

THE INFLUENCE OF VIBRATION-ROTATION INTERACTION ON BAND INTENSITY PARAMETERS FOR ZrO AND CuH*

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ABSTRACT

Effects of vibration-rotation interaction have been studied on the band intensity parameters of ZrO and CuH molecules. Band strengths have been calculated for the ZrO $\alpha(C^3\Delta-X^3\Delta)$ band system, and, in the absence of an electronic transition moment function, Franck-Condon factors and \bar{r} -centroids are reported for the ZrO β , γ , A , and B and the CuH ($A^1\Sigma^+-X^1\Sigma^+$) band systems. RKR and Morse potentials are given for all the electronic states involved.

Subject headings: molecular processes — transition probabilities

I. INTRODUCTION

In this paper we report an investigation of the effect of vibration-rotation interaction upon the Franck-Condon factors (FCF) and \bar{r} -centroids of CuH ($A-X$) and ZrO (α , β , γ , A , and B) band systems, and upon the band strength of ZrO (α) band. The ZrO molecule is known to be an important component of the late type stars, and its spectrum is of considerable importance in distinguishing M and S stars as shown by Keenan and Morgan (1951). The renewed interest in the study of electronic transitions of the ZrO band system has been justified by Schoonveld and Sundaram (1974). Hauge (1971) showed the existence of the 0-0 band of the CuH ($A^1\Sigma^+-X^1\Sigma^+$) system in the sunspot spectrum. He also reported, with considerable uncertainty, the presence of the 1-1 band. Recently Wojslaw and Perry (1976) have identified the 0-0 band together with the 1-0 and 1-1 bands of this system in the spectrum of 19 Piscium. They have also reported the peculiar J -variation of the observed intensities of the 0-0 band. In a recent review Nicholls (1977) stressed the importance of reliable FCFs and related quantities of astrophysically important molecules, including CuH. Previous calculations of FCFs for ZrO (Singh and Pathak 1967*a, b*; Nicholls and Tyte 1967; Liszt and Smith 1971; Schoonveld and Sundaram 1974) did not include the effect of molecular rotation which is important in deriving excitation temperatures (Learner 1962) and isotopic abundances (Keenan and Morgan 1951). For CuH, to our knowledge, there are no FCFs available in the literature. Therefore we undertake this study of the effect of molecular rotation on the band intensity parameters for both ZrO and CuH molecules. The rotational dependences have been studied for vibrational quantum numbers up to 10 and high J (0-100 for ZrO and 0-60 for CuH, with an increment of 5).

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II. THEORY

The integrated intensity of a band of frequency $\nu^{v'J'}_{v''J''}$ cm^{-1} due to an electronic transition between upper level $v'J'$ and lower level $v''J''$, in emission, is given by

$$I^{v'J'}_{v''J''} = \frac{kN_{v'J'}}{w} (\nu^{v'J'}_{v''J''})^4 S^{v'J'}_{v''J''} \frac{S_{J'J''}}{2J' + 1}, \quad (1)$$

where $N_{v'J'}$ is the population of the upper state, k is a constant, w is the degeneracy of the upper state, and $S^{v'J'}_{v''J''}$ is the band strength, given by

$$S^{v'J'}_{v''J''} = \left| \int_0^\infty \Psi_{v'J'} R_e(r) \Psi_{v''J''} dr \right|^2. \quad (2)$$

The factor $S_{J'J''}$, called the Hönl-London factor, is well known for the most important electronic transitions and can be found, e.g., in a paper by Tatum (1967). The band strength $S^{v'J'}_{v''J''}$ is an average with respect to upper and lower wave functions, $\Psi_{v'J'}$ and $\Psi_{v''J''}$, respectively, of the electronic transition moment $R_e(r)$, which is given by

$$R_e(r) = \int \Psi_U^*(\Sigma - er) \Psi_L d\tau_e, \quad (3)$$

and which is also an average of electronic dipole moment with respect to upper (Ψ_U) and lower (Ψ_L) electronic wave functions.

