S. representative and technical expert in the areas of uranium resources,
69 uranium resource estimation, and particularly the geology of sandstone-hosted uranium deposits.
70 In this capacity, Mr. Finch was privileged to visit many of the major uranium deposits of the
71 world. Mr. Finch published extensively, including the highly cited 1967 USGS professional
72 paper "Geology of epigenetic uranium deposits in sandstone in the United States," which is still
73 recognized as a definitive work on the subject (Finch 1967). This publication was the
74 culmination of many years (1949–1961) devoted to his career-long fascination with the uranium
75 geology and uranium resources of the Colorado Plateau region, which continue to be explored
76 today.

77 Samples of finchite are deposited in the mineralogical collections of the Natural History
78 Museum of Los Angeles County, 900 Exposition Boulevard, Los Angeles, CA 90007, USA,
79 catalogue numbers 66476 and 66477.

80 OCCURRENCE

81 Finchite was found in surface outcrops approximately 21 miles south–southeast of
82 Lamesa, Texas, on the eastern edge of Sulfur Springs Draw, Martin County, Texas. A calcrete-

83 type uranium deposit, the Sulfur Springs Draw Deposit, was identified in this area by the Kerr-
84 McGee Corporation in the late 1970s by aerial radiometric surveys of the region (Van Gosen and
85 Hall 2017; Hall et al. 2019). Uranium mineralization is concentrated just above the modern water
86 table in a 30-meter-thick section of calcareous siltstones and fine-grained sandstones capped by
87 pedogenic calcrete up to 6 meters thick. The deposit is partially exposed along the edge of Sulfur
88 Springs Draw by a farm road that was cut into caprock to access the draw. USGS geologists
89 located the exposed mineralization in 2015 and collected samples of yellow uranyl vanadates
90 that coat grains, fill vugs, and line fractures in a calcareous, very fine-grained to fine-grained
91 sandstone and massive carbonate (Figure 1).



92

93 *Figure 1. Finchite and carnotite coating dolomite, Sulfur Springs Draw, Texas.*

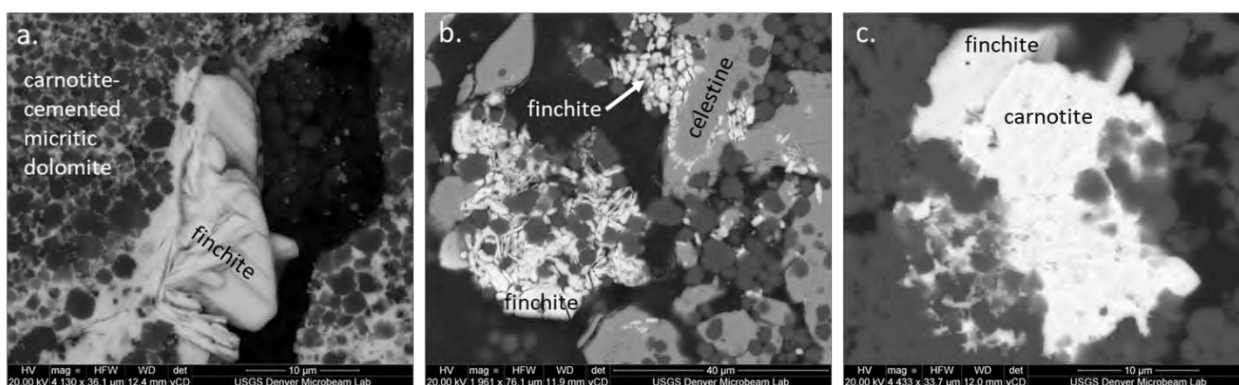
94 Finchite is found in the late Pleistocene Tahoka Formation (Hall et al. 2019), which is
95 thought to be lacustrine based on regional facies relationships and fossil evidence (Frye 1968;
96 Van Gosen and Hall 2017). The Tahoka Formation is exposed rimming approximately 30 large

97 saline lakes of the Southern High Plains. It is a fine-grained, locally calcareous and gypsiferous
98 sandstone that grades laterally into gravel deposits. In the exploration model employed by Kerr-
99 McGee, the lacustrine strata that host the Sulphur Springs Draw and nearby Buzzard Draw
100 deposits were genetically associated with a large Pleistocene lake located downstream. This large
101 prehistoric saline lake has been named Lake Lomax and is the largest Pleistocene-age lake
102 identified in the Southern High Plains region (Frye 1968; Van Gosen and Hall 2017).

