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X-ray diffraction spectrum and fourier transform study of lead iodide crystals grown in gel under electricfield, magneticfield, ultraviolet and infrared radiations

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ABSTRACT

It is presented the infrared (FTIR) spectroscopic investigations of the lead iodide samples grown in pure, electricfield, magnetic field, ultraviolet and infrared radiations. The study of structural, optical and technological importance of lead iodide crystal. Lead Iodide (PbI_2) is a promising candidate for the manufacturing of semiconductor gamma-ray detectors. In addition, the growth of crystals in UV and IR radiations were discussed. Crystallographic measurements were made using XRD spectrum of the pure sample. Lead halides have structures of mainly ionic character based on close-packing of the halide ions.

KEYWORDS

Metals;
Halides;
Optical materials;
Crystal growth;
Infrared Spectroscopy.

INTRODUCTION

Lead iodide has been previously studied by several technique including optical absorption, transmission, ellipsometry using FPLMTO method with spin orbit coupling[1]. In this paper we studied the characterization of PbI_2 using X-ray diffractometry and Fourier transform infrared spectroscopy. It is a wide –band-gap semiconductor (Eg>2eV) with high environmental stability efficiency[2-5]. Recently, its band gap energy and thermal properties were determined by photo acoustic spectroscopy[5-6]. The purpose of this work is to obtain growth kinetics of PbI_2 in gel technique and benefits of its high band gap. It has a hexagonal layered crystal structure with a relatively low melting point of 408°C. TABLE 2 lists important physical and electronic properties of PbI_2. PbI_2 is a promising detector material due to its high resistivity, good charge transporter, and good stability. X-ray detectors are generally fabricated from PbI_2 crystals using ohmic contacts such as Pd or graphite[7]. Since many requirements such ac high resistivity, low noise and good electron transport are also necessary for optical detectors, PbI2 is a potential candidate as a photo detector in scintillation studies. PbI_2 is a P-type semiconductor and crystallizes in an hexagonal cadmium iodide like structure: atoms are located in layers in layers of Pb and I perpendicular to c-axis in the succession I-Pb-I-I-Pb-I, on account of Van der Wall's bonding between the iodine atoms, the cleavage of PbI_2 normal to the c-axis is very easy. Henisch et al. have reported that the crystals like calcium tartrate, calcium tungstrate and lead iodide can be grown by gel technique. The similar

method has been used to grow the crystals of lead iodide by DENNIS et al. HENISCH, PATEL et al. It has been decided to grow the crystals by gel technique, as the gel technique is especially valuable for crystals which because of their low dislocation temperature or low solubility (or both) cannot readily be grown by other method, since the crystals in any one growth system grow competitively, control of nucleation processes in many cases a key to the practical utility of the method. The peculiarity of this material are high resistivity, ability to work in a wide range of temperatures and chemical stability. DAWOOD et al. have reported that Lead Iodide have an application in the fields image recording and high-resolution photography, and on its reaction to bombardment by nuclear particles as investigated by CHADDERTON.

EXPERIMENTAL

Analytical reagent (AR) chemicals were used for the growth and conducted the experiments at room temperature and pressure. Continuous agitation with a magnetic stirrer, this mixture is allowed to set for gel. 20ml. of 0.75M potassium iodide then placed on the top The PbI_2 crystals have been grown by silica gel method. Dissolve 244g of sodium metasilicate in 500ml. of double distilled water to obtain the stock solution.7.5ml. of stock solution is diluted with equal quantity of water. Then 15ml. of 2M acetic acid and 6ml. of 1M lead acetate are combined with of the gel. Five such systems are prepared to get the samples in strong electric field of 20V. magneticfireld 1tesla, boiling test tube placed in front of a UV lamp and another test tube placed in front of a infrared lamp at a distance10cm apart, see Figure 1, good hexagonal plates of lead iodide(PbI2) grow within about three weeks at ordinary temperature and pressure. Amoung other lead compounds so far prepared is lead iodide which have been grown in acidic lead acetate gels, and in the presence of infrared radiation produces good crystal samples for application purpose. The present research work may provide new insights into the morphology-controlled synthesis of metal iodide as well as other inorganic materials. X-ray diffractogram were recorded as shown in Figure 2, for pure PbI_2 to study the crystallography of the crystal. Then observations of the faces of these crystals revealed that they have grown by layer as well as spiral mechanisms. TABLE 2 provides the corresponding properties of lead iodide from literature review. The crystals which results from these

Figure 1 : Synthesis of lead iodide crystals in pure, electrifield, magneticfield, ultraviolet and infrared radiation grown samples

