ESRF	**Experiment title:** Structure determination of Cs metal above 10 GPa	**Experiment number:** HS490
Beamline: ID9	**Date of Experiment:** from: 24 Apr. 1998 to: 27 Apr. 1998	**Date of Report:** 31 Aug. 1998
Shifts: 9	**Local contact(s):** M. Hanfland	Received at ESRF: 01 SEP. 1998

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Report:

The experiment was very successful. Solving the crystal structure of the phase Cs-V was possible thanks to the excellent resolution at ID9. The main results are illustrated in Figs. 1 and 2. The electronic structure and chemical bonding in Cs-V is currently investigated by first-principle calculations.

A paper has been written on the crystal structure results for Cs-V, which was accepted for publication in Physical Review Letters. The abstract reads as follows:

The crystal structure of cesium-V

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The crystal structure of the high-pressure phase cesium-V was investigated using monochromatic synchrotron x-ray diffraction. Full profile refinements of powder diffraction data resulted in a solution with space group Cmca and 16 atoms in the orthorhombic unit cell. The Cs-V structure can be viewed as a distorted fcc structure. Atoms occupy two different Wyckoff positions with 10- and 11-fold coordination, respectively. This new structure type is considered a possible candidate for high-pressure phases of other elemental metals.

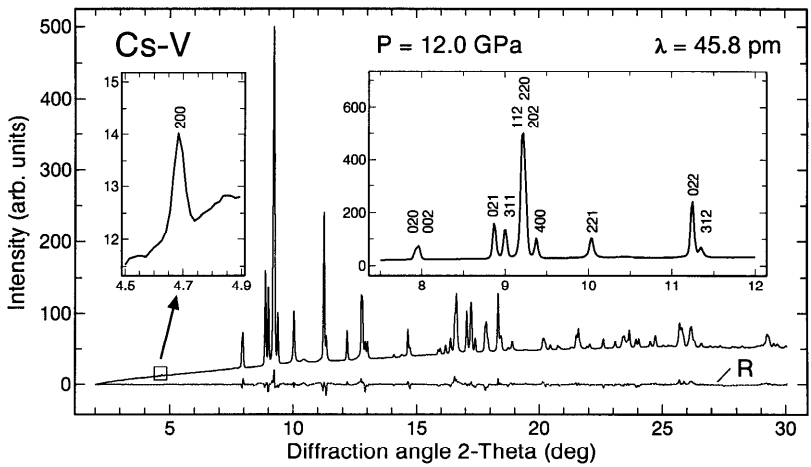

Fig. 1: High-resolution angle-dispersive diffraction diagram of cesium-V at 12 GPa measured at the ESRF. The pattern is indexed in the orthorhombic system. The curve marked 'R' represents the difference between experimental data and the result of a full-profile Rietveld refinement in space group Cmca.

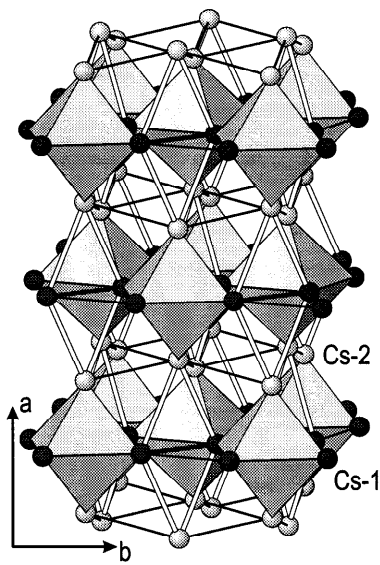

Fig. 2: View of the orthorhombic crystal structure of cesium-V (SG Cmca). There are 1(atoms in the conventional unit cell.