103 At Sulfur Springs Draw, finchite occurs intimately with carnotite and appears as disseminated
104 pore fill and as cross-cutting veinlets in the micritic dolomite host (Figure 2). Paragenetically
105 later than carnotite, finchite occurs predominantly as bladed crystals and crystal aggregates up to
106 approximately 10 μm in width, and as late-stage space fill of powdery masses (Figure 2a–c).
107 Crystals exceeding 10 μm are rare, which is likely due to the low solubility of finchite, causing it
108 to precipitate in very fine-grained crystals. In places, finchite coats earlier carnotite and (Figure
109 2c) and is intergrown with celestine (Figure 2b), the later indicating that the fluids that formed
110 finchite had become rich in Sr. Finchite likely formed under evaporative conditions from fluids
111 at approximately ambient surface temperatures (Ranalli and Yager 2016), which is supported by
112 the presence of accompanying dolomite and celestine. Other associated minerals include quartz,
113 illite, and an unidentified amorphous Sr-rich carbonate species.

114

115



116

117 *Figure 2. a. Backscatter SEM image of finchite crystals (Sulfur Springs Draw) filling a vug within micritic carnotite-cemented*
118 *dolomite. b. Finchite intergrown with celestine in micritic dolomite. C. Finchite associated with carnotite.*

119 Crystals of finchite were subsequently discovered underground in the Pandora mine, La
120 Sal, San Juan County, Utah, where it occurs as coatings on pandoraite-Ca and pandoraite-Ba, on
121 sandstone (Figure 3). The Pandora mine is located within the Paradox Valley district which was
122 formed by uplift and erosion of a salt anticline resulting in exposure of ore-bearing sandstone
123 (Carter and Gualtieri 1965). Significant bleaching alteration has been observed in this area
124 evidenced by gas fields in the Paradox Valley region, and petrographically through hematite
125 crystals preserved by quartz overgrowth. Bleaching alteration is intimately associated with
126 uranium and vanadium deposits here and has been proposed to either reduce hematite to pyrite or
127 reduce hematite and lead to dissolved Fe^{2+} and subsequent mobility away from host rocks.
128 Regardless of the mode of bleaching, the presence of hydrocarbons is believed to be the
129 mechanism responsible for alteration (Barton et al. 2018). Uranium and vanadium
130 mineralization at the Pandora mine was deposited under reducing conditions as solutions
131 containing these elements contacted accumulations of carbonaceous material, depositing
132 uraninite and montroseite- corvusite ore (Kampf et al. 2019). Post mining oxidation of these
133 montroseite-corvusite ores led to crystallization of finchite. At the Pandora mine, finchite
134 specimens occurs as aggregates and individuals reaching up to 100 μm in width (Figure 3).

135



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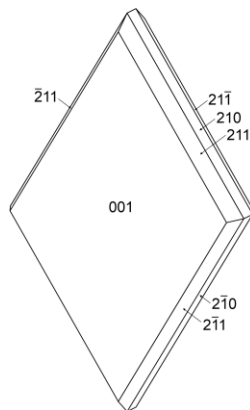
137 *Figure 3. Finchite and pandoraite-Ca from the Pandora Mine, La Sal Mining District, San Juan County, Utah. Horizontal field*
138 *of view is 1.13 mm.*

139

PHYSICAL AND OPTICAL PROPERTIES

140 Finchite crystals from both localities are bright yellow with a light-yellow streak and a pearly,
141 transparent luster. Based on scratch tests, the Mohs hardness of finchite is approximately 2, and
142 crystals are characterized by brittle tenacity, irregular fracture, perfect cleavage on (001) (Figure
143 4), and parting was not observed. Finchite does not fluoresce under short or long wave ultraviolet
144 light. Optically, finchite from the Pandora mine is biaxial (-), with $\alpha = 1.70(1)$, $\beta = 1.85(1)$, and
145 $\gamma = 1.90(1)$ (measured in white light). The $2V$ measured directly on a spindle stage is $53(1)^\circ$; the
146 calculated $2V$ is 55.9° . Dispersion is $r < v$, slight. The mineral is pleochroic: $X =$ colorless, Y and
147 Z are yellow; $X < Y \approx Z$. The optical orientation is $X = \mathbf{c}$, $Y = \mathbf{a}$, and $Z = \mathbf{b}$. Note that the
148 murkiness of the crystals required them to be split into thin cleavage fragments for the index of
149 refraction measurements, which made the measurement of α particularly difficult because it is
150 oriented perpendicular to the cleavage.

