ΛΌΓΟΣ

THE ART OF SCIENTIFIC MIND

COLLECTION OF SCIENTIFIC PAPERS

WITH MATERIALS OF THE INTERNATIONAL SCIENTIFIC-PRACTICAL CONFERENCE

DEVELOPMENT OF MODERN TECHNOLOGIES AND SCIENTIFIC POTENTIAL OF THE WORLD

JULY 29, 2019 • LONDON, GREAT BRITAIN

VOLUME 3

ISBN 978-617-7171-80-4

UDC 001(08)
D 49

EOI: 10.11232/2019.07.29.03

D 49 **Development of modern technologies and scientific potential of the world** : coll. of scientific papers «ΛΌΓΟΣ» with materials of the International scientific-practical conf., London, July 29, 2019. London : NGO «European Scientific Platform», 2019. V.3. p. 134.

ISBN 978-617-7171-80-4

Papers of participants of the International scientific-practical conference «Development of modern technologies and scientific potential of the world», held in London, July 29, 2019, are presented in the collection of scientific papers.

The collection is dedicated to students, graduates, postgraduates, PhDs, young specialists, lecturers, scientists and others interested persons, as well as for a wide range of readers.

Bibliographic description of the materials of the conference is presented in «Google Scholar». Conference is approved by ResearchBib.

UDC 001 (08)

© Participants of the conference, 2019
© Collection of scientific papers «ΛΌΓΟΣ», 2019
© NGO «European Scientific Platform», 2019

ISBN 978-617-7171-80-4

SECTION 13.
CHEMICAL SCIENCES

THE CARCASS-ELECTRON MODELS OF BISMUTH (III) OXYCHLORIDE BiOCl

Ph.D. in Chemistry, Associate professor Kozma Anton

Uzhhorod National University
Ukraine

The BiOCl has valuable photocatalytic [1] and photoelectrochemical properties [2], and also it is used as a component of cosmetics [3]. At the same time, in work [4] it is indicated a possibility of receiving perspective thermoelectrics on the basis of composites with participation of bismuth (III) oxychloride BiOCl and bismuth (III) selenide Bi_2Se_3. Considering that Bi_2Se_3 is a part of a number of effective thermoelectric materials and acts as a component of perspective systems in which such alloys can be formed [5-14], the comprehensive investigation BiOCl is of particular interest.

In the previous work [15] three are established crystal energetics properties BiOCl: structural fragility (ω), energy of a crystal lattice (U) and energy of atomization (E_α). In this work for the first time for bismuth (III) oxychloride it is determined additional crystal energetic parameter – energy coupling of atomic carcass and the connecting electrons (W).

Precision establishments of value W needs preliminary creations and checks of correctness of the maximum quantity possible for chosen the Carcass Electron models compounds. Zuev V.V. et al. [16] for such check suggested to use microhardness value. In this work, on an example BiOCl, for identification of an optimal variant of the carcass-electron models it is for the first time used alternative parameter – specific isobaric heat capacity C_{pm}.

Variants of the carcass-electron models for bismuth (III) oxychloride were developed according to recommendations from [16]. Values of molar (W) and specific (W_m) energy coupling of carcass and the electrides and also specific heat capacity (C_{pm}) counted behind the expressions, known from a source [16].

Necessary for connection BiOCl values of potentials of ionization of the making atoms accepted with [17], and energy of its atomization – with [15]. At realization of calculations with true considered value isobaric molar heat capacity (C_p) of bismuth (III) oxychloride at 298.15 K which is given in a source [18].

Results of the carried-out work are grouped in table 1.

Table 1

Variants of the carcass-electron models structure and are established for their help parameters of BiOCl

№	Variant of the carcass of crystal lattice	Σe^-	W, MJ/mol	W_m, MJ/g	C_{pm}, kJ/(kg×K)	Δ, %
1	$[Bi^{3+}][O^{2+}][Cl^{+}]$	6	11.679	0.056	0.245	-30.85
2	$[Bi^{3+}][O^{2+}][Cl^{3+}]$	8	17.799	0.085	0.302	-14.76
3	$[Bi^{3+}][O^{2+}][Cl^{5+}]$	10	29.498	0.141	0.389	9.80

