

APPENDICES

APPENDIX A – The Fortran Code for the Statistical Thermodynamical Calculations

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! *****
PROGRAM StWater
! *****
!
! This program:
!
! - Calculates the partition functions for 1-, 2-, 3-, 4- H-bonded
!   and non-bonded water species at given mole fractions and
!   temperature.
! - Finds the optimum values for the mole fractions of above given
!   species by maximizing the natural logarithm of the canonical
!   partition function of the whole system with respect to ice-like
!   patch-size "g", H-bond formation probability "p" and the mole
!   fraction of ice-like water molecules "Xi".
! - Calculates the the chemical potentials and molar volumes of the
!   ice, liquid water and hypothetical lattice defect phases.
! - Writes out the results of calculations in a separate ".txt" file.*
!
!           For the subroutine DAT.for refer to :
!           Numerical Implementation and Oceanographic Application
!           of the Gibbs Potential of Ice
!           by R.Feistel, W.Wagner, V.Tchijov, C.Guder
!           Ocean Science, 1 (2005), 29-38
!
! *****

IMPLICIT REAL *8 (A-I,L-Z)

DOUBLE precision, Parameter :: NA = 6.022D+23
DOUBLE precision, Parameter :: pi = 3.1415926535

DOUBLE precision :: PartFunc
DOUBLE precision :: T, Tc, pascal
! --> T: Temperature in Kelvin
! --> Tc: Temperature in Celcius
DOUBLE precision :: pf_0, pf_1, pf_2, pf_3, pf_4
DOUBLE precision :: deg, logZ
DOUBLE precision :: g, g2, g3, g4
! --> g is the patch size in terms of number of constituting
! --> ice-like water molecules.
DOUBLE precision :: xi, p
DOUBLE precision :: f, f0, f1, f2, f3, f4
DOUBLE precision :: g_2_3, g_2_4, g_3_4, n2, n3, n4
DOUBLE precision :: n_T, h1, h2, h3, h4, h0
DOUBLE precision :: patch_size, cnn, fr_ice, lnZ, xu, x1, x2, x3,x4

DOUBLE precision :: Vm, Vm_ice, Vm_blk, vblk, n_p, n_b
DOUBLE precision :: Mu_Ice, Mu_Liq, delta_Mu, Mu_BlK, radius

INTEGER :: i, j, k
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COMMON /INPUT/ T

! --> Initialization of necessary parameters:
CALL DAT
T = 237.15
Tc = T - 273.15
pascal = 101325.D0
lnZ = 0.00

! --> Calculate partition function terms at a given temperature T:
pf_0 = PartFunc(0)
pf_1 = PartFunc(1)
pf_2 = PartFunc(2)
pf_3 = PartFunc(3)
pf_4 = PartFunc(4)

! --> Maximize the canonical partition function
! --> with respect to mol fractions of different H-bonded species:
DO i = 1, 3000

g = 13.0 + 1.0 * i
g2 = 2.621 * g**(1.0/3.0)
g3 = 3.434 * g**(2.0/3.0) - 5.241 * g**(1.0/3.0)
g4 = g - g2 - g3

DO j = 1, 99

P = 0.01 * j
! --> p is the H-bond formation probability of the bulk molecules.
! --> Calculate the fraction of j bonded molecules in the bulk.
f0 = (1.0 - p)**4.0
f1 = 4.0 * p * (1.0 - p)**3.0
f2 = 6.0 * p**2.0 * (1.0 - p)**2.0
f3 = 4.0 * p**3.0 * (1.0 - p)
f4 = p**4.0

! --> Re-calculate the H-bonding states of molecules
! --> on the surface of the patches.
g_2_3 = 2.0 * p * g2 * (1.0 - p)
g_2_4 = g2 * p**2.0
g_3_4 = g3 * p

n2 = g2 - g_2_3 - g_2_4
n3 = g3 - g_3_4 + g_2_3
n4 = g4 + g_2_4 + g_3_4

DO k = 1, 99

xi = 0.01 * k
! --> xi is the mole fraction of molecules belonging to ice-like
! --> patches.

! --> Calculate the final mole fractions of each H-bonding species
h0 = (1.0 - xi) * f0
h1 = (1.0 - xi) * f1
h2 = (1.0 - xi) * f2 + xi * (n2/g)
h3 = (1.0 - xi) * f3 + xi * (n3/g)
h4 = (1.0 - xi) * f4 + xi * (n4/g)

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deg = NA*(log(NA) - 1.0) - NA*h1*(log(NA * h1) - 1.0)
deg = deg - NA*h2*(log(NA * h2) - 1.0) - NA*h3*(log(NA * h3) - 1.0)
deg = deg - NA*h4*(log(NA * h4) - 1.0) - NA*h0*(log(NA * h0) - 1.0)

logZ = deg + NA*h4*log(pf_4) + NA*h3*log(pf_3) + NA*h2*log(pf_2) +
      NA*h1*log(pf_1) + NA*h0*log(pf_0)

IF (lnZ < logZ) THEN
  lnZ = logZ
  patch_size = g
  fr_ice = xi
  cnn = p
  xu = h0
  x1 = h1
  x2 = h2
  x3 = h3
  x4 = h4
END IF

END DO
END DO
END DO

!*****
! --> Calculate the molar volume of ice:
Vm_ice = ice_specific_volume(T, pascal) ! --> in m**3/kg
Vm_ice = Vm_ice * 18.015/1000.0 ! --> in m**3/mole

! --> Calculate the molar volume Vm of supercooled liquid water
! --> in cubic meters at a given temperature T:
Vm = 0.99986 + 6.69D-5*Tc - 8.486D-6*Tc**2.0 + 1.518D-7*Tc**3.0
Vm = Vm - 6.9484D-9*Tc**4.0 - 3.6449D-10*Tc**5.0 - 7.497D-12*Tc**6.0 ! in g/ml
Vm = 18.015D-6 / Vm ! in m**3

! --> Calculate the molar volume of the bulk
! --> molecules in cubic meters:
Vm_blk = (Vm - Vm_ice * fr_ice) / (1.0 - fr_ice)

!*****
! --> Calculate the chemical potential of ice:
Mu_Ice = ice_g (T, pascal) * 18.015D-6 ! --> in kJ/mol

! --> Calculate the chemical potential of water:
delta_Mu = (210368.0 + 131.438*T - 3.32373D6/T - 41729.1*log(T)) * 1.0D-3 ! -
-> mIce - muL, kJ/mol

! --> Calculate the chemical potential of water (ST calculations):
Mu_Liq = -1.38D-23 * T * lnZ * 1.0D-3

! --> Calculate the chemical potential of bulk (ST calculations):
h0 = (1.0 - cnn)**4.0
h1 = 4.0 * cnn * (1.0 - cnn)**3.0
h2 = 6.0 * cnn**2.0 * (1.0 - cnn)**2.0
h3 = 4.0 * cnn**3.0 * (1.0 - cnn)
h4 = cnn**4.0

deg = NA*(log(NA) - 1.0) - NA*h1*(log(NA * h1) - 1.0) - NA*h2*(log(NA * h2) - 1.0)
deg = deg - NA*h3*(log(NA * h3) - 1.0) - NA*h4*(log(NA * h4) - 1.0) - NA*h0*(log(NA * h0) - 1.0)

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logZ = deg + NA*h4*log(pf_4) + NA*h3*log(pf_3) + NA*h2*log(pf_2) +
NA*h1*log(pf_1) + NA*h0*log(pf_0)

Mu_Blck = -1.38D-23 * T * logZ * 1.0D-3

!*****
! Calculate the hard-sphere radius of ice (half the O-O distance):
radius = Vm_ice * 1.0D7 / (6.02 * 4.0 * pi)
radius = radius**0.3333

! --> Calculate the packing volume of a bulk molecule in A**3:
vblk = Vm_blk*1.0D7/6.02

!*****

! --> number of bulk molecules per ice-like patch:
n_b = (1.0 - fr_ice) * patch_size / fr_ice

!*****
! --> Write out the results of the computations to a file:

OPEN (10, file = "results.txt", status = 'unknown')
WRITE (10, ' (A) ') 'Results of the statistical thermodynamical calculations'
WRITE (10, ' (A) ') 'on the structure of water:'
WRITE (10, ' (A) ') '-----'
WRITE (10, ' (A) ') ' '
WRITE (10, ' (A, F6.2) ') 'Temperature = ', Tc
WRITE (10, ' (A, E10.4) ') 'Vm-ice = ', Vm_ice
WRITE (10, ' (A, E10.4) ') 'Vm-liq. = ', Vm
WRITE (10, ' (A, E10.4) ') 'Vm-blk. = ', Vm_blk
WRITE (10, ' (A, F8.4) ') 'Hard-sphere radius of an ice molecule = ', radius
WRITE (10, ' (A, F8.4) ') 'Packing volume of a bulk molecule = ', vblk
WRITE (10, ' (A) ') 'Mole fraction of molecules belonging'
WRITE (10, ' (A, F5.3) ') 'to ice-like patches = ', fr_ice
WRITE (10, ' (A, F7.1) ') 'Avg. patch size= ', patch_size
WRITE (10, ' (A, F8.2) ') 'Number of bulk molecules per ice-like patch = ', n_b
WRITE (10, ' (A, F4.2) ') 'H-bond formation prob. (bulk) = ', cnn
WRITE (10, ' (A) ') ' '

