IJCRT.ORG ISSN : 2320-2882

INTERNATIONAL JOURNAL OF CREATIVE RESEARCH THOUGHTS (IJCRT)

An International Open Access, Peer-reviewed, Refereed Journal

SYNTHESIS AND CHARACTERISATION OF SRBR$_2$ DOPED POTASSIUM CHLORIDE SINGLE CRYSTALS

A.Ancy[1] Dr.M.Maria Lenin[2]

Annai VelanKanni College of Arts and Science, Tholyavattam

Abstract:

Undoped and doped KCl single crystals have been successfully grown by slow evaporation method. The effects of dopant $SrBr_2$ on structural and optical properties were investigated by a number of techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier Transform Infrared analysis, UV-visible (UV). X-ray diffraction study was performed on the title compound. The presence of functional groups and modes of vibrations for A4MBS was interpreted using FT-IR spectrum. The optical quality and percentage of transmission was assessed using UV-Vis analysis. The crystalline perfection of grown crystal was evaluated by high resolution X-ray diffractometry.

Keywords: Crystal growth, PXRD, FTIR, UV, SEM

Introduction:

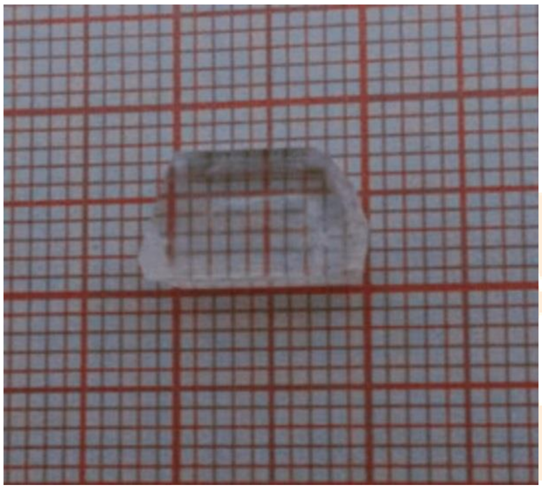
$SrBr_2$ as the best candidate among 125 free standing salts [1]. Extensive studies were performed yet on $SrBr_2$ in heat storage systems [2]. Other salts can be considered when they are supported by a matrix, but at the expense of their heat storage density [3]. For SrBr2 as well, a better stability is observed when it is supported by mesoporous silicage[4]. Two possible processes for $SrBr_2$ production are presented: one is the assumed current process for small scale, the other is a new process expected to reduce the costs and the impacts. Secondly, this process is investigated experimentally. Finally, the sustainability of the proposed process is discussed

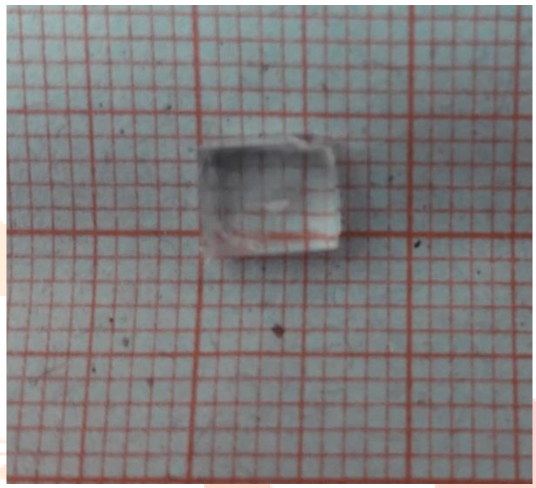
A wide query in Scopus® database on “SrBr2” or “strontium bromide” gives < 100 entries, mostly on the physical, chemical or pharmacological properties of SrBr2, and on its applications in heat storage or lasers. Strontium bromide is a promising material for heat storage applications, especially in the case of low temperature residential heating. The interest in crystal growth process has been increased particularly in the field of technological application [5-7]. Recent research is focused on the search for suitable materials displaying excellent second order nonlinear optical properties for potential application in optoelectronics, telecommunication, and optical storage device [8].

