TABLE 1

The parameters and constants used in the calculation of lattice thermal conductivity of Si to study the role of three phonon normal processes

$$\tau_B^{-1} = 2\cdot0 \times 10^6 \ sec^{-1}$$
$$A = 2\cdot47 \times 10^{-45} \ sec^3$$
$$E = 3\cdot4 \times 10^{-24} \ sec \ deg^{-3}$$
$$v_s = 6\cdot53 \times 10^5 \ cm/sec$$
$$\theta = 658° \ K.$$

For $\tau_N^{-1} < \tau_R^{-1}$, eq. (1) is used to calculate phonon conductivity for the four different values of 'a' (0·001, 0·01, 0·1 and 1·0). Similarly for $\tau_N^{-1} > \tau_R^{-1}$, lattice thermal conductivity is calculated for 'a' = 10, 100, 1,000 using eq. (2). The result is shown in Fig. 1. From Fig. 1, it can be seen that the Callaway theory gives excellent agreement between calculated and experimental results of phonon conductivity of Si for $\tau_N^{-1} < \tau_R^{-1}$ when 'a' is approaching to 10^{-3}. However for $\tau_N^{-1} > \tau_R^{-1}$, the theory fails to yield the correct temperature dependence of the phonon conductivity.
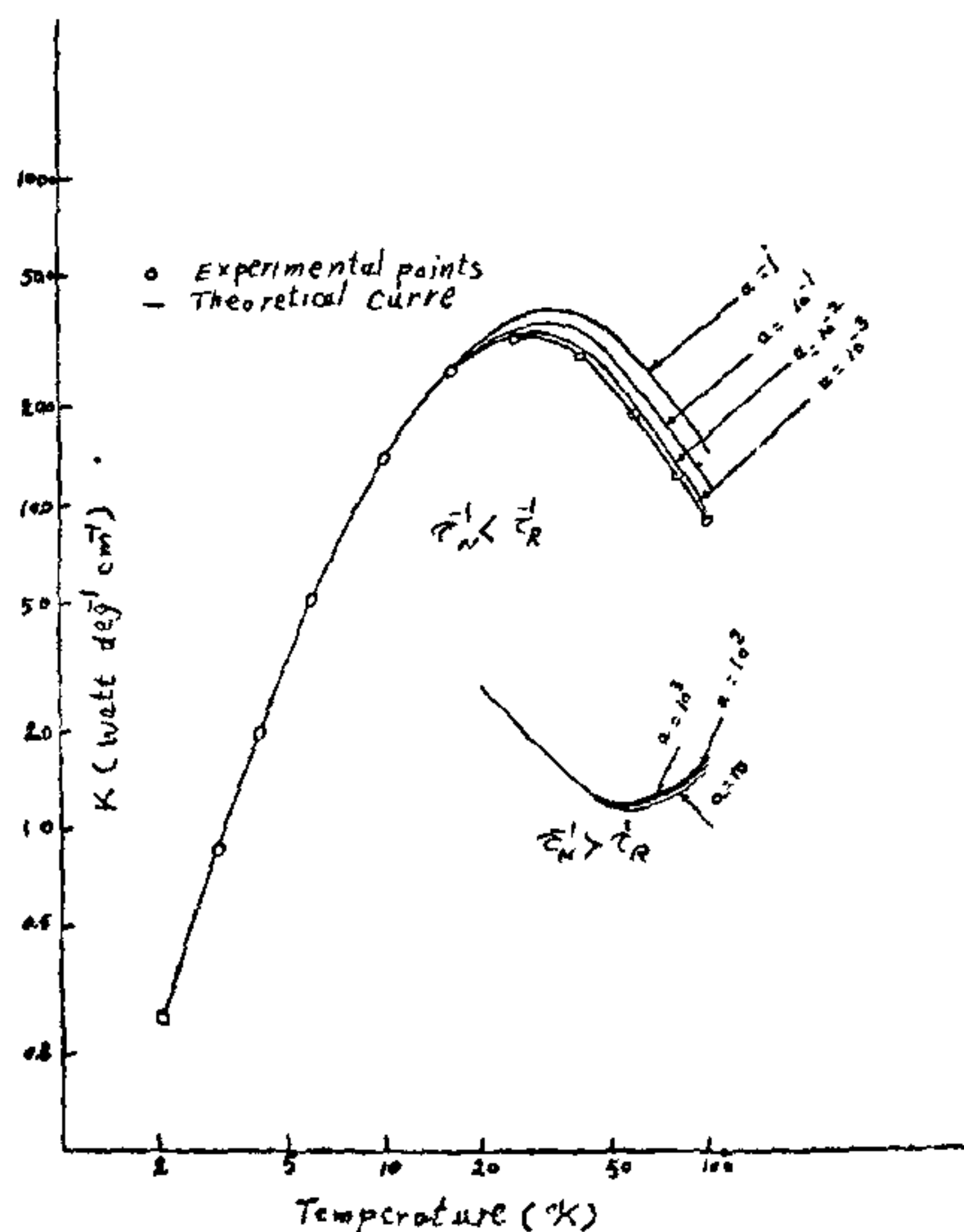