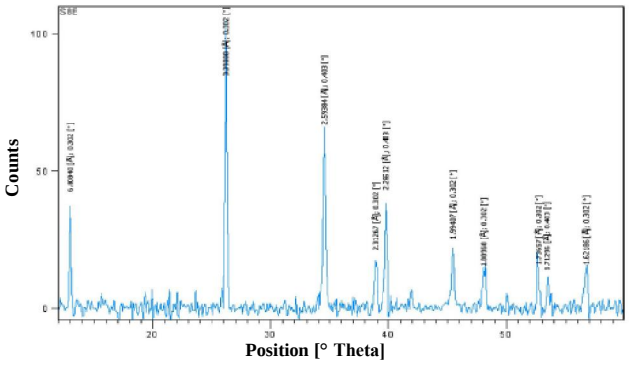

Figure 2 : XRD pattern of pure Lead Iodide Crystal

five conditions were subjected to all possible optical studies and morphological investigations. The FTIR

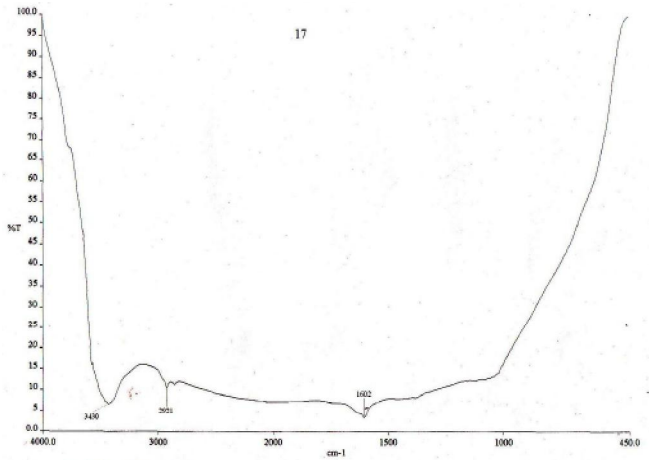

Figure 3 : FTIR of pure PbI_2

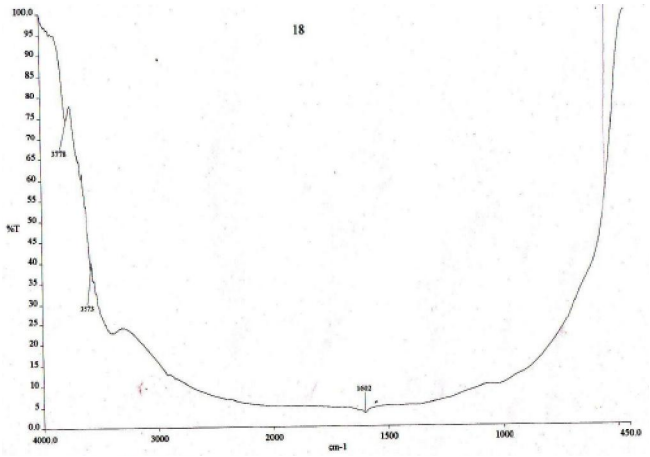

Figure 4 : FTIR of UV grown PbI_2

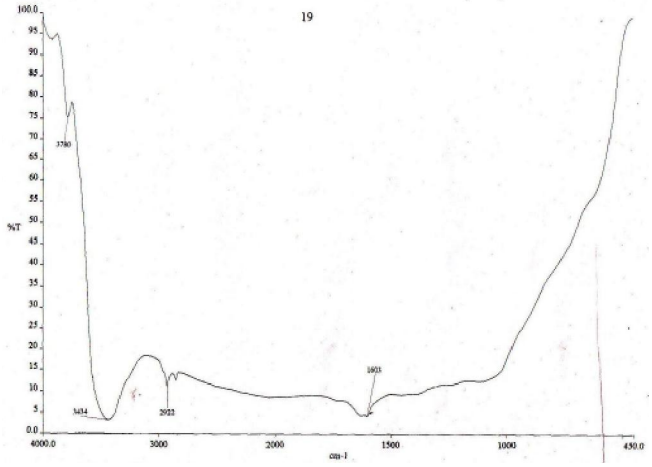

Figure 5 : FTIR of IR grownPbI_2

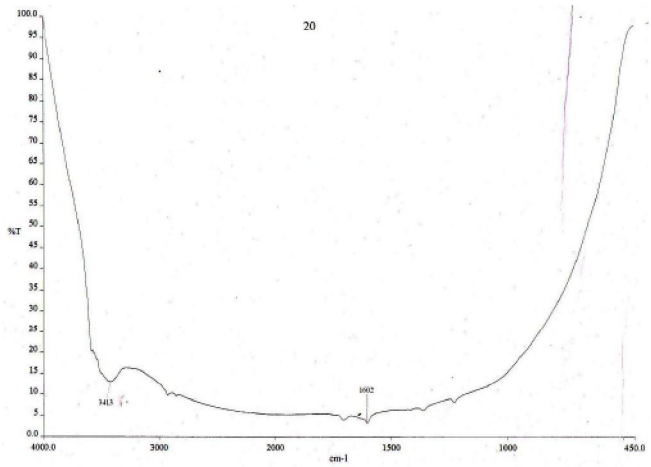

Figure 6 : FTIR of Electric field grown PbI_2

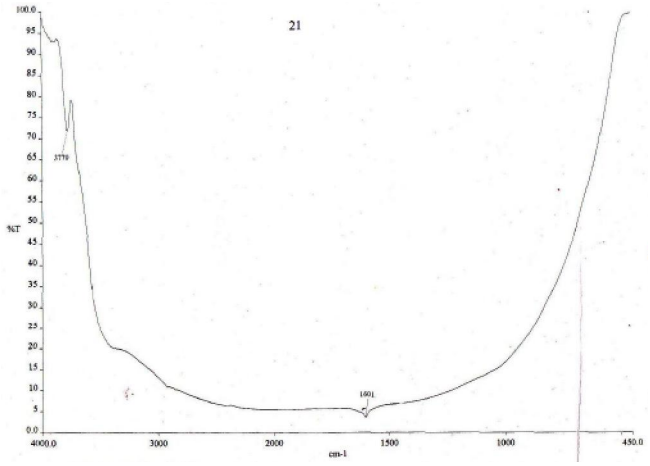

Figure 7 : FTIR of magnetic field grown PbI_2

spectra of all samples prepared by the same gel method are presented in 3,4,5,6 and 7. The analysis of vibrational bands are as shown in TABLE 1. The optical spectra are as a result of interband transition which is negligible for PbI_2. The asymmetric stretching of water is at 3779 cm^{-1}, 3778, 3789 cm^{1} for magnetic field, UV and IR samples while for pure this frequency is only 3430 cm-1. The peaks are of very low intensity because of high band gap of PbI_2. The vibrational mode at around 1600cm-1 is due to Pb-I (ligand) mode of vibration which is present almost in the same region for all the samples. The FTIR analysis of pure, electricfield, magneticfield, UV and IR grown crystals confirms the fundamental functional groups and their vibrational modes of PbI_2. The symmetric stretch in IR, UV and magnetic field grown samples show high %T. The first reports of light ef-

Measurement Conditions:	
Dataset Name	S8E
File name	C:\X'Pert Data\External\04 september 2008\Lillibai\S8E.xrdml
Sample Identification	S8E
Comment 4:00:11 PM	Configuration=conf.flat sample stage, Owner=User-1, Creation date=5/30/2005
PM	Goniometer=PW3050/60 (Theta/Theta); Minimum step size 2Theta:0.001; Minimum step size Omega:0.001 Sample stage=PW3071/xx Bracket Diffractometer system=XPERT-PRO Measurement program=Lillibai, Owner=User-1, Creation date=9/17/2008 2:36:10
	5 to 60(6 minutes)
