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Synthesis and crystal structure studies of 3,3-bis(methylthio)-1-(4-(trifluoromethyl) phenyl)prop-2-en-1-one and 3,3-bis(methylthio)-1-(thiophen-2-yl)prop-2-en-1-one derivatives

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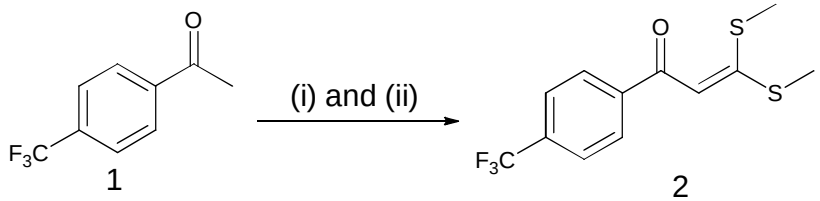
ABSTRACT

The title compounds of 3,3-bis(methylthio)-1-(4-(trifluoromethyl) phenyl)prop-2-en-1-one (J1) and 3,3-bis (methylthio)-1-(thiophen-2-yl)prop-2-en-1-one (J2) were synthesized and characterized by single crystal X-ray diffraction method. The structure was confirmed by X-ray diffraction studies. The compound (J1) crystallizes in monoclinic system under the space group $P2_1/c$, with cell parameters a = 11.8403(8)Å, b = 8.5517(7)Å, c = 11.7986(10)Å, β = 115.158(5)º and Z=4. Similarly, compound (J2) crystallizes in monoclinic system under the space group $P2_1/n$, with cell parameters a = 12.962(2) Å, b = 8.1006(11) Å, c = 13.348(2) Å, β = 114.945(9)º and Z=4. Crystal structure (J1 and J2) stabilized by an C2—H9.O7 and intramolecular C(7)--H(6).O(12) hydrogen bonds.

Graphical Abstract:



1 2

Reaction condition: (i) Pottasium-*tert*-butoxide, *tert*-butanol, CS_2, room temeprature, 4h; (ii) MeI, 0 ℃ to room temeperature, 6h.

Keywords: Ketene dithio acetals, Crystal structure, C-H…O interaction.