s11.m1.p1 Substitution of $Fe^{3+}+O^{2-} \Leftrightarrow Co^{2+}+(OH)^-$ and ordering of the Bi toms in $Bi_2Fe(Fe,Co)(O,OH)_2(OH)_2(AsO_4)_2$ minerals neustädtelite and cobaltneustädtelite. H. Effenberger, *Institut für Mineralogie und Kristallographie, Universität Wien, Althanstraße 14, A-1090 Wien, Austria*, W. Krause, *Henriette-Lott-Weg 8, D-50354 Hürth, Germany*, H.-J. Bernhardt, *Institut für Mineralogie, Ruhr-Universität Bochum, Universitätsstraße 150, D-44780 Bochum, Germany*, C. McCammon, *Bayerisches Geoinstitut, Universität Bayreuth, D-95440 Bayreuth, Germany*.
Keywords: neustädetelite, cobaltneustädtelite, order-disorder.

Crystals of neustädtelite / cobaltneustädtelite, $Bi_2Me1Me2(O,OH)_2(OH)_2(AsO_4)_2$, Me1 = Fe^{3+}, Me2 = (Fe^{3+},Co^{2+}) / (Co^{2+},Fe^{3+}), were investigated optically, by electron-microprobe analyses, Mössbauer spectroscopy, powder and single-crystal X-ray diffraction: space group P, $a = 4.568 / 9.170$, $b = 6.156 / 6.162$, $c = 8.971 / 9.350$ Å, a = 95.35 / 83.18, ß = 99.42 / 70.75, ? = 92.93 / 87.09°, V = 247 / 495 $Å^3$, Z = 1 / 2. The refinements on F^2 converged at wR2(F^2) = 0.104 / 0.199 and R1(F) = 0.047 / 0.075 for 796 / 1450 reflections and 95 / 183 variable parameters. On the average, both minerals have the same crystal structure. Neustädtelite is isostructural with medenbachite, Me2 = Cu^{2+} (Krause W., Bernhardt H.-J., Gebert W., Graetsch H., Belendorff K., Petitjean K., *Amer. Mineral.* **81**, 505-512, 1996). Neustädtelite and cobaltneustädtelite were found on dumps near Schneeberg-Neustädtel, Saxony, Germany. Associated minerals are bismutite, preisingerite, and quartz. The crystals are strongly pleochroitic (brown to pale yellow).

The Bi atoms in neustädtelite are in a [3+4] and [2+5] coordination. They exhibit a site disorder. The separation amounts ~0.5 Å. In cobaltneustädtelite partial ordering cause that half of the Bi atoms are on a fully occupied position and only half of them are on a split position. The partial ordering is induced by three OH groups p.f.u. in cobaltneustädtelite instead of only two in neustädtelite.

Fe^{3+} and Co^{2+} atoms occupy two Me positions. In neustädtelite and cobaltneustädtelite both their coordination figures are moderately distorted octahedra. The average bond lengths <Me1—O> are slightly shorter than <Me2—O> indicating that Me1 = Fe^{3+} and Me2 = (Fe^{3+},Co^{2+}). In medenbachite $Me1O_6 = Fe^{3+}O_6$ forms a comparable octahedron; the $Me2O_6$ polyhedron features a tetragonal bipyramid occupied by Cu^{2+} atoms (Jahn-Teller-effect). One of the two O atoms not belonging to AsO_4 represents a hydroxyl group which links a $Me1O_6$ and a $Me2O_6$ polyhedron, its Bi—O are ≥ 2.77 Å. The other one represents an oxo-oxygen atom or a hydroxyl group with two Bi—O bonds ≤ 2.21 Å. The mixed occupation O^{2-}:(OH)$^-$ is required for charge balance according to the ratio $Fe^{3+}:Co^{2+}$. For compensation of the bond valences the Bi—O bond lengths are adopted by shifting the Bi atoms. Layers in (001) are formed by corner connection of the MeO_4 chains running parallel [010] (formed by edge-sharing MeO_6 polyhedra) with the arsenate tetrahedra. The Bi atoms are interchalated; they are intensely connected to columns parallel [010].

s11.m1.p2 Compressibility and high presussure chemistry of metamict Zircon $ZrSiO_4$. P. Simoncic, M. Kunz, U. Schaltegger. *Laboratory of Crystallography ETH Zentrum, Zurich*
Keywords: compressibility, high pressure, zircon.

Zircon ($ZrSiO_4$) is a very common accessory mineral in igneous and metamorphic rocks. Trace amounts of U allow its use for age determination based on the U-Pb decay. Its structural behavior under high-pressure condition as they exist within the Earth's crust is of interest because of possible pressure effects on radiation damage and U-Pb mobility. Previous studies at high pressure focused on natural non-metamict zircons[1]. However, nothing is known about the structural behavior during compression of a U-bearing zircon with radiation damage.

Powder synchrotron X-ray diffraction ($\lambda = 0.8$ Å) were performed on a partially metamict zircon containing 500 to 900 ppm U. NaCl was used as internal pressure standard. Pressure was applied using a diamond anvil cell. Diffraction cones were recorded using the Mar-image plate system of SNBL at ESRF. Maximal pressure attained during this experiment was 6 GPa. LeBail profile refinements were applied to the diffraction pattern to determine the unit cell parameters. Selected patterns were refined using the Rietveld method.

The volume of the U-bearing zircon before the experiment was determined as 267.78(9) $Å^3$, This is in accordance with the unit cell of a zircon with radiation damage. The decrease of the unit cell for the U-bearing sample shows a conspicuous stepwise collapse-behavior, with a very soft behavior at low pressures and increasingly stiff ranges between the collapse-regions. Therefore, no reasonable bulk modulus can be calculated for the metamict zircon on the compressive branch. During decompression, the increase of the volume is continuous and returns to an ambient pressure value of 264.41(8) $Å^3$, i.e. significantly smaller than the starting value. The P-V curve on decompression can be modeled with a Birch-Murnaghan equation of state with values of K_0 = 236(1) GPa, V_0 = 264.185(8) (K' fixed at the value of 6.5). These results are slightly higher compared to the values of Hazen and Finger (1979)[1], (K_0 = 227(2) GPa, V_0 = 260.79 (4), K' 6.5 fixed). We interpret the stepwise compression behavior and the difference in volume before and after compression as an indication for two different types of structural damages, which are healed upon compression. Pressure is thus able to at least partially recrystallise a radiation-damaged zircon.

[1]Hazen and Finger (1979):Crystal structure and compressibility of zircon at high pressure American Mineralogist, 64, pages 196-201.