test facility but will be put back into regular user mode operation shortly. BL 14.1 has recently been upgraded with an MD2-microdiffractometer including a kappa-geometry option and an automated sample changer. Additional user facilities include office space adjacent to the beam lines, a sample preparation laboratory, a biology laboratory (safety level 1) and high-end computing resources. On the poster, a summary on the experimental possibilities of the beam lines and the provided ancillary equipment for the user community will be given.

[1] Heinemann U., Büssow K., Mueller, U. & Umbach, P. (2003). *Acc. Chem. Res.* 36, 157-163.

Keywords: Macromolecular Crystallography, Synchrotron Radiation, Beam Line

FA1-MS01-P15

Crystal Structure of Dichloridobis[5-nitro-1-trimethylsilylmethyl-1H-benzimidazole-κN^3] cobalt (II) N,N-dimethylformamide solvate.

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Benzimidazole compounds are imported because of their metal complexes and their versatile properties such as biological activities and catalytic activities of their metal complexes in many organic syntheses [1]. We were investigate Crystal structure of benzimidazole compounds due to this important feature by single crystal X-ray diffraction.
Benzimidazole is a heterocyclic aromatic organic compound. This bicyclic compound consists of the fusion of benzene and imidazole.
The title compound, $[CoCl_2(C_{11}H_{15}N_3O_2Si)_2].C_3H_7NO$, was synthesized from 5-nitro-1-trimethylsilylmethyl-1H-benzimidazole and cobalt(II) chloride in dimethylformamide. The Co^{II} atom is coordinated in a distorted tetrahedral environment by two Cl atoms and two N atoms. In the crystal structure, there are a number of C—H...Cl and C—H...O hydrogen-bonding interactions between symmetry-related molecules.

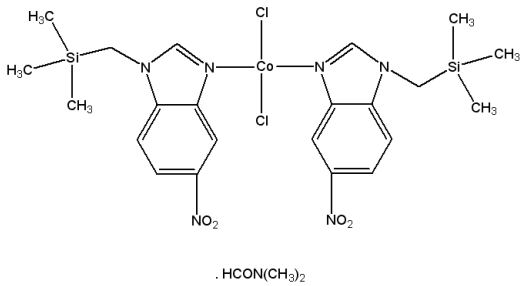

Fig 1: The molecular scheme of the title compound.

Using Stoe IPDS II diffractometer system, it was found that crystal system of $[CoCl_2(C_{11}H_{15}N_3O_2Si)_2]$ is triclinic, space group P-1, a = 9.8982(4)Å, b = 11.6936(5)Å, c = 15.9293(6)Å, α = 106.041(2)°, β = 107.408(2)°, γ = 99.040(3)°, Z = 2, D = 1.428 $M.gm^{-3}$, μ = 0.81 mm^{-1}, R = 0.053, $wR(F^2)$ = 0.123, S = 1.02.
Crystal structure were solved by direct methods using Shelxl 97 Sir97. A refinement was carried out by the full–matrix least–squares method using Shelxl 97. For molecular graphics, ORTEP-3 for Windows [2] (Farrugia, 1997) and PLATON program was used.

[1] Çetinkaya, B.; Çetinkaya, E.; Küçükbay, H.; Durmaz, R.,Arzneim.Forsch. Drug Res., (1996), 46, 1154–1158. [2] Farrugia, L. J. J. Appl. Cryst. (1999), 32, 837–838.

Keywords: Benzimidazole, Single Crystal X-ray Study, N,N-dimethylformamide

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MAIN 2010: finalizing the structure by validation driven structure improvement

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At the final stages of crystal structure determination conformations of side chains, peptide bond orientations considering electron density maps as well as hydrogen bonding networks and electrostatic stability and packing of conformations need to considered before the structure can be considered final and ready for deposition in PDB.
In MAIN a procedure has been developed for automated improvements and completion of the structure. The procedure includes side chain and peptide bond density fitting combined with flipping in a combinatorial manner. At first the current state of the model, termed starting model, is validated towards density maps. Dead end elimination, exhausted, rotational search is used to fit atoms into electron density maps followed by the energy minimization. Next side chains of branched residues ILE, VAL, THR and LEU are flipped and adjusted to density by fragment and side chain fitting, each followed by minimization. Each state is validated and compared to the starting model. When local improvement is achieved, the geometry of the modified part replaces that of the starting model. A similar procedure considering peptide bond orientation follows. After an optimal fit to density maps is achieved combinatorial search considering packing of short range (below 4A) electrostatic and vdw interactions as well as hydrogen bond network is considered. To enable this explicit hydrogens are used. Side chain and residue flipping is at this stage applied to electrostatically asymmetric residues HIS, ASN, GLN, and solvent molecules in a combinatorial manner. Each of the states is saved together with their packing energy. The lowest energy state is at the end of procedure transferred to the working model, which is again energetically minimized - as always using real space refinement procedure. The structure can then be refined against crystallographic targets and the cycle repeated unless the structure is considered done.

Keywords: Macromolecular Crystallography, Structure Refinement, Validation, Automated