Synthesis and crystal growth technique

Analytical grade $SrBr_2$ doped KCl single crystals was dissolved in double distilled water. In order to grow good quality crystals, it is essential to increase purity up to a respectable level. In the present study, the commercially available salt was dissolved in water and purified by the repeated recrystallisation process, and the recrystallised material was used to prepare the saturated solution. The resulting aqueous solution was filtered and allowed to evaporate under optimized conditions to grow crystals by slow evaporation method at room temperature (30 C). After a period of 10 days, optically good quality single crystals are harvested.

Result and Discussion:



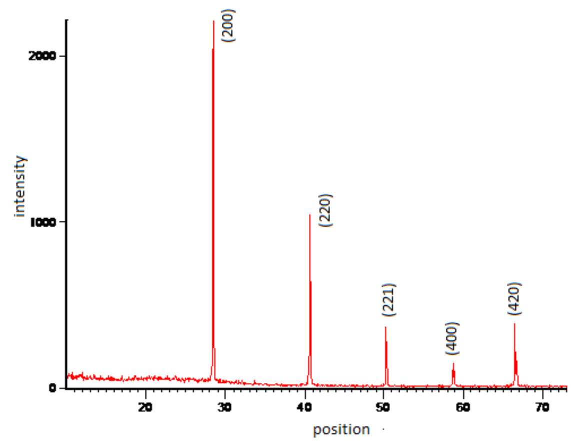


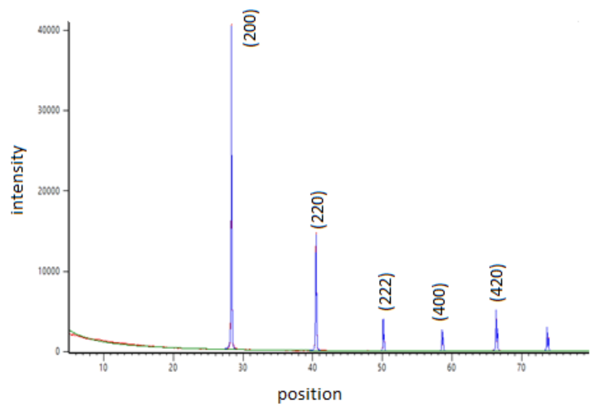
Pure KCl **$SrBr_2$ doped KCl**

Intensity %	Angle in degrees (2θ)	d spacing (Å)	Miller indices (hkl)	Lattice Parameter
100	28.2938	3.15429	(200)	a = 6.308
34.79	40. 4845	2.2282	(220)	
8.4	66.3216	1.40942	(420)	
4.99	58.5604	1.5763	(400)	
4.37	50.1714	1.81836	(222)	

Intensity %	Angle in degrees (2θ)	d spacing (Å)	Miller indices (hkl)	Lattice Parameter
100.00	28.3095	3.14997	(200)	a = 6.411
40.50	40.4833	2.22642	(220)	
11.06	50.1393	1.81795	(420)	
8.48	58.5870	1.57434	(400)	
14.33	66.3357	1.40798	(222)	

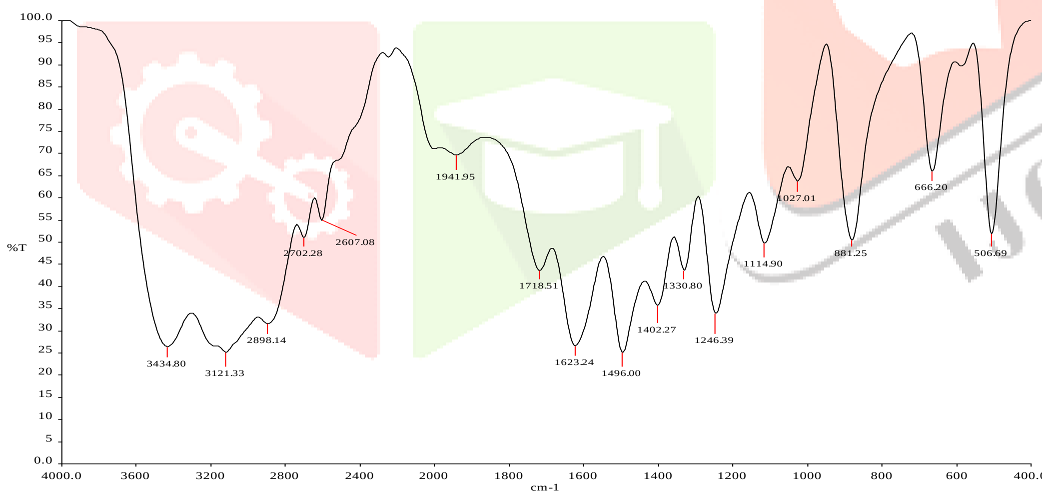
Powder X – ray Diffraction:



