TABLE I

Chemical formula	$C_{22}H_{26}N_2O$
Molecular weight	334·45
	$a = 15{\cdot}99 \pm 0{\cdot}04$ Å
	$b = 15{\cdot}91 \pm 0{\cdot}02$
	$c = 7{\cdot}66 \pm 0{\cdot}02$
	$\beta = 91 \pm 1°$
Space group	$p2_1/c$
	$Z = 4$
	$\rho_c = 1{\cdot}14$ gm . cm^{-3}
	$\rho_m = 1{\cdot}14$ gm . cm^{-3}
	(Flotation in aqueous KI solution)
	μ for copper K_α radiation $= 5{\cdot}61$ cm^{-1}.

The structure was solved by the direct methods followed by Fourier synthesis. The positional as well as the isotropic thermal parameters of all non-hydrogen atoms were refined to R = 0·145 by block-diagonal structure-factor least-squares procedure using 1654 observed reflections. Further refinement of the structure is in progress.

Figure 1 gives the projection of the structure in the *bc*-plane. The molecules associate in pairs about centres of inversion, the two molecules in

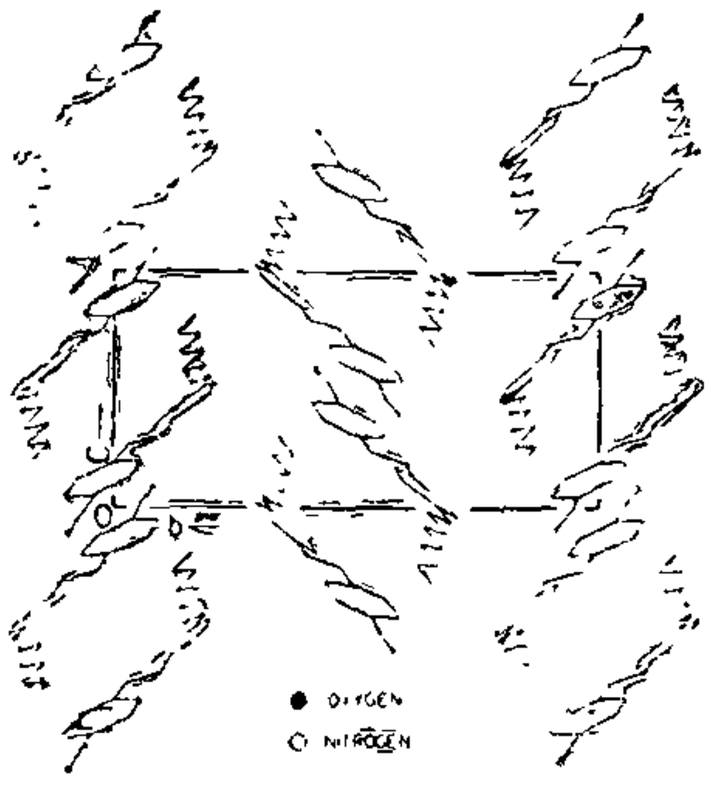

FIG. 1. Projection of the crystal structure in the *bc*-plane.

each pair being anti-parallel to each other. Along the *a*- and *c*-directions, adjacent pairs are related by cell translation and along the *b*-direction they are related by the 2_1 screw axes and the glide planes. Results of further refinement and the detailed description of the structural features will be discussed elsewhere.

The authors thank Prof. S. Chandrasekhar and Dr. S. Ramaseshan, for their kind interest. They also thank Dr. S. Venugopalan for giving the crystals.

Liquid Crystals Laboratory, G. V. VANI.
Raman Research Institute,
Bangalore 560 006,
and
Materials Science Division, KALYANI VIJAYAN.
National Aeronautical Laboratory,
Bangalore 560 017, *March* 30, 1976.

