

# **$A_5[Fe_3O_6]$ ( $A = Rb, Cs$ ), $Cs[FeO_2]$ und $Cs_8[Fe_2O_7]$ :**

## **Neue Oxoferate der schweren Alkalimetalle**

$A_5[Fe_3O_6]$  ( $A = Rb, Cs$ ),  $Cs[FeO_2]$  and  $Cs_8[Fe_2O_7]$ : New Oxoferates of the Heavy Alkaline Metals

Gero Frisch und Caroline Röhr

Institut für Anorganische und Analytische Chemie, Univ. Freiburg, Albertstr. 21, D-79104 Freiburg

Sonderdruckanforderungen an Prof. Dr.-Ing. C. Röhr. E-mail: caroline@ruby.chemie.uni-freiburg.de

Z. Naturforsch. **59b**, 771 – 781 (2004); eingegangen am 16. März 2004

The title compounds were synthesized at a temperature of 775 K *via* reaction of  $Fe_2O_3$  with elemental cesium and rubidium alone or in combination with their hyperoxides  $AO_2$  where required by stoichiometry. The structures of the dark-red crystals have been determined by single crystal x-ray diffraction ( $Cs[FeO_2]$ : cubic, space group  $Fd\bar{3}m$ ,  $a = 839.2(2)$  pm,  $Z = 8$ ,  $R1 = 0.0547$  and  $A_5[Fe_3O_6]$  ( $A = Cs$ : orthorhombic, space group  $P2_12_12_1$ ,  $a = 861.8(2)$ ,  $b = 870.7(2)$ ,  $c = 1658.7(3)$  pm,  $Z = 4$ ,  $R1 = 0.0617$  and  $A = Rb$ : tetragonal, space group  $I\bar{4}2d$ ,  $a = 862.01(8)$ ,  $c = 1504.7(2)$  pm,  $Z = 4$ ,  $R1 = 0.0334$ ). These three compounds contain three-dimensional networks  $[FeO_2]$ , in the case of the ideal stuffed cristobalite composed of corner-sharing tetrahedra  $[FeO_{4/2}]$ , in the case of the new mixed valence compounds  $A_5[Fe_3O_6]$  formed by corner-sharing of tetrahedra  $[Fe^{III}O_{4/2}]$  and triangles  $[Fe^{II}OO_{2/2}]$  in a 1:2 ratio. The crystal structure of the cation rich compound  $Cs_8[Fe_2O_7]$  (monoclinic, space group  $P2_1/c$ ,  $a = 722.32(12)$ ,  $b = 1789.0(3)$ ,  $c = 733.88(12)$  pm,  $\beta = 118.976(3)^\circ$ ,  $Z = 4$ ,  $R1 = 0.0287$ ) exhibits di-ferrate anions  $[Fe_2O_7]^{6-}$  composed of two corner-sharing  $[Fe^{III}O_4]$  tetrahedra with a linear Fe-O-Fe bridge.

*Key words:* Ferrates, Oxoferates