In cases where the electronic transition moment $R_e(r)$ is independent of r , or the dependence is unknown, equation (2) can be written as

$$S^{v'J'}_{v''J''} = R_e^2 q^{v'J'}_{v''J''}, \quad (4)$$

where $q^{v'J'}_{v''J''}$ is known as the Franck-Condon factor (FCF) with the vibration-rotation interaction, and is given by

$$q^{v'J'}_{v''J''} = \left| \int_0^\infty \Psi_{v'J'} \Psi_{v''J''} dr \right|^2. \quad (5)$$

TABLE 1
SPECTROSCOPIC CONSTANTS FOR ZrO AND CuH USED IN THIS WORK*

Electronic State	ω_e (cm ⁻¹)	$\omega_e x_e$ (cm ⁻¹)	B_e (cm ⁻¹)	α_e (cm ⁻¹)	r_e (Å)
ZrO:					
$C^3\Delta$	819.83	3.150	0.39373	0.0021	1.775
$B^3\Pi$	845.58	3.602	0.40395	0.0023	1.755
$A^3\Phi$	856.12	3.430	0.40459	0.0022	1.752
$X'^3\Delta$	937.36	3.487	0.41575	0.0021	1.728
$d^1\Delta$	839.2	2.56	0.399	0.0017	1.764
$c^1\Delta$	938.1	1.80	0.417	0.0012	1.725
$b^1\Sigma^+$	943.75	3.15	0.395	0.0020	1.772
$X^1\Sigma^+$	976.51	3.462	0.423608	0.001954	1.712
CuH:					
$A^1\Sigma^+$	1698.4	44.0	6.875	0.263	1.5721
$X^1\Sigma^+$	1940.4	37.0	7.938	0.249	1.4631

* $\mu_{ZrO} = 13.5836$; $\mu_{CuH} = 0.992242$.

In previous publications (Chang and Karplus 1970; Chakraborty, Pan, and Chang 1971; Gallas, Grieneisen, and Chakraborty 1978) analytical expressions—i.e., working equations to calculate FCFs, \bar{r} -centroids, and band strengths—have been reported in detail and are not reproduced here. For this purpose we particularly refer to the article of Gallas, Grieneisen, and Chakraborty (1978).¹ The calculation of the FCFs is based on the assumption of a Morse-Pekeris molecular potential and in the use of asymptotic expansion techniques to evaluate expression (2). It is worthwhile to mention that expression (2) was used to calculate the band strength, without the usual \bar{r} -centroid approximation.

III. DISCUSSION

The molecular data needed to calculate the intensity parameters are given in Table 1; the electronic states

¹ Note in this reference that the expressions for E_0 and E_1 following equation (6) should read

$$E_0 = 3b_4/4b_2^2 - 15b_3^2/16b_2^3,$$

$$E_1 = -[a_1(3b_3/4b_2 + 1/4t_0) + a_2(3b_3\rho_0/2b_2 + \rho_0/2t_0 + 1/2a't_0)] \times [a't_0b_2R_e(\rho_0)]^{-1}.$$

involved in the α , β , γ , A , and B band systems of ZrO can be seen in Table 2. Spectroscopic constants for the ZrO triplet states ($C^3\Delta$, $B^3\Pi$, $A^3\Phi$, $X'^3\Delta$) are taken from the recent critical analysis of available experimental data made by Schoonveld and Sundaram (1974). For the d , c , and b singlet states we use the constants given by Nicholls and Tyte (1967). The B_e values for these singlet states given in Table 1 were calculated through

$$B_e = \{\mu(0.243559r_e)^2\}^{-1}, \quad (6)$$

and the α_e were calculated using Pekeris's relation

$$\alpha_e = 6B_e^2\{(\omega_e x_e/B_e)^{1/2} - 1\}/\omega_e. \quad (7)$$

Previously the lower electronic state of the ZrO A band system was designated by Uhler and Åkerlind (1956) as an $a(^1\Sigma$ or $^1\Delta)$ state. This state has been recently studied by Balfour and Tatum (1973) in connection with a new $^1\Pi$ - $^1\Sigma$ transition, and by Phillips and Davis (1976a) in connection to another new $^1\Sigma$ - $^1\Sigma$ transition. This state, now called $X^1\Sigma^+$, is presently thought to be the ZrO ground state (Veits *et al.* 1974). Therefore, in calculating the intensity parameters for the A band system of ZrO we used the

