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COUNCIL FOR THE CENTRAL LABORATORY
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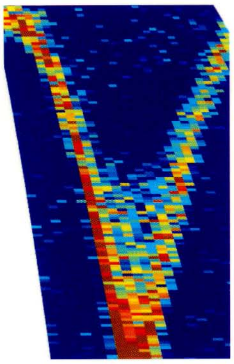
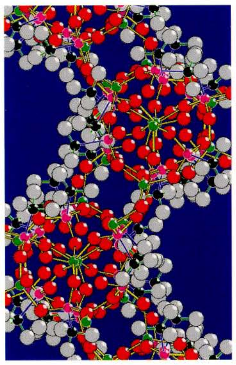
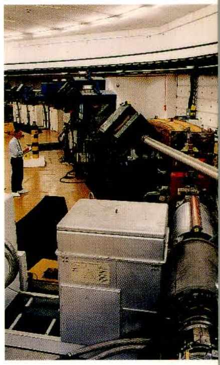
ISIS 99

The Rutherford Appleton Laboratory
ISIS Facility Annual Report
1998-99





ISIS

Foreword

MAPS – the most complex neutron scattering instrument yet developed.

ISIS, with its innovative technical developments, its widely acknowledged 'scientific culture' and its outstanding User Community, is an undisputed jewel in the UK Science Base. On the brink of the new millennium, ISIS finds itself riding high on the crests of many waves.

In September, the ISIS Review, chaired by Sir Michael Thompson, reported to Council. By all measures, ISIS passed with flying colours. The Review recognised that ISIS had greatly exceeded its original expectations and confirmed the outstanding scientific and technical achievements of the facility and its community. The Review endorsed our policy of planned refurbishment and strongly recommended the construction of a Second Target Station and its associated instrument suite. It is now up to us and the community to take these recommendations forward to the Research Councils and to our overseas Partners for timely funding of this crucial development.

A long overdue accelerator development programme is now well established. The RFQ test stand - critical for front end developments for both ISIS and the ESS – is now ready for operation. Good use has been made of internal Laboratory funding to initiate the R&D phase of the ISIS 300 μA upgrade – a necessary first step on the path to the Second Target Station. In collaboration with accelerator physicists from KEK and Argonne, the first of four dual harmonic rf cavities will be installed in ISIS early next year to test beam trapping and the first stages of high intensity acceleration.

The instrument development programme at ISIS is a truly outstanding achievement. MAPS – arguably the most complex neutron scattering instrument ever built – is beginning scientific commissioning, and the massive GEM detector array is growing daily. As the previous wave of developments – HiPr, TOSCA and OSIRIS - establish themselves in the scheduled programme, it is excellent to be able to announce the next generation of ISIS instruments: an advanced strain scanner, ENGIN-X; a factor ten enhancement to the SXD detector array; the EU-funded VESUVIO enhancement for eVS; a major upgrade for the HRPD 90° detector array; and the equally important advanced sample environment initiative.

Although I am personally sorry to say goodbye (at least temporarily) to my friend and colleague Colin Carlile, I know that at ILL he will continue to fight – as he has done so effectively at ISIS – for the neutron cause. Bon Voyage, Colin, and Haste Ye Back !

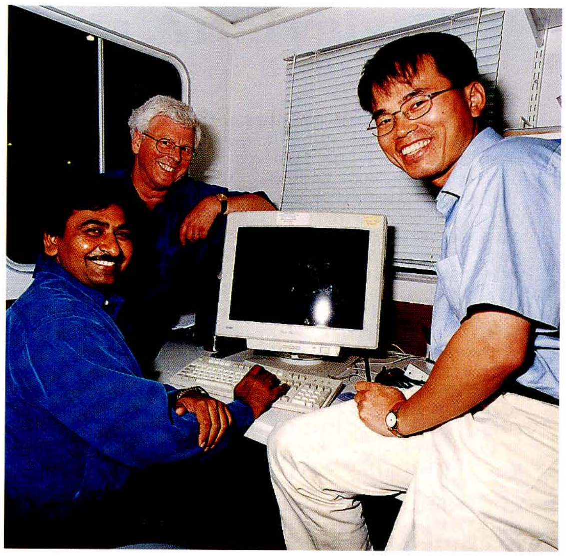
Top left: HRH The Duke of Kent learns about ISIS from Uschi Steigenberger during his visit to the Laboratory in December (98RC5871).

