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|-------------------------|---|
| Title:                  | Structure-property correlation of halogen substituted benzothiazole crystals  |
| Authors:                | Singla, Labhini (/jspui/browse?type=author&value=Singla%2C+Labhini)<br>Choudhury, Angshuman Roy (/jspui/browse?type=author&value=Choudhury%2C+Angshuman+Roy)  |
| Keywords:               | Mechanical properties<br>Benzothiazole crystals   |
| Issue Date:             | 2021  |
| Citation:               | Journal of Molecular Structure, 1243, 130765.   |
| Abstract:               | We have synthesized 3 benzothiazole crystals (1–3) based on existing knowledge of combining flexibility and optical properties towards achieving applications for flexible optoelectronics. However, one crystal was found to be elastically bendable and was found to comply necessary packing features for elasticity. Other two crystals do not obey packing features for elasticity hence they are brittle in nature. Further, Hirshfeld analysis illustrates that elastic crystal 1 possess more number of weak and dispersive interactions compared to other crystals. These interactions were instrumental in invoking elasticity. Moreover, crystals 1–3 were found to be fluorescent as well at specific excitation wavelengths. Therefore, among these crystals, particularly crystal 1 is considered as more promising candidate for flexible optoelectronics. |
| Description:            | Only IISER Mohali authors are available in the record.  |
| URI:                    | <a href="https://www.sciencedirect.com/science/article/pii/S002228602100898X?via%3Dihub">https://www.sciencedirect.com/science/article/pii/S002228602100898X?via%3Dihub</a><br>( <a href="https://www.sciencedirect.com/science/article/pii/S002228602100898X?via%3Dihub">https://www.sciencedirect.com/science/article/pii/S002228602100898X?via%3Dihub</a> )<br><a href="http://hdl.handle.net/123456789/5016">http://hdl.handle.net/123456789/5016</a> ( <a href="http://hdl.handle.net/123456789/5016">http://hdl.handle.net/123456789/5016</a> )   |
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