STRUCTURE OF DL-ASPARTIC ACID

V. AMIRTHALINGAM AND G. N. RAMACHANDRAN

Dept. of Physics, University of Madras, Guindy, Madras-25

In a recent report,[1] Saito, Cano-Corona and Pepinsky have reported the structure of L-asparagine monohydrate, [$CO(NH_2).CH_2.CH(NH_2).COOH, H_2O$] in which they find that no cyclic structure is formed by internal hydrogen bonding, although such a structure has been suggested by Steward and Thompson[2] on the basis of the chemical properties of the compound. Aspartic acid [$COOH.CH_2.CH(NH_2).COOH$] is very similar in constitution and it is possible for a six-membered ring to be produced by one of the hydrogens of the amino group being attached to an oxygen of the carboxyl group by a hydrogen bond. In fact, such a structure has been postulated from chemical considerations by Stehlik and Liskova[3] for aspartic acid.

TABLE I

Co-ordination of atoms in DL-aspartic acid structure

	x	y	z
C_1 ..	0·038	0·161	0·049
C_2 ..	0·079	0·094	0·134
C_3 ..	0·000	−0·017	0·199
C_4 ..	0·027	0·047	0·290
O_1 ..	0·106	0·114	−0·011
O_2 ..	−0·092	0·236	0·094
O_3 ..	0·134	−0·060	0·308
O_4 ..	−0·058	0·154	0·312
N ..	−0·133	0·081	0·208