151



152

153 *Figure 4. Crystal drawing of finchite from the Pandora mine; clinographic projection in nonstandard orientation, [100] vertical.*

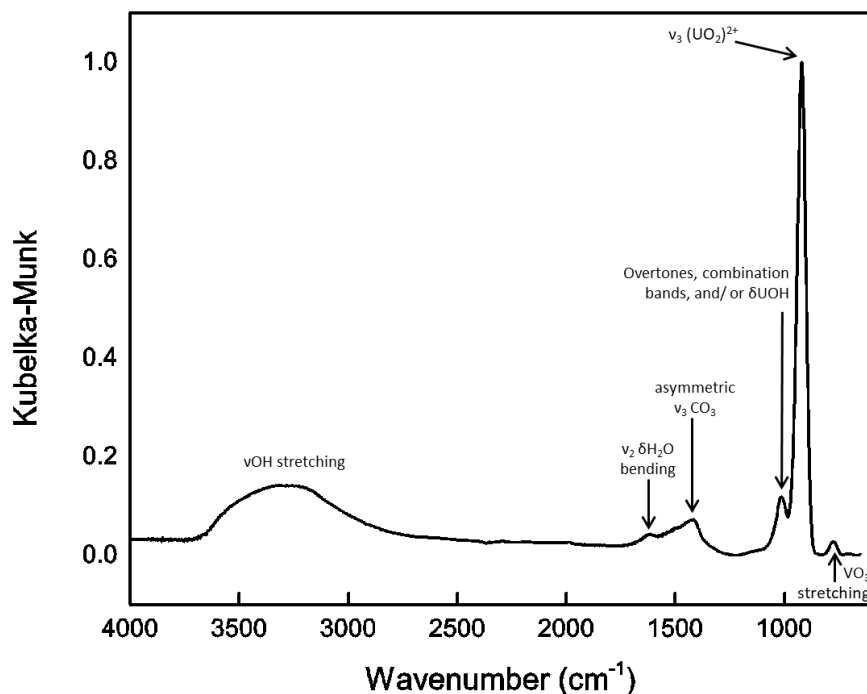
154 The calculated density of finchite is 4.429 and 4.352 g*cm⁻³ based on the empirical and
155 ideal formulae, respectively. The density could not be measured directly because it is higher than
156 that of Clerici solution. The predicted average index of refraction based upon the Gladstone–
157 Dale relationship is 1.85, using $k(\text{UO}_3) = 0.134$ under the assumption that vanadates are
158 analogous to uranyl phosphates and arsenates (Piret and Deliens 1989).

159

INFRARED SPECTROSCOPY

160 Attenuated total reflectance Fourier transform infrared spectra were obtained using a liquid N₂-
161 cooled SENSIR Technologies IlluminatIR mounted to an Olympus BX51 microscope. An
162 attenuated total reflectance objective was pressed into crystals of finchite and the spectrum was
163 measured from 4000 to 650 cm⁻¹ (Figure 5). The ν OH stretching vibrations of interstitial H₂O
164 groups occur between ~2800 and 3600 cm⁻¹, with a maximum intensity occurring at 3282 cm⁻¹.
165 Approximate O–H···O hydrogen bond lengths calculated from the observed stretching
166 frequencies lie within the range 2.9 to 2.6 Å using the correlation function given by Libowitzky
167 (1999). The medium strong band at 1615 cm⁻¹ is assigned as the ν_2 (δ)-bending vibrations of
168 interstitial water molecules. The band located at 1415 cm⁻¹ may be a combination band but likely

169 corresponds to the asymmetric stretching of $\nu_3 \text{CO}_3$, originating from the close association of
170 finchite with dolomite (Gunasekaran et al. 2006).