WRITE (10, ' (A) ') 'Mole fractions of different H-bonded species:'
WRITE (10, ' (A) ') '-----'
WRITE (10, ' (A, F5.3) ') 'x1 = ', x1
WRITE (10, ' (A, F5.3) ') 'x2 = ', x2
WRITE (10, ' (A, F5.3) ') 'x3 = ', x3
WRITE (10, ' (A, F5.3) ') 'x4 = ', x4
WRITE (10, ' (A, F5.3) ') 'xu = ', xu
WRITE (10, ' (A) ') '-----'
WRITE (10, ' (A, E11.5) ') 'ln Z = ', lnZ
WRITE (10, ' (A, F8.5) ') 'Mu(Ice) (kJ/mol) = ', Mu_Ice
WRITE (10, ' (A, F8.5) ') 'Mu(Ice), (ST Calculations), (kJ/mol) = ', delta_Mu +
Mu_Liq
WRITE (10, ' (A, F8.5) ') 'Mu(Ice) - Mu(liq) = ', delta_Mu
WRITE (10, ' (A, F10.5) ') 'Mu Liq. (ST-calculations), (kJ/mol) = ', mu_Liq
WRITE (10, ' (A, F10.5) ') 'Mu Bulk (kJ/mol) = ', mu_Blck

CLOSE (10)

END PROGRAM

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!*****
DOUBLE PRECISION FUNCTION PartFunc(i)

DOUBLE precision, Parameter :: h = 6.626D-34           !J.s
DOUBLE precision, Parameter :: k_bz = 1.38068D-23      !J.K-1
DOUBLE precision, Parameter :: R = 8.314472           !J.K-1.mol-1
DOUBLE precision, Parameter :: pi = 3.1415926535
DOUBLE precision, Parameter :: m_Wat = 2.99236134174693D-26 !kg

INTEGER                :: j

DOUBLE Precision      :: E_H(0:4), nu(0:4,1:6) !J.mol-1, s-1

DATA E_H /11.0352D+3, 8.28432D+3, 5.5229D+03, 2.7614D+03, 0.0/

DATA nu(0,1:6) /4.35D+12, 5.25D+12, 0.0, 0.0, 0.0, 0.0/
DATA nu(1,1:6) /1.7988D+12, 4.3470D+12, 4.7967D+12, 4.7967D+12, 5.2464D+12/
DATA nu(2,1:6) /4.3470D+12, 4.7967D+12, 4.7967D+12, 4.7967D+12, 5.2464D+12, 1.3491D+13/
DATA nu(3,1:6) /6.2956D+12, 6.2956D+12, 6.2956D+12, 1.4990D+13, 1.9487D+13, 2.3983D+13/
DATA nu(4,1:6) /6.2956D+12, 6.2956D+12, 6.2956D+12, 1.4990D+13, 1.9487D+13, 2.3983D+13/

DOUBLE precision      :: T, f, I_z, V_f

COMMON /INPUT/ T

I_z = 1.92D-47      !kg.m2
V_f = 4.40D-31     !m3
f = 1.0

IF (i == 0) Then
  DO j =1,2

    f = f/(1.0 - exp(-h * nu(i,j) / (k_bz * T)))

  END DO

  f = f *pi * (2.0*pi*I_z*k_bz*T/h**2.0)**0.5
  f = f * (2.0*pi*m_Wat*k_bz*T/h**2.0)**1.5 * V_f
ELSE

  DO j=1,6

    f = f/(1.0 - exp(-h * nu(i,j)/(k_bz * T)))

  END DO

END IF

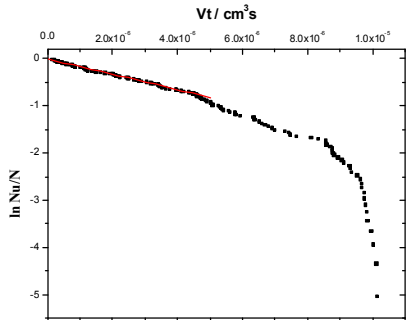
PartFunc = f * exp(-E_H(i)/(R*T))

RETURN
END FUNCTION PartFunc
!*****

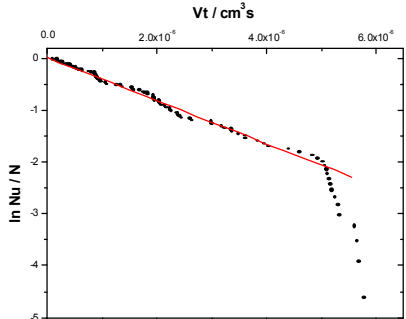
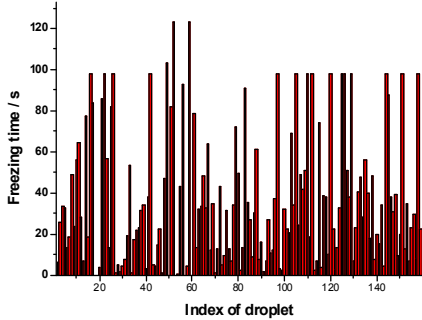
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Appendix B – In N vs Vt Diagrams for tri-distilled Water

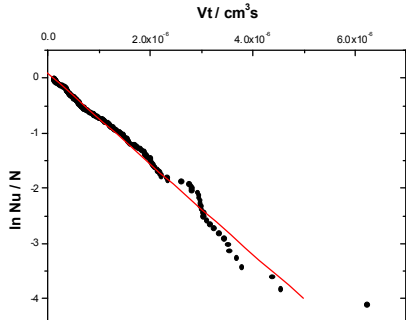
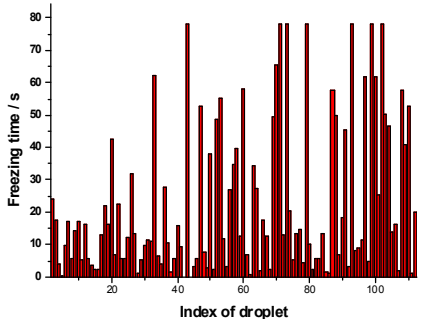
Experiments performed in trap A



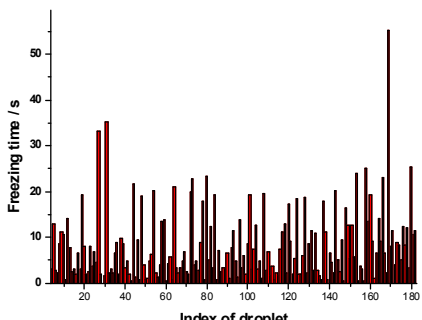
T-meas.: -35.66 °C, J = 1.62 E5

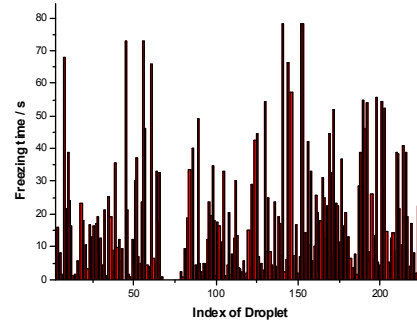
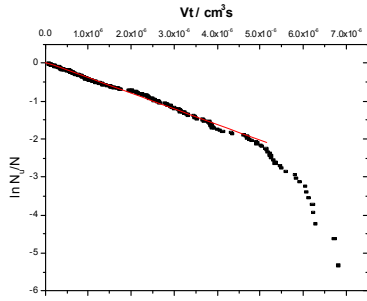


T-meas.: -35.67 °C, J = 4.16 E5

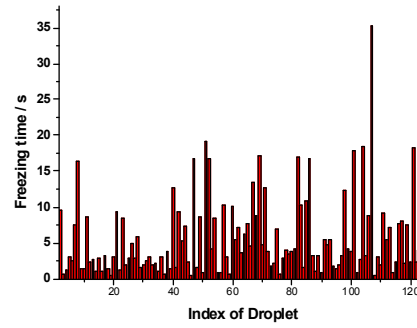
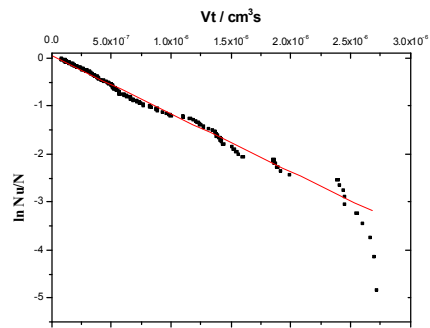


