21stEUROPEANCRYSTALLOGRAPHIC MEETING

DURBAN, SOUTHAFRICA, 24-29 AUGUST 2003

SecondAnnouncement--Callforpapers

Main Conference Information (website: www.sacrs.org.za/ecm21)

YouarecordiallyinvitedtoattendECM-21inDurba

ECM-21 will be held 1 km from the beachfront at the International Convention Centre (ICC) in Durban, in the heart of the Zulu kingdom, Kwazulu-Natal. For the first time an ECM will convene in South Africa -- and indeed Africa. The South African currency (ZAR; South African Rand; 1Euro ca. ZAR9) strongly favours tourism and the conference fees are modest. Participants should at worst not pay more than for a typical ECA meeting at a European destination. Interested participants are encouraged to contact Conference Call (confcall@yebo.co.za) or André Roodt (aroo@rau.ac.za).

Organising Committee

André Roodt (Chairman), RAU, Johannesburg Dave Billing, WITS, Johannesburg Demi Levendis, WITS, Johannesburg Thomas auf der Heyde, TWR, Johannnesburg Susan Bourne, UCT, Cape Town Luigi R. Nassimbeni, UCT, Cape Town Jan Dillen, US, Stellenbosch Gert J. Kruger, RAU, Johannesburg Jan C.A. Boeyens, UP, Pretoria Johan de Villiers, UP, Pretoria Gert Kruger, UN, Durban Paul Boucher, CSIR, Pretoria Åke Oskarsson, LU, Lund, Sweden Jacek Groshowski, JU Krakow, Poland Claude Lecomte, ECA & UHP Nancy, France Manuel Fernandes, WITS, Johannesburg Dave Liles, UP, Pretoria

Programme Committee

Jan Boeyens (Chairman), South Africa Paul Beurskens, Netherlands Mino Caira, South Africa Johan de Villiers, South Africa Eleanor Dobson, United Kingdom Karimat El-Sayed, Egypt Giovanni Ferraris, Italy Gastone Gilli, Italy John Helliwell, United Kingdom Sven Hofmoeller, Sweden Ted Janssen, Netherlands Mikhail Kovalchuk, Russia Gert J. Kruger, South Africa Demetrius Levendis, South Africa Finn Krebs Larsen, Denmark Claude Lecomte, France Eric Mittemeijer, Germany Luigi Nassimbeni, South Africa Alain Polian, France Andreas Roodt, South Africa Trevor Sewell, South Africa Ton Spek, Netherlands Abelmalek Thalal, Morocco Pam Thomas, United Kingdom Peet van Rooyen, South Africa Chick Wilson, United Kingdom Andrew Venter, South Africa Svetlana Zheludeva, Russia Xiaodong Zou, China

Weather & Tourist Attractions

Spring starts in South Africa at the end of August, and temperatures are very mild (min/max: 10 - 25 °C) in Durban (subtropical city). Special visits to game parks are planned, as well as normal pre- and post-conference tours that will be available to experience South Africa's wealth of wild-life (& the big FIVE!), plant diversity and mineralogical phenomena. (Further information, see website & below)

Important Note

Late winter / early spring is a very good time of the year to view game. ALL participants will be treated to a one day excursion (Friday 29 Aug) *INCLUDED IN CONFERENCE FEE*, to a Game Park, replacing the normal midweek excursion. Scientific programme will thus run non-stop for four days (25-28 Aug).

Preliminary Programme

Sunday, 24 Aug: Registration/Welcome Mon-Thu (25-28 Aug): Scientific Programme Thursday Eve (28 Aug): Closure & Dinner Friday, 29 Aug: Game Park Visits

Important Dates & Deadlines

Applications: Financial Assistance: 28 February 2003
Details: www.sacrs.org.za/ecm21
Abstract submission: 31 March 2003

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Early bird Registration: 30 April 2003
Accommodation: 15 July 2003
Deadline: Registration: 15 July 2003

Scientific Programme:

(a) Plenary Lectures: Eight sequential lectures by experts covering a wide selection of topics (confirmed, see below).

