PD. X–1 OLIGONUCLEOTIDE CONFORMATION AND DRUG BINDING. By Andrew H.-J. Wang and A. Rich, Department of Biology, Massachusetts Institute of Technology, Cambridge, MA 02139, USA.

The recent availability of synthetic oligonucleotides of defined sequence has changed our views in the understanding of the nucleic acids. We can now crystallize fragments of nucleic acids and analyze their structure by single crystal X-ray diffraction analysis, which often produces data at atomic or near-atomic resolution. Examples will be discussed of both right-handed and left-handed double helical structures as well as structures containing both RNA and DNA. In addition, the structure of several drug-nucleic acid complexes will be described. It shows in great detail the manner in which these drug molecules have both intercalating components, which bind to the minor groove of B-DNA, as well as hydrogen bonding components which anchor the drug to DNA through its interaction with base pairs on either side of the intercalative site. Analysis at this level makes it possible to contemplate the rational design of molecules such as daunomycin as well as triostin A so that they would interact more strongly as well as more specifically with particular nucleic acid sequences.

PD. X–2 NEUTRON DETECTION SYSTEMS FOR SPALLATION SOURCES. By J B Forsyth, Neutron Division, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon, OX11 0QX, United Kingdom.

The particular qualities of spallation neutron sources which influence the design of suitable neutron detection systems are outlined with reference to the characteristics of the traditional fission reactors. The principal differences include the pulsed nature of most spallation sources, which ensures that all scattering experiments involve time of flight measurements. The need to preserve a short pulse duration means that the spallation neutrons are undermoderated with a consequent increase in the number with epithermal as compared to thermal energies; new scattering instruments are being developed to exploit these shorter wavelength neutrons and detectors which are sensitive in the 0.1–10.0 eV are required. Some of the spallation sources now being designed or built have a brightness which significantly exceeds that of the best research reactors, and this can produce very high instantaneous and/or mean count rates in the detection system for the scattered beam. The area over which detection is required is frequently large to make full use of the white incident beam. Since observations are always made over a wide range of incident neutron energies, incident beam monitors must provide intensity versus energy information to allow normalisation to be carried out.

Recent developments in scintillation detectors are reviewed, including the discrete element, fibre-optic coded assembly and the neutron Anger camera. The principle of resonance detection is described and the potential of foil detectors, especially in the epithermal region, is discussed.

Specialised fast electronics must be provided in most detection systems to cope with the high counting rates and the possible need to veto counts resulting from a particular source pulse or pulses. An example of such a system, developed for instruments at the SNS, Rutherford Appleton Laboratory, is described.

17.1–1 SEARCH FOR A FRAGMENT OF KNOWN GEOMETRY BY INTEGRATED PATTERSON AND DIRECT METHODS. By Ernst Egert and George Sheldrick, Anorganisch-Chemisches Institut der Universität Tammannstraße 4, D-3400 Göttingen, F.R.G.

Patterson search methods have been shown by various authors to be a powerful tool for solving difficult light-atom structures when part of the molecular geometry is known (Egert, Acta Cryst. (1983) A39, 936 and references therein). They employ chemical information directly, and so can compensate for mediocre precision and resolution of the X-ray data. Nevertheless, they are not nearly as popular as direct methods, which owe part of their success to automation and superior computational efficiency. We have developed a procedure which tries to combine the merits of both methods in an attempt to exploit *all* the *a priori* available information. Whilst the orientation of a known fragment is determined by a conventional but highly automated Patterson rotation search, its position in the unit-cell is found by maximising the sum of the cosines of a small number of strong translation-sensitive triple phase invariants, starting from random positions. For those solutions which do not give rise to short intermolecular contacts a weighted Patterson minimum function is calculated. This procedure avoids the time-consuming refinement in Patterson space and should be especially efficient for large structures. Finally the best solutions are sorted according to a figure-of-merit based upon the agreement with the sharpened Patterson function, the triple phase consistency and an R-index involving E(obs) and E(calc).

This method has been implemented as a FORTRAN program which is valid and efficient for all space groups in all settings, and is compatible with SHELX-84. The rotation search can find the orientation of fragments of any size, and allows one degree of torsional freedom. The translation search may locate two independent search fragments of any size (including single atoms) taking into account (heavy) atoms at known fixed positions (if any). Tests with about 30 known structures of different size and complexity, using search fragments taken from other published structures or from force-field calculations, indicate that this novel combination of Patterson and direct methods is reliable and widely applicable. It thus offers an alternative strategy for solving large problem structures if chemical information is available.

It is hoped to make the program available on the same tape as SHELX-84. It has already been shown to be compatible with a wide range of computers, provided that sufficient memory (*at least 40K words*) may be addressed directly and that the word length is *at least 32 bits*.