

Realistic Franck-Condon Factors and r-Centroids for the α -X Bands of CS Molecule

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Abstract: The Franck Condon Factors (FCFs) and r-centroids have been evaluated for the electronic transition $\alpha^3\Pi_r - X^1\Sigma^+$ of Carbon monosulfide $^{12}\text{C}^{32}\text{S}$, based on Morse and Rydberg-Klein-Rees (RKR) potentials by a numerical integration procedure, and the reliability of the obtained values is verified by comparing the results of five different programs used for computing the FC factors. The physical significances of these FC factors and r-centroids have also been discussed, which would be helpful in the verification of the presence CS molecule in interstellar medium and other celestial bodies. Based on the calculated FCFs values the appearance of the bands in this system is also discussed.

Keywords: Transition Probability Parameters, Franck-Condon Factors, r-centroids, CS.

I. Introduction

Franck-Condon factors (FCFs) are important parameters for every molecular band system, since they are involved in the calculation of the relative band intensities, which is a significant source of information in quantitative spectroscopy, high-temperature chemistry and astrochemistry. They are also important for the determination of the molecular structure, population of the v -levels in the upper electronic state involved in transition and also in the calculations of radiative lifetimes, vibrational temperature, kinetics of energy transfer, etc [1]. The FC factors are also useful in the studies of radiative transfer in the atmospheres of stellar and other astronomical objects, which contain molecular species [2]. The concept of r-centroid, which was discovered by Jarman, and demonstrated for the first time by Fraser [3], and further developed by Jarman and Nicholls [4-5], also have been found of much importance as it is used in the interpretation of intensity measurements of many band systems of astrophysical important molecules. Besides this the concept has wide applications in atmospheric physics, space physics, and chemical physics to determine the variation of the electronic transition moment with internuclear separation, and thereby to derive band strengths, and other molecular transition probability parameters [6]. The smooth relationship between r-centroids and wavelengths (or wave numbers) provides a useful relation between experimental measurements and theoretical calculations [5].

The Carbon monosulphide CS molecule has been detected at 3.95 μm in the spectra of C-type stars. [7]. It was also observed radioastronomically through rotational transitions in the circumstellar envelopes of several oxygen-rich stars [8]. CS molecule is observed in Ultraviolet and optical spectra [9]. It has been found in molecular clouds [10], in interstellar space [11], and is identified in an interstellar medium, [12].

In this paper, we report the array of the values of FCFs and r-centroids for the $\alpha^3\Pi_r - X^1\Sigma^+$ band system of the $^{12}\text{C}^{32}\text{S}$ molecule using different programs. Prior to this only information is available in the literature is of Reddy [13], where they reported FCFs without r-centroids and that for few bands. The inconsistency regarding the value of the intense (0, 0) band was also noticed. Furthermore they used only Morse wave function for the calculation of FCFs. Therefore we have undertaken the detailed study of FCFs and r-centroids of this system.

II. Franck-Condon Factors And R-Centroids

Within the framework of the Born-Oppenheimer approximation, the expression for band intensities in emission is given in [14] as

$$I_{\text{em}}(v'v'') = \frac{64}{3}\pi^4 C N_{v'} v^4 \overline{R_e(r)}^2 \left[\int \psi_{v'}(r) \psi_{v''}(r) dr \right]^2 \quad \dots (1)$$

Where C is velocity of light, $N_{v'}$ is number of molecules in v' th level, v is the wave number of radiation of the $v' \rightarrow v''$ vibronic transition; and $\overline{R_e(r)}$ is the average transition moment, which is commonly represented as a function of internuclear distance r. $\psi_{v'}(r)$ and $\psi_{v''}(r)$ are the wave functions which correspond to the rotationless ($J = 0$) vibrational levels in the upper and lower electronic states, respectively. They satisfy the time-independent Schrödinger radial wave equation:

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V(r) \right] \psi_v(r) = E_v \psi_v(r) \quad \dots (2)$$

in which r is the inter nuclear distance, \hbar is Planck's constant, μ is the reduced mass of the two atoms forming the molecule and $V(r)$ is the potential energy .

For many band systems, $R_e(r)$ can be well approximated by a constant or a linear function of r . Since the wave-mechanical formulation of the Franck-Condon principle rests on the assumption that this variation is slow. In such a situation, the r -centroid approximation can be employed. The quantity in the square bracket appearing in eq. (1) is the square of overlap integral known as Franck-Condon factor which is usually denoted by $q_{v'v''}$ and determines how the intensity is distributed among the vibrational bands of a band system. It is expressed as,

$$q_{v'v''} = \left[\int \psi_{v'}(r)\psi_{v''}(r) dr \right]^2 \quad \dots (3)$$

r -Centroid is the r -coordinate of the centroid of the area represented by the overlap integral and defined as,

$$\bar{r}_{v'v''} = \frac{\int \psi_{v'}(r) r \psi_{v''}(r) dr}{\int \psi_{v'}(r) \psi_{v''}(r) dr} \quad \dots (4)$$

