

**SIMPLIFIED CALCULATION OF DIPOLE MOMENTS AND POLARIZABILITIES FROM VAPOR-PHASE MEASUREMENTS OF DIELECTRIC CONSTANT AND REFRACTIVE INDEX**

VAPOR-PHASE measurements of dipole moments and polarizabilities, though more difficult to carry out experimentally, are able to yield much more accurate values for these quantities than measurements on liquids or solutions, due to the absence of induced dipoles and intermolecular polarizations.

A well-known method for calculating dipole moments of polar molecules in the liquid state or in solution of a non-polar solvent is that of Debye<sup>1</sup>, using the corresponding molar polarization  $P_m$  and the molar refraction,  $R_m$ , where  $P_m = [(\epsilon - 1)/(\epsilon + 2)] V_m$  and  $R_m = [(n_D^2 - 1)/(n_D^2 + 2)] V_m$  in which  $\epsilon$  is the dielectric constant of the polar liquid,  $n_D$  its refractive index using the Na-D line radiation, and  $V_m$  is the molar volume ( $M/\rho$ ) under the conditions of measurement. Debye's final widely used<sup>2</sup> equation is

$$\mu_D = \left[ \left( \frac{9kT}{4\pi N_0} \right) (P_m - R_m) \right]^{1/2} = 0.0128 \sqrt{T (P_m - R_m)}, \quad (1)$$

where  $\mu_D$  is the desired dipole moment (in D units),  $k$  is Boltzmann's constant,  $N_0$  Avogadro's number, and  $T$  is in °K.

If, instead, gas-phase measurements of these quantities are used, thereby avoiding to a great extent intermolecular interactions, one can arrive at a very simple equation, and avoid the intermediate calculation of  $R_m$  and  $P_m$ .

The new equation is obtained by noting that  $V_m$  is  $2.24 \times 10^4 \text{ cm}^3$  for all gases† at standard T and P, and that  $(\epsilon + 2)$  and  $(n_D^2 + 2)$  are both very close<sup>1,2</sup> to 3. One then has under these conditions

$$P_m - R_m = \frac{V_m}{3} (\epsilon - n_D^2) = \frac{4\pi N_0 \mu_D^2}{9kT} \quad (2)$$

and therefore

$$\mu_D = \left[ \frac{3V_m RT}{4\pi N_0^2} (\epsilon - n_D^2) \right]^{1/2} = \left[ \frac{3V_m^2}{4\pi N_0^2 P} (\epsilon - n_D^2) \right]^{1/2}. \quad (3)$$

Since  $V_m$  is a constant to 3 significant figures for all gases at STP<sup>6</sup>, and  $P \equiv 1 \text{ atm}$ , equation (3) can be simplified to

$$\mu_D = 18.4 \sqrt{\epsilon - n_D^2} (\times 10^{-18} \text{ esu. cm}). \quad (4)$$

Noting also that  $n_D^2 = 2n_D - 1$  for  $n_D \geq 1$ , the actual calculation can be further simplified by writing

$$\mu_D = 18.4 \sqrt{\epsilon + 1 - 2n} \text{ (Debye units)}. \quad (5)$$

The accepted<sup>2,7</sup> dipole moments obtained by various methods, including eq. (1) for seven common molecules are given in Table I along with the values of  $\epsilon$  and  $n_D$  measured for the gases at 1 atm and 0°C. The fifth column shows the values computed from eqs. (4) or (5), and these are seen to compare quite favorably with the accepted values, despite the simplifying assumptions made in arriving at eq. (5).

Making the same simplifying assumptions as above, one obtains the following simple equation for calcu-

**TABLE I**  
*Dielectric constants,<sup>3</sup> refractive indices,<sup>4</sup> polarizabilities,<sup>5</sup> dipole moments,<sup>7</sup> and calculated values from eqs. (4), (5) and (7)*

Gas*	$\epsilon$ (STP)	$n_D$ (STP)	$\mu_D$ (D units)		$10^{-24} \alpha$ (cm <sup>3</sup> )	
			(Lit.) <sup>6</sup>	Eq. (4) or 5	(Lit.)	Eq. (7)
N <sub>2</sub>	1.000580	1.000295	0	0	1.74 <sup>a</sup>	1.74
CO <sub>2</sub>	1.000921	1.00046	0	0	2.65 <sup>b</sup>	2.71
CO	1.00070	1.000338	0.11	0.1**	1.99 <sup>a</sup>	1.99
N <sub>2</sub> O	1.00113	1.00515	0.17	0.18	3.00 <sup>b</sup>	3.04
HCl	1.00460	1.000449	1.08	1.08	2.63 <sup>a, b</sup>	2.64
NH <sub>3</sub>	1.00720	1.00038	1.48	1.48	2.24 <sup>a</sup>	2.24
H <sub>2</sub> O	1.0126	1.00026	1.94 <sup>c</sup>	2.04	1.59 <sup>b</sup>	1.53

