Yellow and Violet Polymorphs of (2Z)-2-(Nitromethylene)-2H-1,4-benzothiazine-3(4H)-one

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The title compound, (2Z)-2-(nitromethylene)-2H-1,4-benzothiazine-3(4H)-one, $C_9H_6N_2O_3S$, was obtained in the reaction of bromonitroacrylate and o-aminothiophenol [1]. In the solid state, two crystalline polymorphic modifications of the title compound were found - monoclinic, (I), and triclinic, (II). Single-crystal structure determination of I and II revealed the closeness of molecular conformations in both polymorphs. Moreover, the molecules in I and II form centrosymmetric dimers via N-H...O hydrogen bonds. The dimers are further linked into the identical ribbons by the weak intermolecular C-H...O interactions. The distinctions in crystal structures and colours, yellow for I and violet for II, are provided by different packing of the ribbons in both polymorphs.

[1] Berestovitskaya V.M., Tafeenko V.A., Makarenko S.V., Sadikov K.D., Chernyshev I.V., Russ. Zh. Obschej Khimii, 2005, submitted.

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