

# ANNUAL REPORT FOR THE PERIOD 1 January 2007 to 31 December 2007

## 1. Executive Summary

Members of the South African Crystallographic Society have been actively involved in the International Union of Crystallography (IUCr) and European Crystallographic Association (ECA) commissions, local and internal conferences, academic teaching, running training courses and workshops and interacting with industry in an advisory capacity. The relatively small society, with fewer than 100 members, many of whom are students, has also been committed to furthering scientific research, with an admirable number of publications in refereed journals.

South African members have contributed significantly to Union activities and have participated in several international conferences. Five South Africans are currently members of IUCr Commissions (listed under item 2 below). Prof. Susan Bourne continues as the ECA councillor for SA. SACrS members, including a number of students, attended more than ten different international conferences and workshops. Among the most important of these were the School on Crystal Engineering in Erice, Italy (June 2007), the Carman National Physical Chemistry Symposium in Cape Town (September 2007), the S A Chemical Institute Inorganic Conference in Langebaan in July 2007 and the European Crystallographic Meeting in Marrakech, Morocco (August 2007). Prof Bourne attended the ECA Council meeting which was held at the ECM.

The National Committee and the executive of SACrS are acutely aware of the need to build the capacity of this specialised area of science in the country, and it is a task that has been taken up almost exclusively by academics at a small number of SA universities. They are doing everything to the best of their ability to train crystallographers, attract black and female students to the science, and support participation in international conferences. Promoting the attendance of conferences by students plays an important role. Over 20 students attended the ECM in Morocco and the Carman Symposium in Cape Town while smaller numbers each attended the Crystal Engineering School in Italy and the Powder Diffraction Workshop in Johannesburg. Student participation has been supported almost entirely by the supervisors' research grants (NRF, University and other grants). The SA universities that are making the major contributions in crystallography and related research presently have about 60 post-graduates in training. More than 20 additional post-graduate students who are using the experimental and computational methods of the field receive training through course work. Recent initiatives have seen two new diffractometers installed at the Universities of the Witwatersrand and Free State.

There are a number of female scientists active in the union or society, productively teaching crystallography at both undergraduate and post-graduate levels: Prof Susan Bourne (University of Cape Town: former president of SACrS and current chair of the national committee), Dr. Catharine Esterhuysen and Dr Delia Haynes (both at University of Stellenbosch); Dr. Melanie Rademeyer (UKZN); Dr. Sabine Verryn (University of Pretoria) and Dr. Ayesha Jacobs (Cape Peninsula University of Technology) to name but a few. The National Committee agreed in 2004 to nominate new members to improve the scope of representation. Dr Catharine Esterhuysen was the first "capacity-building nominee" in 2004; her status as a researcher is now so well established that she is the current deputy-chair of the committee. Dr Ayesha Jacobs and Mr Siyanda Lubhelwana are the current capacity-building representatives on the committee. The composition of the national committee has changed substantially over the past 5-7 years.

Gender equity has been successfully addressed, while equity in terms of race is an ongoing challenge. However, the profile of graduate students currently being trained in crystallographic theory and techniques is an encouraging sign.

SACrS has supported a number of workshops and symposia (listed in the table below). Two companies dealing with diffraction equipment, BRUKER and PanAlytical, have also had a long term association with the SA Crystallographic Society. They regularly invite SACrS members to present talks at their functions and support the SACrS events.

The high standard of the scientific output from society members is remarkable. Although exact figures could not be obtained, over 100 publications in international, refereed journals (not including conference proceedings) were produced in 2007. A selected list is attached. In addition, at least 70 presentations were made at local and international conferences.

The services and expertise of the SA Crystallographic Society are also of use to both the academic and industrial sectors of the SA community. The crystallographic services provided, primarily by 8 SA universities, have been invaluable to SA chemistry departments (as well as other disciplines). Services that have been provided include x-ray diffraction data collection and crystal structure solution (single crystals), characterization of polymorphism and phase transformations and distribution of the Cambridge Structural Database. WITS, the National Affiliated Centre, distributes the database to other African countries such as Ivory Coast and Senegal. Local (and international) pharmaceutical companies, fine chemical industries and mining companies benefit from the research and specialist knowledge of SA crystallographers and structural/solid-state chemists. There is an increasing participation of biochemists, biologists and medicinal scientists.

In conclusion the South African Crystallographic Society is a small but vibrant society that has a considerable involvement in international organizations and conferences, makes a remarkable scientific output, and plays an essential role in supporting science and technology in Southern Africa.

Headings	Activities completed- January to December 2007		Activities planned- January to December 2008
2. Background & Composition of National Committee	The National Committee is approved by the SA Crystallographic Association (SACrS): It comprises the president of SACrS, IUCr Commission Committee members, as well as other elected members (including a Capacity Building representative)	Prof. Susan Bourne (Chairman) Prof. Demi Levendis Dr Andrew Venter Dr David Billing Prof Andre Roodt Prof Len Barbour Dr Catharine Esterhuysen Ms Esna du Plessis Prof Jan Dillen Dr Ayesha Jacobs (capacity building rep) Dr Melanie Rademeyer Dr Johan de Villiers Mr Siyanda Lubhelwana (capacity building rep) Prof. Jan Boeyens (consultant) Prof. Gert Kruger (consultant) Prof. Luigi Nassimbeni (consultant)	The National Committee is appointed for a three year term, to coincide with the General Assembly of the IUCr. The next General Assembly will be held in Japan in August 2008.
3. Participation by South Africans in Union activities	<ul style="list-style-type: none"> <li>The main participants are from Chemistry Departments in SA Universities, but geologists, physicists, biologists and materials scientists participate in specialist events. SA company representatives also attend courses and workshops.</li> </ul>		<ul style="list-style-type: none"> <li>Discussions with a large SA society, the SA Chemical Institute around agreements on affiliate membership.</li> </ul>
3.1. Size of local community	<ul style="list-style-type: none"> <li>About 100 members</li> </ul>		<ul style="list-style-type: none"> <li>The SACrS elected a new committee in 2005 who are exploring ways to attract members of other specialist groups, such as physics, biochemistry, pharmaceuticals, mineralogy, materials.</li> </ul>
3.2 South Africans serving on Unions or its subsidiary bodies	<ul style="list-style-type: none"> <li>IUCr commission on Structural Chemistry: Prof. Demi C Levendis</li> <li>IUCr commission on Crystallographic Teaching: Prof. Susan A Bourne</li> <li>IUCr commission on Journals: Prof. Andre Roodt and Dr Catharine Esterhuysen</li> <li>IUCr commission on Neutron Diffraction: Dr Andrew Venter</li> <li>European Crystallographic Association (ECA) Councillor for SA: Prof. Susan Bourne</li> </ul>		<ul style="list-style-type: none"> <li>Commissions were elected at the IUCr assembly in 2005 and will serve through 2008.</li> </ul>

