Refinement of the crystal structure of potassium *catena*-carbonato-argentate(I), K[Ag(CO₃)]

Y.-Q. Zheng^{*I}, L.-X. Zhou^I, J.-L. Lin^I and S.-W. Zhang^{II}

^I Ningbo University, Chemistry Department, Institute for Solid State Chemistry, Ningbo, Zhejiang, 315211 P. R. China

^{II} Zhejiang University, Chemistry Department, Hangzhou, Zhejiang, 310028 P. R. China

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Abstract

AgCKO₃, orthorhombic, *Ibca* (No. 73), *a* = 20.389(3) Å, *b* = 5.775(1) Å, *c* = 5.944(1) Å, *V* = 699.9 Å³, *Z* = 8, *R*_{gt}(*F*) = 0.050, *wR*_{ref}(*F*²) = 0.119, *T* = 293 K.

Source of material

Colorless, slender needle-like crystals were grown according to [1, 2].

Discussion

The crystal structure of K[AgCO₃] established on the basis of the photographic data by Barclay & Hoskins in 1963 [2] indicated an abnormal carbonate group with the shortest and largest C—O bonds of 1.24 Å and 1.33 Å, respectively, in comparison with our observations [3]. In order to ascertain the anomaly, it is necessary to refine the crystal structure.

The crystal structure contains zigzag chains of [Ag(CO₃)₂]¹⁻ complex anions parallel [010] which are arranged in layers parallel to (100). In the 2D layers, the Ag atoms form a 3⁶ network with the bridging CO₃²⁻ groups perpendicular above and below. The Ag atoms are linearly bonded to two O atoms with *d*(Ag—O) = 2.085(3) Å and they are coordinated by six close Ag neighbors at 2.972 Å (2×), 3.199 Å (2×) and 3.299 Å (2×) which indicates some Ag—Ag interactions [3]. The C—O bond lengths are 1.272(7) Å for the uncoordinated O atom and 1.283(4) Å (2×) for the coordinated ones. The angle AgO—C—OAg is about 123.4°. Each K⁺ cation is surrounded by nine O atoms at the corners of a twisted mono-capped tetragonal antiprism (K—O: 2.665 Å (1×), 2.832 Å (2×), 2.855 Å (2×), 2.893 Å (2×), 2.977 Å (2×)). The layers are linked via strong K—O1 interactions along [100] (2.665 Å) forming a 2D fragment of the TII structure.

Table 1. Data collection and handling.

Crystal:	colorless, needle-like, size 0.09 × 0.11 × 0.44 mm
Wavelength:	Mo K _α radiation (0.71073 Å)
μ:	67.66 cm ⁻¹
Diffractometer, scan mode:	Bruker P4, θ/2θ
2θ _{max} :	54.96°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	582, 404
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 355
<i>N</i> (<i>param</i>) _{refined} :	31
Programs:	SHELXL-97 [5], ATOMS [6]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Ag	8e	0	1/4	0.13427(9)	0.0188(6)	0.0221(6)	0.0178(7)	0.0061(1)	0	0
K	8c	-0.18032(6)	0	1/4	0.0177(7)	0.0137(7)	0.0216(7)	0	0	-0.0001(4)
C	8c	0.1266(3)	0	1/4	0.016(2)	0.010(2)	0.019(2)	0	0	-0.006(2)
O(1)	8c	0.1890(2)	0	1/4	0.013(2)	0.019(2)	0.035(3)	0	0	0.003(2)
O(2)	16f	0.0967(1)	0.1349(5)	0.1124(4)	0.020(1)	0.021(2)	0.021(1)	0.003(1)	0.001(1)	0.004(1)

* Correspondence author (e-mail: zhengcm@nbu.edu.cn)

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