

Thursday, June 14<sup>th</sup>, 2007

7<sup>30</sup> - 9<sup>00</sup> Registration of participants

## MORNING SESSION

9<sup>00</sup> Opening of the Meeting

Chairpersons: S. Popović, I. Leban

## PLENARY LECTURE

Chairperson: M. Luić

9<sup>15</sup> – 10<sup>15</sup> C. Giacobazzo, A. Altomare, R. Caliendo, M. Camalli, C. Cuocci, A. G. G. Moliterni, R. Rizzi 1

*EXPO2007: A TOOL FOR CRYSTAL STRUCTURE SOLUTION  
AND REFINEMENT FROM POWDER DATA*

10<sup>15</sup> – 10<sup>35</sup> Coffee Break



## SHORT CONTRIBUTIONS

Chairpersons: B. Modec, S. Tomić

10<sup>35</sup> – 10<sup>55</sup> K. F. Fischer, A. Kirfel, H. Zimmermann 5

*HIGH RESOLUTION STRUCTURE DETERMINATION  
WITHOUT FOURIER INVERSION: SOME STEPS TOWARDS  
APPLICABILITY*

10<sup>55</sup> – 11<sup>05</sup> W. Gille 6

*INTERRELATIONS BETWEEN THE SECOND MOMENTS OF  
THE CHORD LENGTH DISTRIBUTIONS OF RANDOM TWO-  
PHASE SYSTEMS; - CONNECTIONS TO THE FIELD OF  
SMALL-ANGLE SCATTERING*

11<sup>05</sup> – 11<sup>25</sup> H. D. Flack 7

*USING AND UNDERSTANDING THE FLACK PARAMETER*

11<sup>25</sup> – 11<sup>35</sup> A. Meden 8

*SYNERGY BETWEEN POWDER CRYSTALLOGRAPHY AND  
QUANTUM CHEMISTRY – AN EXAMPLE*

11<sup>35</sup> – 11<sup>45</sup> L. H. Rees 9

*GEMINI – LEADING THE WAY IN MULTI-  
WAVELENGTH CRYSTALLOGRAPHY*



11<sup>45</sup> - 12<sup>00</sup> S. Petriček 9a  
*CRYSTAL STRUCTURES OF LANTHANIDE BROMIDE  
COMPLEXES WITH DIETHYLEN GLYCOL DIMETHYL ETHER  
[LnBr<sub>3</sub>(diglyme)L] (Ln = Gd, Ho)*


12<sup>15</sup> Welcome drink 

## AFTERNOON SESSION

### PLENARY LECTURE

Chairperson: S. Petriček

16<sup>00</sup> – 17<sup>00</sup> N. Tomašić, V. Bermanec, A. Gajović, M. Rajić Linarić 2  
*METAMICT MINERALS: INSIGHT INTO RELIC CRYSTAL  
STRUCTURES*

17<sup>00</sup> – 17<sup>20</sup> Coffee Break 

### SHORT CONTRIBUTIONS

Chairpersons: B. Prugovečki, P. Šegedin

17<sup>20</sup> – 17<sup>35</sup> P. Makreski, G. Jovanovski, B. Kaitner, A. Gajović 10  
*COMPLEMENTARY USE OF POWDER XRD AND  
VIBRATIONAL SPECTROSCOPY FOR IDENTIFICATION OF  
PYROXENE AND PYROXENOID MINERALS FROM  
MACEDONIA*

17<sup>35</sup> – 17<sup>45</sup> Ž. Žigovečki, V. Bermanec, M. Rajić Linarić 11  
*OVERGROWTH OF CARBONATE MINERAL PHASES WITH  
DIFFERENT CRYSTAL STRUCTURES FROM TREPČA, STARI  
TRG MINE, KOSOVO*

17<sup>45</sup> – 17<sup>55</sup> U. Kolitsch, F. Brandstätter 12  
*A NEW SALT-INCLUSION SULPHATE PHASE FROM A  
BURNING COAL DUMP: CRYSTAL-STRUCTURAL, CHEMICAL  
AND RAMAN-SPECTROSCOPIC CHARACTERISATION*