Lower left: Roger Stewart (Reading University), Chairman of the ISIS User Committee, with Colin Carlile (99RC3174).

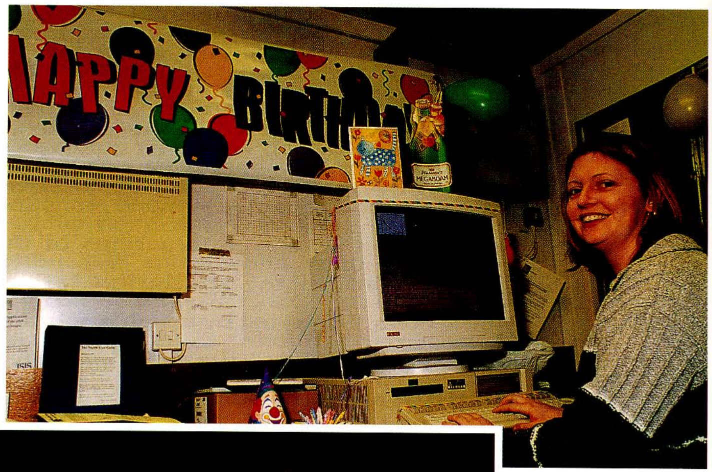
Top right: Bob Eisenstein, Director for Maths, Physics and Chemistry at the NSF, Washington, in discussion with Gavin Williams (99RC1544).

Centre: John Taylor, Director General of the Research Councils, with Andrew Taylor and Gordon Walker (99RC1417).

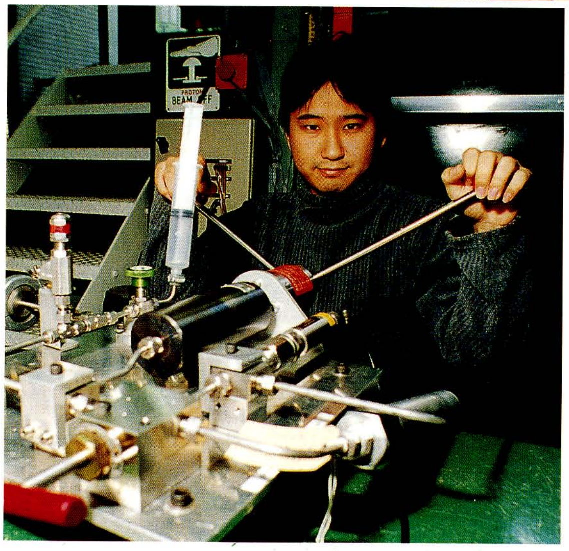
Above right: Sir Brian Fender, Chairman of the Higher Education Funding Council, tours ISIS with Andrew Taylor. Sir Brian received his knighthood for 'services to the University of Keele and HEFCE' in the Queen's Birthday Honours List. ISIS was proud to learn that Andrew Taylor had been awarded an OBE at the same time for 'services to neutron scattering' (98RC1834).

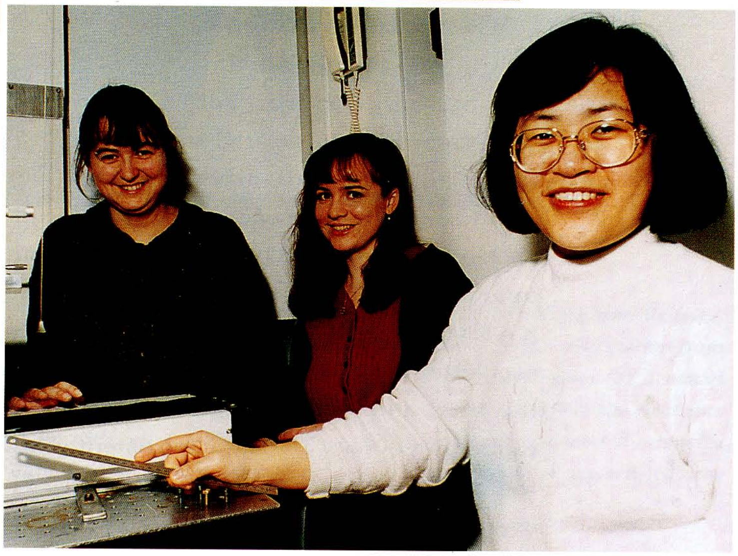


Left: Keith McEwen (UCL), DT Adroja (St. Andrew's) and Je-Geun Pak (Juhu University, Korea) studying non-Fermi liquid scaling in $CeRh_{0.8}Pd_{0.2}Sb$ on HET (99RC3619). Below: Marcy Lumsden (McMaster University) celebrated her birthday whilst investigating superconductivity in Sr_2RuO_4 on MuSR (99MC1168).