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	<ul style="list-style-type: none"> <li>A Roodt, as member of the Exco of the ECA, attended the Exco Meeting in Manchester, Feb 2007, as well as the Exco and Council meetings in Marrakech, Morocco, Aug 2007</li> </ul>	
<p>3.3 Attendance of International Congresses/Workshops</p> <ul style="list-style-type: none"> <li>Number of conferences attended</li> <li>Number of South African delegates</li> <li>Number of papers presented</li> </ul>	<p>The major conferences in 2007 which were of interest to members:</p> <ul style="list-style-type: none"> <li>The School on Crystal Engineering in Erice, Italy (June 2007). Prof Susna Bourne presented a keynote lecture and a further five South African delegates attended. PhD student Vincent Smith (UCT) won the prize for the “best participation by a young scientist.”</li> <li>The European Crystallographic Meeting held in Marrakech, Morocco in August 2007. This was only the 2<sup>nd</sup> time this meeting was held in Africa; the first time was in Durban in 2003 which was largely organised by members of the Society. Prof Len Barbour presented a plenary lecture, Prof Susan Bourne an oral presentation and there were some 22 poster presentations by the remainder of the South African delegates.</li> <li>The Carman National Physical Chemistry Symposium of the South African Chemical Institute was held in September 2007 in Cape Town. One afternoon was devoted to a symposium organised by the SACrS.</li> </ul>	<ul style="list-style-type: none"> <li>The Congress and General Assembly of the International Union of Crystallography will be held in Osaka, Japan in August 2008. As this is the main business meeting of the Union (held every 3 years), the South African delegates have been selected by the SACrS and approved by the national committee. They are Prof Susan Bourne and Prof David Billing.</li> </ul>
<p>3.4 Capacity Building with regard to Membership of National Committee and involvement of young scientists in International Meetings</p>	<ul style="list-style-type: none"> <li>The National Committee agreed (in 2004) to nominate new members to improve their range of representation. Dr Catharine Esterhuysen was the first “capacity-building nominee” in 2004; her status as a researcher is now so well established that she is the current deputy-chair for the committee. Dr Ayesha Jacobs and Mr Siyanda Lubhelwana are the current capacity-building representatives on the committee.</li> <li>A number of SA universities are making major contributions in crystallographic related research; all are training between 2 and 6 post-graduates each in this specialist field, giving a total of around 40 full-time graduate students (while at least 20 other post-graduates use the experimental and computational methods of the field in their own projects). Full details are not easily available, but women and black students are well-represented among these.</li> <li>The composition of the national committee has changed substantially over the past 5-7 years. Gender equity has been successfully addressed, while equity in terms of race is an ongoing challenge. However, the profile of graduate students currently being</li> </ul>	<ul style="list-style-type: none"> <li>Continued efforts are to be made by SACrS executive and individual members to attract new students to the field, train scientists in other disciplines and also those working in industry, and nominate black or female members who are active in the field to the national committee</li> </ul>

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	<p>trained in crystallographic theory and techniques is an encouraging sign.</p> <ul style="list-style-type: none"> <li>• Dr Andrew Venter has presented lectures on Diffraction as part of the Masters in Applied Radiation Science and Technology, North West University. He is also Study leader for an MSc student in Materials Science, University of the Western Cape (which lacks in-house crystallographic expertise)</li> </ul>	
3.5 Organisation of Union related Conferences in South Africa	<ul style="list-style-type: none"> <li>• A Powder X-Ray Diffraction Workshop was organised at the University of Johannesburg in October 2007. This advanced course on powder diffraction used the facilities in the departments of chemistry and geology and the Spectrau laboratories at UJ, and the diffractometers at Wits. The format consisted of lectures in the morning and practical hands-on sessions in the afternoons. The topics covered included: basic crystallography and diffraction, modern instrumentation, sample preparation, databases, multiple-technique search-match, Rietveld refinement, phase quantification, structure determination, strain and crystallite size. Davor Balzar from the University of Denver was a special guest lecturer, taking care of the Strain and Size topics. The other lecturers included Johan de Villiers, Sabine Verryn, Dave Billing, L L Coetzee, Esna du Plessis and Gert Kruger. A detailed programme for the workshop is provided in the appendix.</li> </ul>	<ul style="list-style-type: none"> <li>•</li> </ul>
3.6 Contribution by members to documents and publications	<ul style="list-style-type: none"> <li>• Over 100 publications in international, refereed journals (not including conference proceedings). A selected list is attached.</li> </ul>	
3.7 Report back on recommendations made during the in depth review	<ul style="list-style-type: none"> <li>• None received</li> </ul>	
4. Value to the Community and Benefit to South Africa	<ul style="list-style-type: none"> <li>• The crystallographic services run by 6 SA universities have been invaluable to SA chemistry departments in particular (as well as other university departments): Services provided by SACrS members at these universities include: data collection and crystal structure solution (single crystals); distribution of the Cambridge Structural Database (Wits is the National Affiliated Centre, and also sends the CSD to Southern Africa countries)</li> <li>• The importance of crystallographic techniques and methods is</li> </ul>	Further interaction is planned with the scientific and technical community in industry or contract research institutions (MINTEK, CSIR, NECSA) through workshops and symposia.