\* It should be noted that  $V_m$  at STP for all these gases is, to 3 significant figures,  $22.4 \text{ lit./mol}^6$  \*\* Only 1 significant figure available from the data. <sup>a</sup> From microwave spectroscopy Stark effect<sup>7</sup>.

lating the molecular electric polarizability,  $a$ , from vaporphase measurements of  $n_D$  at STP :

$$R_{st} = \frac{n_D^3 - 1}{n_D^3 + 2}, V_m = \frac{2V_m}{3}(n - 1) = \frac{4}{3}\pi N_0 a \quad (6)$$

from which

$$a = \frac{V_m(n - 1)}{2\pi N_0} = 5.90 \times 10^{-21}(n - 1) \text{ cm}^3. \quad (7)$$

The  $a$  values calculated from eq. (7) are shown in the last column of Table I.

In summary it should be reiterated that the principal advantages of using the new equations given here [eqs. (5) and (7)], aside from their great simplicity, is that work at varying  $T$ 's need not be performed, densities of the sample need not be experimentally determined, and, of most importance, the values so obtained can be regarded as *intrinsic* moments and polarizabilities, free from intermolecular distortions and therefore comparable to the results obtained from the Stark effect.

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† For example  $V_m = 22.41$  for  $O_2$ ,  $22.41$  for  $CO_2$ ,  $22.42$  for  $NH_3$ , and  $22.39$  for  $H_2O$ °.

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### ON THE OCCURRENCE OF SYNTECTONICALLY FILLED VEINS IN THE ROCKS EAST OF BARWAHA CITY, WEST NIMAR DISTRICT, MADHYA PRADESH

DURING the course of structural investigations in a part of the West Nimar District of Madhya Pradesh, the authors have come across the occurrence of syntectonically filled veins containing sigmoidal crystals. Such occurrence is perhaps reported for the first time from the deformed rocks along the Narmada valley.

Both syntaxial and antitaxial veins<sup>1,2</sup> have been found, the former in predominantly calcareous rocks invaded by felsite porphyry sills near Koteswar temple ( $22^\circ 15' : 76^\circ 06'$ ) on both the banks of the river, and the latter about 400 m north of the Sortipura tank ( $22^\circ 16' : 76^\circ 04'$ ), about 5 kms east of the Barwaha city.

Both syntaxial and antitaxial veins have been shown to contain<sup>3</sup> sigmoidal crystals of various mineral species, the commonest being quartz, calcite, chlorite, albite clinozoisite etc. While the growth of crystals is from the walls toward the centre in syntaxial veins, it is reverse in the antitaxial type. In syntaxial veins the crystals grow by diffusion of material from the wall rock while in the antitaxial type, the vein material is foreign to the host rock. The crystals are sigmoidal but bear no signs of fracturing or internal strain and therefore it can be deduced that they were born with a curved form<sup>2</sup>. The crystals have acicular form, unlike their normal crystal habit. This suggests that there were no actual cavities for vuglike growth but the growth initiates in microscopic cracks and continues in the directions of incremental dilations in veins. Durney<sup>3</sup> first recognised such structures in the Helvetic nappes of the External Swiss Alps. By a careful analysis of such structures he was able to show that the Morcles nappe and the Wildhron nappe, the lowest two nappes in the Helvetic pile were forced into the Winstubel depression.

The syntaxial veins found in the area contain sigmoidal crystals of quartz, calcite and plagioclase, the host rocks being predominantly calcareous ones. (Fig. 1). The antitaxial veins contain crystals of calcite in finegrained sandstone (Fig. 2).

The crystals in veins always grow in the direction of principal incremental extension (Fig. 3) and as the latter changes, the path of crystal growth also changes and eventually a sigmoidal geometry results. The degree of sigmoidality depends upon the stage at which the cracks open during the deformation process and the amount of rotational component of strain during a non-coaxial<sup>3</sup> deformation. These crystals enable the deformation paths to be computed<sup>4</sup> and incremental and finite strains to be measured<sup>5</sup>. Further work on these veins is in progress,