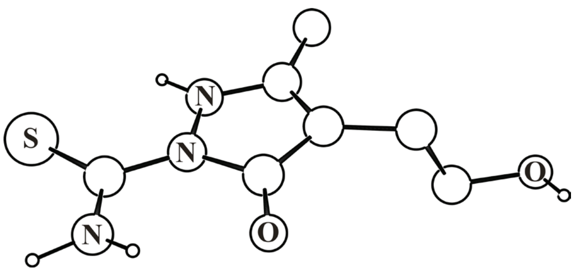
work we present the crystal structure of the potential ligand molecule where R1=(CS)NH_2, R2=H, and R4=CH_2CH_2OH, with emphasis on the mode of molecular association in the crystal lattice. The crystal structure of the parent 3-Methyl-3-pyrazolin-5-one was reported in two polymorphic forms [1,2]. Comparison of the title compund with the structure of the parent molecule, shows that the most significant difference in the pyrazole ring geometry is extension of the N1-C5 bond for ≈0.1Å. This difference could be attributed to the perturbation in the electronic strucutre caused by the presence of thiocarboxamide substituent on the N1. The pyrazole ring is nearly planar: the largest deviation from the mean plane of the ring is 0.010(2). The mean planes of the thiocarboxamide substituent and of the pyrazole ring form dihedral angle of 4.0(2)°. Hydroxyl group is placed so that the normal distance between the mean plane of the pyrazole ring and the O atom is 1.485(2)Å (Fig). Association of molecules in the crystal lattice is determined by the spatial relationships between the hydrogen bond donors and acceptors, which are placed in a neighbouring positions. This enable extension of dimeric hydrogen bonded units into the molecular chains. These chains are connected by weaker N(pyr)-H...OH bond. Due to sterechemical properties of the title molecule, the neighbouring chains are positioned in the aproximately orthogonal fashion.



[1] De Camp W.H., Stewart J.M., *Acta Cryst*., **1971**, B27, 1227.
[2] Zhang Z., Jin S, Wang S., Liu B., Guo J., *Acta Cryst*. **2004**, E60, 315.

Keywords: pyrazolon; X-ray structure

FA4-MS05-P39

Calculation of the Raman spectra of the polymorphic forms of $Y_2Si_2O_7$. Daniel M. Többens[a], Reinhard Kaindl[a], Volker Kahlenberg[a]. [a]*Institute of Mineralogy and Petrography, University of Innsbruck, Austria.*
E-mail: daniel.toebbens@uibk.ac.at

$Y_2Si_2O_7$ forms a number of polymorphs. Three building principles can be distinguished based on the conformation of the silicate groups. Forms β and γ are composed of Si_2O_7 dihedra with the SiO_4 tetrahedra in staggered orientation. In δ, ε, and ζ the two tetrahedra in the dihedra are in eclipsed orientation. The forms α and η contain both monohedra and eclipsed trihedra. Experimental Raman spectra were obtained for the forms α, β, γ, η. Calculations of the vibrational spectra were conducted for all forms but η, which has a very large unit cell. For the *ab initio* calculations the program CRYSTAL06 [1] was used. Calculations were done using DFT with both local and hybrid functionals. Various basis sets taken from the CRYSTAL website were tested (www.crystal.unito.it). For the simple spectrum of form β, unequivocal assignment of all lines was possible. From this, a simple correction of the calculated frequencies could be derived, which helped in the assignment of the more complex spectra. After application of these corrections, the different basis sets give very similar results. Basis sets specifically optimized for this problem reached a slightly better agreement with the observed line positions without correction. However, the calculation times necessary for this are disproportionally longer, and no qualitative changes result. For all polymorphs, the most characteristic lines of the Raman spectra are observed in the range 600 - 900 cm^{-1}. In all cases, these are Si-O stretching and bending modes. An inspection of the underlying structural mechanisms shows the crucial influence of the different conformations of the silica groups especially in this region of the spectra. Pure O-Y-O bending modes were found to be located below 200 cm^{-1}. The lines in the range from 200 cm^{-1} to 520 cm^{-1} are generally O-Y-O bending modes, but contain some degree of distortion of the SiO_4 tetrahedra. Those observed modes involving Y-O stretching were found to be weak.

[1] Dovesi, R. *et al*. Crystal06 User's Manual. Università di Torion, Torino, 2006.

Keywords: rare-earth compounds; raman spectroscopy; ab-initio calculations

FA4-MS05-P40

Structure de Di(4,4',5,5'-Tetramethyl-1,3-Dithia-1',3'-Diselenafulvalene) Tetrafluoroborate: (TMDTSDF)2BF4. Mhanni Allal[a], Ouahab Lahcen[a]. [a]*Laboratoire de Thermodynamique et Modélisation moléculaires, Faculté de Chimie, USTHB, BP : 32 El-Alia, Bab Ezzour 16111, Alger, Algérie.*
E-mail: mhannia@yahoo.fr

(C10H12S2Se2)2 BF4, Mr = 795.31, triclinic, P1, a = 7.208 (16), b = 7.571 (5), c = 13.068 (4) Å, α= 85.65 (4)°, β= 86.88 (7), γ= 70.46 (8)˚, V = 669.9Å^3, Z = 1, Dx = 1.971 g cm-3, F(000) = 385. (Mo K) = 0.71073Å, = 57.59 cm^{-1}, = 293K, = 0.044 based on 1206 observed reflections with. The F atoms of the tetrahedral BF-4 unit are disordered as already observed in such an union. However, the B atom is located at the origin of the unit cell, in contrast with its distribution on both sides of the origin in (TMTCF)2BF4, C=S and Se. The heteroatoms (S and Se) also present a statistical disorder. The bond distances (specially C-S/Se: 1.80 -1.85Å), The interplanar separation (3.59 and 3.62Å) between adjacent organic molecules and the intermolecular heteroatom contacts are midway between those observed in (TMTTF)2BF4 and (TMTSF)2BF4.

Keywords: electrocristallisation; magnétisme; crystallography