LETTER TO THE EDITOR

Detection of infrared fluorescence of carbon dioxide in R Leonis with SOFIA/EXES

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ABSTRACT

We report on the detection of hot CO2 in the O-rich asymptotic giant branch star R Leo based on high spectral resolution observations in the range 12.8–14.3 μm carried out with the Echelon-cross-Echelle Spectrograph (EXES) mounted on the Stratospheric Observatory for Infrared Astronomy (SOFIA). We found >240 CO2 emission lines in several vibrational bands. These detections were possible thanks to a favorable Doppler shift that allowed us to avoid contamination from telluric CO2 features. The highest excitation lines involve levels at an energy of ≳7000 K. The detected lines are narrow (average deconvolved width ≲2.5 km s−1) and weak (usually ≤10% of the continuum). A ro-vibrational diagram shows that there are three different populations, warm, hot, and very hot, with rotational temperatures of ≳550, 1150, and 1600 K, respectively. From this diagram, we derived a lower limit for the column density of ≳2.2 × 1010 cm−2. Further calculations based on a model of the R Leo envelope suggest that the total column density can be as large as 7.0 × 1017 cm−2 and the abundance with respect to H2 ≳2.5 × 10−5. The detected lines are probably formed due to the de-excitation of CO2 molecules from high energy vibrational states, which are essentially populated by the strong R Leo continuum at 2.7 and 4.2 μm.

Key words. stars: AGB and post-AGB – stars: individual: R Leo – stars: abundances – circumstellar matter – line: identification – surveys

1. Introduction

Extensive work has been done in recent decades to characterize the molecular content of the circumstellar envelopes (CSEs) of asymptotic giant branch (AGB) stars. This huge effort has been fruitful, having found more than 90 different molecular species, not counting isotopologues (McGuire 2018), most of which were detected for the first time in the carbon-rich star IRC+10216 (e.g., Ridgway et al. 1976; Betz 1981; Goldhaber & Betz 1984; Bernath et al. 1989; Cernicharo et al. 2000; Agúndez et al. 2008, 2014). Oxygen-rich (O-rich) stars are less chemically active than carbon stars. Among them, we can find ubiquitous species such as CO, HCN, SiS, SiO, or CS as well as other molecules typically found in O-rich environments such as H2O, SO, SO2, H2CO, or NO (e.g., Velilla Prieto et al. 2017).

Most of these molecules have been found in the millimeter range, where molecules without a permanent dipole moment cannot be observed due to their lack of a pure rotational spectrum. One of them is CO2, which is predicted to be an abundant parent species by chemical models (e.g., Cherchneff 2006; Agúndez et al. 2020) with abundances related to H2 of 10−8–10−4. The detections in AGB stars carried out to date have only been done from space with the Infrared Space Observatory (ISO) and the Spitzer Space Telescope (e.g., Justtanont et al. 1996, 1998; Ryde et al. 1997; Tsuji et al. 1997; Yamamura et al. 1999; Cami et al. 2000; Markwick & Millar 2000; Sloan et al. 2010; Smolders et al. 2012; Reiter et al. 2015; Bayliss–Aguirre et al. 2020) as a consequence of the extremely high atmospheric opacity.

Chemical models indicate that a large fraction of the initially available oxygen atoms are locked into CO2, either through the two-body chemical reactions of CO with H2O and OH, or the three-body reaction of CO and atomic oxygen assisted by a catalyst, which is efficient in high density environments. Consequently, the formation efficiency of other O-bearing species is hampered by the formation of CO2. Despite this, CO2 emission has been poorly analyzed in detail.

R Leo is one of the closest O-rich stars, with a distance of 70–85 pc, and it has a low mass-loss rate of ≲1.0 × 10−7 M⊙ yr−1. The terminal velocity of its expanding gas is ≳6–9 km s−1 (De Beck et al. 2010; Ramstedt & Olofsson 2014). The central star pulsates with a period of ≃310 days, its effective temperature is ≳2500–3000 K, and its angular diameter is ≃0″052–0″030 (e.g., Perrin et al. 1999; Fedele et al. 2005; Wittkowski et al. 2016). The molecular observations carried out in the millimeter, submillimeter, and infrared ranges (e.g., Hinkle & Barnes 1979; Bujarrobaj et al. 1994; Etoka & Le Squeren 1997; Bieging et al. 2000; González-Delgado et al. 2003; Ohnaka 2004; Schöier et al. 2010) indicate that CO, H2O, OH, SiO, SO, SO2, and HCN exist with significant abundances, but CO2 has not yet been detected toward R Leo.