Measurement Date / Time	9/17/2008 2:52:10 PM
Operator	Centre For Earth
Raw Data Origin	XRD measurement (*.XRDML)
Scan Axis	Gonio
Start Position [°2Th.]	5.0448
End Position [°2Th.]	59.8968
Step Size [°2Th.]	0.0840
Scan Step Time [s]	67.0828
Scan Type	Continuous
PSD Mode	Scanning
PSD Length [°2Th.]	2.12
Offset [°2Th.]	0.0000
Divergence Slit Type	Automatic
Irradiated Length [mm]	0.50
Specimen Length [mm]	10.00
Measurement Temperature [°C]	25.00
Anode Material	Cu
K-Alpha1 [Å]	1.54060
Generator Settings	30 mA, 40 kV
Diffractometer Type	0000000083005153
Diffractometer Number	0
Goniometer Radius [mm]	240.00
Dist. Focus-Diverg. Slit [mm]	100.00
Incident Beam Monochromator	No
Spinning	No

Peak List:				
Pos. [°2Th.]	Height [cts]	FWHM [°2Th.]	d-spacing [Å]	Rel. Int. [%]
12.9926	39.17	0.3024	6.80840	36.90
26.2041	106.15	0.3024	3.39808	100.00
34.5517	63.73	0.4032	2.59384	60.04
38.9114	17.59	0.3024	2.31267	16.57
39.7622	39.64	0.4032	2.26512	37.34
45.4483	21.81	0.3024	1.99407	20.55
48.1126	11.77	0.3024	1.88968	11.09
52.6643	12.63	0.3024	1.73657	11.90
53.4473	10.48	0.4032	1.71296	9.87
56.7119	12.57	0.3024	1.62186	11.84

fects on nucleation in solution date from 1900, and similar effects in gels have also been reported from time to time (Henisch et al., 1965, Dennis, 1967). It is tempting to envisage a new and intriguing quantum process('Photo nucleation'). Under irradiation by ultraviolet or visible light, the ion uptake is inhibited, and the resulting crystals are deep yellowish. The chemistry involved in the processes given below:

$$Pb(C_2H_3O_2)_2 + 2KI\ PbI_2 + K_2(C_2H_3O_6)_2$$

TABLE 1 : Vibrational band assignments of lead iododе single crystals

Pure, PbI2	Magnetic field, PbI2	Electric field, PbI2	Ultraviolet radiation, PbI2	Infrared radiation, PbI2	Assignments
-	3779s	-	3778s	3780s	Symmetric stretch, H-O-H
3430w	-	3413bw	3573s	3434w	Symmetric stretch of O-H
2912w (split)	-	-	-	2922w(split)	overtones vibrations of O-H
1602	1601	1602	1602	1602	H-O-H, deformation vibrations of free water

