**SUPPLEMENTARY MATERIALS – ДОПОЛНИТЕЛЬНЫЕ МАТЕРИАЛЫ**

**Crystal structure and optical properties of new hybrid halobismuthates of 2,2'-bipyridinium derivatives**

**Кристаллическая структура и оптические свойства новых гибридных галовисмутатов производных 2,2’-бипиридиния**

**S. P. Balabanova, P. A. Buikin, A. B. Ilyukhin, A.Yu. Rudenko, P. V. Dorovatovskii, A. A. Korlyukov, V.Yu. Kotov**

**C. П. Балабанова, П. А. Буйкин, А. Б. Илюхин, А. Ю. Руденко, П. В. Дороватовский, А. А. Корлюков, В. Ю. Котов**

**Russian Journal of Inorganic Chemistry**

**Журнал неорганической химии**

**Table of contents**

[**Table S1.** Crystal data and structure refinement for **I-V**. 2](#_Toc87634255)

[**Fig. S1.** X-ray Rietveld refinement profiles for **I**-**III** and **VI** 4](#_Toc87634256)

[**Fig. S2.** The reflectance spectra of **I**, **III** and **VI** 5](#_Toc87634257)

[**Fig. S3.** The fragment of structure **I** 6](#_Toc87634258)

Table S1. Crystal data and structure refinement for **I-V**.

**Таблица S1.** Основные кристаллографические данные и результаты уточнения структур **I**-**V**.

Identification code **I II III IV V**

Empirical formula C40H36Bi2Br10N8 C10H9BiBr4N2 C39H44Bi2Br12N6O C28H32Bi2I10N4 C50H62Bi3Br17N8O3

Formula weight 1845.83 685.81 1989.68 2111.53 2808.48

Temperature, K 150(2) 296(2) 150(2) 150(2) 150(2)

Wavelength, Å 0.71073 0.71073 0.71073 0.71073 0.71073

Crystal system Triclinic Monoclinic Orthorhombic Monoclinic Triclinic

Space group P-1 C2/c Pccn P21/n P-1

a, Å 13.275(2) 11.9894(3) 22.2572(10) 20.3914(9) 10.0709(4)

b, Å 13.851(3) 17.7949(5) 15.3294(7) 11.8272(5) 13.3048(5)

c, Å 13.916(3) 7.3991(2) 15.7019(7) 20.8858(9) 13.8748(5)

α, ° 89.267(16) 90 90 90 86.5710(10)

β, ° 75.687(19) 94.6080(10) 90 117.4500(10) 84.6510(10)

γ, ° 85.37(2) 90 90 90 82.732(2)

Volume, Å3 2471.2(9) 1573.50(7) 5357.3(4) 4470.0(3) 1833.96(12)

Z 2 4 4 4 1

D (calc), Mg/m3 2.481 2.895 2.467 3.138 2.543

µ, mm-1 15.235 21.344 15.547 14.794 16.482

F(000) 1696 1224 3656 3696 1286

Crystal size, mm 0.16 x 0.12 x 0.10 0.10 x 0.10 x 0.02 0.08 x 0.04 x 0.02 0.18 x 0.18 x 0.06 0.10 x 0.10 x 0.02

θ range, ° 2.079, 25.349 2.053, 30.553 2.070, 28.381 2.043, 30.032 2.046, 30.048

Index ranges -15<=h<=15 -17<=h<=17 -29<=h<=29 -28<=h<=28 -14<=h<=14

 -16<=k<=16 -25<=k<=25 -20<=k<=20 -16<=k<=16 -18<=k<=18

 -16<=l<=16 -10<=l<=10 -20<=l<=20 -29<=l<=29 -19<=l<=19

Reflections collected 37751 12826 124151 50091 30377

Independent reflections, Rint 9022, 0.1188 2422, 0.0477 6703, 0.1354 13075, 0.1093 10695, 0.0610

Completeness to θ = 25.242° 99.9 % 99.9 % 100.0 % 100.0 % 99.8 %

Absorption correction Semi-empirical Semi-empirical Semi-empirical Semi-empirical Semi-empirical

 from equivalents from equivalents from equivalents from equivalents from equivalents

Max,. min. transmission 0.0916, 0.0516 0.7461, 0.1456 0.0962, 0.0558 0.1067, 0.0476 0.099, 0.0506

Refinement method Full-matrix Full-matrix Full-matrix Full-matrix Full-matrix

 least-squares on F2 least-squares on F2 least-squares on F2 least-squares on F2 least-squares on F2

Data / restraints / parameters 9022 / 288 / 541 2422 / 8 / 133 6703 / 6 / 276 13075 / 0 / 397 10695 / 0 / 384

Goodness-of-fit 1.254 1.126 1.066 1.195 0.980

R1, wR2 [I>2sigma(I)] 0.0679, 0.1177 0.0309, 0.0739 0.0539, 0.1326 0.0734, 0.1096 0.0411, 0.0666

R1, wR2 (all data) 0.1320, 0.1320 0.0350, 0.0762 0.0899, 0.1500 0.0858, 0.1149 0.0765, 0.0769

Largest diff. peak and hole, e.Å-3 2.627, -1.824 1.356, -1.772 1.934, -2.513 2.465, -1.610 1.160, -1.055



a

b

c

d

Fig. S1**.** X-ray Rietveld refinement profiles for **I** (a), **I** and **II** mixture(b), **III** (c). The refinement of **VI** profile (d) was performed with hkl phase. All profiles were recorded at RT. Red and blue lines correspond to the calculated profile and experimental pattern respectively. The bottom trace shows the difference curve.

**Рис. S1.** Результаты уточнения по Ритвельду дифрактограмм соединений **I** (а),смеси **I** и **II** (b), **III** (c). Дифрактограмму соединения **VI** (d) уточняли c использованием hkl фазы. Красные и синие кривые отвечают рассчитанным и экспериментальным профилям соответственно. Разностная кривая изображена под графиками.

 

 a b



c

Fig. S2**.** The reflectance spectra of **I** (a, Eg = 2.84 eV), **III** (b, Eg = 2.88 eV) and **VI** (c, Eg = 2.11 eV).

**Рис. S2.** Спектры диффузного отражения **I** (a, Eg=2.84 эВ), **III** (b, Eg = 2.88 эВ) и **VI** (c, Eg = 2.11 эВ).



a



b

Fig. S3**.** The fragment of **I** (a) and the projection along a axis (b).

**Рис. S3.** Фрагмент структуры **I** (a) и проекция вдоль оси a (b).