The gas phase spectra of hydrogen fluoride (HF) and carbon oxide (CO) mixtures are investigated using the Fourier transform infrared (FTIR) broadband spectroscopy technique for the region from 3838 to 3854 cm⁻¹. The OC–HF complex bands, that can correspond to the excited intermolecular (complex) stretching and bending, are observed for the partial mixture pressures of 20 Torr of HF and 30 Torr of CO and higher. The corresponding hot bands of the second harmonic for the bending mode are observed at the total pressure of 100 Torr at -15 degree Celsius (corresponding to 26 Torr of HF and about 90 Torr of CO at room temperature). The observed hot bands are assigned with the help of the fitted spectra for a slightly non-rigid linear molecule. The fitting for the model linear molecule with the experimental data produced the following parameters for the excited states v₁, v₁ + v₂, and v₁ + v₃: v₁ = 3844.030345 cm⁻¹ with B(v₁) = 0.104181 cm⁻¹ and D(v₁) = 3.447151 × 10⁻⁷ cm⁻¹; v₁ + v₂ = 3931.406563 cm⁻¹ with B(v₁ + v₂) = 0.105090 cm⁻¹ and D(v₁ + v₂) = 3.31263 × 10⁻⁷ cm⁻¹; v₁ + v₃ = 3960.722190 cm⁻¹ with B(v₁ + v₃) = 0.102764 cm⁻¹ and D(v₁ + v₃) = 3.059578 × 10⁻⁷ cm⁻¹, respectively.

1. Introduction

OC–HF complex was the subject of a quite large number of both experimental and later theoretical investigations. A significant number of reviews and books have also been published, by detailing the application of experimental methods, particularly those that are spectroscopic [see, for example, [1–5], as well as the development of appropriate computational methods [6–14]. Most of the experimental and theoretical investigations of OC–HF (CO–HF) complexes were carried out under isolated conditions (gas mixtures rarefied to a few Torrs at temperatures below -30 Celsius or supersonic jet expansions). The detailed theoretical studies are still primarily concerned with simple isolated complexes [15], [16]. The pairwise interactions are particularly important for the accurate prediction of properties of the intermolecular interaction, such as equilibrium and vibrational state-specific geometries, dissociation energies, transition frequencies, etc. Such an approach facilitates the determination of the fundamental properties of simpler prototypical systems without emphasizing the process of creation of complexes that can involve three-body interactions or an additional, “out of bound state”, interaction characteristic.

The OC–HF complex was first observed experimentally, using pulsed supersonic jet Fourier transform microwave spectroscopy [1, 17]. These studies indicated that the equilibrium geometry was linear with the atoms configured in the non-linear ground configuration as in Fig. 1. In addition, electric and magnetic properties of OC–HF have also been studied in [18, 19]. We tried to achieve some progress in characterizing the properties of two small covalent molecules quite close distanced. This has been particularly done, by using high resolution spectroscopic techniques, especially in the gas phase. Some important spectroscopic characteristics, like the dependence of a line intensity on the molecular densities, can be found, by using Fourier transform infrared (FTIR) technique. Certain features in the dependence of complex band intensities on molecular densities can help to understand more deeper the nature of the weak bonding. We will discuss it in what follows.