17<sup>55</sup> – 18<sup>05</sup> K. Matošević, D. Matković-Čalogović, D. Medaković 13  
*BIOMINERALS IN THE MUSSELS *Mytilus galloprovincialis* L.*

18<sup>05</sup> – 18<sup>15</sup> A. Jaklin, D. Medaković, Ž. Skoko, S. Popović, A. Borčić, D. M. Lyons 14  
*MINERAL COMPONENTS IN THE OPISTHOBRANCH  
GASTROPOD SHELL *APLYSIA* SPP.*

18 <sup>15</sup> – 18 <sup>25</sup>	<u>A. Jaklin</u> , H. Posilović, A. Borčić, D. Medaković, V. Bermanec	15
	<i>SEM INVESTIGATION OF THE MORPHOLOGY AND STRUCTURE OF THE OPISTHOBRANCH GASTROPOD SHELL APLYSIA SPP.</i>	
18 <sup>25</sup> – 18 <sup>30</sup>	Break	
18 <sup>30</sup> – 18 <sup>45</sup>	M. C. Burla, R. Caliendo, M. Camalli, B. Carrozzini, G. L. Casciarano, L. De Caro, <u>C. Giacovazzo</u> , G. Polidori, D. Siliqi, R. Spagna	16
	<i>IL MILIONE: A SUITE OF COMPUTER PROGRAMS FOR CRYSTAL STRUCTURE SOLUTION OF PROTEINS</i>	
18 <sup>45</sup> – 18 <sup>55</sup>	<u>Milan Melnik</u>	
	<i>ISOMERS IN THE CHEMISTRY OF TIN COORDINATION COMPOUNDS</i>	
18 <sup>55</sup> – 19 <sup>10</sup>	<u>A. Višnjevac</u> , M. Luić, B. Žinić	17
	<i>TAUTOMERIZATION OF 1-TOSYLCYTOSINE PROMOTED BY METAL COMPLEXATION</i>	
19 <sup>10</sup> – 19 <sup>25</sup>	<u>G. Pavlović</u> , Ž. Soldin, Z. Popović	18
	<i>MERCURY(II) COMPLEXES WITH QUINOLINE-2-CARBOXYLIC ACID</i>	
19 <sup>25</sup> – 19 <sup>35</sup>	<u>M. Cetina</u> , A. Nagl, L. Barišić, V. Rapić	19
	<i>CONFORMATION AND HYDROGEN BONDS IN BENZYL 1'-CARBOXY-1-FERROCENE-CARBAMATE MONOHYDRATE</i>	
19 <sup>35</sup> – 19 <sup>45</sup>	<u>A. Blagus</u> , B. Kaitner	20
	<i>CRYSTAL AND MOLECULAR STRUCTURE OF (N,N'-1,2-PHENYLENE-BIS(2-HYDROXY-1-NAPHTYLIDENE-IMINATO-κ<sup>2</sup>N,N'-κ<sup>2</sup>O,O'))-NICKEL(II)</i>	

**Friday, June 15<sup>th</sup>, 2007**

## MORNING SESSION

### PLENARY LECTURE

Chairperson: D. Matković-Čalogović

8 <sup>30</sup> – 9 <sup>30</sup>	<u>R. Kužel</u> , V. Cherkaska, Z. Matěj, M. Janeček, J. Čížek, M. Dopita	3
	<i>STRUCTURAL STUDIES OF SUBMICROCRYSTALLINE MATERIALS OBTAINED BY SEVERE PLASTIC DEFORMATION</i>	

