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Using diffuse reflectance spectroscopy (DRS) for qualitative examination of iron minerals formed in a hydromorphic soil

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The method of diffuse reflectance spectroscopy (DRS) allows a large number of measurements in a rapid, non-destructive mode and does not require complex sample preparation. Based on the recorded wavelength-reflectance spectra, the simultaneous investigation of various soil parameters such as colour, mineral composition, organic matter and moisture content is possible. Several publications have presented results of the qualitative and quantitative analysis of iron-oxides containing trivalent iron (primarily hematite, goethite) by DRS. These iron minerals are usually formed in soils and sediments under surface conditions. Nevertheless in the case of hydromorhic soils water saturation can result iron mineral formation in the absence of oxygen. However, the related soil forming process leads to the appearance of ferrous iron-hydroxides (green rust) in the soil profile, in the literature no reference was found discussing the investigation of samples from reduced soil conditions by DRS method. Our aim was to reveal if DRS is suitable to perform qualitative characterization of both ferrous and ferric iron-oxide and hydroxide minerals of waterlogged soils.
In the present study samples from a sandy meadow soil (calcic, gleyic Phaeozem ferric, arenic) profile were examined in the laboratory using an UV-Vis-NIR spectrophotometer with a diffuse reflectance attachement. Pedogenic iron minerals were characterized through spectral transformations and by comparison with spectrum database and literature data. The results were compared with data obtained from widely used routine methods. X-ray powder diffraction (XRD) for the determination of mineral composition, X-ray fluorescence spectroscopy (XRF) for total iron content and selective chemical dissolution (SCD) for the amorphous and crystalline iron content were presented.
Although iron oxide minerals are usually at low concentrations (approx. 0,1%) or present in a poorly crystalline form, our results show that the presence of iron oxide minerals can be detected based on their characteristic absorption pattern appearing in the visible range (400-700 nm) of the diffuse reflectance spectra. Thus DRS may be a useful complement to the XRD measurements.
Based on our results the mineral transformation processes driven by the valence changes of iron can also be studied by DRS. Accordingly, this method can be suitable for the investigation of hydromorphic soils, where iron minerals are usually present in a poorly crystalline form and containing iron in different oxidation states.

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