

**P09.05.53***Acta Cryst.* (2008). A64, C490**Cocrystal formation between trimethoprim and sulfamethoxazole by sealed-heating method**Erizal Zaini<sup>1</sup>, Cahyati Sumirtapura Yeyet<sup>1</sup>,  
Nurono Soewandhi Sundani<sup>1</sup>, Halim Auzal<sup>2</sup><sup>1</sup>Bandung Institute of Technology, School of Pharmacy, farmasi@itb.ac.id, Bandung, West Java, 40132, Indonesia, <sup>2</sup>Faculty of Pharmacy, Universitas Andalas, Indonesia, E-mail: erizal\_faua@yahoo.co.id

Equimolar cocrystal formation between trimethoprim and sulfamethoxazole by sealed heating methods was carried out. When trimethoprim and sulfamethoxazole were heating at a molar ratio 1:1, new powder X-ray diffraction (PXRD) interferences peaks were observed in addition to PXRD interference peaks of each component. Effect of heating time on trimethoprim-sulfamethoxazole equimolar cocrystal was investigated by using PXRD, differential scanning calorimetry (DSC) and Fourier transform infrared spectroscopy. Cocrystal obtained by sealed heating method at temperature 160 °C had the same PXRD pattern and DSC thermogram with cocrystal from cocrystallization and melting method. These result indicated that heating could induced the formation of cocrystal.

Keywords: trimethoprim, sulfamethoxazole, cocrystal

**P10.01.01***Acta Cryst.* (2008). A64, C490**First report of natural oxyallanite: Oxidation and dehydration during welding of volcanic tuff**Mihoko Hoshino, Mitsuyoshi Kimata, Norimasa Nishida,  
Masahiro Shimizu, Takeshi AkasakaUniversity of Tsukuba, Earth Evolution Sciences, Tennoudai 1-1-1,  
Tsukuba, Ibaraki, 305-8572, Japan, E-mail: hossy716@geol.tsukuba.ac.jp

The oxidation of Fe<sup>2+</sup> to Fe<sup>3+</sup>, the release of H<sub>2</sub>, and the concomitant replacement of OH<sup>-</sup> by O<sup>2-</sup> would produce an oxy-equivalent of allanite (CaREEAl<sub>2</sub>Fe<sup>2+</sup>Si<sub>3</sub>O<sub>11</sub>O(OH)) (Dollase 1973). The reaction Fe<sup>2+</sup> + OH<sup>-</sup> - Fe<sup>3+</sup> + O<sup>2-</sup> + 1/2H<sub>2</sub> is formally equivalent to the oxy-reaction observed in other hydrous Fe<sup>2+</sup>-bearing silicate minerals, such as mica and amphiboles (e.g., Hogg & Meads 1975; Ferrow 1987). However, occurrence of oxyallanite (CaREEAl<sub>2</sub>Fe<sup>3+</sup>Si<sub>3</sub>O<sub>11</sub>O(O)) in natural environment has never been reported. The purpose of the present study is to discuss occurrence of natural oxyallanite. Chemical compositions and crystal structures of the allanites from two rhyolitic rocks--(1) Youngest welded tuff from Toba (YTT), Sumatra, Indonesia and (2) volcanic ash from SK100 (SK100-VAB), Niigata, Japan--were determined by electron microprobe analysis and single crystal diffractometer, respectively. Despite the close similarity, in chemical composition, between YTT allanites and SK100 ones, their unit-cell parameters are distinct from each other. The former has shorter *b* axis and longer *c* axis and larger  $\beta$  value in comparison with cell parameters of the latter. FT-IR analysis shows that YTT allanites have both the smaller OH-absorption band area and the shift of its bands to higher wavenumbers as compared to SK100 ones. Welding of the ash flow tuff including the allanites preformed in Youngest Toba welded tuff would cause them to undergo oxidations, dehydration and replacement. The sequential reaction would result in producing the present YTT allanite, namely oxyallanite. Although oxyallanite was only obtained by heating the natural allanite (e.g., Armbruster et al. 2006), this study first reports that oxyallanite may commonly occur in welded rocks at high temperatures.

