

atom positions based on the response ratio show that there are 1.1 % excited-state species in the crystal in which the I-I distance (3.82(2) Å) is contracted from the ground states (4.41(1)Å). While in the case of the discrete dimer complex [Cu<sub>2</sub>I<sub>2</sub>(PPh<sub>3</sub>)(pyz)<sub>2</sub>], two iodine atoms tend to move out of the {Cu<sub>2</sub>I<sub>2</sub>} plane with opposite direction each other. This indicates that the {Cu<sub>2</sub>I<sub>2</sub>} rotates around an axis containing two Cu atoms. This variety of the motions of {Cu<sub>2</sub>I<sub>2</sub>} frameworks will be concerned with the geometry of the frame at the ground state and solid-state luminescent properties.

Keywords: synchrotron crystallography, photochemistry coordination compound, diffraction under non-ambient condition

## P20.07.34

*Acta Cryst.* (2008). A64, C616

### Structural changes in YBaCo<sub>4</sub>O<sub>7+δ</sub> monitored by variable temperature neutron powder diffraction

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In 2006 it was reported that YBaCo<sub>4</sub>O<sub>7</sub> [1] (Y-114) is not oxygen-stoichiometric but absorbs oxygen up to  $\delta = 1.5$  and then releases it upon heating (even in O<sub>2</sub> atmosphere) in a single, sharp step below 400 °C [2]. The oxygen storage capacity of Y-114 substantially exceeds those for the known oxides; CeO<sub>2</sub>-ZrO<sub>2</sub>: 1.50 mmol-O/ g<sub>catalyst</sub> (500 °C) [3], Y-114: 1.88-2.82 mmol-O/ g<sub>catalyst</sub> (340 °C). By means of in situ X-Ray Diffraction the unit cell of the oxygen-rich phase was identified [4]. This cell (o) is a super cell of the parent cell (h) where  $a_o \approx \sqrt{3}a_h$ ,  $b_o \approx c_h$ , and  $c_o \approx a_h$ . This finding confirmed that oxygen absorption in Y-114 is, as expected, not based on a filling of crystallographic vacancies but rather an adaption of the structure to the increased temperature in presence of oxygen. These findings are confirmed in a very recent paper by Chmaissen et al. [5], where the determination and refinement of YBaCo<sub>4</sub>O<sub>8.1</sub> structure is reported for the first time. Here, we will present our results on structural changes during oxygen intake and release in YBaCo<sub>4</sub>O<sub>7+δ</sub> as monitored by variable temperature neutron powder diffraction.

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Keywords: neutron powder diffraction, variable temperature, oxygen absorption

## P20.09.35

*Acta Cryst.* (2008). A64, C616

### Lattice parameter of microcrystalline gold in a broad temperature range

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The physicochemical properties of gold make that, despite its low abundance and high price, this precious metal has a number of important applications in technology. Moreover, It is one of standards used in X-ray diffraction for pressure and temperature calibration. The accuracy of temperature calibration depends on the knowledge of temperature variation of lattice parameter. Accurate knowledge of lattice-parameter temperature dependence leads to determination of thermal expansion behaviour. Up to now there was no detailed study of the gold lattice parameter covering the low and high temperature range. In the present study, the lattice parameter and the thermal expansion coefficient for the microcrystalline gold polycrystals were studied in detail in the broad temperature range, 10 - 1050 K, using a powder diffractometer at the B2 beamline (DORIS III Synchrotron Ring, Hasylab, DESY). The apparatus configuration allowed for collection of data with high resolution and low background. The wavelength was calibrated in situ, using a diamond standard. A commercial micrometer-size gold powder was mounted within thin-wall capillaries. The experimental value of the measured lattice parameter at 300 K is 4.07818 Å. The study provides reliable data on lattice-parameter temperature dependence, as supported by the close agreement of the derived thermal-expansion data, and of the resulting value of Debye temperature, with those reported in literature.

Keywords: lattice parameter, thermal expansion, gold

## P20.10.36

*Acta Cryst.* (2008). A64, C616-617

### Magnetic ordering in Dy<sub>1-x</sub>Ca<sub>x</sub>BaCo<sub>2</sub>O<sub>5.5</sub> for x = 0.0 and 0.1

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The crystal and magnetic structures of Dy<sub>1-x</sub>Ca<sub>x</sub>BaCo<sub>2</sub>O<sub>5.5</sub> for x = 0.0 and 0.1 have been studied by neutron powder diffraction in the temperature range from 20 to 365 K. The crystal structures of both compounds were found to be best described in space group *Pm3m* on a  $2a_p \times 2a_p \times 2a_p$  unit cells where  $a_p$  refers to the lattice parameter of the cubic perovskite unit cell. The *a*- and *b*-axes were found to decrease and increase abruptly between 315 and 350 K as the temperature increases and the unit cell volumes exhibit signs of excess thermal expansion in the temperature range from 260 to 315 K. Dy<sub>0.9</sub>Ca<sub>0.1</sub>BaCo<sub>2</sub>O<sub>5.5</sub> orders antiferromagnetically for  $T \leq 305$  K into a G-type magnetic structure with a  $2a_p \times 2a_p \times 2a_p$  magnetic unit cell. The magnetic behaviour of DyBaCo<sub>2</sub>O<sub>5.5</sub> was found to be more complex as it exhibits two magnetically ordered phases. DyBaCo<sub>2</sub>O<sub>5.5</sub> orders into a G-type magnetic structure at 260 and 290 K. A  $2a_p \times 2a_p \times 4a_p$  magnetic unit cell was needed for indexing of the magnetic