T-meas.: -35.77 °C, J = 8.19 E5

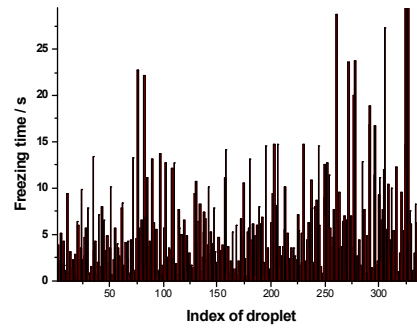
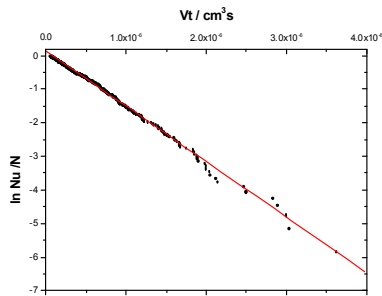




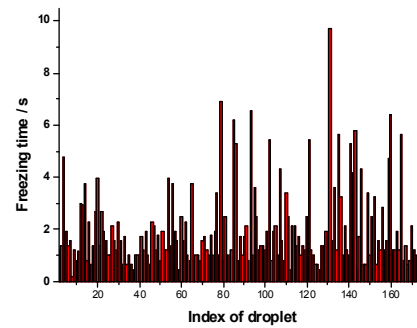
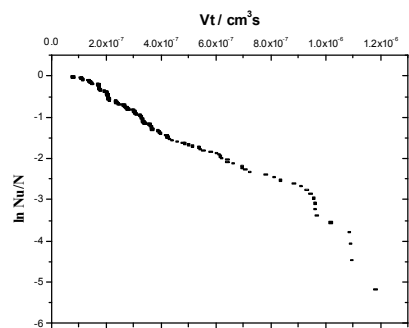
T-meas.: -35.82 °C, J = 4.12 E5



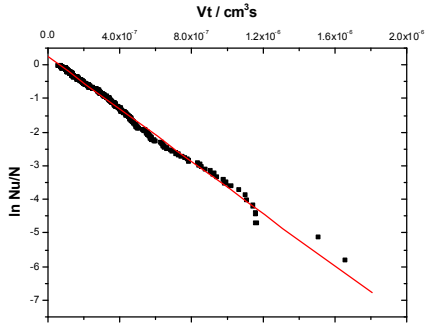
T-meas.: -35.89 °C, J = 1.21 E6



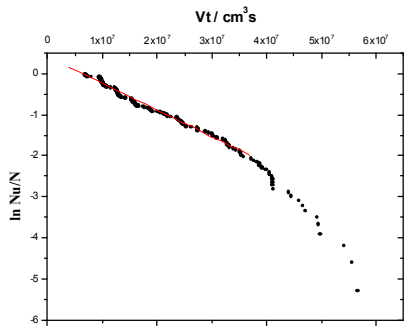
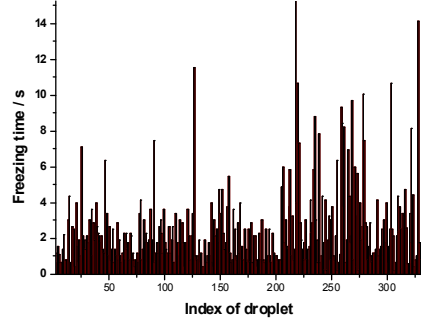
T-meas.: -36.03 °C, J = 1.65 E6



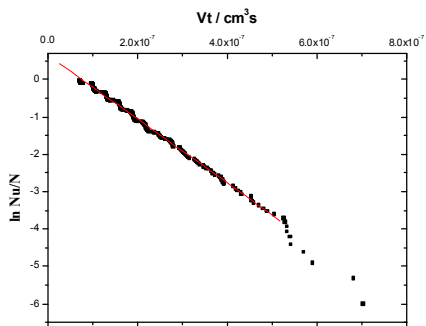
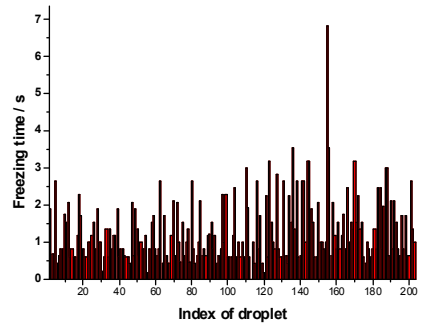
T-meas.: -36.10 °C, J = N.A.



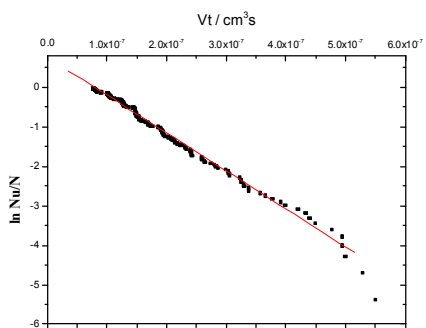
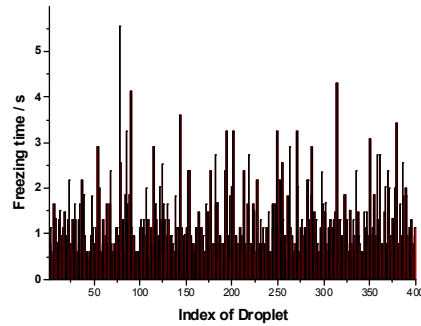
T-meas.: -36.16 °C, J = 3.89 E6



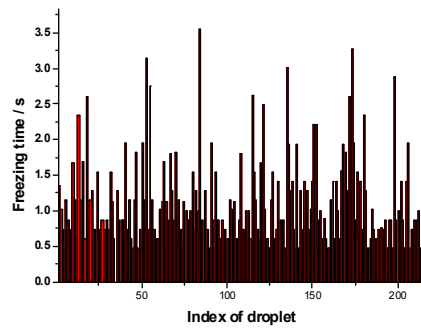
T-meas.: -36.28 °C, J = 6.52 E6

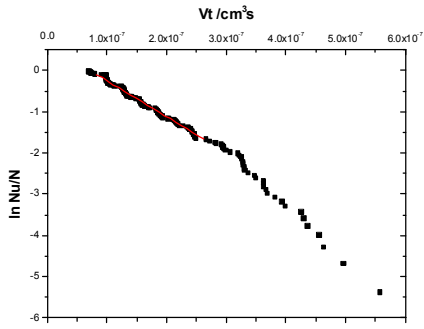


T-meas.: -36.38 °C, J = 8.7 E6

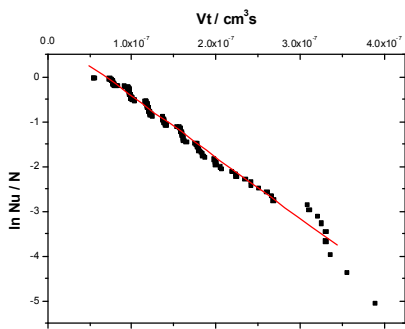
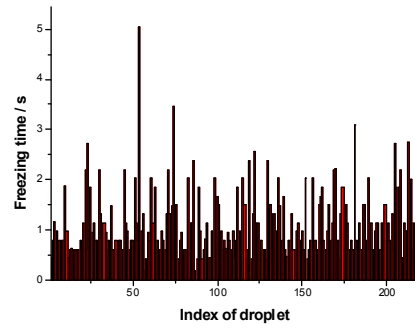


T-meas.: -36.60 °C, J = 9.60 E6

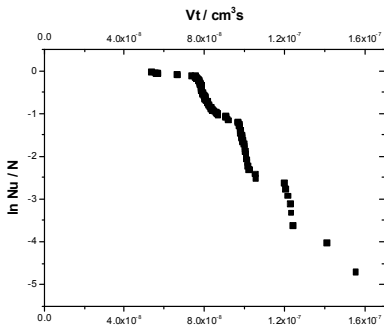
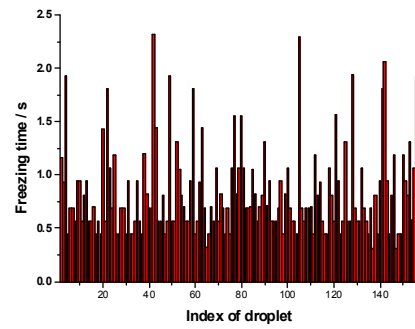




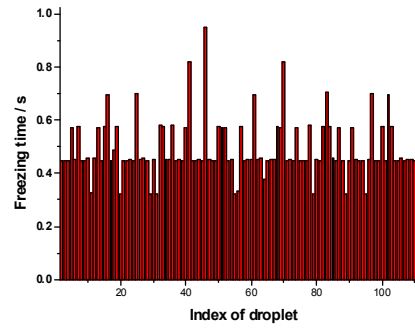
T-meas.: -36.66 °C, J = 8.60 E6



T-meas.: -36.76 °C, J = 1.37 E7

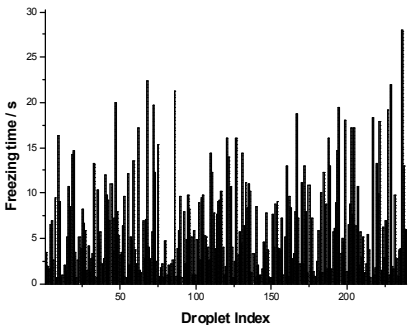
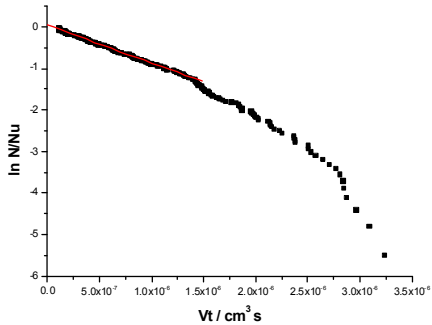


T-meas.: -37.16 °C, J = N.A.

