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

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List of Symbols

- 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 the 4 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_{Hf} :** 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.
- g_2 :** 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.
- g_3 :** 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.
- g_4 :** The number of 4 H-bonded molecules in an ice-like patch.
- $g_{2\rightarrow 3}$:** Number of 2-bonded molecules becoming 3-bonded with the attachment of a non-bonded molecule from the interphase in between the patches.
- $g_{2\rightarrow 4}$:** Number of 2-bonded molecules becoming 4- bonded with the attachment of a non-bonded molecule from the interphase in between the patches.
- $g_{3\rightarrow 4}$:** 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 certain 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 of 1-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 of 4-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.
v_d:	Mole fraction of hypothetical defect phase in liquid water.
n₄:	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 inner-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.
Δμ_{ice-liq} (or Δμ):	μ _{ice} - μ _{liq}
σ:	Symmetry number.
σ_{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.
<τ>:	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.

- $V_m(\mathbf{d})$:** Molar volume of the hypothetical defect phase.
- V_{ice} :** Packing volume of a water in ice.
- $V_m(\mathbf{ice})$:** 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
- $Z(\mathbf{avg})$:** Canonical partition function of an ice embryo, with the most probable size.
- $Z(\mathbf{n})$:** Canonical partition function of an ice embryo, which consists of n water molecules.