

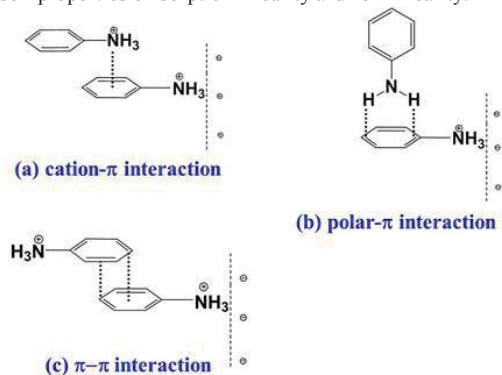
## Sorption of cationic amines to soils and soil minerals: Role of intermolecular interactions.

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### Introduction and Project Goals

Numerous chemicals containing cationic amine functional groups, such as antibiotics, herbicides, and antidepressant drugs, have been detected in surface and ground waters, and some of these pose risks to humans and ecosystems. Understanding and predicting the extent of sorption under a wide range of environmental conditions is key to anticipating potential contamination of groundwater by these chemicals. Cation exchange, the primary mechanism for cationic amine sorption has been well studied. However, there is a lack of knowledge about potential secondary mechanisms of sorption that may result in non-linear sorption isotherms and about the soil characteristics that may facilitate secondary, intermolecular interactions between amines sorbed to the surface and adjacent amines in solution. By examining the sorption of a series of model compounds that represent important sub-structures of antibiotics and pesticides, this study addresses three significant gaps in current understanding of cationic amine fate: (i) the influence of compound structural criteria on amine cation sorption, (ii) secondary interactions mechanisms that contribute to non-linearity in sorption phenomena, and (iii) effect of soil properties on sorption linearity and non-linearity.



**Figure 1:** Hypothesized intermolecular interactions contributing to sorption isotherm non-linearities.

### Results and Conclusions

On evaluating the sorption of several substituted anilines, benzylamines and cyclohexane methyl amine to Ca- and Na-montmorillonite, we established that the primary sorption mechanism, cation exchange, is influenced by the charge density on the amine moiety and compound hydrophobicity. In addition, we found that the presence of a  $\pi$  system, orientation of the molecule on the surface, and electron density at the center of the aromatic ring influenced the extent of intermolecular interaction between a sorbed amine and an adjacent amine. Furthermore, on evaluating cation amine sorption to a wide range of soils, we established that soils with higher density and closer proximity of negatively charged sites (i.e., soils with high cation exchange capacities) may facilitate secondary intermolecular  $\pi$  interactions.

## Evolution of the Strange Lake pluton: Insights from melt and fluid inclusions

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The Mid-Proterozoic Strange Lake pluton (Québec-Labrador, Canada) hosts economic rare earth element (REE) and high field strength element (HFSE) mineralization. The richest zones are confined to the most altered areas within subsolvus granite and associated pegmatites. The main HFSE mineral, the zirconosilicate, gittinsite, is commonly accompanied by armstrongite, kainosite-(Y), bastnäsite, gagarinite-(Y), monazite, pyrochlore and gadolinite.

Previous data on fluid inclusions from quartz pseudomorphs after elpidite and narsarsukite, quartz veins and pegmatitic quartz [1] revealed the importance of late Ca-metasomatism for the REE/HFSE mineralization of the Strange Lake pluton. Two fluids were found to contribute to the mineralization, a high salinity magmatic aqueous liquid containing a reduced carbonic component [2], and a Ca-rich meteoric fluid. Fluid mixing caused oversaturation of the fluid with fluorite and its precipitation, which triggered precipitation of Zr, Y and REE minerals as a result of decreased ligand concentration.

This study reports the results of observations of fluid and melt inclusions characterising progressive stages of the melt-to-fluid evolution. Quartz phenocrysts contain melt inclusions trapped during the very early stage of formation of the Strange Lake granites and pegmatites. A later population of magmatic quartz hosts melt inclusions representing more evolved magmas. Early fluorite included in late magmatic quartz and late arfvedsonite contains two types of inclusions, devitrified melt inclusions and NaCl- and possibly FeCl<sub>2</sub>-rich fluid inclusions. This association presents evidence of the timing of exsolution of fluid from the magma. The next stage of melt-to-fluid evolution is preserved in quartz from miarolitic cavities, which contains abundant aqueous inclusions of variable salinity. The final stage of hydrothermal activity, which is associated with REE/HFSE mineralization, involved Ca-rich aqueous fluids, which were trapped as primary fluid inclusions in late hydrothermal fluorite and secondary inclusions in pegmatitic quartz.

The study of melt and fluid inclusions is permitting reconstruction of the melt-to-fluid evolution of the Strange Lake pluton from the very earliest magmatic stage to the latest stage of mineralization, thereby providing a deeper understanding of the REE/HFSE mineralizing processes at Strange Lake.

[1] Salvi&Williams-Jones (1990) *Geochim. Cosmochim. Acta* **54**, 2403-2418.

[2] Salvi&Williams-Jones (2006) *Lithos* **91**, 19-34.