Table 1. Atomic coordinates and ADPs in $(K_{0.3}Rb_{0.8})$-β-ferrite.
(a) Model 1 (*R*=0.0397 , *wR*=0.1225)

	site	occupancy	x	y	z	Uiso (Å)
O5	2c	1	1/3	2/3	1/4	0.021(2)
Rb1	6h	0.280(2)	0.6830(4)	0.3170(4)	1/4	0.0056(8)
K1	6h	0.099(9)	0.8824(15)	0.1176(15)	1/4	0.016(5)

(b) Model 2 (*R*= 0.0402 , *wR*=0.1236)

	site	occupancy	x	y	Z	Uiso (Å)
O5	2c	1	1/3	2/3	1/4	0.020(2)
Rb1	6h	0.263(4)	0.6829(4)	0.3171(4)	1/4	0.0055(8)
K1	6h	0.037(4)	0.6829(4)	0.3171(4)	1/4	0.0055(8)
Rb2	6h	0.015(8)	0.8826(15)	0.1174(15)	1/4	0.016(6)
K2	6h	0.065(8)	0.8826(15)	0.1174(15)	1/4	0.016(6)

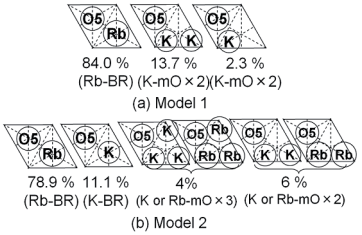

Fig.1 Distributions of K^+ and Rb^+ in $(K_{0.3}Rb_{0.8})$-β-ferrite.

[1] H. Watarai, K. Fujimoto, S. Ito, *ICC3* **2010**, S1-P0245.

Keywords: structure refinement, mixed alkali beta-ferrite

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Structural analysis of a new complex containing tetrapropionatodirhodium units

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Rhodium dinuclear complexes with metal-metal bond with a variety of architectures, properties and different scientific approaches have been reported [1]. Although most of these compounds are based on discrete units, rhodium dimetallic species are currently used as building blocks to achieve an increasing number of coordination polymers with promising properties, mostly one-dimensional chains. However, many interesting arrangements based on dirhodium paddlewheel molecules can be obtained. In this abstract, we present a new dirhodium tetrapropionate with formula $\{K_2[Rh_2(O_2CEt)_4(I)_2]\cdot H_2O\}$. In order to understand the structure of this compound a topological analysis has been carried out.

A good geometrical analysis of molecule-based structural types needs to answer, at least, two questions: the type of building blocks found in the structure, and the way in which these building blocks are connected. Sometimes, the resulting three-dimensional arrangement can be very complicated, and a conventional approach cannot clearly explain the arrangement in the solid state. In these intricate structural types, it is often more illustrative to find the topological parameters that can describe the building blocks and explain their connectivity.

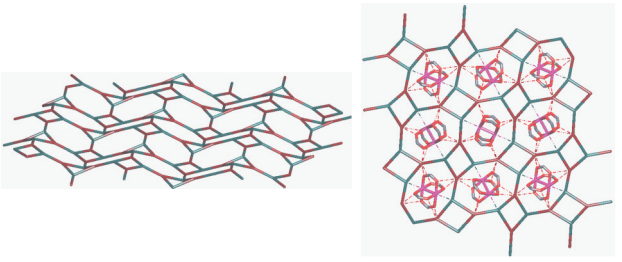

Figure 1. KI subnet (left) and simplified perpendicular view of a $\{K_2[Rh_2(O_2CEt)_4]I_2\bullet H_2O\}_\infty$ layer (right).

Single crystal X-ray diffraction of $\{K_2[Rh_2(O_2CEt)_4(I)_2]\cdot H_2O\}$ displays a complex arrangement of $[Rh_2(O_2CEt)_4]$ paddlewheel molecules with the two axial positions occupied by two iodine atoms. However, the long Rh-I distance, which is higher than the sum of ionic radii, indicates the ionic nature of this interaction. The crystal structure can be described as a stacking of $\{K_2[Rh_2(O_2CEt)_4]I_2\bullet H_2O\}_\infty$ layers parallel to the (-111) crystallographic plane. These layers consist of an undulated two-dimensional ionic network of KI, which can be topologically described as a 3-connected uninodal Shubnikov plane net (4.8^2). The dirhodium units are located inside the 8-member rings, displaying Rh-I and K-O ionic interactions with the inorganic framework. There are also weak hydrogen bonds between adjacent layers through the oxygen atoms from the water molecules bonded to the K^+ cations.

[1] F.A. Cotton, C.A. Murillo, R.A. Walton, *Multiple Bonds between Metal Atoms*, **2005**.

Keywords: rhodium, coordination, crystallochemistry

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Low temperature form of layer silicate RUB-15-LT, $[Si_{24}O_{48}(OH)_8][N(CH_3)_4]_8$*$20H_2O$

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RUB-15 [1] is an interesting layer silicate with layers made up of 4- and 6-rings forming a puckered sheet of interconnected cups which point alternatively up and down. The cups can be described as one half of a sodalite cage with tetramethylammonium (TMA) cations intercalated between layers. Neighboring silicate layers are interconnected through additional hydrogen-bonded water mole-cules. This generates a 3-dim. bonding network consisting of layer like silicate ions and water molecules.

RUB-15 was synthesized at 130°C from a reaction mixture of SiO_2 / TMAOH / H_2O. Synchrotron powder diffraction data were collected between 295 and 150 K at HASYLAB, Hamburg to monitor the phase transition. For a structure analysis of RUB-15-LT a complete powder diffraction data set was collected at 150 K using a Bruker D8 diffractometer with MoKα radiation. To investigate hydrogen bonds ^{1}H Solid-State MAS NMR spectra were recorded at RT on a Bruker ASX400 spectrometer.

RUB-15 shows a phase transition at ca. 200 K from ortho-rhombic to monoclinic symmetry. Upon cooling the unit cell volume shrinks from 2702.4 Å^3 (295 K) to 2631.3 Å^3 (150 K),