ABSTRACTS

DEPARTMENT OF PHYSICS

1. ABSOLUTE VALUES OF PARAMAGNETIC RESONANCE ABSORPTION IN CRYSTALLINE COPPER SULPHATE. Miss K. Sundaramma and G. Suryan, *Curr. Sci.*, 1957, **26,** 80.

Paramagnetic resonance absorption in absolute units was measured in crystalline copper sulphate pentahydrate, by the method of comparing the peak resonance absorption of single crystals of copper sulphate in various directions with that of a standard substance.

2. DISPERSION OF PHOTOELASTIC CONSTANTS OF FUSED SILICA. E. S. Jog and R. S. Krishnan, *Nature*, 1957, **179,** 540.

The piezo-optic constants, q_{11} and q_{12} and the stress optical coefficient $C = [n^3/2\,(q_{12} - q_{11})]$ of fused silica have been measured for the range of wavelengths 2250–5700 Å. The quantity $q_{12} - q_{11}$ exhibits a dispersion of about 10% in the region of wavelengths studied.

3. AN ANALOGUE COMPUTER FOR DOUBLE FOURIER SUMMATION FOR X-RAY CRYSTAL STRUCTURE ANALYSIS. G. Suryan, *Acta Cryst.*, 1957, **10,** 82.

An outline is given of the analogue computer under construction in the laboratory, based on the general principles of the synchronous magnetic recorder. The salient points of the computer and its advantages over the more expensive ones are indicated.

4. THE CRYSTAL STRUCTURE OF AMMONIUM PERCHLORATE NH_4ClO_4. K. Venkatesan, *Proc. Ind. Acad. Sci.*, 1957, **46,** 134.

The crystal structure of ammonium perchlorate has been redetermined. The orthorhombic cell with space-group *Pnma* has four molecules in a unit cell of dimensions $a = 9{\cdot}13$ Å, $b = 5{\cdot}79$ Å and $C = 7{\cdot}47$ Å. The values of the atomic co-ordinates have been refined by double Fourier series methods and the final atomic positions determined are accurate to 0·02 Å. The positions of the hydrogen atoms have been obtained by the use of difference projection along the *b*-axis. In the structure, each chlorine is surrounded tetrahedrally by four oxygen atoms at a mean distance of 1·46 Å. Each ammonium ion is surrounded by twelve oxygen atoms at distances varying from 2·89 to 3·39 Å. The four hydrogens surrounding each nitrogen form weak N–N.O bridges with the nearest oxygen atoms. Tables are given for various atomic co-ordinates and interatomic distances.

5. The Use of Anomalous Scattering for the Determination of Crystal Structures—$KMnO_4$. S. Ramaseshan, K. Venkatesan and N. V. Mani, *Proc. Ind. Acad. Sci.*, 1957, **46**, 95.

The decrease in the scattering factor when the incident radiation is close to the absorption edge of an atom has been utilised for determining the structure of the centrosymmetric crystal $KMnO_4$. Multiple film zero-layer Weissenberg photographs were taken with CuK_α, CoK_α and FeK_α radiations, all of which are quite close to the K-absorption edge of the Mn atom. After reducing these data to the same relative scale, an Anomalous Difference Patterson (A.D.P.) map was computed with $(|F_{Cu}|^2 - |F_{Fe}|^2)$ as coefficient and it was found to have striking resemblance to the Isomorphous Difference Patterson map made with $(|F_{Cu}{}^{KMnO_4}|^2 - |F_{Cu}{}^{KClO_4}|^2)$ as coefficient. The structure was recovered from the A.D.P. diagram by means of the Buerger Vector shift method. An interesting offshoot of this technique is that the position of the excited atom could be directly determined by making a Patterson with $(|F_{Cu}| - |F_{Fe}|)^2$ as coefficient. From the knowledge of the position of the anomalously scattering atom and also its scattering factors for the different radiations, it was possible to assign the signs of as many as 50% of the reflexions. Commencing with these the structure was determined and the atomic parameters were refined. The final R-factor for the *(h0l)* and *(hk0)* projections were respectively 0·145 and 0·153. The parameters found are appreciably different from those reported earlier.

