How to use UltraFine+® Next Gen Analytics VNIR data

What is VNIR-SWIR (NIR) data?

Reflectance spectral soil properties provide important information about your soil samples that relate to landscape settings and can potentially be used to help identify false positive geochemical anomalies in mineral exploration. When you submit your soil samples to the UltraFine+® Next Gen Analytics project via LabWest, you will receive 17 spectral soil parameters. Materials interact with wavelengths of light differently across the electromagnetic spectrum, but human eyes can only interpret a small region of the electromagnetic spectrum. Hyperspectral instruments can see into the infrared and can pick up mineral and chemical differences between materials due to how the light interacts with the crystal structures and molecular compounds of the soil materials. The visible to shortwave infrared (350-2500 nm) reflectance of ultrafine materials give relative abundances of spectrally active minerals, their mineral chemistry and an indication of the key minerals present in the sample.

What does this data mean?

Parameter	Definition	Applications & Limitations
MinGrp1	Main mineral-group detected in the shortwave infrared region	Report of the dominant mineral-group present, which may be deemed to have contributed >51% to the spectral unmixing algorithm. Uses mineral-groups rather than individual minerals (i.e., white mica rather than muscovite). Only reports mineral-groups which are spectrally active in the 1300-2500 nm wavelength region, thus does not report iron oxide minerals. See section below this table for more information.
MinGrp2	Secondary mineral-group detected in the shortwave infrared region	May make up <49% of the predicted mineral-group in the sample and reported the same as MinGrp1.
FeOx	Relative abundance of iron oxide based on the strength of the iron oxide absorption around 900 nm	Indicates the presence of iron oxides and may indicate that the original material was iron-rich. Typically, as this is a surface technique it can disproportionally represent coatings on grains, but with UltraFine samples the material is typically fine grained. Ranges are <0.01 very low; 0.01 - 0.02 = low; 0.02 - 0.2 = moderate; >0.2 = high amounts of iron oxide.
Hem_Goe	Iron oxide species (measurement of the wavelength in nanometres of the iron oxide absorption, which relates to the hematite or goethite proportion)	Hematite absorption is ~890 nm whereas goethite is ~920 nm. Thus, lower numbers represent more hematitic materials, whereas higher values mean the material is more goethitic. Can indicate the type of weathering that has occurred and redox conditions. In some regions can be used to differentiate palaeoenvironments during deposition. Can also include less common iron oxide and oxyhydroxide minerals (such as acid rock drainage minerals: jarosite, schwertmannite, ferrihydrite etc. and lepidocrocite). Magnetite and maghemite are not spectrally active in this wavelength region.
Kln_abun	Relative abundance of kaolinite	Main absorption features coincide with white mica and aluminium smectite and can be influenced where both minerals exist. Ranges are 0.1 - 0.15 = low; 0.2 - 0.25 = moderate; >0.25 = high amounts of kaolinite.
Kln_cryst	Kaolinite crystallinity	Useful for regolith mapping of soils (poorly crystalline = transported vs. highly crystalline = *in-situ*). Ranges are <1.004 = disordered/mixture with smectite; 1.025 - 1.004 = moderate; >1.04 = high. Note very low numbers <0.97 could be dickite.

