FTIR Interpretation of Sample A

FTIR spectrum interpretation with literature-backed band assignments

Summary

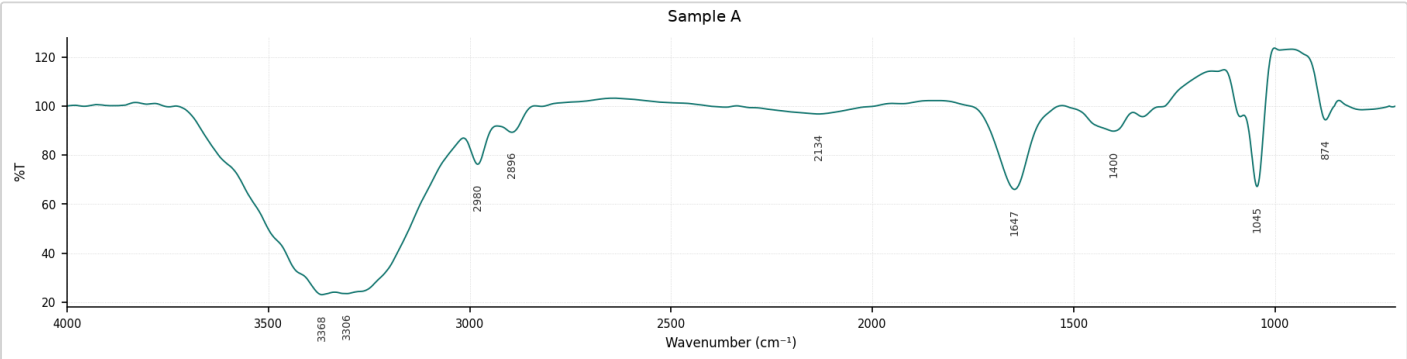
- All nine bands we picked match water and ethanol. The spectrum looks like an ethanol–water solvent, not like the sample material.
- Ethanol shows at 2980 and 2896 cm^{-1} (C–H stretching), 1045 cm^{-1} (C–O stretching) and 874 cm^{-1} (C–C stretching) [1, 2].
- Water shows as the broad O–H band at 3300–3370 cm^{-1}, the H–O–H bend at 1647 cm^{-1} [1] and a weak band at 2134 cm^{-1} [3].
- No band from Sample A constituents can be told apart from the solvent bands. To study the sample compounds, the extract should be dried and measured again.

Sample and Data

Spectrum S1	Sample A — file: sample_A.txt (Tabular text spectrum; y-axis: %T; 700–4000 cm^{-1}; 2301 points)
Customer request	Interpret the submitted FTIR spectrum and provide literature-backed band assignments for research reference.

We received one spectrum as a text file (700–4000 cm^{-1}, %T) and a screenshot of the instrument software. We converted %T to absorbance, picked peaks with the same routine used on FTIR.fun, and compared each band with published FTIR data. Each assignment in the table below gives the reference, the literature band position and the sentence from the paper.

Spectrum (as received, detected peaks marked)



Data Quality Notes

- Large parts of the spectrum are above 100 %T (up to 124 %T). This comes from the multipoint baseline correction shown in the screenshot. Band heights in those ranges are not reliable, and weak bands may be lost.
- The 1300–1800 cm^{-1} range overlaps the water bending region, so small bands there, such as the one at 1400 cm^{-1}, are hard to read.

Band Assignments with Literature Evidence

Evidence grade: A = band and assignment reported for the same material; B = closely related material or spectroscopy handbook; C = general group frequency from a different material. '–' means the literature band lies 5–10 cm^{-1} from the measured band; Δ = |measured − literature|, cm^{-1}. Band strength: s / m / w = strong / medium / weak relative to the strongest band.

Spectrum S1 — Sample A

Band (cm^{-1})	Component / assignment	Functional group / bond (mode)	Evidence	Reference, location, literature band and excerpt (verbatim)
3368 s	Water O–H stretching of hydrogen-bonded water (high-wavenumber side of the broad O–H band)	hydroxyl (H-bonded) *O–H (stretching)*		*No literature assignment within 10 cm^{-1} was found.*
	Ethanol O–H stretching of hydrogen-bonded ethanol, overlapping the water band	hydroxyl (H-bonded) *O–H (stretching)*		*No literature assignment within 10 cm^{-1} was found.*
3306 s	Ethanol O–H stretching of hydrogen-bonded ethanol (low-wavenumber side of the broad O–H band)	hydroxyl (H-bonded) *O–H (stretching)*		*No literature assignment within 10 cm^{-1} was found.*
	Water O–H stretching of hydrogen-bonded water, overlapping	hydroxyl (H-bonded) *O–H (stretching)*		*No literature assignment within 10 cm^{-1} was found.*
2980 m	Ethanol CH3 asymmetric stretching of ethanol	methyl *C–H (asymmetric stretching)*	A Δ 2.8 A Δ 0.8	[1] Section 4.1, p. 6 — 2983 cm^{-1} "This band gradually blueshifts from 2974 cm-1 to 2983 cm-1 as a function of the water content in the mixture." [2] Section 3, ethanol consumption difference spectra — 2981 cm^{-1} "We also observed the rising of negative bands at 2981 and 2900 cm −1 from CH stretching vibrations"
2896 w	Ethanol C–H stretching of ethanol (CH2/CH3)	methylene / methyl *C–H (stretching)*	A Δ 4.4	[2] Section 3, ethanol consumption difference spectra — 2900 cm^{-1} "We also observed the rising of negative bands at 2981 and 2900 cm −1 from CH stretching vibrations"
2134 w	Water bend + libration combination band of liquid water	water *H–O–H (bending + libration combination)*	A Δ 3.6	[3] Abstract — 2130 cm^{-1} "The relatively weak bend+libration water combination band (centered at 2130 cm–1)"
1647 m	Water H–O–H bending of water	water *H–O–H (bending)*	A Δ 2.2	[1] Section 4.2, p. 9 — 1645 cm^{-1} "the peak centered at 1645 cm-1, which corresponds to the H-O-H bending vibration"
1400 w	Ethanol C–H bending of CH2/CH3	methyl / methylene / hydroxyl *C–H and C–O–H (bending)*		*No literature assignment within 10 cm^{-1} was found.*