(b) Micro-symposia & Posters (See Below): The scientific programme is divided in five parallel sessions addressing Five FOCUS AREAS: i.e., [F1] Biological and Macromolecular Crystallography, [F2] Materials and Minerals, [F3] Experimental and Computational Techniques, [F4] Chemical Crystallography, [F5] Special techniques. These Focus Areas will also be covered by *Poster Sessions*.

Abstracts

One page Abstracts in English are invited covering all aspects of crystallography and closely related fields of interest: (i) For micro-symposia and topics see Programme below. (ii) Online submission via website (www.sacrs.org.za/ecm21) -- submission by 31 March 2003. (iii) With submission <u>please indicate under which micro-symposium / topic the Abstract is submitted</u>, e.g., F56 indicates topic of 'Polymorphism' with Chair & co-chair Bernstein & Caira. **Please Note**: Small changes in the programme, dependent on the number of Abstracts received for different micro-symposia, may occur.

Exhibitors

Excellent venue to ensure maximum interaction with delegates & reasonable rates -- information & arrangements based on ECA recommendations via website (www.sacrs.org.za/ecm21). Information: confcall@yebo.co.za

Registration & Accommodation

Electronically – request documents from conference organisers: confcall@yebo.co.za or, download from website

(www.sacrs.org.za/ecm21) **or** fax Registration Form given below.

Travel Arrangements: via Internet.

Booking flights using South African Travel agents will result in significant saving on flights from Europe. The official Travel agent of ECM-21 is ASTRA/ SURE Travel. Block bookings by e.g., student groups, can result in even larger savings.

<u>Detailed Information</u>: Johan le Roux: Tel. +27-51-4476352: Fax: +27-51-4476665; **johanlr.astraho@galileosa.co.za**

The Organizing Committee of ECM-21 shall observe the basic policy of nondiscrimination and affirms the rights of scientists throughout the world to adhere or to associate with international scientific activity without restrictions based on nationality, race, color, age, religion, political philosophy, ethnic origin, citizenship, language, or sex, in accordance with the Statues on the International Council of Scientific Unions. At this meeting (or symposium etc) no barriers will exist which would prevent the participation of bona fide scientists.

Programme:

A.PlenaryLectures

| Tom Blundell | Structural biology of multiprotein complexes involved in cell signalling. | Robert McGreevy | Measuring and modelling atomic and magnetic disorder in crystals |
|------------------|---|-----------------|---|
| Ted Janssen | Quasicrystals | Bill David | Structure determination from powders - crossing the 100-atom threshold. |
| Emil Makovicky | The wonderful world of crystal structures of sulfosalts | Wim Hol | Drug targets in tropical diseases |
| Gilberto Artioli | Tools for mineralogical crystallography | Yu. A. Ossipyan | Space materials research. Present status and perspectives |

