



	Experiment title: The low temperature charge density wave structure of $K_xP_4W_8O_{32}$ ($x = 1.3$)	Experiment number: HS-1111
Beamline: BM01A	Date of experiment: from: 3 May to: 9 May 2000	Date of report: 23-10-2000
Shifts: 18	Local contact(s): Dr. P. Pattison	<i>Received at ESRF:</i>
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Report:

Since their original discovery, the phosphate bronzes $(PO_2)_4(WO_3)_{2m}$ with $m = 2, \dots, 14$ have been studied extensively [1]. The interest in these compounds derives from their low-dimensional electronic properties and the development of Charge-Density Waves (CDWs) at low temperatures [2]. An appealing feature is that the thicknesses of the conducting layers WO_3 are proportional to m , and that the transition temperatures of the CDW transitions increase with m too.

The compounds $K_x(PO_2)_4(WO_3)_{2m}$ are an intercalated variant of the phosphate bronzes, with the potassium atoms located in the hexagonal tunnels bordered by the phosphate groups. They also exhibit CDW transitions, with transition temperatures dependent both on m and x [2]. We believe that the knowledge of the low-temperature superstructures in their CDW states is an essential ingredient to fully understand the CDW properties and the mechanism of the CDW transition. For example, the modulation amplitudes for the different atoms gives an indication about the location of the CDW in the crystal structure.

The compounds $K_xP_4W_8O_{32}$ ($m = 4$) with $0 < x < 2$ have been studied in more detail [3,4]. For $x = 1.3$ a CDW transition has been observed at $T_{CDW} = 170$ K by electrical conductivity experiments [3]. Below T_{CDW} superstructure reflections in diffraction were reported at the positions defined by a modulation wavevector $q = 0.5 a^*$ [2].

The aim of the present experiment is to determine the superstructure of $K_xP_4W_8O_{32}$ ($x = 1.3$) in its CDW state. We have used the six-circle KUMA diffractometer in its four-circle

mode to measure the integrated intensities of the Bragg reflections below T_{CDW} at a temperature of $T = 110$ K. The experiment was successful. The superlattice reflections were observed at the expected positions. We measured the integrated intensities of about 3000 Bragg reflections by ω -scans. Half of them were superlattice reflections. Due to the decision of Dr. Lüdecke to continue his career in the industrie, the structure has not been solved yet. A structure solution with the measured data is scheduled for January-March 2001, when Dr. Dusek will be in Bayreuth. Data processing has convinced us, that the quality and amount of observed intensities is sufficient for a successful structure solution.

- [1] P. Roussel, Ph. Labbé and D. Groult (2000) *Acta Crystallogr.* **B56**, 377.
- [2] J. Dumas, U. Beierlein, S. Drouard, C. Hess, D. Groult, Ph. Labbé, P. Roussel, G. Bonfait, E. Gomez Marin, and C. Schlenker (1999) *J. Solid State Chem.* **147**, 320.
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- [4] P. Roussel, D. Groult, A. Maignan, and Ph. Labbé (1999) *Chem. Mater.* **11**, 2049.