Comparison of Two FTIR Spectra: Sample A and Sample B

Consistency comparison of two FTIR spectra

Result

Same main components, with clear differences

Both samples contain nitrocellulose and calcium carbonate, but in very different amounts. The sample B is mostly calcium carbonate with little nitrocellulose, and it contains a wax-like material that the sample A does not show.

- Both samples contain the same two main materials: nitrocellulose, a common ink binder, and calcium carbonate (calcite), a common filler [3, 1, 5].
- The ratio is very different. In the sample A (A), nitrocellulose gives the strongest bands. In the sample B (B), calcium carbonate dominates and the nitrocellulose bands are weak.
- Only A shows an ester C=O band at 1735 cm^{-1} and bands at 794 and 462 cm^{-1} that may come from silica. Only B shows a sharp C–H pair at 2915/2849 cm^{-1} from a wax-like long-chain material [2].
- The deposit is consistent with material from sample A, mostly its filler, but it is not the same as the sample A film.

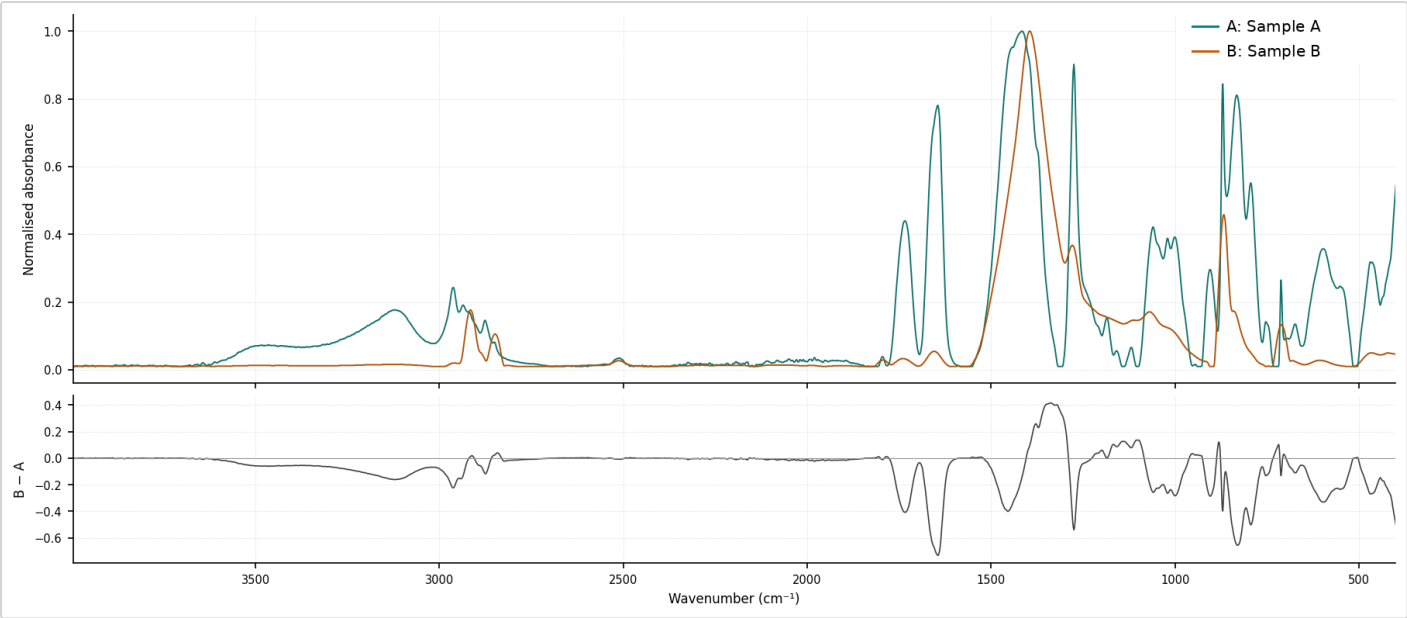
Samples and Data

A	Sample A — file: spectrum_A.dpt (Tabular text spectrum; y-axis: %T; 398–3997 cm^{-1}; 2.05 cm^{-1} point spacing)
B	Sample B — file: spectrum_B.dpt (Tabular text spectrum; y-axis: %T; 398–3997 cm^{-1}; 2.05 cm^{-1} point spacing)
Customer request	Compare the two spectra, see their differences and similarities.
Sample use	Inks
Sample form	Solid/Powder
Stated composition	Ink resin/additives

We received two spectra (Bruker .dpt, 400–4000 cm^{-1}, transmittance). We converted both to absorbance, picked peaks with the FTIR.fun routine, and paired bands that lie within 10 cm^{-1} of each other. For the overlay and the correlation values, both spectra were baseline-corrected and scaled to the same range, using the same steps as FTIR.fun search. Each assignment in the table gives the reference, the literature band and the sentence from the paper.

