

where  $D$  = dissociation energy and  $a$  is a constant, we have computed wave functions for the  $A^2\Pi - X^2\Sigma^+$  transition of CN and used these wave functions to evaluate Franck-Condon factors and  $r$ -centroids defined by the following relations :

$$\text{Franck-Condon factor} = \left[ \int \psi_{v'}^* \psi_{v''} dr \right]^2$$

(FC factor)

$$r\text{-centroid} = \frac{\int \psi_{v'}^* r \psi_{v''} dr}{\int \psi_{v'}^* \psi_{v''} dr}$$

( $\bar{r}_{v', v''}$ )

These results have been tabulated in Table I.

TABLE I

Band	FC Langer (Rydberg potential)	FC Klein- Dunham potentials	RC $\bar{r}_{v', v''}$ Langer (Rydberg potential)	RC $\bar{r}_{v', v''}$ Klein- Dunham potentials
(0, 0)	0.490	0.488	1.212	1.206
(0, 1)	0.377	0.378	1.252	1.252
(0, 2)	0.118	0.115	1.303	1.305
(0, 3)	0.019	0.018	1.372	1.365
(1, 0)	0.333	0.325	1.164	1.165
(1, 1)	0.045	0.0414	1.221	1.223
(1, 2)	0.357	0.348	1.261	1.261
(1, 3)	0.220	0.224	1.351	1.313
(2, 0)	0.129	0.130	1.131	1.128
(2, 1)	0.250	0.237	1.185	1.173
(2, 2)	0.013	0.0125	1.194	1.189
(2, 3)	0.216	0.210	1.262	1.271
(3, 0)	0.035	0.041	1.149	1.095
(3, 1)	0.211	0.195	1.133	1.135
(3, 2)	0.105	0.0983	1.193	1.184
(3, 3)	0.097	0.089	1.215	1.214

In the same table FCs and  $\bar{r}_{v', v''}$  s obtained with the use of Klein-Dunham potential by McCallum and Nicholls<sup>2</sup> have been given for comparison.

As one can see from the table there is very good agreement between our sets of FCs and  $\bar{r}_{v', v''}$  s with those of McCallum and Nicholls at low vibrational quantum numbers. For bands with higher quantum numbers the agreement is not so good. This is as it should be, for, it is known that Langer's procedure holds good only at low quantum numbers.

The advantage of Langer's method consists in its applicability to any potential which can be expressed in closed form. Thus one could use such different analytic potentials and compare their suitability or

otherwise for a given transition. Work on these lines is in progress in our laboratories.

Department of Physics,  
Karnatak University,  
Dharwar 580 003,  
Karnataka State, India,  
September 5, 1977.

D. C. PATIL.  
V. M. KORWAR.

1. Langer, R. E., *Phys. Rev.* 1949, **75**, 1573.
2. McCallum, J. C. and Nicholls, R. W., *Spectroscopic Reports, C.R.E.S.S.*, York University, Toronto, Canada, 1972.

### NQR IN CERTAIN ORGANIC SOLIDS

NUCLEAR Quadrupole Resonance (NQR) frequency of <sup>35</sup>Cl has been measured in five organic solids, using an NQR spectrometer consisting of a frequency modulated, self-quenched superregenerative oscillator-detector. The resonance frequencies were measured with a digital frequency counter with an accuracy of  $\pm 2$  KHz.

The measured NQR frequencies for the five solids at room temperature and at 77° K are given in Table I.

TABLE I

Sl. No.	Name of the solid	<sup>35</sup> Cl NQR frequency (MHz)	
		at 77° K	at 301° K
1.	2-amino-5-chloropyridine	35.630 <sup>a</sup>	
		35.628	35.126
2.	2, 4-dichlorobenzoic acid	35.528 <sup>b</sup>	
		35.527	35.032
		37.432 <sup>b</sup>	
		37.429	36.868
3.	4-chloro-2-nitrobenzoic acid	36.114	35.531
4.	5-amino-2-chlorobenzo-trifluoride	36.391	35.548
5.	2-amino-5-chlorobenzo-trifluoride	35.308	*

<sup>a</sup> Bray *et al.*<sup>1</sup>; <sup>b</sup> Bray and Barnes<sup>2</sup>.

\* The compound is a liquid at room temperature.

