espectroFTIR

SPECTROSCOPIC ANALYSIS REPORT (FTIR)

ABSTRACT

This report presents the Fourier transform infrared (FTIR) spectroscopic analysis of sample Etanol desnaturado, líquido (exemplo), performed by espectroFTIR from numerical spectrum data. Absorption bands were detected by prominence and assigned to functional groups using general literature ranges. 8 bands detected, from 879 a 3318 cm^{-1}. 8 were assessed for confidence (8 high, 0 medium and 0 low). The band pattern is compatible with the class aliphatic alcohols (broad ν O–H, distinct aliphatic ν C–H and ν C–O near ~1000–1090 cm^{-1}, few C–O bands). No reference-spectrum comparison was performed. Data suitability was classified as good.

Keywords: FTIR. Infrared spectroscopy. Band assignment. Spectrum quality. Aliphatic alcohols.

1 INTRODUCTION

This report presents the results of Fourier transform infrared (FTIR) spectroscopic analysis of sample Etanol desnaturado, líquido (exemplo). The aim is to describe observed absorption bands, suggest vibrational assignments to functional groups and compound classes and, when reference spectra are available, measure similarity between the sample and those references.

The analysis was performed automatically by espectroFTIR 2026.10 (ARIS c4fca424), using numerical spectrum data, on November 4, 2026. Section 2 describes the sample, equipment and data treatment; section 3 presents results and discussion; section 4 provides the conclusion. Processing traceability is given in Appendix A.

2 MATERIALS AND METHODS

2.1 Sample identification

Box 1 identifies the sample and analyzed file, with the source of each item of information.

Field	Information	Source
Sample / item	Etanol desnaturado, líquido (exemplo)	User
Request / project	not reported	User
Analysis date	05/10/2026	User
Spectrum file	Branco_EtOH.csv	File

Box 1 – Sample identification

Source: user-provided information and data read from the submitted file; espectroFTIR (2026).

Source: User = provided by you, not verified by the platform; File = read from the submitted file; Algorithm = calculated by espectroFTIR.

2.2 Equipment and acquisition conditions

Spectrum acquisition conditions are listed in Box 2.

Field	Information	Source
Instrument	Spectrometer Espectrofotômetro FTIR	User
Sampling technique	ATR com cristal de diamante	User
Spectral range	4000 a 650 cm^{-1}	User
Scans / resolution	16 scans / 4 cm^{-1}	User
Acquisition software	not reported	User
Instrument qualification (OVP)	Not specified	User

Box 2 – Equipment and acquisition conditions

Source: user-provided information.

2.3 Data treatment and band detection

The spectrum was assessed from exported numerical data. Absorption bands were detected automatically by a computational routine using prominence, with a minimum threshold of 3.0% of chart height and an adaptive floor of 6 times the noise estimated from the spectrum itself (0.11%), with a minimum band separation of 12 cm^{-1}.

Vibrational assignments use general functional-group ranges from the literature (PAVIA et al., 2010), compiled in the software's internal database (ESPECTROFTIR, 2026a), with a position tolerance of ±4 cm^{-1} (software parameter, a ser confrontado com a exatidão de wavenumber do instrumento utilizado). Intensity is relative to the most prominent band in the spectrum (very strong > 90%; strong 70–90%; medium 40–70%; weak to medium 25–40%; weak 10–25%; very weak < 10%).

2.4 Data suitability

Spectral data suitability was classified as good. Box 3 summarizes the items assessed.

Item	Assessment	Source
Data source	numerical spectrum data	File
Spectral range	648 to 3998 cm^{-1}; covered regions: 4000–2500, 2500–1800, 1800–1500, 1500–650	File
Sampling interval	2.06 cm^{-1}	File
Noise (estimate)	0.11% of spectrum height (MAD of the moving-average residual)	Algorithm
Spectral quantity	transmittance, reported by the user	User
Preprocessing	moving average of 3 points applied only to band detection; the original trace is preserved; no baseline correction or normalization in the displayed spectrum	Algorithm
Instrumental resolution (reported)	4 cm^{-1} (declarada pelo usuário, não verificada)	User
Bands near the detection threshold	~805 cm^{-1} (between 60% and 100% of the detection threshold; not included in the band tables; check on the spectrum)	Algorithm
Baseline (estimate)	level ≈ 6.9% of the height at 2600–2000 cm^{-1}; difference of ≈ 0.9% between 4000–3800 and 2600–2000 cm^{-1}; no baseline correction	Algorithm
Saturation / signal clipping	no clear signs	Algorithm
Absolute amplitude	deepest band at 57.8 %T (absorbance ≈ 0.375): strong (from 15 %T)	Algorithm
Baseline slope, absolute	8.0 %T between 4000 and 600 cm^{-1}, about 0.1 times the deepest band: low	Algorithm

