been reported. Among examples, can be named the fo-lowing ones: anilinium nitrate [7], anilinium hydrogenphosphite and anilinium hydrogenoxalate [8]. This structure may be described as formed by alternating sheets of cations and anions which are held together with four five centered N-H…O bonds to form $C_4^4(10)$ $C_4^4(10)$ infinite chains running through the c direction. Moreover, strong O-H…O hydrogen bonds observed between bisulfate anions generate $C_2^2(8)$ chains in the *a* axis direction. The infinite chains resulting from anion-anion and anion-cation interactions can be described as zigzag layers parallel (ac) plans. The crossing of these chains builds up different rings with $R_3^3(10)$ and $R_5^4(16)$ graph set motifs [9].

[1] S.C. Zimmerman, P.S. Corbin, *Struct. Bond*. **2000,** *96*, 63–94. [2] G.R. Desiraju, T. Steiner, *The Weak Hydrogen Bond in Structural Chemistry and Biology*, 507. New York: Oxford University Press. **1999.** [3] J. Bernstein, R.E. Davis, L. Shimoni, N.-L. Chang, *Angew. Chem. Int. Ed. Engl*. **1995**, *34*, 1555–1573. [4] N. Benali-Cherif, H. Boussekine, Z. Boutobba, N. Dadda, *Acta Cryst*. **2009**, *E65*, o2744. [5] N. Benali-Cherif, W. Falek, A. Direm, *Acta Cryst*. **2009,** *E65*, o3058–o3059. [6] K. Jayaraman, A Choudhury C.N.R. Rao, *Solid State Sci.* **2002**,.413–422. [7] M. Rademeyer, *Acta Cryst*. **2004**, *E60*, o958–o960. [8] J.A. Paixao, A. Matos Beja, Ramos, M. Silva, J. Martin-Gil, *Acta Cryst*. **2000 ,** *C56*, 1132–1135. [9] M.C. Etter, J.C. MacDonald, J. Bernstein, *Acta Cryst*. **1990**, *B46*, 256–262.

Keywords: graph theory, hybrid compounds, hydrogen bonds.

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Thiodiazolo[2,3-a](py) as an oxidative cyclization of (py)carbamothioyl by Cu^{2+}

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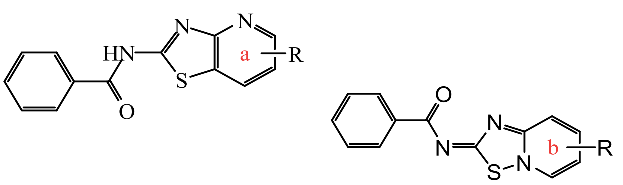
Some compounds are worth from different aspects. The existences of specific functional groups cause unique properties for them. Reaction of benzoyl chloride, potassium thiocyanate with 2-aminopyridine and 2-aminopicoline in one pot produces carbamothioyl benzamide derivatives. These compounds possess various sites to react with numerous reactants.

When 2-aminopyridine was used in above reaction, N-(pyridine-2-ylcarbamothioyl) benzamide was formed. This compound and the other synthesized derivatives were characterized by CHN, IR-, ^{1}HNMR- and ^{13}CNMR spectroscopies. Also their crystal structures were determined.

The reaction of 2-aminopyridine and 2-aminopicoline with Cu(II) salts resulted in oxidative cyclization. There are two possibilities of oxidative cyclization and two different structures (**a** & **b**) for these compounds. The products were characterized CHN, IR-, ^{1}HNMR- and ^{13}CNMR spectroscopies.

The obtained crystals and x-ray single crystal diffraction confirmed the structure b is correct. The structure **b** of different derivatives is able to act as anti cancers.

Increasing of the anti cancer property of these products will be researched by changes and replacement of various groups and functions in both of aromatic rings.



Keywords: oxidative cyclization, thiadiazolo[2,3-a]pyridine

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mosquito® Crystal: fast, reliable automation of Protein Crystallization drop set-up

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Automation of protein crystallography screening has contributed significantly to the rapid progress of crystallography based structural biology. Automation allows samples to be screened using smaller volumes of both protein and screen solutions, reducing costs and saving valuable protein. Additional benefits include increased throughput and accuracy.

One of the challenges to automating this process is the necessity to accurately pipette solutions of varying viscosities. Another challenge is that of drop positioning. The low volume drops have to be placed extremely accurately in order that protein and screen drops coalesce and are not distorted by the edge of the crystallization plates' subwell.

The ability of mosquito® Crystal to address these issues and to automate both micro batch and vapour diffusion methods of protein crystallography (sitting drop, hanging drop) without instrument configuration change offers ultimate flexibility for the crystallography laboratory.

Keywords: Screening-1, Pipetting-2, Mosquito-3

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Ion substitution in tourmaline with chromophore elements growning in hydrothermal conditions

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Unique physical properties of tourmaline crystals (pyroelectric, piezoelectric) and possibility of their use in jewelry makes the growing of synthetic tourmalines a topic of the most immediate interest. Our work is devoted to the crystal chemistry of synthetic tourmalines doped by transition metal (3d) elements (Ni, Cr, Co, Fe, Cu) which are identified as coloring agents (table 1).

Table 1. Characteristic of growing tourmalines.

Smp	Color	3d-elements cont., wt.%	Unit cell parameters, Å		R_F
			a	c	
1	green	NiO-7.4 FeO-5.3	15.897(5)	7.145(2)	0.038
2	green	NiO-13.4 Cr_2O_3-10.2 FeO-0.3	15.945(5)	7.208(2)	0.051
3	pink	CoO-14.4	15.753(8)	7.053(3)	0.057
4	blue	CuO-8.4	15.840(4)	7.091(1)	0.041