ScO ($X^2\Sigma^+$: $v = 0$): $N = 2-1$

The Pure Rotational Spectrum of the ScO ($X^2\Sigma^+$) Radical

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Abstract

The rotational spectrum of ScO ($X^2\Sigma^+$) has been measured in the gas phase in the frequency range 30 – 493 GHz using a combination of Fourier transform microwave/millimeter-wave (FTM/mmW) and submillimeter direct absorption methods. This work is the first pure rotational study of this radical. Both the ground vibrational and $v = 1$ states were observed. ScO was created from the reaction of metal vapor, produced either by a laser ablation source or a Broida-type oven, and N_2O , in the former case heavily diluted in argon. Extensive hyperfine structure was observed in the FTM/mmW data, although the spin-rotation splitting was found to be small (~ 3 MHz). In the mm-wave spectra, however, the fine and hyperfine structure was blended together, resulting in broad, single lines for a given transition $N + 1 \leftarrow N$. The data were analyzed in a combined fit using the very accurate hyperfine measurements of Childs and Steimle (1988), employing a Hund's case b Hamiltonian, and an improved set of **rotational and centrifugal distortion** constants were determined. **These measurements improve the accuracy of predicted frequencies for astronomical searches by 14 – 18 MHz, or 16 – 20 km/s, in the 1 mm region – a difference of half to a full linewidth for certain interstellar sources.** This work also demonstrates the capabilities of the FTM/mmW spectrometer at 61 GHz.

1. Introduction

Simple metal-containing molecules such as diatomic oxides and hydrides have been observed in stellar atmospheres via their electronic transitions for over 100 years. Such molecules are important because they have provided an avenue for spectral identification. For example, TiO and VO bands dominate the far-optical portions of the spectra of late M-type stars, but in cooler dwarfs, they are replaced by those of metallic hydrides [1]. CrH infrared spectra are in fact used as a distinct indicator of L class brown dwarfs [2]. Alkaline earth and rare earth metal oxides such as BaO, LaO, and CeO have also been observed in M-type stars, as well as in sunspots [3]. Supergiants such as VY Canis Majoris (VY CMa) are known to exhibit electronic transitions of AlO, TiO, VO, and YO in their atmospheres as well [4].

ScO is also a well-known stellar constituent. Optical spectra of this molecule have been observed in the atmospheres of M-type stars, supergiants, and eruptive variables. For example, the $A^2\Pi_r-X^2\Sigma^+$ transition of this oxide near 6000 Å has been observed in β Peg, o Cet, and supergiant VY CMa, as well as the explosive stars V4332 Sgr and V838 Mon [5-11]. All of these objects are thought to be oxygen-rich, and Kimeswenger [9] has even suggested that ScO is an effective signature of very O-rich ejecta. In addition, the $B^2\Sigma^+-X^2\Sigma^+$ transition near 4800 Å has been detected in sunspots [5,6,12,13].

The spectrum of ScO has been well-studied in the laboratory both at low and high resolution. The optical spectrum of ScO was first investigated with an arc-flame spectrograph by Fowler [14], who measured bands in the 4700 – 6600 Å range. Meggers & Wheeler [15] subsequently observed spectra from 4500 Å to 7200 Å and identified both the $A^2\Pi_r-X^2\Sigma^+$ and $B^2\Sigma^+-X^2\Sigma^+$ electronic transitions. These bands were heavily studied thereafter by a series of investigators, starting with Adams, Klemperer, & Dunn [16]. In 1972, Stringat et al. [17]

measured the $A^2\Pi_r-X^2\Sigma^+$ transition with high spectral resolution and determined rotational parameters for the molecule, while Childs & Steimle [18] used molecular-beam optical/radio frequency double resonance techniques to establish precise values of fine and hyperfine constants of the ground state from magnetic-dipole allowed transitions. These parameters were also measured for the ground state by an electron spin resonance (ESR)/argon matrix study of Knight et al. [19]. The $A^2\Pi_r-X^2\Sigma^+$ band was additionally investigated by optical Stark methods [20], in which the ground state dipole moment was determined to be $\mu = 4.55$ D. Recently, Mukund et al. [21] used laser-induced fluorescence (LIF) to record the $B^2\Sigma^+-X^2\Sigma^+$ transition with high-resolution, substantially improving the rotational constants for $v = 0, 1$, and 2 levels in the $X^2\Sigma^+$ state. In addition to the experimental work, theoretical calculations have also been performed concerning the low-lying electronic states of ScO [22-24].

