Table 1. *Coordinates of the carbon atoms of* 15,15′-*dehydro-β-carotene*

| Atom number | $y$ | $r = z-x$ | $x$ | $z$ |
|---|---|---|---|---|
| 1 | $0{\cdot}172_4$ | $0{\cdot}554_9$ | −0·703 | 0·852 |
| 2 | $0{\cdot}206_3$ | $0{\cdot}670_4$ | −0·673 | 0·997 |
| 3 | $0{\cdot}243_7$ | $0{\cdot}565_1$ | −0·558 | 0·007 |
| 4 | $0{\cdot}229_4$ | $0{\cdot}425_1$ | −0·340 | 0·085 |
| 5 | $0{\cdot}191_0$ | $0{\cdot}312_9$ | −0·340 | 0·973 |
| 6 | $0{\cdot}165_2$ | $0{\cdot}371_9$ | −0·513 | 0·859 |
| 7 | $0{\cdot}130_1$ | $0{\cdot}271_2$ | −0·528 | 0·743 |
| 8 | $0{\cdot}130_2$ | $0{\cdot}075_8$ | −0·438 | 0·638 |
| 9 | $0{\cdot}095_6$ | $0{\cdot}986_6$ | −0·440 | 0·547 |
| 10 | $0{\cdot}097_9$ | $0{\cdot}797_1$ | −0·338 | 0·459 |
| 11 | $0{\cdot}062_5$ | $0{\cdot}677_7$ | −0·312 | 0·366 |
| 12 | $0{\cdot}069_2$ | $0{\cdot}495_1$ | −0·205 | 0·290 |
| 13 | $0{\cdot}036_1$ | $0{\cdot}373_5$ | −0·172 | 0·202 |
| 14 | $0{\cdot}044_6$ | $0{\cdot}193_2$ | −0·068 | 0·125 |
| 15 | $0{\cdot}013_9$ | $0{\cdot}054_4$ | −0·015 | 0·039 |
| 16 | $0{\cdot}184_3$ | $0{\cdot}155_6$ | −0·122 | 0·034 |
| 17 | $0{\cdot}185_0$ | $0{\cdot}516_8$ | −0·883 | 0·634 |
| 18 | $0{\cdot}132_2$ | $0{\cdot}662_8$ | −0·780 | 0·883 |
| 19 | $0{\cdot}054_5$ | $0{\cdot}089_1$ | −0·548 | 0·541 |
| 20 | $-0{\cdot}012_9$ | $0{\cdot}439_9$ | −0·237 | 0·203 |

*trans* configuration of Fig. 1(*b*) to the *cis* form of Fig. 1(*c*). (The *trans* configuration of Fig. 1(*b*) is reported to occur in *trans*-β-ionylidene crotonic acid (MacGillavry *et al.*, 1951).) The last Fourier projection is shown in Fig. 2, with a superimposed projection of the molecule drawn from the parameters determined by the least-squares refinement. The atomic coordinates $y$ and $r$, where $r = z-x$, are listed in Table 1, along with preliminary $x$ and $z$ coordinates determined from models and from measurements in the three-dimensional Patterson.

Three-dimensional Fourier and least-squares refinements are in progress. A more precise description of the structure and the details of its solution and refinement will be reported later.

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## The unit cell, powder pattern, and space group of phenyl carbonate.

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About a year ago, structure investigations of certain organic carbonates were begun in this Laboratory. The study of ethylene carbonate had proceeded to the point of verification of parameters, when its complete structure was reported (Brown, 1954). Cell dimensions obtained in this Laboratory were

$$a = 8{\cdot}95,\ b = 6{\cdot}285,\ c = 7{\cdot}04\ \text{Å},\ \beta = 99°\ 43',$$

in excellent agreement with the reported values. The space group was verified as $C2/c$, and predicted parameters were close enough to those of Brown that the study was not continued.

A preliminary X-ray survey of phenyl carbonate, $(C_6H_5)_2CO_3$, has determined the unit cell and space group from precession photographs of two specimens of its orthorhombic, lath-shaped crystals.

$$a = 7{\cdot}52,\ b = 6{\cdot}09,\ c = 23{\cdot}47\ \text{Å}.$$

These data lead to a calculated density of 1·323 g.cm.$^{-3}$ for 4 molecules in the unit cell, to be compared with the reported specific gravity of 1·272. The only absent types of reflections are the odd orders of the three pinacoids. Accordingly, the space group is uniquely determined as $P2_12_12_1$. Atomic positions (exclusive of the hydrogen atoms) for the four molecules in the cell are thus fixed by 48 parameters.

The powder pattern of phenyl carbonate was recorded with nickel-filtered copper radiation in a Debye–Scherrer camera of 57·3 mm. radius. After measuring the $d$ spacings with the appropriate Nies scale, line intensities were obtained by comparing microphotometer traces of the powder pattern and a graded intensity scale. These data are presented in Table 1.

Table 1. *Principal lines of the powder pattern of phenyl carbonate*

| $d$ | $I/I_0$ | $d$ | $I/I_0$ |
|---|---|---|---|
| 11·5 | < 5 | 2·82 | 20 |
| 7·2 | 25 | 2·72 | 15 |
| 6·3 | 50 | 2·48 | 10 |
| 5·8 | 65 | 2·40 | 5 |
| 5·3 | 15 | 2·32 | 15 |
| 4·7 | 95 | 2·17 | 10 |
| 4·35 | 90 | 2·10 | 10 |
| 4·00 | 80 | 2·00 | 10 |
| 3·70 | 50 | 1·91 | 10 |
| 3·55 | 100 | 1·88 | 15 |
| 3·35 | 30 | 1·81 | 5 |
| 3·18 | 70 | 1·77 | 5 |
| 3·05 | 15 | 1·74 | 5 |
| 2·92 | 5 | | |

Because of the non-centrosymmetric space group observed, the effort necessary for a complete structure determination did not seem warranted at this time.

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