6. On the Rate of Ultrasonic Emulsification—By E. S. Rajagopal, *Curr. Sci.*, 1957, **26**, 142.

7. The Crystal Structure of Potassium Perchlorate—$KClO_4$. N. V. Mani, *Proc. Ind. Acad. Sci.*, 1957, **46**, 143.

The crystal structure of $KClO_4$ has been completely redetermined. The atomic parameters are found to be different from those reported previously for this crystal. The crystals are orthorhombic with space-group *Pnma* and 4 molecules in a cell of edges $a = 8{\cdot}83$ Å, $b = 5{\cdot}65$ Å and $c = 7{\cdot}24$ Å. The analyses of the structure and the refinement of parameters were carried out by the iteration process of difference synthesis technique. The very prominent diffraction effects encountered in the present case has been pointed out. A procedure involving removal of heavy atom contributions from the structure factors and the computation of Fourier map utilising these coefficients, was adopted to confirm the existence of these diffraction effects. The final discrepancy index calculated for the *(h0l)* and *(hk0)* zones were found to be 0·156 and 0·145 respectively. This value estimated after the removal of the heavy atoms K and Cl from the structure, amounted to 0·235. *In the structure each chlorine atom* is surrounded by 4 oxygens at a mean distance of 1·46 Å which lie at the corners of a nearly regular tetrahedron with Cl at the centre. Each K ion is surrounded by 12 oxygen atoms at an average distance of 3·1 Å. Tables are given for the various atomic co-ordinates and inter-atomic distances. Similarity of this structure to its two isomorphs has been pointed out.

8. ADIABATIC PIEZO-OPTIC COEFFICIENT OF HEAVY WATER. C. K. Narayanaswamy, P. S. Narayanan and R. S. Krishnan, *Nature*, 1957, **180**, 497.

The adiabatic piezo-optic coefficient of heavy water was determined by employing a Rayleigh Zeiss refractometer for sodium D line. It is concluded that while association may influence considerably the piezo-optic behaviour of liquids, it is the local anisotropy of the field around any molecule and the consequent changes in the polarisability of the molecules that should be taken into consideration in any theory for the optical properties of liquids.

9. COMPLEX MAGNETIC PERMEABILITY TENSOR AND PARAMAGNETIC RESONANCE ABSORPTION IN $CuSO_45H_2O$. Miss K. Sundaramma, *Proc. Ind. Acad. Sci.*, 1957, **46**, 232.

The paper presents the result of work done in order to investigate the intensity and comparison of intensities in paramagnetic resonance absorption in several directions of a single crystal of copper sulphate. It was the object of this investigation to see if the absorption tensor was also represented by an ellipsoid of revolution and if so to find the principal values of the tensor. It is found that the peak absorption is not represented by an ellipsoid of revolution. The total or integrated absorption is uniaxial and almost spherical.

10. PULSE SPREAD IN A PROPORTIONAL COUNTER. V. S. Venkatasubramanian and R. S. Krishnan, *Bull. Nat. Inst. Sci., India*, 1957, **9**, 35.

The 4π type of counter has the advantages of practically cent per cent. efficiency and avoidance of corrections due to back scattering. A simple form of 4π counter consisting of a cylinder with two off-axis wires equidistant from a diametral plane is considered. Expressions are derived for the pulse spread in such a counter, due to variation in gas amplification for particle tracks of varying directions. It is found that the spread is not significant enough to affect the counting characteristics.

11. PRELIMINARY REPORT ON THE STRUCTURE OF DIBARIUM CUPRIC FORMATE. Miss K. Sundaramma, K. Vedam and R. V. G. Sundara Rao, *Curr. Sci.*, 1957, **26**, 315.

12. THE USE OF ANOMALOUS SCATTERING WITHOUT PHASE CHANGE IN CRYSTAL STRUCTURE ANALYSIS. S. Ramaseshan and K. Venkatesan, *Curr. Sci.*, 1957, **26**, 352.

It has been pointed out that wherever one uses the isomorphous replacement method for the determination of non-centrosymmetric structures one could substitute the method of anomalous scattering without change of phase.

13. A CONTOUR GENERATOR FOR X-RAY CRYSTAL STRUCTURE ANALYSIS. S. Krishnan, *J. Sci. and Ind. Res.*, 1957, **16 B**, 432.

An electronic device has been developed for the presentation of a two-dimensional function as a contour map on the screen of a cathode-ray oscillograph to be used in conjunction with an analogue computer for X-ray crystal structure analysis. The function to be plotted is fed as an electrical voltage to one pair of plates of a cathode-ray tube in front of which a system of slits and a photomultiplier are placed. The pulse output from the photomultiplier intensifies the spot on a second oscillograph whose x and y time-bases are properly synchronised with the scanning of the function. The image photographed from the second cathode-ray tube is the contour map.