FIG. 1. Phonon conductivity of Si in the temperature range 2–100° K. Solid lines are the calculated value. Circles are the experimental points. 'a' is the relative scattering strength of three phonon normal and umklapp processes.

A similar result was also reported by Dubey and Verma[6] for Ge in the temperature range 2–100° K. Thus, one can say that the role of three phonon normal processes is similar in the phonon conductivity of Si and Ge at low temperatures.

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CRYSTAL STRUCTURE OF METAMIZOL

1-PHENYL-2, 3-dimethyl-5-pyrazolone-4-methylamino-methane-sulphonate sodium, $C_{13}H_{16}N_3O_4S$. Na, known variously as metamizol, methampyrazone or novalgin, is a well known pain relieving drug. Here we give a preliminary account of the x-ray analysis of this compound carried out as part of a programme of structural studies on analgesics and their interactions.

The crystals were grown by the slow diffusion of ethanol vapour into an aqueous solution of the compound. The space group and the unit cell dimensions of the crystals were determined from oscillation, Weissenberg and Precession photographs, and the density was measured by flotation in a mixture of benzene and carbon tetrachloride. The density indicated the presence of one water molecule per formula unit. The cell dimensions were subsequently refined on a four circle diffractometer.

Crystal data : Space group $P2_1/c$.

a 9·143 (3), b 49·50 (2), c 7·314 (2) Å; β 90·2 (1) ; D   1·388 ± 0·005, D   1·40) gm/c.c., Z   8.

The intensity data were collected on a Picker four circle diffractometer. The structure was solved by the direct methods and refined isotropically to a

R value of 0·17. The positions of the crystallographically independent atoms in the structure are showing in Fig. 1.

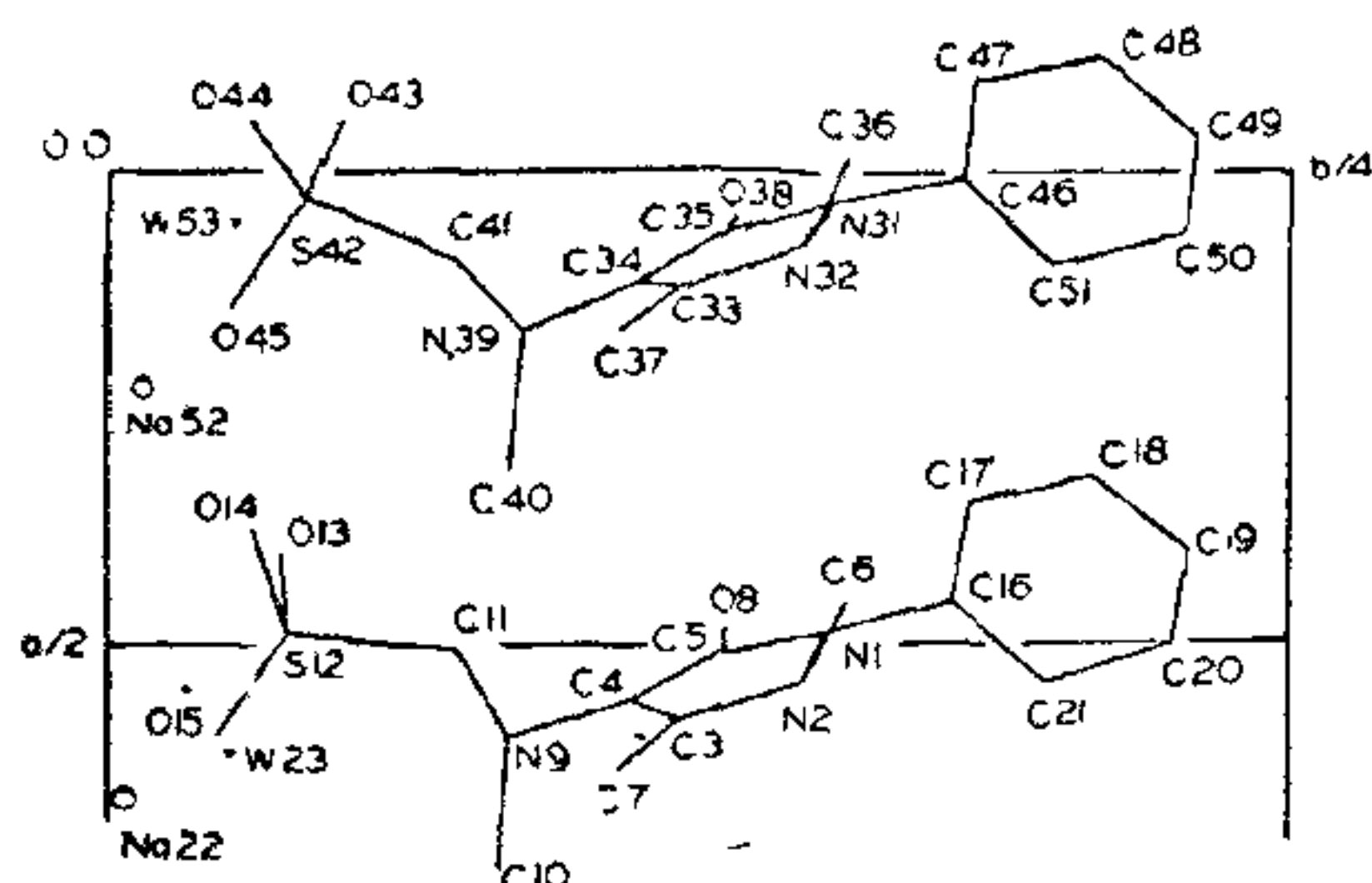
FIG. 1. Positions of the crystallographically independent atoms in the structure as viewed along the c-axis.

