## **Poster Presentation**

## Negative thermal expansion in isostructural Zn(II) and Co(II) L-malates

Anna Krawczuk<sup>1</sup>, Adrianna Chojnacka<sup>1</sup> <sup>1</sup>Faculty Of Chemistry, Jagiellonian University, Krakow, Poland E-mail: krawczuk@chemia.uj.edu.pl

Thermal expansion is a phenomenon that could be described as a deformation of a crystalline material caused by the temperature change at constant pressure. The volume of such a structure usually increases while it is being heated, and this process is reversible, which means that the volume decreases if the temperature is being lowered. However, not all materials expand on heating. Since thermal expansion of a crystal depends on the strength and type of its interatomic forces, in some cases specific structural features may cause contraction of the material. For example, in polymers thermal expansion is usually small and positive along the polymeric chain, whereas in the perpendicular direction, due to lateral vibrations in the chain which produce an effective contraction by bending motions, the thermal expansion coefficient becomes negative.

Here we present two isostructural complexes of zinc and cobalt L-malates, in which, thermal expansion becomes either positive or negative depending on the crystallographic direction. We have proven that thermal expansion is negative along [010] up to 258K and positive above, while the effect is positive in the temperature range of 143-350K along [100] and [001]. It is a result of the existence of one-dimensional pseudo-polymer chains in the studied structures built of the mixture of coordinate and covalent bonds. The presence of coordination bonds in pseudo-polymer chains causes that at a certain point, as an effect of heating, the atoms are more likely to move, which results in the change of the thermal expansion from negative to positive.

[1] Chojnacka A. et al. (2017), to be published.

- [2] Pryde A.K.A. et al. (1996) J. Phys.: Condens. Matter, 8, 10973-10982.
- [3] Barrera G.D. et al. (2005) J. Phys.: Condens. Matter, 17, R217-R252.





1 dimensional pseudo-polymeric chains along [010] in zinc L-malate.

Quadric representation of thermal expansion in zinc L-malate (green color refers to positive values, red to negative values)

Keywords: thermal expansion, crystal structure-property correlation, isostructural complexes