FREQUENCY (cm-1)
s-strong band, w -weak band, bw-broad and weak

TABLE 2 : Properties of lead iodide

PROPERTY	VALUE
BAND GAP	2.3 eV
CRYSTAL STRUCTURE	hexagonal
VAPOUR PRESSURE AT 2000C	10^{-3}torr
DIEELECTRIC CONSTANT	21
DENSITY	6.2g/cm^3
RESISTIVITY	$>10^{13}$ohm-cm
ELECTRON, PRODUCT	10^{-5}
HOLE PRODUCT	2×10^{-4}cm^2/V
MELTING POINT	408^0c

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RESULT

Our results, are summarized according to the analysis in TABLE 1. Comparing our results for five samples the total number of molecular vibrational motion of lead iodide crystal enhanced by the use of IR radiation during growth. Further, interactions could occur between rotational, translational and low-lying internal modes. It is difficult to explain the observed spectra of powdered samples due to the complex nature of the metal-oxygen linkages and the distortions present in the metal-oxygen polyhedral. However, it is possible to make symmetry assignments by comparison with the normal modes of the molecules. We shall test this approximation when the polarized Raman spectrum of PbI_2 is also at our disposal. Pale yellow, hexagonal plates appeared within a few hours and grew to about 10mm diameter. One side of the crystals was smooth, the other showed ridges along the diagonals between corners of the hexagon and along only one direction of the c-axis. XRD results about PbI2 shown in TABLE 3 and TABLE 4.

TABLE 3

No.	Pos. [°2Th.]	FWHM [°2Th.]	Area calc.	Assignment	h	k	l	Multiplicity	F obs.	F calc.	Area [cts*°2Th.]	Derivation	Backgr. [cts]	d-spacing [Å]	Height [cts]	K-A2 / K-A1 Ratio	Matched	Matched by	Rel. Int. [%]	Source	Status
1	12.9926	0.3024	0	Search Unit Cell Result 1	3	0	0	-	0	0	15.79	Pure K-Alpha1	0	6.8084	39.17	-	TRUE	01-075-0983	36.9	Search Peaks	Included
2	26.2041	0.3024	0	Search Unit Cell Result 1	6	0	0	-	0	0	42.8	Pure K-Alpha1	0	3.39808	106.15	-	TRUE	01-075-0983; 03-065-2225	100	Search Peaks	Included
3	34.5517	0.4032	0	Search Unit Cell Result 1	6	5	0	-	0	0	34.26	Pure K-Alpha1	0	2.59384	63.73	-	TRUE	01-075-0983; 03-065-2225	60.04	Search Peaks	Included
4	38.9114	0.3024	0	Search Unit Cell Result 1	1	0	1	-	0	0	7.09	Pure K-Alpha1	0	2.31267	17.59	-	TRUE	01-075-0983; 03-065-2225	16.57	Search Peaks	Included
5	39.7622	0.4032	0	Search Unit Cell Result 1	9	0	0	-	0	0	21.31	Pure K-Alpha1	0	2.26512	39.64	-	TRUE	03-065-2225	37.34	Search Peaks	Included
6	45.4483	0.3024	0	Search Unit Cell Result 1	10	2	0	-	0	0	8.79	Pure K-Alpha1	0	1.99407	21.81	-	TRUE	01-075-0983; 03-065-2225	20.55	Search Peaks	Included
7	48.1126	0.3024	0	Search Unit Cell Result 1	10	4	0	-	0	0	4.75	Pure K-Alpha1	0	1.88968	11.77	-	TRUE	01-075-0983; 03-065-2225	11.09	Search Peaks	Included
8	52.6643	0.3024	0	Search Unit Cell Result 1	6	5	1	-	0	0	5.09	Pure K-Alpha1	0	1.73657	12.63	-	TRUE	03-065-2225	11.9	Search Peaks	Included
9	53.4473	0.4032	0	Search Unit Cell Result 1	8	1	1	-	0	0	5.64	Pure K-Alpha1	0	1.71296	10.48	-	TRUE	01-075-0983; 03-065-2225	9.87	Search Peaks	Included
10	56.7119	0.3024	0	Search Unit Cell Result 1	9	0	1	-	0	0	5.07	Pure K-Alpha1	0	1.62186	12.57	-	TRUE	03-065-2225	11.84	Search Peaks	Included

