Crystal Structure of 2-Nitro-3,4,4-trichloro-1-mono(dodecyl thio)-1-mono[(4-fluorophenyl)piperazine]-1,3-butadiene Compound

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Some thio substituted halodiene derivates show an excellent biological activities such as herbicides, insecticides, fungucides etc. from US-Patent [1]. It is known that piperazine compounds are important chemicals of clinical chemistry. Also, piperazine compounds were used in gen-transfer [2].

The aim of this work is to synthesis and to determine the crystal structure of 2-Nitro-3,4,4-trichloro-1-mono(dodecylthio)-1- mono [(4fluorophenyl) piperazine]-1,3-butadiene compound.

Crystal structure of 2-Nitro-3,4,4-trichloro-1-mono(dodecyl thio)-1-mono[(4-fluorophenyl)piperazine]-1,3-butadiene compound was mounted on an Rigaku R-AXIS Rapid-S Diffractometer with a graphite monochromatized MoKα radiation (λ= 0.71073 Å). The structure was solved by direct method with SIR92 and refined with Crystals [3].

Crystal data : $C_{26}H_{37}Cl_3FN_3O_2S$, triclinic, P-1, a= 7.0933(8), b= 8.3802(6), c= 27.40930(10), α= 76.418(4), β= 77.526(4), γ= 71.231(4) V= 1481.955 (5), Z= 2, Dx= 1.302 g/cm^3, F(000)= 612, μ(MoKα)= 4.13 cm^{-1}.

[1] Diamond Alkali Company (Ert.H.Bluestone), U.S. Pat. 3021370, *Chem.Abst.,* 1962, **57**, 3293c. [2] Zhao S., Miller A.K., *TetrahedronLett*., 1996, **37**, 4463. [3] Altomare A., Cascarano G., Giacovazzo C., Guagliardi A., Burla M., Polidori G., Camalli M., SIR92, *J.Appl.Cryst,*, 1994, **27**, 435.

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