Table 1

№	Variant of the carcass of crystal lattice	Σe^-	W, MJ/mol	W_m, MJ/g	C_{pm}, kJ/(kg×K)	Δ, %
5	$[Bi^{3+}][O^{4+}][Cl^{+}]$	8	24.449	0.117	0.354	-0.08
6	$[Bi^{3+}][O^{4+}][Cl^{3+}]$	10	30.569	0.146	0.395	11.49
7	$[Bi^{3+}][O^{4+}][Cl^{5+}]$	12	42.267	0.202	0.465	31.25
8	$[Bi^{3+}][O^{4+}][Cl^{7+}]$	14	62.648	0.300	0.567	60.04
9	$[Bi^{3+}][O^{6+}][Cl^{+}]$	10	48.765	0.233	0.500	41.13
10	$[Bi^{3+}][O^{6+}][Cl^{3+}]$	12	54.885	0.263	0.531	49.88
11	$[Bi^{3+}][O^{6+}][Cl^{5+}]$	14	66.584	0.319	0.585	65.12
12	$[Bi^{3+}][O^{6+}][Cl^{7+}]$	16	86.964	0.416	0.668	88.55
13	$[Bi^{(3+2)+}][O^{2+}][Cl^{+}]$	8	21.449	0.103	0.310	-12.50
14	$[Bi^{(3+2)+}][O^{2+}][Cl^{3+}]$	10	27.569	0.132	0.376	6.13
15	$[Bi^{(3+2)+}][O^{2+}][Cl^{5+}]$	12	39.268	0.188	0.449	26.73
16	$[Bi^{(3+2)+}][O^{2+}][Cl^{7+}]$	14	59.648	0.285	0.553	56.09
17	$[Bi^{(3+2)+}][O^{4+}][Cl^{+}]$	10	34.219	0.164	0.419	18.27
18	$[Bi^{(3+2)+}][O^{4+}][Cl^{3+}]$	12	40.339	0.193	0.455	28.43
19	$[Bi^{(3+2)+}][O^{4+}][Cl^{5+}]$	14	52.037	0.249	0.516	45.65
20	$[Bi^{(3+2)+}][O^{4+}][Cl^{7+}]$	16	72.418	0.347	0.610	72.18
21	$[Bi^{(3+2)+}][O^{6+}][Cl^{+}]$	12	58.535	0.280	0.548	54.68
22	$[Bi^{(3+2)+}][O^{6+}][Cl^{3+}]$	14	64.655	0.309	0.575	62.30
23	$[Bi^{(3+2)+}][O^{6+}][Cl^{5+}]$	16	76.354	0.365	0.625	76.41
24	$[Bi^{(3+2)+}][O^{6+}][Cl^{7+}]$	18	96.734	0.463	0.704	98.71

As we see from table 1, the slightest error (Δ= -0.08 %) in calculation of C_{pm}(BiOCl) №5 option gives: $[Bi^{3+}][O^{4+}][Cl^{+}]$. From this it follows that can consider the specified option carcass-electron models for bismuth (III) oxychloride the most exact. It should be noted that the used approach of Zuev V.V. et al. [16], on the shown example BiOCl, gives the highest precision (more than 99.9%), the majority of the known semi-empirical methods are characterized much above by an error [19]. Thanks to received result, the offered model of carcass the crystal lattice of bismuth (III) oxychloride can consider optimum. Possibly, it is also expedient to use it for forecasting of other physicochemical properties of BiOCl. At the same time will serve as basic parameter energy value coupling of carcass and elektrides established to *W*=24.449 MJ/mol. Other offered options of carcass-electron models are characterized noticeably by the highest misses if to determine on their help specific heat capacity of bismuth (III) oxychloride. However on the basis of the analysis of these options it was succeeded to establish optimum the carcass-electron model of BiOCl and to calculate for it value of energy coupling of atomic carcass and the connecting electrons.

Conclusions.

The first time for bismuth (III) oxychloride it is offered to the 24th options of carcass-electron models and value of energy coupling of atomic carcass and the connecting electrons is calculated with their help. For the first time for establishment of optimum model is used known value of isobaric heat capacity.

References:

1. Lei Y., Wang G., Song Sh., Fan W. and Zhang H. Synthesis, characterization and assembly of BiOCl nanostructure and their photocatalytic properties. *CrystEngComm.* 2009, 11, 1857–1862.
2. Stephenson J., Celorrio V., Tiwari D., Hall S.R., Green D.C., Fermín D.J. Photoelectrochemical properties of BiOCl microplatelets. *Journal of Electroanalytical Chemistry.* 2018, 819, 171–177.