171

172 *Figure 5. The infrared spectrum (attenuated total reflectance) of finchite.*

173 The strong antisymmetric uranyl stretch, $\nu_3 (\text{UO}_2)^{2+}$, occurs at 920 cm^{-1} , and VO_3
174 stretching modes are visible at 773 cm^{-1} (Cejka 1999). The uranyl cation bond length inferred
175 from the 920 cm^{-1} mode of finchite using the empirical relations given by Jones (1958) and
176 Glebov (1982) is 1.79 \AA , which is in excellent agreement with our X-ray crystallographic results.

177 No evidence is found for the presence of the IR-forbidden symmetric $\nu_1 (\text{UO}_2)^{2+}$ stretch.
178 However, a weak band at 1011 cm^{-1} may be attributed to $\delta\text{-U-O}$ modes of equatorial O atoms, or
179 to combination bands or overtones (Cejka 1999).

180

CHEMICAL ANALYSIS

181 Chemical analyses on crystals from both localities were performed using a JEOL JXA-8900
182 electron microprobe operating at an accelerating voltage of 15 kV, with a beam current of 20 nA
183 and 1 μm spot diameter. Matrix effects were accounted for using the $\phi(\rho z)$ correction routine
184 (Armstrong 1988). The empirical formula is calculated on the basis of 17 O and 2 U *apfu*.
185 Finchite from the Sulfur Springs Draw Deposit contains appreciable U, V, and Sr, with Ca and
186 minor Mg, Fe, Al, and K, with analytical results listed in Table 1. Owing to the small crystal size
187 and intimate association of finchite with carnotite and dolomite, the measured Ca concentrations
188 are likely higher than the actual content of finchite. Furthermore, significant dehydration
189 occurred upon contact of finchite with the microprobe beam leading to anomalously high totals
190 for all elements. Normalized data are also provided in Table 1. Because of the limited amount of
191 material available, the H₂O content was not measured and is instead calculated by stoichiometry
192 with respect to the structure, which on the basis of 17 O *apfu*, provided the empirical formula
193 $(\text{Sr}_{0.88}\text{K}_{0.17}\text{Ca}_{0.10}\text{Mg}_{0.07}\text{Al}_{0.03}\text{Fe}_{0.02})\Sigma_{1.20}(\text{UO}_2)_2(\text{V}_{2.08}\text{O}_8) \cdot 5\text{H}_2\text{O}$. The normalized values are in good
194 agreement with the ideal formula $\text{Sr}(\text{UO}_2)_2(\text{V}_2\text{O}_8) \cdot 5\text{H}_2\text{O}$ calculated from X-ray crystallographic
195 results, which requires SrO 10.96, UO₃ 60.35, V₂O₅ 19.19, and H₂O 9.50, totaling 100 wt%.

196 Crystals of finchite from the Pandora mine, which were much larger, presented less
197 difficulties during chemical analysis. The empirical formula (calculated on the basis of 17 O *apfu*)
198 is $(\text{Sr}_{0.50}\text{Ca}_{0.28}\text{Ba}_{0.22}\text{K}_{0.05})\Sigma_{0.94}(\text{U}_{0.99}\text{O}_2)_2(\text{V}_{2.01}\text{O}_8) \cdot 5\text{H}_2\text{O}$.

199

X-RAY CRYSTALLOGRAPHY AND STRUCTURE DETERMINATION

200 Single-crystal X-ray diffraction data were collected for finchite from Sulfur Springs Draw using
201 a Bruker Apex II CCD-based detector mounted on a three-circle Bruker Apex II Quazar
202 diffractometer with a microfocus source utilizing monochromated MoK α radiation ($\lambda =$

203 0.709 Å). Reflections were integrated and corrected for Lorentz, polarization, and background
204 effects using the Bruker program SAINT. A multiscan semiempirical absorption correction was
205 applied using equivalent reflections in SADABS-2012 (Bruker 2009). An initial structure model
206 was obtained by the intrinsic phasing method using SHELXT (Sheldrick 2015a) in the space
207 group *Pcan*. Refinement proceeded by full-matrix least-squares on F^2 using SHELXL-2016
208 (Sheldrick 2015b). Additional refinement details for Sulfur Springs Draw and Pandora Mine
209 samples are included in Table 2.