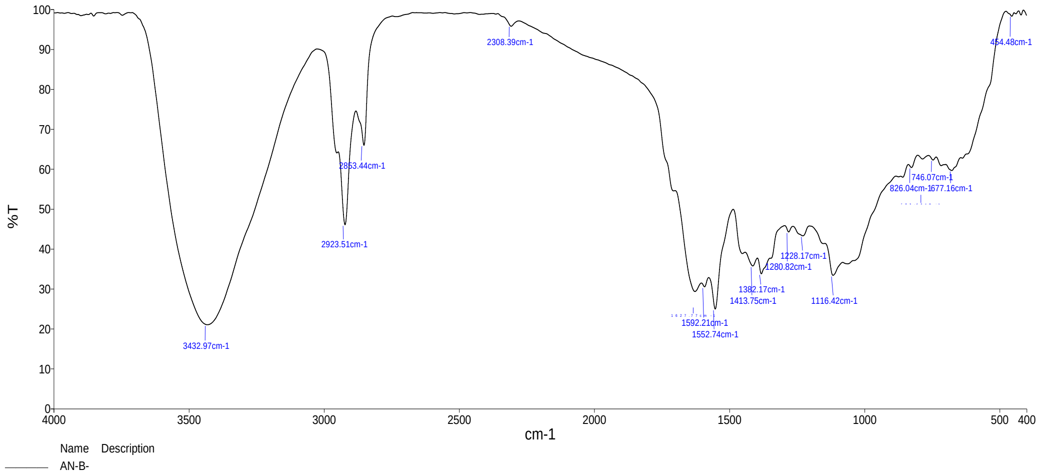


The powder X – ray diffraction patterns of pure and doped $SrBr_2$ are shown in Figure Well defined Bragg peaks are obtained at specific 2θ angles. The ‘d’ spacings and (h k l) values for prominent peaks in the spectrum are identified. Good crystallinity of the grown material is confirmed by the appearance of sharp peaks [9]. This may be due to the absorption or substitution of doped atom in lattice sight. There is slight variation in the lattice parameters depending upon the impurity addition and at the same time, the total crystal structure is not affected.

FTIR analysis

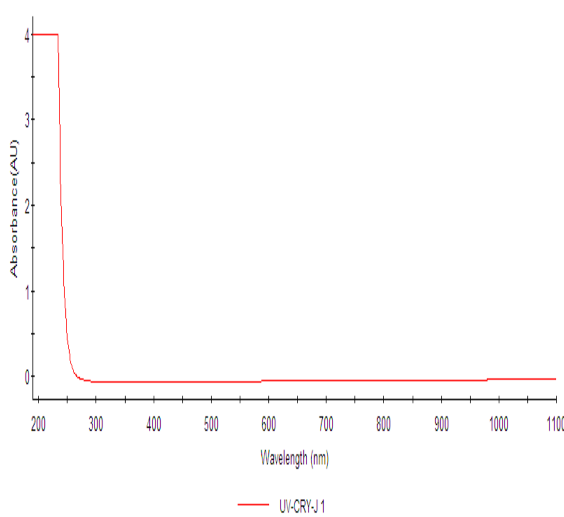


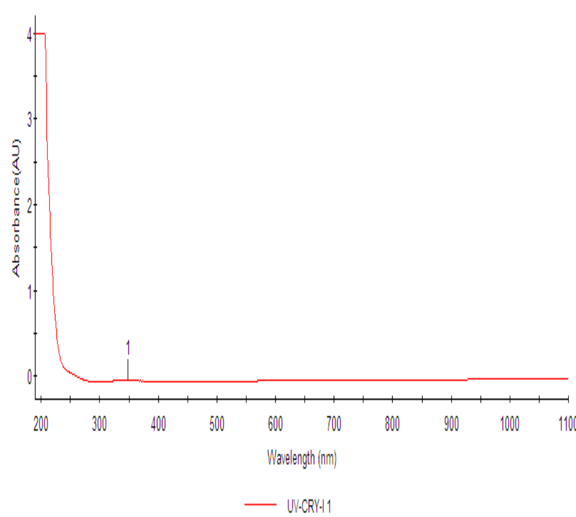
:



