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Conditions of formation of cometary ices

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Was obtained of the nebula gas phase composition which agree best with the experimentally measured chemical compositionn of Hartley 2 comet.

Key words: Solar system, evolution, cometary ices

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The obtained data for the comet Hartley 2 on isotopic composition of water ice [*Hartogh et al., 2012*] are evidence to it was evaporated under nebula conditions. At *T* ~ 100 K a hydrogen isotopic composition of ice was changed according to the chemical reaction

$$HD_{gas} + H_2O_{gas} \leftrightarrow HDO_{gas} + H_{2\ gas}\ ,$$

which passes more efficiently in the gas phase than in the heterogenious system “Ice–$H_{2\ gas}$”.. During next cooling, H_2O_{gas} was condensed into solid clathrate hydrates of various gases. If our assumptions are correct, we can reconstruct a composition of the part of the nebula, where the ice of the comet was formed. Such reconstruction is based on experimental data on composition of Hartley 2 comet [*Meech et al., 2011, Meech et al., 2011; Weaver, 2001; Dello Russo, 2011*] and methods of equilibrium thermodynamics. Variations of *PT* conditions in the nebula at radial distances from Sun ~ 4–10 A.U. according to the model [*Dorofeeva, Makalkin, 2004]* are shown in Fig.1. *PT* conditions of gas hydrates formation from a gas of solar composition are shown in Fig. 2.

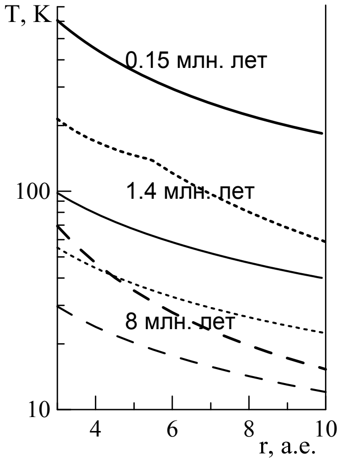

Fig. 1. Variations of *PT* conditions in the nebula at radial distances from Sun ~ 4-10 A.U. Bold lines answer $P = 10^{-6}$ bar, more thin - $P = 10^{-9}$ bar

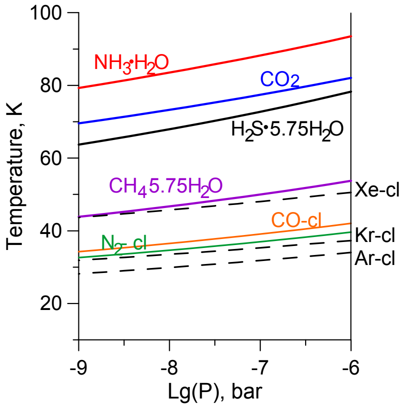

Fig. 2. *PT* conditions of gas hydrates formation from a gas of solar composition according to [*Lunine, Stevenson,* 1985]

The bulk chemical element composition of the nebula was taken as solar abundances according to [*Lodders,* 2010], and a component composition of the gas phase was varied taking into account it’s uncertainty. Necessary temperature dependencies of the equilibrium constants of corresponding heterogeneous reactions were derived by summarizing experimental data on conditions of formation of solid gas hydrates and gas ices obtained [*Lunine, Stevenson,* 1985; *Fray et al.*, 2010]. For calculations we used CHEMEQ code [*Mironenko et al.*, 2008], which applies minimization of Gibbs free energy of the system under liner mass-balance restrictions. Some results of calculations are presented in Fig.3.

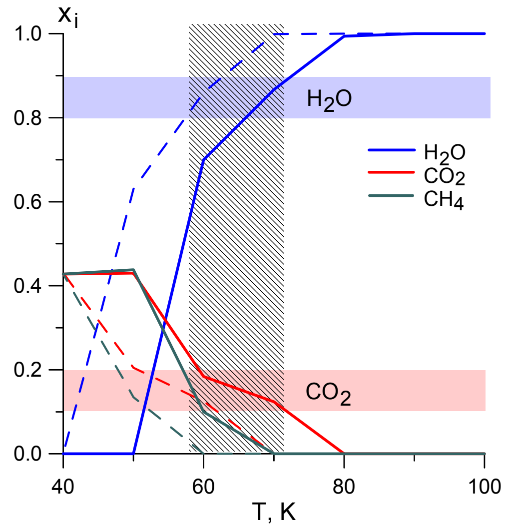

Fig. 3. Variations of the condensed phase composition at the gas phase cooling. Solid lines – correspond the pressure of $P = 10^{-6}$ bar, dashed lines correspond the pressure of $P = 10^{-9}$ bar. Regiong, of H_2O (blue) and CO_2 (pink) correspond the mole phase relations in the comet Hartley 2. The temperature region of stability field of CO_2 and CH_4 clathrate hydrates is shown by dashed lines for pressure interval of $P = 10^{-6}$–10^{-9} bar

As a result of calculations, we obtained C-bearing species ratios of $CO_2 : CO : CH_4 = 1 : 8 : 1$ and N-bering species ratio of $NH_3 : N_2 = 1 : 50$, which agree best with the experimentally measured chemical composition of Hartley 2 comet.

Conclusions

There were regions in Solar nebula, where initially amorphic water ice was evaporated, and as a result of isotopic exchange with $H_{2\ \mathrm{gas}}$, it's D/H was significantly decreased.

During next nebula cooling, H_2O_{gas} was condensed as crystal modifications with a possibility of formation of clathrates of various gases under *P*-*T* conditions of *r* = 4–10 A.U.

Stone-icy bodies (comets) with high contents of volatilities may be formed at near Jupiter orbits, which can be considered as a source of water and other volatilities, including nitrogen, for terrestrial planets.

Probably, the main mechanism of volatilities accumulation in comets, which were formed in Neptunian zone and in Kouiper Belt (*r* > 15–20 A.U.), was their sorption by water ice.

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