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	<p>reflected in the recent acquisition of modern diffraction equipment by two further universities since 2004 (bringing the total of active crystallographic research units at SA universities to 8)</p> <ul style="list-style-type: none"> <li>• Local (and international) pharmaceutical and fine chemical industries benefit from research and from specialist knowledge of SA crystallographers and structural/solid-state chemists</li> <li>• Mining companies also benefit from research and from specialist knowledge (Mineralogists and materials scientist members)</li> <li>• There is an increasing participation of biochemists, biologists and medicinal scientists, especially since the installation of the diffractometer at UWC and introduction of Structural Biology courses.</li> </ul>	
<p>5. Public Society Interfaces and Outreach Programmes – self initiated or facilitated by ICSU</p>	<ul style="list-style-type: none"> <li>• Presentations on crystal growth at Grahamstown Science festival (by members from UCT and Univ. Stellenbosch)</li> <li>• Individual talks to schools and visits to crystallography facilities by school teachers and learners</li> </ul>	<p>Continued presentations at science festivals and schools</p>
<p>6. Research Highlights/ New Initiatives in South Africa</p>	<ul style="list-style-type: none"> <li>• Dr Andrew M Venter and Dr Esna du Plessis serve on the South African Synchrotron Roadmap Implementation Committee: A South African beam line at an already existing synchrotron source would serve as an important step to bridging this divide and greatly expand opportunities for South African scientists to access synchrotron radiation and train them in its use. Designing, building, and commissioning such a beamline (3-5 years) would also provide experience essential to the success of a future African light source. The South African Government has developed the NSI as the guiding framework for major new initiatives in science. A South African beam line at a premier international synchrotron can deliver massively to the Core Missions and Strategic Priorities of the NSI, i.e. human resource development, knowledge generation, utilisation of research results, technology transfer and innovation and provision of state-of-the-art-research equipment infrastructure. The strategic priorities are to redress and equity (race and gender), adherence to quality, internationalisation of research, focus on Africa, positioning the NRF within the National System of Innovation (NSI) and organisational transformation. The Synchrotron Roadmap Implementation Committee was formed and currently consists of the following members: Chair: Simon Connell;</li> </ul>	<ul style="list-style-type: none"> <li>•</li> </ul>

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	<p>Deputy: Giovanni Hearne; Officer - Accelerator Physics: Tony Joel; Officers - Life Sciences: Trevor Sewell, Raymond Sparrow; Officer - Geo / Env Sciences: Wojciech Przybylowicz; Officer - Heritage Sciences: Leon Jacobson; Officers - Material Sciences: Margit Haertig, Danie Hattingh; Officer - Industry Esna du Plessis. The following activities are planned for 2008: * School for Synchrotron based Techniques in Research: 24-26 March 2008; * Users Meeting and Research Workshop: 27-29 March 2008; * Planning Workshop: 30 March 2008</p> <ul style="list-style-type: none"> <li>• The University of the Witwatersrand has acquired a rotating anode generator and large CCD detector suitable for protein crystallography. This will allow South African scientists (chemists, biochemists and crystallographers) access to this exciting current field of research interest.</li> <li>• A NRF grant was awarded to Dr Andrew Venter (under the Research Infrastructure Support Program) for the purchase of a D8 Discover with GADDS instrument for residual stress investigations. This is the first Bruker instrument in SA equipped with a Hi-Star multi wire area detector.</li> <li>• AM Venter elected as a steering committee member for the Materials Engineering Research Initiative Using Advanced Diffraction Methods.</li> </ul>	
7. Science Education	<ul style="list-style-type: none"> <li>• Prof Bourne, as a member of the Crystallographic Teaching commission of the IUCr, was part of the organising committee of an Introductory Crystallography School which was held in Italy in July 2007.</li> </ul>	<ul style="list-style-type: none"> <li>•</li> </ul>

<b>Headings</b>	<b>Activities completed- January to December 2007</b>	<b>Activities planned- January to December 2008</b>
8. Financial assistance received by South Africans direct from ICSU bodies during 2007	<ul style="list-style-type: none"> <li>• None</li> </ul>	<ul style="list-style-type: none"> <li>•</li> </ul>

## ADDENDUM-1:

### REPORT TO THE ICSU NATIONAL BOARD ON THE ACTIVITIES OF THE NATIONAL COMMITTEE FOR THE IUCr, 2007

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#### A SELECTION OF PEER REVIEWED PUBLICATIONS BY SACrS MEMBERS (2007)

(Note: this list was compiled from information readily available to the chair; it is not exhaustive)

1. du Plessis, H. E., Kruger, G. J., & de Villiers, J. P. R. Re-determination of the crystal structure of chi-Hägg carbide. *Z. Kristallogr.* (2007) **222**, 211-217
2. du Plessis, H. E., Kruger, G. J., & de Villiers, J. P. R. "Kristalstrukture van ysterkarbiede" *SA Tydskrif vir Natuurwetenskap en Tegnologie*, Jaargang 26 No. 2: Junie 2007.
3. Horvath, U. E. I. & Raubenheimer, H. G. (2007). *Acta Cryst.* E63, m567-m568.
4. Jacobs, T. & Bredenkamp, M. W. (2007). *Acta Cryst.* E63, o4444.
5. Sheng, X., Strasser, C. E., Raubenheimer, H. G. & Luckay, R. C. (2007). *Acta Cryst.* E63, o4361.
6. Lakomska, I. & Dobrzanska, L. (2007). *Acta Cryst.* E63, m2367.
7. Jacobs, T., Bredenkamp, M. W. & de Vries, E. J. C. (2007). *Acta Cryst.* E63, o3736.
8. de Jongh, L.-A. , Strasser, C. E., Cronje, S. & Raubenheimer, H. G. (2007). *Acta Cryst.* E63, m2137-m2138.
9. Potts, S., Bredenkamp, M. W. & Gertenbach, J.-A. (2007). *Acta Cryst.* E63, o2887.
10. Murray, P., Willans, C., Bredenkamp, M. W. & Gertenbach, J.-A. (2007). *Acta Cryst.* E63, o224-o225.
11. Strasser, C. E., Cronje, S. & Raubenheimer, H. G. (2007). *Acta Cryst.* E63, m2915-m2916.
12. le Roex, T.; Nassimbeni, L.R. and Weber, E. "Clathrates with Mixed Guests", *Chem. Commun.*, 2007, 1124.
13. Inclusion by a Xanthenol Host: Relating Structure to the Kinetics of Desolvation and Guest Exchange., A. Jacobs, N. Faleni, L.R. Nassimbeni, and J.H. Taljaard, *Crystal growth and Design*, 2007, 7, 6, 1003-1006.
14. Inclusion of pyridine and acetone by a diol host: structure, thermal stability and kinetics of desolvation, A. Jacobs, N. L. Masuku, L.R. Nassimbeni and J.H. Taljaard, *Crystengcomm.*, accepted, published as an advanced article on the web.
15. Inclusion with Mixed Guests: Structure and Selectivity, A. Jacobs, K.L. Nohako, L.R. Nassimbeni, H. Su and J.H. Taljaard, *Crystal growth and Design*, In Press.
16. The Search for a Predicted Hydrogen Bonding Motif – A Multidisciplinary Investigation into the Polymorphism of 3-Azabicyclo[3.3.1]nonane-2,4-dione. Ashley T. Hulme, Andrea Johnston, Alastair J. Florence, Phillipe Fernandes, Kenneth Shankland, Colin T. Bedford, Gareth W.A. Welch,

