

s11.m33.p5 **High Pressure Crystallographic Study of L-Cysteine: The Route to a New Polymorph.** S. Moggach, S. Parsons and D.R. Allan, *School of Chemistry, University of Edinburgh, Edinburgh, UK. E-mail: s.moggach@ed.ac.uk*

**Keywords: Cysteine; Pressure; Organic**

Cysteine is a simple amino acid found in many proteins and is an important compound in living cells and in many biochemical oxidation-reduction reactions in which the thiol group of cysteine can be converted to a disulfide link, important for determining the overall shapes of proteins.

There are two known polymorphs of cysteine, one is monoclinic [1] and crystallises in the space group  $P2_1$ , and the other is orthorhombic [2] and crystallises in the space group  $P2_12_12_1$ . Although a room temperature neutron study [2] has been performed on the orthorhombic form under ambient pressure conditions, no study has been done under high hydrostatic pressure.

Under these conditions the usually disordered thiol group at room temperature and pressure was ordered, and was closely followed by an unusually large reduction in volume, until at much higher pressure (c.a. 40kbar) a single crystal to single crystal phase transition was detected.

The new phase of cysteine is still orthorhombic and still crystallises in the space group  $P2_12_12_1$ , however the cell dimensions and packing are significantly different. Even more unusually, the torsion angle about the sulphur atom has rotated by approximately  $120^\circ$ , and is more representative of the torsion angle observed in the monoclinic polymorph.

Such studies are informative when looking at biologically important building blocks such as cysteine to understand the significance of hydrogen bond interactions in these simple organic molecules.

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s11.m33.p6 **High-temperature modification of dicopper divanadate.** R.G. Zakharov,<sup>a</sup> S.A. Petrova,<sup>a</sup> T.I. Krasnenko<sup>b</sup> and M.V. Rotermel<sup>b</sup>,<sup>a</sup>*Institute of Metallurgy, Urals' Division of the Russian Academy of Science, 101 Amundsena str., Ekaterinburg, 620016, Russia, and* <sup>b</sup>*Institute of Solid State Chemistry, Urals' Division of the Russian Academy of Science, 90 Pervomayskaya str., Ekaterinburg, 620219, Russia. E-mail: danaus@mail.ru*

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There are well known two structural modifications of the copper (II) pyrovanadate between the room temperature and its melting point at  $780^\circ\text{C}$  [1]. The temperature of  $\alpha$ - $\beta$  phase transition was determined as  $712^\circ\text{C}$ .  $\beta$ - $\text{Cu}_2\text{V}_2\text{O}_7$  was obtained by rapid quenching from  $750^\circ\text{C}$  [2].

High-temperature X-ray analysis of the  $\alpha$ - $\text{Cu}_2\text{V}_2\text{O}_7$  was carried out at Dron-Uml diffractometer (CuK $\alpha$ -radiation, monochromator of pyrolytic graphite on diffraction beam) using high-temperature attachment UWD-2000 in the temperature range of  $25^\circ$ - $770^\circ\text{C}$ . It was established a phase transition from the  $\alpha$ - $\text{Cu}_2\text{V}_2\text{O}_7$  into the new phase near  $725^\circ\text{C}$ .

X-ray analysis of the samples quenched from  $730^\circ$ - $750^\circ\text{C}$  revealed the mixture of  $\alpha$  and  $\beta$  phases in different ratio depending on cooling rate. The new phase can be indexed in monoclinic lattice  $C2/c$  with unit cell parameters  $a=7.325(1)\text{\AA}$ ,  $b=8.214(1)\text{\AA}$ ,  $c=10.190(1)\text{\AA}$ ,  $\beta=111.78(1)\text{deg}$ . (Table 1). The crystal structure of the new high-temperature phase conditionally called  $\beta'$ - $\text{Cu}_2\text{V}_2\text{O}_7$  is also isostructural to  $\alpha$ - $\text{Zn}_2\text{V}_2\text{O}_7$  and was preliminary refined with Rietica [3].

The copper (II) ion,  $\text{Cu}^{2+}$  ( $d^9$ ), occupying the oxygen polyhedron induce a distortion of it upon quenching due to the Jahn-Teller effect which results in the  $\beta' \rightarrow \beta$  phase transition during cooling the sample to room temperature.

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