

Their improved stability at +160 °C was observed in [3]. Herein, the structural behaviour of the CsLiB<sub>6</sub>O<sub>10</sub> was studied in a wide temperature range using a combination of single crystal X-ray diffraction (-120 °C – r.t.), powder X-ray diffraction (-120 – +700 °C), differential scanning calorimetry (DSC, -100 – +40 °C), and synchrotron powder diffraction (r.t., +300 and +600 °C). Our powder investigations testify the thermal stability of the compound over the whole range of the study. Synchrotron data collected at room temperature show no peak splitting that would indicate a hidden lower symmetry, but a high asymmetry of peaks is observed. Using single-crystal data sets at various temperatures, the crystal structure [1] was refined; empirical absorption corrections ( $\mu = 3.79 \text{ mm}^{-1}$ ) were applied. The results are characterized by significant peaks of residual electron density. A splitting of the Cs position similar to the one suggested in [4] was considered, but it did not change significantly on cooling. Other possibilities for the high residual electron density might be a non-resolved disorder problem or an insufficient absorption correction. For the hydrated samples a reversible partial transition to a new phase was observed at -30 ( $\pm 5$ ) °C. The peaks of the new phase grew till -70 °C and did not change further till -120 °C. After several cooling cycles the crystal was broken. The new phase is likely to be formed on the surface of the crystal, where water molecules attack the crystal, as a first step of its decomposition. The temperature dependencies of the lattice parameters obtained by single-crystal X-ray diffraction are slightly curved at about -70 °C. This correlates to the temperature at which the new phase stopped to grow. Surprisingly, no considerable changes of cell parameters were observed after a slight hydration of powder samples at room temperature. Addition of more water to the sample leads to a formation of a mixture of CsLiB<sub>6</sub>O<sub>10</sub> and both modifications of CsB<sub>5</sub>O<sub>6</sub>(OH)<sub>4</sub>×2H<sub>2</sub>O, i.e.  $\alpha$  and  $\beta$ . Probably, Cs<sub>2</sub>B<sub>10</sub>O<sub>16</sub>×8H<sub>2</sub>O observed in [5, 6 and Ref. therein] as a hydrolytic product of CsLiB<sub>6</sub>O<sub>10</sub>, was actually CsB<sub>5</sub>O<sub>6</sub>(OH)<sub>4</sub>×2H<sub>2</sub>O. Thus, under the action of water, CsLiB<sub>6</sub>O<sub>10</sub> decomposes with a formation of CsB<sub>5</sub>O<sub>6</sub>(OH)<sub>4</sub>×2H<sub>2</sub>O via the intermediate new phase.

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#### FA4-MS35-T04

**Pressure-induced phase transitions in L-alanine, revisited.** Nikolay Tumanov<sup>a</sup>, Elena Boldyreva<sup>b</sup>, Alexander Kurnosov<sup>a,c</sup>, Raul Quesada Cabrera<sup>d,e</sup>.  
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The effect of pressure on L-alanine has been studied by X-ray powder diffraction (up to 12.3 GPa), single-crystal X-ray diffraction (up to 6 GPa), Raman spectroscopy and optical microscopy (up to 6.4 GPa). No structural phase transitions in L-alanine have been observed. At about 1.5-2 GPa (close to the pressure of the previously reported phase transition into a tetragonal phase, 2.3 GPa [1], [2]), the cell parameters  $a$  and  $b$  become accidentally equal to each other, but without a change in the space group symmetry. Neither could be a polymorphic transformation into a monoclinic phase at about 9 GPa confirmed, the changes in the cell parameters till the highest measured pressures being continuous and the cell metrics remaining orthorhombic. Our Raman experiments confirmed the effects described previously for the spectra of L-alanine [1], but we have shown that the spectral changes are continuous and are not related to structural phase transitions. During a slow decompression of L-alanine single crystal (in a methanol-ethanol 4:1 mixture as a pressure-transmitting liquid) from about 6 GPa, a new phase crystallized in the diamond anvil cell in the pressure range between 3-5 GPa, which dissolved at about 2 GPa. This previously unknown phase was characterized by powder X-ray diffraction and Raman spectroscopy and seems to be a solvate L-alanine. The study was supported by a grant from RFBR (09-03-00451), a BRHE grant RUX0-008-NO-06) and a FASI Contract (№ 02.740.11.5102).

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#### FA4-MS35-T05

**Do organic solid-state reactions occur in a concerted manner?** Manuel A. Fernandes, Demetrius C. Levendis. *Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, PO WITS, 2050, Johannesburg, South Africa.*  
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The photochemical solid-state reactions have been heavily studied over the last fifty years leading to the topochemical postulates and other solid-state reaction concepts. In general for reactions that genuinely occur under lattice control, the structure of the product is directly derived from the orientation and structure of the reactants in the starting crystal. Using irradiation methods that encourage single-crystal-to-single-crystal photodimerizations one can often discover the way the molecules (both reactant and product) adapt to their changing environment. However, is it possible to extract information on how the reacting environment affects the solid-state reaction by examination of close contacts? Do random pairs of molecules in the crystal react when exposed to UV light or do the reactions occur in a concerted/relatively ordered manner? In this work we report on the solid-state photochemistry of two polymorphs of *o*-ethoxy-*trans*-cinnamic acid - one which undergoes photodimerization despite the reacting double bonds being about 4.6Å apart, while the other adopts different reaction pathways depending on whether the reaction was carried out at room temperature or at 60°C. In both cases the reactions show convincing evidence for cooperativity between reacting molecules, in that molecules in one unit cell site react