

The mobility of organic molecules in clays

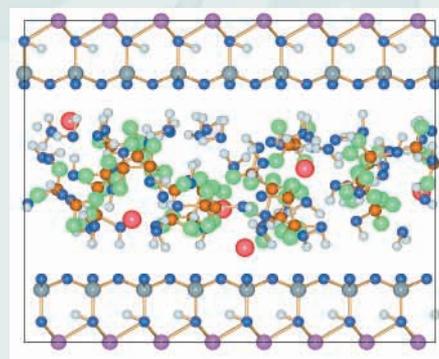
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Understanding and predicting the diffusion of organic molecules in soils and rocks is extremely important in environmental and earth sciences, and is also a key for locating and extracting oil and natural gas. Neutron scattering is a very powerful tool in this context, because it enables us to 'see' individual types of molecule even in very complex systems. To do this, we exploit the different scattering properties of isotopes of the same element, in a technique known as isotopic labelling. For organic molecules and water it is particularly

useful that the isotopes hydrogen (H) and deuterium (D) have very different neutron scattering properties. In our experiments we have labelled the molecules of interest (typically the organics) with H, and everything else with D. Inelastic neutron scattering on IRIS was then used to follow the motion of the H atoms - and therefore the organic molecules. What we find from this is that glycol and phenol are surprisingly mobile in the confined geometries they encounter in clays, when compared with bulk liquids.

Further information:

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NT Skipper et al., *Chemical Geology* (accepted) 2005.



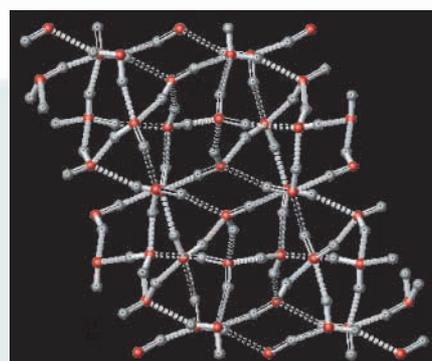
Glycol and water absorbed in the pore of a clay mineral at 325K. We used isotopic labelling to follow the motion of the green-coloured hydrogen atoms on glycol.

More new phases of ice!

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In the twelve known crystalline phases of ice, individual water molecules are tetrahedrally bonded to their neighbours via hydrogen bonding, so that each molecule can adopt six different orientations. In 1933, Linus Pauling showed that the connectivity of the lattice reduces but not altogether suppresses these degrees of freedom, resulting in residual disorder and hence non-zero entropy at zero temperature. Complete ordering is extremely difficult to achieve for most phases of ice, due to a dramatic slowing down of the

reorientation kinetics as temperature falls and thus hydrogen-disorder is frozen-in. We have discovered a new method to induce hydrogen ordering through doping, resulting in the formation of two novel ice phases, provisionally named ice XIII and XIV, which are ordered variants of ice V and XII, respectively. Proton (and deuterium) ordering that was suggested by thermodynamic and spectroscopic methods has been directly confirmed by neutron powder diffraction data collected on GEM. The ice XIII and XIV crystal structures have been solved based on these data, the former being the most complex known arrangement for crystalline water.



a-c plane projection of the crystal structure of fully-ordered ice V (provisionally named ice XIII). The monoclinic structure contains 28 water molecules per unit cell, and is the most complex known arrangement of crystalline water.

Further information:

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JL Finney, *Interdisciplinary Science Reviews* 29 (2004) 339.