Synthesis, Structure and Magnetic Properties of $La_2SrBi_2S_7$

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Abstract

A new phase with the composition $La_2SrBi_2S_7$ has been synthesised by the standard ceramic method. X-ray diffraction studies show that the phase crystallizes in the RP-type (n=3) structure with tetragonal unit cell (a=4.886Å and c=26.160Å). The phase is diamagnetic and magnetic susceptibility is temperature independent.

Keywords: $La_2SrBi_2S_7$, RP-type, XRD studies. Magnetic Properties.

Introduction:

Ruddlesden-Popper-type sulphide phases have been subject matter of intense studies for their wide range of properties. These phases are represented by the composition $A_{n+1}B_nS_{3n+1}$ where usually B-site is occupied by one or more transition metal ion (s). Phases of Zr and Hf with n=1,2 and 3 are known in literature [1-5]. It has been observed that these phases, generally crystallise in the phase group 14/mmm or Fmmm with tetragonal or orthorhombic unit cell. As compared to the corresponding oxides of Ruddlesden-Popper type phases, the cell dimensions of sulphides are much extended and transition metal atoms are unusually in distorted octahedral geometries with varying M-S distances. $Ba_3Zr_2S_7$ is reported to have space group Cccm with orthorhombic unit cell, while Ba-Zr-S (n=3) phase crystallizes in the space group Fmmm with orthorhombic unit cell [2].

In the present paper, synthesis of a new RP-type phase with the composition $La_2SrBi_2S_7$ has been reported. The deficiency in sulphur is the result of loss of S (3) with position co-ordinates (0, 0.5, 0.096). However the other S-position remains unaffected as a result of this structural deformation. Its crystal structure has been determined from the power X-ray diffraction data.

Experiment:

Synthesis

Aldrich make Lanthanum (La) Strontium (Sr) Bismuth (Bi) and Sulphur (S) elements (purity 99.9%) have been used for synthesis of the new phase. The constituent elements weighed corresponding to the stoichiometry $La_2SrBi_2S_7$, were mixed and homogenised by grinding in cyclohexane. The dried and homogenised mixture, pressed into pellets in hydraulic press was placed in quartz tube and evacuated to $\sim10^{-5}$ Torr, vacuum sealed and was heat- treated at 1273K for 72 hours. The mixture during the heat treatment was subjected to a number of intermediate grindings, pelletizing and sealing under same conditions for the completion of the reaction. The final product was pulverised to fine powder for further investigations [6-8].

Elemental Analysis

The phase was further analysed by atomic absorption spectrophotometry, which is one of the most prevalent methods for the trace element analysis [9-11]. The results of chemical elemental analysis [12, 13] and the atomic absorption spectrophotometry are in good agreement. The data are given in Table 1.

Table 1: Analytical data of the phase ($La_2SrBi_2S_7$).
The theoretical value is given parenthesis. Analysis (%)

Phase	La	Sr	Bi	S
$La_2SrBi_2S_7$	27.45 (27.56)	8.51 (8.69)	41.33 (41.47)	22.14 (22.26)

X-ray Diffraction studies

Room temperature powder X-ray diffraction data of the product were recorded on a Stoe-powder diffraction system and a Philips diffractometer at a scanning speed of 1deg./minute in the 2θ range using CuKα and FeKα radiations [14-18]. The X- ray diffraction data are given in the Table 2, while the X-ray pattern, intensity, versus 2θ is drawn in the figure1.