1. Kalyani Vijayan and Vani, G. V., *Pramāna Supplement*, 1975, 1, 75.

K-SHELL PHOTOELECTRIC CROSS-SECTIONS AT 32·879 keV IN INTERMEDIATE Z-ELEMENTS

IN order to supplement the existing data on K-shell photoelectric cross-sections, measurements at 32·879 keV in elements Y, Zr, MO, Ag, Cd and Sn have been made. The method used was similar to the one reported earlier[1]. Photons of energy 32·879 keV were obtained from the K-conversion of 662 keV level in Ba^{137m}. The results obtained are compared with the available theoretical calculations[2-4] (Table I) and are found to agree with the

TABLE I

Comparison of experimental data with theoretical calculations

z	Element	K-shell photoelectric cross-sections at 32·879 keV	
		Present measurements	Theoretical values
39	Y	2200 ± 190	(*a*) 2300
40	Zr	2700 ± 230	(*a*) 2450
42	Mo	2600 ± 220	(*a*) 2900 (*b*) 2900
47	Ag	4600 ± 390	(*a*) 4400 (*b*) 4350
48	Cd	4600 ± 390	(*a*) 4550
50	Sn	5300 ± 450	(*a*) 5350 (*b*) 5300 (*c*) 5300

(*a*)—Scofield; (*b*)—Schmickley-Pratt;
(*c*)—Rakavy-Ron.

theoretical calculations within the experimental uncertainties. The present results prove that the use of the theoretical values of the K-shell photoelectric cross-sections in our earlier determination[5] of the L-shell cross-section at 32·879 keV from the comparison of the intensity of L-shell fluorescent X-rays

with that of the K-shell fluorescent X-rays is justified.

Nuclear Science Laboratories, K. L. ALLAWADHI.
Department of Physics, S. L. VERMA.
Punjabi University, B. S. SOOD.
Patiala 147 002, *March* 29, 1976.

1. Allawadhi, K. L. and Sood, B. S., *Phys. Rev.*, 1975, 11 A, 1928.
2. Rakavy, G. and Ron, A., *Ibid.*, 1967, 159, 50.
3. Schmickley, R. D. and Pratt, R. H., *Lockhead Research Laboratories Report*, L.M.S.C. 5–10–67–11 NYO–3839–9.
4. Scofield, J. H., *Lawrence Livermore Laboratory Report*, 1973, UCRL 51326.
5. Allawadhi, K. L., Mohanjit Singh and Sood, B. S., *Curr. Sci.*, 1973, 42, 86.

OBSERVED CORRELATION BETWEEN COMPOSITION AND MOLECULAR WEIGHT OF AMINO ACIDS IN PROTEINS

THE composition of various proteins, in particular, the distribution of amino acids has been a topic of considerable interest. Early work[1,2] quoted in Meister[3] would appear to yield some general conclusions, although some of these need revision in the light of recent analysis (Dayhoff[4]) which is based on primary sequence analysis. The latter analysis has yielded the relative frequency of occurrence of the amino acids according to the classification of polar, apolar, heterocyclic (and aromatic) and ionisable types.

The randomness or otherwise of the occurrence of these amino acids has been treated statistically[5-7] and tables are available to assist in assessing whether or not their occurrence in a particular protein may be considered as random. Other statistical studies[8-16] are aimed at the analysis of the relative frequency of occurrence of residues in relation to the characteristic secondary structure of the protein chain, with a view to using them in algorithms for predicting protein structure from the given sequence. So also analysis from the point of view of volume occupied by side chain is also available[17]. However as far as we are aware of, no study seems to have been made on the relative abundance of the amino acids in relation to the molecular weight of the constituents.

We have done this and the simple linear correlation that has been observed, is felt to be sufficiently interesting to merit reporting here. Though Dayhoff's Table D 23[4] includes 108 proteins, a few fibrous proteins and also some small peptides have been included in it. In view of this we have selected 32 proteins whose structure by x-ray crystallographic methods have been reported and hence the sequence is uniquely known. This we believe is a sufficiently good sample to yield statistically meaningful result. Figure 1 shows the relation between relative frequency of occurrence and the molecular weight.

