

in TiO_2 . These factors cause the induced dipole moment of the fluorine ions to be an order of magnitude less than that of the oxygen ions in TiO_2 . This leads to an energy correction of about 0.4% in the cases of the fluorides, which is not enough to bring the theoretical and experimental results into agreement.

In conclusion it should be emphasized that these results are at best approximate owing to the fact that the electric field varies both in magnitude and direction over the diameter of an oxygen ion in TiO_2 . It has been assumed here that the polarizing field is that at the center of the ion.

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A simple method for finding the plane of a planar, or partly planar, molecule. By J. L. LAWRENCE* and S. G. G. MACDONALD, *Carnegie Laboratory of Physics, University of Dundee, Dundee, Scotland*

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The plane of a molecule may be found simply by calculating the equations of all planes passing through the origin and two of the peaks in Patterson space, and the distances of all other peaks from each such plane. From the results, the approximate equation of the molecular plane will be obvious, and may be improved by least-squares techniques. This method has the advantage over the $I(\theta, \varphi)$ method that it requires only a small computer and little computer time.

A method of determining the orientation of the planar part of a molecule has been described by Tollin & Cochran (1964). In this method a disc is placed with its centre at the origin of Patterson space, its orientation being determined in terms of the spherical polar angles θ and φ which define the normal to the plane of the disc. The sum of the Patterson function over the disc, $I(\theta, \varphi)$, is calculated as the disc is rotated, and the orientation of the disc when this sum is a maximum is taken to correspond to the plane of the molecule. In this paper a simpler method for determining the molecular plane is described.

A list is made of all peaks in Patterson space which lie within such a distance from the origin as to include all intramolecular vectors. The equations of all planes passing through the origin and two of these peaks, and the distances of all other peaks from each such plane, are calculated. Many of the resulting planes will have approximately the same equation and will have many peaks situated close to them. The best-fit plane through all such peaks, defined as that plane for which the sum of the squares of the distances from the peaks to the plane is a minimum, is then calculated. This should be a good estimate of the plane of the molecule.

This method was used to determine the molecular plane of $\alpha\gamma$ -dimethyltetronic acid, $\text{C}_6\text{H}_7\text{O}_3$, which was believed to be almost wholly planar. The space group is $P2_1/c$, and the cell dimensions are $a=6.66$, $b=14.18$, $c=6.58 \text{ \AA}$, $\beta=100.3^\circ$. The molecular plane was found by the method described to be

$$0.18x + 0.98y + 0.00z = 0.$$

The equation obtained from the $I(\theta, \varphi)$ calculation was

$$0.275x + 0.960y + 0.004z = 0,$$

and the final equation of the plane obtained after determination of the structure was

$$0.284x + 0.958y - 0.038z = 0.$$

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Comparison of the equations of the two planes initially obtained with the equation of the plane in the final structure shows that the method of Tollin & Cochran gave a slightly better estimate of the molecular plane. The plane obtained from the $I(\theta, \varphi)$ calculation is less than 1° away from the final plane while the other plane was 4° off.

The main source of error in the determination of the molecular plane by the method described is probably due to including peaks which, although they lie near to the plane of the molecule, are not due to vectors between atoms in the planar parts of the molecule. If the molecule is large and only partly planar, there may be a number of such peaks. These peaks will also contribute to the $I(\theta, \varphi)$ calculations, but should not alter the position of the maximum. Further, since the latter method involves the summation of the Patterson function over a plane, the peaks are effectively weighted according to their height. The adoption of a weighting scheme may improve the method described here.

There is also the difficulty of deciding where the centre of a Patterson peak is situated, and whether the peak is a single or multiple one.

The advantage of the method is that it involves a very short and simple computer program while the $I(\theta, \varphi)$ calculation requires a complicated program run on a computer having a large storage capacity, even though the full Patterson function does not need to be calculated. Where access to a large computer is not available, and where computer time is at a premium, the method described will yield a starting point for a structure determination very quickly. It might even be possible in some cases to obtain the approximate molecular plane by visual inspection of the Patterson function, after which the least-squares plane may be calculated for the peaks near this plane, no computer being necessary.

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