Right: Anna Llobet (CNRS) and Carlo Kaiser (TU Delft) preparing thin films of lanthanum calcium manganese oxide for study on CRISP (99RC3612). Lower left: Kenji Watanabe (Fukuoka University) studying methanol water mixtures on SANDALS (99MC1150). Lower right Tsueu-Ju Su, Becky Green and Jackie Brewer (University of Surrey) investigating protein adsorption using SURF (99MC2432).





Structure of Immunoglobulin A, a biological macromolecule

Antibody or immunoglobulin molecules play a critical role in our body's immune defence against bacteria and viruses. Immunoglobulin A (IgA) is not only present in blood but is also the predominant antibody class found in the mucosal surfaces of the lung and the gastrointestinal tracts, so forms a critical first line of defence against many invading pathogens. However, despite the abundance and importance of IgA, surprisingly little is known about the three-dimensional structures of the different IgA forms and how these relate to their unique roles in immunity. Small-angle diffraction using neutrons or X-rays is an ideal means to determine their solution structures; measurements on LOQ are helping to reveal the intermolecular arrangement and this in turn provides a better understanding of IgA's functional properties.

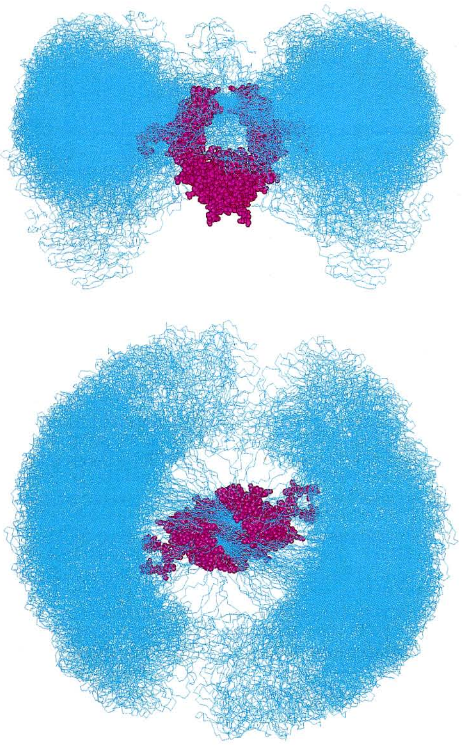


Figure F10.1. The best-fit models for the recombinant tailpiece-deleted IgA1 structure. Two orthogonal views of the 104 best-fit models for IgA1 are shown. The Fc fragment is shown in purple at the centre, while the 104 pairs of Fab fragments are shown in cyan. Adapted from Boehm et al (J. Mol. Biol., 1999) with permission.

Like other immunoglobulins, IgA has a basic monomeric structure composed of two heavy chains and two light chains, arranged into two identical Fab arms and one Fc region, separated by a flexible hinge region. The tips of the Fab arms are responsible for recognizing and binding to structures (antigens) on the surface of foreign cells or molecules. The Fc region interacts with specific receptors on the surface of phagocytic immune cells to trigger mechanisms such as engulfment and cell killing to eradicate the invaders.

IgA exists in a number of different molecular and polymeric forms. In humans, two different subclasses IgA1 and IgA2, have marked differences in their hinge regions. The IgA1 hinge possesses a stretch of 13 amino acids to which sugar groups are attached but this is missing from IgA2. In blood, IgA is mainly in monomeric form, and IgA1 predominates. However, in mucous, IgA is present chiefly as a dimer, and the relative concentrations of the two subclasses are more similar.