TABLE 4

Pos. [°2Th.]	Iobs [cts]	Pos. [°2Th.]	Iobs [cts]	Pos. [°2Th.]	Iobs [cts]	Pos. [°2Th.]	Iobs [cts]	Pos. [°2Th.]	Iobs [cts]
5.0448	0	6.1368	0	7.2288	5.1555	8.3208	0.7123	9.4128	-0.1648
5.1288	2.6808	6.2208	0.3063	7.3128	0.6415	8.4048	0.7174	9.4968	-1.0051
5.2128	0	6.3048	0.2408	7.3968	3.0654	8.4888	-0.2832	9.5808	0
5.2968	2.8136	6.3888	5.7139	7.4808	0.0236	8.5728	0	9.6648	-1.9304
5.3808	1.1545	6.4728	0	7.5648	2.3289	8.6568	-1.0726	9.7488	4.243
5.4648	0	6.5568	0.1725	7.6488	2.5858	8.7408	2.6564	9.8328	1.9659
5.5488	0.7118	6.6408	0	7.7328	1.688	8.8248	3.2212	9.9168	0.3246
5.6328	0.7175	6.7248	3.2373	7.8168	-0.9448	8.9088	0	10.0008	1.5547
5.7168	2.0434	6.8088	0	7.9008	0	8.9928	1.8498	10.0848	0.1766
5.8008	0	6.8928	-2.6495	7.9848	0.1384	9.0768	2.8638	10.1688	0
5.8848	0.8689	6.9768	0.3563	8.0688	0.4806	9.1608	0	10.2528	-2.8929
5.9688	0.8993	7.0608	2.341	8.1528	0.4633	9.2448	-2.8107	10.3368	0.2734
6.0528	0.3833	7.1448	0	8.2368	2.9135	9.3288	-0.9851	10.4208	5.2368

Pos. [°2Th.]	Iobs [cts]	Pos. [°2Th.]	Iobs [cts]	Pos. [°2Th.]	Iobs [cts]	Pos. [°2Th.]	Iobs [cts]	Pos. [°2Th.]	Iobs [cts]
10.5048	1.0409	14.2008	0.4038	17.8968	-0.223	21.5928	-1.1428	25.2888	-0.0265
10.5888	0	14.2848	0	17.9808	-0.0001	21.6768	-1.1317	25.3728	1.427
10.6728	-4.2212	14.3688	-1.3033	18.0648	0.0715	21.7608	1.5147	25.4568	1.8178
10.7568	-1.7222	14.4528	2.819	18.1488	2.592	21.8448	-0.3907	25.5408	-0.6012
10.8408	0.2394	14.5368	1.705	18.2328	-4.7509	21.9288	-0.2435	25.6248	-1.7454
10.9248	-0.5702	14.6208	0	18.3168	1.9974	22.0128	5.7801	25.7088	2.3266
11.0088	0	14.7048	-0.5714	18.4008	-1.0186	22.0968	-2.2796	25.7928	5.9423
11.0928	-1.0844	14.7888	2.5659	18.4848	1.1278	22.1808	-3.9882	25.8768	7.2358
11.1768	-1.6148	14.8728	0.1782	18.5688	1.7909	22.2648	-2.6118	25.9608	-0.1116
11.2608	0	14.9568	0	18.6528	-1.7647	22.3488	2.8794	26.0448	20.3778
11.3448	0.1932	15.0408	-0.0476	18.7368	-2.2227	22.4328	2.0764	26.1288	67.9517
11.4288	1.4056	15.1248	0	18.8208	0.3267	22.5168	0.6046	26.2128	104.7075
11.5128	1.4323	15.2088	-0.7853	18.9048	0.6225	22.6008	1.2692	26.2968	36.7156
11.5968	1.0135	15.2928	-1.2143	18.9888	2.3087	22.6848	0.7502	26.3808	5.1268
11.6808	0.5248	15.3768	2.6328	19.0728	0.0008	22.7688	0.1248	26.4648	-0.203
11.7648	-2.3884	15.4608	0.6928	19.1568	-4.3528	22.8528	0.5634	26.5488	0.3484
11.8488	0	15.5448	0.225	19.2408	1.2814	22.9368	1.2182	26.6328	-1.2231
11.9328	-1.4028	15.6288	5.7398	19.3248	5.8727	23.0208	0.4821	26.7168	0.9285
12.0168	-0.2521	15.7128	2.9327	19.4088	-1.3843	23.1048	-1.7411	26.8008	1.2863
12.1008	-0.3437	15.7968	0.9947	19.4928	1.9134	23.1888	-0.9122	26.8848	0.906
12.1848	3.7513	15.8808	1.6875	19.5768	2.8804	23.2728	2.1955	26.9688	-1.3102
12.2688	1.7693	15.9648	3.0368	19.6608	-2.0597	23.3568	-0.7553	27.0528	-0.3945
12.3528	0.8322	16.0488	0.895	19.7448	-0.0708	23.4408	-0.8256	27.1368	-0.5073
12.4368	0.8188	16.1328	1.0524	19.8288	-0.8631	23.5248	-0.8185	27.2208	-0.0356
12.5208	-0.8351	16.2168	-0.4387	19.9128	6.6616	23.6088	6.4593	27.3048	0.393
12.6048	0	16.3008	-1.9229	19.9968	-4.6229	23.6928	-1.3722	27.3888	-0.2219
12.6888	0.418	16.3848	-0.3496	20.0808	0.1867	23.7768	2.3955	27.4728	1.4827
12.7728	0.3193	16.4688	0.5001	20.1648	1.2195	23.8608	-3.319	27.5568	-2.0985
12.8568	3.7771	16.5528	0.2499	20.2488	-2.0644	23.9448	-0.4286	27.6408	0.4277
12.9408	26.8022	16.6368	-1.0904	20.3328	2.3655	24.0288	0.243	27.7248	1.2708
13.0248	37.2495	16.7208	2.9283	20.4168	-2.4982	24.1128	1.3607	27.8088	0.9777
13.1088	7.0067	16.8048	-0.6811	20.5008	-0.3801	24.1968	-3.2627	27.8928	2.5511
13.1928	0	16.8888	-1.1772	20.5848	-0.2858	24.2808	0.073	27.9768	-1.5235
13.2768	-3.0407	16.9728	-1.3572	20.6688	1.761	24.3648	1.3345	28.0608	-2.5451
13.3608	-1.8259	17.0568	-3.5636	20.7528	-1.0093	24.4488	1.2	28.1448	-0.6194
13.4448	2.033	17.1408	-4.2143	20.8368	-1.0697	24.5328	-2.6	28.2288	0.5346
13.5288	3.0909	17.2248	-0.2933	20.9208	1.9928	24.6168	-1.5256	28.3128	-0.7381
13.6128	2.7872	17.3088	1.7039	21.0048	-1.1658	24.7008	0.2424	28.3968	0.9046
13.6968	0.4751	17.3928	-1.1937	21.0888	-3.229	24.7848	0.3832	28.4808	2.5476
13.7808	0.3133	17.4768	1.5005	21.1728	0.6495	24.8688	-0.1792	28.5648	-1.1943
13.8648	1.7011	17.5608	-0.047	21.2568	3.9798	24.9528	1.4494	28.6488	-1.5238
13.9488	0	17.6448	0.4287	21.3408	-2.4634	25.0368	-2.4059	28.7328	-0.4974
14.0328	-3.2208	17.7288	0.357	21.4248	6.8242	25.1208	1.9642	28.8168	-0.9999
14.1168	-2.8592	17.8128	0.5357	21.5088	-5.3714	25.2048	0.3978	28.9008	-2.524