TABLE 2
FRANCK-CONDON FACTORS FOR SOME BANDS OF α , β , γ , A , AND B BAND SYSTEMS OF ZrO

Band System	J	0-0	0-1	1-0	1-1	2-3	3-5	4-5	6-6
α , $C^3\Delta$ - $X'^3\Delta$...	0	0.6753	0.2674	0.2618	0.2473	0.3282	0.2281	0.1737	0.1067
	50	0.6689	0.2715	0.2654	0.2373	0.3252	0.2317	0.1653	0.1126
	100	0.6497	0.2834	0.2757	0.2086	0.3147	0.2417	0.1402	0.1285
β , $B^3\Pi$ - $X'^3\Delta$...	0	0.8742	0.1166	0.1179	0.6497	0.2691	0.0733	0.3264	0.0474
	50	0.8697	0.1206	0.1218	0.6383	0.2750	0.0771	0.3286	0.0386
	100	0.8555	0.1327	0.1337	0.6037	0.2915	0.0894	0.3325	0.0176
γ , $A^3\Phi$ - $X'^3\Delta$...	0	0.8993	0.0948	0.0957	0.7153	0.2322	0.0492	0.3064	0.1349
	50	0.8958	0.0980	0.0989	0.7060	0.2381	0.0518	0.3111	0.1218
	100	0.8847	0.1079	0.1085	0.6778	0.2552	0.0600	0.3233	0.0866
A , $b^1\Sigma^+$ - $X^1\Sigma^+$	0	0.5161	0.3492	0.3319	0.0584	0.1901	0.2507	0.0105	0.1380
	50	0.5103	0.3514	0.3335	0.0539	0.1838	0.2488	0.0081	0.1343
	100	0.4933	0.3576	0.3378	0.0418	0.1654	0.2419	0.0029	0.1221
B , $d^1\Delta$ - $c^1\Delta$	0	0.7539	0.2110	0.2127	0.3780	0.3346	0.1836	0.2285	0.0674
	50	0.7483	0.2149	0.2166	0.3672	0.3334	0.1876	0.2199	0.0740
	100	0.7310	0.2266	0.2288	0.3347	0.3283	0.1994	0.1929	0.0942

TABLE 3

MORSE AND RKR TURNING POINTS FOR DIFFERENT VIBRATIONAL LEVELS OF THE $b^1\Sigma^+$ AND $X^1\Sigma^+$ STATES OF ZrO*

Electronic State	v	U (cm ⁻¹)	Morse r_{\min}	RKR r_{\min}	Morse r_{\max}	RKR r_{\max}
$b^1\Sigma^+$	0	421.09	1.7205	1.7205	1.8292	1.8292
	1	1258.54	1.6852	1.6851	1.8740	1.8739
	2	2089.69	1.6621	1.6620	1.9066	1.9065
	3	2914.54	1.6440	1.6439	1.9342	1.9341
	4	3733.09	1.6289	1.6287	1.9590	1.9588
	5	4545.34	1.6158	1.6155	1.9819	1.9816
	6	5351.29	1.6041	1.6038	2.0034	2.0030
	7	6150.94	1.5935	1.5931	2.0238	2.0234
	8	6944.29	1.5839	1.5834	2.0435	2.0430
	9	7731.34	1.5750	1.5744	2.0624	2.0619
10	8512.09	1.5667	1.5660	2.0809	2.0802	
$X^1\Sigma^+$	0	487.39	1.6633	1.6632	1.7642	1.7642
	1	1456.96	1.6303	1.6301	1.8057	1.8055
	2	2419.64	1.6087	1.6084	1.8359	1.8356
	3	3375.38	1.5919	1.5914	1.8615	1.8610
	4	4324.19	1.5777	1.5771	1.8843	1.8837
	5	5266.08	1.5654	1.5647	1.9054	1.9046
	6	6201.05	1.5545	1.5535	1.9252	1.9243
	7	7129.09	1.5446	1.5435	1.9441	1.9430
	8	8050.21	1.5355	1.5343	1.9621	1.9609
	9	8964.40	1.5272	1.5257	1.9796	1.9781
10	9871.67	1.5194	1.5177	1.9965	1.9949	

* All r values are given in Å.

$X^1\Sigma^+$ molecular constants given by Phillips and Davis (1976*b*). The r_e presented for this electronic state in Table 1 was calculated using equation (6). For the CuH $A^1\Sigma^+$ and $X^1\Sigma^+$ states we used spectroscopic constants given by Herzberg (1950).