In this Letter, we report on the detection of hot CO2 toward the O-rich star R Leo that was performed from the Stratospheric...
Observatory for Infrared Astronomy (SOFIA; Temi et al. 2018) with the high spectral resolution Echelon-cross-Echelle Spectrograph (EXES; Richter et al. 2018).

2. Observations

Observations of R Leo were carried out with SOFIA/EXES on November 1, 2018 (UT). Two settings in the high-low instrument configuration were taken, which yield a full range of 701.0–782.6 cm$^{-1}$ (12.77 to 14.27 μm). These observations were conducted while SOFIA flew at an altitude of 13.1 km. For both settings, the slit length was ~2″ long and we chose the 2″ wide slit. An additional high-low setting centered around 1335 cm$^{-1}$ (7.5 μm) will be discussed elsewhere.

All EXES data were reduced using the Redux pipeline (Clarke et al. 2015). The median spectral resolving power, $R = \lambda/\Delta\lambda$, was empirically determined from telluric ozone (O$_3$) lines to be about 70,000 for both settings. The resulting spectral resolution is thus $\approx 4.3$ km s$^{-1}$. We calculated the radial velocity of R Leo with respect to Earth during the observing flight to be $-22.4$ km s$^{-1}$, which imparts a blue-shift to the stellar features by $\approx 0.055$ cm$^{-1}$ ($\approx 0.001$ μm) at 740 cm$^{-1}$ ($\approx 13.514$ μm).

These observations were complemented with photometric data from the Infrared Astronomical Satellite Point Source Catalog (IRASPSC), Wide-field Infrared Survey Explorer (WISE), Cosmic Background Explorer Diffuse Infrared Background Experiment Point Source Catalog (DIRBEPSC), Two Micron All-Sky Survey (2MASS), Gaia Data Release 2 (Gaia DR2), and HIPPARCOS catalogs. Additional measures acquired with Johnson filters were also used. All measures were taken from Vizier$^1$.

3. Results

The thinness of the atmosphere at 13 km along with the high excitation of these lines significantly reduced the opacity of the telluric CO$_2$ features and highly increased the atmospheric transmission in the observed spectral range. Lines from seven ro-vibrational bands of the main isotopeologue were detected (01$^1$0$_1$–00$^2$0$_1$, 10$^1$0$_0$–01$^2$0$_1$, 02$^2$0$_0$–01$^0$0$_1$, 11$^0$0$_0$–10$^2$0$_0$, 11$^1$0$_0$–02$^0$0$_1$, 20$^0$0$_0$–11$^1$0$_1$, 20$^2$0$_0$–11$^0$0$_2$, and 11$^0$0$_2$–10$^2$0$_1$; Figs. 1 and B.1 – see a brief description of CO$_2$ in Appendix A). Lines of the hot bands 10$^0$0$_0$–01$^2$0$_1$ and 11$^1$0$_0$–02$^0$0$_1$ of $^{13}$CO$_2$ were also detected (not included in Figs. 1 and B.1 for the sake of clarity). No lines of $^{17}$CO or $^{18}$CO were found, as expected given the low abundance of the oxygen isotopes ($^{13}$C/$^{12}$C $\approx 10$, $^{16}$O/$^{17}$O $\approx 450$, and $^{16}$O/$^{18}$O $\approx 550$; Hinkle et al. 2016).

The observed lines are only seen in emission with a maximum intensity of 10% above the continuum. They are found in the blue-shifted wings of the telluric CO$_2$ features, which are usually much stronger and always in absorption. The same settings were used during the observation of other sources in the same observing campaign, and no similar feature stood out. Hence, they are not instrumental artifacts but real lines that were separated from their telluric counterparts thanks to a high Doppler shift during the observing run.

