

MARCH 1988

SOCIETY OF CRYSTALLOGRAPHERS IN AUSTRALIA

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MESSAGE FROM THE SCA PRESIDENT

Perceptions and memories of last year's IUCr meeting in Perth are many and varied. For those of us who simply attended and participated with the many international guests, it stands as a splendid occasion, scientifically and socially. For those whose lives were seriously disrupted by organisational tasks, the Congress, as an event, is only now coming into focus as the dust settles. We congratulate Ted Maslen and Hans Freeman, and the many others particularly in the Perth and Sydney labs, for putting it all together.

Thanks and congratulations are one thing, but something of greater substance has emerged from this occasion. You will see in Ted Maslen's preliminary report to the Society in this Newsletter that the Congress was a financial success, far in excess of expectations. If used wisely, these financial resources could serve the Society in perpetuity. The proposal which I favour is to deploy all of the profit of the Congress into a special fund, and to draw only on the earnings to support three different activities. The first would be 'The 1987 Scholarship' to allow Australian postgraduate students to travel to IUCr meetings. The second would be 'The 1987 Studentship' in support of student travel to SCA meetings. Finally, 'The 1987 Fellowship' might fund attendance of international speakers at SCA meetings. Although the capital sum is substantial, its earning capacity is not enormous, and some thought needs to be given to balancing the support for the different awards. The membership is invited to offer comments and suggestions on these or other proposals that would ensure that the crystallographic community enjoys long-term benefit from the successes of the 1987 Perth meeting.

Peter Colman



XIVth INTERNATIONAL CONGRESS AND GENERAL ASSEMBLY INTERNATIONAL UNION OF CRYSTALLOGRAPHY PERTH, AUSTRALIA AUGUST 12-20, 1987.

Financial report

During the SCA meeting at the Congress the financial estimates indicated that income would exceed expenditure by a considerable margin. An unexpected surge of late enrolments boosted that margin substantially. The figures as of 31st December 1987, which are close to final, showed a net balance of \$105 854.46 on Congress operations.

Of several factors contributing to this result, the most significant was extensive use of volunteer labour at all stages of the Congress organisation. The surplus on the Commercial Exhibition \$32 000, was three times the budget figure. The use of desktop publishing for preparing Congress documents reduced costs by half, saving \$17 000. Earnings from interest were larger than expected because of high interest rates in the months prior to the Congress. Finally high temperature superconductors were discovered at an ideal time, boosting registrations to 915 plus 189 accompanying members. This was more than 200 higher than the budget figure.

Allowing for inflation the surplus is roughly comparable with the result of the XIIth Congress in Canada. It is large enough to provide the SCA with a modest annual income of 5000+ in addition to the amount needed to ensure that the value of the principal is not eroded by inflation. That will of couse require that the funds be carefully invested – a matter which will require the attention of the S.C.A. Committee.

E.N. (Ted) Maslen

5 12 16

Chairman of the Organizing Committee

COUNCIL NEWS

A Business Meeting of the SCA was held during the Perth Congress on the 18th August 1987. Some important points raised at that meeting were as follows.

Ted Maslen reported on the favourable financial situation of the IUCr Congress (see Ted's report elsewhere in this Newsletter for an up-to-date position), and recommended that after refunds of ca. \$7000 and \$10000 were made to the IUCr and the SCA respectively, the remainder be used to enable student crystallographers to attend future SCA meetings. The numbers attending the Congress were

794 full registrations

121 student registrations

189 accompanying registrations

1104 total attendance

The recommendation from Maureen Mackay and Sandy Mathieson that the next SCA meeting be held at Erskine House, Lorne, in February 1989 was accepted. The suggestion was made that Crystal 16 abut the protein meeting also to be held in Lorne.

Syd Hall detailed the member countries of the Asian Crystallographic Association (AsCA). Initially, the main task is to produce two newsletters per year. Membership cost to the SCA is \$240 per annum.

A motion was carried to the effect that the SCA continue membership of the Federation of Australian Scientific and Technical Societies (FASTS), but that the case be reconsidered at the next Business Meeting. Richard Welberry is currently representing the SCA on FASTS. The concern is that the SCA may not be getting value for the (significant) sum of dollars which it costs in membership dues. However, the other side of the coin is that perhaps the SCA is remiss in allowing FASTS (not to mention the outside world in general) to remain ignorant of what crystallography is all about.