- Ghazala Sadiq, Delia A. Haynes, W. D. Samuel Motherwell, Derek A. Tocher, Sarah L. Price, *Journal of the American Chemical Society*, 2007, 129, 3649-3657.
17. L Sreenivas Reddy, Prashant M Bhatt, Rahul Banerjee, Ashwini Nangia, and Gert J Kruger. Variable-Temperature Powder X-ray Diffraction of Aromatic Carboxylic Acid and Carboxamide Cocrystals. *Chemistry - An Asian Journal*, 2(4), (2007), 505-513.
  18. G J Kruger & C van Blerk. Butane 1,4-diammonium dibromide. *Acta Cryst.* E63, (2007), o342-o344.
  19. Roy, S.; Bhatt, P. M.; Nangia, A.; Kruger, G. J. Stable polymorph of venlafaxine hydrochloride by solid-to-solid phase transition at high temperature. *Crystal Growth & Design*, (2007), 7, 476-480.
  20. van Blerk, C. & Kruger, G.J. Octane-1,8-diammonium dichloride monohydrate, *Acta Cryst.*, (2007), E63, o4289.
  21. van Blerk, C. & Kruger, G. J. Synthesis and structural characterization of butane-1,4-diammonium sulphate. *Journal of Chemical Crystallography*, ONLINE FIRSTTM, 2 November 2007.
  22. G J Kruger, D G Billing & M Rademeyer. Polymorphism in the Long-chain n-Alkylammonium Halides and Related Compounds. Chapter in the book: *Models, Mysteries and Magic of Molecules*; edited by: Jan C A Boeyens and John F Ogilvie ; Collected papers of the contributions to the conference: Indaba5 held at Berg-en-Dal from 20 to 25 August 2006, In press.
  23. D.B.G. Williams, T. Traut, F.H. Kriel and W.E. van Zyl Bidentate amino- and iminophosphine ligands in mono and dinuclear gold(I) complexes, *Inorganic Chemistry Communications*, 2007, 10, 538-542.
  24. Venter AM, van der Watt MW, Wimpory RC, Schneider R, Mc Grath PJ. Topic M. "Neutron strain investigations of laser bent samples". Accepted for publication in *Material Science Forum* (2008).
  25. Reddy L, Alberts HL, Strydom AM, Prinsloo ARE, Venter AM. "Quantum critical behaviour in the (Cr86Ru14)1-xVx system". Accepted for publication in *Journal of Magnetism and Magnetic Materials* (2008).
  26. Zhang SY, Venter AM, Vorster WJJ, Korsunsky AM. "High energy synchrotron x-ray analysis of residual plastic strains induced in shot peened steel plates". Accepted for publication in *Journal of Strain Analysis* (2008).
  27. Korsunsky AM, Vorster WJJ, Zhang SY, Topic M, Venter AM. "A beam-bending eigenstrain analysis of residual elastic strains in multi-scan laser-formed steel samples", *Proceedings of the Institution of Mechanical Engineers, Part C, Journal of Mechanical Engineering Science*, 2007. Accepted for publication.
  28. Topic M, Mc Grath P, Vorster W, Zhang SY, Bucher R, Venter AM, Korsunsky AM. "Multi-scan laser forming: Synchrotron strain scanning and microstructure evolution", *Journal of Strain Analysis* 42 (2007) 497.

29. Underwood JH, de Swardt RR, Venter AM, Troiano E, Hyland EJ, Parker AP. "Hill stress calculations for autofrettaged tubes compared with neutron diffraction residual stresses and measured yield pressure and fatigue life", International Journal for Pressure Vessels and Piping 2007. PVP2007-26617.
30. Troiano E, Underwood JH, de Swardt RR, Venter AM, Parker AP, Mossey C. "3D finite element modeling of the swage autofrettage process including the Bauschinger effect", International Journal for Pressure Vessels and Piping 2007. PVP2007-26743.
31. [1,1'-Bis(diphenylphosphino)ferrocene-K2P,P']dichloroplatinum(II) chloroform solvate, 2007, Acta Cryst., Vol. E63, pp m210-m212, A Muller.
32. Benzyldiphenylphosphine selenide, 2007, Acta Cryst., Vol. E63, pp o317-o318, A Muller.
33. Bicyclic phosphines as ligands for cobalt catalysed hydroformylation. Crystal structures of [Co(Phoban[3.3.1]-Q)(CO)3]2 9(Q = C2H5, C5H11, C3H6NMe2, C6H11), 2007, Dalton Transactions, Nr. 27, pp 2876-2884, PN Bungu, S Otto.
34. Steric and electronic properties in bicyclic phosphines. Crystal and molecular structures of Se = Phoban-Q(Q = C2, C3Ph, Cy and Ph), 2007, J. of Organometallic Chemistry, Vol. 692, pp 3370-3379, PN Bungu, S Otto.
35. cis-[2,6-Bis(di-tert-butylphosphino-methyl)cyclohexyl-κ3P,C1,P']bromido-palladium(II), 2007, Acta Crystallographica Sec. E, Vol. E63, pp m1969, D Olsson, JM Janse van Rensburg, OF Wendt.
36. Tetraphenylphosphonium aquatetracyano-nitridorhenate(V) pentahydrate, 2007, Acta Crystallographica Sec. E, Vol. E63, pp m80-m82, TN Mtshali, W Purcell, HG Visser.
37. Tris(1-naphthyl) phosphite, Acta Crystallographica Sec. E, Vol. E63, pp o2828-o2830, L Kirsten, G Steyl, A Roodt.
38. (Diphenylmethoxyphosphane-κP)(di-phenylphosphanito-κP)(3,5,7-tribromo-tropolonato-κ2O,O') palladium(II) methanol solvate, 2007, Acta Crystallographica Sec. E, Vol. E63, pp m2613-m2614, G Steyl.
39. Tris[diphenyl(4-tolyl)phosphane]-1κ2P,2κP-μ-di-iodido-1:2κ4I-dicopper(I), 2007, Acta Crystallographica Sec. E, Vol. E63, pp m2522, G Steyl.
40. Tetraaqualithium(I) bis(tropolonato-κ2,O,O')lithate(I), 2007, Acta Crystallographica Sec. E, Vol. E63, pp m2343, G Steyl.
41. Carbonyl(3,7-dichlorotropolonato)(triphenyl-phosphine)rhodium(I), 2007, Acta Crystallographica Sec. E, Vol. E63, pp m23-m25, G Steyl.
42. 1-(4-Methoxybenzyl)pyridinium p-toluenesulfonate, 2007, Crystallographica Sec. E, Vol. E63, pp o4326, MC Achilonu, JM Janse van Rensburg, JH van der Westhuizen, A Roodt.
43. Kinetic investigation of a ruthenium metathesis catalyst, 2007, J. of Organometallic Chemistry, Vol. 692, pp 5508-5512, S Booyens, A Roodt, OF Wendt.
44. (Acetylacetonato-κ2O,O')carbonyl-(cyclohexyldiphenylphosphine-κP)-rhodium(I), 2007, Vol. E63, pp m2831-m2832, A Brink, A Roodt, HG Visser.

