

(c) The vanishing of CESR below T_c can not possibly be due to the reasons put forth by Venkataraman *et al.*

(i) Similar results were obtained for samples measured near their T_c . Moreover, the CESR results of Schultz *et al.*⁹, where Al was in the forced normal state, provide a strong credence to our contention. In fact the reported Knight shift data of A-15s¹⁰ and magnetic susceptibility measurements of Ekbote *et al.*¹¹ on Nb₃Sn and V₃Si single crystals are more readily explained in terms of our model.

(ii) The spin lattice relaxation time at low temperature, in superconducting state has been fully discussed by various theorists and they have shown that it is not much different from the normal state¹⁰.

(iii) The skin depth in superconductor has been well discussed by Pippard¹² and others more than 30 years ago. The skin depth is of the same order as the penetration depth λ and our samples are approximately $\lambda/2$ thick. Thus, this satisfies the conditions given by the theorists^{13,14} for observing CESR in superconductors.

(iv) The dielectric properties of the present materials are not altered at low temperatures so that the question of change in the microwave configuration inside the cavity does not arise.

In the light of the above we believe that the points raised by Venkataraman *et al.* are not responsible for the vanishing of the CESR. Finally we may mention that some of the other features, which we believe are important to the present study, are discussed in our comprehensive work on CESR and spin waves in various A-15 materials possessing a range of T_c values from non-superconducting to 22.65 K, which is being published elsewhere¹⁵.

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A SIMPLE METHOD OF CALCULATING THE VOLUME OF ANY DISTORTED COORDINATION POLYHEDRON IN CRYSTAL STRUCTURES

USUALLY during the analysis of crystal structures, the shapes of the coordination polyhedra occurring in them are identified and the metal-ligand distances and related angles are listed. But very rarely are the volumes of such polyhedra calculated and their values presented. The volumes comprise additional information that is useful in many ways, for example, in explaining the relative stabilities among the different phases of some crystal structures and probably in explaining the occurrence of a particular polyhedron among the various possible polyhedra for a given coordination number.

In text-books on solid geometry, formulae are available for calculating the volume of many regular convex polyhedra. For distorted convex polyhedra, the volume can be calculated by dividing them into many tetrahedra and finding the volumes of the tetrahedra. This method, though not entirely new, is presented here for the simple reason that it is not found in ready reference books such as *International Tables for X-ray Crystallography*.

All convex polyhedra can be resolved into tetrahedra, one of the triangular faces of which becomes a face (or part of it) of the polyhedron. The volume of a tetrahedron OABC constructed with the origin O and the points A (x_1, y_1, z_1), B (x_2, y_2, z_2) and C (x_3, y_3, z_3) as the vertices is equal to one-sixth of the value of the determinant formed with the coordinates of the points A, B and C as the rows of the determinant. It should be noted here that the coordinates should be in Å referred to an orthogonal coordinate system and also that the volume of the tetrahedron thus calculated is always signed (either positive

or negative). The volume of the polyhedron is then the modulus of the algebraic sum of the volumes of the various tetrahedra. Suitable modifications can be made in the standard bond scan programs to obtain the information concerning the volume also.

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THE DIPOLE MOMENT OF *n*-BUTANOL-CARBONYL ADDUCTS

THE dielectric polarization studies of the molecular interaction in liquid phase can be used to determine the dipole moment of the complexes and hence the change of the dipole moment defined as,

$$\Delta\mu = \mu_{\text{complex}} - (\mu_a + \mu_b)$$

where μ_a and μ_b are the dipole moments of the *a* and *b* components, which reflect the charge redistribution along the X-H...Y bond. Several investigations¹⁻³ have been carried out to ascertain the nature of complexes by fixing the most favourable structures of the complexes. Presently the dielectric polarization studies of a few *n* butanol vs. carbonyl systems are used to determine the most favourable structures of the complexes formed.

The WTW dipole meter was used for dielectric measurements at 2 MHz with the cell maintained at 30°C ± 0.01°C. From the dielectric constant measurements of the solutes in the mixed solvent of *n*-butanol and carbontetrachloride, the dipole moment of the 1:1 complexes of *n*-butanol and carbonyls formed were calculated employing the method of Huysken's *et al.*⁴ based on Onsager theory. The results are given in Table I.

The most favourable position for the maximum interaction between the lone pair atomic dipole and O-H bond is that position for which the hydrogen bonds formed, by carbonyl compounds should be along sp^2 lone pair⁵ direction of the carboxyl group. This means that the angle between the C=O axis and O-H bond should be 60°. In the case of ketones and acetates the *trans* and *cis*-structures are given in Fig. 1. The dipole moments μ_{ab} of the complex for both structures are presented in Table I.

