



Ammonium bismuth chromate dichromate monohydrate

A Riou, Y Gerault, Yannick Cudennec

► To cite this version:

A Riou, Y Gerault, Yannick Cudennec. Ammonium bismuth chromate dichromate monohydrate. Acta Crystallographica Section C: Crystal Structure Communications [1968-2013], 1990, 46, pp.1915 - 1916. 10.1107/s0108270190004310 . hal-03229401

HAL Id: hal-03229401

<https://hal.science/hal-03229401>

Submitted on 18 May 2021

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Ammonium Bismuth Chromate Dichromate Monohydrate

By A. Riou, Y. Gerault and Y. Cudennec

Laboratoire de Chimie des Matériaux Inorganiques et de Cristallographie, Institut National des Sciences Appliquées, 20 avenue des Buttes de Coesmes, 35043 Rennes CEDEX, France

(Received 26 December 1989; accepted 2 April 1990)

Abstract. $\text{NH}_4\text{Bi}(\text{CrO}_4)(\text{Cr}_2\text{O}_7)\cdot\text{H}_2\text{O}$, $M_r = 577.01$, triclinic, $P-1$, $a = 6.916$ (2), $b = 7.249$ (3), $c = 10.798$ (3) Å, $\alpha = 80.28$ (3), $\beta = 90.52$ (2), $\gamma = 86.49$ (3)°, $V = 532.5$ (6) Å³, $Z = 2$, $D_m = 3.58$ (1), $D_x = 3.598$ Mg m⁻³, $\text{Mo K}\alpha$, $\lambda = 0.71073$ Å, $\mu = 19.938$ mm⁻¹, $F(000) = 528$, room temperature, $R = 0.052$ for 1942 observed reflections. The compound is isotypic with $\text{KBi}(\text{CrO}_4)(\text{Cr}_2\text{O}_7)\cdot\text{H}_2\text{O}$.

Experimental. The preparation of single crystals of $\text{NH}_4\text{Bi}(\text{CrO}_4)(\text{Cr}_2\text{O}_7)\cdot\text{H}_2\text{O}$ has been reported in our previous publications (Cudennec, Lecerf, Riou & Gerault, 1981). Crystals were obtained from a mixture composed of 1 mol of $\text{NH}_4\text{Bi}(\text{CrO}_4)(\text{Cr}_2\text{O}_7)\cdot\text{H}_2\text{O}$ and 4 mol of CrO_3 in a large quantity of water. After reaction, the system containing BiOHCrO_4 was slowly evaporated at room temperature over several days without stirring. Orange parallelepipedal crystals of $\text{NH}_4\text{Bi}(\text{CrO}_4)(\text{Cr}_2\text{O}_7)\cdot\text{H}_2\text{O}$ appeared in the solution. A suitable crystal of 0.20 x 0.15 x 0.09 mm was mounted on an Enraf-Nonius CAD-4 diffractometer. Density was measured by immersion in bromobenzene at room temperature. The unit-cell dimensions were determined and refined on the basis of 25 carefully selected reflections in the angular range $5 < 2\theta < 30^\circ$. Data were collected in the ω - 2θ scan mode with ω -scan width $(2.00 + 0.50\tan\theta)^\circ$ and slit amplitude $(1.00 + 0.35\tan\theta)$ mm. 2700 reflections were measured. The hkl range was $0 \leq h \leq 9$, $-9 \leq k \leq 9$, $-14 \leq l \leq 14$ ($2\theta < 56^\circ$). A periodic check of three standard reflections showed no significant intensity variations. The internal consistency index, R_{int} was 0.024. Reflections were merged to a unique set of 2563. 1942 reflections were considered as observed with $I > \sigma(I)$. Data were corrected for Lorentz and polarization effects and absorption corrections were applied according to the procedure of Walker & Stuart (1983). The structural determination was carried out on a PDP 11/60 computer using the SDP package (Frenz, 1978). Scattering factors were from Cromer & Waber (1965). The structure was determined on the basis of isomorphism with $\text{KBi}(\text{CrO}_4)(\text{Cr}_2\text{O}_7)\cdot\text{H}_2\text{O}$. Refinement was started with atomic coordinates reported by Riou, Gerault & Cudennec (1982). Full-matrix least-squares refinement was based on F and the function minimized was $\sum w(|F_o| - |F_c|)^2$, where $w(F) = 1/\sigma^2(F)$. The weighting scheme had a non-Poisson contribution with $p = 0.050$. Corrections were made for anomalous-dispersion and secondary-extinction effects ($g = 4.0 \times 10^{-7}$). During the last refinement cycle, the r.m.s. shift/e.s.d. was 0.07. The final difference Fourier map showed no peaks higher than 1.5 e \AA^{-3} . In these conditions, the final R was 0.052 and $wR = 0.064$. Final atomic coordinates, except H atoms, and

equivalent isotropic temperature factors are given in Table 1.* The comparison between these atomic coordinates and those of the $\text{KBi}(\text{CrO}_4)(\text{Cr}_2\text{O}_7)\cdot\text{H}_2\text{O}$ structure confirms their isomorphism.