45. Carbonyl(5-chloroquinolin-8-olato- $\kappa$ 2N,O)[tris(4-chlorophenyl)phosphine- $\kappa$ P]rhodium(I), 2007, Acta Crystallographica Sect. E, Vol. E63, pp m3015-3016, JM Janse van Rensburg, A Muller, A Roodt.
46. Di- $\mu$ -thiocyanato-bis[bis(tri-p-tolyl-phosphine)silver(I)] acetonitrile disolvate, 2007, Acta Crystallographica Sect. E, Vol. 63, pp m3076-m3077, GJS Venter, R Meijboom, A Roodt.
47. Carbonyl(5-chloroquinolin-8-olato- $\kappa$ 2N,O)[tris(4-chlorophenyl)phosphine- $\kappa$ P]rhodium(I), 2007, Acta Crystallographica Sect. E, Vol. E63, pp m3015-m3016, JM Janse van Rensburg, A Muller, A Roodt.
48. Racemic dipotassium di- $\mu$ -2-hydroxido-bis[[N,N-bis(carboxylatomethyl)leucinato- $\kappa$ 4N,O,O',O"]-cobaltate(III)] tetrahydrate, 2007, Acta Crystallographica Sect. E, Vol. E63, pp m2998-m2999, HG Visser, W Purcell, A Muller, JM Janse van Rensburg, P Molosia.
49. cis-[2,6-Bis(di-tert-butylphosphinomethyl)cyclohexyl- $\kappa$ 3P,C1,P']bromidopalladium(II), 2007, Acta Crystallographica Sect. E, Vol. E63, pp m1969, D Olsson, JM Janse van Rensburg, OF Wendt.
50. 1-(4-Methoxybenzyl)pyridinium p-toluenesulfonate, 2007, Acta Crystallographica Sect. E, Vol. E63, pp o4326, MC Achilonu, JM Janse van Rensburg, JH van der Westhuizen, A Roodt.
51. (Acetylacetonate- $\kappa$ 2O,O')carbonyl-(cyclohexyldiphenylphosphine- $\kappa$ P)-rhodium(I), 2007, Acta Crystallographica Sect. E, Vol. E63, pp m2831-m2832, A Brink, A Roodt, HG Visser.
52. Bis(tetraphenylarsonium) tricyanidonitrido-(quinoline-2-carboxylato- $\kappa$ 2N,O)rhenate(V) dihydrate, 2007, Acta Crystallographica Sect. E, Vol. E63, pp m1037-m1038, TN Mtshali, W Purcell, HG Visser, SS Basson.
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#### **A SELECTION OF CONFERENCE PRESENTATIONS BY SACrS MEMBERS (2007)**

**(Note: this list was compiled from information readily available to the chair; it is not exhaustive)**

1. Nobathembu Faleni, .A Jacobs, L. R. Nassimbeni, J.H. Taljaard Inclusion Behaviour of a Xanthenol Host Compound: Thermal stability, Kinetics of Desolvation and Guest Exchange. SACI 2006 , 38th Convention of the South African Chemical Institute, Durban, South Africa, 3-8 December 2006. Poster presentation
2. B Breedt, H.E. du Plessis, M.J. Overett, J.J. Retief, A.M. Saib, J. van de Loosdrecht, "In situ XRD analysis of wax encapsulated catalyst", Poster presented at Catsa2007, 11-14 November 2007, at Richards Bay.
3. du Plessis, H.E., Kruger, G. J., & de Villiers, J. P. R. "Powder XRD and neutron diffraction study of Hägg carbide", Lecture at the 1st South African School on Science at Synchrotrons at iThemba labs, 4 - 8 February 2007.
4. du Plessis, H.E "In situ XRD study of reactions of iron carbides during Fischer-Tropsch synthesis" Lecture at the Carman symposium, 23 - 27 September 2007
5. Rietveld school at University of Johannesburg, lectures by Johan de Villiers, Gert Kruger, Dave Billing, Davor Balzar, Sabine Verryn, Louis Coetzee and Esna du Plessis: 29 October - 2 November 2007. Prof Davor Balzar presented 1 day school on crystallite size and strain analysis.
6. 11 delegates from University of Stellenbosch attended the ECM24 in Marrakech Morocco, 22-27 August, where Len Barbour presented a plenary lecture, and the other 10 delegates presented posters. Of these, Bettinah Chipimpi was awarded an IUCr poster prize, and Tia Jacobs was awarded a CCDC poster prize.