FTIR has made energy limited region more accessible. It has made the middle infrared (400-4,000cm-1) also more useful. It is an important technique in organic chemistry. It is an easy way to identify the presence of certain functional groups in a molecule. FTIR spectra have been recorded by using IFS BRUKKER 66V spectrophotometer in the range of 400cm-1 -4000cm-1 in order to find the presence of various functional groups. The FTIR spectrum are taken for all the samples to study the spectroscopic properties of the grown crystals. The force constant value depends on the absorption maximum wave number. The force constant increases, when the absorption maximum wave number increases.

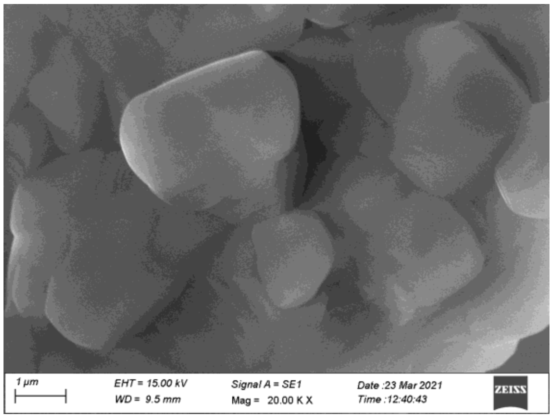
UV-Vis-NIR Spectroscopy:

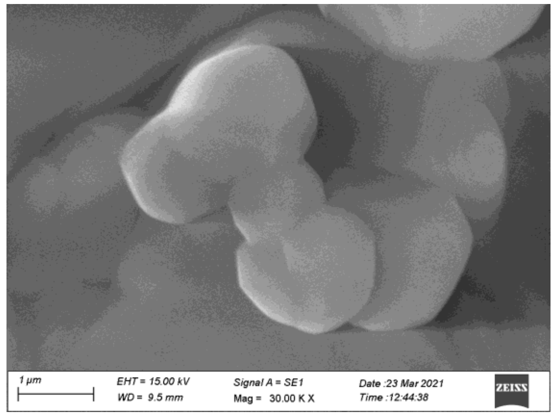


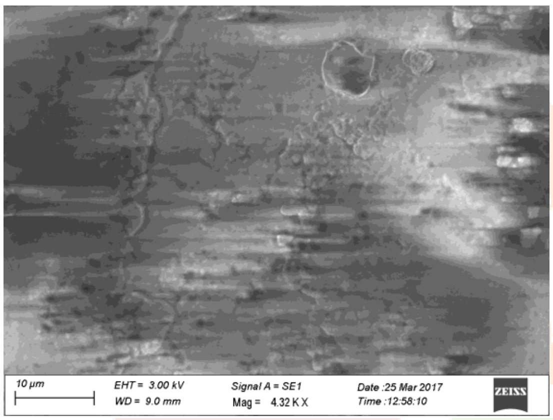


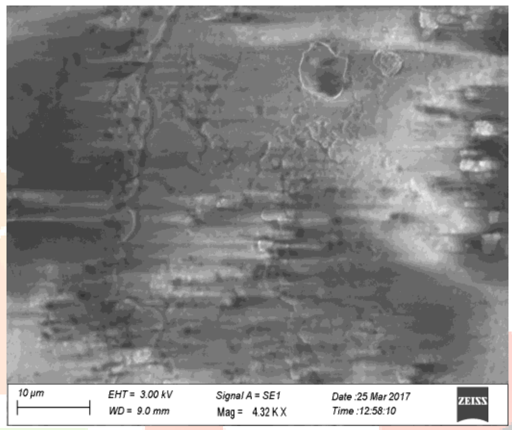
The optical absorption spectra of pure KCl and doped $SrBr_2$ crystals are recorded in the wavelength range 200-800 nm using UV-2600 series in the UV-visible scanning spectrometer. The recorded absorption spectrum is shown in Figure. The UV cut off wavelength of pure KCl is already reported as 218 nm [10] whereas (KCl : $SrBr_2$) crystal has the UV cut off wavelength at 235 nm. Hence it is clear that the presence of KCl in $SrBr_2$ crystal improves its optical transmission and there is no considerable absorption is found in the range 220 nm to 800 nm. This clearly indicates that the $SrBr_2$ doping has increased the optical window of pure KCl crystal.