WM_AS_abun	Relative abundance of white mica and/or aluminium smectite	This result is excluded if the material contains a kaolin absorption feature at 2160 nm >1.005. Ranges are <0.05 = low; 0.07 - 0.14 = moderate; >0.14 = high amounts of white mica/Al-smectite.
WM_AS_comp	White mica and/or aluminium smectite composition (amount of Al-substitution based on wavelength in nanometres)	This result is excluded if the material contains a kaolin absorption feature at 2160 >1.005. Typically indicates less weathered material, or soils from parent rocks. May indicate shallow depth of cover/subcrop or colluvial transport of material from outcrop upslope. Changes in the wavelength (chemistry) of white micas has been linked to alteration and has been used as a vector for mineralisation. Lower values are Al-rich (<2200 nm to - 2208 nm = muscovite), whereas higher values are Al-poor white mica (>2209 nm = phengite) or Al-smectite (~2209 nm = montmorillonite, >2215 nm = palygorskite).
Fe_Kln	Relative abundance of iron substitution in kaolinite	Iron substitution in kaolinite has been found in highly weathered materials over mafic materials and can indicate the parental materials were originally iron-rich. Ranges are 0.01-0.056 = low; 0.016 - 0.03 = moderate; >0.03 = high. This result is excluded if the material contains chlorite.
Chl	Relative abundance of chlorite and dark mica (biotite and phlogopite)	Requires a high proportion of chlorite or biotite to be present, where white mica and kaolinite are absent. This parameter can also falsely include palygorskite (compare to Paly parameter below). Biotite is spectrally dark and can be difficult to detect. Uncommon in highly weathered soils but may occur close to exposures of fresh rocks or very shallow cover. Ranges are 0.01 - 0.015 = low; 0.015 - 0.025 = moderate; >0.025 = high.
FeMgClay	Relative abundance of iron and magnesium smectite	Indicates the presence of Fe and Mg smectite minerals, such as nontronite and saponite, which are associated with the weathering of mafic materials. Ranges are 0.01 -0.014 = low; 0.014 - 0.022 = moderate; >0.022 = high.
OH_mafic	Mafic minerals with OH (i.e., amphiboles) relative abundance as well as Fe/Mg smectites	Indicates the presence of significant amounts of OH-bearing mafic minerals and carbonates, where there is a lack of kaolin and white mica. Ranges are 0.06 – 0.08 = low; 0.08 - 0.12 = moderate; >0.12 = high,
Paly*	Palygorskite	Palygorskite (also known as attapugite) is a Mg Al clay mineral often associated with alkaline conditions and inland lakes. It is highly absorbent and may be associated with elevated metal concentrations. Ranges are 0.04 – 0.07 = low; 0.07 - 0.17 = moderate; >0.18 = high.
Colour	Munsell Colour; results from the spectral data in standard "hue value/chroma" Munsell notation, typically used for describing soil and regolith materials colour	Colour can be related to the mineralogy and organic content.
Hue	A numerical (0 - 360) representation of the colour wheel of Red-Yellow-Green-Cyan-Blue-Magenta(-Red); hues around 0 are red, whereas yellows are ~40 - 60	Gives an indication of the colour of the material.
Saturation	Refers to how washed out or pure the hue is, with low values appearing greyer; values range from 0 - 1	
Intensity	Also known as Value on the HSI or HSV scale of colour or Luminance and refers to how light or dark a hue is; values range from 0 - 1.	Dark material may contain organic carbon or dark minerals, whereas lighter material may contain highly weathered materials or carbonates.

*Only reported in data processed by TSG 3.2 (November 2022); VNIR data processed with the previous TSG version 3.1 does not report palygorskite

What are the minerals in Mineral Group 1 and 2 and how reliable are they?

The Mineral Groups 1 and 2 are automated results of the major and minor minerals, based on a spectral reference library. Not all minerals have diagnostic features in the SWIR and thus are not identifiable. For example, quartz is not directly detectable in the SWIR region but can be diagnostically detected in the thermal infrared using FTIR (Fourier transform infrared) spectroscopy (see How-to FTIR). The Mineral Group 1 represents the major SWIR-active mineral component of the reflectance spectra, whereas Mineral Group 2 is the secondary component and can constitute up to 49% of the match to the spectral library. Where only one mineral group is reported there is either no other mineral-groups in the library that match the sample, or it constitutes less than 15 % of the match. Such spectra will appear as NULL in the raw data and as NOMATCH in the UltraFine+® Next Gen outputs. Carbonates, although detectable by SWIR in high abundances will often not be detected in soil samples, where they have been coated by other materials. Carbonates are also reported in FTIR data allowing cross reference and confirmation of key changes observed in the spectral output delivered in the UltraFine+® data.

