

Poster Presentation

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Crystal structure analysis of organic compound $C_{18}H_{13}ClO_4S$

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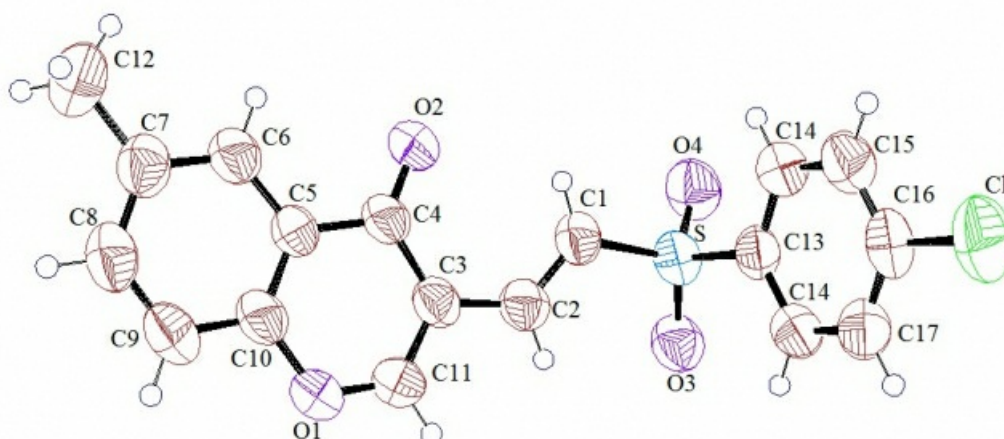
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The crystal structure analysis of organic compound, $C_{18}H_{13}ClO_4S$ was performed by using single crystal X-ray diffraction technique. The title organic compound contains three nearly planar segments (the benzopyranone group, the chlorophenyl ring and the ethene group). The sulfonyl plane is inclined at 52.8(2) degrees to the plane of the chlorophenyl group and at 48.9 (2) degrees to the plane of the benzopyranone group. Crystals obtained from 2 propanal by slow evaporation are monoclinic, $a = 12.91(7)$, $b = 9.708(6)$ and $c = 14.372(4)$ Å, $\beta = 112.54(2)$; $V = 1655.1(3)$ Å³, $M_w = 360.81$, $\lambda(\text{MoK}\alpha) = 0.71073$ Å. The independent reflections were collected by using Bruker Smart diffractometer and the structure was solved by direct methods and refined by full matrix least squares using SHELXL-97.

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Keywords: [organic compound](#), [sulfonyl plane](#), [monoclinic](#)