space efficiently. Higher-level languages are extravagant in storage space and hence generally excluded, making it necessary to use low-level language to program small computers.

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Molecular Modelling and Computer Graphics

By C. D. BARRY and A. C. T. NORTH. (*Laboratory of Molecular Biophysics, Department of Zoology, University of Oxford, South Parks Road, Oxford OX1 3PS, U.K.*)

Computer graphics is a new and rapidly growing branch of computer technology. Its bearing on problems involving molecular structure seems obvious. This communication seeks to examine the field of molecular graphics and aims to outline the achievements and the hardware cost involved.

Specific uses of an interactive graphics system considered include: the display and manipulation of a computer-generated protein model and its application to the crystallographic determination of protein structure; the production of animated sequences and graphs illustrating chemical reactions and mechanisms for teaching purposes; and the use of programs capable of generating trial conformations for small molecular structures starting from input in the form of chemical formulae.

These examples indicate some current applications. There are many fields in which a graphical form of output is more readily comprehended than a digital one, and the true potential of the technique is likely to be limited only by the ingenuity of the user.

On-Line Applications in X-Ray Crystallography

By O. S. MILLS. (*Department of Chemistry, University of Manchester, Manchester M13 9PL, U.K.*)

The relative merits of consoles, terminals, computing terminals and graphical units are discussed in the context of application to crystallographic computation. In all these, there is a play-off between effectiveness, convenience, priority and intrinsic cost. The use to which terminal consoles, whether simple computing or allied with graphical facilities, will be put is discussed.

Computer Control of Mechanical Experiments on Muscle

By R. H. ABBOTT. (*Agricultural Research Council Unit of Muscle Mechanism, Department of Zoology, University of Oxford, Parks Road, Oxford OX1 3PS, U.K.*)

The special property of insect fibrillar flight muscle which enables it to contract rhythmically without synchronous nervous stimulation is the delayed component of the tension that results from an imposed length change. We have been investigating this phenomenon by using small bundles of glycerol-treated fibres of giant tropical water bugs. They are glued between a fixed-tension transducer and a moving-coil vibrator, and are bathed in a solution containing ATP and inorganic ions. The vibrator is mounted on a micro-manipulator to allow changes of mean fibre length, and is itself used to impose only periodic changes of length on the muscle fibres. If sinusoidal length changes are imposed, the delay appears as a phase lag between length and tension changes. Analysis of the change of this phase relationship with frequency shows that the delay is exponential, and its magnitude and time constant can be evaluated.

Information about the contractile mechanism may be obtained by measuring these characteristics under different mechanical and chemical conditions. To obtain a useful amount of information from a single preparation, the manipulation of the apparatus and logging of results must be done as fast as possible, and a human operator is unequal to the task. We have interfaced a PDP8/I computer to all the necessary devices, namely (i) a Solatron JM 1600 oscillator and resolved-component indicator to provide the sinusoidal drive and measure the phase and amplitude of the tension changes, (ii) a stepping motor drive attached to the micro-manipulator that adjusts mean muscle length, and (iii) a mechanism for changing the solution in which the fibres are immersed. The software allows the machine to be controlled by typing individual commands on the on-line teletype. These are single letters followed in some cases by a number. More usually, however, the commands are stored in the computer memory for automatic sequential execution. In this way the computer may be programmed with great simplicity to run an experiment lasting several hours without any manual intervention. A record of the experiment is printed on the on-line teletype, and a codified form of the results may be produced on paper tape.

It is known from other experiments that both Ca^{2+} and an increase of mean fibre length will activate the fibres in the sense of increasing their oscillatory work output. Closer analysis of their effects, by using the apparatus described, has revealed that, although both increase the magnitude

of the delayed component of tension, only Ca^{2+} has an effect on the time-constant of its development.

