Synthesis, Crystal Structure and Some Physical Properties of 2(1',2',2',2'-tetrafluoroethylidene)-3,3-bis-Trifluoromethyl-2,3-dihydrobenzo[4,5]-imidazo[2,1-b]-thiazole

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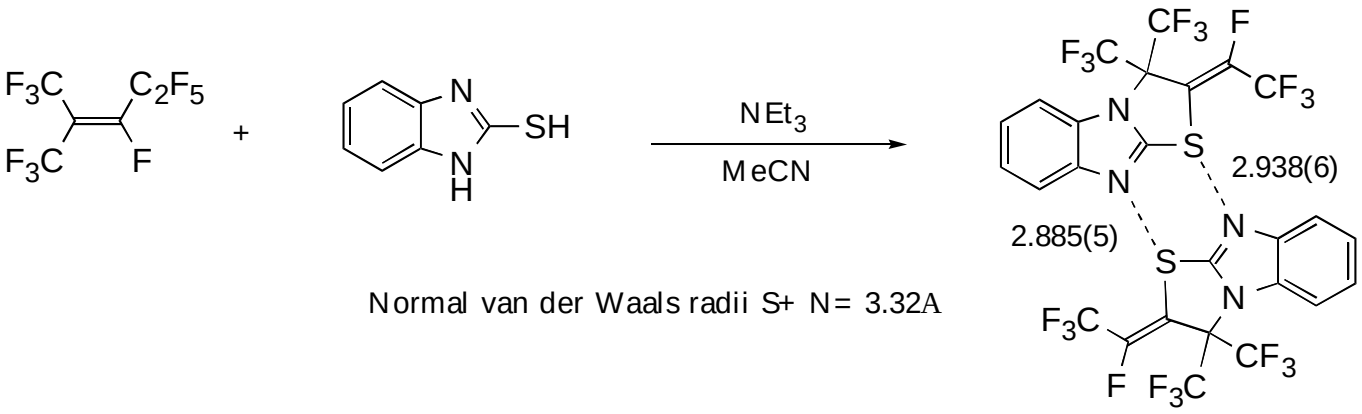
Synthesis of structural analogs of known biologically active compounds is a useful way of improving their properties. One such attempt is synthesis of tetramizol (active antihelmintic) analog by the reaction of perfluoro-2-methyl-pentene-2 with benzimidazol-2-thiole in the presence of triethylamine giving rise to the titled compound.



Normal van der Waals radii S+ N= 3.32A

The obtained compound shows very unusual properties. In contrast to precursors, it is easily soluble almost in any common solvent, ranging from methanol to hexane and even **perfluoro-2-methyl-pentene-2** (**!**). The highest solubility may be attributed to superlipophilicity of entered perfluoroalkyl groups. Compound is extremely volatile, so that X-ray analysis was difficult. According to X-ray data dimers are formed. To rationalize this we assumed that sulfur atom becomes acceptor (Lewis acid) under the effect of electron-withdrawing perfluoroalkyl group, but nitrogen is still keeping Lewis basicity. Dimers topology is so similar to guanine-cytozine and adenine-thymine pairs topology in DNA and RNA that it seems to be possible the influence of titled compound on the processes with participation of the last-mentioned.