9<sup>30</sup> – 9<sup>50</sup>

Coffee Break



## SHORT CONTRIBUTIONS

Chairpersons: G. Pavlović, A. Meden

9 <sup>50</sup> – 10 <sup>00</sup>	<u>I. Leban</u> , G. Giester, N. Lah	21
	<i>A NEW COPPER(II) BASIC SULFATE: POLY[3-AMINOPYRIDINIUM M<sub>3</sub>-HYDROXIDO-DI-M<sub>3</sub>-SULFATO-BIS[AQUASULFATOCOPPER(II)]]</i>	
10 <sup>00</sup> – 10 <sup>10</sup>	<u>N. Lah</u> , I. Leban	22
	<i>THE ASSEMBLY OF DINUCLEAR CU(II) ALKOXIDES TO FORM TETRANUCLEAR AND POLYNUCLEAR COMPOUNDS</i>	
10 <sup>10</sup> – 10 <sup>20</sup>	M. Čuskić, A. Golobič, <u>P. Šegedin</u>	23
	<i>CRYSTAL STRUCTURES OF [CuBr<sub>2</sub>(3-OHpy)<sub>2</sub>], 1 AND [CuBr<sub>2</sub>(3-OHpy)<sub>4</sub>], 2, 3-OHpy=3-HYDROXYPYRIDINE</i>	
10 <sup>20</sup> – 10 <sup>30</sup>	<u>K. Starič</u> , T. Menič, A. Golobič, P. Šegedin	24
	<i>CRYSTAL STRUCTURE OF [Cu<sub>2</sub>(O<sub>2</sub>CH)<sub>4</sub>(nia)<sub>2</sub>], nia=NICOTINAMIDE</i>	
10 <sup>30</sup> – 10 <sup>40</sup>	<u>N. Judaš</u> , D. Matković-Čalogović	25
	<i>PYRAZINE AS A DITOPIC LIGAND TO STEER THE MOLECULAR SELF-ASSEMBLY OF COPPER(II) B-DIKETONATE BUILDING BLOCKS</i>	
10 <sup>40</sup> – 10 <sup>50</sup>	<u>G. Jovanovski</u> , P. Naumov	26
	<i>ON THE ORIGIN OF THE OVERSHORT C–O BOND IN THE BINUCLEAR COPPER(II) IMIDAZOLE SACCHARINATO COMPLEX</i>	
10 <sup>50</sup> – 11 <sup>00</sup>	M. Jurić, <u>B. Perić</u> , N. Brničević, P. Planinić, D. Pajić, K. Zadro, G. Giester, B. Kaitner	27
	<i>SUPRAMOLECULAR CONTACTS BETWEEN DIAMAGNETIC AND PARAMAGNETIC [M(bpy)<sub>3</sub>]<sup>2+</sup> ENTITIES IN [M(bpy)<sub>3</sub>]<sub>2</sub>[NbO(C<sub>2</sub>O<sub>4</sub>)<sub>3</sub>]Cl·nH<sub>2</sub>O (M = Fe<sup>2+</sup>, Co<sup>2+</sup>, Ni<sup>2+</sup>, Cu<sup>2+</sup> AND Zn<sup>2+</sup>; n = 11, 12) COMPOUNDS</i>	
11 <sup>00</sup> – 11 <sup>10</sup>	Break	
11 <sup>10</sup> – 11 <sup>20</sup>	B. Modec	28
	<i>STRUCTURAL PROPERTIES OF OXOMOLYBDATES WITH GLYCOLATO LIGANDS</i>	

11 <sup>20</sup> – 11 <sup>30</sup>	B. Modec, <u>J. V. Brenčič</u>	29
	<i>STRUCTURAL PROPERTIES OF TWO MONONUCLEAR CITRATO MOLYBDATE COMPLEXES</i>	
11 <sup>30</sup> – 11 <sup>40</sup>	<u>M. Kasunič</u> , B. Modec	30
	<i>STRUCTURAL PROPERTIES OF A DINUCLEAR MOLYBDATE(VI) COMPLEX WITH DIANION OF 2-HYDROXY-2-PHENYL-3-NITROPROPANOIC ACID</i>	
11 <sup>40</sup> – 11 <sup>50</sup>	<u>N. Kitanovski</u> , A. Golobič, B. Čeh	31
	<i>STRUCTURES OF MOLYBDENUM(V) OXO COMPLEXES WITH BIS(3,5-DIMETHYLPYRAZOL-1-YL)ACETATE</i>	
11 <sup>50</sup> – 12 <sup>00</sup>	<u>M. Đaković</u> , Z. Popović, G. Giester	32
	<i>NICKEL(II) THIOCYANATE COMPLEXES WITH PYRIDINE MONOCARBOXAMIDES</i>	
12 <sup>00</sup> – 12 <sup>15</sup>	<u>A. Pevec</u> , M. Erčulj, S. Petriček, A. Demšar	33
	<i>CRYSTAL STRUCTURES OF THREE NEW ZINC PIVALATE COMPLEXES</i>	
12 <sup>15</sup> – 12 <sup>25</sup>	<u>E. Goresnik</u> , Z. Mazej, M. Tramšek, T. Bunič, B. Žemva	34
	<i>STRUCTURAL INVESTIGATIONS OF INORGANIC FLUORIDES CONTAINING POLY-HYDROGEN FLUORIDES OR HF MOLECULES COORDINATED TO METAL CENTER</i>	