Scanning Electron Micoscope:









To characterize such materials the scanning electron Microscope now uses a wide range of operating conditions to target the desired sample volume, sophisticated modeling techniques to interpret the data. It also uses novel imaging modes to derive new types of information. These include depth resolved three dimensional data, and spatially resolved crystallographic data.

Conclusion:

Good optical quality of single crystals $SrBr_2$ doped Potassium Chloride single crystals were grown by slow evaporation solution growth method at room temperature. The powder X-Ray diffraction study confirms the lattice parameter value. The lattice parameters have been found by single crystal X-ray diffraction technique. X-Ray diffraction. . The presence of functional groups in $SrBr_2$ doped Potassium Chloride has been identified by FT-IR spectral analysis. From the UV spectrum, the $SrBr_2$ doped Potassium Chloride crystal is found to be transparent in the UV region and it could be a useful candidate for optoelectronic applications in visible and infrared region. The morphology of all the grown samples were analysed through SEM images.

References

[1] N'Tsoukpoe K, Schmidt T, Rammelberg H, Watts B and Ruck W. A systematic multi-step screening of numerous salt hydrates for low temperature thermochemical energy storage. Applied Energy 124; 2014: 1-16.

[2] Michel B, Mazet N, Mauran S, Stitou D and Xu J. Thermochemical process for seasonal storage of solar energy: Characterization and modeling of a high density reactive bed. Energy 47; 2012: 553-563

[3] Aristov Y, Tokarev M, Cacciola G and Restuccia G. Selective water sorbents for multiple applications, 1. CaCl2 confined in mesopores of silica gel: Sorption properties. Reaction Kinetics and Catalysis Letters 59; 1996: 325-333.

[4] Courbon E, D'Ans P, Permyakova A, Skrylnyk O, Steunou N, Degrez M and Frère M. A new composite sorbent based on SrBr2 and silica gel for solar energy storage application with high energy storage density and stability. Applied Energy 190; 2017: 1184-1194

[5] Baraniraj ,T ., Philominathan, P, "Growth, Thermal, mechanical and dielectic studies of International Journal of Materials Science ISSN 0973-4589 Volume 12, Number 2 (2017) © Research India Publications http://www.ripublication.com 279 Glycine doped Pottassium acid phthalate single crystals", (2011),J. Minerals & material Characterization & Engineering, 10-9, 805-815.

[6] Dillip, R., Madhukar Reddy, C., Deva Prasad Raju , B: Growth and characterization of Nonlinear optical material. J. Minerals & materials Characterization & Engineering", (2011). 10-12, 1103-1110.

[7] Anjelin Ursula Portia,S., Jayanthi , K., Ramamoorthy ,K : Growth and Characterization of pure and disodium hydrogen phosphate mixed with potaddium dihydrogen phosphate crystal using slow evaporation technique. American J. biological and Pharmacetual research. 1-2, 77-82(2014).

[8] Yakushkin, E.D.,.Efremova, E.P ., Baranova, A.I, "Growth conditions and electrical properties of KDP crystals: II Dielectric permittivity measurements, (2001), crystallography reports, 46-5, 904-908.

[9]. Arumanayagam T, Ananth S et al. (2012). Studies on growth, spectral, optical and mechanical properties of new organic NLO crystal: guanidinium L- glutamate (GuGL). Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, vol 97, 741–745.

[10]. Babu R R, Ramesh R (2010). Growth, structural, spectral, mechanical and optical properties of pure and metal ions doped sulphamic acid single crystals, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, vol 76(5), 470 – 475