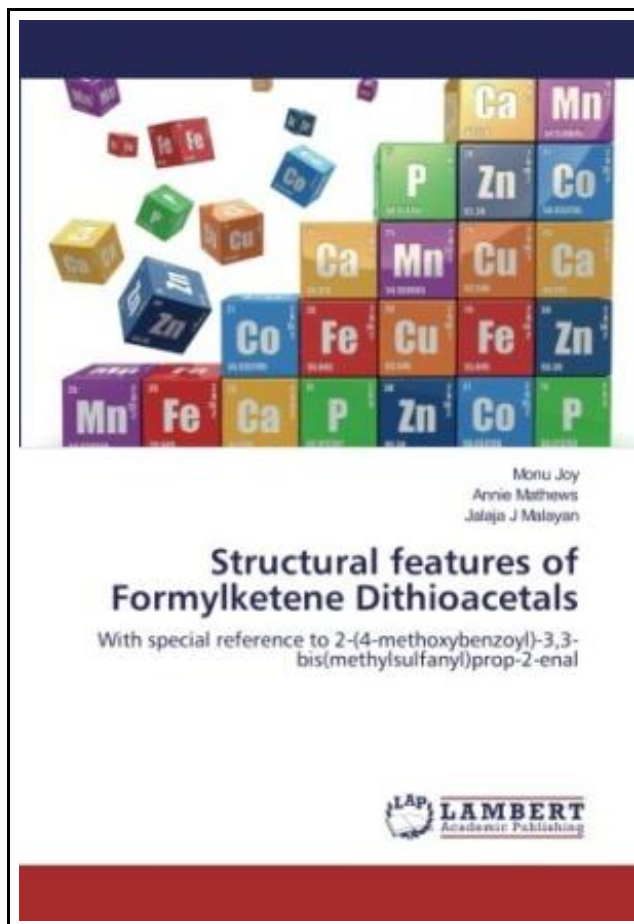


## Structural features of Formylketene Dithioacetals



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Condition: New. Publisher/Verlag: LAP Lambert Academic Publishing | With special reference to 2-(4-methoxybenzoyl)-3,3-bis(methylsulfanyl)prop-2-enal | In this work, a formylketene dithioacetal derivative was synthesized by using a reported method and its crystal structure study was carried out by means of Single Crystal XRD in order to determine the molecular conformation and to understand the influence of aroyl groups on the stereo chemistry by using Brucker Kappa Apex II Diffractometer and with WinGX software. We are reporting the FT-IR, FT-Raman and FT-NMR spectral characterizations of 2-(4-methoxybenzoyl)-3,3-bis(methylsulfanyl)prop-2-enal, a push-pull butadiene derivative with potential applications. Number of similar aroyl formylketene dithioacetals from acetophenone derivatives are semisolids. Therefore we assume that the methoxy substitution on the benzene ring do influence the crystalline nature of the compound. The structural and spectroscopic data of the molecule in the ground state were calculated by using ab initio (HF/6-31G) and DFT (B3LYP/6-31G(d)) methods. The optimized geometrical and spectroscopic parameters were comparable with experimental as well as literature values. | Format: Paperback | Language/Sprache: english | 84 pp.



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