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| D.IVI | B.Micro-symposia(Chair/co-chairindicated)[NOT ENUMBERING:e.g.,F56indicates'Polymorphism'Cha ir/co-chairBernstein&Caira] | | | | | | | | |
|-------|---|-------------------------------------|---|--|--|--|--|--|--|
| | [F1]: Macromolecular and | []F2]: Materials and Minerals | [F3]: Experimental and Computational | [F4]: Chemical Crystallography | [F5]: Special techniques | | | | |
| | Biological Crystallography | | Techniques | | | | | | |
| 1 | Crystallisation | New developments in the structure | Electron crystallography and real | Synergy of experiment and theory in studies of | Powder diffraction in applied and industrial | | | | |
| | | determination of quasicrystals | structures | charge, spin and momentum densities | mineralogy | | | | |
| | T. Bergfors / T Unge | G. Chapuis / W. Steurer | S. Hovmöller / I. Dodony | P. Becker / C. Gatti | J. de Villiers / I. Madsen | | | | |
| 2 | Synchrotron radiation and | Electron crystallography on beam | High photon energy techniques | Impact of charge and spin density studies on | Fast diffraction - high energy and high | | | | |
| | radiation damage | sensitive samples | | molecular sciences | throughput powder diffraction | | | | |
| | E. Garman / M Weik | U. Kolb / C. Kübel | ?? / P. Suortti | F.K. Larsen / N. Ghermani | R. Dinnebier / S. Verryn | | | | |
| 3 | Structure refinement and analysis | Electron crystallography on | Grazing angle techniques | Rooted in nature: compounds -chirality, | Materials for energy storage and the | | | | |
| | | inorganic materials | | absolute structure, absolute configuration | environment | | | | |
| | ?? / G. Murshudov | ?? / M. Gemmi | J Daillant / G. Fragneto | J. Grochowski / T. Auf der Heyde | L Nazar / ?? | | | | |
| 4 | Atomic resolution | Mineralogical mrystallography | Automatic structure determination: | Towards the unification of shared-proton | Structure determination from powder | | | | |
| | | | Challenges for the future | interactions | diffraction data | | | | |
| | C. Jelsch / V. Lamzin | T. Balic-Zunic / S. Krivovichev | A.L. Spek / D. Billing | G. Gilli / L. Nassimbeni | L. McCusker / G.J. Kruger | | | | |
| 5 | Proton and electron transfer | Modular aspects of inorganic | Can modern programming languages | Molecular interactions at extreme conditions | Joint powder diffraction and non-diffraction | | | | |
| | processes | crystals – in memory of Boris B | and techniques lead to higher reliability | | techniques | | | | |
| | | Zvyagin | and programmer productivity? | | | | | | |
| | M.A. Carrondo / S. Mc Sweeney | S. Merlino / M. Nespolo | L. Cranswick / J. Dillen | E. Boldyreva / G. Hearne | K. Shankland / C. Frampton | | | | |
| 6 | HIV/ AIDS (Infectious diseases) | From minerals to materials science | Diffraction image processing and data | Inclusion compounds and intercalates: | Polymorphism | | | | |
| | | | quality | Structure and application | | | | | |
| | A. Wlodawer / T. Sewell | E. Scandale / J. Kreisel | E. Dodson / S. Parsons | S. Bourne / S. C. de Sanctis | J. Bernstein / M. Caira | | | | |
| 7 | Large systems | Relaxor ferroelectric materials | Algorithms of the future | Structure-properties relationship in molecular | Use of synchrotron and neutron powder | | | | |
| | | | | crystals | diffraction | | | | |
| | A. Yonath / ??? | P. Thomas / ?? | D. Watkin / S. Urzhumtsev | C. Wilson / D.C. Levendis | A. Hewat / A. Fitch | | | | |
| 8 | Enzyme catalysis | Charge/orbital ordering in strongly | High resolution X-ray diffraction at new | Core chemical crystallography | Indexing powder diffraction patterns: | | | | |
| | | correlated electron systems | European SR sources | | Opportunity for new heuristic and global | | | | |
| | | | | | optimisation methods | | | | |
| | G. Dodson / R. Hilgenfeld | P. Bordet / A. Guehria- Laidoudi | M.V. Kovalcuk / B. Capelle | F. Lahoz / J. Rutherford | R. Shirley / C. Rademeyer | | | | |
| 9 | Transcription and translation | Crystallography in Africa | Crystallography at extreme conditions: | From structural knowledge to chemical | Time resolved spectroscopy | | | | |
| | | | recent results and new developments | reactivity | | | | | |
| | A. Liljas / ?? | A. Thalal / G. Kamau | J.P. Itié / M. Catti | C. Mealli / P.H. van Rooyen | ?? / S. Techert | | | | |
| 10 | Molecular recognition in | Perovskites ancient and modern - in | Crystallisation techniques frontier | Structural applications in coordination | Spectroscopy - an approach to local | | | | |
| | molecules and macromolecules | memory of Helen D Megaw | | complexes | structure | | | | |
| | ?? / C. Kenyon | M. Glazer / P. Boucher | N. Chayen / H Einspahr | A. Roodt / P. Comba | E. Libowitzky / A. Beran | | | | |

Satellite Meetings: To ensure maximum attendance all aspects of crystallography will be adequately covered by the ECM programme. Only two satellite meetings are scheduled:

(a) Neutron Diffraction:

(b) Indaba4

21-22 August at Centurion/ Pretoria with visits to the Safari-1 research reactor at Pelindaba. Organised by Chick Wilson (C.C.Wilson@rl.ac.uk) & Andrew Venter (amventer@aec.co.za).