- Both spectra cover the same range with the same point spacing, so they can be compared directly.
- A has a broad weak band around 3100–3500 cm^{-1} (O–H or N–H) that was not picked as a peak; B has almost none. This may come from moisture or from a minor component and was not used for the result.

Overlay and Similarity



Top: both spectra after the same baseline correction and normalisation used by FTIR.fun search. Bottom: difference spectrum B − A.

Metric	Value
Correlation coefficient, whole common range (400–3996 cm⁻¹)	0.692
Correlation coefficient of first-derivative spectra	0.369
Correlation coefficient, 2500–4000 cm⁻¹ (X-H stretching region (O-H, N-H, C-H))	0.355
Correlation coefficient, 1800–2500 cm⁻¹ (triple-bond / cumulated double-bond region)	0.290
Correlation coefficient, 1500–1800 cm⁻¹ (double-bond region (C=O, C=C, H-O-H bend, NO2 asym.))	0.219
Correlation coefficient, 400–1500 cm⁻¹ (fingerprint region)	0.642

Correlation coefficients describe overall shape similarity (1 = identical shape). They do not decide sameness on their own; the band-by-band comparison below does.

Band-by-band Comparison

Shared = present in both spectra; A only / B only = present in one spectrum; relative intensity = band absorbance ÷ strongest band of the same spectrum. Evidence grade: A = same material in the literature; B = closely related material or handbook; C = general group frequency from a different material; '–' = literature band 5–10 cm⁻¹ away; Δ = |measured − literature|, cm⁻¹.

A (cm⁻¹)	B (cm⁻¹)	Rel. int. A / B	Observation	Component / assignment	Literature evidence (verbatim excerpt)
2962	—	0.20 / —	A only Medium in A (0.20); not resolved in B, where the C–H bands sit at 2915/2849 instead.	**Nitrocellulose (cellulose nitrate)** C–H stretching of the binder *aliphatic C–H; C–H (stretching)*	A Δ 3.8 [1] Table 1, CN membrane column — 2966 cm⁻¹ (A 2962) “2966 2963 2958 νC-H”
—	2915 / 2849	— / 0.21 / 0.14	B only Sharp pair in B (0.21 / 0.14); not present in A.	**Long-chain hydrocarbon (wax-like)** CH2 asymmetric and symmetric stretching of long hydrocarbon chains *methylene (–CH2–)n; C–H (stretching)*	B Δ 2.0 [2] Section on blooming, p. 50 — 2917 cm⁻¹ (B 2915) “The two strong and sharp bands at 2917 and 2849 cm-1 can be assigned to the asymmetric and symmetric stretching vibration of the methylene group (-CH2-) respectively.”

