

## Measurement of the grain size of HgClBr- nano form of HgClBr

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### ABSTRACT

Grain size measurement has acquired importance on account of the emergence of nano-research. We have produced HgClBr by the two methods. We find HgClBr has been produced in nano-form by one of the two methods. The details are reported here.

**Key words:** Grain size measurement, nano-form of HgClBr.

### INTRODUCTION

Nano science is the most revolutionary emerging field of Science and Technology Materials, the grain size of which lies between 1nm and 100nm ( $1\text{nm} = 10^{-9}\text{m}$ ), are called nano-materials. These have interesting properties, not found in the non-nano-form. Because of their interesting properties, these find wide applications in Science and Technology.

Whether a material is of nano-form or not can be determined only by measuring the average grain size of the material. It has been found that only in some ways of the preparation of a compound, it is produced in the nano-form, otherwise, by most other methods, it is produced in non-nano-form.

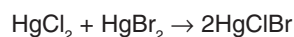
We have produced HgClBr in nano-form.

Section-2 reports two methods of

producing HgClBr. Section 3 gives the particle size measurement of the product HgClBr, as prepared by the two methods. In one of these, the HgClBr is formed in nano-form.

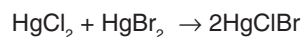
#### Section -2 Method I

HgClBr is formed by heating a solid equimolar mixture of  $\text{HgCl}_2$  and  $\text{HgBr}_2$ , in an oven at  $80^\circ\text{C}$  for 48 hours:



#### Method II

In the method of preparation, suggested by D.C. Parasher, formerly Head Chemistry Division, NPL, New Delhi, a saturated solution of  $\text{HgCl}_2$  and  $\text{HgBr}_2$  mixed in 1:1 ratio, is kept in a desiccator over  $\text{CaCl}_2$  until crystals separate out:



**Table 1: Calculation of grain size of the compounds**

S.No.	Name of Compound	$2\theta$	$\text{Cos } \theta$	$\beta_{2\theta}$	grain size (nm)
1.	HgClBr (1 <sup>st</sup> Method)	19.26	0.98	$\sim 1 \times 10^{-3}$	$\sim 136$
2.	HgClBr (2 <sup>nd</sup> Method)	4.530	0.99	$2.18 \times 10^{-3}$	66

Table 1(a): HgClBr (I method)

Angle [°2 $\theta$ ]	d-values $\alpha$ 1[°A]	d-value $\alpha$ 2[°A]	Peak Intensity [Counts]	Rel. int [%]
3.280	26.9146	26.9814	20	22.9
19.265	4.6034	4.6149	88	100
20.860	4.2549	4.2655	35	39.4
25.325	3.5139	3.5227	25	28.3
28.330	3.1477	3.1555	71	79.9
31.870	2.8056	2.8126	34	38.1
35.630	2.5177	2.5240	12	13.9
40.685	2.2158	2.2213	23	26.1
42.415	2.1293	2.1346	13	14.7
43.660	2.0715	2.0766	19	21.9
45.440	1.9944	1.9993	26	29.4
49.525	1.8390	1.8436	11	12.3
58.280	1.5819	1.5858	10	10.9

Table 1(b): HgClBr (II method)

Angle [°2 $\theta$ ]	d-values $\alpha$ 1[°A]	d-value $\alpha$ 2[°A]	Peak Intensity [Counts]	Rel. int [%]
4.530	19.4902	19.5386	112	89.6
5.635	15.6705	15.7094	50	40.2
14.445	6.1268	6.1420	45	35.8
16.725	5.2964	5.3095	12	9.2
18.510	4.7894	4.8014	42	33.7
19.375	4.5775	4.5889	92	73.5
20.985	4.2298	4.2403	26	20.7
22.225	3.9966	4.0065	17	13.4
25.350	3.5105	3.5192	22	17.6
26.840	3.3189	3.3272	20	16.1
28.075	3.1757	3.1836	123	98.2
28.440	3.1357	3.1435	125	100
29.760	2.9996	3.0070	35	27.8
31.910	2.8022	2.8092	32	25.9
35.635	2.5174	2.5236	14	11.5
40.565	2.2221	2.2276	14	11.5
42.490	2.1258	2.1310	21	16.9
43.700	2.0697	2.0748	46	36.9
45.530	1.9906	1.9956	21	16.9
49.825	1.8286	1.8332	7	5.8
58.920	1.5662	1.5701	14	11.5
67.355	1.3891	1.3936	6	5.0

In both the above methods 99.9% purity, Merck chemicals are used.

