Structural Features of Some Schiff Base Disulfide Compounds

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Schiff bases bearing imine N and anionic S atoms constitute an important class of polydentate ligands and their metal complexes have previously been used as models for biological systems. The molecule and crystal structure of a new synthesized disulfide compound $[C_{30}H_{22}F_6N_2O_2S_2]$ has been undertaken with a view to obtaining accurate structural parameters of interest in disulfide compounds. Crystal data:M=620.62, Triclinic, a=7.639(2)Å, b=8.526(8)Å, c=23.349(5)Å, α =89.04(4)°, β =89.99(2)°, γ =63.41(4)°, V=1359.6(9)Å³, Pī, R=0.0538, Rw=0.0944. The structure was solved by direct methods and refined by least squares on F_{obs}^2 by using SHELX-97.

In the second phase of the study, structural results have been compared with the values found in our previous studies related at least four Schiff base disulfides [1-4]. The molecular conformation around central S-S bond has been affected by trifloromethyl groups in the molecule. High electronegativity in the CF₃ groups has been cause to conformational changes in the torsion angle of C-S-S-C [77.8(4)°]. Two strong intramolecular hydrogen bonds [O-H···N, O···N: 2.612(9) and 2.612(8)Å] have been observed and cause to increasing of the planarity in the main parts of the molecule.

[1] İde S., Öztaş G., Ancın N., Tüzün M., Acta Cryst., 1997, C53, 376-378. [2]
Özbey S., Temel A., Ancın N., Öztaş S.G., Tüzün M., Z. Kristallogr., 1998, 213, 207-208. [3]Candan M.M., İde S., Kendi E., Öztaş G., Ancın N., Spectroscopy Letters, 1998, 31(4), 891-900. [4] İde S., Ancın N., Öztaş S.G., Tüzün M., Pharm. Acta. Helv., 1998, 72, 291-294.

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