Item	Assessment	Source
Noise by region	3600–3000 cm^{-1}: 0.015 to 0.028 %T (clean region)	Algorithm
Low-confidence zones	none	Algorithm
CO_2 and water vapor	no clear CO_2 bands; no water-vapor lines	Algorithm
Band confidence	8 high, 0 medium and 0 low (depth from the baseline; provisional criterion)	Algorithm

Box 3 – Spectral data suitability

Source: espectroFTIR (2026b).

3 RESULTS AND DISCUSSION

3.1 Spectrum

Figure 1 shows the submitted spectrum, with vertical lines at detected peaks and functional-group ranges. Eight bands were detected, from 879 to 3318 cm^{-1}. Figure 2 repeats the spectrum with numbered bands (the numbers of Table 3) and the low-confidence zones shaded; Figure 3 enlarges the fingerprint region.

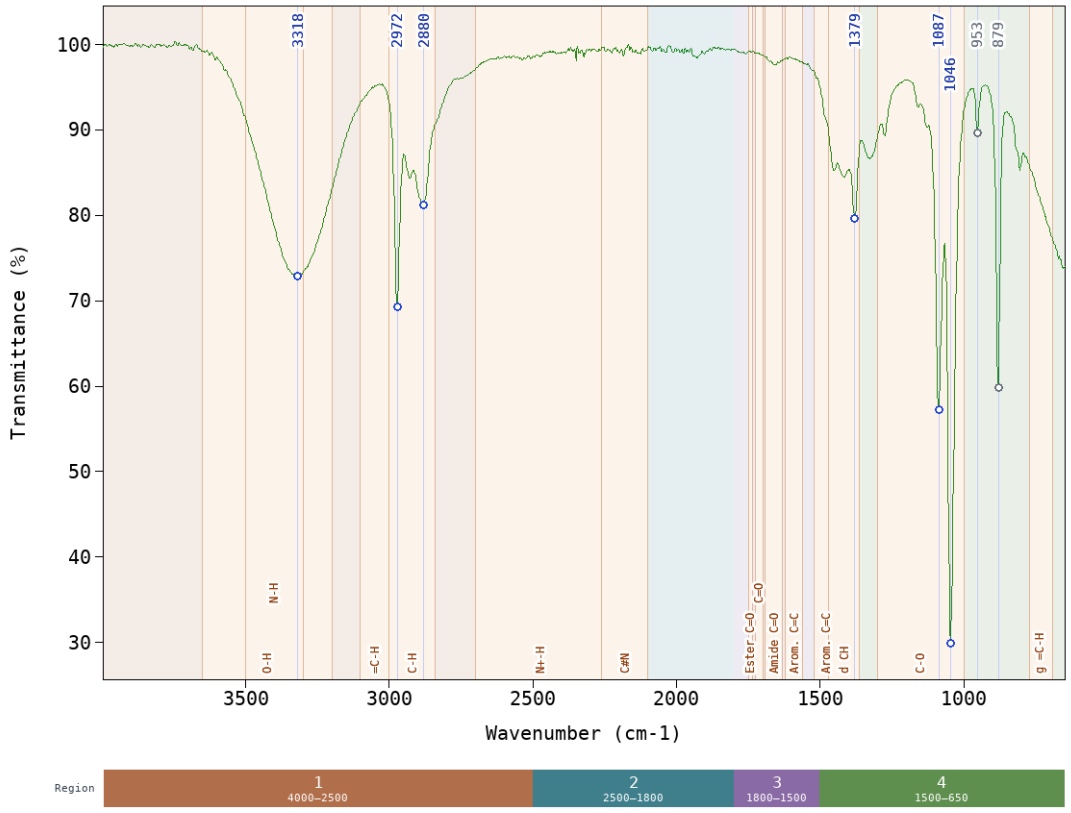


Figure 1 – FTIR spectrum with vertical lines at detected peaks and functional-group ranges; the lower strip numbers regions 1 to 4 of Table 2; gray labels indicate bands with no corresponding range in the general table

Source: espectroFTIR (2026b), from the spectrum of sample Etanol desnaturado, líquido (exemplo).

