lytic-like protease. In contrast, the high-resolution crystal structures of another prokaryote serpin, tengpin, reveals that the serpin domain of this molecule folds spontaneously and rapidly to most stable (i.e. relaxed) conformation. This is an exciting result, since tengpin represents the first serpin identified to date that obeys Anfinsen's conjecture. Furthermore, the X-ray crystal structures of tengpin reveals the structural basis for a novel mechanism for loop-C-sheet serpin-polymerisation. Analysis of the structural data provides striking insight into the mechanism of serpin metastability and the structural basis for serpin polymerisation.

[1] a) Irving J.A., et al., *Structure 2003*; b) Fulton K.F., et al., *J Biol Chem*, 2005.

Keywords: serpin, folding, polymerisation

MS03 CHIRAL AND NON-CENTROSYMMETRIC STRUCTURES

Chairpersons: Shiv P. Halasyamani, Reiko Kuroda

MS03.24.1

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Spontaneous Resolutions in Halogen Bonded Fluorinated Networks

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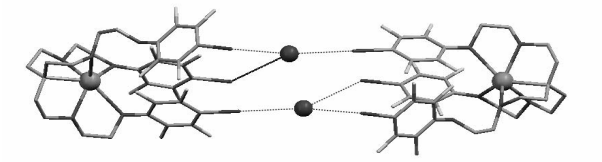
Halogen bonding is an efficient tool for self-assembling halo-perfluorocarbons (PFC) and hydrocarbons (HC) [1]. Its particular ability to control spontaneous resolution in hybrid PFC-HC systems has been discovered only recently [2]. Up to now we observed spontaneous resolutions in four cases affording chiral cocrystals, space group $P2_12_12_1$. Three of them involved long-chain iodo-PFC's (C_8-C_{10}) with either QUATS or *N,N,N',N'*-tetramethyl-*p*-phenylendiamine as bases. Their different features with regard to the segregation behaviour and the conformation of the PFC chains will be outlined. The X-ray structure of a chiral alkali halide complex **1** (Figure) involving a tripodand will also be presented.



1

[1] Metrangolo P., Neukirch H., Pilati T., Resnati G., *Acc. Chem. Res.*, 2005, *in press.* [2] Neukirch H., Guido E., Liantonio R., Metrangolo P., Pilati T., Resnati G., *Chemm. Commun.*, 2005, 1534.

Keywords: halogen bonding, chiral resolution, molecular cocrystals

MS03.24.2

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Invariom Modeling for Improving Absolute Structure Determination

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A reliable determination of the Flack parameter [1] for structures of organic molecules, containing only the elements H, C, N, and O usually fails. The reason for this is the very weak anomalous signal obtained from the light atoms [2]. Recently we have introduced invariom [3] and here we try to improve the absolute structure determination by replacing the independent atom model with the aspherical invariom scattering model. The determination of the Flack parameter was included in the program XDLSM [4]. Alternatively, its calculation has been attempted via a hole-in-one procedure. A precise data set on a steroid compound was collected using copper radiation and CCD detection, and first results are reported.

[1] Flack H. D., *Acta Cryst*., 1983, **A39**, 876. [2] Flack H. D., Bernardinelli G., *J. Appl. Cryst.*, 2000, **33**, 1143. [3] Dittrich B., Koritsanszky T., Luger P., *Angew. Chem. Int. Ed.*,2004, **43**, 2718. [4] Koritsanszky T., Richter T., Macci P., Gatti C., Howard S., Mallinson P.R., Farrugia L., Su Z.W., Hansen N.K., *XD*, Freie Universitat Berlin, Berlin, 2003.

Keywords: Invarioms, Flack parameter refinement, chiral structures

MS03.24.3

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Optical Topographies of Chiral Structures

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Can optical rotatory power, a phenomenon typically associated with chirality or handedness, be used as a contrast mechanism in microscopy? Chiroptical imaging techniques have not heretofore been implemented. This neglect has created a hole in the science of molecular chirality, particularly with respect to complex, heterogeneous, organized media. We built a circular extinction imaging microscope to examine chromophores in anisotropic hosts. With this instrument, images of crystals were made via two mechanisms, intrinsic circular dichroism (CD) and a new effect that was discovered and called anomalous circular extinction (ACE). Through these new chirality "spectacles" we have observed left and right handed twinning in crystals of a dye that was masked by all previous methods of analysis, Figure 1 [1]. However, when turned onto unusual dyed crystals, we observed optical effects that mimic those due to chirality.

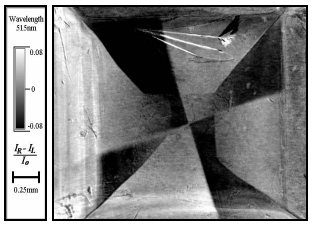

Figure 1. Circular Dichroism in 1-8-Dihydroxyanthraquinone.

[1] Claborn K., Puklin-Faucher E., Kurimoto M., Kaminsky W., Kahr B., *J. Am. Chem. Soc.*, 2003, **125**, 14825-14831.

Keywords: chirooptical properties, circular dichroism measurement, dyes

MS03.24.4

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Nonlinear Optical Properties of Chiral Polymers and Systems

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We present the nonlinear optical properties of different thin film films of chiral (conjugated) polymers. These systems exhibit large magnetic dipole nonlinearities, in some cases larger than the effects linked to electric dipole interactions. The nonlinear optical effects observed indicate the links between magnetic hypersusceptibilities and chirality. We also investigated supramolecular assemblies of helicenes where the nonlinear optical effects are exclusively described by electric dipole interactions. In the crystalline liquid state the chirality, as expressed by nonlinear CD effects, of these helicene assemblies could be switched by the application of an electric field.

Keywords: polymers, chirality, nonlinear optics

MS03.24.5

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Some Reminiscences of Non-centrosymmetric Structures

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In the "neanderthal" age of crystallography, a light atom non-centrosymmetric crystal was usually relegated to the skeleton collection of unsolvable structures. The development of MULTAN