

Title compound will be good intermediates to synthesise various pharmacologically active compounds.

The compound crystallizes as colourless plates in monoclinic with space group $P2_1/n$ and cell dimensions $a=8.493(7)\text{\AA}$, $b=17.071(1)\text{\AA}$ and $c=11.875(1)\text{\AA}$. The structure was solved by SHELX97 program (Sheldrick 1997) and refined to a R factor of 0.0597. The details of the weak interactions are discussed in this paper.

Keywords: X-ray crystallography, small molecules, organic compounds

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Structure of 2-[4-(Dimethylamino)phenyl]-4,5-diphenyl-1H-imidazole Isopropanol Solvate

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Different types of organic compounds have been synthesized using microwave-assisted organic synthesis [1] and Usovitsky & Khmel'nitsky [2] have reported the use of this technique in the preparation of 2,4,5-substituted imidazoles. Their synthetic procedure involved the condensation of 1,2-diaryethandienones with aldehydes and ammonium acetate as the source of ammonia with an acidic support (acidic silica) in a microwave oven. We synthesized 2-[4-(dimethylamino)phenyl]-4,5-diphenyl-1H-imidazole using a similar technique in the absence of the acidic support media. Recrystallization of the reaction product from isopropanol afforded the title compound, as shown by single-crystal X-ray structure determination. The title compound, $C_{23}H_{21}N_3 \cdot C_3H_8O$, crystallizes with two independent molecules and two solvent molecules in the asymmetric unit. These are connected through hydrogen bonds between the NH group of the imidazole ring and the O atom of the isopropanol solvent molecule, as well as between the N atom of the imidazole ring and the OH group of the isopropanol solvent molecule.

[1] Lidström P., Tierney J., Wathey B., Westman J., *Tetrahedron*, 2001, 57, 9225-9283. [2] Usovitsky A. Ya., Khmel'nitsky Y., *Tetrahedron Lett.*, 2000, 41, 5031-5034.

Keywords: microwave materials, organic structures, hydrogen bonds

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Substituents at Oxygen Influence N,O-Distances in Thiohydroxamates

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The N,O bond in O-derivatives of N-(hydroxy)thiazole-2(3H)-thiones may selectively be cleaved upon thermal (60–80 °C) or photochemical (300–350 nm) excitation. This circumstance along with additional useful chemical properties causes N-oxy-substituted thiazolethiones to be unprecedentedly versatile and efficient precursors for the generation of reactive intermediates such as carbon or oxygen centered radicals [1].

In view of the fact that N-alkoxycarbonyloxy-, N-acyloxy-, and N-alkoxy-derivatives of thiazole-2(3H)-thiones differ significantly in their stability, selected candidates of each set of thiones (a total of 14 compounds) were investigated by single-crystal X-ray diffraction at temperatures ranging between 298 K and 100 K.

The results of the study indicate that the N,O bond length in N-oxy-substituted thiazole-2(3H)-thiones increases along the series of substituents at oxygen H ~ alkyl < acyl < alkoxy-carbonyl [2,3].

[1] Hartung J., Schwarz M., Svoboda I., Fuess H., Duarte M.T., *Eur. J. Org. Chem.*, 1999, 1275. [2] Hartung J., Schneiders N., Bergsträsser U., *Acta Cryst.*,

2005, E61, o421. [3] Hartung J., Bergsträsser U., Schneiders N., Altermann S., Svoboda I., Fuess H., *in preparation*.

Keywords: heterocyclic compounds, single-crystal X-ray diffraction, nitrogen oxygen bond

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X-ray Induced Radiation Damage in Taurine – a Combined X-ray and Raman Study

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Taurine is one of the lesser-known amino acids, nevertheless, it plays a role in the body and is essential to newborns of most mammal species, and it also protects our bodies against damage from radiation. Along with methionine, cystine and cysteine, it is a sulphur amino acid. The taurine molecule ($\text{NH}_3^+-\text{CH}_2-\text{CH}_2-\text{SO}_3^-$) is small and therefore a well suited model compound for this family of amino acids, as well as for describing the radiation damage in more complex sulphur containing amino acid systems.

Taurine exposed to ⁶⁰Co gamma rays have been shown to produce traces of different radicals [1], which are detectable with EPR. However, when taurine is irradiated with x-rays, an anisotropic change in the lattice constants is observed, where the crystal expands mainly along the c-axis of the unit cell. The system has been investigated with single crystal diffraction data at 120K and at room temperature, and separately with time resolved high resolution powder diffraction in combination with Raman spectroscopy. The Raman spectra reveal a red shift of the S-O stretching frequency as a function of exposure time. The single crystal data show a continuous rise of charge located approximately 1Å away from one of the oxygen atoms. This finding along with the Raman observation suggest the existence of an x-ray induced proton transfer within the taurine crystals rather than pure radical formation.

[1] Bulut A., Karabulut B., Tapramaz R., Koksall F., *Radiat. Phys. Chem.*, 2000, 58(2), 149-52.

Keywords: diffraction, radiation damage, Raman spectroscopy

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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 derivatives show an excellent biological activities such as herbicides, insecticides, fungicides 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[(4-fluorophenyl) 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 MoK α radiation ($\lambda=0.71073\text{\AA}$). 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, $P\bar{1}$, $a=7.0933(8)$, $b=8.3802(6)$, $c=27.40930(10)\text{\AA}$, $\alpha=76.418(4)$, $\beta=77.526(4)$, $\gamma=71.231(4)^\circ$ $V=1481.955(5)$, $Z=2$, $D_x=1.302\text{ g/cm}^3$, $F(000)=612$, $\mu(\text{MoK}\alpha)=4.13\text{ cm}^{-1}$.

[1] Diamond Alkali Company (Ert.H.Bluestone), U.S. Pat. 3021370, *Chem. Abst.*, 1962, 57, 3293c. [2] Zhao S., Miller A.K., *Tetrahedron Lett.*, 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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