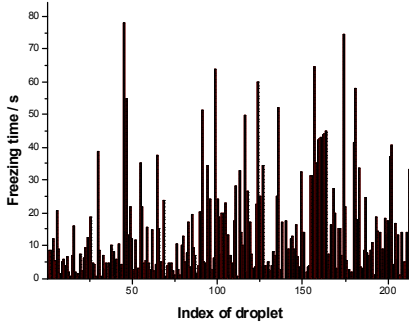
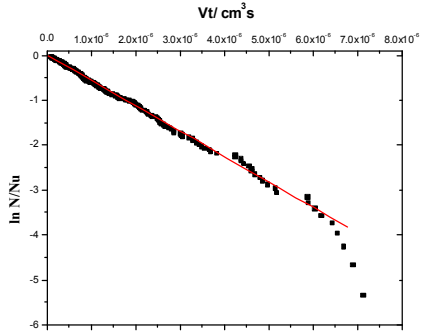


Appendix C – In N vs Vt Diagrams For Aqueous Mixtures at Low Solute Concentrations

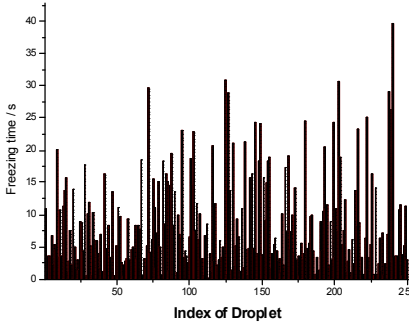
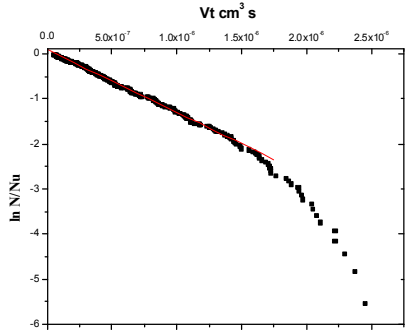
Water + 1, 4-Dioxane Binary Liquid Mixture - $x_{\text{diox}} = 0.002$



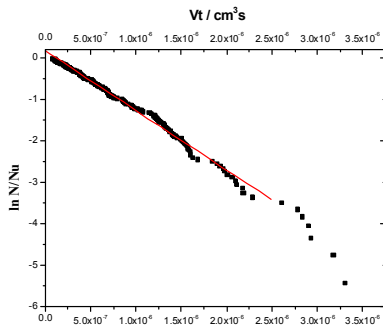
T-meas.: -36.26 °C, J = 9.12E5



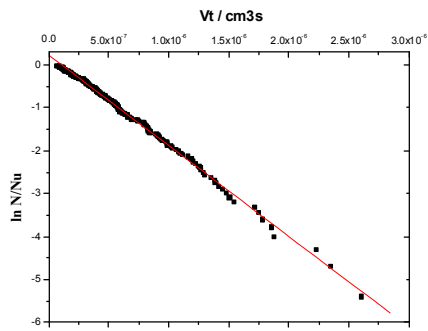
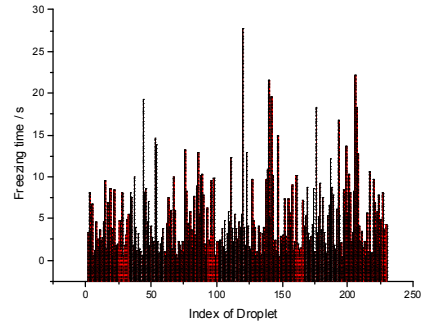
T-meas.: -36.32 °C, J = 5.66E5



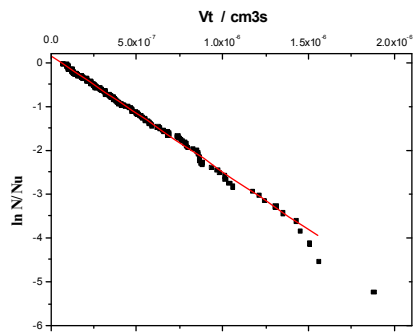
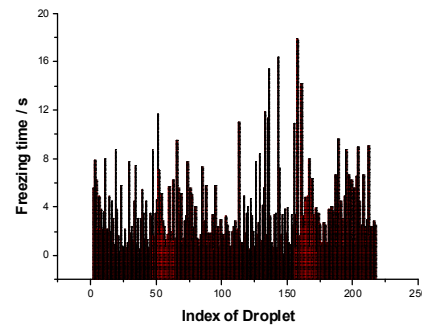
T-meas.: -36.40 °C, J = 1.39E6



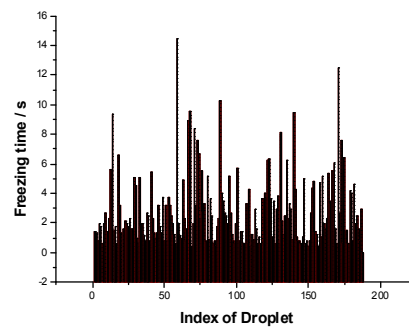
T-meas.: -36.50 °C, J = 1.45E6

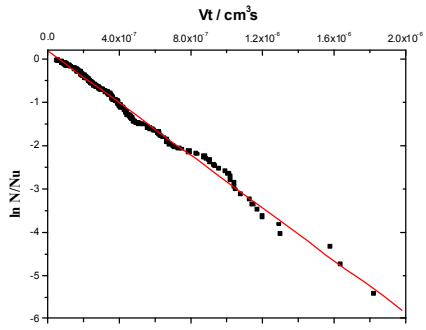


T-meas.: -36.55 °C, J = 2.11E6

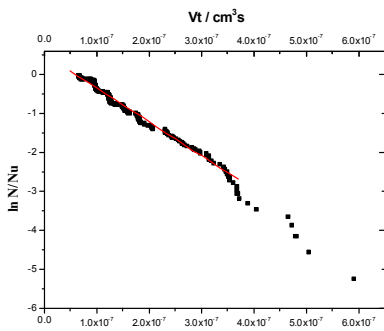
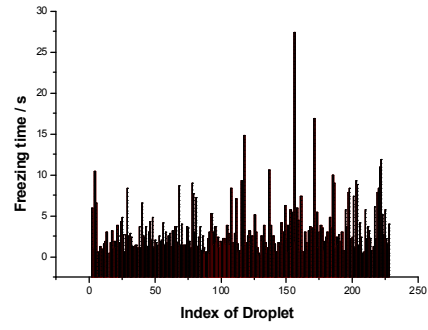


T-meas.: -36.59 °C, J = 2.65E6

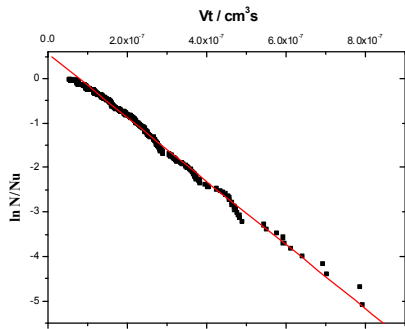
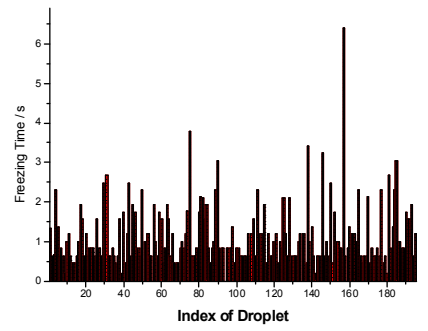




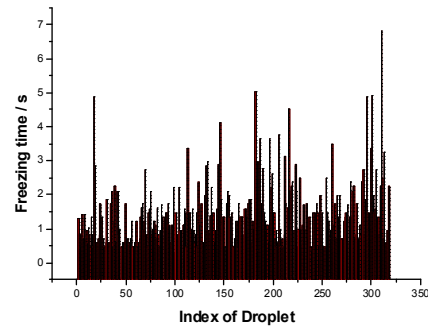
T-meas.: -36.76 °C, J = 3.03E6



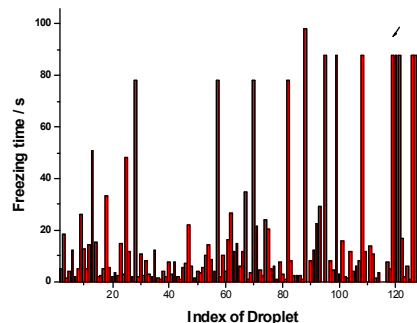
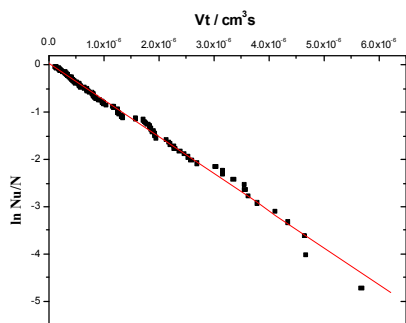
T-meas.: -36.83 °C, J = 8.70E6