Fig. 1. Geometry of the complex OC-HF in its ground states. The sketch is based on data provided in [1], [20]: Planar OC–HF complex ground state geometry: R = 365 pm is the distance between the centers of masses of OC and HF monomers; ϕ = 14°, θ = 22°. Approximately, in a monomer OC, the distance between atoms O and C is r₁ = 113 pm; in a HF monomer, the distance between atoms H and F is r₂ = 92 pms. The relative radius of each atom in the monomers above is taken as the covalent radius from the table of covalent radii in [21]. The angles ϕ and θ usually correspond to the angles θ₁ and π–θ₂, respectively.
OC–HF dimer is a weaker member of the group with medium-strength hydrogen-bonded interaction [12]. An isolated OC–HF dimer is relatively well characterized by high-resolution spectroscopy. It was initially identified using pulsed-nozzle Fourier transform microwave spectroscopy and was one of the first complexes investigated by ro-vibrationally resolved gas phase infrared spectroscopy [1, 22, 4]. Based on ground state microwave spectroscopy, OC–HF was determined to be linear in its equilibrium geometry with the monomers bonded through the carbon atom. In the ground vibrational state, it is a very nearly prolate asymmetric top, in which only $K = 0$ transitions are observed. The complex has since been a subject of the extensive further spectroscopic characterization. Such analysis included, most importantly, a precise experimentally determined dissociation energy, a study of the state-specific vibrational predissociation and a simulated analysis of the third harmonic of the HF vibration at 10894.46(1) cm$^{-1}$ that is significantly greater than the ground state dissociation energy determined to be 732(2) cm$^{-1}$ [23, 24]. It is also a system that has been a subject of the extensive previous computational study as a prototypical hydrogen-bonded dimer involving first row atoms [25, 39]. The approaches developed in [40] for OC–HF are based on adaptations of the previously developed potential compound-model (PCM) and the compound-model morphing (CMM) techniques [41, 42]. We use the obtained predictions to compare with our experimental results.

The characteristic frequencies of spectra obtained in this work are compared with the theoretically predicted by the compound-model “morphing” with radial shifting (CMM-RS) approach [40] and those obtained by the supersonic beam and color center laser spectrometer [5]. The CMM-RS methodology presented in work [40], based on \textit{ab initio} potential grids, uses the reproducing kernel Hilbert space [43] fitting functions, giving raise in the dipole-dipole interaction at quite long distances, to interpolate the radial coordinates of the six-dimensional potential for OC–HF. The experimental data, used to “morph” the intermolecular potential energy surface of OC–HF in [40], include 24 points from [1–5] (such like rotational constants $B_{\text{ground}}$, $B(v_1)$, $B(v_1 + v_2)$; frequencies of the band centers $v_1$, $v_1 + v_2$; $v_1 + v_3 - v_3$, etc.).

The corresponding potential surface [40] does not possess a local maximum above the “zero” level with respect to the distance between the monomers, therefore, leaving the open question about the processes that “make the complex happened”. Hence, if we consider the complex structure in Fig. 1 with the attractive dipole-dipole interaction between the monomers, such kind of hydrogen bonding potential should have significant enough contributions from the rotationally induced distortion energy and/or the item of ionic interaction as in examples 6 and 7 in Fig. 2, where some possible potential curves $V(r)$ ($r$ denotes the distance between the centers of masses of monomers) are depicted.

Respectively, our paper consists of the two main parts: experimental observations and the discussion of the obtained results.

2. Experimental Results

The values of the $v_1$, $v_2$, and $v_1^4$ modes of vibrational frequencies were initially determined to be 3789.3(3) cm$^{-1}$, 2162.4(3) cm$^{-1}$ and 389.5(5) cm$^{-1}$, using infrared spectra in solid argon matrices [44]. Analysis of the intramolecular bands $v_1$ and $v_2$ located at 3844.0294(50) cm$^{-1}$ and 2167.69904(11) cm$^{-1}$ under isolated equilibrium gas phase and slit jet expansion conditions were reported using a single-frequency mode hop color center laser [22] and diode laser spectroscopy [4], respectively. A reinvestigation of the sub-Doppler reso-
The vibrational frequency $v_1 + v_3 - v_1$ hot band is at 3849.4416 cm$^{-1}$; theoretical $v_1 + v_3 - v_3$ hot band is at 3851.972 cm$^{-1}$; where the bending $v_3 = 81.97997$ cm$^{-1}$; rotational constant in the ground state $B(GS) = 0.10221$ cm$^{-1}$; in the excited state $v_1$: $B(v_1) = 0.10304$ cm$^{-1}$; in the excited state $v_3$: $B(v_3) = 0.09958$ cm$^{-1}$; in the excited state $v_1$: $B(v_1) = 0.10426$ cm$^{-1}$; in the excited state $v_1 + v_3$: $B(v_1 + v_3) = 0.10510$ cm$^{-1}$; in the excited state $v_1 + v_3$: $B(v_1 + v_3) = 0.10178$ cm$^{-1}$. In the sense of the provided possible assignment, we can see the corresponding P-heads at approximately 3839.12 cm$^{-1}$ in Fig. 7 for the $v_1$ H-F stretching fundamental in the OC-HF, 3844.5 cm$^{-1}$ for $v_1 + v_3 - v_3$, and 3847.85 cm$^{-1}$ for $v_1 + v_3 - v_3$, with new unassigned 3850.07 cm$^{-1}$, and 3852.05 cm$^{-1}$ lines (the heads of bands).

