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"Latent" phase clusters-kvatarons – and water condensation

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The results of numerous experimental investigations of supersaturated solutions and vapor phases indicate their microheterogeneous structure. In particular, such results were obtained with using Raman spectroscopy. Some recent data have appeared which indicate that even in saturated media a considerable portion of substance is bound into clusters. However, these facts are in direct conflict with the classical theory of nucleation. In this connection, we proposed a new nucleation model for the formation and stable existence of nanodimensional cluster in saturated and supersaturated media. In this model the energy, required for the cluster formation with radius r, is determined by the expression:

$$\Delta G = \frac{4}{3}\pi r^2 \sigma_0 \left(1 - \frac{4\delta}{r}\right) - \frac{1}{3}\frac{(Ze)^2}{\pi\varepsilon\varepsilon_0 r},$$

were σ_0 is the specific surface energy, Ze is the charge, ε is the dielectric permittivity, ε_0 is the electric constant. The parameter δ represents the diameter of cluster-forming molecules (for water it is equal to the proton-proton distance in a water molecule, δ can be taken to be 0,3 nm). This formula differs from classical Gibbs formula for the energy of nucleus formation in that it allows for non-activation ($\Delta G \leq 0$) formation of clusters with radius $r \leq 4\ \delta$. These are the clusters that we called kvatarons. Because of the absence of energy barriers in kvatarons formation, they arise at the rate several orders more than that classical nucleation. In the context of our model, the analogue of the Kelvin equation relating supersaturation ln p/p_0 to the radius of kvatarons has the form:

$$\ln\frac{p}{p_0}=\frac{2\sigma_0 V_m}{RTr}\left(1-\frac{\delta}{r}\right)-\frac{V_m\left(Ze\right)^2}{16\pi^2\varepsilon\varepsilon_0 r^4 RT}$$

Therefore, even at the absence of supersaturation in vapor phase clusters (kvatarons) with $r\approx\delta$ are formed and can exist. At the highest possible (limiting) supersaturation kvataron radius $r=2\delta$. The finite size of spontaneously forming kvatarons is 4δ. Kvatarons typically have a quasispherical shape and icosahedral symmetry (fullerene-like structures). It should be mentioned that kvatarons are rather large particles. Thus if $r=\delta$, the number of molecules in a water kvataron is 8 (when they dense) and 16 (it they are empty and molecules locate only on the sphere surface). When $r=4\delta$, the number of molecules in kvataron is 256 and 512. However, kvatarons are not actual new-phase nuclei. They cannot be described in terms of known states of substance. Actually kvatarons represent a separate intermediate phase that arises at the nanolevel under nonequilibrium conditions. Kvatarons are clusters a new species of the atom-molecular organization of substance, a new state. This state referred to as a “latent” phase. The “latent” phase clusters-kvatarons transforms in to crystalline or liquid nuclei only at achieving certain critical sizes ($r=4\delta$).

The kvataron model allows for a novel interpretation of many percularities of atmospheric water existance and condensation, of clouds formation, of interaction between water-clusters and impurity particles, especially CO_2, etc. An interesting consequence of the model is that it predicts a possibility of formation of two phases of liquid water, which are distinguished by the sizes of regions of short range order and physical-chemical properties. The first phase (“amorphous”) is formed by condensation of kvatarons, 2δ in radius; the second “crystalline”, one by condensation of kvatarons $r=4\delta$ in radius. The region of short-range order in “amorphous” water is equal to 54 molecules, for “crystalline” water – 380. Calculations indicate that the common water is a 2:1 mixture of both phases. This ratio is a consequence of preservation of “molecular memory” about the formation mechanism.

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