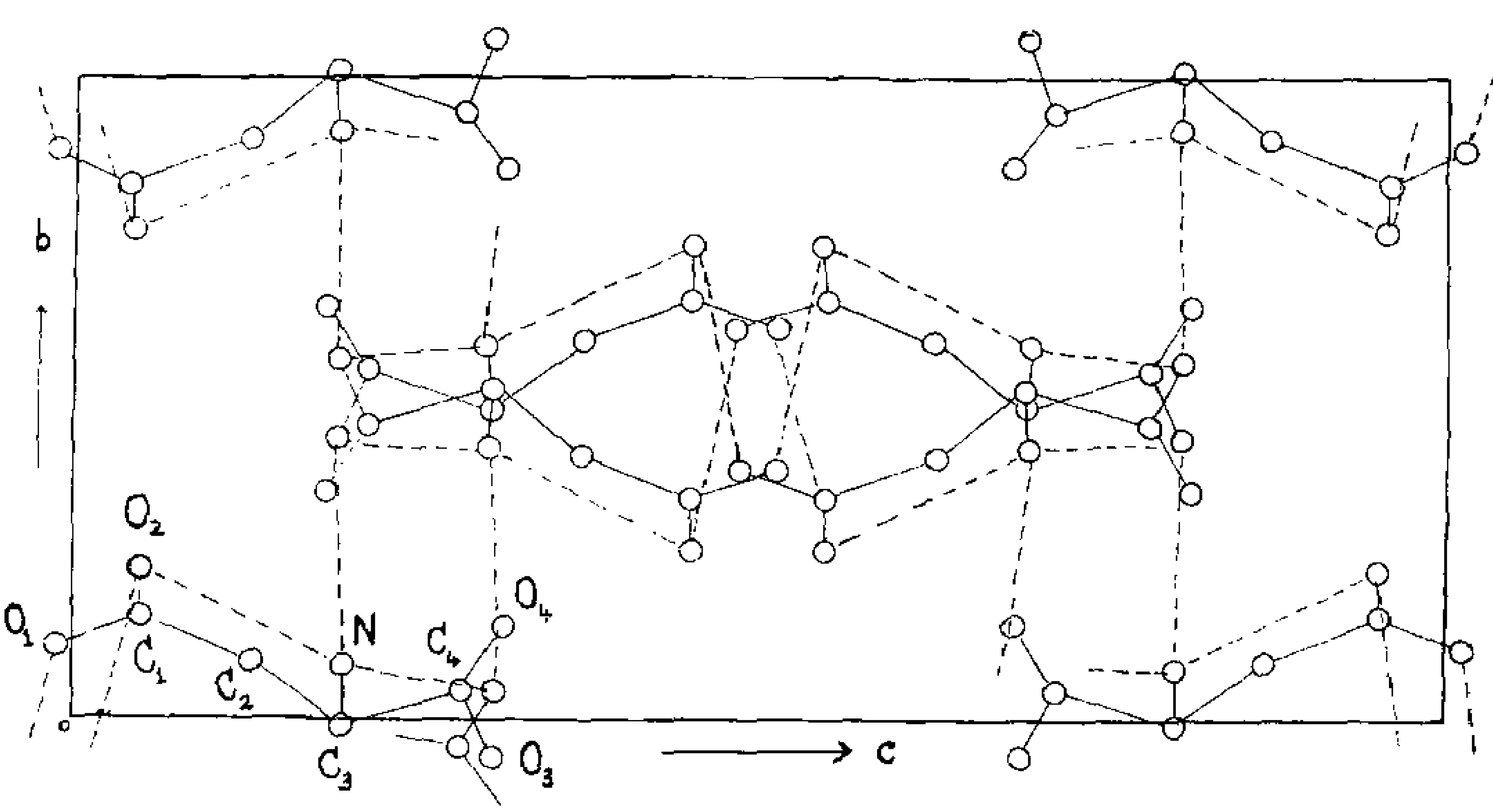

FIG. 1. Projection of structure on (100) plane.

The crystal structure of DL-aspartic acid has been determined by X-ray methods and it is found that an integral hydrogen bond definitely exists in this compound. The crystal is monoclinic with $a = 9\cdot18$A, $b = 7\cdot49$A, $c = 15\cdot79$A, $\beta = 96°$ and belongs to the space group I $2/a$ with 8 molecules per unit cell.[4] The structure was determined by a combination of trial and error methods making use of models, with the Patterson projection along a and b axes and signs determined by inequality methods. Both Fourier projections have large overlaps of atoms and the final positions of atoms were fixed from considerations of bond lengths and bond angles and by making use of an error synthesis. Table I gives the co-ordinates finally chosen; the positions of atoms are expected to be correct to 0·1A. The symbols for the atoms in this table are the same as those marked in Figs. 1 and 2, which give the projections of a unit cell on the (100) and (010) planes. The hydrogen bonds are indicated by dotted lines. The agreement between calculated and observed structure factors is fairly satisfactory, the R-values being 0·25 and 0·20 for the a and b projections.

As will be seen from the figure, (i) the molecule of aspartic acid has the zwitterion structure with three hydrogens attached to the nitrogen; (ii) one of the three hydrogen atoms is internally hydrogen bonded to the oxygen atom O_2 while the other two are bonded to