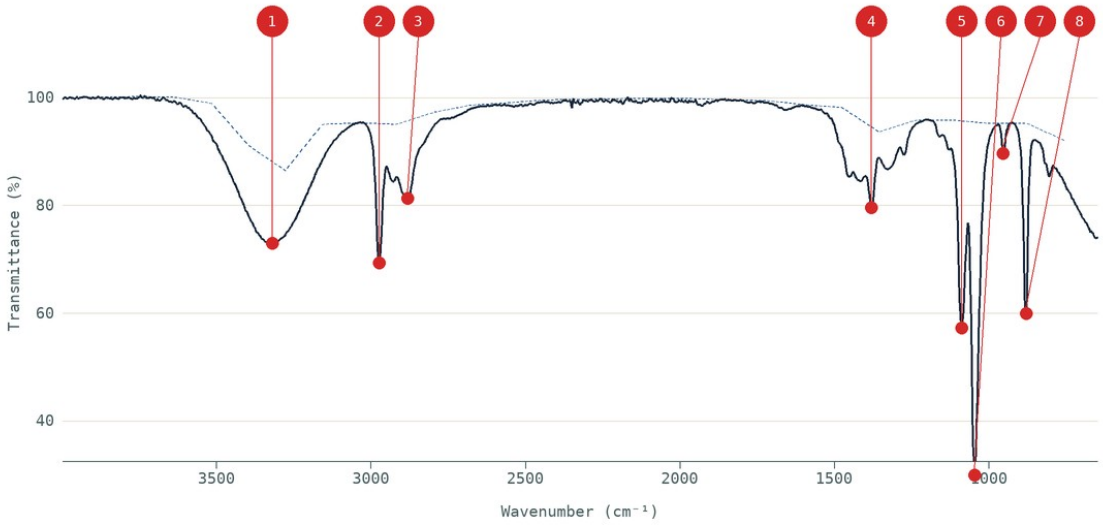


Figure 2 – Spectrum with numbered bands (same numbers as Table 3); red: high or medium confidence; gray: low; dashed: estimated baseline; orange bands: low-confidence zones

Source: espectroFTIR (2026b), from the spectrum of sample Etanol desnaturado, líquido (exemplo).

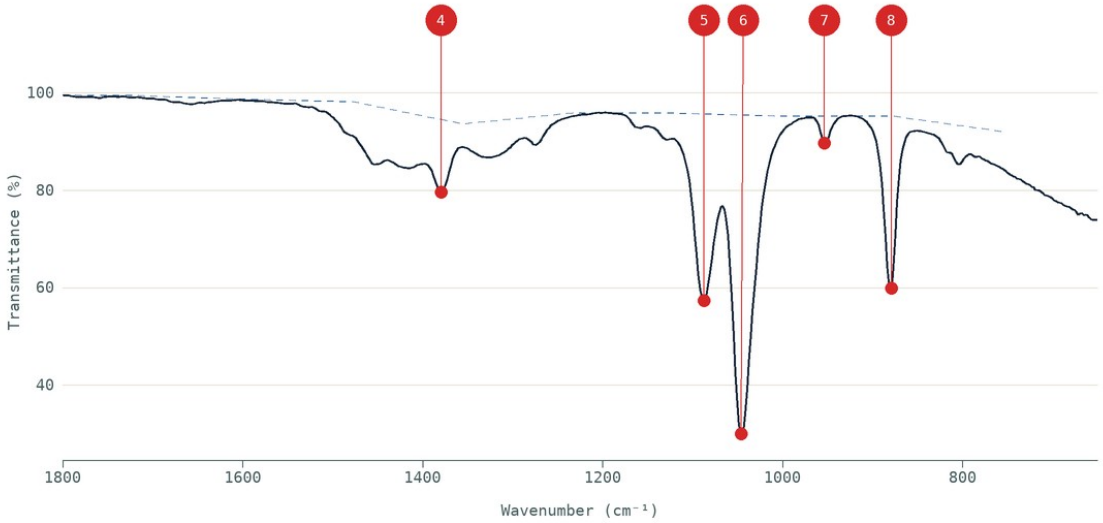


Figure 3 – Fingerprint region (1800 to 650 cm^{-1}) with the numbered bands of Table 3

Source: espectroFTIR (2026b), from the spectrum of sample Etanol desnaturado, líquido (exemplo).

3.2 Observed absorption bands

Table 1 lists observed bands, with position, relative intensity, width and the main suggested assignment, as well as possible alternatives and supporting bands.