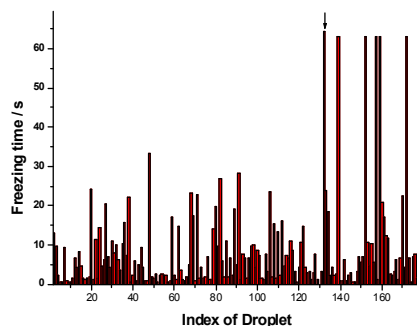
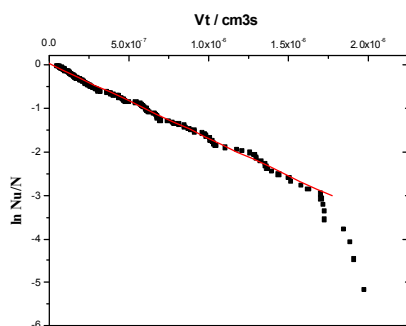
T-meas.: -36.85 °C, J = 7.18E6



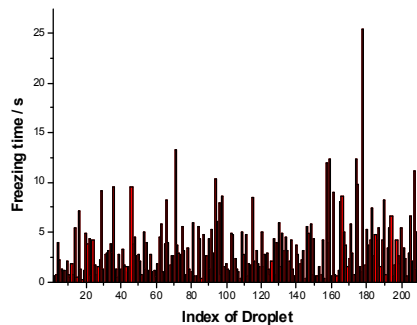
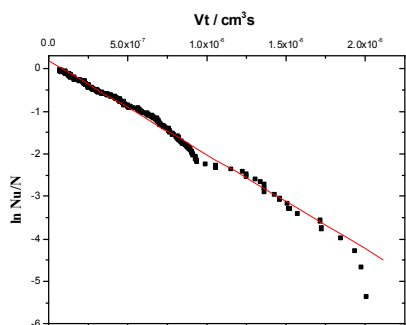
Water + Ethanol Binary Liquid Mixture – $x_{eth} = 0.002$



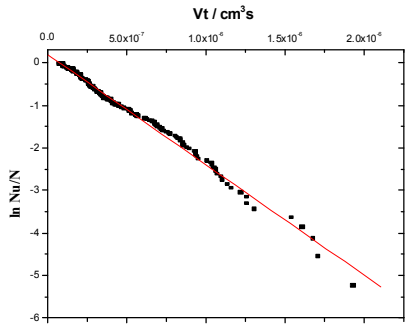
T-meas: $-36.03 \text{ }^\circ\text{C}$, $J = 7.82 \text{ E}6$ (Trap A)



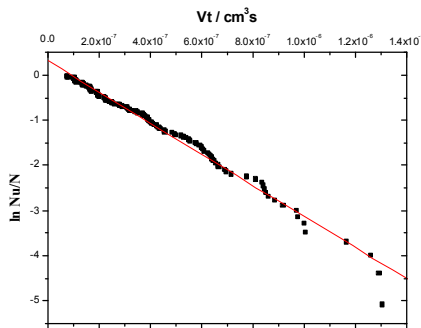
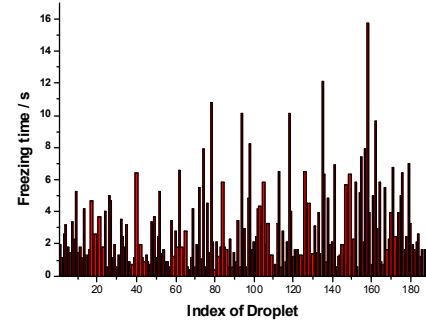
T-meas: $-36.13 \text{ }^\circ\text{C}$, $J = 1.71 \text{ E}6$ (Trap A)



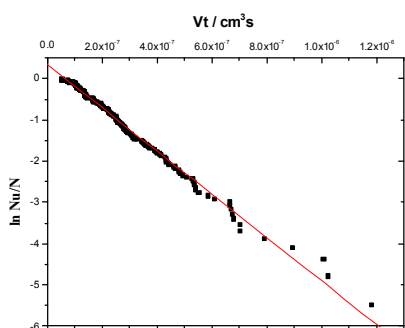
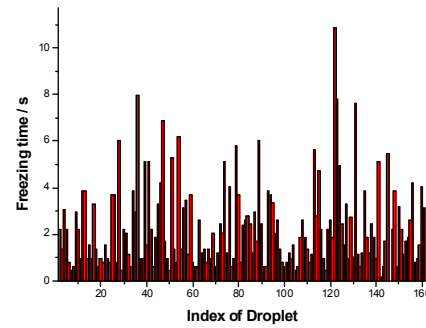
T-meas: $-36.23 \text{ }^\circ\text{C}$, $J = 2.21 \text{ E}6$ (Trap A)



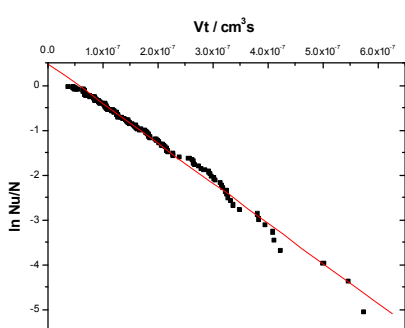
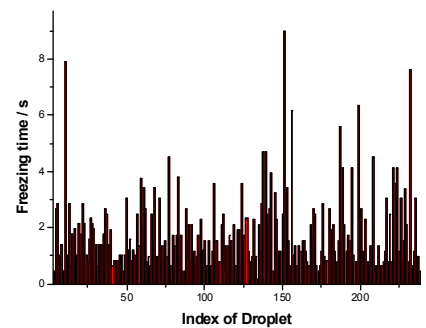
T-meas: -36.28 °C, J = 2.60 E6 (Trap A)



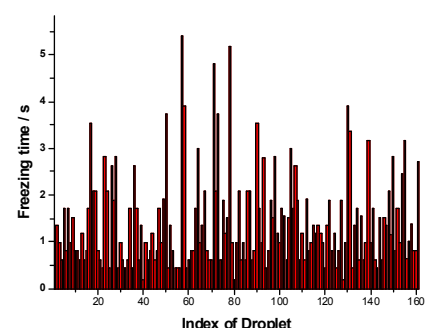
T-meas: -36.36 °C, J = 3.4 E6 (Trap A)



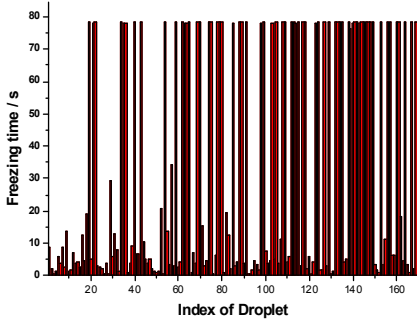
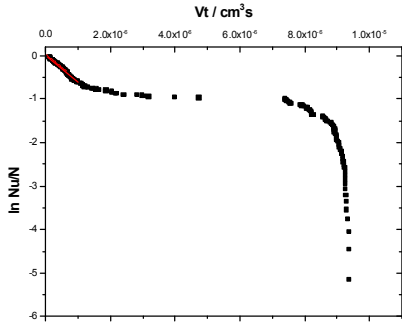
T-meas: -36.43 °C, J = 5.24 E6 (Trap A)



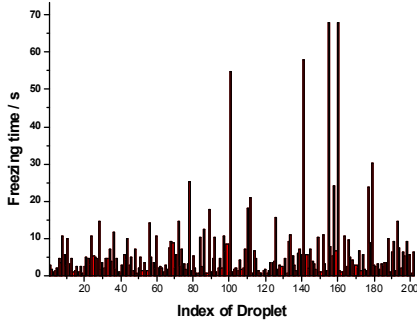
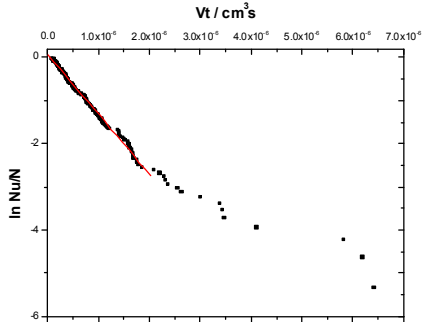
T-meas: -36.49 °C, J = 8.93 E6 (Trap A)



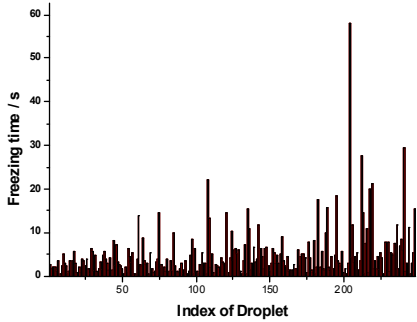
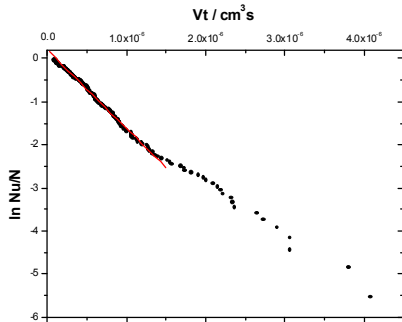
Water + Isopropanol Binary Liquid Mixture – $x_{\text{isoprop}} = 0.002$