					B Δ 0.3 [2] Section on blooming, p. 50 — 2849 cm⁻¹ (B 2849) “The two strong and sharp bands at 2917 and 2849 cm-1 can be assigned to the asymmetric and symmetric stretching vibration of the methylene group (-CH2-) respectively.”
1735	—	0.37 / —	A only Medium in A (0.37); not detected in B.	**Ester carbonyl compound (plasticiser or ester resin)** Ester C=O stretching, typical of a plasticiser or ester resin used with nitrocellulose *ester carbonyl; C=O (stretching)*	B- Δ 6.6 [3] Background, p. 2 — 1728 cm⁻¹ (A 1735) “A smaller peak due to the carbonyl group of the plasticizer is observed at 1728 cm −1 .”
1648	1655	0.61 / 0.08	Intensity change Present in both; strong in A (0.61), weak in B (0.08). In B the band is 6 cm⁻¹ higher.	**Nitrocellulose (cellulose nitrate)** Nitrate ester, NO2 asymmetric stretching *nitrate ester (O–NO2); N=O / NO2 (asymmetric stretching)*	A Δ 3.4 [3] Methods, PCA, p. 6 — 1645 cm⁻¹ (A 1648) “Loading plots were overlayed onto the reference IR spectra of CN and PVAc to identify correlation between areas of positive or negative deviation and the diagnostic IR peaks of PVAc (1729, 1225 and 1018 cm −1) and CN (~1645, 1280 and 840 cm −1)” A Δ 1.4 [3] Discussion, p. 11 — 1656 cm⁻¹ (B 1655) “Camphor and DBP have a characteristic carbonyl peak at 1738 and 1720 cm −1 respectively, which are located at a slightly higher energy than the nitrate peak of CN at ~1656 cm −1 .”
1412	1394	0.90 / 1.00	Shifted Present in both; strong in A (0.90) and the strongest band of B (1.00); maximum 18 cm⁻¹ lower in B.	**Calcium carbonate (calcite)** Carbonate asymmetric stretching (v3) *carbonate (CO_3^{2-}); C–O (asymmetric stretching)*	A- Δ 7.7 [4] Section 3, p. 7 — 1420 cm⁻¹ (A 1412) “the main differences were observed for three absorption bands at 1420, 875 and 712 cm-1, corresponding to vibrations of carbonate groups (CO3), which constitute calcium carbonates” A- Δ 6.1 [5] Section 3.1, p. 5 — 1400 cm⁻¹ (B 1394) “characteristic IR absorptions associated with the fundamental vibrations of the carbonate group observed around ~1400 cm-1 (broad peak), 872 cm-1 and 712 cm-1”
1275	1279	1.00 / 0.43	Intensity change Present in both; strongest band of A (1.00), medium in B (0.43).	**Nitrocellulose (cellulose nitrate)** Nitrate ester, NO2 symmetric stretching *nitrate ester (O–NO2); NO2 (symmetric stretching)*	A Δ 3.2 [1] Table 1, CN membrane column — 1278 cm⁻¹ (A 1275) “1278 1276 1277 ν s NO 2 in CN” A Δ 0.9 [1] Table 1, CN membrane column — 1278 cm⁻¹ (B 1279) “1278 1276 1277 ν s NO 2 in CN” A Δ 1.1 [6] Section 2 (experimental), p. 2146 — 1280 cm⁻¹ (B 1279)

					“Nitrocellulose can be identified by the characteristic IR band of the nitric group at 1660 (ν as) and 1280 (ν s)”
1061	1070	0.67 / 0.25	Shifted Present in both; 8 cm⁻¹ higher and weaker in B (0.67 in A, 0.25 in B).	**Nitrocellulose (cellulose nitrate)** C–O–C / C–O stretching of the cellulose ring *glucose ring ether / alcohol; C–O–C, C–O (stretching)*	A Δ 0.3 [1] Table 1, CN membrane column — 1061 cm⁻¹ (A 1061) “1061 1051 1045 ν a O-C-C attached to the NO 2 group [38], νCOC of the cellulose ring in CN [18]” A- Δ 8.5 [1] Table 1, CN membrane column — 1061 cm⁻¹ (B 1070) “1061 1051 1045 ν a O-C-C attached to the NO 2 group [38], νCOC of the cellulose ring in CN [18]”
905 / 595	—	0.46 / 0.58 / —	A only Medium to strong in A (0.46 / 0.58); not detected in B.	Not assigned; no literature band within 10 cm⁻¹ was found for a component that fits the rest of the spectrum *unknown; unknown*	*Not used for the result; no citation given.*
870	868	0.87 / 0.51	Shared Present in both at nearly the same position (870 / 868).	**Calcium carbonate (calcite)** Carbonate out-of-plane bending (v2) *carbonate (CO_3^{2-}); CO3 (out-of-plane bending)*	A Δ 1.6 [5] Section 3.1, p. 5 — 872 cm⁻¹ (A 870) “characteristic IR absorptions associated with the fundamental vibrations of the carbonate group observed around ~1400 cm-1 (broad peak), 872 cm-1 and 712 cm-1” A Δ 3.7 [5] Section 3.1, p. 5 — 872 cm⁻¹ (B 868) “characteristic IR absorptions associated with the fundamental vibrations of the carbonate group observed around ~1400 cm-1 (broad peak), 872 cm-1 and 712 cm-1”
831	—	0.84 / —	A only Strong in A (0.84); no separate band in B.	**Nitrocellulose (cellulose nitrate)** N–O stretching of the nitrate ester *nitrate ester (O–NO2); N–O (stretching)*	A Δ 4.4 [1] Table 1, CN membrane column — 827 cm⁻¹ (A 831) “827 828 827 ν-NO in CN” A- Δ 8.6 [3] Methods, PCA, p. 6 — 840 cm⁻¹ (A 831) “Loading plots were overlayed onto the reference IR spectra of CN and PVAc to identify correlation between areas of positive or negative deviation and the diagnostic IR peaks of PVAc (1729, 1225 and 1018 cm −1) and CN (~1645, 1280 and 840 cm −1)”
794 / 462	—	0.66 / 0.69 / —	A only Strong in A (0.66 / 0.69); not detected in B.	**Silicate or silica** Si–O–Si symmetric stretching (794) and bending (462), possibly silica (tentative) *siloxane (Si–O–Si); Si–O (stretching, bending)*	A- Δ 5.6 [7] Section 3, p. 5 — 800 cm⁻¹ (A 794) “at 800 and 465 cm-1 ascribable to asymmetric and symmetric Si-O-Si stretching and bending vibrations” A Δ 3.1 [7] Section 3, p. 5 — 465 cm⁻¹ (A 462)