In calculating the transition probability parameters for the ZrO α , β , and γ band systems, i.e., the transitions involving the triplet states, Schoonveld and Sundaram (1974) found the Morse potential to be an excellent representation of the true potential of the aforementioned band systems of ZrO. In order to test the reliability of the Morse potential for the ZrO A and B and CuH ($A^1\Sigma^+$ - $X^1\Sigma^+$) band systems we have also calculated the Rydberg-Klein-Rees (RKR) potentials for the involved electronic states, and compared with the Morse potentials. The energies for each vibrational level are given in Tables 3, 4, and 5 together with the turning points. From the result of this comparison one can also expect the Morse potential to be valid for ZrO A and B and CuH ($A^1\Sigma^+$ - $X^1\Sigma^+$) band systems. These energy curves are given for the rotationless case, but the Morse potential is expected to give reliable results for high rotational levels also. In order to come to this conclusion we have checked the orthogonality of the wave functions for all transitions, by equating the spectroscopic constants of the upper and lower electronic states. We found the diagonal matrix elements to differ from unity by less than 10^{-6} and the off-diagonal elements to be in the 10^{-14} to 10^{-20} range. Morse and RKR potential curves were also calculated for the ZrO triplet electronic states and found to agree up to high vibrational levels. Since part of the turning points are given by Schoonveld and Sundaram (1974), we shall not repeat them here. However, they are available on request.

TABLE 4

MORSE AND RKR TURNING POINTS FOR DIFFERENT VIBRATIONAL LEVELS OF THE $d^1\Delta$ AND $c^1\Delta$ STATES OF ZrO*

Electronic State	v	U (cm ⁻¹)	Morse r_{\min}	RKR r_{\min}	Morse r_{\max}	RKR r_{\max}
$d^1\Delta$	0	418.96	1.7113	1.7113	1.8202	1.8202
	1	1253.04	1.6755	1.6754	1.8646	1.8645
	2	2082.00	1.6519	1.6517	1.8967	1.8965
	3	2905.84	1.6335	1.6332	1.9238	1.9236
	4	3724.56	1.6179	1.6176	1.9480	1.9477
	5	4538.16	1.6044	1.6040	1.9703	1.9699
	6	5346.64	1.5924	1.5919	1.9912	1.9907
	7	6150.00	1.5815	1.5809	2.0110	2.0104
	8	6948.24	1.5714	1.5707	2.0299	2.0292
	9	7741.36	1.5622	1.5614	2.0482	2.0474
10	8529.36	1.5535	1.5526	2.0659	2.0650	
$c^1\Delta$	0	468.60	1.6752	1.6752	1.7782	1.7782
	1	1403.10	1.6406	1.6406	1.8192	1.8192
	2	2334.00	1.6176	1.6177	1.8486	1.8486
	3	3261.30	1.5995	1.5995	1.8732	1.8732
	4	4185.00	1.5842	1.5841	1.8950	1.8950
	5	5105.10	1.5707	1.5707	1.9150	1.9149
	6	6021.60	1.5587	1.5587	1.9335	1.9335
	7	6934.50	1.5477	1.5477	1.9510	1.9510
	8	7843.80	1.5376	1.5376	1.9677	1.9677
	9	8749.50	1.5283	1.5282	1.9837	1.9836
10	9651.60	1.5195	1.5194	1.9991	1.9990	

* All r values are given in Å.

FCFs for the ZrO band systems have been reported in Table 2 for some transitions. As expected, the factors do not differ very much for the 0-0 transition even when $J = 100$, because of the similarity of the spectroscopic constants of the ZrO band systems. However, the effect appears beyond 1-1 transitions and is pronounced in the weaker but still observable