Of the four proposals to amend the Constitution, two (Honorary Life Membership and Newsletter Editor) required a postal ballot of all members. In secret ballots at the meeting, the necessary majorities were obtained in both cases allowing the postal ballots to proceed (see results below). Two other amendments, to instigate penalties for late payment of membership dues, and to abolish all standing committees with the exception of the Nominations Committee, were passed. As a result of the amendment, the relevant section of the SCA Constitution regarding membership dues now reads: 'The annual membership subscription shall be \$20. The annual subscription for students shall be \$3. The annual subscription for corporate members shall be \$130. Members who pay the subscription by April 1st of the year in which it applies will be entitled to a discount of \$5 (full), \$1 (student) or \$30 (corporate)'.

The high cost of the Cambridge database was discussed together with the need for a unified front to formally request the Cambridge database to lower the fee. A request was made to the new executive to take appropriate action. Rates should come down as the Australian dollar is down! See section below for the current position.

Needs were expressed for support for junior crystallographers to attend future SCA conferences and for the formation of a temporary standing committee to investigate funding of 'big science' and the setting of priorities for the procurement of large capital items.

RESULTS OF POSTAL BALLOTS. In the postal ballots carried out in November/December 1987 to amend the Constitution of the SCA, both amendments were overwhelmingly supported. Out of a total of 158 members eligible to vote, 62 returned formal votes for both proposals. In each case, there were 60 votes in favour of the amendment and 2 votes against. Therefore, the Constitution is duly amended to include the provision for Honorary Life Membership of the SCA, and to allow for the formal position of Newsletter Editor on Council.

A meeting of the SCA Council was held in Melbourne on the 25th February 1988. At that meeting, a proposal to establish an investment account to handle the surplus funds from the Perth Congress was accepted. A request from the organisers of Crystal 16 for \$2500 to support the attendance of Prof. Jack Dunitz at the meeting was supported, and it was suggested that Prof. Dunitz be the first '1987 Fellowship' recipient.

FORTHCOMING MEETINGS

May 16-20, 1988. Centenary Conference of ANZAAS, Sydney. Contact the ANZAAS office, 10 Martin Place, Sydney.

August 14-19, 1988. Australian X-Ray Analytical Association, 7th National Conference 'New Horizons in Analytical Science', University of W.A. Contact AXAA-88, P.O. Box 479, Claremont, W.A. 6100

August 15-19, 1988. The Twelfth International Liquid Crystal Conference, The University of Freiburg, F.R.G. Contact Dr. G. Baur, Fraunhofer-Institut IAF, Eckerstr. 4, D-7800 Freiburg, Federal Republic of Germany.

September 15-24, 1988. Summerschool on Crystallography and its Teaching, Tianjin, China. Contact Prof. Xiao-Lan Liu, Dept. of Chemistry, Tianjin Normal University, Tianjin, China.

February 16-19, 1989. SCA Crystal 16 Meeting of Crystallographers, Erskine House, Lorne, Victoria. Contact Dr. M.F. Mackay, Dept. of Chemistry, La Trobe University, Bundoora, Vic. 3083.

July 2-7, 1989. International Conference on Coordination Chemistry, Gold Coast, Queensland. Contact ICCC Secretariat, UniQuest Limited, University of Queensland, St. Lucia, Qld. 4067.

MISCELLANEA

A few copies of the new (1986) World Directory of Crystallographers remain and these will be offered on a first-come basis at the bargain rate of \$5 each. Please make cheques payable to the SCA, and forward to Geoff Williams (ARL, Yallambie 3085).

Membership - at present we number just over 150 strong, but there must be quite a few new students and others in crystallography centres who would be keen to join once the benefits of membership of the SCA are explained to them. Please put them in touch with the secretary. To make it easy for you, some of the benefits are as follows:

keep in touch with people and with the issues that concern us as crystallographers (we aim for two newsletters per year):

participate in the national CRYSTAL conferences and workshops (first held in 1961 and now 15 in number);

exert formal influence over the public view of crystallography (including Government support and recognition) both directly as a member of the SCA, and indirectly through the SCA's membership of the Federation of Scientific and Technological Societies (FASTS);

receive 50% discount on subscriptions to SEARCH (through FASTS).

Incidentally, invitations to join the SCA have now been sent to all those 90 people listed in the World Directory of Crystallographers who are not already SCA members.

And a reminder to any member who has not yet sent his 1988 membership fee to Colin Kennard, that this year for the first time a penalty will be incurred for payments made after April 1st.