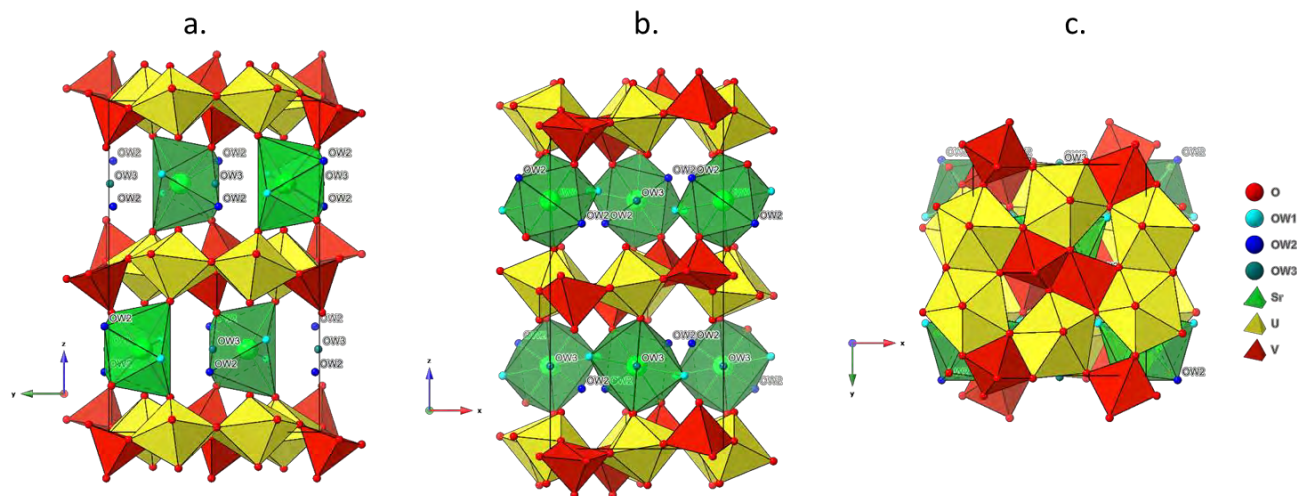
210 DESCRIPTION OF THE STRUCTURE

211 The structure solution of finchite from both localities located one U, one V, and six O sites that
212 make up a uranyl vanadate sheet, as well as one interstitial cation site occupied predominantly by
213 Sr (Figure 6). Chemical analyses indicate finchite from Sulfur Springs Draw contains
214 appreciable Ca and K at this site as well, and that finchite from the Pandora mine contains
215 significant Ca and Ba substitution. Three O atoms belonging to H₂O groups were also located
216 between the uranyl vanadate sheets. Positional and anisotropic displacement parameters were
217 successfully refined for all non-H atoms; however, a subsequent difference-Fourier synthesis did
218 not provide plausible H atom sites. Atomic coordinates and displacement parameters for each
219 refinement are contained in Supporting Information Tables S1 and S2, with selected bond
220 distances in Tables S3 and S4, and results of bond valence analyses in Tables S5 and S6 for
221 Sulfur Springs and Pandora finchite samples, respectively.

222 During refinement of finchite from Sulfur Springs draw, an initial model was produced
223 using free refinement of the interstitial cation site occupancy as only Sr. This resulted in an
224 occupancy of 1.05 Sr, suggesting that a heavier element may be present, or indicating a non-ideal
225 absorption correction. Instead, we forced the interstitial cation occupancies to match those

226 measured by electron microprobe. When modeled this way, the structure remains nearly identical
227 to our initial solution, yielding only a slight improvement in the agreement index.

228 During the refinement of the Pandora mine finchite structure, attempts to model the
229 interstitial site as $(\text{Sr}, \text{Ca}, \text{Ba}) = 1$, yielded a site containing very little Ca, ~ 0.8 Sr, and ~ 0.2 Ba.
230 Resultingly, we forced the site composition and occupancy to match that determined by EMPA
231 ($\text{Sr}_{0.5}$, $\text{Ca}_{0.28}$, and $\text{Ba}_{0.22}$) giving an agreement index of $R1 = 0.06$, $wR2 = 0.17$, slightly worse
232 than our refinement with only Sr and Ba present. This could indicate that the crystal used for
233 structure determination possesses slightly higher Sr and Ba content, and no Ca relative to the
234 crystal examined with EMPA. However, it is likely that substitution introduces positional
235 disorder, given the large differences in the ionic radii and bonding requirements of Ca, Sr, and
236 Ba, such that these atoms do not sit precisely at the site defined by the EAXY, EADP position
237 and ellipsoid.