The fourth in the multidisciplinary Indaba series of the Structural Chemistry Commission of the IUCr. This meeting takes place at Skukuza, in the Kruger National Park, 17-22 August 2003 -- Attendance limited to about 120 delegates. Theme for Indaba4: 'Patterns in Nature'. Enquiries to Peet van Rooyen: pvrooyen@scientia.up.ac.za: www.sacrs.org.za/indaba4

Workshops: Three workshops are scheduled, free of charge, on a first come first serve basis. These will be full-day workshops and will run in parallel on Sunday, 24 Aug 2003. Please reserve place via email to confcall@yebo.co.za -- Further detail on website (An additional workshop or two, based on substantial delegate interest might be included – consult website on regular basis for updated information)

Title and Coordinator **Participants** 40

70

40

- 1. Cambridge Structural Database (F Allen: UK; allen@ccdc.cam.ac.uk)
- 2. Single Crystal and Powder Diffraction Software Workshop (L Cranswick: UK; l.m.d.cranswick@ dl.ac.uk)
- 3. Introduction to Protein Crystallography (E Dobson: UK; ccp4@ysbl.york.ac.uk)

REGISTRATIONFORM

21st European Crystallographic Meeting, Durban, South A frica,24-29August2003 ElectronicversionsofThisRegistrationFormcanb edownloadedfromthewebsiteorrequestedelectron icallyfromConferenceCall PleasereturnthisformtotheConferenceOrganiser Secretariatuseonly CONFERENCECALLSOUTHAFRICA Tel:+27312662384 Reg.No PostnetSuite29,PrivateBagX3 Fax:+27312662380 Westville, Durban, 3630 E-mail: confcall@yebo.co.za **PARTICIPANTATTENDANCEINFORMATION** Note: Please contact your nearest South African Embassy forVisainformation Pleaseprovideinformationasyouwishittoappear onvourbadgeandinthelistofparticipants.A copyofthis ONEPAGE registrationform shouldbecompletedfor <u>eachactiveparticipant</u>.PleasecompleteonyourPCorTypewriterorbyw ritinginblockletters Title:Mr/Ms/Dr/Prof FamilyName/Surname Address: FirstName PresentPosition Institution/Organisation State: Phone Country: Fax Code: E-mailaddress ACCOMPANYINGPERSON/SPOUSE(Notparticipatingin themeeting) FamilyName/Surname FirstName SPECIALDIETARYREQUIREMENTS:(PleaseSpecify) Other(pleasespecify) Halaal Vegetarian SOCIALFUNCTIONSINCLUDEDINTHEREGISTRATIONFEE(Pleaseindicateifyouwillattendthefollowingso cialfunctions) ClosingBanquetDinner(28/8/02) DayTourtoGameReserveforSafari(29/8/03) WelcomeCocktailReception(24/8/03) **CAPACITYINWHICHATTENDINGTHEMEETING:**(Indicate One) Fullparticipant Student AccompanyingPerson/Spouse REGISTRATIONFEES:PricesQuotedin **EURO, PERPERSON** Paidonorbefore30April2003: After30April2003 1.ParticipantRegistration 310.00 370.00 75.00 120.00 2.Students 100.00 130.00 3.Accompanyingperson/spouse ck&bag,refreshmentbreaksoneachday,2specia leveningevents/socialfunctionsincluding Costincludesentrancetosessions, registration pa entreandbackagaineachday $and transport from official hotel stocon ference \\ c$ dinner, day tour to agamere serve including lunch, ECIALEVENTS, AREEXCLUDEDANDAREFORYOURÓWNACC LUNCHES/DINNERSDURINGTHECONFERENCE, EXCEPTATSP OUNT. CANCELLATIONNOTICE: 70% of Registration fees will be payable if cancellation and the control of ellationisreceivedAFTER31July2003. **REGISTRATION PAYMENT METHOD -- Pleaseindicate** Banktransfer CashonArrival Creditcardonarrival Toqualifyfordiscountedregistrationfee,please arrangefordirectbanktransfer/draftintotheC onferencea/c(detailsoverleaf) HOTEL RESERVATION REQUEST (Attached is a list of hotels with rates quoted in EURO) -- In order to qualify for the discounted rate, all reservation requests must be sent to Conference Call. Accommodation is assigned based on the information furnished on this form on a first-come first-served basis. Credit card information is requested in order to guarantee your reservation, and deductions may be made 5-7 days prior to arrival. If you do not have a credit card, then full prepayment for your hotel reservation will be required 2 weeks prior to arrival and deposited into the conference account. If you do not occupy your room by check-out time of the day following your confirmed check-in date, the room will be released and the non-occupancy night charged to your credit card. Modifications or cancellations must be made in writing to Conference Call SA. 2ndchoice PreferredHotel:1 st choice Requirements: SingleRoom Double/TwinRoom(2personssharing) Ifsharingwithwhom DateofArrival: August2003 DateofDeparture August2003 **HOTELPAYMENTMETHOD--**Pleaseindicate Banktransfer CashonArrival Creditcardonarrival