Most members will be aware that the First Ewald Prize for outstanding contributions to the science of crystallography was awarded by Theo Hahn, then-president of the IUCr, to Professor J.M. Cowley and Dr. A.F. Moodie at the Opening Ceremony of the Perth Congress on 12 August 1987. After the Perth Congress, Theo Hahn passed through Sydney on his way home to Europe, and presented Hans Freeman with signed originals of the Ewald Prize citation to Alex Moodie and the Ewald Medal citation to Mrs. Ella Ewald. Hans has very kindly passed the Alex Moodie citation to the SCA for preservation in the archives, and the other citation will be framed for permanent display in the School of Chemistry at The University of Sydney. As Hans indicates, these are clearly collector's items which should be preserved, and it is the SCA's intention also to frame the citation. Many thanks, Hans!

Budding crystallographers? My two daughters, Gretel (7) and Naomi (5) were inquisitive on a recent trip to the beach to know where the large piles of salt at the salt-works came from. So a simple experiment was planned and a supply of salt water was collected for subsequent evaporation in two (most important - one for each!) shallow containers sitting in the sun. After several weeks, they discovered some fine large shining crystals, and spent a happy half hour collecting some magnificent specimens (and eating a few too). They have undoubtedly discovered that appreciation that all crystallographers have for the beauty of nature in the crystalline world. (ed.)

PEOPLE

All those who have been welcomed to AINSE at Lucas Heights over the years by a smile from Bill Palmer will be sad to hear of his impending retirement in August. From all of us, thanks and good luck, Bill!

Man on the move! John Parise has resigned his position as lecturer in chemistry at the University of Sydney to take up a teaching and research position at the crystallographic lab. of the Department of Earth and Space Sciences, State University of New York at StonyBrook. We suspect some of the appeal of this new position is the proximity of the Brookhaven Synchrotron - Congratulations John!

Neil Isaacs has escaped Melbourne's summer by spending six months with Dr. Guy Dobson at York. Also accompanying Neil is Sandra Cowan who is completing her Ph. D. studies. Neil will be returning at the end of March.

Steve Wilkins will be escaping Melbourne's autumn to spend four months from mid-March at The Photon Factory, Tsukuba, Japan.

And perhaps smartest of all, Rod Hill will be escaping Melbourne's winter by taking nine months study leave in the Federal Republic of Germany, at the Mineralogical Institute, University of Wurzburg. Rod will be working with Prof. E. Tillmanns, on a Ludwig Leichhardt Fellowship, starting late June.

Around October, David Stuart and Yvonne Jones from the Molecular Biophysics Laboratory, Oxford, will be visiting CSIRO Protein Chemistry and Materials Science (Melbourne) on Bicentennial Fellowships.

Congratulations to Peter Colman for winning the 1988 Lemberg Medal from the Australian Biochemical Society for his work on influenza viruses!

Bob Cheary will be brushing up his skiing (if winter comes early) on the slopes around Grenoble from July to October. He also hopes to have some spare time to work with Alan Hewitt at the ILL. Then it will be back to fish and chips with a spell at the Daresbury synchrotron until January '89.

We welcome two new members - Nicholas Calos is a 2nd year Ph.D. student with Colin Kennard at the Dept. of Chemistry, University of Queensland. Nicholas is using the Rietveld Method for the determination of the crystal structures of some local minerals. And John Watts, of CSIRO Division of Mineral Products in Port Melbourne, has an interest in studying complex sulpho-salts and rare-earth mineral structures.

Sadly, we note the deaths of two SCA members - Mr. Janis Fridrichsons and Dr. John Sanders. Sandy Mathieson and Alex Moodie have kindly written the following obituaries.

The world of crystallography has been greatly diminished by the untimely death, on the 3rd of December 1987, of John Veysey Sanders.

John Sanders was born in Adelaide in 1924 and attended school and university in that city, graduating with honours in physics in 1947. He started his long and distinguished career in research as a CSIR student, working in Cambridge in the Laboratory of the Physics and Chemistry of Rubbing Solids which, at that time, was directed by Dr. Philip Bowden. John's work on the application of the methods of electron diffraction to surface layers on metals led to the award of a Ph.D. by the University of Cambridge in 1949. Even at this early stage the distinctive Sanders' style can be detected in the directness of the approach and the clarity of the analysis.