### **14<sup>30</sup> (sharp) - MEETING EXCURSION**

#### **Zadar and Nin**

Archaeological Museum/St. Donatus' Church,  
St. Mary's Church "The Gold and Silver of Zadar",  
Sea Organs

Meeting point: in front of the Hotel

Light refreshments in the Arsenal

**20<sup>00</sup> – Return to the Hotel**




Saturday, June 16<sup>th</sup>, 2007

MORNING SESSION

PLENARY LECTURE

Chairperson: J. V. Brenčič

8<sup>30</sup> – 9<sup>30</sup> B. Kozlevčar 4  
*STRUCTURAL ANALYSIS OF COPPER(II) COORDINATION  
COMPOUNDS AND CORRELATION WITH THEIR MAGNETIC  
PROPERTIES*

9<sup>30</sup> – 9<sup>50</sup> Coffee Break 

SHORT CONTRIBUTIONS

Chairpersons: N. Lah, M. Cetina

9<sup>50</sup> – 10<sup>00</sup> T. Đorđević 35  
*CRYSTAL STRUCTURE OF M1CO(OH)(ASO<sub>4</sub>) (M1 = SR<sup>2+</sup>,  
CD<sup>2+</sup>), TWO NEW MEMBERS OF THE DESCLOIZITE AND  
ADELITE GROUPS*

10<sup>00</sup> – 10<sup>10</sup> K. Schwendtner, U. Kolitsch, E. Tillmanns 36  
*OCTAHEDRALLY COORDINATED ARSENIC SUBSTITUTING  
FOR M<sup>3+</sup> CATIONS – M<sup>1+</sup>M<sup>3+</sup><sub>2</sub>AS(HASO<sub>4</sub>)<sub>6</sub> VERSUS  
M<sup>1+</sup>M<sup>3+</sup>(HASO<sub>4</sub>)<sub>2</sub>*

10<sup>10</sup> – 10<sup>25</sup> M. Wierzbicka, U. Kolitsch, E. Tillmanns 37  
*FLUX SYNTHESIS AND CRYSTAL STRUCTURE OF THE  
NEW MIXED SILICATES NA<sub>4</sub>SR<sub>2</sub>M<sup>3+</sup><sub>2</sub>(Si<sub>2</sub>O<sub>7</sub>)(SiO<sub>4</sub>)<sub>2</sub> (M<sup>3+</sup> = Y,  
IN, SC)*

10<sup>25</sup> – 10<sup>35</sup> S. Bosnar, C. Kosanović, B. Subotić, D. Bosnar, N. Tomašić, Z. Kajcsos, P. Major, L. Lohonyai, L. Liskay, K. Lázár, K. Havancsák, P. Gordo 38  
*FREE-VOLUME STUDIES IN ALUMINOSILICATE CERAMICS*

10<sup>35</sup> – 10<sup>45</sup> J. Popović, B. Gržeta, E. Tkalčec, S. Kurajica 39  
*EFFECT OF COBALT DOPING ON ZINC ALUMINATE  
STRUCTURE*

10<sup>45</sup> – 10<sup>55</sup> K. Demšar, A. Meden, S. D. Škapin, D. Suvorov 40