Mineral	Definition (example minerals)	Applications & Limitations
Kaolin	Kaolinite, halloysite, dickite, nacrite minerals	Kaolinite is a common mineral in weathered terrains, the crystallinity can indicate transported vs. *in situ* material. Halloysite has a very similar spectral appearance to a mixture of kaolinite + montmorillonite.
Smectite	Montmorillonite, nontronite and magnesium clays (saponite)	Commonly found in alluvial settings (montmorillonite) and weathering close to mafic rocks (nontronite/saponite), as well as in weathering of volcanic rocks.
White-Mica	Muscovite, phengite, paragonite, illitic varieties of white mica	Commonly found associated with shallow soils near or adjacent to granitic material. May also be associated with feldspar, which is not detected by SWIR.
Amphibole	Hornblende, tremolite, actinolite, riebeckite	Uncommon, but may be associated with shallow soils near or adjacent to mafic material.
Chlorite	Clinochlore, chamosite	Associated with shallow soils near or adjacent to chlorite bearing rocks, particularly where they are fresh.
Dark-Mica	Biotite and phlogopite	Dark micas tend to weather rapidly once exposed and are uncommon.
Other_ALOH	Group of other Al-bearing minerals	Pyrophyllite, prehnite, diaspore and gibbsite. Of these, gibbsite is the most likely to be seen in soils, particularly in highly weathered terrains (gibbsite can be cross checked against the FTIR data).
Other_MgOH	Group of other Mg-bearing minerals	Indicator for Talc and hornblende. Not commonly seen as a major component of soils.
Carbonate	Calcite, dolomite, magnesite	May be present where calcrete occurs, but SWIR is less reliable than the thermal infrared wavelength regions used by the FTIR for detecting carbonate. Carbonates can be easily coated by other materials which are active in the SWIR, making them less detectable. Due to the carbonate region overlapping with other minerals, sometimes white mica, chlorite and FeMg clays can be misinterpreted as carbonate (cross check with FTIR carbonate data).
Sulfate	Gypsum, alunite, jarosite	Gypsum can be found near salt lakes and saline soils; the other minerals are uncommon outside of acid rock drainage environments.
NOTAROK	Anything that is not a mineral, this could be plastic, wood, etc.	
OTHERMINS	Other rare minerals for UltraFine soil	Minerals that occur only very rarely in UltraFine soils. One example could be serpentine that may be a product of weathering of ultramafic rock.
NOMATCH	No mineral-groups in the library match the sample	NULLs reported in the Mineral Groups 1 and 2 are translated to NOMATCH as these are minerals that have no match in the current library. NOMATCH will not appear in raw data from LabWest and will only be present in machine learning outputs.

Why are there so many NULLs in my data?

NULL values indicate the sample may lack a significant enough diagnostic absorption feature for that parameter, which would indicate that the mineral pertaining to that parameter is not present or cannot be spectrally detected (possibly due to the mineral being coated with another mineral). Much of the soils in Australia contain minerals associated with weathered materials, but some areas may contain minerals more associated with primary rock minerals (e.g., lithosols in the Australian Soil Classification System), particularly where close to exposures of outcropping rock. Because of this, the machine learning workflow replaces NULLs in Mineral Groups 1 and 2 with NOMATCH, to indicate that a mineral may be present, but cannot be reliably identified from the shortwave infrared spectral library. For example, a sample with high amounts of Fe oxides and quartz will produce NULLs for the Mineral Groups.

How do I use VNIR-SWIR data?

In addition to the raw data you receive from LabWest that you can plot and interrogate as you wish, you will also receive a shape file of your VNIR-SWIR data that can be dropped into ArcGIS®. We recommend plotting Mineral Groups and Colour as categories and all other data as quantities.

Example of VNIR-SWIR data application for surface exploration

The concentration of many metals in soil samples is related to their mineral composition, such as the of abundance iron oxides and clay minerals. VNIR-SWIR parameters can aid the identification of patterns, and in downgrading or upgrading target areas, as well as identifying areas of unique soil types to better interpret potential anomalies. Which parameters to use may be dependent on soil type, landscape context and deposit style.

Example 1: Normalisation of Au concentration by relative iron oxide abundance

Many trace metals are readily adsorbed to clay mineral and iron oxides. Given the high adsorption capacity of iron oxides, it is worth considering whether an anomaly of a metal of interest is present in iron oxide-rich or -poor soils and normalise the geochemical data accordingly to up- or downgrade targets.

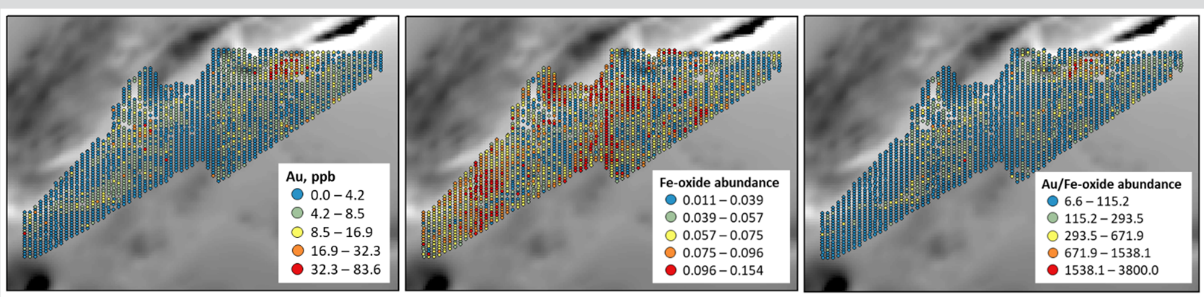

***Figure** 1: Au concentration, relative iron oxide abundance, and Au normalised by relative iron oxide abundance over gravity (grey scale). The normalisation has effectively reduced the Au target size over a very large survey area.*