The low-J lines of the fundamental band are blocked by the atmosphere, but a few lines with $J \geq 70$ can be identified in the spectrum. The detected lines of the hot and combination bands, for which the Earth’s atmosphere is more transparent, involve ro-vibrational levels with $J \geq 5$. The highest excitation ro-vibrational level involved in the detected lines is at $\approx 7000$ K. Additional emission lines were detected in the spectrum but not identified. They are probably produced by even higher excitation bands of CO$_2$ (e.g., 03$^3$0$_0$–02$^2$0$_1$, 12$^2$0$_2$–03$^0$0$_1$, 31$^0$0$_0$–22$^2$0$_1$, 31$^0$0$_2$–22$^0$0$_2$, or 20$^0$1$_2$–11$^1$1$_2$) or $^{13}$CO$_2$ that cannot be unambiguously identified.

The CO$_2$ emission lines are not systematically accompanied by noticeable blue-shifted absorption features above the detection limit. It probably occurs because the population of the upper vibrational states of each detected band is very high and the emission covers the absorption component. This effect could be a consequence of the strong radiation field emitted by R Leo and the dusty component of the envelope (see Sect. 4).

The comparison of different lines of bands 11$^0$0$_1$–10$^0$0$_1$, 10$^0$0$_1$–01$^0$0$_1$, and 01$^1$0$_0$–00$^0$0$_1$ (Fig. 2) suggests that there is not a significant velocity difference between them. They are roughly single-peaked lines that are approximately centered at the systemic velocity and totally delimited by the terminal gas expansion velocity. The average full width at half maximum (FWHM) of the emission lines is $\approx 5$ km s$^{-1}$. Considering that the spectral resolution of our observations is $\approx 4.3$ km s$^{-1}$, the average deconvolved FWHM is $\approx 2.5$ km s$^{-1}$, but the broadest lines show a deconvolved FWHM of $\approx 5$ km s$^{-1}$. Therefore, the lines are formed at the beginning of the acceleration region, where the gas expands at velocities up to $\approx 2.5$ km s$^{-1}$. The low-J lines of band 11$^0$0$_1$–10$^0$0$_1$ seem to comprise two components: a very narrow peak centered at the systemic velocity and a flat-topped contribution, which probably comes from already accelerated gas.

We analyzed the strongest CO$_2$ bands with a ro-vibrational diagram (Fig. 3; Appendix C). The continuum intensity was estimated by fitting the photometric data beyond 0.7 μm (Fig. 4a). The mass-loss rate of R Leo is relatively low ($\approx 1.0 \times 10^{-7} M_\odot$ yr$^{-1}$; e.g., Ramstedt & Olofsson 2014), hence the dust grain density is also low. Nevertheless, they contribute significantly to the continuum emission, which can be described to the first approximation as two black-bodies: a compact one at $\approx 2400$ K mainly associated with the central star and a more extended black-body at a temperature of $\approx 850$ K. The warm black-body seems to represent the bulk of dust emission, which comes from a region with a diameter of $\approx 0\farcs09$. This value is a lower limit since dust emission would be better described by a more extended gray-body in a more detailed model.

The CO$_2$ lines can be grouped into three different populations, namely warm, hot, and very hot, with approximate temperature populations of 550, 1150, and 1600 K, respectively. The dispersion of the data set related to the 11$^0$0$_1$–02$^2$0$_1$ band is high, and the uncertainty of the rotational temperature derived from the fit could be underestimated. Assuming only a warm population is the most conservative approach. Interestingly, the bands involving higher energy vibrational states (11$^0$0$_1$–10$^0$0$_1$ and 11$^1$0$_0$–02$^0$0$_1$) show lower rotational temperatures (Sect. 4).

The emitting region related to each population can be roughly determined in the envelope. The lack of a pure rotational spectrum for CO$_2$ prevents an efficient radiative rotational relaxation and implies that CO$_2$ is rotationally under local thermodynamic equilibrium (LTE) throughout the entire envelope. The kinetic temperature for the CSE of R Leo is not well known but we can assume it to follow the power-law $\propto \alpha^{-7}$, where $\alpha \approx 0.7$. This exponent is commonly used to analyze the emission of O-rich stars (e.g., Decin et al. 2006; Velilla Prieto et al. 2015; Sánchez Contreras et al. 2015) and is very similar to that derived from observations of the outer envelope of the carbon-rich star IRC+10216 ($\alpha=0.68$; Guélin et al. 2018), where the gas is expected to be as rarefied as in the envelope of R Leo. Therefore,