	and C–O–H bending of ethanol (tentative)			
1045 m	Ethanol C–O stretching of ethanol (coupled with O–H bending)	primary alcohol *C–O (stretching)*	A Δ 0.6 A Δ 0.6 B Δ 0.6	[2] Section 3, ethanol consumption difference spectra — 1044 cm⁻¹ "Negative bands at 1044 and 877 cm −1 indicate consumption of ethanol (solid lines) and are due to the C-O stretching and C-C stretching vibrations of ethanol respectively" [1] Section 4.1, p. 6 — 1044 cm⁻¹ "two intense peaks appear at 1086 cm-1 and 1044 cm-1 which correspond to O-H bending coupled to C-O stretching vibrations and O-H bending coupled to C-C stretching vibrations, respectively." [4] Section 3, p. 11 — 1044 cm⁻¹ "The highest peaks at 1086 and 1044 cm-1 are ascribed to the C-O stretch absorption bands, which are important regions for ethanol"
874 w	Ethanol C–C stretching of ethanol	ethyl skeleton *C–C (stretching)*	A Δ 4.2 A Δ 3.2	[1] Section 4.1, p. 6 — 878 cm⁻¹ "The last band that can be observed to belong to ethanol is a band at 878 cm-1, which corresponds C-C stretching vibrations." [2] Section 3, ethanol consumption difference spectra — 877 cm⁻¹ "Negative bands at 1044 and 877 cm −1 indicate consumption of ethanol (solid lines) and are due to the C-O stretching and C-C stretching vibrations of ethanol respectively"

What the Spectrum Indicates

Water — Water is clearly present. The broad band at 3300–3370 cm⁻¹ is O–H stretching. The band at 1647 cm⁻¹ is the H–O–H bend [1], and the weak band at 2134 cm⁻¹ is a combination band seen only in liquid water [3].

Ethanol — Ethanol is clearly present. The C–H bands at 2980 and 2896 cm⁻¹, the strong C–O band at 1045 cm⁻¹ with a shoulder near 1086 cm⁻¹, and the C–C band at 874 cm⁻¹ all match ethanol in water [1, 2, 4].

Sample A constituents — We could not find bands from the sample itself. Extracts often show C=O bands near 1700–1740 cm⁻¹ and aromatic bands near 1510–1610 cm⁻¹. Neither is resolved here. If the sample compounds are present, they are at a level that the solvent bands cover.

Conclusion

The spectrum is that of an ethanol–water mixture. This fits a liquid ethanolic extract measured before the solvent was removed. From this spectrum alone we cannot name the functional groups of the Sample A compounds. The result does not mean the extract is empty; it means the solvent is much stronger than the dissolved material.

Limitations

- The three bands at 3368, 3306 and 1400 cm⁻¹ are assigned from general band positions. We did not find a published band within 10 cm⁻¹ for them, so the table lists them without a reference.
- The baseline correction pushed the signal above 100 %T in many ranges, which can hide weak bands.

- We do not know how the sample was prepared or measured (liquid or dried, ATR or KBr). If this differs from what we assume, please tell us and we will check again.

Recommended next steps

- Dry the extract fully (for example, evaporate the ethanol and dry at low heat or under vacuum) and measure the solid residue by ATR or as a KBr pellet.
- Export the raw spectrum without baseline correction, or use a baseline that keeps all points below 100 %T.
- Also measure the pure solvent the same way. Subtracting it from the extract spectrum helps to show the sample bands.

References

1. Zeinalipour-Yazdi, C. D.; Loizidou, E. Z. An experimental FTIR-ATR and computational study of H-bonding in ethanol/water mixtures. Chemical Physics 2021, 550, 111295. https://doi.org/10.1016/j.chemphys.2021.111295
2. Kumar, S.; Barth, A. Following Enzyme Activity with Infrared Spectroscopy. Sensors 2010, 10(4), 2626–2637. https://doi.org/10.3390/s100402626
3. Verma, P. K.; Kundu, A.; Puretz, M. S.; Dhoonmoon, C.; Chegwidden, O. S.; Londergan, C. H.; Cho, M. The Bend+Libration Combination Band Is an Intrinsic, Collective, and Strongly Solute-Dependent Reporter on the Hydrogen Bonding Network of Liquid Water. The Journal of Physical Chemistry B 2018, 122(9), 2587–2599. https://doi.org/10.1021/acs.jpcb.7b09641
4. Anjos, O.; Martínez Comesaña, M.; Caldeira, I.; Pedro, S. I.; Eguía Oller, P.; Canas, S. Application of Functional Data Analysis and FTIR-ATR Spectroscopy to Discriminate Wine Spirits Ageing Technologies. Mathematics 2020, 8(6), 896. https://doi.org/10.3390/math8060896

This report interprets the spectrum supplied by the customer and is for research and reference use. FTIR identifies functional groups and material classes; exact composition needs the confirmatory tests listed above.

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