An atomic structure is only available for a murine IgA Fab fragment by crystallography, and none at all for an Fc region or an intact IgA, since antibodies are not easy to crystallize for reason of their size and flexibility. To help determine solution structures, measurements were made (using LOQ at ISIS and Stations 2.1 and 8.2 at Daresbury,) on monomeric IgA1 and a recombinant IgA1 (PTerm455) lacking a tailpiece (the 18 amino acid C-terminus of the heavy chain) on the Fc region.

A medium resolution structure to a precision of about 1 nm was developed by a novel highly-constrained technique in which molecular dynamics simulations of the IgA1 hinge peptides were used to create 12,000 randomised IgA1 models. Each one was

An ordered stack of spin valves in a layered magnetoresistive perovskite

In the past few years there has been a huge revival of interest in manganese oxides with cubic perovskite structure, $RE_{1-x}A_xMnO_3$ (RE = La, Pr, Nd and A=Ca, Ba, Sr, Pb), because of the very large magnetic field-induced changes in electrical resistance they can display. This phenomenon is known as colossal magneto-resistance (CMR). The magnetic fields are typically several Tesla, however, which limits applications in technologies such as magnetic memory and sensors. One approach for production of low-field magnetoresistance is to make ceramics with crystal structures that consist of multilayers of ferromagnetic manganite sheets separated by insulating material. This approach has recently succeeded with $La_{2-2x}Sr_{1+2x}Mn_2O_7$ for x=0.3. To determine the mechanism for this low temperature magnetoresistance magnetic neutron diffraction has been performed on single crystal samples using the IRIS and OSIRIS spectrometers.

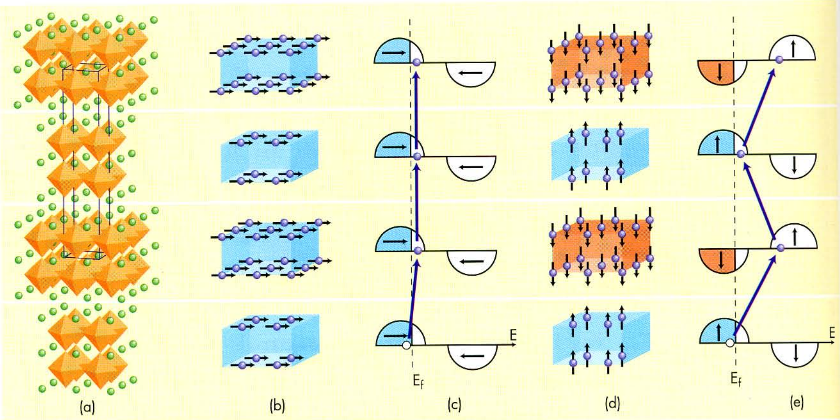
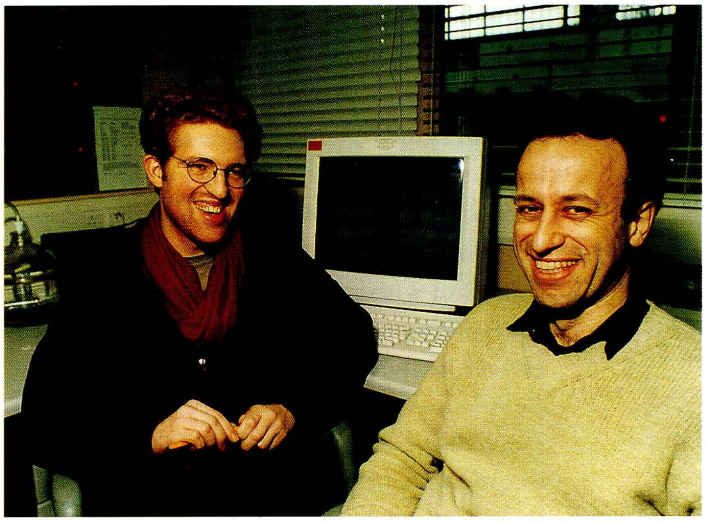