Nuclear quadrupole resonance has been observed for the first time in the three solids, namely, 4-chloro-2-nitrobenzoic acid, 5-amino-2-chloro-benzotrifluoride and 2-amino-5-chlorobenzotrifluoride (liquid at room temperature). For the other two solids, 2-amino-5-chloropyridine and 2, 4-dichlorobenzoic acid, the NQR frequency has been reported earlier at 77° K only by Bray *et al.*<sup>1</sup> and Bray and Barnes<sup>2</sup>. We have measured

NQR frequency in these two solids both at 77 K and at room temperature. Two resonance lines have been observed in 2,4-dichlorobenzoic acid due to chemically inequivalent sites.

The resonance frequency of 5-amino-2-chlorobenzo-trifluoride is higher than that of 2-amino-5-chlorobenzo-trifluoride. This may be explained by the fact that chlorine occupying the ortho position will have a higher resonance frequency when compared to the chlorine occupying the meta position (Nagarajan and Murthy<sup>3</sup>). Similarly, when the resonance frequency of 4-chloro-2-nitrobenzoic acid is compared with that of 4-chloro-3-nitrobenzoic acid (37.483 MHz—Bray and Barnes<sup>2</sup>) and 4-chlorobenzoic acid (34.673 MHz—Meal<sup>4</sup>), we observe that the introduction of nitro group increases the resonance frequency. Also, 4-chloro-3-nitrobenzoic acid has a higher resonance frequency than 4-chloro-2-nitrobenzoic acid. This is because when the chlorine occupies the ortho position with respect to the nitro group a higher resonance frequency will result as compared with the chlorine in the meta position (Ref. 3).

The authors wish to thank Professor K. N. Kuchela for his interest and encouragement in this work. One of the authors (N.D.) is grateful to the University Grants Commission, Government of India, for the award of a research grant.

Department of Physics,  
Bangalore University,  
Bangalore 560 001,  
August 3, 1977.

S. P. BASAVARAJU.  
N. DEVARAJ.

1. Bray, P. J., Moskowitz, S., Hooper, H. O., Barnes, R. G. and Segel, S., *J. Chem. Phys.*, 1958, 28, 99.
2. — and Barnes, R. G., *Ibid.*, 1957, 27, 551.
3. Nagarajan, V. and Murthy, C. R. K., *Ind. J. Pure and Appl. Phys.*, 1963, 1, 168.
4. Meal, H. C., *J. Am. Chem. Soc.*, 1952, 74, 6121.

### IN-SITU MEASUREMENT IS A MUST FOR SIZE EFFECT STUDIES OF THIN METAL FILMS\*

THE anomalous behaviour of the size dependence of the electrical transport properties in metals, semi-metals, semiconductors, alloys etc., may be associated with the anomalous conditions in the structure of thin films which should depend very much on the method and environment of deposition. So the experimental conditions should be the same as those which have been postulated when deriving relations in the theory of size effects (Fuchs<sup>1</sup>, Sondheimer<sup>2</sup>). It has been

observed (Garcia *et al.*<sup>3</sup>) that the film properties change drastically when the film is removed from high vacuum. So according to them, for accurate results the measurements should be done without removing the film from the high vacuum (*i.e.*, *in-situ*). Here the resistivity values for each of silver and copper films measured under *in-situ* and not *in-situ* conditions and deposited under extremely controlled evaporation conditions have been reported. In an earlier paper (Pal *et al.*<sup>4</sup>) we have reported the *in-situ* measurements of resistivity of silver films (300 Å to 2000 Å) at room temperature. In the present paper, the resistivity ( $\rho$ ) of the silver films is discussed as a function of thickness ( $t$ ) of the film at 30°C by keeping the films both inside (*in-situ*) and outside (not *in-situ*) the high vacuum (Fig. 1). The resistivity of the films was found to increase drastically, especially for the thinner ones when they were removed from high vacuum. Thinner films are affected more.

In the present paper, the effect of residual atmosphere on copper films has been studied at room temperature (Fig. 2) by exposing a thin copper film (thickness = 300 Å) prepared at a pressure  $1.33 \times 10^{-3}$  Newton/metre<sup>2</sup> to  $1.33$  Newton/metre<sup>2</sup>,  $1.33 \times 10^2$  Newton/metre<sup>2</sup> and  $1.013 \times 10^5$  Newton/metre<sup>2</sup> (*i.e.*, atmospheric) pressure by admitting air slowly. The method of preparation of the copper films was discussed in our earlier paper (Pal *et al.*<sup>5</sup>). From  $1.33 \times 10^{-3}$  Newton/metre<sup>2</sup> to  $1.33$  Newton/metre<sup>2</sup> pressure, there is practically no change in the resistivity  $\rho$  of the copper film. The resistivity very slowly changes up to  $1.33 \times 10^2$  Newton/metre<sup>2</sup> and finally increases abruptly as the film is exposed to atmospheric pressure. This change is very fast and the film stabilises within a few seconds. Even after annealing the previously exposed film at 120°C for about two hours at  $1.33 \times 10^{-3}$  Newton/metre<sup>2</sup>, the resistivity value remained 25% higher than that obtained with the fresh sample at  $1.33 \times 10^{-3}$  Newton/metre<sup>2</sup>. Murgulesch and Ionescu<sup>6</sup> also observed a change of 6% to 16% in the resistivity value of continuous copper films owing to adsorption of oxygen. Thus it may be concluded that one should make *in-situ* measurements on thin films in order to derive meaningful informations on size effect.

