in the fibers. The strain applied to the fibers has been modeled by an integrated texture-stress model inside the program as well.

[1] http://www.ing.unitn.it/~luttero/maud [2] Ischia G., Wenk H.-R., Lutterotti L., Berberich F., *J. Appl. Cryst.*, 2005, **38**, 377.
Keywords: structure determination, texture, polymer

P.11.09.1
Novel Structure of 1,1'-Disubstituted Ferrocene Derivative
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Some of the 1,1'-disubstituted ferrocene derivatives (bMAF-*n*, *n* is the carbon number in the flexible spacer) show liquid crystallinity. It was reported that bMAF-5 had S-typed molecular structure [1]. The S-shaped one of the other derivative was already reported by the other workers [2]. Recently, new U-typed one was found out in bMAF-10 [3].

In this study, the crystal structure of bMAF-2 was analyzed by single crystal X-ray diffraction method. All measurements were made by Rigaku AFC-5R diffractometer with graphite monocromatized CuKα radiation. The crystal structure obtained in this study was a monoclinic with space group *C2/c*. The residual R and wR converged on 0.036 and 0.067, respectively. The feature of the structure was very unique, because the two substituent had a bent structure around a *gauche* conformation. This molecular structure was given a name to Z-shape, which was different from those of bMAF-5 (S-shape) and 10 (U-shape).

Liquid crystallinity will be discussed from structural point of view.

[1] Nakamura N., et al, *Mol. Cryst. Liq. Cryst.*, 2005, *in press*. [2] Khan A.M., et al., *Liq. Cryst.*, 1989, **5**, 285. [3] Nakamura N., et al, *Chem. Lett.*, 2004, **33**, 358.
Keywords: ferrocene compounds, liquid crystal, crystal structure

P.11.09.2
Crystal Structure of 1,24-Dibromotetracosane
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The crystal structure of 1,24-dibromotetracsane was analyzed by single crystal X-ray diffraction method. The compound crystallized in a monoclinic system (a = 5.482 (3)Å, b = 5.381 (2)Å, c = 43.859 (2)Å, β = 93.07 (2)°, Z = 2) with a space group $P2_1/c$. The molecule is centrosymmetric and its skeleton has an all-*trans* conformation including both terminal Br atoms. In the crystal, the molecules form layers with a thickness of *c*/2. In the layer, the molecules inclined to the basal plane of Br atoms. The layers are arranged in a zigzag manner between the neighboring layers making a herringbone motif just like the smectic C_A structure of liquid crystals.

The molecular and crystal structures of 1,24-dibromotetracosane are similar to those of the homologs with an even number of C atoms, *vis*. 1,12-dibromododecane[1], 1,14-dibeomotetradecane[2], 1,16-dibromo -hexadecasne[3], 1,18-dibromooctadecane[4], 1,20-dibromoicosane[5], and 1,26-dibromohexsacosane[6].

[1] Kulpe S., et al, *Cryst. Res. Technol.*, 1981, **30**, 349. [2] Uno K., et al, *Acta Cryst.*, 2003, **E59**, o708. [3] Kobayasi H., et al, *Cryst.Res. Technol.*, 1995, **30**, 275. [4] Nakamura N., et al, *Cryst. Res. Technol.*, 1993, **28**, 953. [5] Nakamura N., et al, *Acta Cryst.*, 2004, **E60**, o1408. [6] Takamizawa K., et al, *Eng. Sci. Rep. Kyushu Univ.*, 1992, **13**, 341.
Keywords: alkyle halide, crystal structure, liquid crystal

P.11.09.3
Crystal Structure of Monosubstituted Ferrocene Derivatives
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A series of monosubstituted ferrocene derivatives, ω-[4-(4-methoxyphenoxy-carbonyl)phenoxycarbonyl]alkyl 4-ferrocenyl benzoate (abbreviated hereafter as MPAF-*n*, *n* = 1~11, where *n* is the number of carbon atoms in the methylene unit) were prepared in our laboratory [1].

In the present study, the crystal and molecular structures of MPAF-10 were determined by X-ray diffraction method using a single crystal. All measurements were made by Rigaku AFC-5R diffractometer with graphite monocrochromatixed CuKα radiation. The crystal structure obtained in this study was orthorhombic (a=8.176(6), b=88.253(7),c=10.140(9)Å,Z=8) with space group Pbca. The residual R and wR converged on 0.056 and 0.128, respectively. Good of fitness is 1.000.

