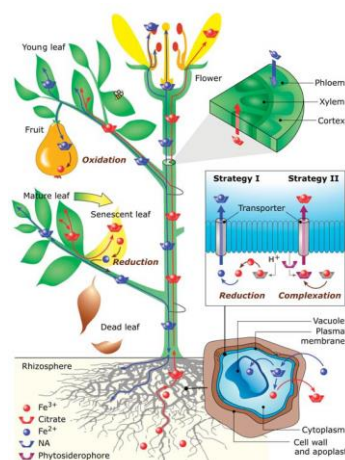


Geochemistry of Non-Traditional Stable Isotopes



Sampling of aerosols in North Kensington



A model of trace element fluxes within the plant

Recent developments in plasma source mass spectrometry have enabled us to determine isotope ratios of heavier elements (>40 amu) with the precision and accuracy needed to study isotope variations in the environment. Following a period of analytical method development and probing possible applications to problems in Earth and Environmental sciences, the community is now trying to understand better the physical, chemical and biological mechanisms leading to isotope fractionation and to develop predictive ab initio models.

One area of special interest to our group is the soil-plant environment and in particular metal pathways from rocks and soils into plants and microorganisms. The aim is to develop the novel stable isotope systems as technique to study nutrient uptake mechanisms *in situ*. We have recently proposed the first conceptual model accounting for observed isotope fractionation of copper and zinc in the plant soil environment based on field experiments. The next step is now to comprehensively test the individual processes proposed in this model using well-constrained laboratory experiments and to develop predictive models. To this end, we are investigating isotope fractionation during complexation with phytosiderophores and organic ligands. We are trying to identify the structural and reactive characteristics that determine isotopic fractionation and we carry out theoretical computations using DFT theory to model equilibrium fractionation mechanisms during complex formation. Future work is aiming to test the proposed fractionation model for other key elements in the plant – microorganisms – soil – rock system such as Mo, Fe, and Co.

A second area of research is developing metal isotopes as source tracers in atmospheric particulates. In particular we aim to test the newly developed hypothesis that non-combustion traffic sources are now the dominant contributor of metals in the urban atmosphere. Recently completed work on aerosols in selected cities around the world (London, Barcelona, Sao Paulo) suggests that this is possible for copper and zinc. If we can confirm this by proving that the underlying mechanisms indeed lead to the signatures observed, then our work would present a major breakthrough in tackling urban pollution. Laboratory experiments, which determine the extent and direction of isotopic fractionation during important industrial processes, include waste combustion, smelting, and galvanization. To this end, we have just recently successfully established a model of isotope fractionation during coal composition for zinc.

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Relevant literature:

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- Marković, T., Manzoor, S., Humphreys-Williams, E., Kirk, G.J.D., Vilar, R. and Weiss, D.J. (2017) Experimental Determination of Zinc Isotope Fractionation in Complexes with the Phytosiderophore 2'-Deoxymugeneic Acid (DMA) and Its Structural Analogues, and Implications for Plant Uptake Mechanisms. *Environmental Science and Technology* 51, 98-107.
- Mondillo, N., Wilkinson, J.J., Boni, M., Weiss, D.J. and Mathur, R. (2018) A global assessment of Zn isotope fractionation in secondary Zn minerals from sulfide and non-sulfide ore deposits and model for fractionation control. *Chem. Geol.* doi.org/10.1016/j.chemgeo.2018.09.033.