On his return to Australia in 1950 he joined the Division of Tribophysics and established in those laboratories the techniques of electron diffraction and, later, electron microscopy.

In his characteristically calm and self-effacing way he set about the development of those experimental methods which have contributed so significantly to our knowledge of the micro structure of surfaces and, in particular, to the understanding of the growth of metallic films on It was this work which brought solid substrates. the international recognition of the originality of his approach and, indeed, many of the results on, for instance, step densities metallic clusters have passed into the scientific canon. He continued to contribute to this field for the rest of his life, but such was the breadth of his interests and the depth of his understanding that his work on high-resolution electron microscopy and in particular, on lattice imaging, would be regarded by many scientists as of even greater significance. His paper with John Allpress and David Wadsley this topic is certainly classical. It effectively opens up a new and highly significant area of crystallographic enquiry, and the succession of papers which follow extend the range of application and consolidate the technique. It is a simple statement of fact that a handful of people in Melbourne changed the course of inorganic chemistry significantly in this period, and that John and David were pivotal in this move.

In later years John was to use lattice imaging in a great variety of investigations ranging over much of solid state chemistry, but perhaps the most sustained and notable were those concerned with the constitution and catalytic activity of the zeolites. This incisive and elegant work is known throughout the scientific world and John was in great demand to lecture on this topic. He, in fact, gave generously of his time to do this and the vividness of his talks comes readily to the minds of those of us fortunate enough to have attended them.

It was on the structure of one of the zeolites that John was working the day before his death.

All of this might well be thought more than sufficient to fill the working life of a scientist even of John's high ability, but throughout most of his career John pursued yet another line of enquiry, namely the origins of diffraction colour in nature. His main

purpose was to unravel the processes that generate colour in gem opal. In this he succeeded in the broadest sense, and further, conveyed his discoveries far outside the scientific community. Gemmologists, miners, prospectors and many members of the lay public found themselves, at first entertained, and then informed by John's vivid exposition. A range of people who are unaware of catalysis and lattices value John's contributions to knowledge derived from the apparently simple observation of accessible material. This has long been a touchstone for the distinguished scientist.

This simplicity of course conceals depth, and no aspiring crystallographer should miss the opportunity of studying in detail John's work on opal. In particular his papers in Acta Crystallographica on his opalimeter and its use in the analysis of stacking faulting, illustrated with colour photographs of his wife Gloria's ring, are in the tradition set by Faraday and Huxley.

In all of these activities John exhibited qualities which might serve as a model, perhaps particularly in these times. First, he pursued science, not power and not status, and he pursued it by individual effort. He was a fine administrator and was in demand for this purpose, but he was never deflected from research. He quickly disposed of his organisational duties and later in the day was to be found in the laboratory.

Secondly he brought a total honesty to his scientific work, claiming only what he had established beyond doubt and, quite oblivious of any considerations of competition, worked calmly towards quantitative understanding.

Finally, he possessed an enviable detachment and humour that endowed his work with a balance and scale, and made collaboration a continuing source of enjoyment.

With such a record John was the subject of many marks of distinction, the listing of which would have been a source of distaste and embarrassment to him but one, at least, must be mentioned, namely his election to the Fellowship of the Australian Academy of Sciences in 1980.

I count it as one of the greatest privileges in my life to have collaborated with John Sanders, a fine scientist and the most unassuming of men, deeply appreciative of the arts and bringing elegance, as well as incisiveness, to the sciences.

A.F. Moodie.

ASBUG LETTER NO 6

Dear Colleague,
following a suggestion I made at the Melbourne SR and more recently while on a visit to the PF, namely Workshop that Australian scientists would welcome an opportunity to be involved in the planning of a new instrument at the PF collaboration with PF staff (hopefully as a precursor to obtaining funding from Australia), I received the attached letter from Masami Ando.

In reply, I have sent some information on designs for a revolutionary state of the art high-resolution XRPD and SAXS instrument based on new types of monolithic x-ray monochromators developed at the Division of Materials Science and Technology. The instrument would incorporate such monochromator(s) matched to the resolution of an appropriate PSD. Also sent was some information from Dudley Creagh on a design for the monochromator system.

Following a recent request from DITAC (Stephen Utick of Bilateral Exchange Section) for information on benefits to precompetitive areas of research (their jargon, not mine) which would result from establishment of an Australian station at the PF, I sent the attached letter plus much supporting information. I believe he is preparing a supportive document for such a proposal which will be widely circulated, and strongly urge as many people as possible to send their own supporting statements plus a brief outline of projects where direct access to FF (in any areas of research, not necessarily, XRPD orSAXS) would be of value to their research, and any potential national benefits. I believe Australia would be able to exchange time on its instrument for time on other instruments such as a protein crystallography or EXAFS station.

