

## CONFERENCE PROGRAMME

**Saturday, September 23, 2000-09-05**

*Aula, Buliding A0 University of Mining and Metallurgy (AGH)*

**11.30:** Conference opening

**Chairman: M. Handke**

**11.45:** Opening lecture

L-1 *A. Müller*

PANDORA'S BOX REVERSED THROUGH CHEMISTRY: AESTHETIC BEAUTY AND NEW MATERIALS

**12.30:** L-2 *L. A. Nafie*

VIBRATIONAL CIRCULAR DICHROISM OF CHIRAL MOLECULES IN THE SOLUTION AND SOLID STATE

**13.05:** L-3 *K. Parlinski*

FIRST-PRINCIPLE CALCULATIONS OF VIBRATIONAL FREQUENCIES IN CRYSTALS

**14.00:** Lunch – *Cafeteria “Krakus”*

**Chairman: H. Ratajczak**

**15.30:** L-4 *E.H. Korte and A. Röseler*

INFRARED SPECTROSCOPIC ELLIPSOMETRY TO CHARACTERIZE ANISOTROPIC SURFACE LAYERS

**16.05:** L-5 *J. Mink*

VIBRATIONAL SPECTROSCOPIC STUDY OF SURFACES

**16.40:** Coffee break

**17.00:** L-6 *Z. Mielke*

APPLICATION OF MATRIX ISOLATION TECHNIQUE TO THE STUDIES OF PHOTOCHEMICAL REACTIONS

**17.35:** L-7 *J. Wilson*

FT-IR MICROSCOPE MAPPING

**CANCEL**

**18.10:** L-8 *M. W. Urban*

INFRARED/RAMAN CHEMICAL IMAGING AND 3-DIMENSIONAL ANALYSIS OF POLYMERIC MATERIALS

**18.15:** Welcome party

**Sunday, September 24, 2000**

11.00-18.00 Trip to Pieskowa Skała and Tyniec

19.00-21.00 **POSTER SESSION**, Cafeteria „Krakus”