Schuster⁶ by the LCAO-MO studies of the hydrogen bonding, between carbonyl and hydroxyl groups

TABLE I
The calculated and experimental dipole moments of *n*-butanol-carbonyl complexes

<i>n</i> -butanol + various carbonyls	μ_{ab}^* (D) (calc.) <i>trans</i> structure	μ_{ab}^* (D) (calc.) <i>cis</i> structure	μ_{ab}^* (D) (obs.)
(a) Methyl ethyl ketone	2.88	4.32	3.19
(b) Cyclohexanone	2.98	4.44	3.36
(c) Methyl acetate	2.09	3.30	2.49
(d) Ethyl acetate	2.10	3.37	2.47

* The values given above are in Debyes unit.

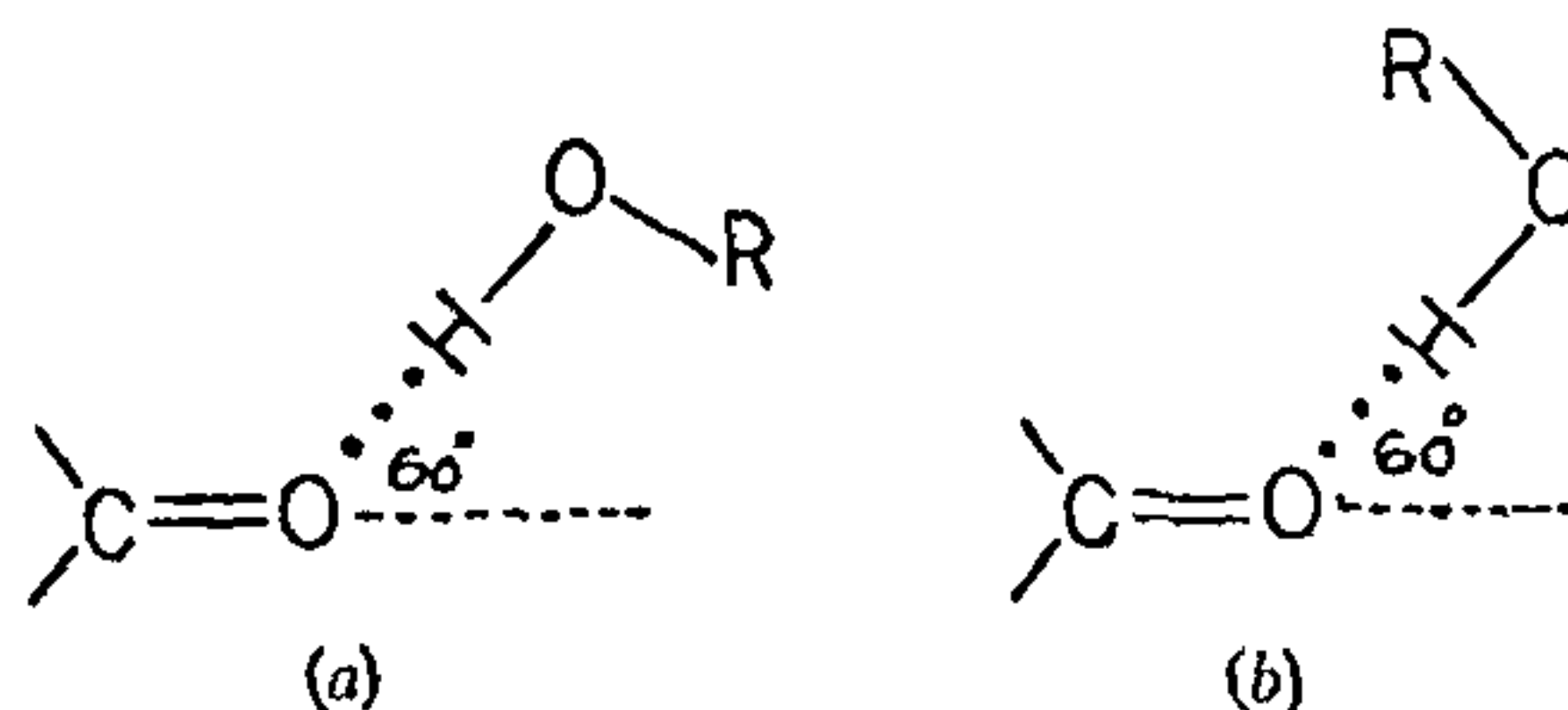


FIG. 1. (a) *Trans* structure; (b) *Cis* structure.

showed that in structures with the same orientation of the functional groups forming the hydrogen bond, the arrangement with the smaller dipole moment had the lower energy. Also the experimentally observed dipole moment is nearer to that of *trans* structure and hence the *trans* form seems to be the most favourable, in all the systems studied here.

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