

Evolution of planet-satellite system due to accumulation of dispersed material from protoplanet cloud

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Recently a hypothesis of the planet-satellite systems formation based on the concept of the rotational collapse of a gas-dust cloud with further growth of the planet embryos by accumulation of the dispersed material was suggested [1-3]. This hypothesis satisfies the geochemical constraints on the Earth and Moon composition, which can not be explained by the Giant Impact hypothesis.

In the presented lecture we investigate the third stage of the planet-satellite system formation, according to the mentioned hypothesis. A combined computational-analytical model of the system evolution is developed. First, the ratio of particles, captured by each body in a planet-satellite system is obtained from the computer simulation. This ratio is obtained as a function of the planet-satellite mass ratio. Then this function is used in the analytical model of the growth of the bodies due to the dispersed material accumulation.

The analysis of the presented model shows, that the greater body (the planet) grows much faster than the smaller one (the satellite). Both bodies are considered to be initially formed in the process of the rotational collapse of the gas-dust cloud. Therefore the high-temperature embryos of the planet and its satellite were equally depleted in iron and volatile elements. Later on, both the planet and its satellite acquired the colder material from the residual part of the cloud. However, the satellite accumulated little, maintaining the iron deficiency, whereas, the planet embryo collected the major fraction of the surrounding material, whereby the composition of the planet became closer to the composition of the cloud as a whole. These results are in a good correspondence with the current composition of the Earth-Moon system, where the Moon has considerably less volatile elements and iron than the Earth.

[1] Galimov *et al.* (2005) *Geochemistry International* **11**, 1137-1149. [2] Galimov *et al.* (2005) *J. Earth Syst. Sci.* **114**, 1-8. [3] Vasilyev *et al.* (2005) *Proc. of APM'2004*, 425-429.

Quantum mechanical calculation of hydrogen isotope exchange thermodynamics and kinetics on organic compounds

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This study has used quantum mechanical methods to calculate the equilibrium isotopic fractionation factors, activation energies and rate constants for H-D exchange on various sites in alkanes. Both isolated alkane molecules and alkane + water exchange have been modeled. Results will be presented for the test system 2-methyl butane to predict the fractionation thermodynamics and kinetics at primary, secondary and tertiary C-H sites. Results on the biomarkers pristane and phytane will also be presented.

The advent of molecular-specific deuterium analyses has provided a powerful and precise means for evaluating organic hydrogen isotopic signatures and the fractionations associated with biological, environmental and geochemical processes. This advance has generated a surge of interest to establish molecular-specific δD values as indicators of paleoclimate. However, studies based on organic-rich sedimentary rocks have demonstrated that the δD signature of branched compounds shifts to more enriched values with increased thermal exposure. The equilibrium fractionation factors and kinetics of H/D exchange are not known for these reactions, so estimating these values will provide constraints on possible modifications of original δD values.

Test calculations for H-abstraction on methane suggest that the thermodynamics of these reactions can be computed to within an accuracy of a few kJ/mol. The activation energy barriers to these reactions have not been measured, so comparison to experimental values for alkanes is not possible at this time, but the thermodynamic accuracy indicates that the energy barriers should be reasonably accurate to estimate H-D exchange rate constants as a function of temperature. Equilibrium isotopic fractionations are calculated more accurately based on the theoretical frequency shifts of C-H bonds with D-substitution.

The results from this computational study can be employed to help interpret molecular H-isotopic data from preserved organic matter. Applications to paleoenvironmental studies will be discussed.