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HOTELOPTIONSANDSPECIALNEGOTIATEDRATES(FORYOU ROWNACCOUNT)

AllratesquotedareinEURO,perperson,pernight inclusiveofBed&Breakfast&GovernmentTourism Levy

| Name of Hotel Rating | | Description; ICC = Conference Centre | Rate € pp/day bed & breakfast | |
|-------------------------|------|--|-------------------------------|---------|
| | | | Single | Sharing |
| Hilton Durban | **** | Upmarket & modern, conveniently next door to the ICC, 1 min walk | 94.00 | 60.00 |
| Royal Hotel Durban | **** | In the City Centre, 1 minute drive from the ICC, 5 star service & facilities | 80.00 | 57.00 |
| Riverside Hotel | **** | Upmarket, modern, overlooking River & Sea, 5 minutes drive to ICC. | 71.00 | 55.00 |
| Holiday Inn North Beach | *** | Modern hotel, on upmarket North beach overlooking ocean, 5 min drive to ICC | 75.00 | 54.00 |
| City Lodge Durban | *** | Limited services, modern hotel, within walking distance from the ICC | 63.00 | 50.00 |
| Tropicana Hotel | *** | Full service hotel on South beach, overlooking ocean, 5 min drive from ICC | 60.00 | 48.00 |
| Beach Hotel | ** | On Beachfront, older hotel with basic furnishings, 5 minute drive from the ICC | 50.00 | 42.00 |
| Protea Hotel | ** | Student accommodation (Fourpersonssharinglargedormitorytyperoom) | | 20.00pp |

PAYMENTTERMS&CONDITIONSFORYOURRESERVATION

1. Pleaseprovideus with credit card details. The "Conference Call" will appear on your credit cards tatement. If this is not acceptable, please advise your card to be deducted ONARRIVAL at the hotel for the full amount due. Receipts will be is sued at the entrangements for entrangements for byour card to be deducted ONARRIVAL at the hotel for the full amount due. Receipts will be is sued at the entrangement of the full amount due. Receipts will be is sued at the entrangement of the full amount due. The full amount due are the fu

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HOTELCANCELLATIONPOLICY: HotelReservationscancelled:

(i) 30 dayspriortoarrival, **INWRITING**, will be accepted without penalty. (ii) 16-29 days priortoarrival, will be liable topay a 25% canc ellation penalty of the Total Reservation Amount; (iii) 0-15 days prior to arrival, will be liable topay a 100 % cancellation penalty of the Total Reservation Amount.

NOTES: RATESMAYINCREASEBYEURO5.00PERPERSON.PERNIG HT.PENDINGFOREIGNEXCHANGEFLUCTUATIONS

(i) All rates quoted are PER PERSON, PER NIGHT, inc making accommodation selection; (iii) No personal c booking agents.

Iuding bed and breakfast; (ii) Attention should be heques accepted; (iv) Rates negotiated and nett; no n-commissionable to other travel or n-commissionable travel or n-commissiona

<u>AIRPORTTRANSFERS(foryourownaccount</u>: €20.00(euro)perperson,returnairporttransfer(airport–hotel–airport) to Conference Call as soon as they are available.

