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Unit cell and space group of sublimed fumaric acid.

By L. G. ROLDAN, F. J. RAHL, and A. R. PATERSON, *Allied Chemical Corporation, Central Research Laboratory, Morristown, N.J., U.S.A.*

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In the course of an investigation of the crystallization of fumaric acid, two different crystalline forms were found.

One is obtained when a water solution is allowed to crystallize. This form was studied by Reis & Schneider (1928) who claimed it to be monoclinic, whereas Yardley (1925) reported it as triclinic. Our experimental data from an identical type of crystallization agree with the Reis & Schneider work.

A second type of crystallization was obtained by sublimation of the previous form at 220–235 °C. This new crystalline form is predominantly composed of needlelike contact twins. The twins are formed by two enantiomorphic structures in which the $(10\bar{1})$ plane is the plane of composition and also the twin-plane. The new cell is triclinic and is not, so far as we know, covered by any publication. Its parameters are:

$a = 4{\cdot}52 \pm 0{\cdot}02$, $b = 7{\cdot}51 \pm 0{\cdot}02$, $c = 5{\cdot}40 \pm 0{\cdot}04$ Å
$\alpha = 136{\cdot}7 \pm 0{\cdot}3°$, $\beta = 110{\cdot}6 \pm 0{\cdot}3°$, $\gamma = 72{\cdot}8 \pm 0{\cdot}3°$.

The number of molecules per unit cell is one. A calculated density of 1·63 g.cm^{-3} agrees with the observed density of 1·60 g.cm^{-3}. The space group $P\bar{1}$ is suggested by the absence of pyroelectric effect.

No further work on this compound is planned.

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Standard deviation of coordinates as a function of the residual and temperature coefficient.

By E. STANLEY, *University of Saskatchewan, Regina Campus, Regina, Saskatchewan, Canada*

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Tables of R, the residual, as a function of the standard deviation of coordinates, $\sigma(r)$, and temperature coefficient, B, have been calculated in two and three dimensions (Stanley, 1964, 1965). It has been suggested that tables in which the standard deviation of coordinates as a function of the residual were tabulated might be more use. These tables have now been prepared by interpolation from those previously published and give the values of $\sigma(r)$ in Å as a function of R and B for carbon atoms of the form suggested by Vand, Eiland & Pepinski (1957) within the limit of the sphere of reflexion of Cu $K\alpha$ radiation. From these tables it is probably more obvious how the data and the symmetry control the value of the residual. For three-dimensional data for a structure in a centrosymmetric space group with zero temperature coefficient, a residual of 5 % corresponds to a standard deviation of coordinates of 0·009 Å. The same residual for two-dimensional data for a structure in a non-centrosymmetric space group and a temperature coefficient of 4 Å^2 corresponds to a standard deviation of coordinates of 0·022 Å.

A comparison with other methods of estimating the standard deviation is interesting. The method of Booth (1947), as might be expected, gives estimates which agree very well with the present work. The [001] projection of triphenyl phosphate (Davies & Stanley, 1962) has a value of $R = 14$ % and a value of $B = 4{\cdot}5$ Å^2. The value of $\sigma(r)$ calculated by Booth's method is 0·04 Å. This agrees very well with the value of 0·04 Å obtained from the tables. Comparison with estimates of standard deviations made from the values of the slopes of the difference map at atomic