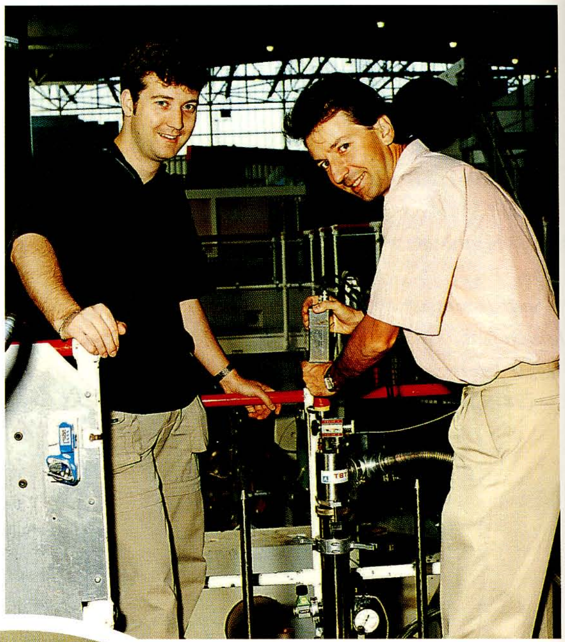
Figure F15.1. (a) $La_{2-2x}Sr_{1+2x}Mn_2O_7$ structure. The Mn ions are at the centre of the MnO_6 octahedra. Circles denote La and Sr. (b),(d): magnetic structure of the Mn sub-lattice with H=1.5T, H=0T. (c), (e): carrier transport for H=1.5 T, H=0T.

$La_{2-2x}Sr_{1+2x}Mn_2O_7$ is constructed from bilayer slices of MnO_2 sheets taken from the cubic perovskite, with the slices separated by insulating $(La,Sr)_2O_2$ layers (figure F15.1). With doping of x=0.3 holes per Mn site the material orders magnetically below T_c=90K. Above T_c the electrical resistivity perpendicular to the plane of the bilayers, ρ_c, follows the semi-conducting behaviour also seen in the cubic manganites, but the in-plane resistivity, ρ_{ab}, remains metallic to 270K (figure F15.2). Below T_c the resistivity is metallic in both directions. As is common for the cubic manganites, the magnetoresistance is greatly enhanced near T_c for currents both parallel and perpendicular to the MnO_2 planes (figure F15.2). What is new in the layered compound is that for temperatures far below T_c, substantial magnetoresistance remains. Furthermore, the low-temperature magneto-resistance is highly anisotropic and saturates at very small fields, as figure F15.3a shows.

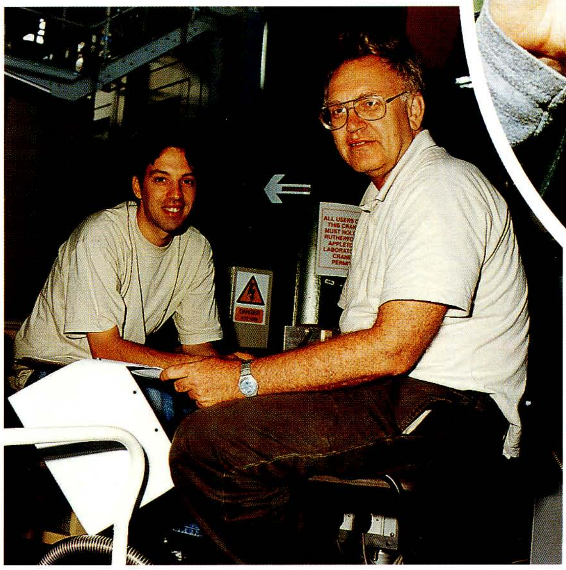
The results from neutron experiments at 4K«T_C = 90K are shown in figures F15.1 (centre, right). In zero applied field, the manganese moments are arranged ferromagnetically within a bilayer, but the bilayers are stacked antiferromagnetically. With an applied field of 1.5 T, chosen to be above the saturation field of 1T in figure F15.3a, the Mn moments remain ferromagnetically ordered within a bilayer, (albeit rotated by 90° from the zero field direction), but now the bilayers are stacked ferromagnetically.