239 *Figure 6. The crystal structure of finchite.*

240 As in other uranyl vanadate minerals and synthetic U(VI) vanadate compounds, U atoms
241 are strongly bonded to two O, giving the approximately linear uranyl ion UO_2^{2+} (Burns et al.

242 1997). Further coordination by five O in the equatorial plane, perpendicular to axial uranyl O
243 atoms, results in pentagonal bipyramidal coordination geometries. Pairs of pentagonal
244 bipyramidal U polyhedra share an edge, forming dimers. Similarly, V in the anionic sheet
245 occupies V_2O_8 dimers, where each V atom forms slightly distorted edge-sharing square
246 pyramidal polyhedra with the apex of each pyramid pointing in opposite directions. Pairs of
247 uranyl pentagonal bipyramids and V_2O_8 dimers form sheets that extend along [100] and [010]
248 (Figure 6), an identical structural unit found in other uranyl sorovanadates (Krivovichev et al.
249 2013; Spano et al. 2017b). In particular, the U & V sheet in finchite is indistinguishable from
250 those of francevillite and curienite (Cesbron and Morin 1968), as well as metatyuyamunite
251 (Burciaga-Valencia 2010). Additionally, chemical analyses indicate that finchite contains K, Ca,
252 Mg, Al, and Fe substituting for Sr. This is unsurprising given the extensive solid solution present
253 in the francevillite–curienite series and the close association of carnotite, tyuyamunite, and
254 strelkinite (K, Ca, and Al uranyl vanadates), respectively, in most U–V-bearing deposits (Finch
255 1967).

256 The uranyl vanadate sheets in finchite are linked through interstitial Sr^{2+} in eightfold
257 coordination as well as by an extensive network of H bonds formed between interstitial water
258 and O atoms of the sheet (Figure 6a–c). Sheets are stacked parallel to [001], corresponding to the
259 observed plane of perfect cleavage (Figure 6c). Four O atoms that coordinate Sr belong to the
260 $[(UO_2)_2(V_2O_8)]^{2-}$ sheets on either side (Figure 6a–b). Two O atoms coordinating Sr are apical O
261 atoms of V_2O_8 units (O6), and an additional two O atoms coordinating Sr are those of the uranyl
262 O atom O4 (Figure 6a–b). The remaining four O bonded to Sr belong to water (O_{w1} and O_{w2})
263 (Figure 6a–b). O_{w1} and O_{w2} likely participate in H bonding among themselves and to interstitial

264 O_{w3} , which is held in place by H bonding only, and the O_{y1} atom O2 located within the
265 $[(UO_2)_2(V_2O_8)]^{2-}$ sheet (Figure 6a–b).

266 Material paucity and the intimate association with carnotite, dolomite, and celestine
267 (Figure 2) precluded collection of powder X-ray diffraction data of finchite from Sulfur Springs
268 Draw, Texas. However, powder diffraction data were collected for a sample of finchite from the
269 Pandora mine, and results are included in Table S7 (supporting information). The powder
270 diffractogram of finchite was also simulated from single crystal data for the Sulfur Springs Draw
271 sample and is compared with experimental powder diffraction data from Pandora finchite in
272 Supporting Information Figure S1. Calculated d values and intensities derived from the single
273 crystal structure are presented in Table S8.

274 **IMPLICATIONS**

275 The uranium deposits in the US Southwest were heavily mined during the Cold War and the
276 many tons of uranium ore that were recovered from this region fueled plutonium-production
277 reactors in Washington and South Carolina. Legacies of this activity include hundreds of inactive
278 mines and their associated tailings (Avasarala et al. 2017; Avasarala et al. 2020), more than 228
279 large underground nuclear waste storage tanks in Washington (Peterson et al. 2008; Stubbs et al.
280 2009; Christensen et al. 2004) and South Carolina (Evans 1992), and extensive subsurface
281 contamination at former nuclear weapon production sites. Modeling the environmental transport
282 of U, radionuclides, and heavy metals, such as Sr, requires a detailed understanding of the
283 minerals that form and limit their mobility.