In the above equation \bar{r} is the r -centroid which is the weighted average with respect to $\psi_{v'} \psi_{v''}$ of the range of internuclear separation r values experienced by the molecule in both states of the $v' \rightarrow v''$ transition [5] or may be looked upon as an effective value of r for the band in much the same way as the v of eqn.(1) constitutes its effective wave number [15]. The r -centroid is the most practical method for calculation of the band strengths for the observed transitions in diatomic molecules .Since it is an approximation, there are limits to its use, according to [5] .The approximation is good to the n th order if

$$\bar{r}_{v'v''}^n = \int \psi_{v'}(r)r^n \psi_{v''}(r)dr / \int \psi_{v'}(r)r^{n-1} \psi_{v''}(r)dr \quad \dots (5)$$

And its accuracy factor that indicates the degree of its applicability given by Drake and Nicholls [16]

$$Y_{v'v''}^{(n)} = \bar{r}_{v'v''}^n / (\bar{r}_{v'v''})^n = \int \psi_{v'}(r) r^n \psi_{v''}(r) dr / (\bar{r}_{v'v''})^n \int \psi_{v'}(r) \psi_{v''}(r) dr \cong 1 \quad \dots (6)$$

When $Y_{v'v''}^{(n)}$ is unity, the approximation implied in eqs.(4)and,(6) are exact. Deviation from unity for ($n \geq 2$) is a measure of the error in the approximation. The accuracy of the calculated FCF and r -centroid values depend on the knowledge of the potential energy functions of the lower and upper electronic states, which are used in the radial Schrodinger equation to solve for the rotationless vibrational wavefunctions $\psi_{v'}(r)$ and $\psi_{v''}(r)$, Commonly used wavefunctions are those of Morse[17] and Rydberg- Klein-Rees (RKR) [18-20] potentials.

III. Computational Method

There are various methods to calculate the overlap integral, the details of the said methods are reported in the literature [21], [22]. Beside these, other workers have also suggested methods to calculate the FCF factors and developed programmes for such calculations., Amongst them are Le Roy [23-25], Telle [26-29], Espy [30] (see also more of its applications) [31-32], Jarman and McCallum [33-35] and Felenbok [36-37]. In the present study, we have used all of these approaches and in the results the names of the authors are mentioned. The order as follow: (1) Le Roy, (2) Telle, (3) Espy, (4) Jarman and McCallum referred as Jarman and (5) is of Felenbok. These programs are modified to be compatible with our PC (except Le Roy's program, in which we made minor modification to calculate r -Centroids). All the constants used in the other programs are updated as in LEVEL8.0 according to [38] and [39]. We computed potential energy curves using the spectroscopic constants given in Table 1.

IV. Results and discussion

The calculated FCFs and r -Centroids for the bands are listed in Tables 2 and 3. The FCFs factors and r -centroids reveal the intensity distribution in these band systems. The small value of $\Delta r = r'_e - r''_e = 0.0338\text{\AA}$ (where r_e is internuclear distance in a particular electronic state), suggests that the Condon parabola must be very narrow [14] .Condon Parabola is a locus of intense bands in v'' progressions which often pass through (0,0) and are not completely symmetric about $v' = v''$ unless the ω'_e and ω''_e s are very close together.[43] F-C factors of such bands are shown in bold in Table 2 . It is clear that the Condon parabola of this system is really very narrow. The magnitude of the FC factors from Table 2 indicates that the sum rule is satisfied for most of upper and lowers state progressions. In the case of the r -centroids the established fact that the sequence difference $\Delta \bar{r} = r_{v'v''} - r_{v'+1,v''+1}$ remains approximately constant for the strong sequences It is found also that r -centroid values increases systematically with increasing wavelength of the corresponding $v' v''$ bands, which is expected for transitions between states with $r'_e > r''_e$ and hence the bands are red degraded. For example the wavelength and wavenumbers versus r -centroids of few bands of $\Delta v = -1$ sequence of this system are displayed in Table 4 and are plotted in Fig.1 which show a linear relationship. Nicholls [5] have shown that $r_{0,0}$ is usually greater than $(r'_e + r''_e)/2$ for systems whose potentials are not very much anharmonic. In the present case $r_{0,0}$ is found to be slightly greater than $(r'_e + r''_e)/2$ by 0.004 ($r_{0,0} = 1.5558$, $(r'_e + r''_e)/2 = 1.5518$), hence the potentials are not much anharmonic. After preparation of this work we found that the FCFs & r -centroids were

calculated for this system [44] in 13×7 arrays and our results are similar to them. However we repeat the calculations for a 15×15 array and Fig. 2 -3 show a 3-D FCFs for this array while Fig. 4 show the PECs for the transition. The complete list of the 10×10 results showing the wave numbers, wavelengths and r-centroids accuracy factors can be obtained from us on request.