A Computer-Based Multi-Channel System for Automatic Chemical Analysis

By M. H. ABERNETHY, G. T. BENTLEY, D. GARTELMANN, P. GRAY, J. A. OWEN and G. D. QUAN SING. (*Department of Biochemistry, Alfred Hospital, Melbourne, Department of Biochemistry, Royal Melbourne Hospital, Melbourne, and Hospital Computer Study Group, Computer Centre, Monash University, Melbourne, Vic., Australia*)

For the past 2 years an on-line computer has been used for hospital biochemistry. Currently the

system covers 80% of the work load of the laboratory (250 000 tests/annum).

Standard AutoAnalyzers are used as basic analytical instruments and these are coupled to a PDP 8/S computer. The system collects data simultaneously from 12 test channels fed from six sample channels. Input of command instructions, the collection and processing of data and the output of results occur as time-shared processes. Results are identified by specimen laboratory accession number entered into the system manually. Each test channel is calibrated in terms of a third-order polynomial expressing the assay value as a function of the peak readings. Correction is applied for calibration drift and specimen interaction. Factors that were considered in the design of the system and the main features of the program are presented and discussed.

COMMUNICATIONS

Oxidation of *cis*- and *trans*-Acenaphthene-1,2-diol by Soluble Preparations from Rat Liver

By ELIZABETH C. DRUMMOND, P. CALLAGHAN and R. P. HOPKINS. (*Department of Biochemistry, St Thomas's Hospital Medical School, London S.E.1, U.K.*)

The dehydrogenation of *cis*- and *trans*-acenaphthene-1,2-diol to acenaphthenequinone by a rat liver microsomal preparation was demonstrated by Drummond & Hopkins (1969). Ayengar, Hayaishi, Nakajima & Tomida (1959) partially purified an enzyme (catechol reductase, EC 1.3.1.5) from acetone-dried rabbit liver powder that dehydrogenates *trans*-1,2-dihydrobenzene-1,2-diol to 1,2-dihydroxybenzene in the presence of NADP^+ , and a similar reaction would be involved in the oxidation of the acenaphthenediols to acenaphthenequinone if 1,2-dihydroxyacenaphthylene were the initial dehydrogenation product.

In the present work a preparation was obtained from acetone-dried rat liver powder that dehydrogenates *trans*-acenaphthene-1,2-diol in the presence of NADP^+ . The preparation was assayed by following the increase in extinction at 340 nm due to the diol oxidation product and NADPH in 50 mm-tris-HCl, pH 9.0, at 37°C. The preparation was made by chromatographing the 100 000g supernatant of a suspension of the acetone-dried powder in 0.15 M-potassium chloride on Sephadex G-25 equilibrated with 10 mm-tris-HCl, pH 8.0. This removes endogenous cofactor-reducing activity. The protein eluate was further chromato-

graphed on DEAE-cellulose equilibrated in the same buffer, the column being eluted with a sodium chloride gradient. A fraction was obtained with nine times the specific activity of the Sephadex G-25 eluate. This preparation differed from the microsomal system in that it catalysed the oxidation of *trans*-acenaphthene-1,2-diol more readily than that of the *cis*-isomer, and required NADP^+ , and not NAD^+ , as cofactor. A preparation with these properties was also obtained from the 100 000g supernatant of a homogenate of rat liver. An almost identical protein elution profile was obtained from the DEAE-cellulose column, and a similar degree of purification was achieved.

After incubation of *trans*-acenaphthene-1,2-diol and NADP^+ at 37°C with a preparation of the soluble enzyme at pH 9.0 for 2 h, acenaphthenequinone was found to be present in the reaction medium, showing that the end product of the reaction was the same as that obtained with the microsomal preparation.

Thus there are at least two systems in rat liver that dehydrogenate acenaphthene-1,2-diol: one in the microsomal fraction and another in the soluble fraction. This appears to be similar to the findings of Billings, Sullivan & McMahon (1970) on the dehydrogenation of indan-1-ol to indan-1-one.

Ayengar, P. K., Hayaishi, O., Nakajima, M. & Tomida, I. (1959). *Biochim. biophys. Acta*, **33**, 111.

Billings, R. E., Sullivan, H. R. & McMahon, R. E. (1970). *Biochemistry, Easton*, **9**, 1256.

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