7. 7 delegates from University of Stellenbosch attended the Carman2007 conference in Cape Town, South Africa, 23-27 September. Len Barbour, Klaus Koch, Catharine Esterhuysen and Delia Haynes all presented talks, while the others presented posters.
8. Inclusion behaviour of a series of xanthenol host compounds., A. Jacobs, N. Faleni, K.L. Nohako, L.R. Nassimbeni, J.H. Taljaard, Carman Symposium, September 2007, Cape Town, Oral presentation.
9. Inclusion chemistry of a diol organic host., R. P. Molete, A.Jacobs, L.R.Nassimbeni, J.H.Taljaard, Carman Symposium, September 2007, Cape Town, Poster presentation.
10. Inclusion of pyridine and DMF by a butterfly host, S. Mokgosi, A.Jacobs, L.R.Nassimbeni, J.H.Taljaard, Carman Symposium, September 2007, Cape Town, Poster presentation.
11. Study of the Inclusion Behaviour and Kinetics of a diol host., L.Z. Masuku, A. Jacobs, L.R. Nassimbeni, J.H. Taljaard, Carman Symposium, September 2007, Cape Town, Poster presentation.
12. Study of the inclusion ability of 9-(1-naphthyl)-9H-xanthen-9-ol, K.L. Nohako, A. Jacobs, L. R. Nassimbeni, J. H.Taljaard, Carman Symposium, September 2007, Cape Town, Poster presentation.
13. D. Haynes: Oral presentation at the International Conference on the Chemistry of the Organic Solid State in Venezuela in July 2007: A series of novel phenylethylamine salts
14. D. Haynes: Oral presentation at the Carman Conference Cape Town in September 2007: Crystal engineering with NH<sub>3</sub><sup>+</sup>: a series of novel salts of aromatic amines
15. D. Haynes: 11th BCA/CCG Intensive Course in X-ray Structure Analysis in Durham, UK in March 2007.
16. 24th European Crystallographic Meeting, Marrakesh, Morocco, 22 – 27 August 2007, "Structural characteristics of the butane-1,4-diammonium dihalide salts", van Blerk, C. & Kruger, G.J – Poster presentation.
17. 24th European Crystallographic Meeting, Marrakesh, Morocco, 22 – 27 August 2007, " Synthesis, characterization and phase transitions in the long-chain n-alkylammonium halides and metal-halides ",Gert J Krugera, Charmaine van Blerka, David G Billingb, Andreas Lemmererb and Melanie Rademeyer - Oral presentation.
18. Annual SACI - CARMAN Physical Chemistry Symposium, V & A Waterfront, Cape Town, South Africa, September 2007, "Structural aspects of hydrated octane-1,8- and decane-1,10-diammonium dichlorides", van Blerk, C. & Kruger, G.J. – Poster presentation.
19. Annual SACI - CARMAN Physical Chemistry Symposium, V & A Waterfront, Cape Town, South Africa, September 2007 " Synthesis, crystal structures, and phase transitions in the n-alkylammonium salts", van Blerk, C. & Kruger, G.J. – Oral presentation.

20. Congresso Nazionale di Chimica e Tecnologie delle Ciclodestrine, Asti, Italy, 6-8 May 2007. Poster presentation: Isostructural solvates and conformation of Peracetyl- $\gamma$ -Cyclodextrin. M R Caira, G Bettinetti, M Sorrenti, L Catenacci, D Cruickshank and K Davies.
21. International Conference on Organic Chemistry, Erzurum, Turkey, 5-9 June 2007. Poster PP-67: Synthesis of unsymmetrical disulfides and thiosulfates. N Stellenboom, R Hunter, M R Caira.
22. 6th AFMC International Medicinal Chemistry Symposium, 8-11 July 2007, Istanbul, Turkey. Oral presentation OP-5: Structural Elucidation of Cyclodextrin Inclusion Complexes of novel Allicin-mimics. M R Caira, R Hunter, S A Bourne, T Qwebani and M Barbieri.
23. Fifth Conference: "Isotopic and Molecular Processes", PIM 2007, September 20-22, Cluj-Napoca, Romania. Invited lecture: Structural elucidation of chemically modified cyclodextrins and their inclusion complexes for medicinal applications. M R Caira.
24. Fifth Conference: "Isotopic and Molecular Processes", PIM 2007, September 20-22, Cluj-Napoca, Romania. Poster presentation:  $^1\text{H}$  NMR Study of Inclusion Complexes of Phenylurea Derivatives in  $\alpha$ -Cyclodextrin. D Bogdan, V Smith, M Vasilescu, M Bogdan, M R Caira, S Simon.
25. Carman National Physical Chemistry Symposium, V & A Waterfront, Cape Town, 23-27 Sept, 2007. Poster presentation: Multiplicity of crystal forms of a  $\beta$ -CD inclusion complex. V J Smith\*, M R Caira and S A Bourne. (\*Winner of prize for best poster)
26. Carman National Physical Chemistry Symposium, V & A Waterfront, Cape Town, 23-27 Sept, 2007. Poster presentation: Polymorphs of the Thiourea Drug Isoxyl. J Li, M R Caira and S A Bourne.
27. Engineering of Crystalline Materials Properties: State-of-the-art in Modelling, Design, Applications. (a NATO-ASI school). Erice, Italy. 7-17 June 2007. Invited keynote lecture: Complementarity: Correlating structural features with physical properties in supramolecular systems. S A Bourne
28. INORG007: SA Chemical Institute Inorganic Chemistry meeting. Langebaan, South Africa. 8-12 July 2007. Invited lecture: Supramolecular coordination chemistry: Design and Analysis of Functional Coordination Compounds. S A Bourne
29. ECM24: European Crystallographic Meeting. Marrakech, Morocco. 23-27 August 2007. Lecture: Reproducibility in inorganic crystal engineering: A cautionary tale. S A Bourne
30. Venter AM, Residual stress investigations with diffraction techniques, Research Workshop during the proceedings of the Science at Synchrotron series of meetings, 9 February, iThemba Labs, Cape Town.
31. Venter AM, Studies of magnetic materials with neutron diffraction, Thematic Workshop during the proceedings of the Science at Synchrotron series of meetings, 8 February, iThemba Labs, Cape Town.
32. Venter AM, Alberts HL, Reddy L, Prinsloo ARE, Neutron diffraction study of the Cr+14at.% Ru system doped with V, European Conference for Neutron Scattering, Lund Sweden, 25 to 29 June 2007.

33. Vorster WJJ, van der Watt MW, Venter AM, Oliver EC, Leo Prakash DG, Korsunsky AM, Quench modeling and investigations into the influence of boiling phase incipient temperatures shifts due to quenchant hydrodynamics on residual stress formation, International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics, 1 – 4 July 2007, Pilansberg South Africa.
34. Vorster WJJ, van der Watt MW, Venter AM, Oliver EC, Leo Prakash DG, Korsunsky AM, Residual elastic strain measurements and modeling of AISI 316L stainless steel cylinders subjected to spray quenching, International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics, 1 - 4 July 2007, Pilansberg South Africa.
35. Troiano E, Underwood JH, de Swardt RR, Venter AM, Parker AP, Mossey C, 3D finite element modeling of the swage autofrettage process including the Bauschinger effect, 2007 ASME Pressure Vessel and Piping Conference, 22 – 26 July 2007, Texas USA.
36. Underwood JH, de Swardt RR, Venter AM, Troiano E, Hyland EJ, Parker AP, Hill stress calculations for autofrettaged tubes compared with neutron diffraction residual stresses and measured yield pressure and fatigue life, 2007 ASME Pressure Vessel and Piping Conference, 22 – 26 July 2007, Texas USA.
37. Venter AM, Residual stress investigations with neutron diffraction and facilities at Necsa, Materials Engineering Research using Advanced Diffraction Methods, Irene SA, 23 August 2007.
38. Venter AM, van der Watt MW, Neutron strain investigations of laser bent samples, MECASENS IV Conference, 24 – 26 September 2007, Austria.
39. Vorster WJJ, van der Watt MW, Venter AM, Oliver EC, Leo Prakash DG, Korsunsky AM, Neutron diffraction measurement and finite element modelling of spray quenching of AISI 316L stainless steel cylinders, MECASENS IV Conference, 24 – 26 September 2007, Austria.
40. Venter AM, Residual stress projects using diffraction techniques at Necsa, Joint Institute of Neutron Research Seminar day, 20 September 2007, Dubna, Russia.