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$^1$ https://vizier.u-strasbg.fr/index.gml
Fig. 1. Spectrum of R Leo in the spectral range 701–742 cm\(^{-1}\) in the rest frequency (i.e., we have corrected for R Leo’s radial velocity with respect to Earth at the time of observation). The detected CO\(_2\) lines are plotted in different colors depending on the band. The red synthetic spectrum is a model to the CO\(_2\) emission (Sect. 4). The gray spectrum is the atmospheric transmission calculated with the ATRAN code (Lord 1992). Only the lines that were clearly detected are marked with arrows. The branches are not indicated for the sake of clarity. An additional spectral range is shown in Fig. B.1.
the CO₂ populations at 1600, 1150, and 550 K are located at 2.2, 3.5, and 10 R₆, from the center of R Leo, respectively. Considering that the gas in these three regions is being accelerated, kinematic effects such as line broadening are expected as the bulk of the line emission comes from higher radii. The dual component detected in the low-J lines of band 11¹⁰⁻¹⁰⁰₁₀ could be evidence of these effects (Fig. 2).

Considering an angular stellar diameter of 0°028, the angular sizes of the emitting regions are ≈0°06, 0°10, and 0°28. The corresponding ratios of beam filling factors are 0.5, 1.4, and 10.5, respectively. Hence, the resulting column densities for the populations in the vibrational states 0¹⁰⁻¹⁰⁰₁₀, 1⁰¹⁰⁻¹⁰⁰₁₀, and 1¹¹⁻¹⁰⁰₁₀ described by the ro-vibrational diagram are (1.3 ± 0.5) × 10¹⁶, (8.6 ± 2.4) × 10¹⁵, and (4.4 ± 0.7) × 10¹⁴ cm⁻², respectively. These partial results only allow us to establish a lower limit for the total column density in the envelope: N(col) ≥ (2.2 ± 0.8) × 10¹⁶ cm⁻². A larger continuum source would increase this lower limit.

4. Discussion and final remarks

The continuum emission peaks around 2.5 µm (Fig. 4a), and it is capable of exciting a significant fraction of the CO₂ molecules up to high energy vibrational states thanks to the strong CO₂ bands 10¹⁻⁰²⁻¹⁰⁰₁₀ and 10¹³⁻¹⁰⁰₁₀, which are at ≈2.7 µm and 0⁰¹⁻⁰²⁻⁰₀₁₀ at ≈4.2 µm (Fig. 4b). The stellar radiation field dominates the excitation of CO₂ up to a few stellar radii beyond the photosphere. States 10¹₁⁻¹⁰⁰₁₀ and 10¹⁻¹⁰⁰₁₀ serve as a bridge to efficiently populate states 10⁰₁₀⁻¹⁰⁰₁₀ and 10⁰⁻¹⁰⁰₁₀ from the ground, strengthening the emission of bands 10⁰⁻¹⁰⁰₁₀ and 10⁰⁻¹⁰⁰₁₀, respectively. The continuum emission peaks around 2.5 µm (Fig. 2). The baseline has been removed. The thick vertical blue lines represent the terminal gas velocity ranging from 6 to 9 km s⁻¹. The spectral resolution is ≈4.3 km s⁻¹. The red fits were done with Gaussians. The blue fits consider a Gaussian and a rectangular function.

Many AGB and semi-regular (SR) stars have shown CO₂ features in ISO and Spitzer observations (Sect. 1), but only the CO₂ column densities and abundances of a handful of them have been estimated. The derived column densities are between 2.0 × 10¹⁶ cm⁻² for R Cas (Markwick & Millar 2000) and 1.0 × 10¹⁹ cm⁻² for EP Aqr (Camia et al. 2000). Hence, a column density of ≈5 × 10¹⁷ cm⁻² can be adopted as typical for AGB and SR stars with a high dispersion of a factor of 20. The column density for the vibrationally excited CO₂ that we derived for R Leo (≈2 × 10¹⁶ cm⁻²) indicates that the amount of CO₂ molecules distributed among other vibrational states could be as high as 80%.

