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Hematopoietic prostaglandin(PG) D synthase(H-PGDS) is responsible for production of PGD_2 as an allergic or inflammatory mediator in mast cells and Th2 cells[1].

We solved the crystal structure of human H-PGDS bound to the cofactor glutathione(GSH) and HQL-79, a novel inhibitor of H-PGDS in the presence of Ca^{2+} or Mg^{2+}, showing the HQL-79 molecule penetrated into the active site between Trp104 and GSH binding site with its biphenyl rings locating at the bottom of the active site, inducing the conformational change of Trp104 with a 60 degree rotation and a 3.7 A movement of the indole ring.

The surface plasmon resonance analysis revealed that the binding affinity (KD) of HQL-79 is accelerated 10-fold in the presence of both Mg^{2+} and GSH, revealing that the GSH molecule strongly bound in the Mg^{2+}-bound form helped the insertion of the HQL-79 molecule, reducing the *Ki* value to be 5 μM with 10-fold in the presence of Mg^{2+}. HQL-79 specifically inhibits H-PGDS activities competitive to the substrate PGH_2, and non-competitive to the cofactor GSH[2].

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Keywords: prostaglandins, anti-inflamatory compounds, X-ray structural analysis

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Polymorphism and Photochromism of Salicylideneaniline

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Organic compounds exhibiting photo- or thermochromicity have been of considerable interests owing to their properties and possible applications. The photochromism of salicylideneaniline (SA) was discovered by Senier *et al.* at the beginning of last century. In 1964, Cohen *et al.* [1] observed polymorphism.

It is generally accepted that the stable form of SA in the ground state is the enol form, with an intramolecular hydrogen bond between the hydroxyl group and the nitrogen atom. Upon photoexcitation of this enol form with UV light, it undergoes an ultrafast proton transfer from the hydroxyl group to the nitrogen, due to the electronic redistribution in the excited state. The proton transfer generates a keto tautomer in the excited singlet state.

Here, we report on the alpha-2-polymorph structure of SA in the ground state [2], already mentioned by Cohen. We shall also described a new polymorph, beta, which features a planar SA molecule and is therefore thermochromic. Then, we revisit the alpha-1-polymorph structure of SA described by Destro *et al.* [3], but reconsidering their hypothesis. We suggest a lowering of the symmetry with the aim to improve the structure solution.

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Keywords: photochromism, polymorphic structures, properties and structure relationships

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Structure, Chemical Bonding and Thermoelectric Performance of Zn_4Sb_3

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Thermoelectricity is due to play an important role in today's energy challenges. The ideal thermoelectric material is a *phonon glass and electron crystal*, i.e. has a low thermal conductivity combined with high electrical conductivity and Seebeck coefficent. Zinc-antimonide, with formal stoichiometry Zn_4Sb_3, nicely fulfills these requirements, but to explain its unusual combination of properties was not possible because its detailed structure remained for a long time unknown. Now, a crystal structure consistent with the observed mass density has been proposed for the first time by structurally refining single-crystal XRD data, and by analysing powder-synchrotron-radiation diffraction data with a Rietveld-MEM technique.[1,2] Zn_4Sb_3 has a regular Sb lattice, while Zn is distributed over several non-equivalent sites with fractional occupancy. To deconvolute the space-time average inherent to XRD we carried out an extensive computational investigation, and we identified the atomistic arrangements through which the system evolves.[2] In this poster, the bonding and atomic properties of these structures are investigated within the formalism of the Quantum Theory of Atoms In Molecules, and contrasted to the proposed Zintl-phase description of Zn_4Sb_3.[1,2] Furthermore, band-structure calculations of the electronic transport properties are performed to unravel how the atomic structure relates to the material's thermoelectric performance.

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Keywords: XRD, ab-initio computations, thermoelectricity

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Synthetic Chrysotile: Effect of Foreign Ions on the Hydrothermal Synthesis

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Conventional and synchrotron radiation X-ray diffraction have been used to characterize chrysotile nano-crystals synthesized under bland hydrothermal conditions. In particular, the effects on the crystallization kinetics of the presence of Al, Fe and Ti species have been evaluated.

Studies were conducted both *in situ* using synchrotron radiation X-ray diffraction at the Daresbury Laboratory station 16.4 and *ex situ* on the material synthesized in a Parr 4652 laboratory reactor.

The synthesis of the material was obtained under conditions usually considered very bland to form complex silicates.

Chemical physical, structural and morphological characterization of the synthesized crystals allowed to know the role of the foreign ions on the observed materials features.

Keywords: nanotubes, chrysotile, hydrothermal synthesis

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Structural Comparisons of Three Intermetallic Antimonide Families

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High quality single crystals of the ternary antimonides $LnNi_xSb_2$ (Ln = Y, Gd – Er; $x \approx 0.6$) and $LnNiSb_3$ (Ln = Pr, Nd, Sm) have been grown from an antimony flux. Their crystal structures have been characterized by single crystal X-ray diffraction experiments. The $LnNi_xSb_2$ compounds adopt the $HfCuSi_2$ structure type and crystallize in the tetragonal space group *P*4/*nmm* with $Z = 2$ and lattice parameters of $a \approx 4.3$ Å, $c \approx 9.3$ Å, and $V \approx 170$ Å^3. These compounds are layered and consist of *Ln*-capped Sb square nets and Ni tetrahedral frameworks arranged in an anti-PbO fashion. The $LnNiSb_3$ compounds adopt the $CeNiSb_3$ structure type and crystallize in the orthorhombic space group, *Pbcm* (No. 57), $Z = 12$, with lattice

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