Keywords: oxyallanite, welded tuff, volcanic ash beds

**P10.01.02***Acta Cryst.* (2008). A64, C490**The effects of F-OH replacement on the compression of super hydrous phase B structure**Takahiro Kuribayashi<sup>1,3</sup>, Toshiro Nagase<sup>4</sup>, Hiroshi Kojitani<sup>2</sup>,  
Masaki Akaogi<sup>2</sup>, Russell Hemley<sup>3</sup>, Ho-k Mao<sup>3</sup>, Yasuhiro Kudoh<sup>1</sup><sup>1</sup>Tohoku University, Department of Earth Science, 6-3, Aramaki Aza Aoba, Aoba-ku, Sendai, Miyagi, 980-8578, Japan, <sup>2</sup>Department of Chemistry, Gakushuin University, Tokyo 171-8588, Japan, <sup>3</sup>Geophysical Laboratory, Carnegie Institution of Washington, Washington DC. 20015, USA, <sup>4</sup>The Tohoku University Museum, Tohoku University, Sendai 980-8578, Japan, E-mail: t-kuri@mail.tains.tohoku.ac.jp

Super hydrous phase B (SUP-B), Mg<sub>10</sub>Si<sub>3</sub>O<sub>14</sub>(OH)<sub>4</sub>, is known as one of dense hydrous magnesium silicate minerals (DHMS) in Earth Science category. Physical properties of SUP-B are investigating to understand the structure of Earth's interior, since lots of previous works on phase study showed that SUP-B is stable under the cold slab conditions. Also, according to previous studies including ourselves, DHMS phases have a simple trend in the relationship between bulk modulus and some indexes such as density, the filling factor and so on. In these relationships, the F-OH replacement effects on the compression of these phases have not been clarified yet. Since F should be included in natural minerals instead of OH, it is important to understand F-OH replacement effects on some physical properties. In this study, for the structure of super hydrous phase B, high-pressure single crystal x-ray diffraction experiments were conducted to investigate the F-OH replacement effects on the compression. Fluorine end member SUP-B phase (F-SUP-B) was synthesized using a multi anvil apparatus installed in Gakushuin University under 21 GPa and 1400C conditions. Single crystal of F-SUP-B (0.04 x 0.04 x 0.03 mm<sup>3</sup>) was used for X-ray diffraction experiments at the BL-10A beam line in Photon Factory, KEK, Japan. Lattice parameters of this phase were measured at 0.0001, 1.5, 2.7, 4.0, 5.0, 6.4 and 7.4 GPa. The isothermal bulk modulus of F-SUP-B, calculated using the Birch-Murnaghan EoS (assuming K'=4), was K=153(3) GPa. This value was slightly larger (7%) than that (K=145(1) GPa) of OH-SUP-B. This is consistent with the predicted values from the case of norbergite which is known as other DHMS. The privation of weak hydrogen bonding in F-SUP-B structure caused its elastic hardening.

Keywords: high-pressure X-ray diffraction, single-crystal X-ray methods, synchrotron radiation

**P10.01.03***Acta Cryst.* (2008). A64, C490-491**Melt inclusion geothermometry and crystallography of calcic-plagioclases**Babita Rani Choudhary, Gajananrao Narayanrao Jadhav  
IITBombay, Powai, Earth Sciences, choudhary.r.babita@gmail.com,  
Mumbai, Maharashtra, 400076, India, E-mail: choudhary.r.babita@gmail.com

Babita Rani Choudhary (choudhary.r.babita@gmail.com) Dr. Gajananrao Narayanrao Jadhav (jadhav@iitb.ac.in) Department of Earth Sciences, IIT Bombay, Powai, Mumbai-400076, Maharashtra, India The crystallizing temperature works as a catalyst to initiate the nucleation of specific type of crystal development. Plagioclase phenocrysts have trapped small mass of magma as melt inclusions in the zoned as well as twinned variety, which indicate the geothermometric sequences of melt inclusions. To observe the kinetics of crystal-thermometry, we examined the zoned calcic-plagioclase phenocryst, from Deccan basalt samples collected from