

aspect could be obtained due to the small number of reflections recorded.

TABLE I

Values of the Debye-Waller factor B , the mean amplitude of vibration $(\bar{u}^2)^{1/2}$ and the Debye temperature θ at room temperature of Gd-Zn and Gd-Mg

Substance	B (\AA^2)	$(\bar{u}^2)^{1/2}$ (\AA)	θ (K)
Gd-Zn	2.665 ± 0.162	0.318 ± 0.010	108 ± 3
Gd-Mg	3.697 ± 0.464	0.375 ± 0.024	101 ± 6

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FRANCK-CONDON FACTORS AND r -CENTROIDS FOR THE ($A^2\Pi - X^2\Sigma^+$) TRANSITION OF CN BY LANGER'S APPROXIMATION METHOD

THE Red band System of CN ($A^2\Pi - X^2\Sigma^+$) transition is well known. Good deal of work, both experimental and theoretical, has been done on this particular system. In the present investigation we have chosen this transition for testing the validity of one of the less known methods of solving the Schrödinger wave equation approximately. This method is due to Langer¹, and very briefly it may be described as follows :

The one-dimensional Schrödinger wave equation is written as

$$\frac{d^2\psi}{dx^2} + \lambda^2 [E - V(x)] \psi = 0 \quad (1)$$

where $\lambda^2 = 2\mu/\hbar^2$, μ = reduced mass, \hbar = Planck's constant, $V(x)$ = Potential energy function.

The variable is changed from x to z through the relation

$$Z = x - x_e - \left(\frac{\sigma}{\lambda}\right) \quad (2)$$

where

$$\sigma = -\frac{2V''(x_e)\lambda E}{9[V''(x_e)]^2} \quad (3)$$

x_e = equilibrium internuclear distance; the primes indicate derivatives with respect to x .

Equation (1) then becomes

$$\frac{d^2\psi}{dz^2} - [\lambda^2\psi_0^2(Z) + \lambda\psi_1(Z) + \psi_2(Z)] \psi = 0 \quad (4)$$

where

$$\psi_0^2(Z) = V(z + x_e)$$

$$\psi_1(Z) = V'(z + x_e)$$

$$\psi_2(Z) = \lambda^2 \left\{ V\left(z + x_e + \frac{\sigma}{\lambda}\right) - V(z - x_e) - V'(z + x_e) \right\}.$$

Finally the solutions will come out as

$$\psi_n = \left[\frac{2V''(x_e)}{\pi} \right]^{1/4} \left(\frac{n!}{2^n} \right)^{1/2} \times \frac{2(-1)^{(n-1)/2}}{\left(\frac{n-1}{2}\right)!} \frac{M_n}{\frac{1}{2} + \frac{1}{4}, -\frac{1}{4}} \quad (\xi)$$

where n is odd

$$\psi_n = \left[\frac{2V''(x_e)}{\pi} \right]^{1/4} \left(\frac{n!}{2^n} \right)^{1/2} \times \frac{(-1)^{n/2}}{(n/2)!} \frac{M_n}{\frac{1}{2} + \frac{1}{4}, -\frac{1}{4}} \quad (\xi)$$

where n is even.

where the M 's are confluent hypergeometric functions.

Using these wave functions and the Rydberg potential defined by

$$V(x) = -D [1 + a(x - x_e)] e^{-a(x-x_e)}$$

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 Nicholls² 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.

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NQR IN CERTAIN ORGANIC SOLIDS

NUCLEAR Quadrupole Resonance (NQR) frequency of ³⁵Cl 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 ± 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	³⁵ Cl NQR frequency (MHz)	
		at 77° K	at 301° K
1.	2-amino-5-chloropyridine	35.630 ^a	
		35.628	35.126
2.	2, 4-dichlorobenzoic acid	35.528 ^b	
		35.527	35.032
		37.432 ^b	
3.	4-chloro-2-nitrobenzoic acid	37.429	36.868
		36.114	35.531
4.	5-amino-2-chlorobenzotrifluoride	36.391	35.548
5.	2-amino-5-chlorobenzotrifluoride	35.308	*

^a Bray *et al.*¹; ^b Bray and Barnes².

* 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.*¹ and Bray and Barnes². We have measured