Related literature. Little is known about chromate dichromate compounds. Such compounds containing Fe^{3+} or Al^{3+} ions were prepared some years ago, and their structures solved (Gerault & Bonnin, 1976; Cudennec, 1977). The structure of a ternary compound containing bismuth has been published recently: $\text{Bi}_2(\text{CrO}_4)_2(\text{Cr}_2\text{O}_7)$ (Gerault, Riou, Cudennec & Bonnin, 1987). The crystal structure of $\text{KBi}(\text{CrO}_4)(\text{Cr}_2\text{O}_7)\cdot\text{H}_2\text{O}$ was reported by Riou *et al.* (1982).

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52978 (14 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

- CROMER, D. T. & WABER, J. T. (1965). *Acta Cryst.* **18**, 104–109.
CUDENNEC, Y. (1977). *J. Inorg. Nucl. Chem.* **39**, 1711–1713.
CUDENNEC, Y., LECERF, A., RIOU, A. & GERAULT, Y. (1981). *C. R. Acad. Sci.* **293**, 369–371.
FRENZ, B. A. (1978). *The Enraf–Nonius CAD-4 SDP – A Real-Time System for Concurrent X-ray Data Collection and Crystal Structure Solution*. In *Computing in Crystallography*, edited by H. SCHENK, R. OLTJOF-HAZEKAMP, H. VAN KONINGSVELD & G. C. BASSI. Delft Univ. Press.
GERAULT, Y. & BONNIN, A. (1976). *Bull. Soc. Fr. Minéral. Cristallogr.* **99**, 197–202.
GERAULT, Y., RIOU, A., CUDENNEC, Y. & BONNIN, A. (1987). *Rev. Chim. Minér.* **24**, 631–640.
RIOU, A., GERAULT, Y. & CUDENNEC, Y. (1982). *Acta Cryst.* **B38**, 1693–1696.
WALKER, N. & STUART, D. (1983). *Acta Cryst.* **A39**, 159–168.

Table 1. *Final atomic coordinates and equivalent isotropic temperature factors for NH₄Bi(CrO₄)-(Cr₂O₇).H₂O*

$$B_{\text{eq}} = (4/3) \sum_i \sum_j \beta_{ij} \mathbf{a}_i \cdot \mathbf{a}_j.$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{eq} (Å ²)
N	0.870 (2)	0.015 (2)	0.313 (1)	2.3 (3)
Bi	0.34412 (7)	0.20675 (8)	0.07529 (6)	1.057 (9)
Cr(1)	0.8369 (3)	0.2462 (3)	0.9581 (2)	0.78 (4)
Cr(2)	0.3523 (3)	0.4710 (3)	0.7435 (2)	1.13 (4)
Cr(3)	0.5892 (3)	0.1930 (3)	0.6098 (2)	1.34 (4)
O(1)	0.919 (1)	0.235 (2)	0.822 (1)	2.2 (2)
O(2)	0.023 (1)	0.203 (1)	0.065 (1)	1.7 (2)
O(3)	0.676 (1)	0.077 (1)	0.000 (1)	1.4 (2)
O(4)	0.721 (2)	0.452 (1)	0.954 (1)	2.2 (2)
O(5)	0.618 (1)	0.332 (1)	0.215 (1)	2.0 (2)
O(6)	0.833 (2)	0.515 (2)	0.348 (1)	2.6 (3)
O(7)	0.676 (1)	0.703 (1)	0.136 (1)	1.6 (2)
O(8)	0.438 (1)	0.587 (1)	0.336 (1)	1.6 (2)
O(9)	0.565 (2)	0.034 (2)	0.734 (1)	2.2 (2)
O(10)	0.795 (2)	0.177 (2)	0.545 (1)	2.7 (3)
O(11)	0.587 (2)	0.814 (2)	0.489 (1)	2.6 (3)
O(<i>w</i>)	0.813 (1)	0.711 (2)	0.712 (1)	2.1 (2)