This compound shows liquid crystallinity. This molecule bents a little around a ester group located in the ferrocene side. The feature of the molecule is not favorable for the liquid crystalline compound. Two molecules, however, associate head to head manner making a rod-like shape. Therefore, this compound exhibits liquid crystallinity.

[1] Hanasaki T., Ueda M., Nakamura N., *Mol. Cryst. Liq. Cryst.*, 1993, **237**, 329.
Keywords: liquid crystal, ferrocene compounds, crystal structure

P.11.09.4
Crystal Structure of a Liquid Crystalline Ferrocene Derivative
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A series of 1,1'-disubstituted ferrocene derivative, 1,1'-bis[ω-[4-(4-methoxyphenoxy-carbonyl)phenoxy]alkoxycarbonyl]ferrocene (abbreviated hereafter as bMAF-*n*, where *n* is the number of carbon atoms in the methylene unit) was prepared, and some of them (bMAF-3,5~12) exhibited liquid crystallinity[1,2]. In this study, the crystal structures of bMAF-3 were determined by the X-ray diffraction method in order to gain an understanding of the interrelation between the crystal structure and some physical properties. The single crystals of the compounds were obtained from a solution with a mixed solvent by the slow evaporation method. The measurement was made on a Rigaku AFC-5*R* diffractometer with graphite monochromatized Cu-*Kα* radiation. The calculation was performed using the *Crystal-Structure* crystallographic software package. The crystal structure was mono-clinic system (*a*=5.857(4)Å, *b*=24.105(3)Å, *c*=14.069(4)Å, *β*=93.15(4)°, *Z*=2) with space group $P2_1$. In generally, rod-like molecules has advantageous structure to show liquid crystallinity. The molecular structures of bMAF-3 could be regarded as rod-like. In fact, they have the advantage of showing liquid crystallinity, and they give rise to liquid crystallinity.

[1] Hanasaki T., Ueda M., Nakamura N., *Mol. Cryst. Liq. Cryst.*, 1994, **250**, 257. [2] Nakamura N., Mizoguchi R., Ueda M., Hanasaki T., *Mol.Cryst. Liq.Cryst.*, 1998, **312**, 127.
Keywords: liquid crystal, ferrocene, rod-like

P.11.09.5
Layer and Molecular Orientation in Electroclinic Liquid Crystals: Dynamic μ-Diffraction
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For the direct determination of the microscopic local layer structure in the smectic liquid crystal under the external field, time-resolved synchrotron X-ray μ-diffraction has become a powerful tool [1]. In this presentation, static and dynamic local layer structures and local molecular orientation in the electroclinic effect of the chiral smectic A (SmA) phase were analyzed with μ-diffraction.

An X-ray beam size was about 3×4 μm^2. The samples were ferroelectric liquid crystals (TK-C101) and measured in the SmA phase. At the high electric field, the compound chevron structure, consisting of the curved vertical chevron and the horizontal chevron, was realized. The molecular orientation measured by the high angle halo-pattern showed the spatially-alternate molecular inclination corresponding to the layer deflection. It was shown that the anchoring effect at the alignment film played an important role for the layer structure. The layer response of the electroclinic effect was similar to that in the high electric field treatment of SmC phase, though the origin of the layer shrinkage was different between them.

[1] a) Takahashi Y., et al, *Jpn. J. Appl. Phys.*, 2001, **40**, 3294; b) *Phys. Rev.* 2003, E**67**, 051706.
Keywords: smectic liquid crystal, time-resolved, X-ray microbeam

P.11.10.1
Growth and Properties of KTiOPO₄ Single Crystals doped with Er and Nd
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KTiOPO₄ (KTP) single crystals are of great interests due to their ferroelectric and nonlinear optical properties. Last time the attention is given to the investigation of KTP-family crystals doped with rare earth and codopant ions as the material for self-doubling [1,2].

In the present work single crystals of KTP codoped with Ln = Er, Nd and Me = Nb, Ta, Ba, Ca, Mg, Bi, Al, Si, KCl were grown by means of flux method and some properties were investigated.

The investigations show that an addition of Nb and Ba leads to decreasing of KTP:Ln:Me optical quality, whereas the quality increases with KCl and Bi and does not markedly depends on Ln.

Maximum luminescence intensity was observed in KTP:Er:Nb crystals. Life time of $^4F_{3/2}Nd^{3+}$ and $^4I_{13/2}Er^{3+}$ has been found as 250 μs and 6 ms for KTP:Nd and KTP:Er respectively. In KTP:Ln:Me the life time changes in the area of 1 - 7 ms for $^4I_{13/2}Er^{3+}$ and 180 - 300 μs for $^4F_{3/2}Nd^{3+}$ depending on the codopant of ion Me.