Here we present the first direct measurement of the pure rotational spectrum of the ScO ($X^2\Sigma^+$) radical in its $v = 0$ and 1 vibrational levels. The spectra were recorded using both Fourier transform microwave/millimeter-wave (FTM/mmW) and direct absorption methods. From these data, combined with the previous hyperfine measurements of Childs and Steimle (1988), an improved set of spectroscopic parameters have been determined, in particular the rotational constants. Some of the data were recorded with the FTM/mmW spectrometer near 61 GHz, further demonstrating its high frequency capability.

2. Experimental

Spectra of ScO ($X^2\Sigma^+$) were first recorded using the Fourier transform microwave/millimeter-wave (FTM/mmW) instrument of the Ziurys group. This machine is a Balle-Flygare type design and operates from 4 – 90 GHz [25,26]. The system consists of a vacuum chamber, evacuated to 10^{-8} Torr by a cryopump, with two spherical mirrors positioned in

a near confocal arrangement, forming a Fabry-Perot cavity. Two different sets of mirrors are used to cover the full frequency range of the instrument. From 4 – 40 GHz, antennas are used for injection and detection of the radiation, while waveguide are employed for this purpose in the 40 – 90 GHz range. The frequency source is a signal generator (Agilent), coupled with various multipliers (Norden Millimeter) for operation above 40 GHz. Detection of time-domain molecular emission (free induction decay or FID) is accomplished with low noise amplifiers (Miteq, Spacek, Norden Millimeter, or NRAO). The FID signals are processed by a computer; where a Fourier transform is performed to generate a spectrum. The instantaneous bandwidth of the spectrometer is ~ 1 MHz; spectral scanning is accomplished by changing the synthesizer frequency while optimizing the cavity response. The molecular beam is injected into the cavity at a 40° angle from the cavity axis using a pulsed nozzle (General Valve). Because of the orientation of the beam with respect to the electric field supported by the cavity, measured transitions have a Doppler doublet structure with a FWHM of about 50 - 100 kHz.

In the FTM/mmW instrument, ScO was created in a supersonic expansion coupled with a laser ablation source. A mixture of 0.1% N_2O in 200 psi of argon, pulsed from the expansion nozzle, was reacted with metal vapor generated by a Nd:YAG laser (532 nm) impinging on a rotating/translating scandium rod. Unlike many of our experiments, a DC discharge was not used to synthesize ScO, as it significantly reduced the spectral signals.

Submillimeter measurements of ScO were subsequently conducted using the high-temperature direct absorption spectrometers of the Ziurys group. This instrument is composed of a radiation source, a double-walled steel gas cell, and a detector [27]. The source consists of various combinations of Gunn oscillators and Schottky diode multipliers that enable coverage from 65 to 850 GHz. The double-pass vacuum chamber is water-cooled and contains a Broida-

type oven, which produces metal vapor through resistive heating. The detector is a helium-cooled, hot electron bolometer, operated at 4 K. The radiation is directed through the system quasi-optically using a feedhorn, several lenses, a polarizing grid, and two ellipsoidal mirrors. Phase-sensitive detection is accomplished by modulating the radiation source at 25 kHz and detected at $2f$, which produces a second-derivative spectrum.

ScO was created in the millimeter/submillimeter system from a mixture of metal vapor, generated by the Broida oven, and N_2O . Because scandium is quite expensive, remaining pieces of rod from the laser ablation source (~ 0.5 g) were used in the experiments. About 30 mTorr of argon carrier gas was introduced into the chamber from beneath the oven, while ~ 3 mTorr of N_2O was added over the top. Again, a DC discharge was not needed in the synthesis.

Transition frequencies of scandium oxide were determined in the submillimeter instrument by recording two scan pairs, 5 MHz in width, one in increasing frequency and the other in decreasing frequency. The spectral features were fit with a Gaussian profile to determine the center frequencies. The line widths were found to be broader than usual - typically 1750 kHz at 461 – 492 GHz. The experimental accuracy is estimated to be ± 50 kHz. For the FTM/mmW studies, transitions frequencies were established by taking the average of the Doppler pairs; estimated experimental accuracy in this case is ± 4 kHz.

