

## Origin of the nodules in the 18.6 ka Sarno plinian eruption of Mt. Somma-Vesuvius (Italy) and their significance

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Nodules (coarse-grain 'plutonic' rocks) were collected from the phreato-magmatic phase of the Sarno eruption in C. Traianello quarry, located on the NE slope of Mt. Somma. Based on the mineral composition the rocks can be classified as monzonite-monzogabbro. They consist of An-rich plagioclase, K-feldspar, clinopyroxene (ferro-diopside), mica (phlogopite-biotite) ± olivine and amphibole. Unlike most of the nodules from the other eruptions, these samples do not have typical cumulative texture, but rather display a porphyrogranular texture. The phenocrysts are large (up to few mm) with variable compositional zoning. The phenocrysts are often partially to completely enclosed by later poikilitic feldspars. Sometimes irregular intergrowths of alkali feldspar and plagioclase and smaller unidentified crystals can be observed. These features are interpreted as crystallized melt pockets. Based on their textures, the nodules may represent the *in situ* crystallizing melt on the walls of the magma chamber. The lack of the interstitial glass, which is common in nodules from similar environments, can be explained by the time difference between the plinian and the phreatomagmatic phase. The time difference might have provided sufficient time for the interstitial melt in Sarno samples to crystallize.

Minerals, especially clinopyroxenes, are abundant in crystallized silicate melt inclusions. The inclusions consist of mica, oxide minerals, clinopyroxene and possibly apatite, feldspar, interstitial glass, bubble. Unlike nodules from other eruptions, all fluid inclusions in Sarno samples are single phase and secondary in origin, and not associated with melt inclusions. The different textures and inclusion populations may indicate different pre-eruptive conditions and processes, compared to other eruptions. Melt inclusions in clinopyroxenes have been analyzed by LA-ICP-MS. The major and trace element compositions of MI are similar to the products erupted during the plinian phase, indicating that they may be co-genetic. Melt inclusions have been rehomogenized for further analyzes to determine the volatile content, in order to estimate a minimum crystallization depth.

## Monte Carlo study of aggregation of alkyltrimethylammonium ions at the montmorillonite-water interface

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Unlike naturally occurring bentonites, organically modified ones exhibit adsorption capabilities not only for cationic but also for anionic contaminants. This property renders them valuable for various environmental and industrial processes like sewage treatment, groundwater remediation, production of nanocomposites, and waste disposal. An additional essential advantage regarding the application of organoclays to the remediation of contaminated groundwater is their effective adsorption of non-polar organic contaminants such as the highly persistent, toxic and carcinogenic polycyclic aromatic hydrocarbons.

The precise molecular structures of organically modified clays as well as the mechanisms determining their observed adsorption properties are still not well understood. To establish a relation between experimental observations and underlying molecular structures, we performed classical molecular simulations of the external montmorillonite surface modified by alkyltrimethylammonium ( $C_nTMA^+$ , with  $n$  being the number of methyl (ene) groups in the alkyl chain).

The adsorption of alkyltrimethylammonium ions at the montmorillonite-water interface and the formation of interfacial  $C_nTMA^+$  aggregates at higher concentrations of adsorbed  $C_nTMA^+$  were studied. The simulations were performed in NVT-ensemble at a temperature of 298 K applying the Metropolis and the configurational-bias Monte Carlo algorithms for increasing surface concentrations of  $C_8TMA^+$ ,  $C_{12}TMA^+$ , and  $C_{16}TMA^+$  ions. The discussion will comprise the arrangement of adsorbed organic and inorganic ions, structure and type of adsorption complexes, conformation of alkyl chains, and the water structure at the organically modified montmorillonite-water interface taking into account findings of previous experimental and simulation studies.