Our experimental data were obtained under certain conditions of the gas phase of the mixture (temperatures, pressures, resolutions, etc.), using a BOMEM DA8 Fourier transform spectrometer system with multipath White cell (a stainless steel chamber about 2 m in length and 0.18 m in diameter) and a cryogenic cooling system, with a detector InSb (1800–14000 cm$^{-1}$), windows CaF$_2$ (1200–8500 cm$^{-1}$), and a “Quartz” light source (2000–25000 cm$^{-1}$). In these experiments, a liquid-nitrogen-cooled InSb detector is used with an instrumental resolution of 0.01 cm$^{-1}$. The temperature gradient along a White cell is measured to be about 5 K between the two extremes of the multipass cell; accordingly, the average temperature is provided. In Figs. 3–7, “ap.” stands for the aperture, “path” means the total pathlength of the transmitted beam, “res.” stands for resolution; other parameters are clear in the notation.
In Fig. 3 A and B, we can see the partially rotational resolved $v_1$ H-F stretching fundamental band of the OC–HF complex near the $P$-head at 3839.12 cm$^{-1}$. On all of them, the possible "P"-head of the $v_1 + v_3 - v_2$ band is visible at 3847.85 cm$^{-1}$.

The latter "P-head" also appears at room temperature (see Fig. 5) with twice higher CO partial pressure. Other "hot" band heads of the OC–HF complex at room temperature as in Fig. 6. In Fig. 6, the strong transition at 3839.12 cm$^{-1}$ and the relative line strengths (relative dipole moments – see the instruction in [46]) for the transition $v_1 \leftarrow 0$, 0.85 for $v_1 + v_3 \leftarrow v_2$, and 0.7 for $v_1 + v_3 \leftarrow v_3$. The fitting (with Boltzmann weight factors) of the model linear molecule with the experimental data gave the following parameters for the excited states $v_1$, $v_2$, and $v_3$: $v_1 = 3844.0325(3)$ cm$^{-1}$ and fundamental $v_1 = 3849.4401(4)$ cm$^{-1}$ bands.

In Fig. 8, we propose a reader to compare the observed spectra (shown in Fig. 3, A) with the simulated spectra based on the experimental data from Fig. 3, A and the approximate values of the constants $B(GR) = 0.101480$ cm$^{-1}$; $D(GR) = 3.8 \times 10^{-7}$ cm$^{-1}$, $B(v_2) = 0.103030$ cm$^{-1}$; $D(v_2) = 3.7 \times 10^{-7}$ cm$^{-1}$, $B(v_3) = 0.100800$ cm$^{-1}$; and $D(v_3) = 3.4 \times 10^{-7}$ cm$^{-1}$.

The state constants determined from an analysis of the fundamental $v_1$, hot $v_1 + v_3 - v_2$, and $v_1 + v_3 - v_3$ bands in [5] are as follows: $B(v_1) = 0.1042511(7)$ cm$^{-1}$; $D(v_1) = 0.04$ cm$^{-1}$; and $D(v_2) = 0.06$ cm$^{-1}$.