<i>CRYSTAL STRUCTURE DETERMINATION OF CALA<sub>4</sub>TI<sub>4</sub>O<sub>15</sub></i>		
10 <sup>55</sup> – 11 <sup>05</sup>	<u>A. Gajović</u> , I. Djerdj, N. Tomašić, A. Šantić	41
	<i>STRUCTURE OF ZIRCONIUM TITANATE CERAMICS FOR HUMIDITY SENSORS</i>	
11 <sup>05</sup> – 11 <sup>15</sup>	<u>A. Šantić</u> , A. Moguš-Milanković, A. Gajović	42
	<i>ENVIRONMENT SENSITIVE ELECTRICAL CONDUCTIVITY OF ZIRCONIUM TITANATE CERAMICS</i>	
11 <sup>15</sup> – 11 <sup>25</sup>	Break	
11 <sup>25</sup> – 11 <sup>35</sup>	<u>G. Štefanić</u> , S. Musić, M. Ivanda	43
	<i>THERMAL BEHAVIOR OF THE AMORPHOUS PRECURSORS OF THE ZRO<sub>2</sub>-SNO<sub>2</sub> SYSTEM</i>	
11 <sup>35</sup> – 11 <sup>45</sup>	<u>M. Ristić</u> , S. Musić	44
	<i>FORMATION OF POROUS <math>\alpha</math>-FE<sub>2</sub>O<sub>3</sub> MICROSTRUCTURE BY THERMAL DECOMPOSITION OF FE(IO<sub>3</sub>)<sub>3</sub></i>	
11 <sup>45</sup> – 11 <sup>55</sup>	<u>M. Žić</u> , M. Ristić, S. Musić	45
	<i><sup>57</sup>FE MÖSSBAUER, FT-IR AND FE SEM INVESTIGATION OF THE FORMATION OF HEMATITE AND GOETHITE AT HIGH PH VALUES</i>	
11 <sup>55</sup> – 12 <sup>05</sup>	<u>T. Jurkin</u> , M. Gotić, S. Musić	46
	<i>SYNTHESIS OF MAGNETITE NANOPARTICLES BY THE <math>\gamma</math>-IRRADIATION OF WATER-IN-OIL MICROEMULSION</i>	
12 <sup>05</sup> – 12 <sup>15</sup>	<u>V. Novosel–Radović</u> , N. Radović, M. Balen	47
	<i>OXIDE SCALES AND HOT ROLLED STEEL STRIP</i>	
12 <sup>15</sup> – 12 <sup>25</sup>	<u>C. Kosanović</u> , B. Subotić, V. Svetličić, T. Mišić	48
	<i>MICRO-VESSELS FROM PSEUDOMORPHISM AFTER THERMAL TREATMENT OF CATION – EXCHANGED ZEOLITES</i>	
12 <sup>25</sup> – 12 <sup>35</sup>	F. Weitzer, H. Chen, <u>J. C. Schuster</u>	49
	<i>RIETVELD REFINEMENT OF THE TRICLINIC TERNARY PHASE CR<sub>4</sub>(AL,SI)<sub>11</sub></i>	
12 <sup>35</sup> – 12 <sup>50</sup>	<u>Ž. Skoko</u> , S. Popović, G. Štefanić	50
	<i>MICROSTRUCTURE OF AL-ZN AND ZN-AL ALLOYS</i>	
12 <sup>50</sup> – 13 <sup>00</sup>	<u>V. Ličina</u> , A. Moguš-Milanković, Ž. Skoko, S. T. Reis, D. E. Day	51
	<i>INFLUENCE OF CRYSTALLIZATION ON THE ELECTRICAL CONDUCTIVITY OF IRON PHOSPHATE GLASSES</i>	


13 <sup>00</sup> – 13 <sup>10</sup>	F. van Meurs	Bruker AXS	52
	<i>RECENT ACHIEVEMENTS IN THE DEVELOPMENT OF SINGLE CRYSTAL DIFFRACTION SOLUTIONS</i>		