TABLE 5

MORSE AND RKR TURNING POINTS FOR DIFFERENT VIBRATIONAL LEVELS OF THE $A^1\Sigma^+$ AND $X^1\Sigma^+$ STATES OF CuH*

Electronic State	v	U (cm ⁻¹)	Morse r_{\min}	RKR r_{\min}	Morse r_{\max}	RKR r_{\max}
$A^1\Sigma^+$	0	838.20	1.4453	1.4456	1.7313	1.7316
	1	2448.60	1.3689	1.3696	1.8756	1.8763
	2	3971.00	1.3233	1.3241	1.9931	1.9940
	3	5405.40	1.2900	1.2900	2.1027	2.1035
	4	6751.80	1.2639	1.2644	2.2100	2.2105
	5	8010.20	1.2426	1.2424	2.3183	2.3181
	6	9180.60	1.2248	1.2236	2.4295	2.4283
	7	10263.00	1.2098	1.2069	2.5457	2.5429
	8	11257.40	1.1969	1.1919	2.6686	2.6636
	9	12163.80	1.1859	1.1779	2.8004	2.7924
10	12982.20	1.1764	1.1646	2.9436	2.9317	
$X^1\Sigma^+$	0	960.95	1.3426	1.3433	1.6094	1.6101
	1	2827.35	1.2680	1.2701	1.7377	1.7398
	2	4619.75	1.2224	1.2258	1.8393	1.8427
	3	6338.15	1.1886	1.1932	1.9315	1.9361
	4	7982.55	1.1616	1.1673	2.0195	2.0253
	5	9552.95	1.1391	1.1459	2.1059	2.1127
	6	11049.35	1.1199	1.1277	2.1921	2.1999
	7	12471.75	1.1033	1.1120	2.2792	2.2879
	8	13820.15	1.0888	1.0982	2.3681	2.3775
	9	15094.55	1.0759	1.0860	2.4597	2.4697
10	16294.95	1.0645	1.0750	2.5546	2.5651	

* All r values are given in Å.

TABLE 6
 \bar{r} -CENTROIDS FOR SOME BANDS OF α , β , γ , A , AND B BAND SYSTEMS OF ZrO

Band System	J	0-0	0-1	1-0	1-1	2-3	3-5	4-5	6-6
α , $C^3\Delta-X'^3\Delta\dots$	0	1.7539	1.8181	1.6977	1.7602	1.8331	1.9005	1.8488	1.8053
	50	1.7577	1.8214	1.7020	1.7641	1.8365	1.9036	1.8522	1.8086
	100	1.7692	1.8313	1.7150	1.7757	1.8466	1.9129	1.8626	1.8186
β , $B^3\Pi-X'^3\Delta\dots$	0	1.7445	1.8518	1.6478	1.7511	1.8671	1.9522	1.8826	1.7558
	50	1.7483	1.8540	1.6532	1.7549	1.8694	1.9543	1.8849	1.7564
	100	1.7596	1.8607	1.6690	1.7664	1.8763	1.9610	1.8921	1.7521
γ , $A^3\Phi-X'^3\Delta\dots$	0	1.7431	1.8628	1.6338	1.7496	1.8784	1.9695	1.8942	1.7702
	50	1.7468	1.8647	1.6392	1.7534	1.8804	1.9718	1.8962	1.7735
	100	1.7580	1.8710	1.6552	1.7648	1.8868	1.9787	1.9027	1.7830
A , $b^1\Sigma^+-X^1\Sigma^+$	0	1.7439	1.7928	1.7016	1.7508	1.8068	1.8616	1.8270	1.7844
	50	1.7475	1.7962	1.7055	1.7545	1.8103	1.8649	1.8319	1.7881
	100	1.7584	1.8064	1.7171	1.7659	1.8207	1.8748	1.8501	1.7992
B , $d^1\Delta-c^1\Delta\dots$	0	1.7464	1.8207	1.6802	1.7510	1.8311	1.9003	1.8403	1.8075
	50	1.7502	1.8237	1.6847	1.7547	1.8342	1.9029	1.8435	1.8105
	100	1.7614	1.8327	1.6982	1.7658	1.8435	1.9106	1.8528	1.8199

bands. The \bar{r} -centroids for the ZrO band systems are given in Table 6. All FCFs and \bar{r} -centroids calculated by us for the rotationless case agree very well with previous values given by Nicholls and Tyte (1967) and Schoonveld and Sundaram (1974).

Since Rai, Dube, and Singh (1971) reported the electronic transition moment of the ZrO $\alpha(C^3\Delta-X'^3\Delta)$ band system to vary as

$$R_e(\bar{r}) = \text{const.} (1 + 0.015\bar{r} + 0.03\bar{r}^2),$$

we have also calculated the relative band strengths for this band system. They are shown in Table 7. It should be noted that these relative band strengths are calculated without use of the usual \bar{r} -centroid approximation.

