

# Direct synthesis and crystal structure of metal(II) thiocyanate complexes with 1-alkyl-1,2,4-triazoles

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In continuation of our previous studies in coordination chemistry of 1,2,4-triazoles [1,2], here we report direct synthesis and characterization of metal(II) thiocyanate complexes with 1-*iso*-propyl-1,2,4-triazole (ptr) and 1-*tert*-butyl-1,2,4-triazole (btr). These triazoles were found to interact with metal powders and ammonium thiocyanate in organic solvents (DMSO, toluene, acetonitrile, alcohols) under heating to give crystalline complexes  $[M(\text{ptr})_4(\text{SCN})_2]$ , where  $M = \text{Co}, \text{Ni}$ ;  $[M(\text{btr})_4(\text{SCN})_2] \cdot \text{btr}$ , where  $M = \text{Cu}, \text{Ni}$ ;  $[\text{Cu}(\text{btr})_2(\text{SCN})_2]_n$  and  $[\text{Cu}(\text{btr})_3(\text{SCN})_2]$ .

Single crystal X-ray analysis showed that ptr and btr acted as monodentate ligands coordinated by metal cations *via* the heteroring  $\text{N}^4$  atoms in all obtained complexes. Complex  $[\text{Cu}(\text{btr})_2(\text{SCN})_2]_n$  was found to be 1D coordination polymer, formed due to bridging thiocyanate anions (Fig. 1a). Other compounds are mononuclear complexes, in which thiocyanate anions are coordinated by metal only through the nitrogen atoms. In complexes  $[M(\text{btr})_4(\text{SCN})_2] \cdot \text{btr}$ , their crystal lattices include also non-coordinated triazole molecules (Fig. b).

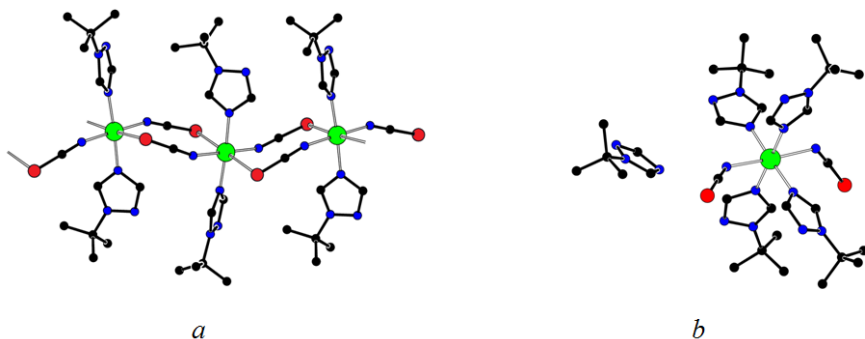


Fig. a) Coordination polymeric chain in the crystal structure of  $[\text{Cu}(\text{btr})_2(\text{SCN})_2]_n$ ; b) complex molecule together with non-coordinated triazole molecule in the crystal structure of  $[\text{Cu}(\text{btr})_4(\text{SCN})_2] \cdot \text{btr}$ . All hydrogen atoms are omitted for clarity.

## References

- [1] S.V. Voitekhovich et al. Z. Anorg. Allg. Chem. (2018) 644: 100
- [2] M.M. Degtyarik et al. J. Belarusian State University. Chemistry (2020) 1: 64.