14. DIPOLE MOMENTS OF SATURATED DICARBOXYLIC ACIDS. P. T. Narasimhan, *Proc. Nat. Inst. Sci.*, 1958.

The dipole moments of oxalic, malonic, succinic, glutaric and adipic acids in dioxan have been reported and discussed in relation to their molecular structure. It is shown that the carboxyl groups of these acids exhibit rotation in dilute solutions in dioxan. The dissociation constants of these acids have also been discussed in relation to their dipole moments.

15. INFRARED INTENSITIES AND THE NATURE OF THE CHEMICAL BOND. P. T. Narasimhan, *Proc. Nat. Inst. Sci.*, 1958.

The differences in the $d\mu/dr$ values (μ=bond dipole moment and r=bond length) obtained from parallel and perpendicular infrared fundamental vibration bands of SO_2, NH_3 and PH_3 are ascribed to changes in the hybridization of the lone pair orbitals which will contribute to the moment derivatives due to stretch in the parallel bands but may not influence the perpendicular bands on account of symmetry. By making use of the plausible assumption that when the bonds in these molecules are stretched (totally symmetric mode) the S character of the lone pair orbitals tends to increase, it has been possible to study the variation of hybridization due to bond stretch from infrared intensity data. A discussion on the method of ascertaining the sign of $d\mu/dr$ of bonds, using the case of H_2O for illustration is also given.

16. STRESS OPTICAL COEFFICIENTS OF DIFFERENT SPECIMENS OF VITREOUS SILICA. R. S. Krishnan, E. S. Jog and R. Srinivasan, *Nature*, 1958, **181**, 692.

Measurements on the stress optical coefficients of two specimens of vitreous silica differing in homogeneity revealed a slightly higher value for the less homogeneous specimen. The two specimens do not differ in their refractive index values or impurity content. The more homogeneous specimen was neutron irradiated and it was found that neutron irradiation causes an increase in the stress optical coefficient of the specimen at all wavelengths. This can be attributed to the increase in the inhomogeneity of the specimen caused by neutron irradiation.

17. Ultraviolet Absorption Bands of Mercury Chloride. V. G. Krishnamurthy, *Zeits. Physik*, 1958, **150**, 287.

The ultraviolet bands of mercury chloride have been excited in uncondensed discharge and photographed with a quartz Littrow Spectrograph. The class II system between λ 2900 to 2700 suggested by Weiland as due to the triatomic molecule has been studied in detail. In addition to the bands already recorded by previous investigators, a number of new bands has been recorded in the present investigation. A new vibrational analysis of these bands is given. The entire bands are ascribed to the longer wavelength component of $^2\pi - {}^2\epsilon$ the other component being the system in the region λ 2650 to 2400 with a $^2\pi$ interval of 3335 cm.$^{-1}$ which is in keeping with the corresponding intervals obtained in the case of HgF and Hgl respectively. The following vibrational constants have been determined.

ν_e	ω_e'	ω_e''
36346 cm.$^{-1}$	385 cm.$^{-1}$	292·5 cm.$^{-1}$

18. Some Algebraic Identities. A. K. Rajagopal, *Math. Gaz.* (*London*), 1957, **41,** 137.

It is shown that some algebraic identities usually solved by cyclic symmetry may be solved, in a very elegant and interesting way.

19. A Curious Triangle. A. K. Rajagopal, *Math. Gaz.* (*London*), 1958, **42,** 40.

A set of problems on medians of a triangle has been extended to the case of the medians of a triangle by M. J. Satterly.

20. On Notes 2023, 2094, 2299. A. K. Rajagopal, *Math. Gaz.* (*London*), 1958, **42,** 43.

A particular sum is proved by a very simple and elementary way differing from the proofs given by three other authors. With the same technique two further results are obtained.

21. The Use of Complex Numbers in Obtaining Trigonometrical Identities. A. K. Rajagopal, *Math. Gaz.* (*London*), 1958, **42.** 53.

Complex numbers are used to combine the sine and cosine rules for a triangle to give a symmetric expression. To show the power of this, half-a-dozen identities are proved as illustration.

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