V. Figures and Tables

Table 1: Spectroscopic constants of the $X^1\Sigma^+$ and $a^3\Pi_r$ states of $^{12}\text{C}^{32}\text{S}$

Constant ^a	$X^1\Sigma^+$	$a^3\Pi_r$
T_e	-641.033	27661.0
T_0	0 ^b	27019.967 ^c
ω_e	1285.15464	1135.10
$\omega_e x_e$	6.502605	7.73
$\omega_e y_e$	3.8873×10^{-3}	-
B_e	0.820043559	0.7851
α_e	0.005918345	0.00720
$r_e(\text{\AA})$	1.534942609	1.568729470

- a. All values are in data units of cm^{-1} , unless otherwise noted.
- b. Adjusted T_e of the X state to give $T_0 = 0 \text{ cm}^{-1}$.
- c. Adjusted T_e of the A state to give the corresponding ν_{00} value of [40]. X-state constants from [41] & a-state constants from [42].

Table 2: FCFs of $a^3\Pi_r - X^1\Sigma^+$ band system of $^{12}\text{C}^{32}\text{S}$

$v' \setminus v''$	0	1	2	3	4	5
0	8.29E-01	1.56E-01	1.46E-02	8.97E-04	3.95E-05	1.30E-06
	8.29E-01	1.56E-01	1.46E-02	8.97E-04	3.95E-05	1.30E-06
	8.29E-01	1.56E-01	1.46E-02	8.97E-04	3.95E-05	1.30E-06
	8.29E-01	1.56E-01	1.46E-02	8.97E-04	3.95E-05	1.29E-06
	8.29E-01	1.56E-01	1.48E-02	9.24E-04	4.13E-05	1.39E-06
1	1.54E-01	5.35E-01	2.65E-01	4.19E-02	3.72E-03	2.19E-04
	1.54E-01	5.35E-01	2.65E-01	4.19E-02	3.72E-03	2.19E-04
	1.54E-01	5.35E-01	2.65E-01	4.19E-02	3.72E-03	2.19E-04
	1.54E-01	5.35E-01	2.65E-01	4.19E-02	3.72E-03	2.19E-04
	1.54E-01	5.35E-01	2.64E-01	4.24E-02	3.82E-03	2.28E-04
2	1.97E-02	2.72E-01	2.63E-01	3.42E-01	9.05E-02	1.17E-02
	1.59E-02	2.59E-01	3.08E-01	3.28E-01	7.90E-02	9.54E-03
	1.59E-02	2.59E-01	3.08E-01	3.28E-01	7.90E-02	9.55E-03
	1.59E-02	2.59E-01	3.08E-01	3.28E-01	7.90E-02	9.53E-03
	1.57E-02	2.60E-01	3.08E-01	3.27E-01	7.96E-02	9.76E-03
3	1.20E-03	4.50E-02	3.15E-01	1.47E-01	3.48E-01	1.22E-01
	1.20E-03	4.50E-02	3.15E-01	1.47E-01	3.48E-01	1.22E-01
	1.20E-03	4.50E-02	3.15E-01	1.47E-01	3.48E-01	1.22E-01
	1.20E-03	4.50E-02	3.15E-01	1.48E-01	3.48E-01	1.22E-01
	1.15E-03	4.47E-02	3.17E-01	1.48E-01	3.46E-01	1.22E-01
4	7.51E-05	4.95E-03	8.34E-02	3.28E-01	4.93E-02	3.32E-01
	7.51E-05	4.95E-03	8.34E-02	3.28E-01	4.93E-02	3.32E-01
	7.51E-05	4.95E-03	8.34E-02	3.28E-01	4.93E-02	3.32E-01
	6.37E-05	4.67E-03	8.19E-02	3.30E-01	5.26E-02	3.31E-01
	6.74E-05	4.78E-03	8.30E-02	3.29E-01	4.95E-02	3.29E-01
5	4.18E-06	4.15E-04	1.25E-02	1.26E-01	3.03E-01	5.32E-03
	4.19E-06	4.15E-04	1.25E-02	1.26E-01	3.03E-01	5.31E-03
	4.19E-06	4.15E-04	1.25E-02	1.26E-01	3.04E-01	5.31E-03
	4.20E-06	4.15E-04	1.25E-02	1.26E-01	3.04E-01	5.31E-03
	3.38E-06	3.79E-04	1.22E-02	1.25E-01	3.06E-01	5.38E-03
6	2.21E-07	2.93E-05	1.35E-03	2.49E-02	1.66E-01	2.54E-01
	2.22E-07	2.93E-05	1.35E-03	2.49E-02	1.66E-01	2.53E-01
	2.22E-07	2.93E-05	1.35E-03	2.49E-02	1.66E-01	2.54E-01
	2.23E-07	2.94E-05	1.35E-03	2.49E-02	1.66E-01	2.54E-01
	1.57E-07	2.46E-05	1.26E-03	2.44E-02	1.66E-01	2.55E-01
7	1.14E-08	1.87E-06	1.18E-04	3.38E-03	4.24E-02	1.98E-01
	1.14E-08	1.87E-06	1.19E-04	3.39E-03	4.24E-02	1.98E-01
	1.14E-08	1.87E-06	1.19E-04	3.39E-03	4.24E-02	1.98E-01
	1.12E-08	1.88E-06	1.19E-04	3.39E-03	4.24E-02	1.98E-01