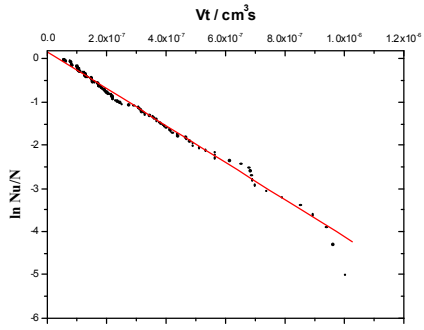
T-meas: -36.04 °C, J = 6.12 E5 (Trap A)



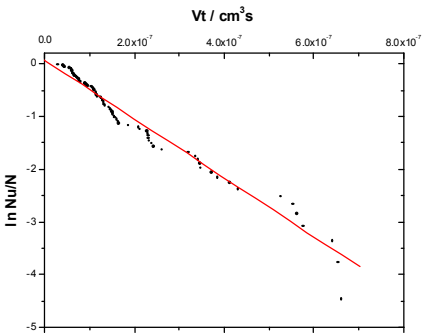
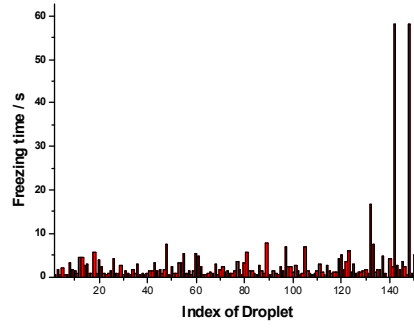
T-meas: -36.09 °C, J = 1.38 E6 (Trap A)



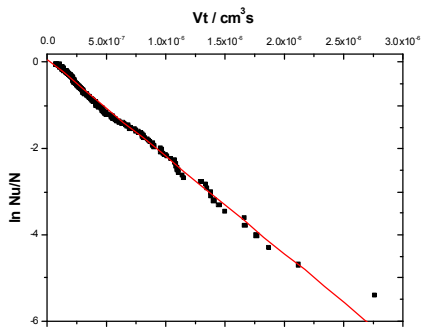
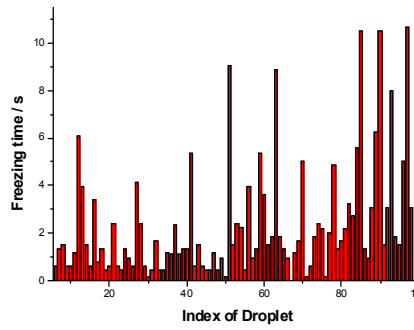
T-meas: -36.14 °C, J = 1.82 E6 (Trap A)



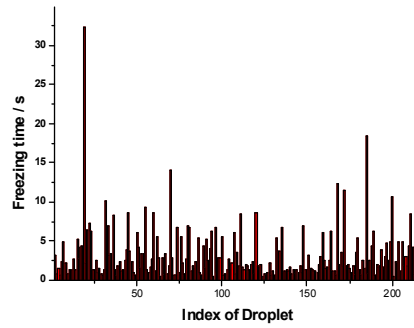
T-meas: -36.24 °C, J = 4.30 E6 (Trap A)



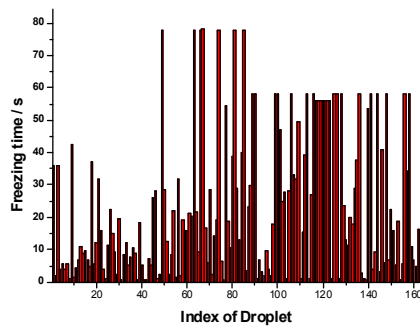
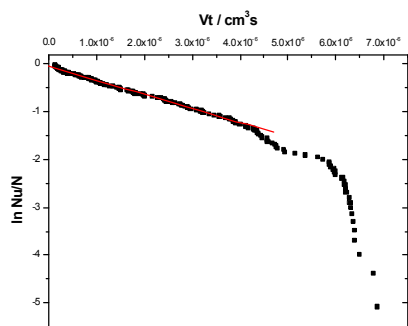
T-meas: -36.34 °C, J = 5.57 E6 (Trap A)



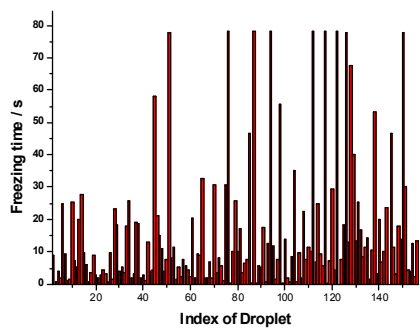
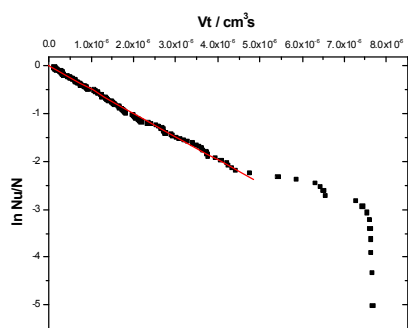
T-meas: -36.38 °C, J = 2.25 E6 (Trap A)



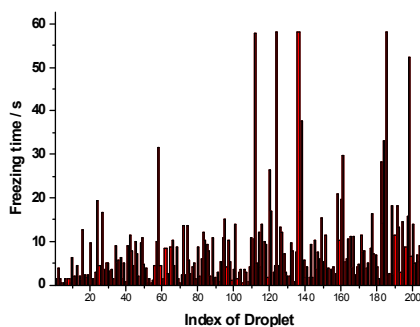
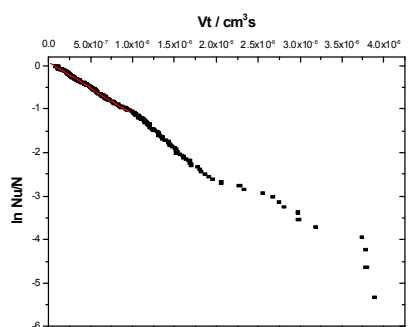
Water + Glycol Binary Liquid Mixture – $x_{gly} = 0.002$



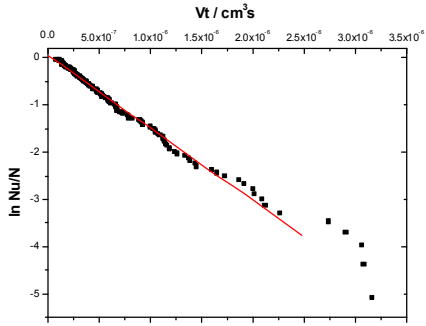
T-meas: -36.16 °C, JL = 2.95 E5 (Trap A)



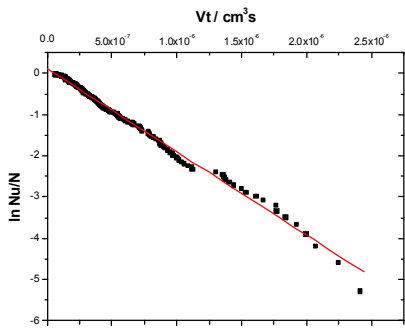
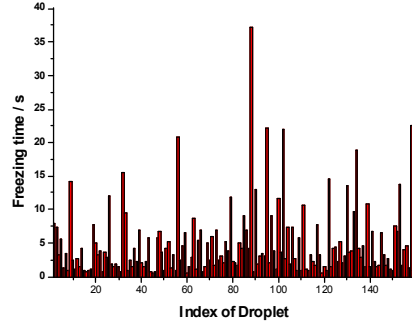
T-meas: -36.22 °C, JL = 4.92 E5 (Trap A)



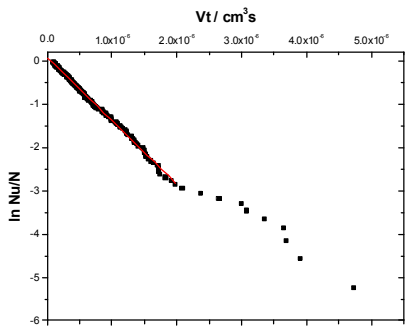
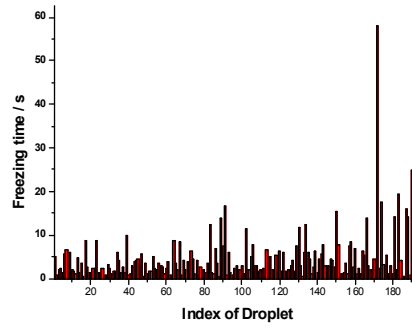
T-meas: -36.36 °C, JL = 1.21 E6 (Trap A)