The dimensions of the two crystallographically independent molecules in the structure are nearly the same. The hetero nitrogen atoms in the five membered ring of each molecule are pyramidal with the attached phenyl and methyl groups lying on the opposite sides of the plane of the ring. The bond lengths and angles in the pyrazolone group are comparable to those observed in the other two analgetic pyrazolone derivatives, namely, antipyrine and amidopyrine[1,2]. The sodium ions in the structure are coordinated by sulphonyl oxygen atoms and water molecules. It is interesting to note that the carbonyl oxygen atom in the pyrazolone group is not involved in metal coordination or hydrogen bonding.

Further refinement of the structure is in progress.

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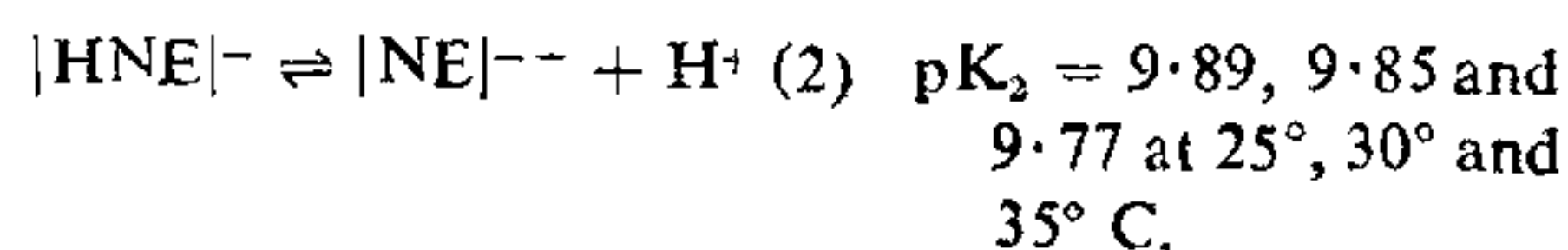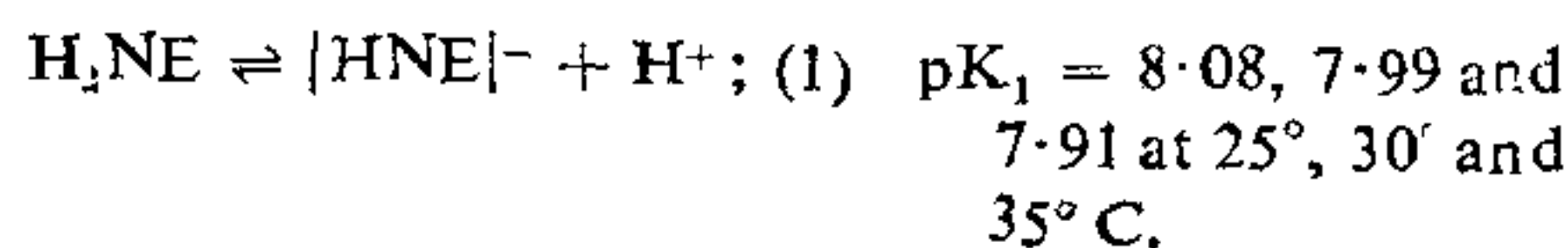2. — and —, *Ibid.*, 1976, 32 B, 2432.