The Lorentzian contribution to a linewidth (full width half maximum) of 0.04 cm$^{-1}$ and the approximate values of the constants $B(v_2) = 0.04$ cm$^{-1}$; $D(v_2) = 0.06$ cm$^{-1}$; $B(v_3) = 0.04$ cm$^{-1}$; and $D(v_3) = 0.06$ cm$^{-1}$.

The approximate values of the constants $B(v_2) = 0.04$ cm$^{-1}$; $D(v_2) = 0.06$ cm$^{-1}$; $B(v_3) = 0.04$ cm$^{-1}$; and $D(v_3) = 0.06$ cm$^{-1}$.
The obtained spectroscopic information allows one to make a further analysis of properties of the gas phase mixture. Some thoughts and ideas of applications of the obtained data are presented in the following section.

3. Discussion of the Experimental Results

The intercomplex frequencies $\nu_{15}$, $\nu_3$, and $\nu_{14}$ correspond to the temperatures 117 K (in terms of $k_B T$ per the two-dimensional mode involved), 156 K (312 K in terms of $1/2 k_B T$ per mode), and 530 K (in terms of $k_B T$ per the two-dimensional mode involved), respectively. Consequently, at the experiment temperatures from 300 K to 260 K, we can most probably observe hot bends corresponding to the frequencies $\nu_{15}$ and $\nu_3$. At this point, the corresponding dipole matrix elements define, which band can be more prominent. It is worth to note that the theoretical dissociation energy found in [40] by the “morphed” adiabatic potential with both monomers in their ground vibrational states is characterized by the equilibrium dissociation energy $D_e = 1310(10)$ cm$^{-1}$ and the ground state dissociation energy $D_0 = 742.5(50)$ cm$^{-1}$. $D_0 = 742.5(50)$ cm$^{-1}$, corresponding to a quite strong binding energy with the “dissociation” temperature 1069 K (in terms of $(1/2)k_B T$). In such a case, one could say that, if there is no some “barrier” to create a stable complex, potentially all monomers (for, example, HF) may exist only in bound states with the other kind of monomers (CO, accordingly). Below, we try to analyze the situation in more details.

The coupled master equation in the case of vibrational-rotational-translational exchange can be solved to find the internal state distribution in a space-homogeneous medium with one-component density num-
ber \( n \)

\[
\frac{\partial}{\partial t} \rho_{iv} = \frac{n}{V} \sum_{jv'} \left[ -\rho_{iv} k(iv \rightarrow jv'; T) + \rho_{jv'} k(jv' \rightarrow iv; T) \right]
\]

(1)

where \( \rho_{iv} \) are the vibrational-rotational populations with \( i \) indexing rotational states and \( v \) – vibrational ones; \( k \) is the state-to-state vibrational-rotational relaxation rate constant. The rate constants can be modeled in different ways (see, e.g., [47]). The transition rate (or, in some sense, the rate coefficient) can be expressed through the equilibrium reaction constant as \( k_{\text{react}} = \nu_D K_2^3 \) with \( \nu_D \) being a characteristic frequency associated with the controlling reaction coordinate. Below in this section, we discuss some possible way to define the equilibrium constant.

