

ОКСОЦЕНТРИРОВАННЫЕ СЛОИ В КРИСТАЛЛИЧЕСКИХ СТРУКТУРАХ
ОКСАГАЛОГЕНИДОВ $\text{Bi}_9\text{P}_2\text{O}_{18}\text{X}$ ($\text{X}=\text{Cl}, \text{Br}$)

Козин М.С. (mkozin1985@yandex.ru), Ментре О. (olivier.mentre@ensc-lille.fr), Сийдра О.И. (siidra@mail.ru), Кривовичев С.В. (skrivovi@mail.ru)
Санкт-Петербургское отделение. СПбГУ

LADDER-OXOCENTERED LAYERS IN CRYSTAL STRUCTURE OF
 $\text{Bi}_9\text{P}_2\text{O}_{18}\text{X}$ ($\text{X}=\text{Cl}, \text{Br}$) OXYHALIDES

Kozin M.S.¹, Mentré O.², Siidra O.I.¹, Krivovichev S.V.¹

¹ Saint Petersburg branch, Saint Petersburg State University

²UCCS, UMR 8181 Equipe de Chimie du Solide Villeneuve d'Ascq, France

A new bismuth oxyhalide of formula $\text{Bi}_9\text{P}_2\text{O}_{18}\text{Br}$ has been synthesized and characterized. Single crystals were prepared as follows. Bi_2O_3 , CoO , WO_3 , BiPO_4 and RbBr were mixed in 7:2:1:4:60 molar ratio. 1 g of the resulted mixture was placed in a gold capsule and sealed. The tube was heated to 850°C for 6 h and maintained for 6 h. Afterward the tube was cooled down to 500°C for 100 h and finally to room temperature for 30 h. The resulted product was slightly crushed and washed with water in the ultrasonic cleaner. Orange single crystals were isolated from the concomitant powder matrix.

The crystal structure of new $\text{Bi}_9\text{P}_2\text{O}_{18}\text{Br}$ oxyhalide has been studied by the means of single crystal x-ray analysis (Bruker X8 APEX2). The structure is monoclinic, $P2_1/n$ ($a = 18.076(2) \text{ \AA}$, $b = 5.4223(7) \text{ \AA}$, $c = 19.198(3) \text{ \AA}$, $\beta = 104.382(7)^\circ$, $V = 1822.69(40) \text{ \AA}^3$). The structure was solved by direct methods and refined to $R_1=0.021$. Generally the crystal structure is similar to $\text{Bi}_9\text{P}_2\text{O}_{18}\text{Cl}$ (Mentre, 1998). Previously, there was an error in the choice of space group is probably related to a lack of data. The crystal structure of $\text{Bi}_9\text{P}_2\text{O}_{18}\text{Cl}$ oxyhalide has been studied by the means of single crystal x-ray analysis (Bruker X8 APEX2). The structure is monoclinic, $P2_1/n$ ($a = 17.9512(6) \text{ \AA}$, $b = 5.3972(2) \text{ \AA}$, $c = 22.9264(6) \text{ \AA}$, $\beta = 125.708(2)^\circ$, $V = 1803.66(10) \text{ \AA}^3$). The structure was solved by direct methods and refined to $R_1= 0.034$. Both structures are based on the ladder-like layers formed by OBi_4 tetrahedra with the large channels occupied by Cl and Br atoms. The comparison and relationship with the similar Bi oxysalts compounds is given.

Mentre O., Abraham F. // J. Solid State Chem. 136, 34-45 (1998).