					"at 800 and 465 cm-1 ascribable to asymmetric and symmetric Si-O-Si stretching and bending vibrations"
710	710	0.44 / 0.24	Shared Present in both at the same position (710).	**Calcium carbonate (calcite)** Carbonate in-plane bending (v4), typical of calcite *carbonate (CO_3^{2-}); CO3 (in-plane bending)*	A Δ 1.7 [5] Section 3.1, p. 5 — 712 cm^{-1} (A 710) "characteristic IR absorptions associated with the fundamental vibrations of the carbonate group observed around ~1400 cm-1 (broad peak), 872 cm-1 and 712 cm-1" A Δ 1.7 [5] Section 3.1, p. 5 — 712 cm^{-1} (B 710) "characteristic IR absorptions associated with the fundamental vibrations of the carbonate group observed around ~1400 cm-1 (broad peak), 872 cm-1 and 712 cm-1"

Components in Each Sample

Component	A	B	Basis
Nitrocellulose (cellulose nitrate) *ink binder*	present	present	A shows the full nitrate ester set at 1648, 1275 and 831 cm^{-1} with the ring band at 1061 cm^{-1} [3, 1]. B shows 1655 and 1279 cm^{-1} only, and they are much weaker [3, 1].
Ester carbonyl compound (plasticiser or ester resin) *ink additive*	present	not detected	One C=O band at 1735 cm^{-1} in A [3]. FTIR alone cannot say which ester it is.
Calcium carbonate (calcite) *filler / extender pigment*	present	present	Carbonate bands near 1400, 870 and 710 cm^{-1} in both spectra [4, 5]. In B it is the main absorbing material.
Long-chain hydrocarbon (wax-like) *wax additive or contamination*	not detected	present	Sharp CH2 pair at 2915/2849 cm^{-1} in B only [2]. The source (paraffin or polyethylene wax, or another long-chain material) cannot be determined from these two bands.
Silicate or silica *possible filler*	present	not detected	Bands at 794 and 462 cm^{-1} in A [7]. The main Si–O band near 1080 cm^{-1} would overlap the nitrocellulose band, so this is not confirmed.

Interpretation

Similarities

- Nitrocellulose bands appear in both: NO2 stretching near 1650 and 1277 cm^{-1} and the ring C–O band near 1061–1070 cm^{-1} [3, 1, 6].
- Calcium carbonate bands appear in both near 1400, 870 and 710 cm^{-1} [4, 5]. The small calcite bands near 1795 and 2512 cm^{-1} are also seen in both overlays.

Differences

- Amount of binder: the nitrocellulose bands are much weaker in B. The strong N–O band at 831 cm^{-1} in A is not resolved in B [1].
- Ester C=O at 1735 cm^{-1} is present only in A. This is typical of a plasticiser or an ester resin used with nitrocellulose [3].

- The carbonate band is the strongest band in B, and its maximum is 18 cm^{-1} lower than in A. This can come from different particle size or packing, or from overlap with other bands in A.
- A sharp C–H pair at 2915/2849 cm^{-1} appears only in B. It points to a long-chain hydrocarbon such as a wax [2]. A shows a C–H band at 2962 cm^{-1} instead.
- Bands at 794 and 462 cm^{-1} (possible silica) [7] and two unassigned bands at 905 and 595 cm^{-1} are present only in A.

The simplest explanation is that the sample B is made mostly of filler particles from sample A, with only a small amount of the binder. A wax is often added to inks, and dust can also pick up wax-like material from nearby surfaces, so the CH2 bands in B may come from either source. FTIR cannot tell these two cases apart.