#### Grain size measurement.

Several methods are available for grain size measurement e.g.<sup>4</sup>. However, we have used the Debye-sherrer formula. It is well observed that the particle size D may be estimated by using Debye-sherrer formula<sup>5</sup>

$$D = \frac{K\lambda}{\beta_{2\theta} \cos \theta}$$

where  $K$  is constant taken as 0.94,  $\lambda$  is  $k\alpha_1$  wave length of the x-ray used ( $\lambda = 1.54 \times 10^{-10}$  m)

and  $\beta_{2\theta}$  is the full, width at half maximum of a very prominent intensity peak of the x-ray diffractogram of the compound,  $\theta$  is the angle at which the particular diffraction peak occurs. The above formula only holds for stress free crystallites. This assumption is generally found to be correct.

The two diffractograms of the HgClBr, prepared by the two methods, are given by figs. 1(a) and 1(b) respectively and the corresponding digital data are given in Tables 1(a) and 1(b). Normally one should take two or three prominent diffraction peaks and get the average grain size. Since visual reducing of the width is a very unsatisfactory procedure, we select the broad peak at  $2\theta = 4.530$ .

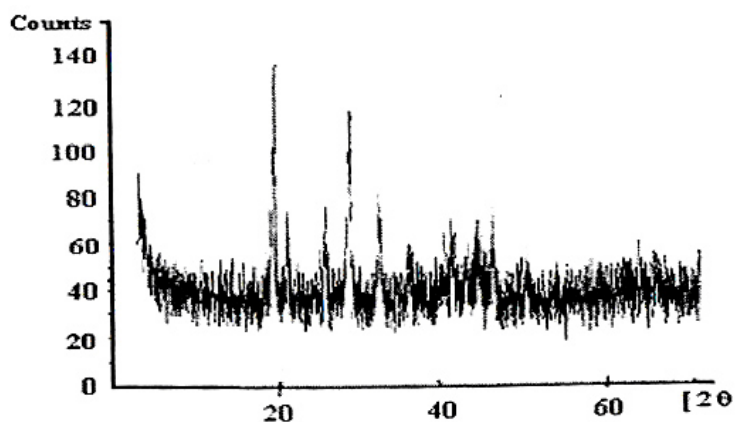


Fig. 1(a): HgClBr (I method)

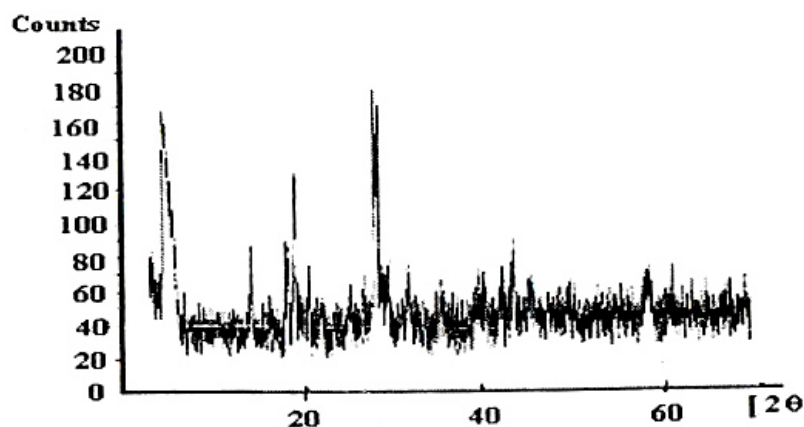


Fig. 1(a): HgClBr (II method)

We see that HgClBr is produced in nano – form by Method – II. It is a white coloured crystalline solid. Independent studies, not being reported here, show that it pure and stable.

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