## AFTERNOON SESSION

### SHORT CONTRIBUTIONS

*Chairpersons: N. Kitanovski, A. Višnjevac*

15 <sup>30</sup> – 15 <sup>50</sup>	<u>M. Jaskolski</u> , O. Pasternak, M. Sikorski, G. Bujacz	53
	<i>CRYSTAL STRUCTURE OF PLANT HORMONE-BINDING PROTEIN IN COMPLEX WITH ZEATIN</i>	
15 <sup>50</sup> – 16 <sup>00</sup>	<u>S. Tomić</u> , I. Dokmanić	54
	<i>DIVALENT METAL CATIONS IN PROTEINS: ABUNDANCE, COORDINATION, FUNCTION</i>	
16 <sup>00</sup> – 16 <sup>15</sup>	<u>M. Luić</u> , Z. Štefanić, D. Vujaklija	55
	<i>STRUCTURAL CHARACTERIZATION OF THE STREPTOMYCES COELICOLOR SINGLE-STRANDED DNA-BINDING PROTEIN</i>	
16 <sup>15</sup> – 16 <sup>30</sup>	<u>K. Lewiński</u> , K. Kurpiewska, J. Font, M. Ribó, M. Vilanova	56
	<i>CRYSTALLOGRAPHIC STUDIES ON STRUCTURAL STABILITY OF RNASE A VARIANTS</i>	
16 <sup>30</sup> – 16 <sup>40</sup>	<u>B. Prugovečki</u> , D. Matković-Čalogović	57
	<i>CRYSTAL AND MOLECULAR STRUCTURE OF THE BROMO INSULIN DERIVATIVE AT ROOM TEMPERATURE</i>	
16 <sup>40</sup> – 16 <sup>50</sup>	<u>D. Milić</u> , D. Matković-Čalogović, T. V. Demidkina, A. A. Antson	58
	<i>DISCRETE DISORDER OF A WHOLE PROTEIN DOMAIN IN THE CRYSTALS OF TYROSINE PHENOL-LYASE</i>	
16 <sup>50</sup> – 17 <sup>00</sup>	<u>A. Vujičić-Žagar</u> , T. Pijning, S. Kralj, W. Eeuwema, L. Dijkhuizen, B. W. Dijkstra	59
	<i>THE FIRST CRYSTAL STRUCTURE OF THE GLYCOSIDE HYDROLASE FAMILY 70 GLUCANSUCRASE GS180-ΔN FROM LACTOBACILLUS REUTERI</i>	

17 <sup>00</sup> – 17 <sup>15</sup>	Coffee Break		
17 <sup>15</sup> – 17 <sup>25</sup>	<u>D. Matković-Čalogović</u> , K. Užarević, I. Đilović, M. Cindrić		60
	<i>FLEXIBLE SUPRAMOLECULAR HOST FOR TRIGONAL ANION GUESTS</i>		
17 <sup>25</sup> – 17 <sup>35</sup>	<u>Z. Štefanić</u> , V. Tomašić		61
	<i>SIMPLIFIED REPRESENTATION OF CRYSTAL STRUCTURES: CHOLIC ACID HOST FRAMEWORKS AS A CASE STUDY</i>		
17 <sup>35</sup> – 17 <sup>45</sup>	<u>D. Cinčić</u> , T. Friščić, W. Jones		62
	<i>ISOSTRUCTURAL HALOGEN-BONDED COCRYSTALS VIA STRUCTURALLY EQUIVALENT DONORS AND ACCEPTORS</i>		
17 <sup>45</sup> – 17 <sup>55</sup>	<u>M. Devčić</u> , A. Kwokal, M. Horvat, E. Meštrović, A. Danilovski		63
	<i>NOVEL FORM OF CELECOXIB</i>		
17 <sup>55</sup> – 18 <sup>05</sup>	<u>D. Šišak</u> , E. Lekšić, E. Meštrović		64
	<i>CRYSTAL FORM OF LAMOTRIGINE AND LAMOTRIGINE – SUCCINIC ACID DMSO SOLVATED COCRYSTAL</i>		
18 <sup>05</sup>	<b>Closing remarks</b>		
		<i>Chairpersons: I. Leban, S. Popović</i>	

20<sup>00</sup> **MEETING DINNER**  
All participants and accompanying persons  
are cordially invited