Conclusion

The two spectra share their main components, nitrocellulose and calcium carbonate, so sample B is consistent with material from this type of ink. They are not identical: sample B has far less binder, no ester C=O band, none of the bands at 794 and 462 cm^{-1}, and an extra wax-like component. These differences point to a deposit that is mostly filler with added or picked-up wax, not a piece of the sample A film.

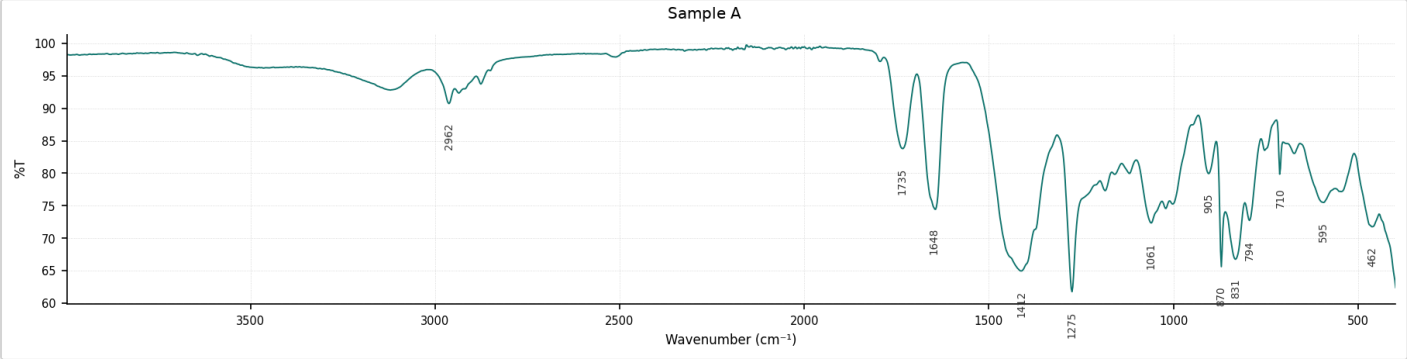
Limitations

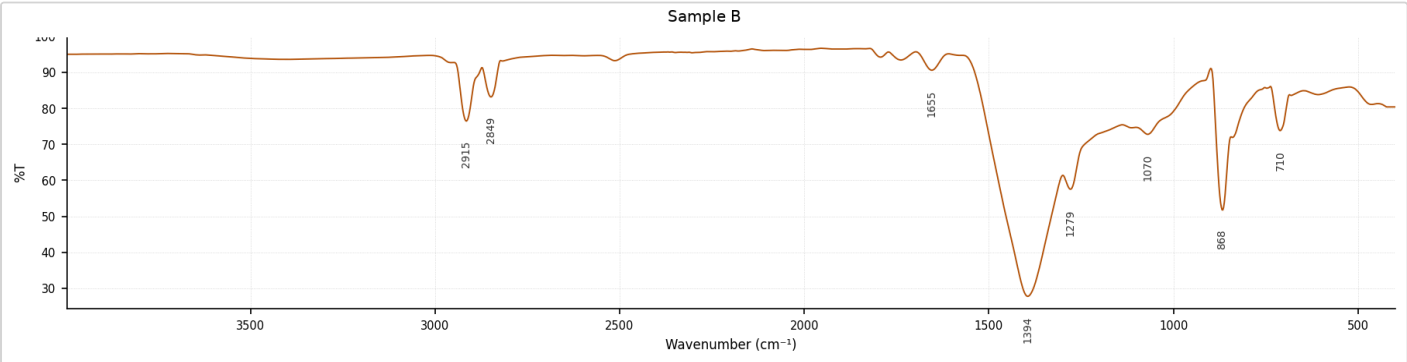
- FTIR shows material classes. It cannot prove that sample B came from this specific ink batch.
- Weak components, under a few percent, may not show in either spectrum.
- The 1061–1070 cm^{-1} band can include other materials, such as silica, so its shift between A and B is not used on its own.

Recommended next steps

- SEM-EDS of sample B to confirm calcium-rich particles and check for silicon.
- A solvent extract of sample B (for example with hexane) measured by FTIR, to see the wax on its own.
- If the dust was collected on a surface, also measure that surface, so contamination can be ruled out.

Appendix: Spectra as Received (detected peaks marked)





References

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This report compares the spectra supplied by the customer and is for research and reference use. FTIR shows functional groups and material classes; confirming exact composition or origin needs the tests listed above.

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