We created a simple model of R Leo to estimate the total column density of CO₂ with the code developed by Fonfría et al. (2008) to model the molecular emission of AGB stars. We adopted a stellar temperature of 2750 K, a mass-loss rate of 1.0 × 10⁻⁷ M_☉ yr⁻¹, a solar He abundance with respect to H₂ (≈0.17; Asplund et al. 2009), a kinetic temperature of 2750(1 R_⋆/r)⁰.⁰ K, CO₂ under rotational LTE, gas accelerated from the photosphere until it reaches 8 km s⁻¹ at 3 R_⋆, after which point it expands at a constant rate, and a thin dusty component outward from 3 R_⋆. A vibrational temperature profile of ≈2750(1 R_⋆/r)⁰.⁰ K, which is steeper than the kinetic temperature, is needed to produce lines of the 0¹¹⁻⁰⁰⁻⁰₀₁₀ band with no absorption component in the observed range. The maximum vibrational temperatures for higher energy states can be as high as 5000 K. The adoption of temperatures similar to that derived from the 0¹⁰⁻⁰₀⁻⁰₀₁₀ band results in lines of bands 10⁰⁻¹⁰⁰₁₀ and 1¹¹⁻¹⁰⁰₁₀, respectively. Hence, the selective population of bands 10⁰⁻¹⁰⁰₁₀ and 1¹¹⁻¹⁰⁰₁₀, which are at ≈2.7 µm and 0⁰¹⁻⁰²⁻⁰₀₁₀, respectively, could be explained by this scenario. However, the vibrational temperatures of bands 10⁰⁻¹⁰⁰₁₀ and 1¹¹⁻¹⁰⁰₁₀, which are at ≈4.2 µm (Fig. 4b), can be as high as 5000 K.
are in unobserved vibrational states. In particular, about 10% of them are in the ground state and thus impossible to observe without a space-based facility. The synthetic spectrum can be seen in Figs. 1 and B.1. This result is similar to the column density found for R Tri ($\approx$5.2 $\times$ 10$^{-17}$ cm$^{-2}$; Baylis-Aguirre et al. 2020), which has the same mass-loss rate ($\approx$1.1 $\times$ 10$^{-7}$ M$\odot$ yr$^{-1}$) as RLeo. The CO$_2$ column density for a Cet, which has a mass-loss rate as high as RLeo, is $\approx$2 $\times$ 10$^{-17}$ cm$^{-2}$, and it is 1.0 $\times$ 10$^{13}$ cm$^{-2}$ for EP Aqr, which has a mass-loss rate of 2.3–3.1 $\times$ 10$^{-7}$ M$\odot$ yr$^{-1}$ (Knapp et al. 1998; De Beck et al. 2010). This discrepancy suggests that either the CO$_2$ column density does not depend strongly on the mass-loss rate, or that it has not been accurately estimated. Thus, a systematic study of the CO$_2$ emission in O-rich stars is needed to understand how this molecule forms.

The detection of the CO$_2$ bands presented in the current work demonstrates the incomparable ability of SOFIA/EXES to observe the infrared spectrum of molecules in space, even when they are highly perturbed by the Earth’s atmosphere, due to the combination of (1) high spectral resolution, (2) the very thin atmosphere that exists above the stratosphere, and (3) a favorable observation date to have the best Doppler shift with respect to the telluric absorption, which is crucial for getting reliable line profiles after the removal of the baseline. Despite the fact that the CO$_2$ column density presented in this work was derived simplistically with substantial uncertainties, a careful analysis that considers CO$_2$ under rotational LTE can improve the accuracy of the results.

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Fig. 4. Effect of the continuum emission of RLeo on the vibrational excitation of CO$_2$. a: continuum emission of RLeo based on photometric observations available in several databases. This data set has been fitted with two black-bodies between 0.8 and 100 m (solid black curve) to represent the star (“eff”) and the dusty component of the envelope (“dust”). The dashed black curve is an extrapolation of this fit below 0.8 m. The $T_X$ and $\theta_X$ are the temperature and the angular diameter of the X emitting region. The vertical gray bands indicate the spectral ranges covered by the strongest CO$_2$ bands. Neither dust opacity nor scattering were considered in our fits. b: low spectral resolution absorption spectrum of CO$_2$ calculated under LTE at a temperature of 1500 K and with a column density of 5 $\times$ 10$^{13}$ cm$^{-2}$. The strongest bands are highlighted in gray. c: vibrational energy diagram of CO$_2$ with the most important vibrational states involved in the observed bands. The possible vibrational transitions are plotted as red lines, with thickness increasing as their $A$-Einstein coefficient grows (dashed lines for the lowest coefficients).
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Appendix A: Brief description of CO₂