3. Results and Analysis

Based on the previous spectroscopic constants from Mukund et al. [21] and Childs & Steimle [18], lines arising from the $N = 1 \rightarrow 0$ transition of ScO near 31 GHz were readily located using the FTM/mmW instrument. Scandium oxide has a $^2\Sigma^+$ ground electronic state, and therefore $S = 1/2$. In a case $b_{\beta J}$ coupling scheme, the rotational angular momentum, indicated by quantum number N , couples with the electron spin angular momentum S to produce fine

structure doublets labeled by J , where $\mathbf{J} = \mathbf{N} + \mathbf{S}$. In addition, scandium has a nuclear spin of $I = 7/2$, which in turn generates hyperfine structure, designated by quantum number F , where $\mathbf{F} = \mathbf{J} + \mathbf{I}$. These couplings generate six strong hyperfine components in the $N = 1 \rightarrow 0$ transition; all were measured. The $N = 2 \rightarrow 1$ was found thereafter, which had an extremely complex hyperfine pattern with 18 favorable hyperfine components. Again, all 18 lines were recorded. In both transitions, several weaker lines arising from the $v = 1$ state were observed as well. The $v = 1$ state lies at an energy of 965 cm^{-1} above ground state [21].

Based on the refined spectroscopic constants from the FTM/mmW data, sub-mm lines of ScO were then recorded near 460 - 490 GHz. At these higher frequencies, both the spin-rotation and the hyperfine splittings were essentially collapsed. The two transitions measured therefore consisted of single, although somewhat broadened, spectral lines. Only two such transitions could be measured because only a small amount of scandium was available for the experiment, which was rapidly vaporized in the Broida oven.

Representative FTM/mmW spectra of the $N = 1 \rightarrow 0$ and $2 \rightarrow 1$ transitions near 30.8 and 61.5 GHz in the ground vibrational state ($v = 0$) are presented in Figure 1. Each transition consists of multiple fine/hyperfine components, partly arising from the scandium nuclear spin. There are five frequency breaks in each spectrum such that multiple features could be displayed. Doppler doublets are indicated by the brackets above each spectral line. Only six of the eighteen favorable hyperfine components are displayed for the $N = 2 \rightarrow 1$ data (lower panel); all six measured for the $N = 1 \rightarrow 0$ transition are shown (upper panel). The scandium hyperfine interactions dominate the spin-rotation coupling, such that hyperfine components arising from different J quantum numbers intermix as in a b_{ps} scheme. Slight Zeeman splitting is also evident

in the two $\Delta F = 0$ components in the $N = 1 \rightarrow 0$ transition, which lie near 30.77 and 30.84 GHz, respectively.

Figure 2 displays four hf components of the $N = 2 \rightarrow 1$ transition of ScO arising from the $v = 1$ state near 61.2 GHz. The lines arise from both spin components, $J = 1.5 \rightarrow 0.5$ and $J = 2.5 \rightarrow 1.5$, as shown in the figure. Each Doppler doublet is indicated by brackets, and there are three frequency breaks in the spectrum. The lines are clearly weaker than those from the $v = 0$ state, despite longer signal averaging (at least a factor of two per line).

The submillimeter spectra of ScO, acquired near 460 – 490 GHz, are displayed in Figure 3. Here the $N = 15 \leftarrow 14$ (upper panel) and $16 \leftarrow 15$ (lower panel) transitions are shown. At these higher frequencies, both the fine and hyperfine structure effectively collapse into a single line. The measured linewidths are somewhat broader (by ~ 500 kHz) than expected for these features, which can be accounted for by the residual fine/hyperfine structure in each transition.

The microwave and submillimeter transition frequencies measured for ScO are listed in Table 1. A total of 26 and 11 individual lines were measured for the $v = 0$ and 1 states, respectively, involving $\Delta J = 0, \pm 1$, and ± 2 and $\Delta F = 0, \pm 1$ transitions.

