International Journal of Chemistry and Applications.
ISSN 0974-3111 Volume 4, Number 1 (2012), pp. 1-8

http://www.irphouse.com

Synthesis, Growth and Spectroscopic Studies of Marine Dye Nlo Material: Disodium 2-(1,3-Dioxoinden-2-Yl)Quinoline-6,8-Disulfonate (Quinoline Yellow) Crystals

M. Jayandran[1] and V. Balasubramanian[2]

[1]Department of chemistry, Mahendra Engineering College,
Namakkal-637 503, India
[2] Department of chemistry, AMET University, Chennai -603112, India

Abstract

Disodium 2-(1,3-dioxoinden-2-yl)quinoline-6,8-disulfonate as a marine dye was synthesized by taking and Quinine reacted with 1,3-Dioxoindan-2-yl and disulfonic acid disodium salt are used to synthesized marine dye like Quinoline Yellow
($C_{18}H_9NNa_2O_8S_2$). It is soluble in water. Single crystals of disodium 2-(1, 3-dioxoinden-2-yl)quinoline-6,8-disulfonate were grown by solution method with slow evaporation technique. The grown crystals were characterized by single crystal X-ray diffraction (XRD) analysis, FTIR studies and UV-visible transmittance studies and the NLO activity of the grown crystal has been checked by Second Harmonic Generation (SHG) test.

Keywords: Disodium 2-(1, 3-dioxoinden-2-yl) quinoline-6, 8-disulfonate; solubility; solution growth; FTIR; XRD; SHG.

Introduction

Nonlinear optical (NLO) materials have gained considerable attention due to their practical applications in the field of optoelectronics(1,2). The development of NLO materials led to compounds potentially suitable for application in frequency conversion, optical telecommunication, image processing, optical computing, and data storage devices(3-6). Disulfonic acid family-type crystals have over the years been subjected to extensive investigation by the researchers for their non-linear optical properties(7, 8). Among the disulfonic acid, quinoline is the simplest molecule with second harmonic generation efficiency of about one-third of that of the well known

KDP (9,10) , it is expected to get improved NLO properties. Keeping this in mind, the Quinoline mixtures have been mixed to form a novel NLO material. disodium 2-(1, 3-dioxoinden-2-yl)quinoline-6,8-disulfonate ($C_{18}H_9NNa_2O_8S_2$)reported the details of crystal structure of Quinoline Yellow and it is observed from the various properties of crystals report. Hence the aim of this paper is to report the growth, spectroscopic studies and NLO activity of disodium 2-(1, 3-dioxoinden-2-yl)quinoline-6,8-disulfonate (Quinoline Yellow) crystals for the first time.

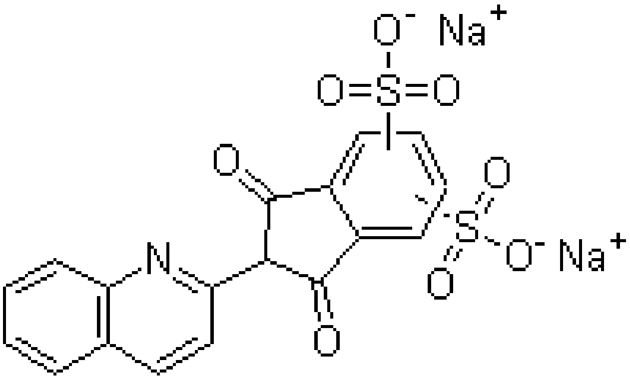

Figure 1: Structure of disodium 2-(1, 3-dioxoinden-2-yl)quinoline-6,8-disulfonate salt

Experimental Methods

Growth of Quinoline Yellow Single Crystals

The purity of the synthesized salt of disodium 2-(1, 3-dioxoinden-2-yl)quinoline-6,8-disulfonate (Quinoline Yellow) has been improved by re-crystallization. Using the solubility data, the saturated solution of disodium 2-(1, 3-dioxoinden-2-yl)quinoline-6,8-disulfonate (Quinoline Yellow) in deionized water was prepared and it was stirred using a magnetic stirrer for about one hour to get homogenious solution.