In order to discuss these matters and to also prepare a proposal for submission to ARC (essentially update of previous ARGS proposal) for the establishment of a National Facility at the PF, I am proposing to hold a meeting in Melbourne

10 AM FRIDAY 19TH FEBRUARY IN THE SCHOOL OF PHYSICS AT THE UNIVERSITY OF MELBOURNE

If you are able to attend could you please contact either me (03-542-2918) or Zwi Barnea (03-344-7074). In order to give as much it is vital that people weight to this proposal as possible, bring or send brief outlines (a paragraph or two) on research proposals and projects to be carried out at PF.

Other items for discussion are:

- i) Prospects for the establishment of a small synchrotron radiation facility in Australia. There are some very exciting and rapid developments in this area and I plan to report on a visit which I made to Oxford Instruments last December where a small superconducting synchrotron is being developed for IBM.
- ii) Other options for direct access to SR facilities, exchange of information and opportunities for collaborative projects. I will be working at the PF for approx 4 months from mid-march '88 and would be happy to act as an intermediary in any proposals/projects. I expect to make several return visits to Australia during that time.

A new bimonthly magazine has been produced by Gordon and Breach entitled

SYNCHROTRON RADIATION NEWS

First issue came out in January and it appears to give a very good account of activities at different facilities, etc.

STEPHEN WILKINS

CAMBRIDGE CRYSTALLOGRAPHIC DATA BASE

Many will already be aware of the dire situation Australian crystallographers are facing regarding the continued availability of access to the Cambridge database and software. In a nutshell, Tony Graddon at CSIRO Information Services will no longer be acting as the Australian Affiliated Centre due to cuts in the CSIRO budget. This means that CSIRO Information Services must return tapes of the 1987 release of the database, and they are not permitted to hold any further copies of the database and software.

The implications for other Australian users are that after a period of three months grace, unless funds are forthcoming from elsewhere, any copies of the Cambridge system held by academic institutions will be recalled and, we understand, satellite access will also be curtailed, effectively cutting off access for all Australian researchers.

Previous to this alarming news, the SCA in conjunction with Tony Graddon wrote to the Cambridge Crystallographic Data Centre putting the case that funds for this service were desperately scarce, and requesting a review of the annual fee charged to the relatively small number of Australian crystallographers.

The response from Dr. Olga Kennard at the CCDC was to indicate that Australia has been charged at the rate of category II countries (i.e. countries having between 100-200 crystallographers listed in the World Directory). However, in view of the special circumstances, Dr. Kennard was prepared to offer a reduced subvention for 1988 of 16,000 Sfr - a 10% increase over the 1987 subvention, with no charge for the new software and enhanced database for which the actual charge should be Sfr 25,000.

Now for the ray of hope. Dr. David Winkler, a molecular designer at the CSIRO Division of Chemicals and Polymers, is keen for his Division to act as the new National Affiliated Centre. This, of course, depends on a sufficient number of users of the database being prepared to put in funds to meet the fee requested (ca. A\$17,000) - 12 users at \$1500 each is one possible solution.

In reality, we have little choice - to lose access Australia-wide would be disastrous, not just for crystallographers but also for those working in molecular design. The person to contact (quickly!) with offers of help is Dr. David Winkler, CSIRO Division of Chemicals and Polymers, GPO Box 4331, Melbourne 3001; tel. (03)647-7222 and FAX (03) 646-1984.

Syd Hall and Ted Maslen also intend to raise this issue later in the year in their capacities as members of the new IUCr Working Party for Crystallographic Information. If you have strong opinions regarding the Cambridge system, or databases/publication of crystallographic data in general, contact Syd or Ted on (09)380-2725.

ADVERTISEMENTS

NEWSLETTER POLICY: As a service to crystallographers and suppliers alike, Council has agreed to experiment with the inclusion of short (half an A4 page maximum), unpaid advertisements from any member of the SCA, as well as from suppliers of specialist crystallographic equipment. It is emphasised that this is an introductory service, and that the policy will be under review. Any supplier of crystallographic equipment or services is welcome to contact the Newsletter Editor with copy for this section; the Editor will have sole discretion as to whether the advertisement is appropriate for inclusion.

