Acta Cryst. (1954). **7**, 595

The crystal structure of triphenylene.*

By V. Vand and R. Pepinsky, *X-Ray and Crystal Analysis Laboratory, The Pennsylvania State University, State College, Pa., U.S.A.*

(*Received* 12 *May* 1954)

Triphenylene, $C_{18}H_{12}$, is orthorhombic, with $a = 13{\cdot}20$ Å, $b = 16{\cdot}84$ Å, $c = 5{\cdot}28$ Å, space group $P2_12_12_1$. A structure has been reported by Klug (1950), who obtained his solution by the use of the Fourier transform method. Klug published two-dimensional Fourier projections on the (001) and (100) planes. His results give abnormally close intermolecular distances (as low as to 2·58 Å). These distances throw doubt on the correctness of Klug's solution.

We have reinvestigated the structure, using the computers X-RAC and S-FAC, and with Klug's observed values of structure factors. It appeared that there exist a number of near-homometric solutions, in which the molecule retains its orientation but is translated in two different directions corresponding to alternate changes of signs of certain groups of strong high-order reflections.

After some preliminary exploration of several such solutions, the physically correct solution has been obtained by forming a system of simultaneous quadratic equations for the important intermolecular approaches, and solving these by successive iterations, until all the distances became $\geqslant 3{\cdot}60$ Å. This solution proved at once to be the correct one when the map was observed on X-RAC, as judged by the roundness and equivalent heights of peaks, and absence of negative background. It is therefore to be concluded that in triphenylene all the intermolecular distances are normal, and there are no powerful bonding forces between the molecules as reported by Klug. The approximate coordinates of the center of the molecule are $x/a = 0{\cdot}20$, $y/b = 0{\cdot}08$, whereas Klug's coordinates were $x/a = 0{\cdot}18$, $y/b = 0{\cdot}14$. The shift amounts to more than 1 Å.

* Research supported by Grant No. A-228 from the National Institute of Health, National Institute of Arthritis and Metabolic Diseases. Computations on X-RAC and S-FAC supported by Contract No. N6onr-26916, T. O. 16, with the Office of Naval Research.

We are grateful to Dr Peter Friedlander of the Johnson Foundation, University of Pennsylvania, for pointing out to us the anomalies of Klug's solution.

Reference

Klug, A. (1950). *Acta Cryst.* **3**, 165.

Acta Cryst. (1954). **7**, 595

Lorentz polarization factors for precession angles of 10°, 15° and 21°.

By Masao Atoji and William N. Lipscomb, *School of Chemistry, University of Minnesota, Minneapolis* 14, *Minnesota, U.S.A.*

(*Received* 1 *June* 1954)

The use of smaller precession angles, 10°, 15° and 21°, is recommended for poorly defined crystals which show high background scattering, and for experimental arrangements which may restrict the precession angle to less than 30°. The ratio of Laue–Bragg reflections to the general background is considerably improved by the use of smaller precession angles, and we have used this method to improve the accuracy of intensity measurements as well as to obtain additional weak reflections. In addition, the presence of a cooling or heating system, the presence of a very large unit cell, or the demands placed upon the accuracy of the precession mechanism by an extremely small crystal are all situations for which smaller precession angles are sometimes useful.

The mathematical expression is that derived* by Waser (1951), and the results are plotted in the form given by Burbank (1952). For the sake of completeness the reader is also referred to the replotting of Burbank's results by Grenville-Wells & Abrahams (1952), and to the zero-level values for angles between 21° and 30° by Dulmage & Lipscomb (*International Tables*, vol. 2, to be published).

Values of $1/(LP)$ are expressed in terms of the cylindrical reciprocal-lattice coordinates, ξ (radial), ζ (axial) and τ (angular). Only values for $\tau = 45°$ are given in

Table 1. *Values of* $(LP)^{-1}$ *for zero level precession photographs at* $\mu = 5°$, 10°, 15° *and* 21° *at* $\tau = 45°$

ξ/μ	5°	10°	15°	21°
0·05	0·40	0·84	1·31	1·91
0·10	0·67	1·64	2·60	3·82
0·15	0·62	2·33	3·83	5·68
0·20	—	2·84	4·97	7·51
0·25	—	3·05	5·96	9·27
0·30	—	2·69	6·76	10·93
0·35	—	—	7·24	12·45
0·40	—	—	7·26	13·79
0·45	—	—	6·50	14·85
0·50	—	—	3·87	15·56
0·55	—	—	—	15·72
0·60	—	—	—	15·04
0·65	—	—	—	12·94
0·70	—	—	—	7·34
$\xi_{max.}$	(0·174)	(0·347)	(0·518)	(0·717)

* Corrected for typographical errors.