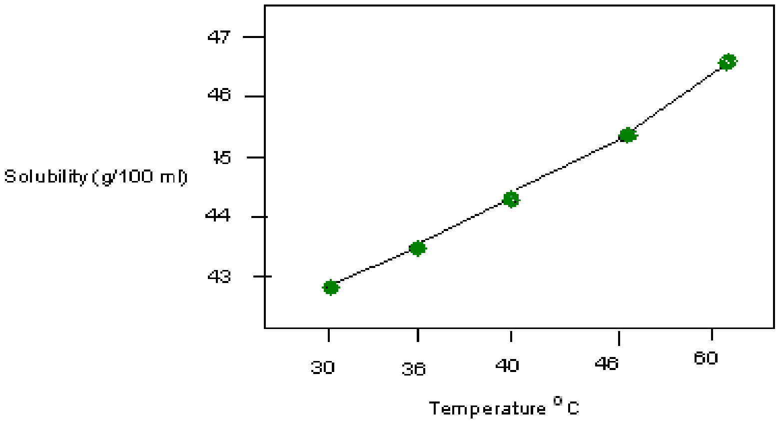

Figure 2: Solubility curve for Quinoline Yellow crystal

The saturated solution was filtered using 4 micro Whatmann filter paper. Then the filtered solution was taken in a beaker and covered by a perforated cover for controlled evaporation. A typical single crystal with size 14 x 13 x 7 mm^3 was obtained within a period of 25-30 days. The grown crystal is shown in the figure 3.

Figure 3: Photograph of as-grown crystal of Quinoline Yellow.

Characterization Single crystal XRD studies

The grown crystals were subjected to single crystal XRD to confirm the crystallinity and also to estimate the lattice parameters by employing Bruker-Nonious MACH3/CAD4 single X-ray diffractometer. From single crystal X-ray diffraction data, it is observed that the disodium 2-(1, 3-dioxoinden-2-yl)quinoline-6,8-disulfonate (Quinoline Yellow) crystal is orthorhombic in structure with space group P212121. The lattice parameters are observed to be a=6.193(2) Å,b=9.931(1) Å, c=11.757(3) Å, α=β=γ=90° and V =723.08(2) Å3. The obtained lattice parameters for disodium 2-(1, 3-dioxoinden-2-yl) quinoline-6, 8-disulfonate (Quinoline Yellow) crystal in this work are found to be in good structure. The peaks in the fig show the crystalline nature of Quinoline Yellow. Further the peaks are indexed. This is shown in fig.4.

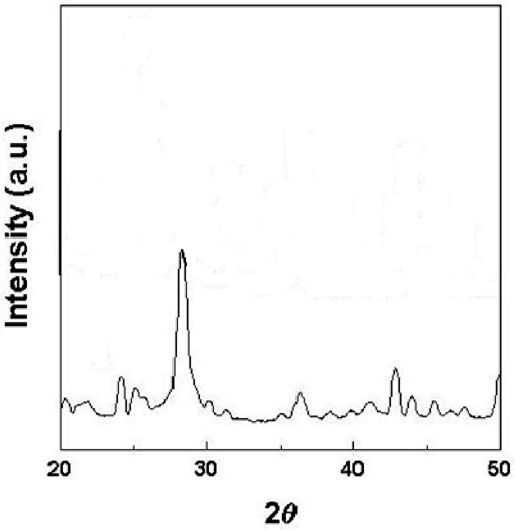

Figure 4: XRD patterns recorded from disodium 2-(1, 3-dioxoinden-2-yl) quinoline-6, 8-disulfonate (Quinoline Yellow) crystal