The used technique to compute the potential energy of the complex is essentially limited by the set of bound states with negative total energy values as, for example, in [40]. The latter does not give understanding the states with negative total energy values as, for example, if put under higher pressures, because a dipole moment is induced by the intermolecular forces. Because of the rapid decrease of intermolecular forces with increasing separation of the molecules, the induced dipole moment is a short-range function of the intermolecular distances. Consequently, the induced transition moment persists only during the time of the collision. Part of the energy of the photon which is absorbed by the collision cluster may appear as an increase in the molecular translational energy after the collision (for all photon energy transformed into translational motion, we have pure translational transitions with \( \Delta J = 0 \) and \( \Delta m = 0 \) or \( \Delta m \neq 0 \) for the orientational transition or “flip-flop” rotational transition in the cluster with \( \Delta J_1 = -\Delta J_2 \)). The noted here especially concerns two unlike gases, when the respective electron clouds are deformed to a different degree during the collision time. In our case, both molecules (HF and CO) possess permanent dipole moment. Although the absorption, corresponding to the permanent dipole moments, gives the largest contribution to the total absorption coefficient, the simultaneous enhancement of the intensity of the dipole-allowed transitions in both kinds of monomers can happen during translational-rotational-vibrational transitions with \( \Delta J \neq 0 \) and \( \Delta J \neq 0 \), for instance. Because the observed distances between two closest “hot band” lines (in the sense of the integrated all rotational transitions in the band) are within 2...6 cm\(^{-1}\) (see Fig. 7), the pre-dissociation transitions, such like ground \( \rightarrow \nu_1 + \nu_{\text{monomer}} \) (\( \Delta J_{\text{CO}} = \pm 1 \)), can be under consideration for the investigated mixtures.

Assuming a thermal equilibrium in the investigated gas mixtures and a quite small source intensity (a change in the upper level population has to be much less than the population value during the time corresponding to the source Rabi frequency (which is supposed to be smaller than the molecule decay rate)), one can estimate the contribution from binary and ternary collisions by investigating the dependence of the absorption coefficient (here, to stay within certain quantum optics principles, we give our edition of the expression [49] cited on the pages 415–416):

\[
\alpha_{f \rightarrow i} = \frac{1}{\text{Linewidth}} \int_{\text{Line}} \alpha(\tilde{\nu}) \tilde{d}\tilde{\nu} = \frac{8\pi^2 \tilde{\nu}_f g'' \exp(-\tilde{\nu}'/k_B T) \left[1 - \exp(-h\tilde{\nu}_f/k_B T)\right]}{4\pi \varepsilon_0 3h c \delta \nu Q} \times S_{f \rightarrow i},
\]

(4)
on particle densities. Here, besides the standard constants $k_B, \hbar, \varepsilon_0$, and $c$ in the IS system of units, $\tilde{\nu}_{if} = \frac{(E_f - E_i)}{\hbar}$ is the transition frequency in Hz; $g^0$ is the degeneracy of the level with energy $E^0$; $\delta \nu$ is the characteristic line width ("non-cyclic" frequency in Hz) giving the fitting of the absorption coefficient with an experimental value and may be defined by the detector characteristic time of reaction and the phase maximum frequency as for the FTIR spectroscopy using a Michelson interferometer (this was not tested with the obtained experimental results). For example, an InSb detector in our experiment has 4\mu s characteristic "delay" time, and the phase maximum frequency is 7899 Hz; $\tilde{Q}$ is the partition function, defined as

$$Q = \sum_n g_n \exp \left( -E_n/k_B T \right),$$

where $E_n$ is the energy, and $g_n$ is the total degeneracy of the state $n$. The line strength $S_{f \rightarrow i}$ of an electric dipole transition is given by

$$S_{f \rightarrow i} = \sum_{\Phi_{int}} \sum_{A=X,Y,Z} |\langle \Phi_{int}' | \mu_A | \Phi_{int} '' \rangle|^2,$$

where $\Phi_{int}$ and $\Phi''_{int}$ are eigenfunctions of the molecular Hamiltonian corresponding to the eigenvalues $E'$ and $E''$, respectively; $\mu_A$ is the component of the molecular dipole moment operator along the $A$ axis ($A = X, Y,$ or $Z$); the $(X,Y,Z)$ axis system has the origin at the molecular center of mass, for example, and a space-fixed orientation. The absorption coefficient per molecule can be expanded in a power series of the number density

$$\alpha_{f \rightarrow i} = \sum_{SP=1}^{2} \left\{ \alpha_{0,SP}^{f \rightarrow i} n(SP) + \alpha_{2,SP}^{f \rightarrow i} n^2(SP) + \ldots \right\}.$$