The following were conference presentations at Rhemantec presenting X-ray results.

41. Bioorganometallic Chemistry of Rhenium and Technetium: Future of <sup>99m</sup>Tc Radiopharmacy. Roger Alberto
42. Review of Tc and Re(V) + (III) chemistry at MU. Hendrik Engelbrecht, Paul Benny , Stephanie Lane, and Silvia Jurisson
43. High-valent Technetium Complexes with Tripodal Ligands. Henrik Braband, Yuji Tooyama and Roger Alberto
44. Towards new rhenium radiopharmaceuticals: rhenium(V) nitride complexes with sulfonamide based dithiocarbamate ligands. Joanne Perils
45. Synthesis, Structure and Reactivity of Half-Sandwich ReIII and TcIII Tricarbonyl Complexes: A Potentially New Prodrug Delivery System? Fabio Zobi, Bernhard Spingler and Roger Alberto
46. Evaluation of several <sup>99m</sup>Tc-ligands for peptide based radiopharmaceuticals. Patricia Antunes, Paul Schmutz, and Roger Alberto

47. Cell Uptake Studies of Bombesin-Intercalator Conjugates of Re/99mTc(CO)<sub>3</sub><sup>+</sup>. Agorastos Nikos, Lubor Borsig, Annabelle Renard and Roger Alberto
48. Rhenium(I) compounds in Nuclear Medicine. Crystallographic and kinetic investigation of different [Re(CO)<sub>3</sub>(L<sub>1</sub>)(L<sub>2</sub>)<sub>n</sub>]- complexes. Marietjie Schutte, Andreas Roodt, Hendrik G. Visser
49. Imido, Amido and Amino Complexes of Re(V) with Multidentate Aromatic Amine. Irvin Booyesen, Thomas Gerber and Peter Mayer
50. Direct syntheses of 99TcVII complexes with the [TcO<sub>3</sub>]<sup>+</sup> core from [TcO<sub>4</sub>]<sup>-</sup> for labeling biomolecule. Y. Tooyama, H. Braband, B. Spingler and R. Alberto
51. Stable ReI/II(CO)<sub>2</sub> complexes: Reflection on a series of new precursors for organometallic chemistry. Lukas Kromer, Bernhard Spingler and Roger Alberto
52. Rhenium(I) carbonyl complexes as model radiopharmaceuticals. Hendrik G. Visser, Gerdus Kemp, Marietjie Schutte and Andreas Roodt
53. The SAMSA group as an alternative bifunctional chelate for labelling biological active moieties with technetium-99m. Otto Knoesen and Marina Rautenbach
54. Pandora's box and Medusa's molecule – dendrimers as drug-delivery vehicles. R. Meijboom
55. A general approach to α, β-diamino propionic acid and its complexes recognized by LAT1. Yu LIU, P. Schmutz, M. Bauwens, J. Mertens, R. Alberto
56. Cytotoxicity studies in bacteria and carcinoma cells of novel Pt-vitamin B12 derivatives. Pilar Ruiz-Sánchez, Bernhard Spingler, Jorge C. Escalante-Semerena, Stefano Ferrari and Roger Alberto
57. Spectroscopic and theoretical investigation of the isomerisation of [Re(O)<sub>2</sub>(Eten)<sub>2</sub>]<sup>+</sup> and related complexes. G. Steyl, A. Roodt and H.P. Engelbrecht
58. Mobile and trapped manganese fragments as key components of π-arene and π-heteroarene complexes and networks. Simon Lotz and Dwight A Sweigart
59. Synthesis and structural features of novel Group VII transition Metal carbene complexes. Daniela I. Bezuidenhout, David C. Liles, Petrus H. van Rooyen and Simon Lotz
60. Synthesis, characterization, reactivity and structural features of Fischer carbene complexes of group 7 transition metals. Marile Landman and Dave Liles
61. Evaluation of ligand and solvent effects on a potential catalyst using a rhodium cupferrate system as model. Johan Venter, Stephen Basson and Walter Purcell
62. Quinoline improving the life of Manganese triad metals, wicked! J. Marthinus Janse van Rensburg, A. J. Muller and A. Roodt

63. Rhodium carboxylato phosphite, phosphinite complexes as catalysts. Leo Kirsten, Gideon Steyl and Andreas Roodt
64. Speciation and interconversion mechanism of mixed fluoro and O,O- and O,N- bidentate ligand complexes of Zirconium. Maryke Steyn , Gideon Steyl and Andreas Roodt
65. Hypoelectronic Clusters: Are They Deviant Clusters or Part of the Same Class? Ipe J. Mavunkal, Bruce C. Noll, Reinout Meijboom, Alfred Muller and Thomas P. Fehlner
66. Synthesis and characterization of Copper(I) O,O-bidentate complexes Righardt du Plessis, Gideon Steyl & Andreas Roodt
67. SolidState Packing Disorders in the Manganese Triad. Alfred Muller
68. Speciation and interconversion mechanism of mixed fluoro O,O' - and O,N- bidentate ligand complexes of Hafnium. J.A Viljoen, A. Muller and A. Roodt
69. Silver(I) coordination with group 15 ligands and the ligand exchange mechanism. Gertruida J.S. Venter, Reinout Meijboom, Andreas Roodt
70. Ring a ring of Rosies, a pocket full of Phosphines. Alice Brink, Nicoline Cloete, Andreas Roodt and Hendrik G. Visser
71. A crystallographic and kinetic studies of the formation of tricyanonitrido( $\kappa^2$ N,O)rhenate(V) ions. Thato Mtshali, Walter Purcell and Stephen Basson
72. Implications for nuclear medicine from mechanistic studies on substitution reactions in complexes of the manganese triad. Andreas Roodt