FTIR analysis

The Fourier Transform Infrared (FTIR) spectrum of disodium 2-(1, 3-dioxoinden-2-yl) quinoline-6, 8-disulfonate (Quinoline Yellow) crystal was recorded in the region 400 - 4000 cm-1 using FTIR SHIMADZU 8400S. Amide functional group appeared at 3440 cm^{-1} with sharp absorption and also giving C=O stretching absorption at 1638 cm^{-1}. It was further confirmed by observing C=O overtone absorption appeared at 3810 cm^{-1} and 3919 cm^{-1}. The strong absorption at 1030 cm^{-1} was assigned to C-O group due to its stretching vibrations. The strong absorption at 1047cm^{-1} confirms the presence of SO_3-Na substitution groups along with the group. Also, strong absorption at 1411 cm^{-1} was due to bending absorption of alkyl group. The sample was prepared by mixing disodium 2-(1, 3-dioxoinden-2-yl) quinoline-6, 8-disulfonate (Quinoline Yellow) with KBr into pellet form. The observed spectrum is shown in the figure-5.And the absorptions were summarized in table-1.

Table 1: Frequencies of the fundamental vibrations of GPC

S. No.	Frequency in wavelength (in $cm^{-1)}$	Assignment of vibration
1	3810 and 3919	C=O Overtone absorption
2	3440	-NH stretching vibration
3	2364	sp^3 asym. Stretching
4	2224	sp^3 sym. Stretching
5	1564	COO asym. Stretching
6	1411	sp^3 alkyl bending
7	1030	C-O stretching
8	1047	C-SO_3

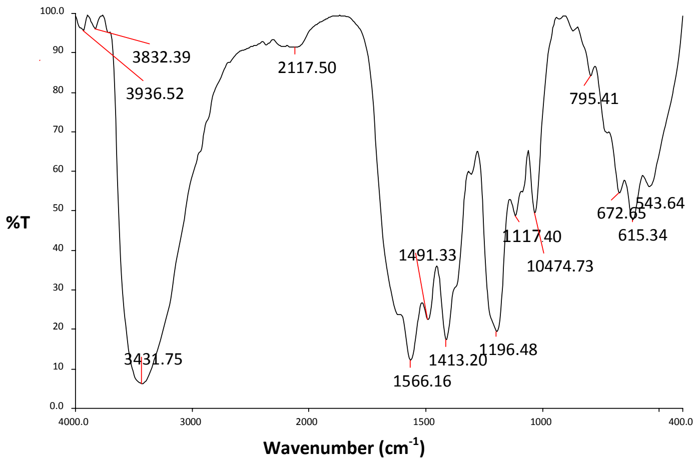

Figure 5: FTIR spectrum of Quinoline Yellow crystal.

Optical transmission spectral analysis

The UV-Visible transmittance spectrum (Fig.6) of disodium 2-(1, 3-dioxoinden-2-yl) quinoline-6, 8-disulfonate (Quinoline Yellow) crystal was recorded in the wavelength range 190-1100 nm, using Lambda 35 spectrometer. Optically polished single crystal of thickness 2 mm was used for this study. This spectral study may be assisted in understanding electronic structure of the optical band gap of the crystal. The study of the absorption edge is essential in connection with the theory of electronic structure, which leads to the prediction of whether the band structure is affected near the band extreme. The peak appeared at 525 nm and 575 nm corresponding to the Quinoline moiety. The UV-Visible transmittance spectrum shown in fig.6.