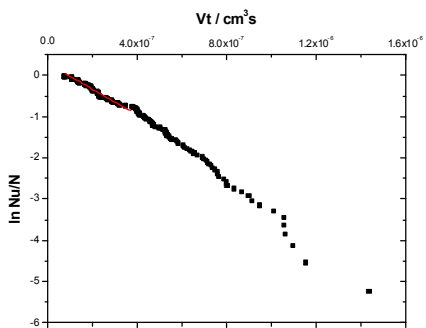
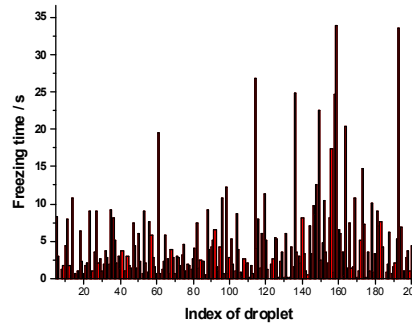
T-meas: $-36.43\text{ }^{\circ}\text{C}$, $J_L = 1.54\text{ E}6$ (Trap A)



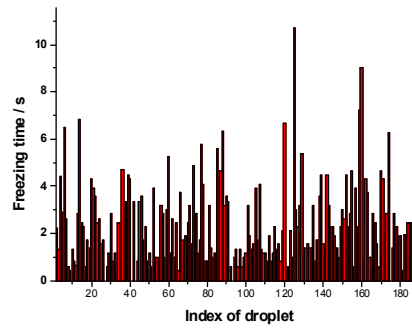
T-meas: $-36.51\text{ }^{\circ}\text{C}$, $J_L = 2.02\text{ E}6$ (Trap A)

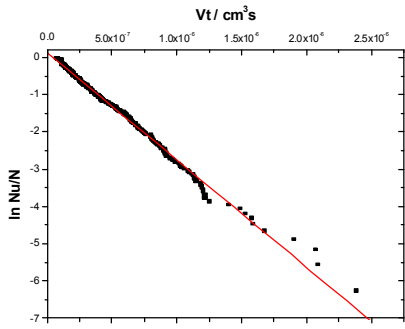


T-meas: $-36.57\text{ }^{\circ}\text{C}$, $J_L = 1.47\text{ E}6$ (Trap A)

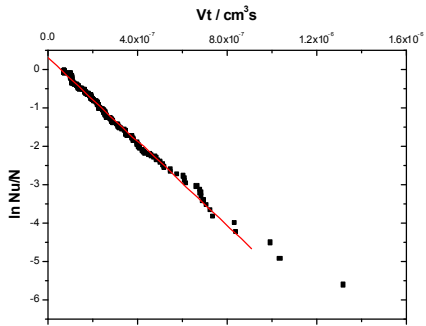
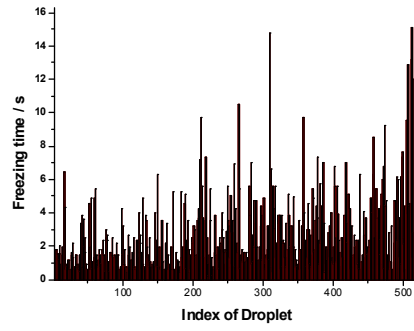


T-meas: $-36.65\text{ }^{\circ}\text{C}$, $J_L = 3.12\text{ E}6$ (Trap A)

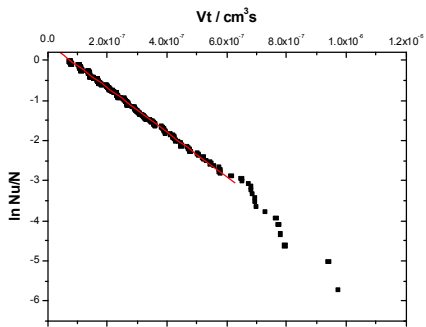
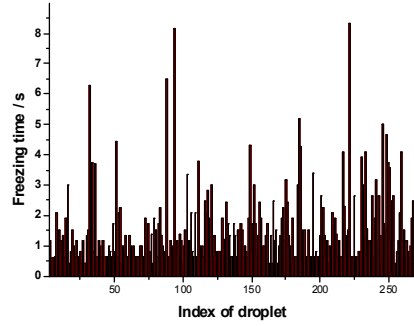




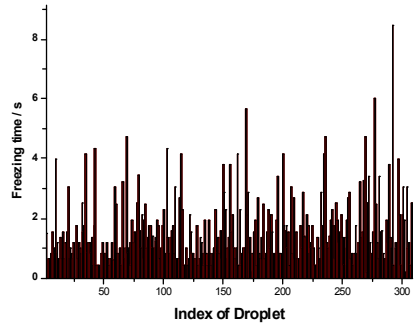
T-meas: -36.71 °C, $J_L = 2.88 \text{ E6}$ (Trap A)



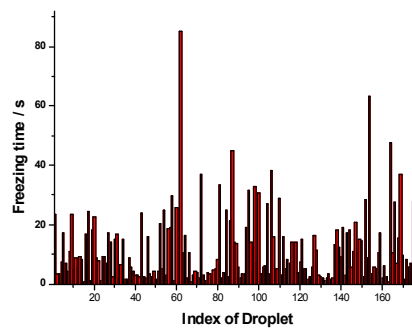
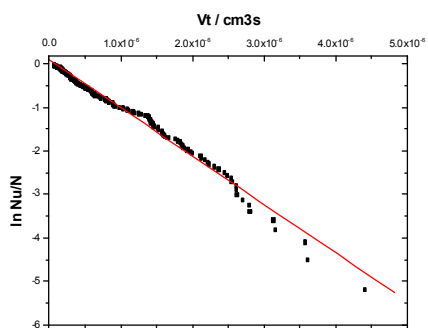
T-meas: -36.74 °C, $J_L = 5.45 \text{ E6}$ (Trap A)



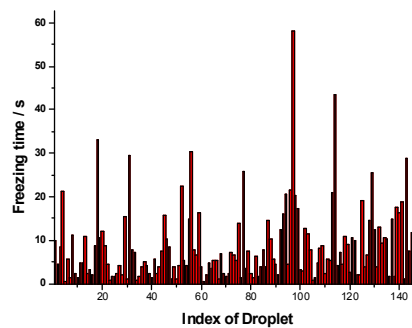
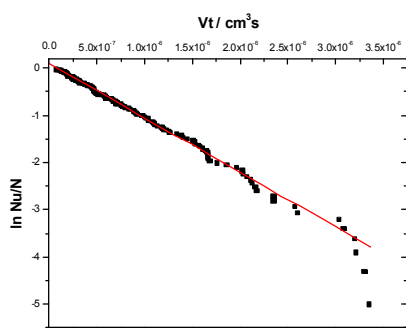
T-meas: -36.81 °C, $J_L = 5.54 \text{ E6}$ (Trap A)



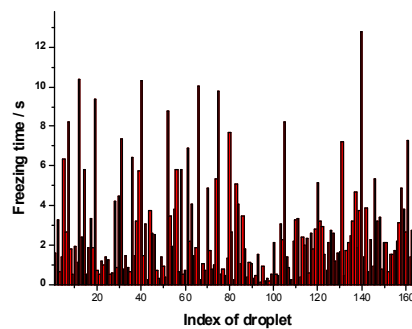
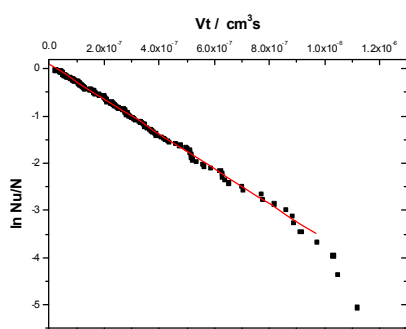
Aqueous Urea Solution – $x_{\text{urea}} = 0.002$



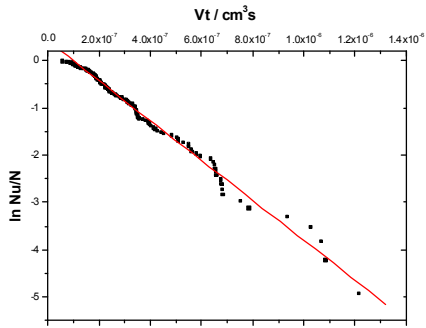
T-meas: -35.96 °C, J = 1.11 E6 (Trap B)



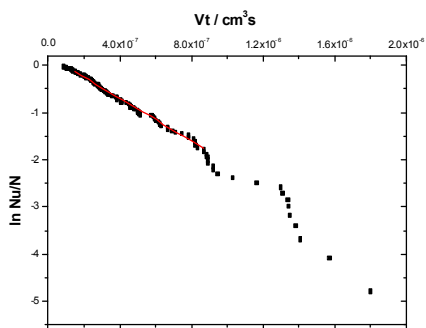
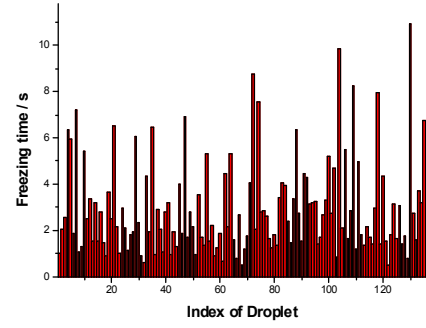
T-meas: -36.01 °C, J = 1.15 E6 (Trap B)



