layer with oxygen and La/Ba atoms is stacked by two types. One is cubic ABCABC stacking for perovskite layer and hexagonal ABAB stacking for junction slabs which is composed three octahedral with face contact. There are three positions for Ba/La ions as follows: *A*1 position with La and Ba is located near vacant octahedron, *A*2 position is located next stacking layer, and *A*3 position is occupied the center of perovskite layer. Structures of $BaLa_4Ti_4O_{15}$ substituted Ca and Sr for Ba are also analyzed. And relationship between structure and properties of them are presented.

Keywords: microwave dielectrics, homologuos compound, hexagonal layered perovskite

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Extraordinary Negative Thermal Expansion in the Smallest Chiral Amino Acid Alanine

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Amino acid construction consists of a carboxylic acid (-COOH) and an amino ($-NH_2$) functional group attached to the same tetrahedral carbon atom, the α-carbon. Every amino acid, with the exception of glycine, comes in two forms, a left-handed (L) and a right-handed (D) version, which are identical mirror images of each other. However, protein chains cannot be formed from a mixture of D and L.

We report on high resolution X-ray and neutron scattering diffraction as well as quasi-elastic neutron (QENS) studies on crystalline L- and D-alanine over a wide temperature range. Our aim is to verify the possibility predicted by the Nobel Laureate A. Salam, that a phase transition, related to a break of the as C α-H bond, occurs in alanine. While no change in the space group symmetry was observed, a negative thermal expansion, by discrete steps, along the **c**-axis is observed till the melting point. Additional anomalies are also noticed in the **a** and **b** lattice constants at 170K. Moreover, the evolution of the mean-square displacement, obtained from the QENS, data shows a steadily increase on heating, but near 150K and again near 200K a deviation from the expected behavior is observed. The results suggest the excitation of new degrees of freedom, possibly due to a progressive conformational change of the NH^{3+} group. The ramifications of this study can be extremely interesting for the understanding of homochirality as well as a breakthrough in molecular mapping via non-traditional sources of information.

Keywords: amino acids, chirality, structure and properties

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Structure Evolution and Magnetoelectricity in BaO-TiO-FeO-CoO System at R .T

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Crystal structures evolution and their transformation with compositions have been studied on BaO-TiO-FeO-CoO system over a composition zone using Rietveld analysis of x-ray powder diffraction data .The phases as appeared after synthesis showed at RT, a combination of perovskite and spinel phases corresponding to piezoelectric [PE] and piezomagnetic [PM]phases as grown in situ leading to a composite magnetoelectric [ME] material. The ME property of such composites at RT have been measured by dynamic method. A quantitative comprehension of the ME property of the composite in terms of the structures of the component phases have established that ME property being the result of mechanical coupling between the PE and PM phases has considerable contribution from their individual structural property which have been evoluted during in-situ preparation.

Keywords: X-ray structural crystallography, magnetoelectric property, composite inorganic phases

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Negative Refraction : an Intrinsic Property of Uniaxial Crystals

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Negative refraction (NR) is a phenomenon where light is refracted to propagate along the same side as the incident light with respect to the normal of the interface, contrary to the normal light refractions. It can be used to realize the "superlense" with a resolution smaller than the wavelength and many other optic applications. Recently, NR has been realized in metamaterials, photonic crystals and traditional crystals. Although the wave vector k does not form a left-handed triplet with the electric field E and magnetic filed H for the light in conventional crystals, the light can be bent on the same side with the incident light. We theoretically and experimentally show that negative refraction can be realized at the surface of uniaxial crystals by orientating the crystals with their optic axes at a certain angle θ_0 to the normal of the light incoming surface. The concept of negative refraction can be extended to be an intrinsic property of all uinaxial crystals. That is, NR can be realized in all the uniaxial crystals including with the tetragonal, hexagonal and trigonal symmetries. It is revealed that the angular range for incident light to yield negative refraction attains its maximum that only depends on the difference of two indices of refraction |ne-no| when $\tan^2\theta_0$=n0/ne. The maximum refracted angle is dependent on the ratio ne/no. The careful experiments on positive uniaxial crystal YVO_4 and negative unaxial crystal calcite ($CaCO_3$)give results in good agreement with the calculated ones.

Keywords: crystal structure properties, optical crystallography, refractive index

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Unravelling the Mechanism of the Bathochromic Shift in the Lobster Carapace

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The colouration mechanism in the lobster carapace was revealed at 3.2Å resolution by a protein crystal structure of β-crustacyanin [1]. The crystals are a vivid blue colour and this colour is provided by two bound molecules of the carotenoid astaxanthin. There are three candidate molecular parameters responsible for the bathochromic shift of astaxanthin, which is famously demonstrated via the colour change of lobsters on cooking, turning from blue/black to orange/red: 1. the coplanarisation of the end rings with the polyene chain, increasing the degree of conjugation; 2. an electronic polarisation effect stemming from H bonding of the keto oxygen atoms of the bound astaxanthins, to histidine and water molecules; 3. an exciton interaction due to the close proximity of the two bound astaxanthins.

In order to investigate these colour tuning parameters further, we have determined four new crystal structures of the carotenoids astaxanthin and canthaxanthin all of which are red. These have allowed us to investigate the atomic environment of the end rings and the crystal packing arrangements of the polyene chains. Further experiments are in progress and will also be reported.

[1] Cianci M., Rizkallah P.J., Olczak A., Raftery J., Chayen N.E., Zagalsky P.F., Helliwell J.R., *PNAS USA*, 2002, **99**, 9795-9800.

Keywords: lobster, colour, carotenoids

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Crystal Structure of Hematopoietic Prostaglandin D Synthase Complexed of HQL-79

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