	7.76E-09	1.41E-06	1.03E-04	3.20E-03	4.18E-02	1.99E-01
8	4.86E-10	1.11E-07	9.00E-06	3.60E-04	7.13E-03	6.46E-02
	4.94E-10	1.11E-07	9.03E-06	3.61E-04	7.14E-03	6.46E-02
	4.86E-10	1.11E-07	9.00E-06	3.60E-04	7.13E-03	6.46E-02
	4.37E-10	1.11E-07	9.03E-06	3.61E-04	7.14E-03	6.46E-02
	5.12E-10	8.18E-08	7.22E-06	3.23E-04	6.84E-03	6.41E-02
9	3.73E-12	5.33E-09	6.10E-07	3.23E-05	9.12E-04	1.33E-02
	4.59E-12	5.50E-09	6.18E-07	3.25E-05	9.14E-04	1.33E-02
	3.55E-12	5.29E-09	6.09E-07	3.23E-05	9.12E-04	1.33E-02
	2.38E-12	5.33E-09	6.15E-07	3.24E-05	9.13E-04	1.33E-02
	5.35E-11	5.83E-09	4.85E-07	2.73E-05	8.40E-04	1.29E-02
10	6.02E-12	6.35E-11	3.33E-08	2.51E-06	9.58E-05	2.02E-03
	4.85E-12	8.75E-11	3.53E-08	2.57E-06	9.68E-05	2.03E-03
	6.40E-12	5.83E-11	3.29E-08	2.50E-06	9.57E-05	2.02E-03
	4.16E-12	6.46E-11	3.37E-08	2.53E-06	9.62E-05	2.03E-03
	8.40E-12	6.06E-10	3.70E-08	2.13E-06	8.47E-05	1.91E-03

Cont...

$v' \setminus v''$	6	7	8	9	10
0	3.37E-08	6.28E-10	1.22E-11	5.68E-14	8.23E-15
	3.37E-08	6.30E-10	1.20E-11	8.26E-14	2.83E-16
	3.37E-08	6.29E-10	1.24E-11	4.92E-14	9.90E-15
	3.42E-08	6.37E-10	1.15E-11	2.37E-13	1.66E-12
	3.53E-08	7.04E-10	1.41E-11	8.09E-14	1.06E-13
1	9.13E-06	2.92E-07	6.61E-09	1.47E-10	1.11E-12
	9.14E-06	2.92E-07	6.65E-09	1.40E-10	1.64E-12
	9.14E-06	2.92E-07	6.61E-09	1.49E-10	9.63E-13
	9.09E-06	3.00E-07	5.65E-09	3.36E-10	1.96E-11
	9.69E-06	3.05E-07	7.33E-09	1.36E-10	1.53E-12
2	9.37E-04	5.10E-05	2.03E-06	5.77E-08	1.37E-09
	7.21E-04	3.73E-05	1.43E-06	3.92E-08	8.81E-10
	7.21E-04	3.73E-05	1.44E-06	3.89E-08	9.85E-10
	7.25E-04	3.65E-05	1.56E-06	2.77E-08	1.84E-09
	7.46E-04	3.92E-05	1.49E-06	4.23E-08	9.12E-10
3	1.93E-02	1.83E-03	1.15E-04	5.25E-06	1.69E-07
	1.93E-02	1.83E-03	1.15E-04	5.24E-06	1.68E-07
	1.93E-02	1.83E-03	1.15E-04	5.26E-06	1.68E-07
	1.92E-02	1.85E-03	1.12E-04	5.24E-06	2.49E-07
	1.97E-02	1.88E-03	1.20E-04	5.42E-06	1.79E-07
4	1.65E-01	3.37E-02	3.93E-03	2.96E-04	1.59E-05
	1.65E-01	3.37E-02	3.93E-03	2.96E-04	1.57E-05
	1.65E-01	3.37E-02	3.93E-03	2.96E-04	1.59E-05
	1.63E-01	3.35E-02	3.76E-03	3.01E-04	1.65E-05
	1.66E-01	3.43E-02	4.03E-03	3.08E-04	1.63E-05
5	2.87E-01	2.04E-01	5.30E-02	7.52E-03	6.72E-04
	2.87E-01	2.04E-01	5.31E-02	7.51E-03	6.70E-04
	2.87E-01	2.04E-01	5.31E-02	7.52E-03	6.72E-04
	2.87E-01	2.04E-01	5.31E-02	7.53E-03	6.74E-04
	2.85E-01	2.04E-01	5.38E-02	7.68E-03	6.95E-04
6	3.61E-03	2.25E-01	2.34E-01	7.69E-02	1.32E-02
	3.62E-03	2.25E-01	2.34E-01	7.69E-02	1.31E-02
	3.62E-03	2.25E-01	2.34E-01	7.69E-02	1.32E-02
	3.63E-03	2.25E-01	2.34E-01	7.69E-02	1.32E-02
	3.58E-03	2.23E-01	2.34E-01	7.79E-02	1.34E-02
7	1.89E-01	3.03E-02	1.57E-01	2.51E-01	1.04E-01
	1.89E-01	3.03E-02	1.57E-01	2.51E-01	1.04E-01
	1.89E-01	3.03E-02	1.57E-01	2.51E-01	1.04E-01
	1.89E-01	3.03E-02	1.57E-01	2.51E-01	1.04E-01
	1.91E-01	3.03E-02	1.55E-01	2.50E-01	1.05E-01
8	2.17E-01	1.23E-01	7.09E-02	9.33E-02	2.52E-01
	2.17E-01	1.23E-01	7.10E-02	9.37E-02	2.53E-01
	2.17E-01	1.23E-01	7.09E-02	9.33E-02	2.52E-01
	2.17E-01	1.23E-01	7.10E-02	9.32E-02	2.52E-01
	2.19E-01	1.24E-01	7.10E-02	9.16E-02	2.51E-01
9	9.02E-02	2.21E-01	6.50E-02	1.12E-01	4.25E-02
	9.02E-02	2.21E-01	6.47E-02	1.12E-01	4.35E-02
	9.02E-02	2.21E-01	6.50E-02	1.12E-01	4.26E-02
	9.02E-02	2.21E-01	6.49E-02	1.12E-01	4.25E-02
	9.00E-02	2.22E-01	6.50E-02	1.12E-01	4.13E-02
10	2.25E-02	1.17E-01	2.08E-01	2.34E-02	1.43E-01