As we reported, to our knowledge the FCFs for CuH ($A^1\Sigma^+-X^1\Sigma^+$) band system are not available in the literature. Therefore we decided to give FCFs for all transitions with v' , $v'' \leq 4$ and for $J = 0, 30$, and 60. For the hypothetical Q -branch they can be found in Table 8. It is noticed that, even for the 0-0 and 0-1 transitions, FCFs differ by 50% while J is increased from 0 to 60. Pronounced effects are seen in 1-1, 2-0,

TABLE 7

RELATIVE BAND STRENGTH FACTORS FOR THE
 ZrO $\alpha(C^3\Delta-X'^3\Delta)$ BAND SYSTEM*

v'	J	$v'' = 0$	$v'' = 1$	$v'' = 2$	$v'' = 3$	$v'' = 4$
0...	0	0.8450	0.3393	0.0654	0.0077	0.0006
	50	0.8376	0.3447	0.0680	0.0082	0.0007
	100	0.8157	0.3606	0.0758	0.0097	0.0008
1...	0	0.3237	0.3099	0.4449	0.1527	0.0262
	50	0.3284	0.2977	0.4471	0.1575	0.0276
	100	0.3421	0.2623	0.4521	0.1722	0.0323
2...	0	0.0662	0.4127	0.0687	0.4178	0.2342
	50	0.0689	0.4133	0.0610	0.4143	0.2400
	100	0.0773	0.4134	0.0409	0.4018	0.2568
3...	0	0.0094	0.1495	0.3737	0.0008	0.3282
	50	0.0101	0.1543	0.3682	0.0001	0.3199
	100	0.0123	0.1683	0.3500	0.0013	0.2939
4...	0	0.0010	0.0310	0.2205	0.2795	0.0225
	50	0.0011	0.0329	0.2252	0.2695	0.0275
	100	0.0015	0.0392	0.2382	0.2392	0.0444

* Calculated using $R_e(\bar{r}) = \text{const.} (1 + 0.015\bar{r} + 0.03\bar{r}^2)$.

TABLE 8

ROTATIONAL DEPENDENCE OF FRANCK-CONDON FACTORS
 FOR THE CuH $A^1\Sigma^+-X^1\Sigma^+$ BAND SYSTEM

v'	J	$v'' = 0$	$v'' = 1$	$v'' = 2$	$v'' = 3$	$v'' = 4$
0...	0	0.7147	0.2609	0.0238	0.0006	0.0000
	30	0.7072	0.2649	0.0270	0.0009	0.0000
	60	0.4155	0.4037	0.1509	0.0273	0.0024
1...	0	0.2101	0.3045	0.4115	0.0709	0.0030
	30	0.2149	0.2863	0.4129	0.0812	0.0045
	60	0.2784	0.0016	0.2787	0.3107	0.1121
2...	0	0.0540	0.2559	0.0823	0.4613	0.1376
	30	0.0558	0.2593	0.0645	0.4482	0.1581
	60	0.1413	0.0863	0.0995	0.0434	0.3091
3...	0	0.0146	0.1100	0.2070	0.0032	0.4275
	30	0.0151	0.1150	0.2005	0.0001	0.3892
	60	0.0682	0.1091	0.0028	0.1273	0.0206
4...	0	0.0043	0.0416	0.1392	0.1222	0.0179
	30	0.0045	0.0444	0.1438	0.1047	0.0359
	60	0.0333	0.0846	0.0073	0.0695	0.0170

and 2-1 transitions. For the 0-2 transitions the FCFs for $J = 60$ differ from that when $J = 0$ by a factor of 6. This leads us to believe that for CuH ($A^1\Sigma^+-X^1\Sigma^+$) band system the vibration-rotation interaction cannot be neglected in calculating FCFs. The \bar{r} -centroids for