The microwave and submillimeter data were combined in a global fit with the rf-optical double resonance data of Childs & Steimle [21] for $v = 0$ and 1, where $\Delta N = 0$. The $v = 0$ and 1 data were analyzed separately using a Hund's case $b_{\beta J}$ Hamiltonian. Terms for rotation, spin-rotation, magnetic hyperfine, electric quadrupole, and nuclear spin-rotation were modeled:

$$\hat{H}_{\text{eff}} = \hat{H}_{\text{rot}} + \hat{H}_{\text{sr}} + \hat{H}_{\text{mhf}} + \hat{H}_{\text{eQq}} + \hat{H}_{\text{nsr}} \quad (1).$$

The results of these analyses are presented in Table 2, along with those from previous works [18,21]. Note that the γ_H term was needed for the $v = 1$ analysis, as these data encompass higher N values than the $v = 0$ set [21]. In comparison, Mukund et al. [18] derived estimates of B , D ,

and the hyperfine b constant from LIF measurements with $\sim 0.1 \text{ cm}^{-1}$ precision, while Childs and Steimle [21] obtained the hyperfine and spin-rotation parameters from magnetic dipole transitions. Our analysis is the first global fit to both the rotational and fine/hyperfine constants. As can be seen in the table, the values of B and D for $v = 0$ and B for $v = 1$ are significantly improved from the past work, and are two orders of magnitude more precise. The hyperfine and fine structure parameters have very similar precision and are in excellent agreement with the previous determinations. The *rms* of the fits to the data are 8 and 3 kHz for $v = 0$ and 1, respectively.

4. Discussion

According to the most recent theoretical work on ScO, this species has an electron configuration of (core) $8\sigma^2 3\pi^4 9\sigma^1$ [24]. The 8σ and 3π are thought to be bonding orbitals. A triple bond is predicted to exist between the scandium and oxygen atoms, composed of a single σ bond and two π bonds. The 9σ orbital, which contains the unpaired electron, is **thought** to be a combination of scandium atomic $4s$ and $3d$ orbitals [24] **or a** mixture of $4s$ and $4p$ orbitals [18]. The amount of Sc $4s$ character can be estimated by comparing the Fermi contact term of ScO to that of atomic scandium. Using the atomic value of $b_F(\text{Sc}) = 2823 \text{ MHz}$ [28], the percent s character in the 9σ orbital is calculated to be 69%.

The remaining $\sim 31\%$ contribution the 9σ orbital could be either $p\sigma$ or $d\sigma$ in composition.

This fraction of orbital character is likely the dominant contributor to the dipolar hyperfine term c . This parameter, defined as:

$$c = \frac{3}{2} g_s \mu_B g_N \mu_N \left\langle \frac{3\cos^2\theta - 1}{r^3} \right\rangle \quad (2),$$

can only be generated by anisotropic orbitals, **such as p or d orbitals**. The angular factor

$\langle 3\cos^2\theta - 1 \rangle$ in the above expression for a $p\sigma$ orbital is 4/5, while for a $d\sigma$ orbital, it is 4/7. From the above equation, the expectation value of $\langle 1/r^3 \rangle$, which provides an estimate of the radial extent of the 9σ orbital, can be calculated. Using $c = 74.4096(68)$ MHz, $\langle 1/r^3 \rangle$ is found to be 1.541 a.u.⁻³ for a $p\sigma$ orbital or 2.157 a.u.⁻³ for a $d\sigma$ orbital contribution to the unpaired electron. The value of $\langle 1/r^3 \rangle$ for free Sc^+ is 1.851 a.u.⁻³ [28], while that for neutral Sc is 0.911 a.u.⁻³ [29]. The value for Sc^+ is almost exactly between that of the two values calculated for ScO from the different orbital mixtures. Thus, both the $3d$ and $4p$ orbitals could be contributing at some level to that of the unpaired electron. The value for neutral Sc, in contrast, is far from both values, which implies that the unpaired electron in ScO has a distribution about the nucleus that is comparable to Sc^+ . Therefore, scandium oxide is highly ionic, as also implied by the large Fermi contact term, and should be considered as Sc^+O^- . This result agrees well with the theoretical calculations by Miliordos & Mavridis [23], who postulated that $0.8 e^-$ is transferred from Sc to O when the molecule is formed.

