Structure and dynamics of water surface in the helium and argon atmosphere: Computer simulation

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Molecular dynamics computer simulation of water films about 40 Å thick was performed. Virtual temperature was about 300 K. Simulated systems contained several thousands of water molecules and up to two hundreds of helium or argon atoms. Both surfaces of the film are very rough. Diffusion coefficient of the surface molecules is noticeably greater than those of the molecules in central region of the film. Diffusion coefficients in the films under the pressure of noble gases are somewhat lower than in the films which are in the equilibrium with water vapour in the absence of any other component. Diffusion of the surface molecules is almost isotropic. Surface molecules form fewer hydrogen bonds than molecules in the bulk water and in centre of the film. Distribution coefficients of the gas atoms between the two phases are in qualitative agreement with experimental data on the solubility of these gases at corresponding temperature and pressure. Surrounding of argon atoms by water molecules does not resemble structure of the clathrate hydrates.

Isotopic markers in wines from Douro region, Portugal

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Food safety is one of Europe's priorities and is becoming a Worldwide demand, due to the mobility of people and provisions. Food supplies traceability must be insured from farmers to consumers. Discrimination of wines from particular regions through trace elements is based on a presumption that its content results essentially from rock to soil and from this to grape. Several works have been developed on isotopic markers as tools towards the geographical authenticity of wines. In order to better understand chemical elements translocation along rock-soil-vine-wine system Sr and 87Sr/86Sr ratio behaviours were studied in vine. Their use as a possible fingerprint of the Douro Controlled Origin of Denomination was evaluated. The study was based on the characterization of two distinct geological regions, Carrazeda de Ansiães (granite) and Alijó/Sabrosa (schist), situated in the Douro Region. All rock, soil, vine organs and red wines were collected in these zones.

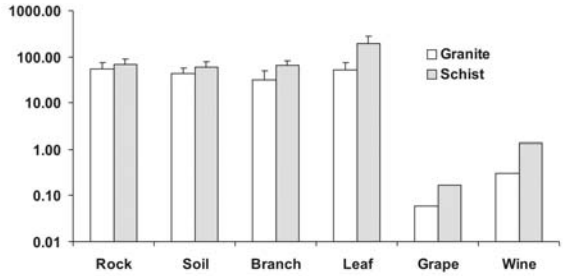

Figure 1: Average Sr content and standard derivation by sample.

$^{87}Sr/^{86}Sr$	Rock	Soil	Grape (must)	Wine
Granite	0.770011	0.779225	0.71799	0.719199
Schist	0.739819	0.740815	0.716083	0.718108

Table 1: Rocks, soils, musts and wines $^{87}Sr/^{86}Sr$ ratio.

The values obtained in this study and in others, including multielement analysis could be useful in wine discrimination according to their geographical provenience and to detect/prevent frauds. The Sr value could be used as fingerprints in the origins of wines, but the wine isotopic ratio is probably controlled by other factors, such as rain water, which need to be studied.