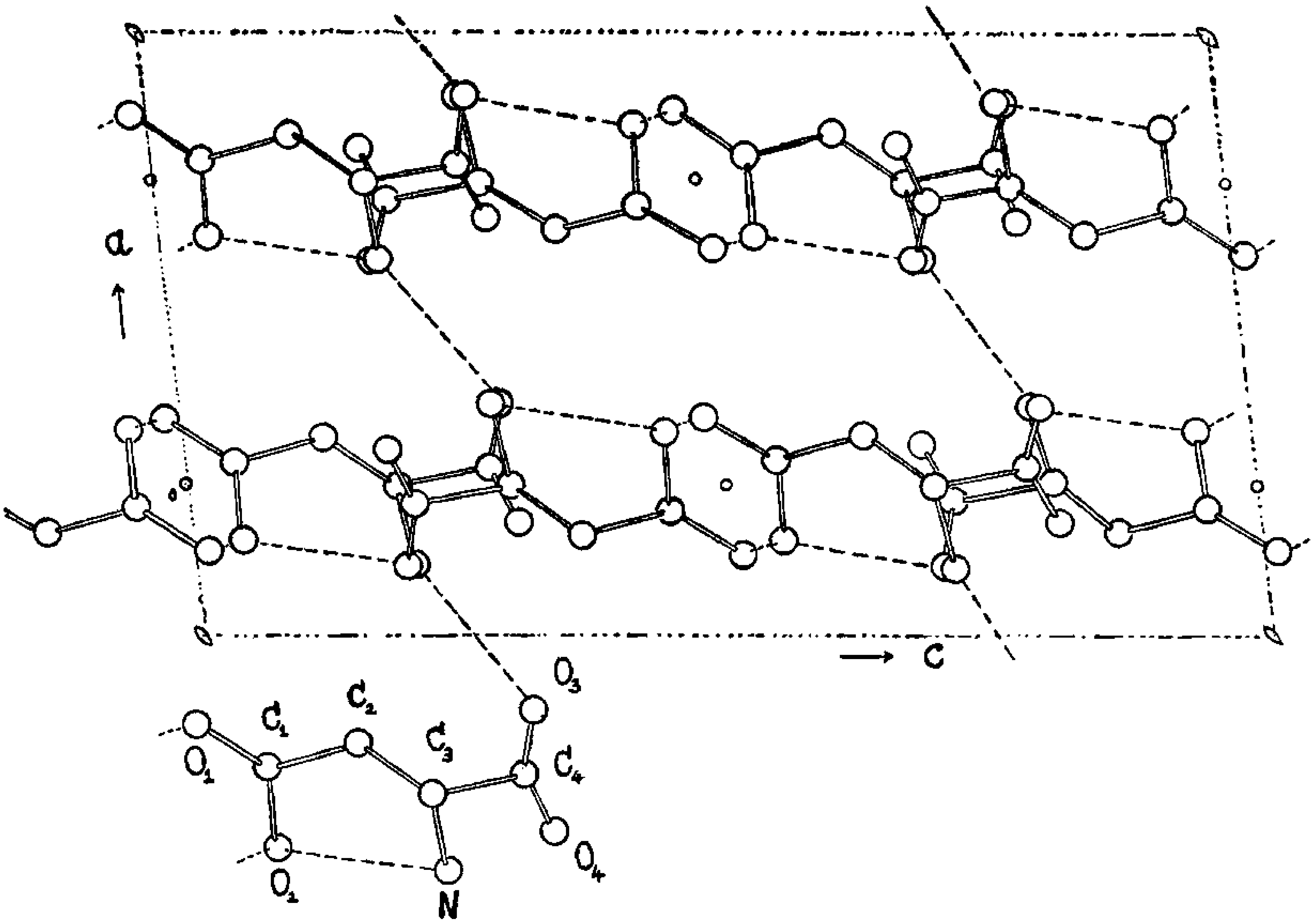

FIG. 2. Projection of structure on (010) plane.

oxygen atoms O_3 of different molecules; (*iii*) the molecule has its chain length nearly parallel to the long axis (*c*) and two molecules in a line are linked together mutually by means of hydrogen bonds formed between their carboxyl groups.

1. Saito, Y., Cano-Corona, O. and Pepinsky, R., *Science*, 1955, **121**, 435.
2. Steward, F. C. and Thompson, J. F., *Nature*, 1952, **169**, 739.
3. Stehlik, B. and Liskova, N., *Chem. Zvesti*, 1950, **4**, 60
4. Dawson, B. and Mathieson, A. McL., *Acta Cryst.*, 1951, **4**, 475.

THE PHOTOSYNTHETIC CYCLE

IN a paper presented before the International Conference on the Peaceful Uses of Atomic Energy, Professor Calvin of the University of California, Berkeley, U.S.A., has described the theory of a "photosynthesis battery" which has resulted from the researches of his group. The use of radioactive carbon to trace the source of chemical reactions in the plant has given insight into the order in which the plant makes chemicals and the way in which it takes energy from the sun and uses it for the chemical reactions.

By developing precise and delicate methods for separating and measuring the radioactive compounds formed by the plant, Prof. Calvin's group have isolated some fifteen compounds and traced the reactions needed for the complete process from CO_2 to sucrose. Compounds made by the plant in the first few seconds, sometimes in amounts less than a fraction of a microgram, were isolated and measured.

Studies of the carbon reduction cycle have led to a new theory as to how the energy absorbed by the chlorophyll from the sun is used to split the water molecule. This theory proposes an arrangement like a tiny battery, made of layers of chlorophyll between the microscopically thin layers of fat and protein. The battery absorbs sunlight and uses the energy of the sunlight to split the water molecule. The electrons freed from the water are held by a compound believed to contain sulfur until they are used by the enzymes in the carbon reduction cycle.

With this detailed knowledge it is claimed that it should be possible not only to increase crop growth but also to vary the kind of products obtained and to use small plants as factories for the production of concentrated fat, protein or sugar, as desired. With more knowledge of the "photo-synthetic battery" it should also be possible to devise more efficient means of converting solar energy to a form which can be used for power or fuel.