	2.25E-02	1.17E-01	2.07E-01	2.29E-02	1.42E-01
	2.25E-02	1.17E-01	2.08E-01	2.34E-02	1.43E-01
	2.25E-02	1.17E-01	2.08E-01	2.32E-02	1.43E-01
	2.21E-02	1.17E-01	2.09E-01	2.31E-02	1.43E-01

The result order is respectively for: (1) Le Roy, (2)Tele, (3)Espy, (4)Jarman, (5)Felenbok.

Table 3: *r*-centroids of $\alpha^3 \Pi_r - X^1 \Sigma^+$ band system of $^{12}C^{32}S$

$v' \setminus v''$	0	1	2	3	4	5
0	1.5558	1.6541	1.7378	1.8134	1.8866	1.9593
	1.5558	1.6540	1.7378	1.8134	1.8866	1.9593
	1.5558	1.6540	1.7378	1.8134	1.8866	1.9593
	1.5560	1.6540	1.7380	1.8130	1.8870	1.9600
	1.5557	1.6539	1.7365	1.8118	1.8850	1.9558
1	1.4693	1.5647	1.6626	1.7453	1.8202	1.8924
	1.4693	1.5647	1.6626	1.7453	1.8202	1.8923
	1.4693	1.5647	1.6626	1.7453	1.8202	1.8923
	1.4690	1.5650	1.6630	1.7450	1.8200	1.8920
	1.4692	1.5644	1.6623	1.7440	1.8185	1.8909
2	1.3741	1.4818	1.5729	1.6712	1.7529	1.8271
	1.3741	1.4818	1.5729	1.6712	1.7529	1.8271
	1.3741	1.4818	1.5729	1.6712	1.7529	1.8271
	1.3740	1.4820	1.5730	1.6710	1.7530	1.8270
	1.3732	1.4816	1.5722	1.6709	1.7516	1.8253
3	1.2670	1.3902	1.4941	1.5791	1.6799	1.7607
	1.2670	1.3902	1.4941	1.5791	1.6799	1.7607
	1.2670	1.3902	1.4941	1.5791	1.6798	1.7607
	1.2670	1.3900	1.4940	1.5790	1.6800	1.7600
	1.2627	1.3893	1.4937	1.5780	1.6795	1.7594
4	1.1449	1.2876	1.4060	1.5062	1.5796	1.6886
	1.1449	1.2876	1.4061	1.5062	1.5796	1.6886
	1.1449	1.2876	1.4060	1.5062	1.5796	1.6886
	1.1220	1.2820	1.4050	1.5060	1.5790	1.6890
	1.1314	1.2840	1.4052	1.5056	1.5778	1.6881
5	1.0070	1.1708	1.3077	1.4216	1.5179	1.5419
	1.0071	1.1709	1.3077	1.4216	1.5179	1.5419
	1.0071	1.1709	1.3077	1.4216	1.5179	1.5418
	1.0080	1.1710	1.3080	1.4220	1.5180	1.5420
	0.9729	1.1602	1.3048	1.4207	1.5171	1.5373
6	0.8569	1.0379	1.1961	1.3273	1.4368	1.5291
	0.8572	1.0380	1.1962	1.3273	1.4368	1.5291
	0.8570	1.0380	1.1962	1.3273	1.4368	1.5291
	0.8580	1.0380	1.1960	1.3270	1.4370	1.5290
	0.7913	1.0117	1.1878	1.3249	1.4360	1.5282
7	0.6910	0.8888	1.0685	1.2207	1.3465	1.4518
	0.6921	0.8891	1.0687	1.2208	1.3465	1.4518
	0.6912	0.8888	1.0686	1.2208	1.3465	1.4518
	0.6828	0.8893	1.0690	1.2210	1.3460	1.4520
	0.6302	0.8391	1.0486	1.2143	1.3445	1.4509
8	0.4135	0.7163	0.9224	1.0987	1.2447	1.3652
	0.4206	0.7180	0.9230	1.0989	1.2448	1.3653
	0.4127	0.7160	0.9224	1.0987	1.2447	1.3652
	0.3509	0.7167	0.9231	1.0990	1.2450	1.3650
	0.5892	0.6724	0.8857	1.0838	1.2398	1.3636
9	-1.8026	0.4356	0.7480	0.9571	1.1282	1.2680
	1.5040	0.4488	0.7512	0.9581	1.1286	1.2682
	-1.8901	0.4323	0.7473	0.9570	1.1282	1.2680
	-2.6300	0.4334	0.7496	0.9577	1.1280	1.2680
	0.7093	0.5962	0.7173	0.9307	1.1174	1.2644
10	1.2908	1.4015	1.4946	1.5506	1.6797	1.2908
	1.2911	1.4017	1.4949	1.5501	1.6785	1.2911
	1.2908	1.4015	1.4945	1.5504	1.6797	1.2908
	1.2910	1.4020	1.4950	1.5510	1.6790	1.2910
	1.2881	1.4004	1.4936	1.5482	1.6785	1.2881