Position (cm^{-1})	Intensity	Width (cm^{-1})	Primary assignment	Possible alternatives	Supporting bands
3318 ± 2	Weak to medium	broad (~251)	ν O–H: Alcohol hydroxyl (hydrogen-bonded O–H)	—	~1046 (ν C–O)
2972 ± 2	Medium	medium (~31)	ν Aliphatic C–H: Carbon chain	—	~1379 (δ CH_2 / CH_3)
2880 ± 2	Very weak	medium (~41)	ν Aliphatic C–H: Carbon chain	—	~1379 (δ CH_2 / CH_3)
1379 ± 2	Weak	medium (~101)	δ CH_2 / CH_3: Carbon chain	—	~2972 (ν C–H)
1087 ± 2	Weak to medium	narrow (~21)	ν C–O: Aliphatic alcohol (alcohol C–O)	—	~3318 (ν O–H)
1046 ± 2	Very strong	narrow (~29)	ν C–O: Aliphatic alcohol (alcohol C–O)	—	~3318 (ν O–H)
953 ± 2	Very weak	narrow (~14)	— (no range in the general table)	—	—
879 ± 2	Medium	narrow (~16)	— (no range in the general table)	—	—

Table 1 – Spectral bands observed in the sample Etanol desnaturado, líquido (exemplo)

Source: espectroFTIR (2026b).

The uncertainty (±) reflects data sampling (wavenumber interval), not the instrument's wavenumber accuracy. Supporting bands are other detected bands that usually accompany the main assignment; their absence weakens but does not exclude the assignment.

Table 2 summarizes detected bands by spectral region, including regions where no band was detected and bands with no matching range in the general functional-group table. Regions 1 to 4 use the same numbering and colors as Figure 1.

N°	Region (cm^{-1})	Detected bands	With a corresponding range	No corresponding range	Observation
1	4000–2500	3	3	0	all with a corresponding range
2	2500–1800	0	0	0	no band detected in this region
3	1800–1500	0	0	0	no band detected in this region
4	1500–650	5	3	2	no corresponding range: ~953, ~879

Table 2 – Bands detected by spectral region in the sample Etanol desnaturado, líquido (exemplo)

Source: espectroFTIR (2026b).

Table 3 shows, for each band outside the low-confidence zones, the depth measured from the baseline, the confidence and the general reading; the numbers are those of Figure 2.

N°	Position (cm^{-1})	Depth (%T)	Confidence	General reading (not tied to any substance)
1	~3318	15.23	High	ν O–H: Alcohol hydroxyl (hydrogen-bonded O–H)
2	~2972	22.06	High	ν Aliphatic C–H: Carbon chain
3	~2880	14.23	High	ν Aliphatic C–H: Carbon chain
4	~1379	13.32	High	δ CH_2 / CH_3: Carbon chain
5	~1087	34.38	High	ν C–O: Aliphatic alcohol (alcohol C–O)
6	~1046	57.84	High	ν C–O: Aliphatic alcohol (alcohol C–O)
7	~953	3.61	High	no range in the general table
8	~879	25.77	High	no range in the general table

Table 3 – Depth and confidence of the bands observed in sample Etanol desnaturado, líquido (exemplo)

Source: espectroFTIR (2026b).

Confidence criterion (provisional): high = depth of 0.8 %T or more, outside a noise zone; medium = 0.4 to 0.8 %T; low = less than that.

3.3 Spectral interpretation by region

Each spectral region presents observations (detected bands), assignments using general functional-group ranges, and automatic-rule inference, which is the least certain part and depends on the whole spectrum.

3.3.1 4000 to 2500 cm^{-1} region (O–H, N–H and C–H)

a) **Observed:** ~3318 (broad, weak to medium); ~2972 (medium); ~2880 (very weak) cm^{-1};

b) **Assignment (general ranges):** ν O–H (~3318); Aliphatic ν C–H (~2972, ~2880);

c) **Inference:** Broad absorption was observed at ~3318 cm^{-1} (hydrogen-bonded ν O–H), together with distinct aliphatic ν C–H and ν C–O at 1000–1150 cm^{-1}, with no carbonyl or defined N–H: this pattern is compatible with an aliphatic alcohol; confirmation depends on the fingerprint region. Aliphatic ν C–H absorption occurs at ~2972 and ~2880 cm^{-1}.

3.3.2 2500 to 1800 cm^{-1} region (triple and cumulated bonds)

a) **Observed:** no band detected in this region;

b) **Assignment (general ranges):** no band to assign;

c) **Inference:** No band attributable to ν C≡N, ν C≡C or an N^+–H envelope (2500–1800 cm^{-1}) was detected under the conditions and within the region evaluated.

3.3.3 1800 to 1500 cm^{-1} region (carbonyl and C=C)

a) **Observed:** no band detected in this region;

b) **Assignment (general ranges):** no band to assign;

c) **Inference:** No band attributable to ν C=O (carbonyl) (1830–1630 cm^{-1}) was detected under the conditions and within the region evaluated.