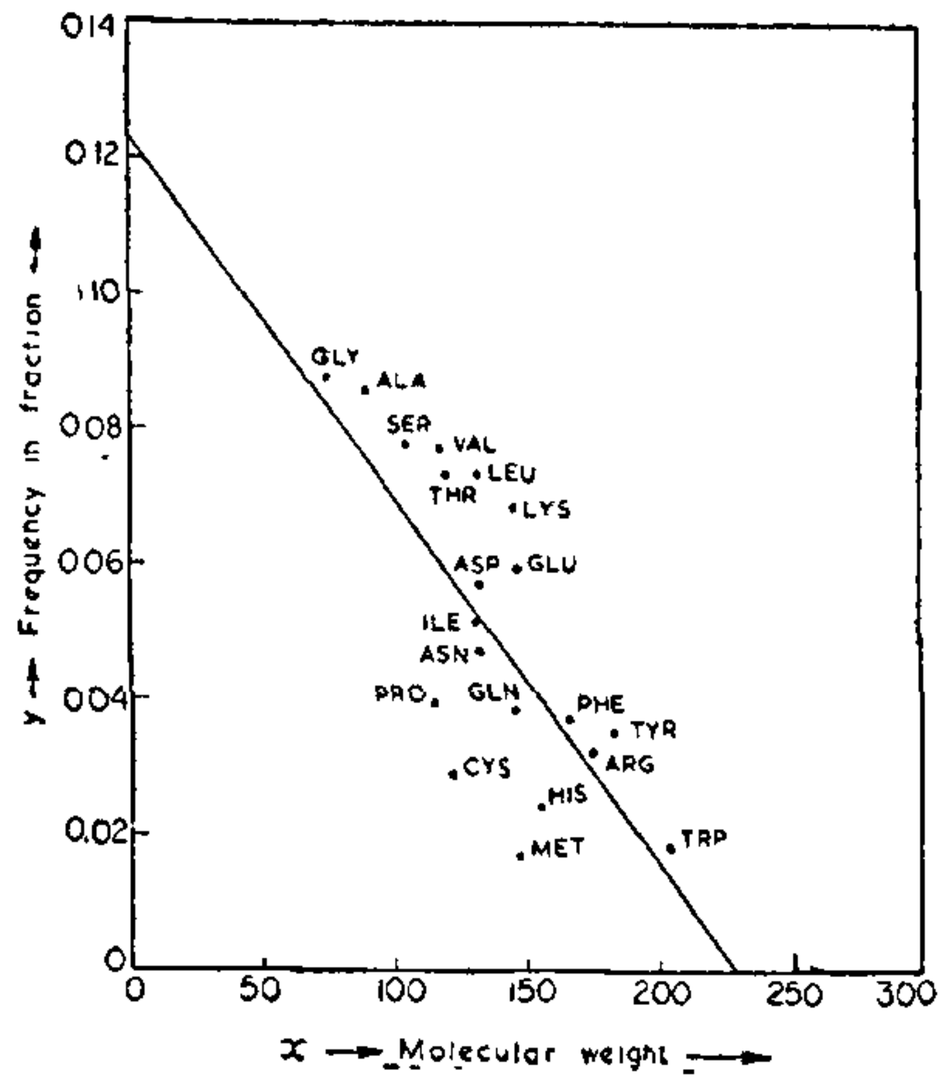

FIG. 1. Plot of molecular weight *vs.* the relative frequency of occurrence of amino acids in 32 proteins.

It is interesting to note that there is an approximately linear relation. The largest deviation from the above line is noticed for methionine and cystine and it is interesting that these two are amino acids containing sulphur. Among the rest, leucine (non-polar), lysine (polar) and histidine (heterocyclic) show somewhat large deviations.

The least squares equation to the line in Fig. 1 :

$$y = -0{\cdot}00054\ x + 0{\cdot}12445.$$

The equation leads to the result that nearly 67% of the amino acids are those having molecular weights less than 137 which is the mean of the 20 amino acids. At the two ends, the relative frequencies work out to be 8·4% for glycine and 1·4% for tryptophan. These are respectively about 70% more and 70% less than the mean (5%) to be expected if all the 20 amino acids are randomly distributed with equal probability.

Further analysis from this angle is in progress and results will be reported in due course.

Dept. of Crystallography and Biophysics, S. S. RAJAN. R. SRINIVASAN.
University of Madras,
Guindy Campus, Madras 600 025,
India, *July* 30, 1976.