Figure F15.3 shows the close correlation between the sharp switching of the resistance perpendicular to the planes and the similarly sharp switching from antiferromagnetic to ferromagnetic ordering on the Mn moments. The low-temperature, anisotropic magnetoresistance is similar to that seen in artificially constructed magnetic





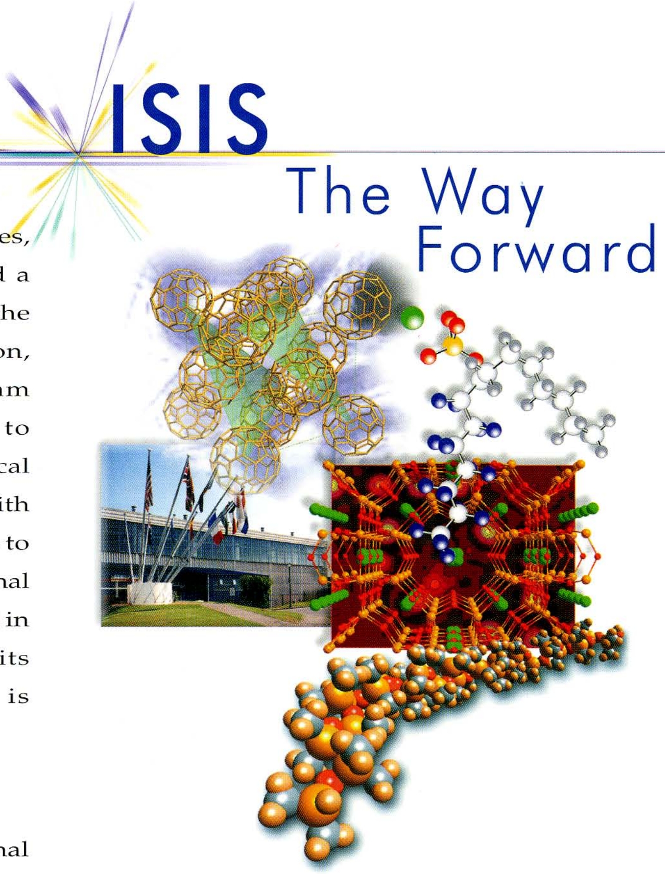
Upper left: Dickon Champion and Steve Bramwell (UCL) unravelling the structure of the pyrochlore $Gd_2Ti_2O_7$ on POLARIS (99MC1423). Upper right: Carlo Kaiser (TU Delft) and Pierre Dalmas de Reotier (CEA Grenoble) using the MuSR dilution refrigerator to study the heavy fermion superconductor UPt_3 (99RC3593). Centre: Sandrine Nave (Bristol) preparing her microemulsion sample for LOQ (99MC1422).



Upper left: Emial Polturak and Tuvy Markovitz (Technion Haifa) using PRISMA to explore solid Helium (99RC3606). Right:Takashi Kamiyama (Hokaido University), Toshiya Otomo, Masa Arai (KEK) and colleague exploring glasses on MARI (99RC3599).

News and Events

Review of ISIS



As part of its strategic audit of facilities, the Council of the CLRC commissioned a review of ISIS in early 1997. Under the chairmanship of Sir Michael Thompson, former Vice Chancellor of Birmingham University, the Review's remit was to consider the scientific output and technical performance of the Facility, together with scope for future improvements, and was to be clearly positioned within the international context. The Review reported to Council in September 1998, and a summary of its conclusions and recommendations is presented here:

Conclusions:

- ISIS has greatly exceeded its original expectations, and provides neutron facilities that are unmatched anywhere else in the world.
- UK university groups using the facility are consistently at the highest levels in international comparisons as revealed by the Funding Council's Research Assessment Exercises.
- The quality and professionalism of ISIS staff provide an exemplary environment for the training of young researchers, who make up the majority of ISIS users.
- Whilst the performance of ISIS has increased year on year over the past decade, it is close to its maximum performance level in terms of available time and source brightness. The current rate of applications for beamtime by well-qualified research groups significantly exceeds the capacity of the facility, a situation which is likely to continue and be exacerbated in the future. In order to satisfy future demand for the facility, there is a strong case for expanding the capability of ISIS to serve more users.

Recommendations

The Review recommends that:

- The CCLRC management should ensure that sufficient resources are given to supporting the ISIS facility in order to maintain the advantage given to UK research groups using neutron scattering.
- A crucial requirement in the near future is the refurbishment or replacement of the older sections of the linear accelerator.
- The financial arrangements for ISIS should be reviewed with the aim of ensuring long term provision for the replacement of capital equipment and plant.
- Owing to current levels of demand and forecasts for future usage of the facility, a second target station and associated instrument suite should be added.

Further information on the Review and its conclusions can be found in the brochure *'ISIS - The Way Forward'* produced by the facility.