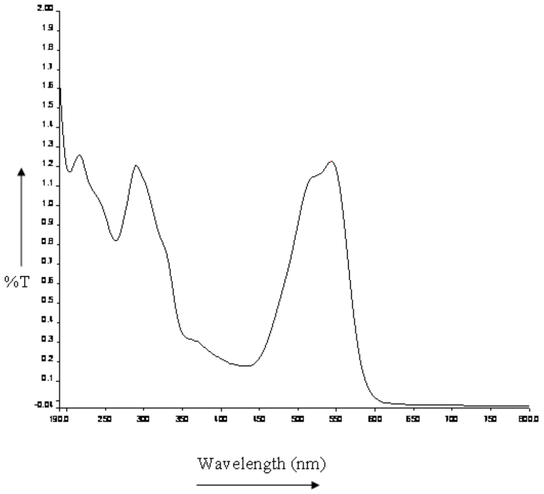

Figure 6: UV-Visible transmittance spectrum for Quinoline Yellow crystal.

Second Harmonic Generation (SHG) test

The Nonlinear Optical (NLO) property of the grown crystal was confirmed by Kurtz-Perry powder technique14. The disodium 2-(1, 3-dioxoinden-2-yl)quinoline-6,8-disulfonate (Quinoline Yellow) crystal was powdered with uniform particle size using a ball mill and it was packed densely between two transparent glass slides. An Nd:YAG laser was used as a light source.This laser device can be operated in two differentmodes. In the single-shot mode, the laser emits an 8 ns pulse. While in the multi-shot mode, the laser produces a continuous train of 8 ns pulse at a repetition rate of 10 Hz. In the present study, a multishot mode of 8 ns laser pulse with a spot radius of 1mm was used. The experimental setup for measuring SHG efficiency is shown in the figure 7.A fundamental laser beam of 1064 nm wavelength, 8 ns pulse with 10 Hz pulse rate was made to fall normally on the sample cell(S). The power of the incident beam was measured using a power meter. The filter F1 removes the 1064 nm light and the filter F2 is a BG-38 filter, which also removes the residual 1064 nm light. F3 is an interference filter with bandwidth of 4 nm and central wavelength 532 nm.The green light was detected by a photomultiplier tube (PMT) and displayed on a Cathode Ray Oscilloscope(CRO). KDP crystal was powdered into identical size as disodium 2-(1, 3-dioxoinden-2-yl)quinoline-6,8-disulfonate (Quinoline Yellow) crystal and it was used as reference material in the SHG measurement. In the NLO process that taking place in the sample, it converts the 1064 nm radiation into green light (λ=532 nm) when Nd:YAG laser light is passed into the sample and this confirms the SHG . It was found that the efficiency of SHG is 0.76 times that of the standard KDP.