Example 2: Normalisation of Au concentration by clay type

Clay minerals can be effective metal sinks in soils. Swelling clays (e.g., smectites) have negatively charged interlayer surfaces, which attracts hydrated cations. Non-swelling clays (e.g., kaolinite) do not attract metals into interlayer spaces. It is therefore worth considering whether an anomaly of a metal of interest is present in a swelling or non-swelling clay and normalise the data accordingly. In this example, the data population was separated by Mineral Group 1 and Au was z-log normalised for each population individually.

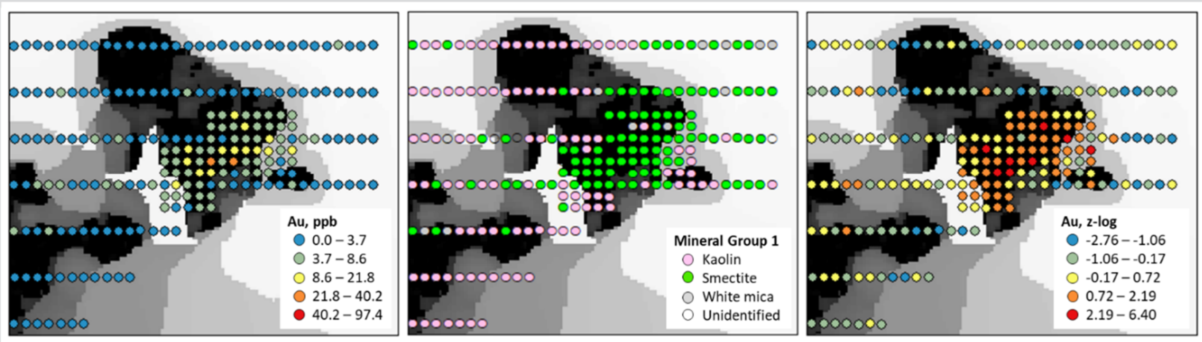

Figure 2: Au concentration, Mineral Group 1 and Au adjusted for Mineral Group 1 (z-log normalised and recombined) over depth of cover (grey scale). The recombined data has effectively highlighted the main Au target over a smaller survey area.

References

1. Berman, M., Bischoff, L., Lagerstrom, R., Guo, Y., Huntington, J., Mason, P., Green, A.A., 2017. A comparison between three sparse unmixing algorithms using a large library of shortwave infrared mineral spectra. IEEE Transactions on Geoscience and Remote Sensing 55, 3588–3610. https://doi.org/10.1109/TGRS.2017.2676816
2. Duke, E.F., 1994. Near infrared spectra of muscovite, Tschermak substitution, and metamorphic reaction progress: implications for remote sensing. Geology, 4, 621-624.
3. Laukamp, C., Rodger, A., LeGras, M., Lampinen, H., Lau, I., Pejcic, B., Stromberg, J., Francis, N., Ramanaidou, E. (2021): Mineral physicochemistry underlying feature-based extraction of mineral abundance and composition from shortwave, mid and thermal infrared reflectance spectra. Minerals, 11(4), 347
4. Wang, R., Cudahy, T., Laukamp, C., Walshe, J.L., Bath, A., Mei, Y., Young, C., Roache, T.J., Jenkins, A., Clarke, F., Baker, A., Roberts, M., Laid, J., 2017. White mica as a hyperspectral tool in exploration for Sunrise Dam and Kanowna Belle gold deposits, Western Australia. Economic Geology, 112 (5), 1153-1176.
5. Yang, K., Huntington, J.F., Cudahy, T.J., Mason P., Scott K.M., 2001. Spectrally mapping the compositional variation of white micas in hydrothermal systems and the application in mineral exploration. Geoscience and Remote Sensing Symposium. IGARSS'01. IEEE 2001 International Volume 7: Sydney, NSW, Australia, 3294–3296.
6. Yang, K., Huntington, J.F., Gemmell, J.B., Scott, K.M., 2011. Variations in composition and abundance of White mica in the hydrothermal alteration system at Hellyer, Tasmania, as revealed by infrared reflectance spectroscopy. Journal of Geochemical Exploration, 108, 143-156.