Corporate advertisers are reminded that the Society of Crystallographers offers corporate membership at the rate of \$100 per annum, and any applications for membership will be most welcome.

EMPLOYMENT

CSIRO Research Scientist (Materials Scientist)

A position to undertake research into the development and application of X-ray diffraction instruments for the microstructural characterisation of brittle materials including ceramics, composites and electronic materials is offered. Techniques to be applied include double-crystal diffractometry, topography and small-angle scattering.

Applicants should possess a Ph. D. degree in physics, materials science or equivalent qualifications and proven research ability in X-ray diffraction physics or a closely related field. A strong background in high-resolution X-ray diffraction techniques, X-ray optics and computing methods, as well as an aptitude for scientific instrument development are highly desirable. Experience in X-ray double-crystal diffraction, small-angle scattering and topographic techniques would be advantageous.

The appointee will be based at the Division of Materials Science and Technology Research Laboratory, Clayton, Victoria. Salary range \$28629 - \$41861. Indefinite tenure. Applications close 8th April 1988. For more information contact Dr. S. Wilkins or Ms. B. Bond on (03)542-2777.

New diffraction tube gives intensity plus resolution

The need to trade-off resolution for optimum peak intensity is a problem familiar to most x-ray diffractionists. So for the best solution has been to select a wide receiving slift to give maximum peak heights for measurement — and to accept the risk that closely spaced lines may not be separated.

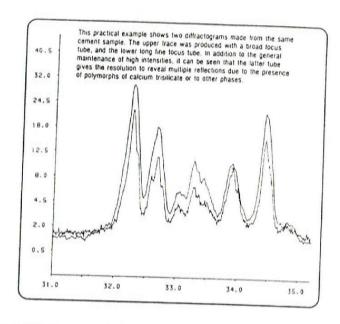
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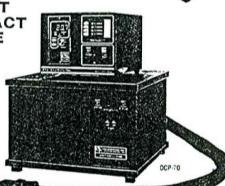
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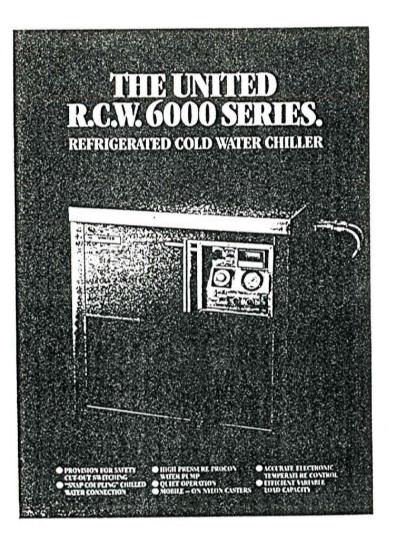
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An important feature of the R.C.W unit is its ability to accurately and efficiently track a set temperature without its its ability to accurately and efficiently track a set temperature without in the connected to multiple pieces of equipment where the total heat houd does not exceed the output of the chiller. Incorporated on the unit's recessed control panel, is an adjustable therm stat with easy to read scale, which is wired into the over-ride safety circuit, together with a low water level switch. Auxiliary contacts are provided on the safety circuit to connect to the load source, so that in the case of failure, supply to the equipment being civiled in the same time activating an alarm or wurning light. The over-ride circuit is designed so that the chiller will not automatically restart.

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nylon casters, providing mobility over reasonably smooth floors.

The top of the boxsing is clear of any components, manufactured of stainless steel to provide a clean work top, and removable to provide access to the chilled water reservoir and control systems. Sound absorbing material and thermal insulation are applied where appropriate in the units construction. CONSTRUCTION.

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and designed to high standards, for operation under extreme conditions.

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COMPRESSOR

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- 2 hp

RESERVOIR CAPACITY (Sunkey seel)

PUMP CAPACITY AT 50 PSI = 15 5 litres min 3-4 guillons min

THERMOSTAT

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TEMPERATURE STABILITY - Plus or minus 0.5"

TEMPERATURE RANGE - +5 to 35°C

POWER REQUIREMENTS = 15 amp 2+0 volt 50 HZ. Single Phas 8"0 x 560 x 895 34%* x 22* x 35%* DIMENSIONS LXWXH

WEIGHT



UNITED REFRIGERATION PTY. LTI

P.O. BOX 114, GREENSBOROUGH 3088, PHONE 435 2333