The presence of Ln ions in KTP:Ln:Me crystals does not strongly affect on ferroelectric phase transition temperature, but suppresses the dielectric permittivity peak caused by the above-named transition.

[1] Sole R., Nikolov V., Koseva I., et al., *Chem. Mater.*, 1997, **9**, 2745. [2] Carvajal J. J., Nikolov V., Sole R., et al., *Chem. Mater.*, 2002, **14**, 3136.
Keywords: crystal growth, KTiOPO₄, ferroelectrics

P.11.10.2
Second-Order Nonlinear Optical Properties of Tetradentate Schiff base Complexes
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Quadratic non-linear optical properties of new unsymmetrical Ni(II), Cu(II), Zn(II) and VO(II) complexes with [N₂O₂] chelate tetradentate ligands are presented. The complexes were synthesized by template condensation of 1-phenylbutane-1,3-dione mono-*S*-methylisothiosemicarbazone with o-hydroxybenzaldehyde or its 5-

phenylazo-derivative. The crystal structure of some complexes was determined by using synchrotron radiation (XRD1 beamline at ELETTRA, Trieste).

Large values of hyperpolarizability, as obtained for these complexes by the solution-phase dc electric-field-induced second harmonic (EFISH) generation method, together with their high stability constants, make them promising candidates for successful applications in the field of optoelectronic technologies.

The values of theoretical hyperpolarizability, calculated through both Finite Field and Time Dependent DFT methods, are also presented.
Keywords: transition-metal complexes, nonlinear optical properties, theoretical calculations

P.11.10.3
Temperature Depence of Refractive Indices in selected Borates
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The knowledge of the temperature dependence of the refractive indices of a nonlinear optical crystal play a key role for its classification as a NLO material. For example, the temperature dependence can be used as a possibility for fine tuning of the phase-matching conditions of a nonlinear optical frequency conversion process. In general it is advantageous to describe the temperature dependence of the refractive indices using the temperature dependence of the polarisation tensor [a_{ij}] (optical dielectric impermeability tensor) $\Delta a_{ij} = b_{ij} \Delta T + c_{ij} \Delta T^2 + ...$, where [$b_{ij}$], [$c_{ij}$],... describe the linear, quadratic, etc. temperature dependence of the polarisation tensor. In most cases (far from phase transitions) the linear approximation turn out to be an adequate description.

In this work we present a technique for the measurement of temperature dependence of refractive indices based on a Jamin interferometer, which allows to measure optical path length differences as a function of temperature (temperature range: 50...280 K). The knowledge of the refractive indices at a reference temperature T_o (e.g. room temperature) including the orientation of the indicatrix, and the knowledge of thermal expansion data in the same temperature range are necessary for the evaluation of the experimental data.

As results we present the [b_{ij}] tensors of the non-centrosymmetric borate crystals: $Zn_4[O(BO_2)_6]$ (PG: $\bar{4}3m$), $Li_2B_4O_7$ (PG: *4mm*), β-BaB_2O_4 (PG: *3m*), PbB_4O_7 (PG: *mm2*), SrB_4O_7 (PG: *mm2*) and BiB_3O_6 (PG: *2*).
Keywords: non-centrosymmetric borates, phase-matching, nonlinear optics

P.11.10.4
Nonlinear Optical Properties of Lithium Sulfate Monohydrate, Li₂SO₄ · H₂O
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Lithium sulfate monohydrate crystallizes in the monoclinic polar space group $P2_1$ [1]. Among the group of non-ferroelectric polar crystals, Li₂SO₄·H₂O possesses the highest pyroelectric coefficient as well as remarkable piezoelectric and electro-optic properties. However, there is only little known about its nonlinear optical properties [2]. Recently, the possibilities of phase-matched second harmonic generation (SHG) in Li₂SO₄·H₂O were analysed in detail [3]. In this work we present the results of our investigation of the SHG. Using the Maker fringe technique and four differently oriented plane slabs of Li₂SO₄·H₂O crystals all eight independent components of the nonlinear optical susceptibility tensor [d_{ijk}] for the fundamental wavelength λ = 1079.5 nm (Nd:YAP laser) were determined. In comparison to other polar properties of Li₂SO₄·H₂O the coefficients d_{ijk} are surprisingly small; they are one order of magnitude smaller than those of commonly used crystals for frequency conversion of laser light, such as KTiOPO₄, β-BaB₂O₄, LiB₃O₅ or BiB₃O₆. The

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