HOMOGENOUS NUCLEATION RATES OF ICE IN SUPERCOOLED BINARY LIQUID MIXTURES OF WATER + NON-ELECTROLYTES: A COMBINED THEORETICAL AND EXPERIMENTAL STUDY

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A: Helmholtz free energy.
A_n: Surface area of an ice-embryo with size n.
b_0: Mole fraction of the non-bonded water molecules in 1 mole of hypothetical defect phase of liquid water.
b_1: Mole fraction of the 1 H-bonded water molecules in 1 mole of hypothetical defect phase of liquid water.
b_2: Mole fraction of the 2 H-bonded water molecules in 1 mole of hypothetical defect phase of liquid water.
b_3: Mole fraction of the 3 H-bonded water molecules in 1 mole of hypothetical defect phase of liquid water.
b_4: Mole fraction of the4 H-bonded water molecules in 1 mole of hypothetical defect phase of liquid water.
c_g: The concentration of the critical ice nucleus in a given volume.
c_{eff}: Effective concentration of the critical ice nucleus, which are able to grow further in a given volume.
Δg^*: Free energy of activation for the diffusion of water molecules (across the ice-water interface).
ΔG_n: Free energy of the formation of an ice-embryo with size n.
ΔG_{n^*}: Free energy of the formation of a critical ice-nucleus.
dr: The thickness of the surface layer on the outer shell of an ice-embryo.
D: Self diffusion constant of liquid water.
E_A: Activation energy of defect formation.
E_H: Apparent H-bond energy per mole of liquid water.
E_i: H-bond energy in 1 mol of i-bonded water molecules.
f: The net flux of water molecules to the surface of a critical ice nucleus.
f_v: Molecular vibrational partition function for water molecules.
f_t: Molecular translational partition function for water molecules.
f_r: Molecular rotational partition function for water molecules.
f_i: Molecular partition function for i-bonded water molecules.
g: Also called as Eadie's patch size .The total number of molecules included in a purely ice-like patch ignoring the molecules of hypothetical defect phase. It counts for the 4-bonded molecules in the bulk of an ice-like patch and the 2- and 3- bonded molecules on the surface of a patch.
G: Gibbs free energy.
g2: The number 2 H-bonded molecules on the surface of an ice-like patch before the interaction of surface molecules with the adhering non-bonded molecules of the interphase.
g3: The number 3 H-bonded molecules on the surface of an ice-like patch before the interaction of surface molecules with the adhering non-bonded molecules of the interphase.
g4: The number of 4 H-bonded molecules in an ice-like patch.
$g_{2\rightarrow3}$: Number of 2-bonded molecules becoming 3-bonded with the attachment of a non-bonded molecule from the interphase in between the patches.
$g_{2\rightarrow4}$: Number of 2-bonded molecules becoming 4- bonded with the attachment of a non-bonded molecule from the interphase in between the patches.
$g_{3\rightarrow4}$: Number of 3-bonded molecules becoming 4- bonded with the attachment of a non-bonded molecule from the interphase in between the patches.
g(y): Combinatorial factor in the partition function, which counts for all possible configurations for a given state of y having composed of ceratin mole fractions of different H-bonded water molecules.
G_2: The number 2 H-bonded molecules on the surface of an ice-like patch after the interaction of surface molecules with the adhering non-bonded molecules of the interphase.
G_3: The number 3 H-bonded molecules on the surface of an ice-like patch after the interaction of surface molecules with the adhering non-bonded molecules of the interphase.
G_4: The number 4 H-bonded molecules on the surface of an ice-like patch after the interaction of surface molecules with the adhering non-bonded molecules of the interphase.
h_0: Fractions of non-bonded water molecules in a 1 mole of liquid water.
h_1: Fractions of1-bonded water molecules in a 1 mole of liquid water.
h_2: Fractions of 2-bonded water molecules in a 1 mole of liquid water.
h_3: Fractions of 3-bonded water molecules in a 1 mole of liquid water.
h_4: Fractions of4-bonded water molecules in a 1 mole of liquid water.
I_z: Moment of inertia about the z axis.
j: Actual number of H-bonds a water molecule forms with its neighbors, which depends on its coordination environments. It varies between 0 and 4.

J: Temperature dependent nucleation rate expressed as number of germs formed per unit volume per unit time.