These new measurements of the rotational spectrum of ScO will be important for astronomical searches of the molecule in circumstellar environments. The best transitions for such searches would be at 1 mm and higher, where the fine and hyperfine structure are effectively collapsed, allowing for an increase in the observed intensity. At 1 mm, the improved rotational constants generate transition frequencies 14 – 18 MHz, or 16 – 20 km/s, higher than those from previous predictions [21]. This shift can correspond to at least half to a full linewidth in multiple astronomical sources. Given the low cosmic abundance of scandium, circumstellar ScO lines will likely be weak. Transitions frequencies accurate to within 1 – 2 MHz are necessary in this case because of the large number of low-level unidentified features present in

high sensitivity, circumstellar radio spectra towards sources where ScO could be found, such as VY CMa or IK Tau. The large dipole moment of 4.55 D [20] should improve the likelihood of detection.

Identification of ScO in the circumstellar shells of evolved stars would be interesting from several aspects. First, it would provide the first information of the chemistry of scandium, which has yet to be observed in an interstellar molecule. Secondly, it would provide a connection between photospheric and circumstellar material, as has been seen for AlO [4]. In circumstellar shells, ScO would most likely be formed by local thermodynamic equilibrium (LTE) chemistry, as the molecule, though a radical, is relatively stable. However, as in the case for AlO [30], shocks might contribute to its synthesis.

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Table 1MW/Submillimeter-wave Transition Frequencies of ScO ($X^2\Sigma^+$)^a

N'	$\leftrightarrow$	N''	J'	$\rightarrow$	J''	F'	$\rightarrow$	F''	$v = 0$		$v = 1$	
									ν_{obs}	$\nu_{\text{o}} - \nu_{\text{c}}$	ν_{obs}	$\nu_{\text{o}} - \nu_{\text{c}}$
1	$\rightarrow$	0	0.5	$\rightarrow$	0.5	3	$\rightarrow$	4	30743.757	0.000	30582.937	0.001
			1.5	$\rightarrow$	0.5	5	$\rightarrow$	4	30767.461	0.000	30608.026	-0.003
			1.5	$\rightarrow$	0.5	3	$\rightarrow$	3	30768.594	0.002	30608.550	0.003
			0.5	$\rightarrow$	0.5	4	$\rightarrow$	3	30791.572	-0.002	30631.165	0.001
			1.5	$\rightarrow$	0.5	2	$\rightarrow$	3	30802.824	0.000	30643.553	-0.001
			1.5	$\rightarrow$	0.5	4	$\rightarrow$	4	30844.122	0.000	30684.026	0.000
2	$\rightarrow$	1	1.5	$\rightarrow$	1.5	3	$\rightarrow$	4	61507.031	0.002		
			2.5	$\rightarrow$	1.5	3	$\rightarrow$	2	61548.342	0.000		
			1.5	$\rightarrow$	1.5	4	$\rightarrow$	4	61549.234	-0.002		
			1.5	$\rightarrow$	0.5	2	$\rightarrow$	3	61553.174	-0.001		
			2.5	$\rightarrow$	1.5	5	$\rightarrow$	4	61554.073	0.001	61234.465	0.000
			2.5	$\rightarrow$	0.5	4	$\rightarrow$	4	61554.785	0.000		
			2.5	$\rightarrow$	0.5	3	$\rightarrow$	4	61559.595	0.003		
			2.5	$\rightarrow$	1.5	2	$\rightarrow$	2	61564.189	0.000		
			2.5	$\rightarrow$	1.5	6	$\rightarrow$	5	61565.724	0.000	61246.285	-0.004
			1.5	$\rightarrow$	0.5	5	$\rightarrow$	4	61574.465	-0.003	61254.009	0.003
			2.5	$\rightarrow$	1.5	4	$\rightarrow$	3	61577.764	-0.003	61257.487	0.001
			2.5	$\rightarrow$	1.5	1	$\rightarrow$	2	61580.776	0.002		
			2.5	$\rightarrow$	1.5	3	$\rightarrow$	3	61582.574	0.000		
			2.5	$\rightarrow$	1.5	2	$\rightarrow$	3	61598.420	-0.001		
			1.5	$\rightarrow$	0.5	3	$\rightarrow$	3	61607.393	-0.001		
			1.5	$\rightarrow$	1.5	4	$\rightarrow$	5	61625.896	-0.002		
			2.5	$\rightarrow$	1.5	5	$\rightarrow$	5	61630.733	-0.001	61310.462	-0.001
			1.5	$\rightarrow$	0.5	4	$\rightarrow$	3	61649.605	0.004		
15	$\leftarrow$	14	^b			^b			461568.033	0.057		
16	$\leftarrow$	15	^b			^b			492304.740	-0.047		

^a In MHz; residuals from global fit with hyperfine data from [18].^b Fine and hyperfine structure unresolved.