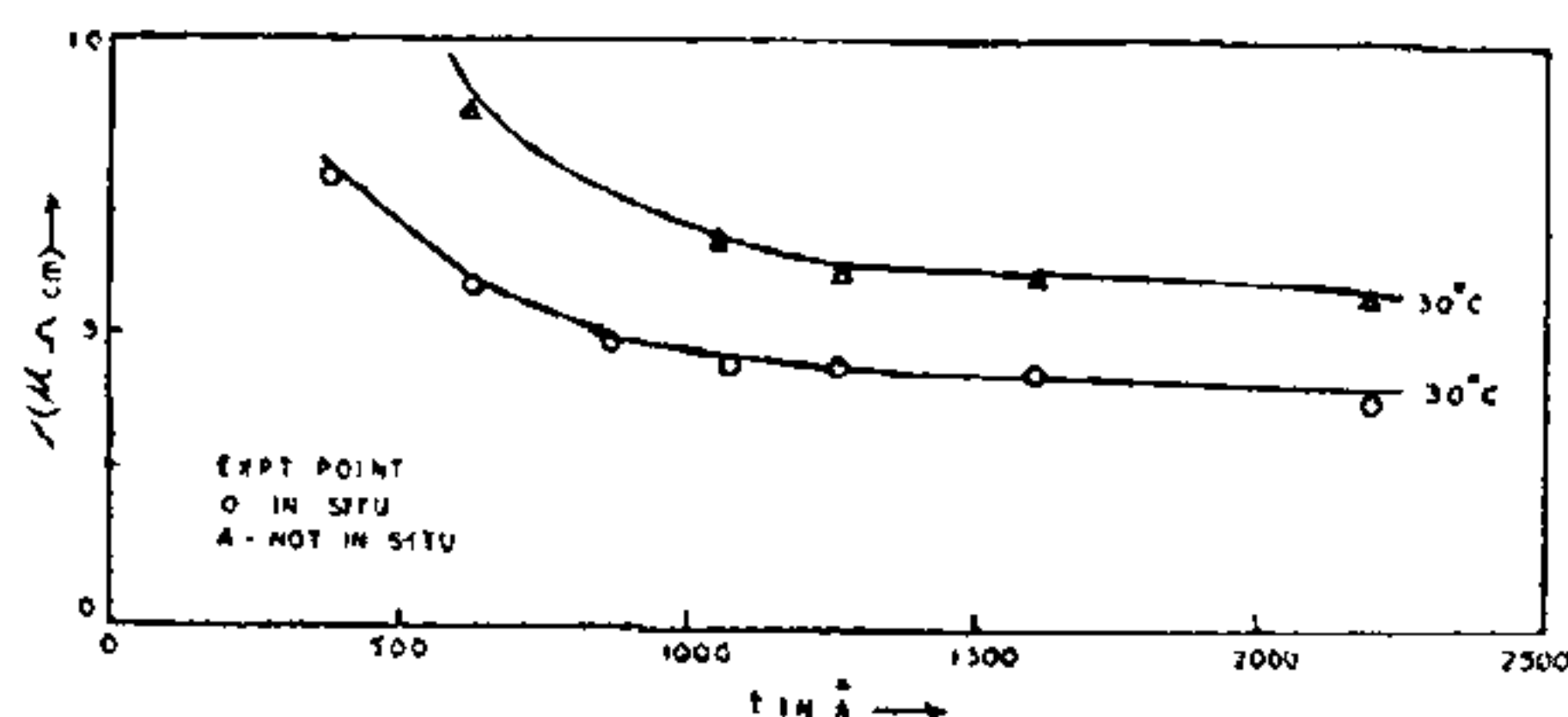


FIG. 1. Resistivity ( $\rho$ ) of silver films as a function of thickness ( $t$ ) at room temperature.

\* This is a part of the Ph.D. work of the author.