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 dieletcric 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,

$$\Delta \vec{\mu} = \vec{\mu}_{complex} - (\vec{\mu}_a + \vec{\mu}_b)$$

where μ_a and μ_b are the dipole moments of the *a* and *b* components, which reflect the charge redistribution along the $X - H \cdots Y$ bond. Several investigations[1-3] 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 measurments at 2 MHz with the cell maintained at $30° C \pm 0.01° C$. 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 pair[5] 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.

Schuster[6] by the LCAO-MO studies of the hydrogen bonding, between carbonyl and hydroxyl groups

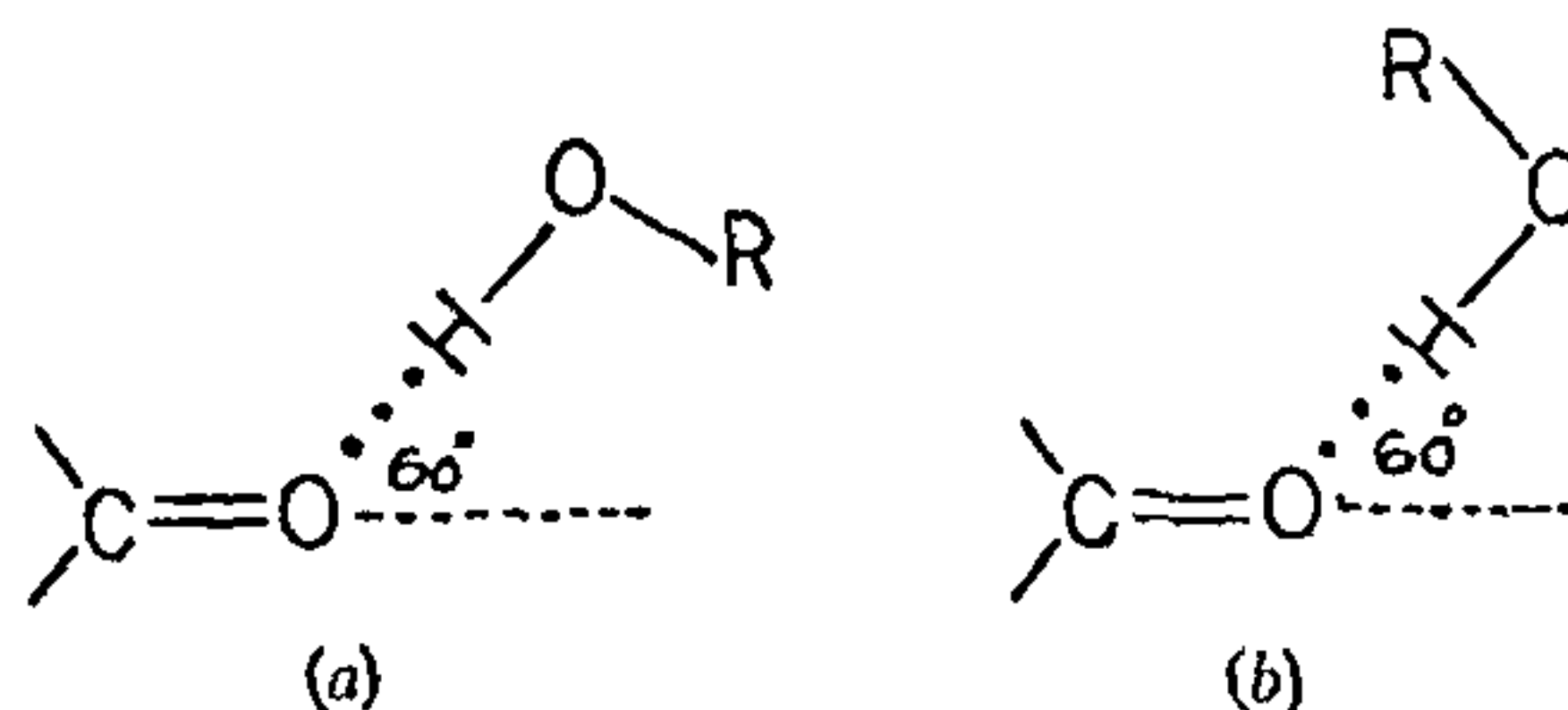| *n* butanol + various carbonyls	μ_{ab}^* (D) (calc.) *trans* structure	μ_{ab}^* (D) (calc.) *cis* structure	μ_{ab}^* (D) (obs.)
(*a*) Methyl ethyl ketone	2·88	4·32	3·19
(*b*) Cyclohexanone	2·98	4·44	3·36
(*c*) Methyl acetate	2·09	3·30	2·49
(*d*) Ethyl acetate	2·10	3·37	2·47

* 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 funtcional groups forming the hydrogen bond, the arrangement with the smaller dipole mowent had the lower energy. Also the experimentaly observed dipole moment is nearer to that of *trans* strutcure and hence the *trans* form seems to be the most favourable, in all the systems studied here.

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1. Cleverdon, D., Collins, G. B. and Smith, J. W., *J. Chem. Soc.*, 1956, p. 4499.
2. Debecker, A. and Huyskens, P., *J. Chim. Phys.*, 1971, 68, 287.
3. Shanmugasundaram, V. and Meyyappan, S. Rm. M., *Z. Phys. Chemie*, 1977, 258, 673.
4. Huyskens, P., Huyskens. Z., Duterme, P. and Clerbaux, T., *J. Chim. Phys.*, 1967, 64, 1326.
5. Murthy, A. S. N. and Rao, C. N. R., *J. Mol. Struct.*, 1970, 6, 253.
6. Schuster, P., *Int. J. Quantum Chem.*, 1969, 3, 851,