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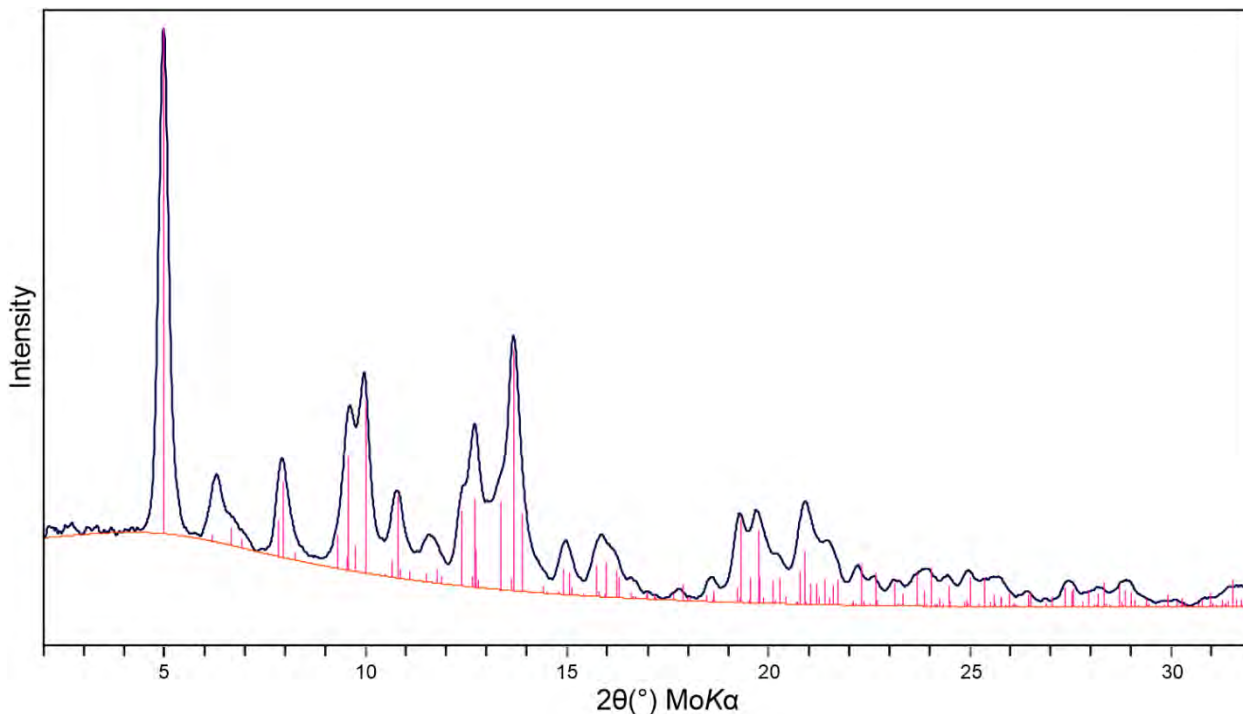
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376 **Supporting Information**

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Figure S1. Simulated powder diffraction data for finchite from Sulfur Springs Draw (red) compared with experimental diffraction data collected for Pandora finchite (blue).

Table 1. Chemical composition (in wt%) for finchite.

Constituent	Sulfur Springs Draw					Pandora mine			
	Mean (10 spots)	Range	Standard Dev.	Standard	Normalized	Mean (11 spots)	Range	Standard Dev.	Standard
K ₂ O	0.91	0.12-2.13	0.88	orthoclase	0.83	0.24	0.09-0.99	0.28	orthoclase
SrO	10.43	9.01-11.32	0.93	celestine	9.46	5.62	5.30-5.97	0.21	SrTiO ₃
CaO	0.65	0.48-0.94	0.19	wollastonite	0.59	1.67	1.48-1.82	0.10	wollastonite
BaO						4.18	3.87-4.46	0.20	barite
MgO	0.16	0.05-0.44	0.13	olivine	0.15				
FeO	0.08	0.00-0.11	0.03	syn. fayalite	0.07				
Al ₂ O ₃	0.19	0.00-0.31	0.08	anorthite	0.17				
V ₂ O ₅	21.57	20.99-22.32	0.41	V ₂ O ₅	19.57	19.74	19.14-20.28	0.38	V metal
UO ₃	65.60	64.49-66.57	1.11	syn. UO ₂	59.53	61.17	59.46-61.93	0.89	syn. UO ₂
H ₂ O*	10.61				9.63	9.75			
Total	110.20				100.00	102.37			