(7)

Here, $\alpha_{0,SP}^{f \rightarrow i}$, $\alpha_{2,SP}^{f \rightarrow i}$, ... are the absorption coefficients per one molecule taking binary, ternary, ... collisions into account, respectively. Because of the following use of the reviewed absorption coefficient per molecule in the expression for the transmission through the passlength $z$:

$$I_{1}(f \leftarrow i) = I_{0}(\tilde{\nu}) \exp \left[ -zn \\alpha_{f \rightarrow i} \right],$$

(8)

where $n$ (OC–HF) is the number of complexes per unit volume, the resulting “binary” (ternary) absorption coefficient per unit passlength

$$\tilde{\alpha}_{f \rightarrow i} = n (\text{CO-HF}) \alpha_{f \rightarrow i} = \tilde{\alpha}_{1}^{f \rightarrow i} n (\text{CO}) n (\text{HF}) + \tilde{\alpha}_{2}^{f \rightarrow i} n^2 (\text{CO}) n (\text{HF}) + \ldots$$

(9)

depends on the density as the square power for binary collisions, more accurately as $n (\text{CO}) n (\text{HF})$, and as the cubic number density for ternary collisions including items proportional to $n^2 (\text{CO}) n (\text{HF})$ and $n (\text{CO}) n^2 (\text{HF})$. The obtained experimental data for the transmittance can possibly answer the question: Which of the contributions from binary and ternary collisions is the most important? This, in turn, can give some picture about the possible channels of the complex creation, which was shortly described above.

For instance, assuming a quite small contribution from higher orders in densities than the 3-rd one, we calculated the three resulting absorption coefficients $\tilde{\alpha}_{1}^{f \rightarrow i}$, $\tilde{\alpha}_{2}^{f \rightarrow i}$ in expression 9 for the intensities averaged over 18 points on the range of frequency from 3839.01 cm$^{-1}$ to 3839.28 cm$^{-1}$, corresponding to the $P$-head of the fundamental $v_1$ band. The three graphs, describing the mixture at room temperature, were chosen (Fig. 5, C and D, and Fig. 6), so that the corresponding averaged relative intensities (transmittance) are 0.045554721, 0.141861727, and 0.538861464. The latter yields the following resulting transmission coefficients: $\tilde{\alpha}_{2} = 8.71 \times 10^{-51}$ m$^2$, $\tilde{\alpha}_{1}^{3} = -1.26 \times 10^{-74}$ m$^3$, $\tilde{\alpha}_{2}^{3} = 6.91 \times 10^{-76}$ m$^3$. The positive numbers potentially tells us about the main mechanism of the creation of OC–HF complexes. Therefore, the two-particle collisions of CO and HF, and the three-particle collisions CO–HF–CO are the main contributors in the complex number density. It is worth to note that the contribution from the ternary collisions CO–HF–CO is by one order lower than that from the binary ones under the provided conditions.

The concentration of the complexes $n_{00}$ (OC–HF) in the ground state can be estimated using the calculated dissociation energy $D_0$. Assuming the main effects are due to the binary interactions as in the example above, the equilibrium reaction $A + B \rightleftharpoons AB$ can be characterized by the equilibrium constant $K_{00}$ (see [50], Chapter 17):

$$K_{00} = \frac{n_{00} (\text{OC–HF})}{n_{00} (\text{OC}) n_{00} (\text{HF})} = V \frac{Z (\text{OC–HF})}{Z (\text{OC}) Z (\text{HF})} =$$
where \( n_{00} \) (OC) and \( n_{00} \) (HF) are the corresponding concentrations in the ground vibrational states of the proton acceptor and the proton donor, respectively; \( \mu \) is the complex reduced mass; \( Z (SP) \) and \( Z_{rot} (SP) \) denote the total partition function and the partition function of rotational energy levels at a certain temperature \( T \) of thermal equilibrium for a \( SP \)-th species, accordingly.