Cont...

$v' \setminus v''$	6	7	8	9	10
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0	2.0233	2.1206	2.0971	2.7721	1.6560
	2.0234	2.1198	2.1044	2.5244	2.7131
	2.0232	2.1190	2.0922	2.8752	1.5448
	2.0190	2.1230	2.0790	0.7131	1.4840
	2.0295	2.1003	2.1046	2.4466	1.5082
1	1.9645	2.0283	2.1214	2.1129	2.5670
	1.9645	2.0284	2.1195	2.1299	2.3225
	1.9645	2.0282	2.1221	2.1073	2.6674
	1.9660	2.0200	2.1860	1.8570	1.0860
	1.9612	2.0329	2.1021	2.1729	2.3217
2	1.8983	1.9698	2.0334	2.1225	2.1309
	1.8983	1.9698	2.0338	2.1193	2.1599
	1.8983	1.9698	2.0332	2.1233	2.1238
	1.8970	1.9760	2.0070	2.2660	1.9090
	1.8969	1.9666	2.0376	2.1069	2.1756
3	1.8341	1.9044	1.9753	2.0387	2.1237
	1.8341	1.9044	1.9752	2.0396	2.1199
	1.8341	1.9044	1.9753	2.0385	2.1251
	1.8350	1.9010	1.9820	2.0380	2.0010
	1.8323	1.9031	1.9722	2.0423	2.1128
4	1.7686	1.8413	1.9107	1.9809	2.0442
	1.7686	1.8413	1.9108	1.9807	2.0461
	1.7686	1.8413	1.9107	1.9810	2.0439
	1.7690	1.8400	1.9170	1.9700	2.0300
	1.7673	1.8394	1.9095	1.9780	2.0474
5	1.6973	1.7767	1.8486	1.9172	1.9867
	1.6973	1.7767	1.8486	1.9174	1.9866
	1.6973	1.7767	1.8486	1.9172	1.9868
	1.6970	1.7770	1.8490	1.9170	1.9870
	1.6967	1.7754	1.8467	1.9160	1.9839
6	1.7114	1.7060	1.7849	1.8561	1.9239
	1.7111	1.7060	1.7849	1.8561	1.9243
	1.7113	1.7060	1.7848	1.8561	1.9238
	1.7110	1.7060	1.7850	1.8560	1.9240
	1.7161	1.7053	1.7836	1.8541	1.9227
7	1.5396	1.6648	1.7145	1.7932	1.8638
	1.5396	1.6647	1.7145	1.7933	1.8638
	1.5396	1.6648	1.7145	1.7932	1.8638
	1.5400	1.6650	1.7140	1.7930	1.8640
	1.5384	1.6655	1.7136	1.7920	1.8617
8	1.4665	1.5486	1.6649	1.7225	1.8016
	1.4665	1.5486	1.6646	1.7225	1.8020
	1.4665	1.5485	1.6649	1.7226	1.8016
	1.4660	1.5490	1.6650	1.7220	1.8020
	1.4656	1.5472	1.6646	1.7213	1.8005
9	1.3836	1.4807	1.5544	1.6712	1.7290
	1.3836	1.4808	1.5544	1.6707	1.7297
	1.3836	1.4807	1.5543	1.6713	1.7292
	1.3840	1.4810	1.5540	1.6710	1.7290
	1.3823	1.4798	1.5527	1.6705	1.7274
10	1.2908	1.4015	1.4946	1.5506	1.6797
	1.2911	1.4017	1.4949	1.5501	1.6785
	1.2908	1.4015	1.4945	1.5504	1.6797
	1.2910	1.4020	1.4950	1.5510	1.6790
	1.2881	1.4004	1.4936	1.5482	1.6785

The result order is respectively for (1) Le Roy, (2)Tele, (3)Espy, (4)Jarmain, (5)Felenbok