TABLE 9

ROTATIONAL DEPENDENCE OF THE \bar{r} -CENTROIDS
 FOR THE CuH $A^1\Sigma^+-X^1\Sigma^+$ BAND SYSTEM

v'	J''	$v'' = 0$	$v'' = 1$	$v'' = 2$	$v'' = 3$	$v'' = 4$
0...	0	1.5381	1.7196	1.9873	2.3786	2.7424
	30	1.6374	1.8321	2.0990	2.4392	2.8017
	60	2.0321	2.2240	2.4342	2.6708	2.9529
1...	0	1.3813	1.5940	1.7558	2.0146	2.3871
	30	1.4761	1.6996	1.8749	2.1328	2.4599
	60	1.9208	2.3650	2.3182	2.5199	2.7518
2...	0	1.2695	1.4235	1.6861	1.7959	2.0452
	30	1.3554	1.5278	1.8031	1.9224	2.1707
	60	1.8328	2.0353	2.1744	2.4612	2.6223
3...	0	1.1888	1.3063	1.4739	2.1780	1.8409
	30	1.2651	1.4037	1.5889	4.8836	1.9759
	60	1.7641	1.9481	1.9337	2.3042	2.3962
4...	0	1.1292	1.2216	1.3488	1.5386	1.4326
	30	1.1973	1.3104	1.4591	1.6674	1.6674
	60	1.7122	1.8867	2.1393	2.2091	2.4989

TABLE 10
FRANCK-CONDON FACTORS FOR THE R AND P BRANCH OF THE CuH ($A-X$) BAND

J''	$R(J'')$				$P(J'' + 1)$			
	0-0	0-1	1-0	1-1	0-0	0-1	1-0	1-1
0.....	0.7138	0.2615	0.2106	0.3030	0.7156	0.2602	0.2097	0.3060
1.....	0.7130	0.2622	0.2111	0.3015	0.7165	0.2595	0.2092	0.3075
2.....	0.7121	0.2628	0.2115	0.3000	0.7173	0.2588	0.2087	0.3091
3.....	0.7113	0.2635	0.2119	0.2985	0.7183	0.2581	0.2083	0.3106
4.....	0.7105	0.2641	0.2124	0.2970	0.7192	0.2574	0.2078	0.3122
5.....	0.7097	0.2647	0.2128	0.2956	0.7201	0.2566	0.2073	0.3138
6.....	0.7088	0.2653	0.2133	0.2941	0.7210	0.2559	0.2068	0.3154
7.....	0.7080	0.2654	0.2137	0.2926	0.7219	0.2551	0.2063	0.3169
8.....	0.7072	0.2665	0.2142	0.2912	0.7229	0.2544	0.2058	0.3185
9.....	0.7064	0.2670	0.2146	0.2897	0.7238	0.2536	0.2054	0.3200
10.....	0.7056	0.2676	0.2150	0.2882	0.7247	0.2529	0.2049	0.3216
11.....	0.7048	0.2682	0.2155	0.2866	0.7256	0.2521	0.2044	0.3231
12.....	0.7039	0.2688	0.2160	0.2851	0.7265	0.2514	0.2039	0.3246
13.....	0.7030	0.2694	0.2164	0.2835	0.7274	0.2507	0.2035	0.3260
14.....	0.7022	0.2700	0.2169	0.2818	0.7282	0.2499	0.2030	0.3274
15.....	0.7012	0.2707	0.2174	0.2801	0.7291	0.2492	0.2026	0.3287

the CuH ($A^1\Sigma^+ - X^1\Sigma^+$) band system are given in Table 9. Regarding these values, we would like to mention that in some cases, where the overlap integral is very small, the \bar{r} -centroids could be unreliable. This is probably the problem with the \bar{r} -centroid $\bar{r}_{33}(J = 30) = 4.8836$. However, it would be interesting to study the criteria of the minimum and maximum \bar{r} -centroids to be used in generating the $R_e(\bar{r})$ functions.

Finally, in Table 10 we give the FCFs for the R and P branches of the 0-0, 0-1, 1-0, and 1-1 bands of CuH ($A^1\Sigma^+ - X^1\Sigma^+$) band system for J up to 15. These factors should be useful, together with Hönl-London factors, in calculating the rotational intensity structure

of these bands. It is interesting to note that for the 0-0 band, for which Wojslaw and Perry (1976) reported a peculiar J -dependence, the FCFs increase with J for the P branch and decrease for the R branch.

In view of the great number of data generated for all the studied band systems, larger vibrational arrays with full rotational dependence are not published here but are available from the authors on request.

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