Table 2. Data collection and structure refinement details for finchite.

Crystal Data	Sulfur Springs Draw	Pandora mine
Diffraction	Bruker Apex II Quazar	Rigaku R-Axis Rapid II
X-ray radiation/power	MoK α ($\lambda = 0.71075$ Å)	MoK α ($\lambda = 0.71075$ Å)
Temperature	100(2) K	293(2) K
Structural Formula	(Sr _{0.88} K _{0.17} Ca _{0.10})(UO ₂) ₂ (VO ₄) ₂ ·5H ₂ O	(Sr _{0.50} Ca _{0.28} Ba _{0.22})(UO ₂) ₂ (VO ₄) ₂ ·5H ₂ O
Space group	<i>P</i> <i>ca</i> <i>n</i>	<i>P</i> <i>ca</i> <i>n</i>
Unit cell dimensions	<i>a</i> = 10.363(6) Å <i>b</i> = 8.498(5) Å <i>c</i> = 16.250(9) Å	<i>a</i> = 10.3898(16) Å <i>b</i> = 8.5326(14) Å <i>c</i> = 16.376(3) Å
<i>V</i>	1431.0(13) Å ³	1451.8(4) Å ³
<i>Z</i>	4	4
Density (for above formula)	4.352 g/cm ³	4.279 g/cm ³
Absorption coefficient	27.246 mm ⁻¹	26.966 mm ⁻¹
<i>F</i> (000)	1619	1612
Crystal size	14 × 10 × 3 μm	150 × 90 × 20 μm
θ range	2.51 to 24.99°	3.09 to 23.24°
Index ranges	-12 ≤ <i>h</i> ≤ 12, -10 ≤ <i>k</i> ≤ 10, -19 ≤ <i>l</i> ≤ 19	-10 ≤ <i>h</i> ≤ 11, -9 ≤ <i>k</i> ≤ 8, -18 ≤ <i>l</i> ≤ 18
Reflections collected/unique	13105/1259; <i>R</i> _{int} = 0.209	4561/997; <i>R</i> _{int} = 0.0793
Reflections with <i>F</i> > 4σ <i>F</i>	736	757
Completeness to θ_{\max}	100%	95.3%
Refinement method	Full-matrix least-squares on <i>F</i> ²	Full-matrix least-squares on <i>F</i> ²
Restraints/parameters	196/102	0/101
GoF (ref/all)	1.022/0.948	1.094/1.094
Final <i>R</i> indices [<i>F</i> > 4σ(<i>F</i>)]	<i>R</i> ₁ = 0.0555, <i>wR</i> ₂ = 0.1240	<i>R</i> ₁ = 0.0600, <i>wR</i> ₂ = 0.1576
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.1172, <i>wR</i> ₂ = 0.1490	<i>R</i> ₁ = 0.0796, <i>wR</i> ₂ = 0.1711
Largest diff. peak/hole	+3.28/-2.28 e·Å ⁻³	+2.58/-1.47 e·Å ⁻³

**R*_{int} = $\Sigma|F_o^2 - F_c^2(\text{mean})|/\Sigma[F_o^2]$. GoF = $S = \{\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)\}^{1/2}$. *R*₁ = $\Sigma||F_o| - |F_c||/\Sigma|F_o|$. *wR*₂ = $\{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$; *w* = $1/[\sigma^2(F_o^2) + (aP)^2 + bP]$ where *P* is $[2F_c^2 + \text{Max}(F_o^2, 0)]/3$, *a* is 0.0538, and *b* is 75.381 from Sulfur Springs Draw. From the Pandora mine, *a* is 0.0725, and *b* is 79.984.