Table 4: r-centroids, Wave numbers and Wavelengths of $\Delta v=-1$ sequence of $\alpha^3 \Pi_r - X^1 \Sigma^+$

(v', u')	$\bar{r}_{v', u'}$ (Å)	$\nu_{v', u'}$ (cm ⁻¹)	$\lambda_{v', u'}$ (Å)
(0,1)	1.6540	26313.50	3800.3
(1,2)	1.6626	26173.95	3820.6
(2,3)	1.6712	26031.89	3841.4

(3,4)	1.6798	25887.29	3862.9
(4,5)	1.6886	25740.13	3885.0
(5,6)	1.6973	25590.40	3907.7
(6,7)	1.7060	25438.06	3931.1
(7,8)	1.7145	25283.10	3955.2
(8,9)	1.7226	25125.49	3980.0
(9,10)	1.7292	24965.21	4005.6

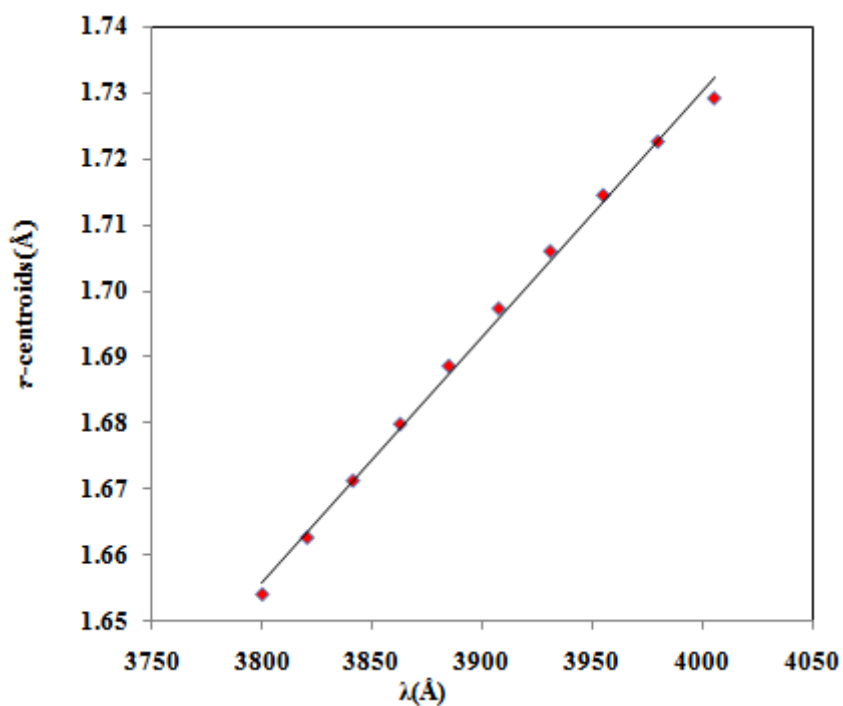


Fig. 1: Variation of r -centroids with λ for $\Delta v=-1$ sequence

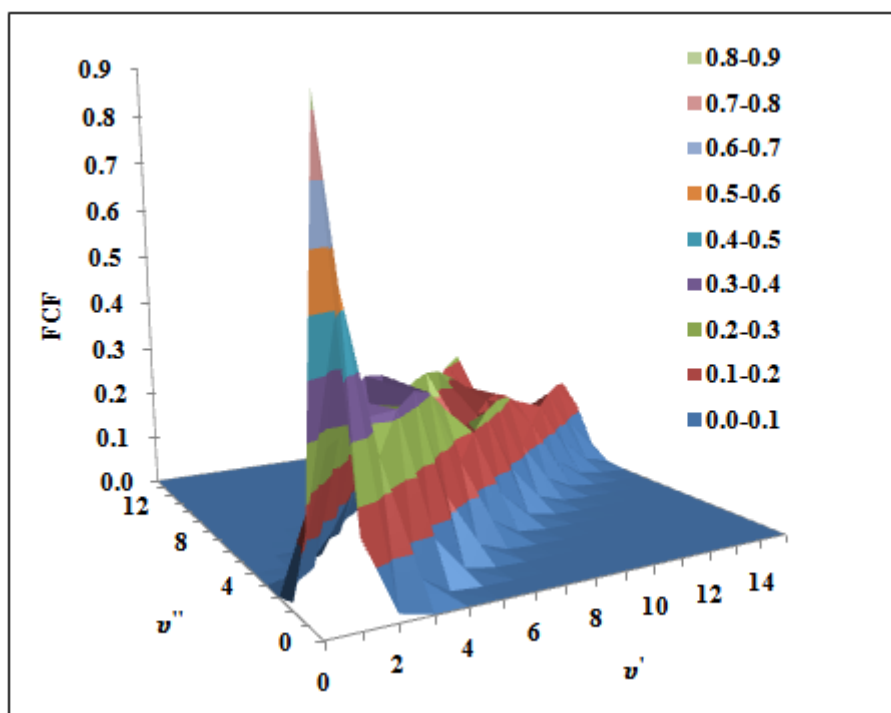


Fig. 2: 3-D Surface of FCF's for the $a^3 \Pi_r - X^1 \Sigma^+$ transition of $^{12}C^{32}S$