**ADDENDUM-2:**

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**2007 PXRD Course (University of Johannesburg)**  
**29 October – 2 November 2007**  
**Programme**

<b>MONDAY – CRYSTALLOGRAPHY &amp; DIFFRACTION</b>		
8:30 - 9:00	Registration and Outline of Course	GJK
9:00 – 9:45	<i>Theory 1:</i> Crystallography Lattices, crystal systems, unit cells, Bravais lattices, planes & indices, lattice transformations	SV
9:45 – 10:30	<i>Theory 2:</i> Diffraction Theory Diffraction of X-rays, neutrons, electrons; Bragg's law	GJK
<b>10:30 - 10:45</b>	<b>Tea</b>	
10:45 – 11:30	<i>Theory 3:</i> Symmetry Crystal symmetry, point groups, space groups, International Tables for Crystallography, crystal structures	GJK
11:30 – 12:15	<i>Theory 4:</i> Information in Diffraction Patterns Reciprocal lattice, Ewald sphere, intensities of diffracted peaks	GJK
<b>12:15 - 13:15</b>	<b>Lunch</b>	
13:30 - 16:30	<i>Practical 1:</i> Crystal structure databases demo Space groups, cell transformations PowderCell demo and exercise HighScore Plus: data import and structure plot Topas: data import and structure plot	GJK GJK SV LLC DGB ++

<b>TUESDAY - POWDER DIFFRACTION AND QUANTITATIVE ANALYSIS</b>		
9:00 – 9:45	<i>Theory 5:</i> Powder Diffraction Powder diffractometer geometry and diffraction pattern capture	DGB
9:45 – 10:30	<i>Demo 1:</i> Instrumentation Sources, sample stages, detectors, alignment, standards, combining diffraction with other techniques	LLC

<b>10:30 - 10:45</b>	<b>Tea</b>	
10:45 – 11:30	<i>Theory 6: Phase Identification by XRD</i> ICDD Powder Diffraction File, Search-match techniques	SV
11:30 – 12:15	<i>Theory 7: Quantitative analysis by XRD</i> Mathematical background, RIR's, full-pattern refinement, presence of amorphous components, gentle intro to Rietveld method.	JDV
<b>12:15 - 13:15</b>	<b>Lunch</b>	
13:30 – 14:15	<i>Theory 8: Sample Preparation</i> Flat-plate, transmission, capillary samples; dealing with micro absorption and preferred orientation	LLC
14:30 - 16:30	<i>Practical 2:</i> PDF reading, Phase identification and Search-Match, Q-XRD	LLC, SV DGB

### WEDNESDAY - RIETVELD REFINEMENT

9:00 – 10:30	<i>Theory 9: Introduction to Rietveld Refinement</i> Overview of profile models and fundamental parameter models, parameters required in the refinement, including background, lattice constants, profile and profile-shape functions, peak asymmetry, line broadening, preferred orientation, etc. Use of constraints and restraints	JDV
<b>10:30 - 10:45</b>	<b>Tea</b>	
10:45 – 11:15	<i>Practical 3: Introduction and demonstration of Topas (data import, refinement setup, output)</i>	JDV, Roy
11:15 – 11:45	<i>Practical 4: Introduction and demonstration of AutoQuan (data import, refinement setup, output)</i>	SV
11:45 – 12:15	<i>Practical 5: Introduction and demonstration of HighScore Plus (data import, refinement setup, output)</i>	LLC

<b>12:15 - 13:15</b>	<b>Lunch</b>	
13:30 - 16:30	<i>Practical 6:</i> Working through a complete refinement of a small inorganic structure. Comparison of different software packages: Topas, Expert +, Topas acad, AutoQuan, GSAS, etc	EDP, LLC JDV, SV
<b>17:00 – 21:00</b>	Social evening – a traditional Braaivleis	

<b>THURSDAY - STRUCTURE DETERMINATION and RIETVELD HINTS AND TIPS</b>		
9:00 – 9:30	<i>Theory 10:</i> Indexing of powder pattern peaks	GJK
9:30 – 10:00	<i>Theory 11:</i> Lattice Refinement - Pawley and Le Bail	EDP
10:00 – 10:30	<i>Theory 12:</i> Structure Determination & Refinement, Obtaining initial structure, completion of the model, error estimation (R-values, etc.).	GJK
<b>10:30 - 10:45</b>	<b>Tea</b>	
10:45 – 11:15	<i>Theory 13:</i> Multiphase analysis and quantification by Rietveld refinement	SV
11:15 – 11:45	<i>Theory 14:</i> Rietveld Practical Aspects Problem cases and difficulties	JDV
11:45 – 12:15	<i>Practical 7:</i> Multiphase analysis and quantification by Rietveld refinement	SV, JDV
<b>12:15 - 13:15</b>	<b>Lunch</b>	
13:30 - 16:30	<i>Practical 8:</i> Le Bail - GSAS and Topas Examples Indexing, structure determination, refinement Topas simulated annealing, charge flipping	DGB, EDP GJK JDV

<b>FRIDAY – PEAK BROADENING – SIZE &amp; STRAIN ANALYSIS</b>		
9:00 – 9:45	<i>Theory 15:</i> Peak broadening and peak shape	DB
9:45 – 10:30	<i>Theory 16:</i> Crystallite size	DB
<b>10:30 - 10:45</b>	<b>Tea</b>	
10:45 – 11:30	<i>Theory 17:</i> Strain and Residual Stress	DB
11:30 – 12:15	<i>Theory 18:</i> Size and Strain modeling in Rietveld Refinement	DB

<b>12:15 - 13:15</b>	<b>Lunch</b>	
13:30 – 14:30	<i>Practical 9:</i> Applications of peak broadening and peak shape analysis.	DB
14:30 – 15:00	<i>Theory 19:</i> Non-ambient XRD	EDP
15:00 - 15:30	<i>Theory 20:</i> Cluster analysis	JDV
15:30 - 15:45	Summary, photo and certificate ceremony	GJK
16:15 – 18:15	Tour of X-ray lab and Cocktail party (sponsored by Bruker) Wits Gate House 8 <sup>th</sup> floor	
<b>Lecturers:</b>		
DB	Davor Balzar	
DGB	Dave Billing	
LLC	El-el Coetzee	
JDV	Johan de Villiers	
EDP	Esna du Plessis	
GJK	Gert Kruger	
SV	Sabine Verryn	