J_L: Nucleation rate calculated from the slope of a linear segment which occurs left to a knick (short-time region) in an ln N_u/N_0 vs $V_d \cdot t$ diagram.

J_R: Nucleation rate calculated from the slope of a linear segment which occurs right to a knick (long-time region) in an ln N_u/N_0 vs $V_d \cdot t$ diagram.

k: Boltzmann constant.

k: Rate constant.

n_d: The number of water molecules in a patch (or on the surface of agglomerates) which belong to the hypothetical phase of defects.

ν_d: Mole fraction of hypothetical defect phase in liquid water.

n_4: Number of 4-bonded molecules in an ice-embryo.

$n_{interface}$: Number of water molecules found in the interphase adherent on the surface of a patch.

n_s: Number of water molecules on a unit area on a patch surface.

n_T: Total number of molecules including the four-bonded molecules in the iner-shell, and defect molecules on the surface, in an ice-embryo.

N: Total number of water molecules in a system.

N_A: Avagadro's number.

$N_{Agg.-S}$: Number of 4-bonded agglomerates (or ice embryos) placed at the surface of a patch.

$N_{Agg.-T}$: Total number of four-bonded agglomerates present in a patch.

N_c: Number of water molecules in contact with the unit surface area of an ice embryo.

N_i: The number of i-bonded water molecules in 1 mole of liquid water.

m: Molecular mass of a water molecule.

μ_{liq}: Chemical potential, i.e. Molar Gibbs free energy of liquid water.

μ_{ice}: Chemical potential, i.e. Molar Gibbs free energy of ice.

μ_d: Chemical potential, i.e. Molar Gibbs free energy of the hypothetical defect phase.

$\Delta\mu_{ice-liq}$ (or $\Delta\mu$): $\mu_{ice} - \mu_{liq}$

σ: Symmetry number.

$\sigma_{i/w}$: Surface tension of the ice-water interface on a growing ice embryo.

P_{diff}: The probability that a molecule will diffuse out is lattice point.

p: H-bond formation probability in the hypothetical phase of lattice defects in liquid water.

p: Pressure.

P_{rel} (n): Probability of finding an ice embryo of size n in a patch

ρ_T(liq): Density of liquid water at a given temperature T.

ρ_T(ice): Density of ice at a given temperature T.

ρ_T(d): Density of hypothetical defect phase at a given temperature T.

$r_{inner-shell}$: Radius of the inner shell of a patch below its adherent interphase.

r_{patch}: Radius of a patch having a spherical geometry.

R_{agg}: The radius of the inner-shell of an ice-embryo.

r(T): Van der Waals radius of the water molecule in ice at a given temperature.

s: Total number of assigned vibrational frequencies for a water molecule, which depends on its H-bonding state.

S: Entropy.

S_T: Total patch size, i.e. Total number of 4-bonded molecules and the molecules with less than 4-Hydrogen bonds which constitutes a patch and its adherent interface.

t_M: Lifetime of the metastable state in liquid water.

t_R: The relaxation time of the metastable state in liquid water.

$<\tau>$: Average mean passage time for the water molecules to leave a surface layer of certain thickness.

T: Temperature

U: Internal energy.

χ_H: The electronegativity of the hydrogen atom.

X_i: Mole fraction of ice-like phase in liquid water.

χ_O: The electronegativity of the oxygen atom.

V_d: Packing volume of a water molecule that belong to the hypothetical defect phase.

V_f: Free volume of a water molecule in a translational motion.

$V_m(d)$: Molar volume of the hypothetical defect phase.
V_{ice}: Packing volume of a water in ice.
$V_m(ice)$: Molar volume of ice.
V_{patch}: Total volume of a patch assuming a spherical geometry.
V_{surf}: The volume of the surface layer of with a thickness dr for a spherical agglomerate.
W_{eff}: Total effective surface area available for the growth of four-bonded agglomerates (ice-embryos) on the surface of a patch.
Ω_{eff}: The effective surface area for the growth of an agglomerate, which lies near to the surface.
Ω_g: The surface area of the critical ice nucleus.
W_{patch}: Surface area of the inner shell of a patch just below its adherent interface.
z: Maximum number of H-bond that water can form with its nearest neighbors in liquid water (z =4).
Z: Canonical partition function of liquid water.
Z: The Zeldovitch factor
Z(avg): Canonical partition function of an ice embryo, with the most probable size.
Z(n): Canonical partition function of an ice embryo, which consists of n water molecules.