STABILITY CONSTANTS OF BIVALENT METAL CHELATES OF 2-(N-α-METHYL, 2-HYDROXY BENZYLIDENEIMINO) ETHANESULPHONIC ACID

HOLM *et al.*[1], and others[2] have recently reviewed the metal chelates of Schiff bases. The Schiff base 2-(N-α-methyl, 2-hydroxybenylideneimino) ethanesulphonic acid (H_2NE) was synthesized by the method reported[3] earlier by the condensation of ortho hydroxyacetophenone and 2-amino ethanesulphonic acid. H_2NE provides three possible coordination sites, *viz.*, $-SO_3H$, $-OH$ and $=N-$groups. The present investigation is concerned with the determination of stability constants of the chelates of Cu(II), UO_2(II) and VO(II) with H_2NE.
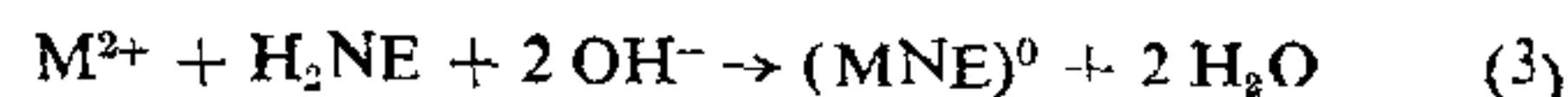
All titrations were carried out at 25° C, 30° C and 35° C by applying Calvin's extension of Bjerrum's method[4]. The following solution mixtures (total volume 40 ml) were prepared and titrated against 0·2 M potassium hydroxide : (A) 10·0 ml 0·02 M H_2NE + 4·0 ml. 1·0 M $NaClO_4$ + 26·0 ml water, (B) 10·0 ml 0·02 M H_2NE + 10·0 ml 0·02 M metal-ion solution + 4·0 ml 1·0 M $NaClO_4$ + 16·0 ml. water, (C) 10·0 ml 0·02 M H_2NE + 5·0 ml 0·02 M metal-ion solution + 4·0 ml 1·0 M $NaClO_4$ + 21·0 ml water.

RESULTS AND DISCUSSION

Metal-H_2NE system.—The appearance of inflections after the addition of 1 and 2 moles of alkali/mole of ligand corresponds respectively to the neutralisation of $-SO_3H$ and $-OH$ groups. The reactions may be stated as :

$$H_2NE \rightleftharpoons |HNE|^- + H^+ ; \quad (1)$$

$$pK_1 = 8·08, 7·99 \text{ and } 7·91 \text{ at } 25°, 30' \text{ and } 35° C.$$

$$|HNE|^- \rightleftharpoons |NE|^{--} + H^+ \quad (2)$$

$$pK_2 = 9·89, 9·85 \text{ and } 9·77 \text{ at } 25°, 30° \text{ and } 35° C.$$

When equimolar concentration of the metal-ion is added, the shape of the free ligand titration curve changes appreciably as a result of chelate formation and two inflections at 2 and 3 moles of alkali/mole of ligands are indicated. The reactions may be represented as :

$$M^{2+} + H_2NE + 2 OH^- \rightarrow (MNE)^0 + 2 H_2O \quad (3)$$

$$(MNE)^0 + OH^- \rightarrow \tfrac{1}{2}[M(NE)_2]^{2-} + \tfrac{1}{2}[M(OH)_2]^0 \quad (4)$$

When the mixture containing metal and ligand in the ratio of 1 : 2 (taking half the concentration of the metal-ion), was titrated against standard alkali, two inflections at 1 and 2 moles of alkali/mole of ligand are observed which may be attributed