3.3.4 1500 to 650 cm^{-1} region (fingerprint)

a) **Observed:** ~1379 (weak); ~1087 (weak to medium); ~1046 (very strong); ~953 (very weak); ~879 (medium) cm^{-1};

b) **Assignment (general ranges):** δ CH_2 / CH_3 (~1379); ν C–O (~1087, ~1046); no range in the general table: ~953, ~879;

c) Inference: δ CH_2/CH_3 was observed at ~1379 cm^{-1}. Bands of ν C–O / C–O–C occur at ~1087 and ~1046 cm^{-1}, compatible with an alcohol or ether (absence of carbonyl argues against an acid or ester). The strongest ν C–O band, at ~1046 cm^{-1}, is typical of a primary alcohol (primary alcohols absorb near 1050, secondary near 1100 and tertiary near 1150 cm^{-1}); together with broad O–H and no carbonyl, it is compatible with a simple aliphatic alcohol. This is the fingerprint region: comparison with a reference obtained under the same conditions is the strongest criterion.

A interpretation acima é gerada automaticamente a partir das posições dos picos detectados (aproximadas; ±4 cm^{-1}, tolerância de atribuição). It describes what was and was not observed and indicates compatible functional groups and classes; it does not identify a substance. Presence or absence of a band must be assessed with the complete spectrum and references obtained under the same conditions.

3.4 Material classes compatible with the bands

Functional-group classes compatible with observed bands according to automatic rules. This is not substance identification: different materials share the same bands, and mixtures combine their components' bands.

a) **Aliphatic alcohols (broad ν O–H, distinct aliphatic ν C–H and ν C–O near ~1000–1090 cm^{-1}, few C–O bands)** (for example ethanol, methanol, isopropanol and other short-chain alcohols, and glycols). Bands: ~3318; ~2972; ~1087; ~1046 cm^{-1}.

3.5 Spectrum quality and guidance for the next measurement

Spectrum quality was classified as good: strong signal, stable baseline and low noise. No adjustments are needed.

What is already good: the region from 3600 to 3000 cm^{-1} came out clean, with very low noise (0.015 to 0.028 %T), and the spectrum has enough points to record broad and narrow bands.

4 CONCLUSION

No reference-spectrum comparison was performed. The report describes observed absorption bands and compatible functional-group ranges. Submit a reference library to compare with references.

The band pattern is compatible with the class aliphatic alcohols (broad ν O–H, distinct aliphatic ν C–H and ν C–O near ~1000–1090 cm^{-1}, few C–O bands).

REFERENCES

ESPECTROFTIR. Internal database of infrared absorption ranges (functional groups and common materials). Parnaíba: [s. n.], 2026a. Database version: that of the software cited in ESPECTROFTIR (2026b). Available at: https://espectroftir.com.br/en/tabela-de-frequencias.html. Accessed: November 4, 2026.

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APPENDIX A – TRACEABILITY

Box 4 provides the data needed to reproduce and check this result.

ARIS (Algorithm for Rule-based Interpretation of Spectra) is the espectroFTIR procedure that detects the bands, assigns functional groups by rules and, when a library is available, compares the spectrum with the reference spectra. The code in brackets on the Software row is the shortened SHA-256 of the code used in this analysis and identifies the version of the algorithm.

Item	Description	Source
Software	espectroFTIR 2026.10 (ARIS c4fca424)	Algorithm
Detection parameters	limiar 3.0% da altura do gráfico; piso de 6× o ruído; distância mínima 12 cm^{-1}; smoothing of 3 pontos; tolerância de atribuição de faixas ±4 cm^{-1}	Algorithm
Quality parameters (provisional)	baseline: mean of the 5 lowest values in 215 cm^{-1} windows (step 120), interpolated; depth = difference from the baseline, with a 9-point moving average; noise per 100 cm^{-1} window from the second difference (1.4826 × MAD); low-confidence zone: noise-dominated window with noise ≥ 5× that of the quietest third and ≥ 10% of the amplitude; band confidence: high ≥ 0.8, medium ≥ 0.4 %T; amplitude: strong ≥ 15, adequate ≥ 5, weak ≥ 2 %T	Algorithm
Analyzed file (SHA-256)	0d7d0bd72de911c6aa096c257d6d2be14a8838b43c491914b163551e8c696c90	File
Issued on	04/11/2026 05:57:06 (Brasília time)	Algorithm

Box 4 – Processing traceability

Source: espectroFTIR (2026b).