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Neustädtelite and cobaltneustädtelite, the Fe^{3+}- and Co^{2+}-analogues of medenbachite

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ABSTRACT

Neustädtelite and cobaltneustädtelite, two new minerals related to medenbachite, were found on samples from the dumps of the Güldener Falk mine near Schneeberg-Neustädtel, Saxony, Germany. The general appearance of the two new minerals is very similar: small tabular crystals up to 0.2 mm in diameter, transparent to translucent, with a brown color and a light brown streak; the lustre is adamantine. Both minerals are optically biaxial negative, $2V = 65(5)°$, $n_x = 2.02(2)$, $n_y = 2.09$ (calc.), $n_z = 2.12(2)$; pleochroism is strong with X = brown to opaque, Y = yellow, Z = pale yellow. Mohs' hardness is 4.5. The cleavage parallel to {001} is good. The chemical compositions were derived by means of electron-microprobe analyses. Average contents for neustädtelite/cobaltneustädtelite are (in wt%): Bi_2O_3 52.58/51.54, PbO 0.08/0.08, CaO 0.15/0.32, Fe_2O_3 13.92/10.90, Al_2O_3 0.29/0.07, CoO 3.35/5.47, NiO 0.34/1.61, ZnO 0.09/0.39, CuO 0.07/0.00, As_2O_5 26.82/25.91, P_2O_5 0.23/0.43, H_2O (calc.) 2.56/3.01, total 100.48/99.73. Mössbauer spectra of cobaltneustädtelite and medenbachite confirmed that all of the iron is trivalent. Based on 12 O atoms, the empirical formulae for the neustädtelite and cobaltneustädtelite type materials are $(Bi_{1.94}Ca_{0.02})_{\Sigma 1.96}Fe_{1.00}(Fe_{0.50}Co_{0.38}Ni_{0.04}Al_{0.05}Zn_{0.01}Cu_{0.01})_{\Sigma 0.99}[(OH)_{2.44}O_{1.40}]_{\Sigma 3.84}[(AsO_4)_{2.01}(PO_4)_{0.03}]_{\Sigma 2.04}$ and $(Bi_{1.91}Ca_{0.05})_{\Sigma 1.96}Fe_{1.02}(Co_{0.63}Fe_{0.16}Ni_{0.19}Zn_{0.04}Al_{0.01})_{\Sigma 1.03}[(OH)_{2.88}O_{1.12}]_{\Sigma 4.00}[(AsO_4)_{1.95}(PO_4)_{0.05}]_{\Sigma 2.00}$, respectively. As derived from chemical analyses and crystal-structure investigations the ideal end-member compositions are $Bi_2Fe^{3+}Fe^{3+}O_2(OH)_2(AsO_4)_2$ (neustädtelite) and $Bi_2Fe^{3+}Co^{2+}O(OH)_3(AsO_4)_2$ (cobaltneustädtelite). Extensive solid solution is observed between these two minerals. Neustädtelite and cobaltneustädtelite crystallize in space group $P\bar{1}$; the cell parameters refined from powder data are $a = 4.556(1)/9.156(1)$, $b = 6.153(2)/6.148(1)$, $c = 8.984(2)/9.338(1)$ Å, $\alpha = 95.43(2)/83.24(1)$, $\beta = 99.22(2)/70.56(1)$, $\gamma = 92.95(3)/86.91(1)°$, $V = 246.9/492.2$ Å^3, $Z = {}^1/_2$, density (calc.) 5.81/5.81 g/cm^3. Structure investigations were performed using single-crystal X-ray data. In both minerals edge-sharing alternating $Fe^{3+}Ø_6$ and $(Fe^{3+},Co^{2+})Ø_6$/$(Co^{2+},Fe^{3+})Ø_6$ octahedra (Ø = O,OH) form chains parallel to [010] that are corner-linked by arsenate tetrahedra to layers parallel to (001). The Bi atoms are linked by O atoms to form columns parallel to [100]; these are sandwiched between layers of composition $^{[6]}M_2(OH)_2(AsO_4)_2$ (M = Fe^{3+},Co^{2+}). In neustädtelite the Bi atoms are site disordered; in cobaltneustädtelite half of the Bi atoms are ordered and half are on a split position. The partial ordering is induced by the presence of three OH groups, as compared to two in neustädtelite. A structural reinvestigation of medenbachite, $Bi_2Fe^{3+}(Cu^{2+},Fe^{3+})(O,OH)_2(OH)_2(AsO_4)_2$, proved isotypy with cobaltneustädtelite; the new cell parameters for medenbachite (refined from X-ray powder data) are: $a = 9.162(2)$, $b = 6.178(1)$, $c = 9.341(2)$ Å, $\alpha = 83.50(2)$, $\beta = 71.04(2)$, $\gamma = 85.15(2)°$, $V = 496$ Å^3, $Z = 2$.