\[
\left( \frac{h^2}{2\pi\mu kT} \right)^{3/2} \frac{Z_{rot} (OC-HF)}{Z_{rot} (OC) Z_{rot} (HF)} \exp (D_0/kT),
\]

4. Conclusion

The simulated spectra and the corresponding vibrational frequencies of the OC–HF complex, described by the statistically weighted (by Boltzmann factors) transitions of the heterodimer modeled as a slightly non-rigid linear molecule (with the frequency transition expression \( \nu = \nu_0 + B''J''(J'' + 1) - D''[J''(J'' + 1)]^2 - B''''J''''(J'''' + 1) + D''''[J''''(J'''' + 1)]^2 \); here, the quantum number \( l \) is zero), are comparable with the experimental data obtained from the FTIR broadband scans of the gas phase mixtures at different total pressures and temperatures. The obtained results can be in use to make the further analysis of the gas phase properties. For example, the obtained dependence of the absorption coefficient on the partial pressures (densities) at room temperature showed the main absorption contribution from the binary collisions. Thus, the problem can be raised about the complex creation in the context of binary interactions.

The Robert A. Welch Foundation is thanked for the financial support in the form of pre-doctoral and post-doctoral fellowships under grant A-747. I also thank Dr. J. Bevan’s group and the Laboratory for Submm/THz Science and Technology at Texas A & M University (College Station, Texas, USA) for providing support and consultations.


ФУР’Є СПЕКТРОСКОПIЯ ГАЗОВОЇ ФАЗИ CO ТА HF СУМIШЕЙ У СЕРЕДНIЙ IНФРАЧЕРВОНIЙ ОБЛАСТI

А.С. Сiжук

Р е з ю м е

Спектри газової фази CO та HF сумiшей було дослiджено за допомогою FTIR спектрометра у дiапазонi частот 3838–3854 см\(^{-1}\). Групи лiнiй комплексу OC–HF, що можуть вiдповiдати збудженим iнтермолекулярним (комплексу) розтягненням та згинам, були спостереженi для парцiальних тискiв 20 Торр HF та 30 Торр СО i вищих. Вiдповiднi “гарячi” групи лiнiй другої гармонiки моди згину були спостереженi для сумiшi, що вiдповiдає повному тиску 100 Торр при \(-15^\circ C\) (що вiдповiдає приблизно 26 Торр HF i 90 Торр CO при кiмнатнiй температурi). Спостереженi групи лiнiй було визначено за допомогою моделi “слабко нетвердої” лiнiйної молекули. Корелiцiя модельної лiнiйної молекули з експериментальними даними вiдтворила такi параметри для збуджених станiв

\[
v_1, \ v_1 + v_3^5,\ v_1 + v_3,\ v_1 + v_3 + v_3^5 = 3844, 30345 \text{ см}^{-1} \text{ з } B(v_1) = 0, 104181 \text{ см}^{-1} \text{ i } D(v_1) = 3, 447151 \cdot 10^{-7} \text{ см}^{-1}; v_1 + v_3 = 3931, 406563 \text{ см}^{-1} \text{ з } B(v_1 + v_3) = 0, 105090 \text{ см}^{-1} \text{ i } D(v_1 + v_3) = 3, 31263 \cdot 10^{-7} \text{ см}^{-1}; v_1 + v_3 + v_3^5 = 3960, 722190 \text{ см}^{-1} \text{ з } B(v_1 + v_3) = 0, 102764 \text{ см}^{-1} \text{ i } D(v_1 + v_3) = 3, 059578 \cdot 10^{-7} \text{ см}^{-1}, \text{ вiдповiдно.}
\]