Pos. [°2Th.]	Iobs [cts]	Pos. [°2Th.]	Iobs [cts]	Pos. [°2Th.]	Iobs [cts]	Pos. [°2Th.]	Iobs [cts]	Pos. [°2Th.]	Iobs [cts]
28.9008	-2.524	32.5968	-0.7751	36.2928	0.2091	39.9888	-3.4532	43.6848	-0.4762
28.9848	-0.9203	32.6808	-1.4939	36.3768	-0.1726	40.0728	0.0142	43.7688	-1.0976
29.0688	0.9629	32.7648	2.5134	36.4608	-0.9975	40.1568	4.5167	43.8528	-0.1874
29.1528	-0.4815	32.8488	1.2282	36.5448	1.9737	40.2408	-1.5754	43.9368	1.0831
29.2368	-0.4577	32.9328	-1.6653	36.6288	-0.8621	40.3248	0.4598	44.0208	-0.3425
29.3208	1.8155	33.0168	-0.4637	36.7128	-0.116	40.4088	0.4481	44.1048	-0.199
29.4048	1.6871	33.1008	0	36.7968	0.9787	40.4928	-0.5105	44.1888	0.4744
29.4888	-1.1934	33.1848	0.7787	36.8808	-2.3522	40.5768	0.9923	44.2728	0.3723
29.5728	-1.0924	33.2688	-0.1696	36.9648	3.8665	40.6608	3.8012	44.3568	-0.6898
29.6568	1.6518	33.3528	-1.5558	37.0488	-1.5837	40.7448	-0.9972	44.4408	-0.5803
29.7408	-0.6925	33.4368	-1.9465	37.1328	3.7425	40.8288	0.1321	44.5248	0.3707
29.8248	-0.7293	33.5208	-1.1196	37.2168	2.1863	40.9128	-0.5141	44.6088	1.1374
29.9088	1.7862	33.6048	0.7178	37.3008	-3.12	40.9968	1.2196	44.6928	1.2066
29.9928	0.0901	33.6888	-0.8378	37.3848	-0.1104	41.0808	1.4818	44.7768	1.935
30.0768	0.9054	33.7728	-1.6636	37.4688	0.9008	41.1648	0.9059	44.8608	2.0368
30.1608	0.2291	33.8568	2.2938	37.5528	-1.383	41.2488	0.0391	44.9448	1.7771
30.2448	-1.3718	33.9408	2.9303	37.6368	-0.9471	41.3328	0.5653	45.0288	1.1321
30.3288	-0.8035	34.0248	5.2855	37.7208	1.0657	41.4168	1.6789	45.1128	4.6573
30.4128	1.1358	34.1088	-0.3503	37.8048	1.6222	41.5008	-1.2363	45.1968	4.7556
30.4968	-1.1463	34.1928	7.9367	37.8888	2.0067	41.5848	0.6462	45.2808	7.1016
30.5808	-2.2143	34.2768	8.9136	37.9728	-0.9697	41.6688	3.558	45.3648	18.0573
30.6648	-2.9052	34.3608	13.1898	38.0568	0.0963	41.7528	-0.4312	45.4488	21.8741
30.7488	-0.858	34.4448	41.9397	38.1408	2.6837	41.8368	5.0451	45.5328	13.0891
30.8328	0.5715	34.5288	66.0684	38.2248	-1.314	41.9208	6.802	45.6168	4.9879
30.9168	0.2142	34.6128	40.9713	38.3088	-2.3334	42.0048	2.059	45.7008	1.0806
31.0008	-0.3193	34.6968	22.4348	38.3928	-2.784	42.0888	0.082	45.7848	1.0083
31.0848	1.9414	34.7808	6.9112	38.4768	-0.6599	42.1728	0.2324	45.8688	1.6691
31.1688	2.9663	34.8648	3.0673	38.5608	1.6441	42.2568	0.1976	45.9528	0.4567
31.2528	0.7612	34.9488	0.7017	38.6448	-1.0674	42.3408	-0.3896	46.0368	1.3876
31.3368	-2.5477	35.0328	-0.2174	38.7288	4.4576	42.4248	-0.6078	46.1208	-0.2133
31.4208	-1.9267	35.1168	1.9211	38.8128	8.7587	42.5088	0.33	46.2048	-1.6806
31.5048	1.0177	35.2008	-1.3237	38.8968	17.3938	42.5928	2.0691	46.2888	1.107
31.5888	0.8132	35.2848	0.2703	38.9808	14.9153	42.6768	-0.8909	46.3728	1.2024
31.6728	-0.7729	35.3688	2.2807	39.0648	6.2555	42.7608	-1.493	46.4568	2.0608
31.7568	0.377	35.4528	-0.1888	39.1488	-1.5768	42.8448	-0.2466	46.5408	-0.1091
31.8408	-1.2699	35.5368	3.5473	39.2328	-0.8396	42.9288	-0.7856	46.6248	-1.5761
31.9248	-0.6017	35.6208	-3.2171	39.3168	-0.6314	43.0128	0.0858	46.7088	0.2137
32.0088	-1.4089	35.7048	-1.2151	39.4008	1.2878	43.0968	0.9233	46.7928	0.3037
32.0928	4.3876	35.7888	-0.9999	39.4848	2.9294	43.1808	-0.3018	46.8768	-0.1661
32.1768	-1.6292	35.8728	1.8461	39.5688	8.5386	43.2648	-0.2403	46.9608	-1.4416
32.2608	-3.4408	35.9568	0.2127	39.6528	14.5258	43.3488	0.1501	47.0448	-1.4522
32.3448	-4	36.0408	2.733	39.7368	38.2024	43.4328	-0.4061	47.1288	0.1776
32.4288	0.3859	36.1248	-0.1657	39.8208	31.7221	43.5168	0.552	47.2128	1.4406
32.5128	-1.8744	36.2088	1.8294	39.9048	15.7413	43.6008	0.7328	47.2968	2.0409