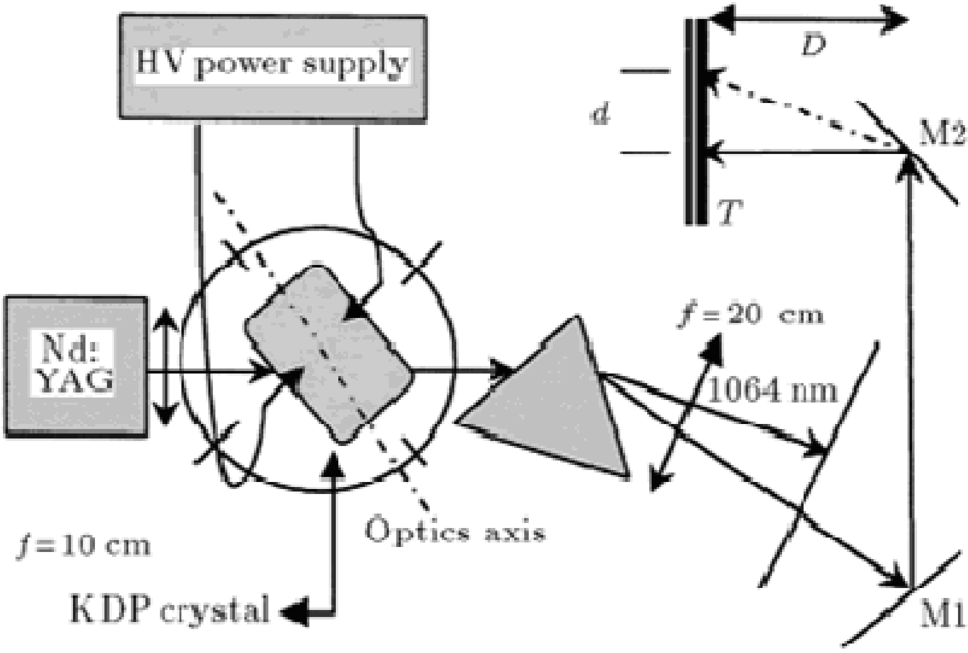

Figure 7: Experimental setup for SHG measurement

Conclusion

Disodium 2-(1, 3-dioxoinden-2-yl) quinoline-6, 8-disulfonate (Quinoline Yellow) salt was synthesized and solubility was determined at various temperatures. Bulk single crystals of Quinoline Yellow salt was grown by solution method. It is observed that the grown crystal is transparent, coloured and has good morphological edges. Single crystal X-ray analysis reveals that the crystal belongs to orthorhombic system with space group P212121. The functional groups present in disodium 2-(1, 3-dioxoinden-2-yl)quinoline-6,8-disulfonate (Quinoline Yellow) crystal are confirmed by the FTIR spectral analysis. The optical absorption study reveals high transparency of the crystal with a UV cut off wavelength of 240 nm. The NLO efficiency of the crystal is found to be 0.81 times that of KDP.

Acknowledgement

The authors are thankful to Mahendra Engineering College and AMET University to do the present work and also very thankful to NIT-Tiruchi for providing to utilize Scanning Electron Microscopy for analysis.

References

[1] X.Q. Wang, D. Xu, M. Lu, D. Yuan, J. Huang, X.Cheng, T. Xie, G.H. Zhang, S.L. Wang, S.Y.Guo, J.R. Liu, Z.H. Yang, P. Wang, J. Crystal Growth 234 (2002) 469.

[2] X.L. Duan, D.R. Yuan, X.Q.Wang, S.Y. Guo, J.G.Zhang, D. Xu, M.K. Lu, Cryst. Res.Technol. 37 (2002) 1066.

[3] C.C. Frazier, M.P. Cockerhamn, E.A. Chauchard,C.H. Lee, J. Opt. Soc. Am. B 4 (1987) 1899.

[4] S.B. Monaco, L.E. Davis, S.P. Velsko, F.T. Wong,D. Eimerl, J. Crystal Growth 85 (1987) 252.

[5] P. Gunter, Ch. Bosshard, K. Sutter, H. Arend, G.Chapuis, R.J. Twieg, D. Dobrowolski, Appl. Phys.Lett. 50 (1997) 486.78

[6] C. Krishnan, P. Selvarajan, T. H. Freeda, Material Letters, 62 (2008) 4414.

[7] M. Kitazawa, R. Higuchi, M.Takahashi, Appl.Phys. Lett. 64 (1994) 2477.

[8] L. Misoguti, A.T. Varela, F. D. Nunes, V.S.Bagnato, F.E.A. Melo, J. Mendes Filho, S.C.Zilio, Opt. Mater. 6 (1996) 147.

[9] B.Suresh Kumar, M.R.Sudarsana Kumar, K.Rajendra Babu, Cryst.Res.Technol. 43(2008)745.

[10] C. Razzetti, M.Ardoino, L. Zanotti, M. Zha, C.Paorici, Cryst. Res. Technol.37 (2002) 456.

[11] K. Yamada, A. Sato, T. Shimizu, T. Yamazaki, S.Yokoyama, Acta Cryst. E64 (2008) o806.

[12] P.Selvarajan, J.Glorium Arul Raj, S.Perumal,J.Crystal Growth 311 (2009) 3835.

[13] G. Socrates, Infrared and Raman characteristic Group Frequencies, 3rd Ed., Wiley, New York (2001).

[14] S. K. Kurtz, T.T. Perry. J. Appl. Phys 39 (1968) 3798.79