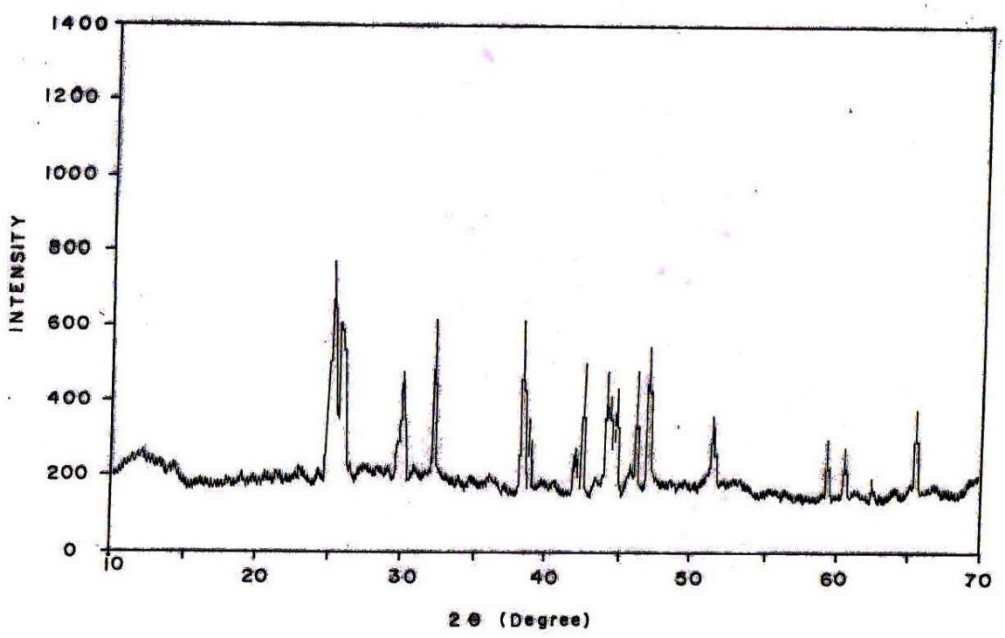

Figure 1: *X-ray Diffraction pattern of $La_2SrBi_2S_7$*

Magnetic Susceptibility Measurement

Magnetic susceptibility of the powdered phase was recorded in a Faraday balance provided with Polytronic Faraday-type electromagnet and a Mettler microbalance. Specially fabricated Dewar flask of the size which could be adjusted within polegaps of electromagnet was used for keeping liquid nitrogen, which surrounded the phase crucible [16, 17]. The phase was held hanging in the inner tube of the Dewar flask with a fine thread. Magnetic susceptibility in the temperature range 77K-300K could be measured by this arrangement.

Results and Discussion

Crystal Structure

The unit cell parameters of the phase were calculated from X-ray diffraction data (Table 2). The indexing of the data shows that it crystallises in the tetragonal unit cell with a=4.886Å and c=26.160Å. In order to determine the crystal structure, the theoretical X-ray diffraction data were generated by Treor and Lazy- Pulverix analysis. The d_{cal} values computed from data are in good agreement with the experimental interplanar distances. The data along with the assigned h k l values are given in the Table 2.

Table 2: Powder X-ray Diffraction Data of $La_2SrBi_2S_7$

h	k	l	d_{obs} (Å)	d_{cal}(Å)	I_{obs}	I_{cal}
1	0	1	4.810	4.802	14	16
1	0	5	3.570	3.571	100	100
1	1	0	3.455	3.450	81	62
0	0	8	3.274	3.270	15	1
1	0	7	2.963	2.968	34	8
1	1	6	2.697	2.707	10	4
0	0	10	2.627	2.616	8	22
2	0	0	2.460	2.443	57	47
2	0	2	2.410	2.401	6	2
2	0	4	2.308	2.288	29	6
1	0	10	2.084	2.085	9	23
2	1	5	2.022	2.016	30	43
2	0	8	1.960	1.957	36	1
2	1	7	1.928	1.886	41	5
0	0	14	1.868	1.868	22	2
1	1	12	1.841	1.843	5	4
2	0	10	1.789	1.485	15	28
2	1	9	1.746	1.746	24	6
2	0	2	1.719	1.712	14	1
1	1	14	1.647	1.643	6	2
0	0	16	1.630	1.635	5	1
3	0	3	1.601	1.601	4	1
3	0	5	1.553	1.555	15	10
2	2	8	1.522	1.527	13	1
2	0	14	1.485	1.484	4	4
2	2	10	1.449	1.441	6	14
3	0	9	1.423	1.420	26	2
3	1	8	1.396	1.397	12	1
2	1	15	1.379	1.363	6	7.0
2	2	12	1.354	1.353	9	3.0

Space group: 14/mmm

a=4.886Å, c=26.160Å

Table. Positional Coordinates for $La_2SrBi_2S_7$

Atom	X	Y	Z	Occupancy
La (1)	0	0	0.5	0.67
La (2)	0	0	0.3148	0.67
Sr (1)	0	0	0.5	0.33
Sr (2)	0	0	0.3148	0.33
Bi	0	0	0.0971	1
S(1)	0	0	0	1
S(2)	0	0	0.190	1
S(3)	0	0.5	0.096	1

Magnetic susceptibility studies

The molar magnetic susceptibility measurements as a function of temperature suggest that the phase is diamagnetic and magnetic susceptibility is temperature independent.

Conclusion

A new phase with the composition $La_2SrBi_2S_7$ has been synthesised by the standard ceramic method. X-ray diffraction studies show that the phase crystallizes in the RP-type (n=3) structure with tetragonal unit cell. The molar magnetic susceptibility measurements as a function of temperature suggest that the phase is diamagnetic and magnetic susceptibility is temperature independent.

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