Pos. [°2Th.]	Iobs [cts]	Pos. [°2Th.]	Iobs [cts]	Pos. [°2Th.]	Iobs [cts]	Pos. [°2Th.]	Iobs [cts]	Pos. [°2Th.]	Iobs [cts]
47.3808	-1.5037	49.9008	-1.2855	52.4208	-0.5747	54.9408	1.4763	57.4608	-1.5436
47.4648	-0.7359	49.9848	5.7259	52.5048	6.3414	55.0248	0.8649	57.5448	-0.1916
47.5488	1.3653	50.0688	3.2607	52.5888	20.4391	55.1088	-0.4579	57.6288	1.1341
47.6328	3.3733	50.1528	-2.5976	52.6728	12.0291	55.1928	-1.25	57.7128	1.7294
47.7168	-0.0657	50.2368	-0.2379	52.7568	6.6002	55.2768	1.9579	57.7968	2.5563
47.8008	1.5448	50.3208	1	52.8408	6.1134	55.3608	2.5201	57.8808	0.5598
47.8848	6.6914	50.4048	-0.9383	52.9248	-3.6333	55.4448	-1.9877	57.9648	-1.9262
47.9688	7.8837	50.4888	1.3217	53.0088	0.3115	55.5288	-0.4581	58.0488	2.0925
48.0528	14.8472	50.5728	1.7348	53.0928	-0.5854	55.6128	0.5359	58.1328	3.5482
48.1368	11.6687	50.6568	-2.2741	53.1768	-1.5226	55.6968	3.3255	58.2168	0.9942
48.2208	15.6477	50.7408	0.1437	53.2608	0.548	55.7808	0.6419	58.3008	-0.7778
48.3048	1.848	50.8248	0.9718	53.3448	1.9145	55.8648	-2.0998	58.3848	-0.7629
48.3888	-0.894	50.9088	-0.1318	53.4288	9.4007	55.9488	0.8555	58.4688	-0.6002
48.4728	0.4671	50.9928	-0.4397	53.5128	11.5334	56.0328	0.9512	58.5528	1.5516
48.5568	-0.861	51.0768	-1.1955	53.5968	6.3758	56.1168	-1.5579	58.6368	3.5425
48.6408	0.5315	51.1608	0.4016	53.6808	1.0731	56.2008	0.6827	58.7208	-0.4599
48.7248	-1.1219	51.2448	-2.4083	53.7648	5.6274	56.2848	-1.4125	58.8048	-0.5159
48.8088	-0.9465	51.3288	-1.9137	53.8488	-3.09	56.3688	1.8152	58.8888	0.3491
48.8928	0.3432	51.4128	0.0049	53.9328	-2.609	56.4528	5.1407	58.9728	-0.3795
48.9768	-0.1415	51.4968	0.9354	54.0168	1.9989	56.5368	5.3415	59.0568	0.1373
49.0608	0.5466	51.5808	-1.1269	54.1008	-0.5402	56.6208	11.5759	59.1408	1.6203
49.1448	0.0886	51.6648	2.3477	54.1848	1.631	56.7048	12.595	59.2248	2.8879
49.2288	-0.9625	51.7488	-2.3964	54.2688	0.6093	56.7888	15.7114	59.3088	-0.0662
49.3128	-0.226	51.8328	-1.1235	54.3528	0.9445	56.8728	3.9072	59.3928	-2.7608
49.3968	1.6072	51.9168	-0.3572	54.4368	-0.4693	56.9568	-4.4463	59.4768	0.4115
49.4808	1.6458	52.0008	0.5396	54.5208	-1.2938	57.0408	0.4322	59.5608	3.1519
49.5648	-2.0665	52.0848	2.3535	54.6048	-0.4085	57.1248	0.9618	59.6448	1.2456
49.6488	0.8152	52.1688	-1.9953	54.6888	-1.9381	57.2088	0.5617	59.7288	-2.2011
49.7328	0.9994	52.2528	-2.2729	54.7728	-0.1423	57.2928	2.0122	59.8128	-0.6581
49.8168	-1.1062	52.3368	0.4788	54.8568	0.7917	57.3768	1.4745	59.8968	-0.0703