3. Химическая энциклопедия: В 5 т.: т. 1: А – Дарзана/Ред-кол.: Кнунянц И.Л. (гл. ред.) и др. – М.: Сов. энцикл., 1988. – 623 с.
4. Evaristo-Vázquez M., Hernández-Pichardo M.L., Rodríguez-González E. Conductivity improvement of topological insulators of Bi_2Se_3 by the p-n heterojunction of Bi_2Se_3/BiOCl. *Revista Mexicana de Ingeniería Química*. 2019, 18(3), 813–823.
5. Kozma A.A., Sabov M.Yu., Peresh E.Yu., Barchiy I.E., and Tsygyka V.V. Thermoelectric Properties of a Eutectic $SnSe_2$–Bi_2Se_3 Alloy. *Inorganic Materials.* 2015, 51(2), 93–97.
6. Козьма А.А., Барчій І.Є., Пореш Є.Ю., Цигика В.В., Беца В.В., Соломон А.М., Сабов М.Ю. Одержання та термоелектричні властивості полікристалічних сполук $TlBiSe_2$ і Tl_9BiSe_6. *Наук. вісник Ужгородського у-ту. Серія «Хімія»*. 2010, 1(23), 22–25.
7. Kozma A.A., Barchij I.E., Peresh E.Yu. Phase relation in the Tl_2SnSe_3–Tl_4SnSe_4–$TlBiSe_2$ quasiternary system. *Chem. Met. Alloy*. 2011, 4(1–2), 94–97.
8. Козьма А.А., Пореш Є.Ю., Барчій І.Є., Сабов М.Ю., Глух О.С., Цигика В.В. Температурна залежність теплоємності сполук $TlSb(Bi)Se_2$ і $Tl_9Sb(Bi)Se_6$. *Наук. вісник Ужгородського у-ту. Серія «Хімія».* 2009, 2(22), 87–91.
9. Козьма А.А., Барчій І.Є., Пореш Є.Ю., Барчій О.І. Тріангуляція квазіпотрійної системи Tl_2Se–$SnSe_2$–Bi_2Se_3. *Proceeding of IV International workshop "RNAOPM'2008". Lutsk, Jine 1–5*, 2008, p. 40–42.
10. Козьма А.А., Пореш Є.Ю., Барчій І.Є., Сабов М.Ю., Беца В.В., Цигика В.В. Термоелектричні властивості евтектичних сплавів систем $TlBiSe_2$–$SnSe_2$ (Tl_2SnSe_3, Tl_4SnSe_4) і Tl_4SnSe_4–Tl_9BiSe_6. *Укр. хім. журн*. 2011, 77(9), 23–26.
11. Козьма А.А., Барчій І.Є., Пореш Є.Ю., Цигика В.В. Фазові рівноваги на квазібінарних перерізах квазіпотрійної системи Tl_2Se–$SnSe_2$–Bi_2Se_3. *Укр. хім. журн*. 2010, 76(4), 80–84.
12. Козьма А.А. Взаємодія компонентів у квазіпотрійній системі Tl_4SnSe_4–Tl_2Se–Tl_9BiSe_6. *Наук. вісник Ужгородського у-ту. Серія «Хімія»*. 2013, 2(30), 15–22.
13. Козьма А.А., Пореш Е.Ю., Барчій І.Є., Сабов М.Ю., Зубака О.В. Термоелектричні властивості евтектичних сплавів квазіпотрійної системи $SnSe_2$–$TlBiSe_2$–Bi_2Se_3. *Наук. вісник Ужгородського у-ту. Серія «Хімія»*. 2016, 1(35), 22–27.
14. Козьма А.А., Барчій І.Є., Пореш Є.Ю., Цигика В.В. Фізико-хімічна взаємодія у квазіпотрійній системі $SnSe_2$–$TlBiSe_2$–Bi_2Se_3. *Наук. вісник Ужгородського у-ту. Серія «Хімія»*. 2009, 1(21), 6–12.
15. Козьма А.А. Кристалоенергетичні властивості бісмут(III) оксид-хлориду BiOCl. *Wiadomości o postępie naukowym i rzeczywistych badaniach naukowych współczesności*: kolekcja prac naukowych «ΛΌΓΟΣ» z materiałami Międzynarodowej naukowo-praktycznej konferencji, Kraków, 17 czerwca 2019 r. Kraków: OP «Europejska platforma naukowa», 2019. Tom 4. S. 63–66.
16. Зуев В.В., Поцелуева Л.Н., Гончаров Ю.Д. Кристаллоэнергетика как основа оценки свойств твердотельных материалов (включая магнезиальные цементы). С-Пб. 2006. 139 с.
17. Волков А.И., Жарский И.М. Большой химический справочник. Минск: *Современная школа*, 2005. 608 с.
18. Barin I. (in collab. with Platzki G.). Thermochemical Data of Pure Substances. 3 ed. Weinheim: *VCH*, 1995. P. 1885.
19. Kozma A.A. Advantages of Using Semi-Empirical Methods in Teaching Students at the Faculty of Chemistry of Uzhhorod National University. *International Journal of Education and Science.* 2019, 2(2), 22.