Carbon dioxide is a linear triatomic molecule that belongs to the $D_{coh}$ group and, hence, displays no permanent dipole moment. Its atoms vibrate according to four normal modes, two of which are degenerate. The other two modes, $\nu_3(\sigma_u^*)$ and $\nu_2(\sigma_u^*)$, are stretching modes. The two degenerate modes are combined into the bending mode $\nu_2(\pi_u)$, which induces a vibrational angular splitting in the ro-vibrational levels with different $e - f$ parity (Brown et al. 1975). The fundamental band associated with the $\nu_1(\sigma_g^*)$ mode is infrared inactive due to the $g - u$ symmetry with respect to the molecular middle plane. The absence of nonzero nuclear spins forbids the rotational levels with even or odd $J$, depending on the symmetry of the vibrational state.

The similarity between the energies of the vibrational states $\nu_1(\sigma_g^*)$ and $2\nu_2(\sigma_u^*)$ and other overtones produces a Fermi resonance that results in groups of significantly perturbed states. For simplicity, we have adopted in this work the notation $\nu_1(\sigma_g^*)$ and $2\nu_2(\sigma_u^*)$ for the vibrational states, where $\nu_1$ is the 1th vibrational number, $l$ is the vibrational angular momentum number related to the bending mode $\nu_2$, and the index $r = 1, 2, \ldots$ orders the vibrational levels of each Fermi resonant group in decreasing order of energy (Rothman & Young 1981). The frequencies of the lines have been taken from the HITRAN Database (Gordon et al. 2017).

Appendix B: Additional observations

The observations covered a total spectral range from 701.0 to 782.6 cm$^{-1}$. Figure 1 shows the range 701.0–741.8 cm$^{-1}$, which includes most of the strongest detected lines. The rest of the total spectral range 741.8–782.6 cm$^{-1}$, contains a lower number of strong features, but there is still a significant amount of weaker CO₂ lines (Fig. B.1).

Appendix C: The ro-vibrational diagram

We made a ro-vibrational diagram for the strongest observed emission lines by using the well-known formula from Goldsmith & Langer (1999), which we adapted to a normalized infrared spectrum:

$$\ln \left[ \frac{W4\pi J_{v,\text{cont}}}{\Lambda_0 g_v hv \nu_0 N_{\text{col,0}}} \right] \approx y_0 - \frac{h \nu E_{\text{rot,up}}}{k_B T_{\text{rot}}}$$

where $W$ is the integral of the observed line over the frequency (cm$^{-1}$), $\nu$ is the rest frequency (cm$^{-1}$), $E_{\text{rot,up}}$ is the rotational energy of the upper level involved in the transition, $T_{\text{rot}}$ is the rotational temperature of the upper vibrational state, and $I_{v,\text{cont}}$ is the continuum emission measured from Earth. The $N_{\text{col,0}}$ is a column density set arbitrarily to $10^{15}$ cm$^{-2}$ to get dimensionless arguments for the logarithms. We define the quantity $y_0$ as:

$$y_0 = \ln \left[ \frac{N_{\text{col,vib}}}{N_{\text{col,0}} Z_{\text{rot}} \theta_{\text{em}}^2 \theta_{\text{cont}}^2} \left( \frac{\theta_{\text{em}}^2}{\theta_{\text{cont}}^2} \right) \right]$$

where $N_{\text{col,vib}}$ is the column density of the upper vibrational state involved in the band, $Z_{\text{rot}}$ is the rotational partition function, and $\left( \theta_{\text{em}}^2/\theta_{\text{cont}}^2 \right)$ is the ratio of the beam filling factors for the line emission and continuum sources. The $\theta_{\text{em}}$ and $\theta_{\text{cont}}$ represent the diameters of the line and the continuum emitting regions, respectively. The $\theta_b$ represents the angular size of the convolution of the point spread function (PSF), the atmospheric seeing, and any possible instrumental effects. In this work, we have assumed that $\theta_b \approx 3''$. 

L15, page 7 of 8
Fig. B.1. Spectrum of R Leo in the spectral range 742–782 cm$^{-1}$. See the caption of Fig. 1.