The role of hydroxyl group (OH) in forming minerals

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There was studied the changes of the pyrrhotites structure when hydroxyl group (OH) is introduced into it. After synthesis (1273 K) the samples were maintained at the room temperature ($\sim 25^{\circ}$ C) for 29 years in atmospheric conditions.

The X-ray and chemical analysis analysis of the samples, which were maintained, showed that there are compounds containing hydroxyl group (OH) in the crystal structure. The samples contained parabutlerite, goethite, szomolnokite, rozenite, rhomboclase, pyrite and pyrrhotite.

For example the influence of hydroxyl group (OH) on the content of the formed szomolnokite was considered on the basis of calculating the thermodynamic potentials using the Bose-Einstein statistics. The theoretical calculations were compared with X-ray phase analysis data (table 1).

S/Fe ratio	Percentage hydroxyl group (OH)	Szomolnokite percentage	
		X-ray	As calculated
1.710	4.25	21.21	16.779
1.684	2.72	12.92	18.533
1.670	4.42	23.70	19.553
1.660	2.38	11.65	20.315
1.580	5.11	25.61	27.586
1.571	5.27	17.36	28.552
1.497	7.99	41.55	41.127
1.382	4.25	26.60	21.780
1.380	9.35	21.04	21.540
1.250	0.85	5.07	10.499
1.158	2.03	6.19	6.314
1.157	1.70	3.29	6.279
1.052	0.34	2.07	3.514

Table 1. The szomolnokite percentage in the samples

As it is shown in the table, tendency to decreasing both with increasing of szomolnokite content with decreasing S/Fe ratio is observed both X-ray data and the theoretical calculation results.

Seasonal magnesium isotope variations in soil solutions reflecting physico-chemical processes controlling soil weathering fluxes

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Chemical weathering supplies base cations controlling the long-term availability of nutrients. Base cations, including magnesium, lost by plant uptake or leaching, are replaced by mineral weathering and partly retained on the soil exchange complex. Despite Mg isotopes being used as a weathering proxy, the fractionation mechanisms in the critical zone are still unclear. Here we report the first look into the seasonal variability of Mg isotope compositions in soil solutions derived from a well-defined protolith, Icelandic basalt, which was exposed to seasonal freeze-thaw cycles. Less weathered freely drained Brown and Glevic Andosol (BA-GA) are compared with more weathered poorly drained Histosol and Histic Andosol (H-HA). The difference in clay content (35 and 48%) and proportions of exchangeable Mg (2 and 7%) in BA-GA and H-HA, respectively, allow for a direct assessment of the processes controlling Mg isotope ratios (δ^{26} Mg relative to DSM-3). Vegetation (-0.30 to -0.18‰) is heavier than parental basalt (-0.31‰) and bulk soils (-0.79 to -0.25‰). Soil solutions (-1.16 to -0.53‰) are relatively lighter than the basalt. Magnesium retention on the soil exchange complex is larger in neutral than in acid soils and discriminates against light Mg isotopes (-0.88 to -0.51‰) contributing towards isotopically lighter soil solutions in BA-GA. Seasonal variations (from June to September) of Mg isotope ratios in soil solutions from organic-rich H-HA are likely to reflect the release of heavier Mg isotopes from the decomposition of plant material during thaw. Our results show that Mg isotopes have a great potential as a proxy for seasonal soil processes, especially in sub-arctic soils where environmental changes would potentially affect vegetation decomposition, CO₂ release, and associated nutrient delivery to the hydrosphere.

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