Table 2
Spectroscopic Constants of ScO ($X^2\Sigma^+$)

Parameter ^a	$v = 0$		$v = 1$	
	This work	Previous work	This work	Previous work
B	15393.39134(87)	15392.35(72) ^b	15313.3839(41)	15312.25(76) ^b
D	0.0173219(74)	0.01719(23) ^b	0.01745(58)	0.01727(24) ^b
γ	3.2149(16)	3.2175(12) ^c	4.43451(75)	4.4344(6) ^c
γ_D	$2.357(10) \times 10^{-4}$	$2.323(12) \times 10^{-4}$ ^c	$2.4315(75) \times 10^{-4}$	$2.432(6) \times 10^{-4}$ ^c
γ_H			$7.9(1.3) \times 10^{-10}$	$7.9(9) \times 10^{-10}$
b_F	1947.3456(74)	1947.339(6) ^c	1948.7336(21)	1948.733(6) ^c
b_{FD}	$5.067(47) \times 10^{-4}$	$4.615(27) \times 10^{-4}$ ^c	$5.037(17) \times 10^{-4}$	$4.542(15) \times 10^{-4}$ ^c
c	74.4096(68)	74.416(6) ^c	74.6545(81)	74.656(6) ^c
c_D	$1.517(55) \times 10^{-4}$	$1.47(3) \times 10^{-4}$ ^c	$1.489(31) \times 10^{-4}$	$1.49(3) \times 10^{-4}$ ^c
eQq	72.247(34)	72.240(15) ^c	71.662(30)	71.663(24) ^c
C_I	0.021826(58)	0.02181(3) ^c	0.022067(70)	0.02208(6) ^c
rms	0.008		0.003	

^a In MHz; errors are 3σ in the last quoted decimal places.

^b Ref. [21].

^c Ref. [18].

Figure Captions

FIGURE 1. – FTM/mmW laboratory spectra of the $N = 1 \rightarrow 0$ (upper panel) and $2 \rightarrow 1$ (lower panel) rotational transitions of ScO ($X^2\Sigma^+$) arising from the $v = 0$ state near 30.7 and 61.5 GHz, respectively. Each rotational transition consists of fine structure doublets, indicated by J , which are further split into several hyperfine components, labeled by F , due to the Sc nuclear spin. The hyperfine couplings dominate the spin-rotation splittings. There are five frequency breaks in both spectra to show multiple features. Doppler doublets are designated by brackets above each individual line. Residual Zeeman splitting is apparent in the $F = 3 \rightarrow 3$ and $4 \rightarrow 4$ components in the $N = 1 \rightarrow 0$ transition. The $N = 1 \rightarrow 0$ and $2 \rightarrow 1$ spectra were each created from six, 600 kHz-wide scans, with 200 and 1000 pulse averages per scan, respectively.

FIGURE 2. – FTM/mmW laboratory spectrum of the $N = 2 \rightarrow 1$ rotational transitions of ScO ($X^2\Sigma^+$) in the $v = 1$ excited vibrational state near 61.2 GHz. Four hyperfine components are displayed in the figure, labeled by F , three arising from the $J = 2.5 \rightarrow 1.5$ spin doublet and the fourth from the $J = 1.5 \rightarrow 0.5$ set. There are three frequency breaks in the figure to show these features. Doppler doublets are indicated by brackets above each individual line. This spectrum was created from four, 600 kHz wide scans, with 2000 pulse averages per scan. Note that despite increased integration time, these spectra are weaker than the $v = 0$ lines.

FIGURE 3. – Submillimeter direct absorption laboratory spectra of the $N = 15 \leftarrow 14$ and $16 \leftarrow 15$ rotational transitions of ScO ($X^2\Sigma^+$) in the ground vibrational state near 461 and 492 GHz, upper and lower panels, respectively. For both transitions, all of the fine/hyperfine components are effectively collapsed into a single feature. Each spectrum is an average of four, 30 MHz-wide scans, each with a duration of about 30 sec.

Figure 1

Figure 2

Figure 3