PLEASE USE YOUR CONFERENCE REGISTRATION NUMBER AS A REFERENCE WHEN CORRESPONDING WITH CONFERENCE CALL'S OFFICES. THIS WILL BE COMMUNICATED TO YOU ON RECEIPT OF THE COMPLETED REGISTRATION & ACCOMMODATION BOOKING FORM.

<u>PRE/POST OR ACCOMPANYING PERSONS TOURS (for your own account)</u>: For further information or to make a tour reservation please contact DHM Tours directly on <u>dhmtours@iafrica.com</u> or visit their website on <u>www.dhmtours.co.za</u>. A description of recommended tours will be listed on the conference website shortly – some examples are given below – **Typical Prices in Euro**; i.e: € 22 = 22 euro. Tour bookings can also be done on ARRIVAL at the Tours desk

- 1. Durban City Tour Half day; € 22 pp. A day filled with excitement and adventure! An opportunity to discover South Africa's holiday Mecca.
- 2. Durban Wildlife Tour 09h00 to 15h00; € 33 pp (Incl. lunch). Combines tranquility of bird life and the intrigue of the ocean's most awesome predator, the shark.
- 3. Valley of 1000 Hills Half day; € 29 pp (excludes lunch). Travel inland exploring the majestic and seemingly never-ending rolling hills typical of KwaZulu Natal.
- 4. Midlands Meander Full day € 59 pp (Incl. lunch). Art studios, country hotels, tea gardens, pottery, weaving workshops, via spectacular Howick Falls.
- Hluhluwe Game Reserve Full day € 75 pp. (Fully inclusive of open game drive and lunch). Travel along the scenic North Coast towards beautiful Hluhluwe/Umfolozi Game Reserve, famed for its rhino conservation and also a haven for the "Big 5".

Longer Tours: For further detail contact DHM Tours.

- 6. Drakensberg Experience 2 Day / 1 Night, € 170 pp (Fully inclusive).
- 9. Kruger Swazi Wild Life 6 nights / 7 days; € 790 pp sharing.
- The "Big 5" Wildlife Tour 1 night / 2 days, € 190 pp (Fully inclusive).
- 10. Cape Experience 3 nights / 4 days; € 510 pp. Does not incl. flight (approx € 220 pp).
- 8. The "Big 5" Wildlife Tour 2 night / 3 days, € 295 pp (Fully inclusive).

WELOOKFORWARDTOWELCOMINGYOUINDURBAN-AGATE WAYTOSOUTHERNAFRICA

Since being sighted by Vasco da Gama in 1497, Durban's natural harbour has given birth to a vibrant, go-ahead and ever changing city. Apart from having the busiest harbour in Africa, Durban is served by its **own international airport** only 15 minutes from its Central Business District Durban is an ideal base from which to explore the beauty and splendours of Southern Africa. Within two hours you could be on a safari at one of the country's renowned **game reserves** - home to some of the world's rarest and most exotic species - or you could be in the **fairest Cape**. Ninety minutes by road and you could be hiking or trout fishing in the magnificent **Drakensberg**. **Other options:** a day or two away could put you at the origins of man in the **Sterkfontein Caves**, or in the midst of a miraculous flower transformation in the **Namaqualand Desert**. You could be etching into memory the glorious sunsets and camp fires of the **Kruger and other National Parks in South Africa**, visit neighbouring Zimbabwe to witness the majesty of the **Victoria Falls**, game parks of **Botswana** or Skeleton Coast in **Namibia**.

There are many faces to Durban - city of great beauty and cultural diversity where you can witness the Dance of the Virgins, a Zulu war dance and attend a performance of the ballet or Opera all in the same day. The only constant is the famous South African weather - and Durban can serve up the best of it, with an average of **320 sunny days** a year. A surfer's paradise and international holiday mecca. Mile upon mile of unspoiled, sun-soaked beaches, bronzed life guards and bikini beauties. Seagulls, pelicans and exotic birds. Colourful rickshas, beautiful parks, sidewalk cafes and restaurants. Here architecture encapsulates the diverse histories and cultures of the people. Graceful Victorian buildings, exotic temples and dignified mosques all stand side by side.