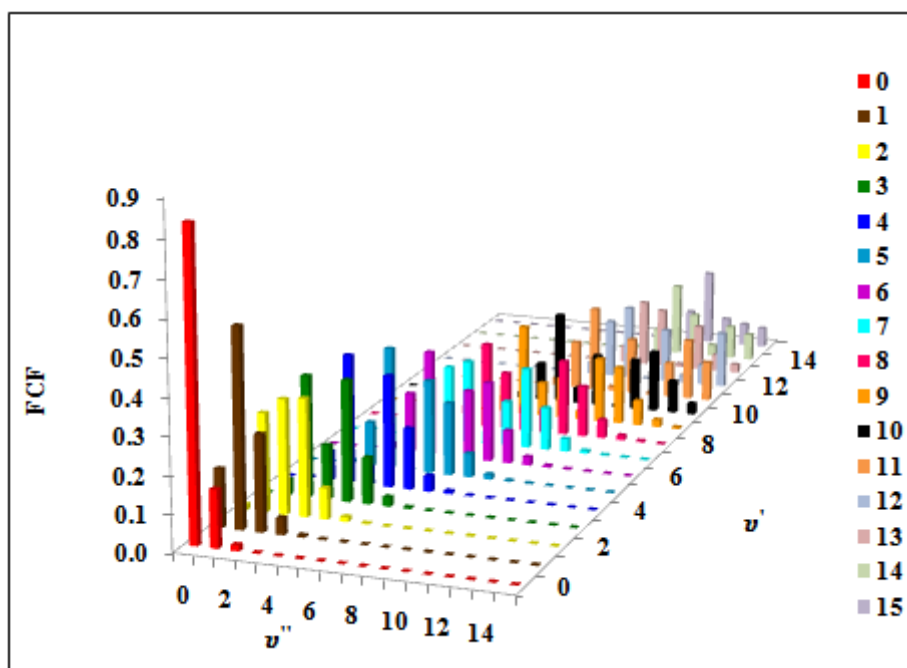


Fig. 3: 3-D Pairs of FCF's for the $a^3 \Pi_r - X^1 \Sigma^+$ transition of $^{12}C^{32}S$

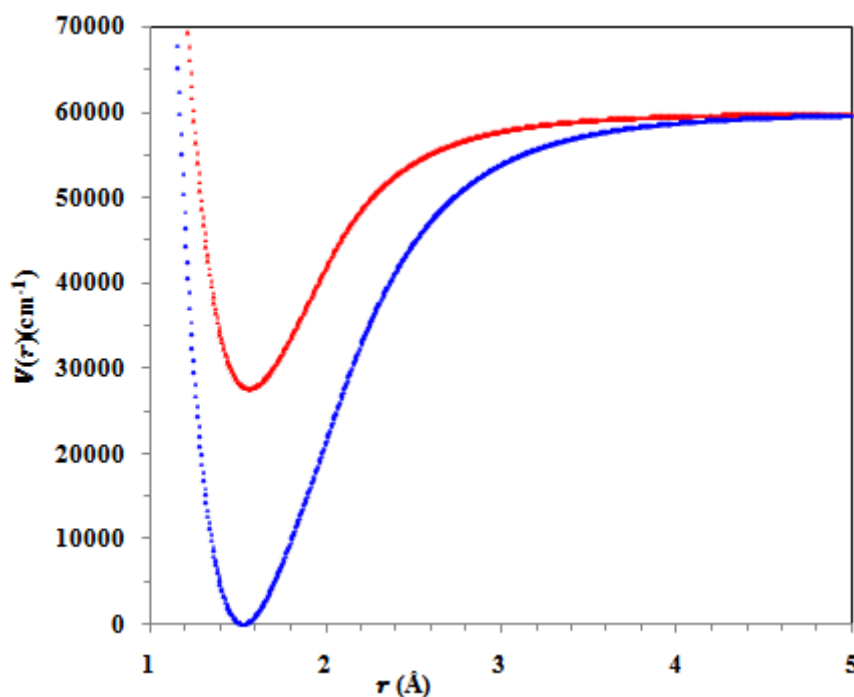


Fig. 4: PECs for $a^3 \Pi_r - X^1 \Sigma^+$ transition of $^{12}C^{32}S$

VI. Conclusion

The FCFs and *r*-centroids for the *a*-X bands of Carbon monosulfide were calculated using Morse and Rydberg–Klein–Rees (RKR) potentials. and it was shown that both agreed fairly well for transitions involving vibrational levels with v' and v'' up to 10, however, at higher levels or (at very small values of FCFs ($<10^{-6}$) small deviations appear which is not surprising since the small FC-factors are more uncertain, and more sensitive with respect to the potential used than the large FC-factors., which, however, do not change the intensity pattern, at least up to $v \approx 10$, and the *r*-centroids approximation may breakdown here as it is clear from Table 3.

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