DISCUSSION

For optical applications, especially for simple harmonic generation (SHG) the material considered must be transparent in the wavelength region of interest. The broad feature of around 1600cm-1seems to occur due to deformation of a free water molecule will be strong in lead iodide. To the best of our knowledge, the lead iodide crystal possess third order non-linearity (Optical Materials). In Pbcl2 and PbBr2 which are isomorphous, lead is nine co-ordinate, while PbI_2 has six-co-ordinate lead in a structure based on CdI_2 layer lattice, since lead normally has a co-ordination of six or more in complexes, it is reasonable to consider that lead halide possess very low solubility. As one can see from the analysis of FTIR spectra large wavelength area was undisturbed resisting the reorientation mobility of a molecular ion. It is obvious in this case, that reorientation parameters are dependent as on the crystal structure and so also on the configuration of the given ion. As for the crystal structure and positional symmetry in the molecule is lowering in the crystal phases preceding the melt due to the substantial thermal activation of the ion mobility as well as the increase in dynamic interaction

between the ions. The habit of PbI_2 crystals that is least affected by external factors. In view of the wide band gap, low vapour pressure, and high resistivity, PbI_2 detectors are capable of low noise operation at elevated temperatures. Successful operation of Lead Iodide X-ray detectors at 100°C has been reported earlier[9]. The high temperature capability of PbI_2 makes it promising for applications such as bore-hole logging and environmental monitoring. Usually the bending mode of water increases in wave number with increased strength of hydrogen bonding. However, this correlation does not always hold. In addition, the ability to obtain an entire broad band or transient spectrum enables one to monitor unusual properties of the transiently excited species and to look for potential sample.

CONCLUSION

It is common observation that PbI_2 can be grown in gel, nucleating very rapidly in the presence of infrared radiation. The NLO effect in the molecule originates from a strong due to the ability to crystallize in non-centrosymmetric structure. Amoung several compounds reported for NLO property, PbI_2 derivatives are noticeable materials for their excellent crystallizability. The FTIR spectra of the compound has been recorded to do the qualitative analysis of the vibrational bands. In the present talk new spectroscopic result of PbI_2 will be discussed. There are very few crystals like PbI_2, which satisfy high melting point, mechanical stability and chemical inertness. Hence the search for new materials seems to be unending. There is a strong need of nonlinear optical crystals to cover near infrared and far infrared wavelength region In the procedures described thus so far, the gel is used as the reaction medium, in which the PbI_2 is chemically formed.

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