**Monday, September 25, 2000**

*Lecture Hall, Building A-4 University of Mining and Metallurgy*

**Chairman: J.Mink**

**8.30:** L-9 *H. Ratajczak*

MOLECULAR HYDROGEN-BONDED CRYSTALS WITH NONLINEAR OPTICAL PROPERTIES: ROLE OF THE HYDROGEN BONDS

**9.05:** L-10 *S. Bratos and J.C. Leicknam*

EARLY TIME DYNAMICS OF HYDROGEN BONDS IN WATER

**9.40:** L-11 *A. M. Yaremko, H. Ratajczak, E.V. Mozdor and J. Baran*

THEORY OF THE PROFILES OF HYDROGEN STRETCHING INFRARED BANDS: FERMI – DAVYDOV RESONANCES IN HYDROGEN – BONDED CRYSTALS

**10.15:** O-1 *M. J. Wójcik*

DYNAMIC INTERACTIONS AND PROTON TUNNELING IN HYDROGEN-BONDED SYSTEMS

**10.35:** O-2 *T. Misiaszek and M. M. Szostak*

VIBRATIONS RECOGNIZED AS A SOURCE OF OPTICAL NONLINEARITY IN THE MOLECULE AND CRYSTAL OF 4-ISOPROPYLPHENOL

**10.55:** Coffee break

**Chairman: S.Turell**

**11.10:** L-12 *J. Baran*

POLARISED VIBRATIONAL STUDIES OF GLYCINE COMPOUNDS CRYSTALS

**11.45:** L-13 *A. Graja*

ELECTRONIC PROCESSES IN TTF - DERIVED COMPLEXES STUDIED BY IR AND NIR SPECTROSCOPIES

**12.20:** L-14 *G. Keresztury and B. Jordanov*

ENHANCING THE RELIABILITY OF VIBRATIONAL ASSIGNMENTS: MEASUREMENT AND CALCULATION OF TRANSITION MOMENT DIRECTIONS

**12.55:** L-15 *L. M. Proniewicz*

RESONANCE RAMAN TECHNIQUES TO STUDY  $\pi$ -CATION AND NONRADICAL SPECIES OF METALLOPORPHYRINS WITH METAL-OXO BOND

**13.30:** Lunch, Cafeteria “Krakus”

**Chairman: G. Keresztury**

**15.00:** L-16 *S. Kokot*

STUDIES OF POLYMERS BY VIBRATIONAL SPECTROSCOPY AND  
CHEMOMETRICS

**15.35:**L-17 *A.J. Barnes, J. Baran, J. Barycki, S. Debrus, H. Ratajczak, Z. Latajka, M. May  
A. Pietraszko*

STRUCTURAL AND VIBRATIONAL STUDY OF A NOVEL NONLINEAR  
OPTICAL MATERIAL: 3-NITROBENZOIC ACID HYDRAZIDE

**16.10:** O-3 *F. Sécheresse, E. Cadot and A. Dolbecq*

SULFUR IN POLYOXOANIONS, TOWARDS A NOVEL CLASS OF  
POLYMETALATES

**16.30:** O-4 *S. Quillard, M. I. Boyer, G. Louarn, B. Corraze, G. Froyer*

VIBRATIONAL CHARACTERISATION OF AN OLIGOANILINE :  
A MODEL COMPOUND OF POLYANILINE

**16.50:** *Coffee break*

**Chairman: J. Van der Mass**

**17.10:** L-18 *I. Gnatyuk, T. Gavrilko, G. Puchkovskaya, O. Yaroshchuk, H. Ratajczak,  
Yu. Goltzov, L. Matkovskaya, G. Peltl and K. Otto*

PHASE TRANSITIONS AND DYNAMICS OF LIQUID CRYSTALS IN  
NANOPOROUS MEDIA

**17.45:** L-19 *R.G. Zhibankov, S.P. Firsov, D.D. Grinshpan, J. Baran, M.K. Marchewka,  
H. Ratajczak*

VIBRATIONAL SPECTRA AND NONVALENT INTERACTIONS OF  
CARBOHYDRATE MOLECULES

**18.20:** O-5 *J. Ryzkowski*

CHELATE COMPOUNDS ADSORPTION ON INORGANIC OXIDES

**CANCEL 18.40:** O-6 *E.N. Shermatov*

SUPERCONDUCTING ENERGETIC SPLIT END VIBRATIONAL SPECTRUM

**Tuesday, September 26, 2000**

*Lecture Hall, Building A-4 University of Mining and Metallurgy*

**Chairman: A. Barnes**

**9.00:** L-20 *H. D. Lutz*

RAMAN AND INFRARED SPECTROSCOPIC STUDIES ON DECOMPOSITION  
OF SPINEL - TYPE SULFIDE SOLID SOLUTIONS

**9.35:** L-21 *C. Kinowski, S. Turrell, L. Hench, J.-M Nedelec and M. Bouazaoui*

STUDY OF THE KINETICS OF DENSIFICATION PROCESSES IN POROUS  
SILICA GELS USING RAMAN SPECTROSCOPY

**10.10:** *Coffee break*

**Chairman: S. Kokot**

**10.30:** L-22 *M. Handke*

VIBRATIONAL SPECTRA OF INORGANIC POLYMERS – SILICATES

**11.05:** O-7 *J. Datka and B. Gil*

HETEROGENEITY OF OH GROUPS IN HZSM-5 ZEOLITES  
*COMPARING OF MICROCALORIMETRIC AND IR RESULTS*

**CANCEL 11.25:** O-8 *W. Gadomski, and B. Ratajska-Gadomska*

RAMAN SPECTROSCOPY OF WATER CLUSTERS DURING THE SOL-GEL  
TRANSITION

**11.25:** O-9 *M. Kozanecki, J. Zientarska, J. Ulański*

*CONFOCAL MICRO-RAMAN INVESTIGATION OF MULTILAYER POLYMER  
COMPOSITES*

**12.05:** *Concluding remarks*

**13.00:** Lunch, Cafeteria “Krakus”