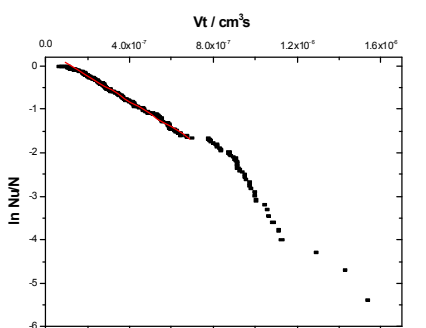
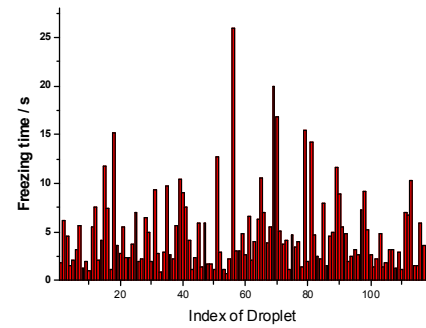
T-meas: -36.13 °C, J = 3.71 E6 (Trap B)



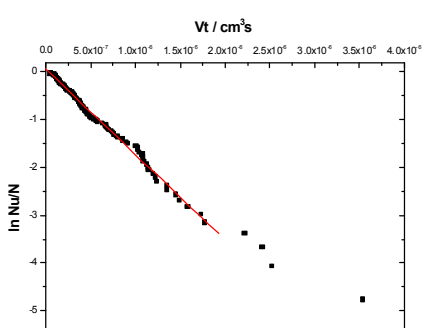
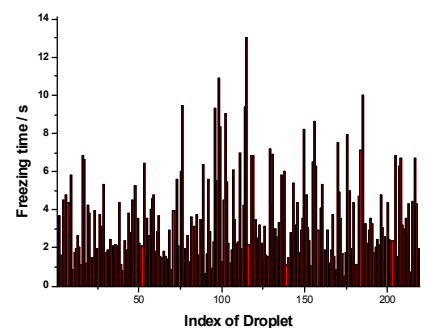
T-meas: -36.17 °C, J = 4.2 E6 (Trap B)



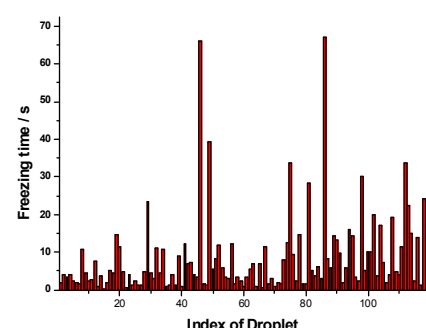
T-meas: -36.18 °C, JR = 2.25 E6 (Trap B)

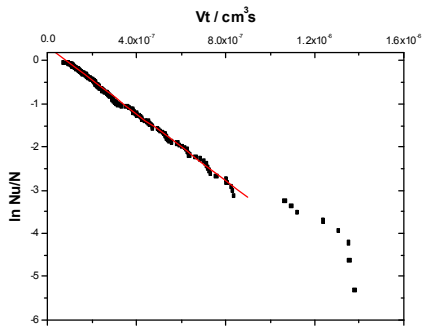


T-meas: -36.28 °C, JL = 2.93 E6 (Trap B)

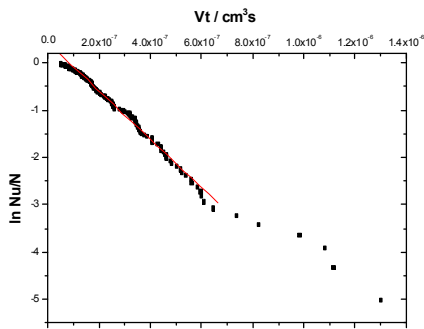
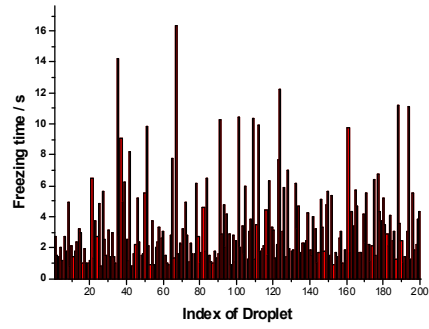


T-meas: -36.33 °C, JL = 1.79 E6 (Trap B)

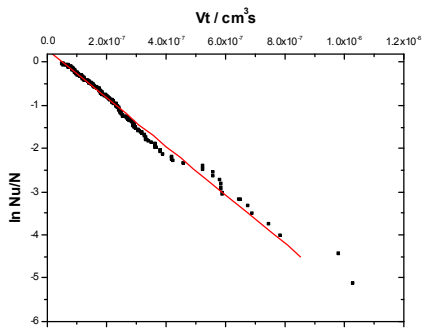
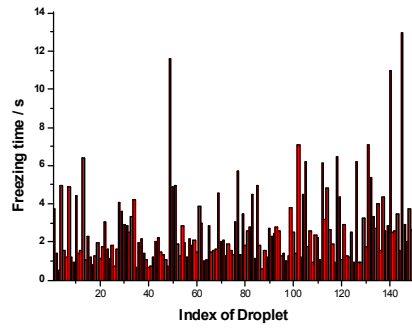




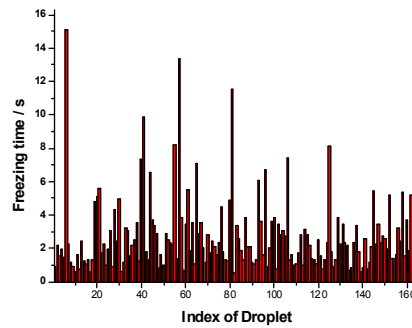
T-meas: $-36.34\text{ }^{\circ}\text{C}$, JR = $3.88\text{ E}6$ (Trap B)

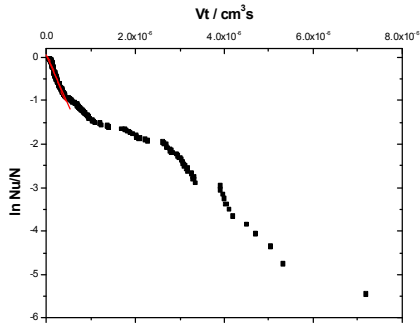


T-meas: $-36.38\text{ }^{\circ}\text{C}$, JR = $5.09\text{ E}6$ (Trap B)

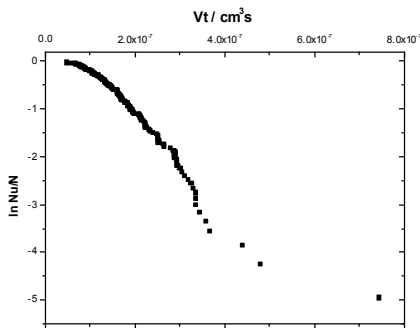
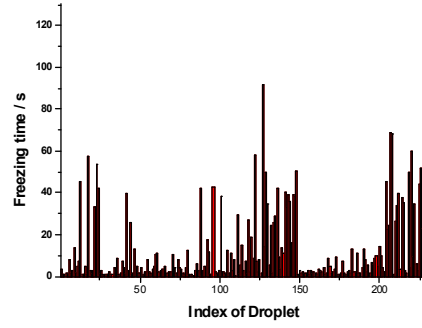


T-meas: $-36.47\text{ }^{\circ}\text{C}$, JL = $5.61\text{ E}6$ (Trap B)

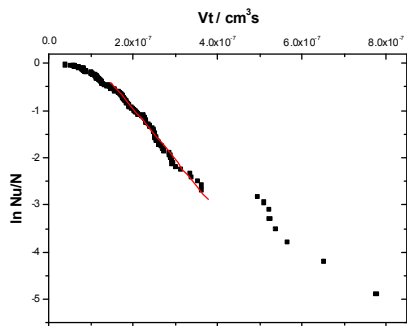
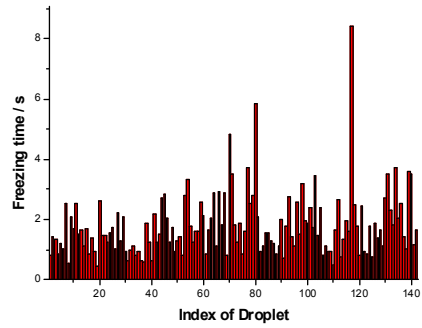




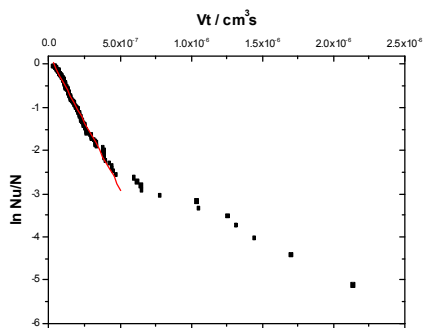
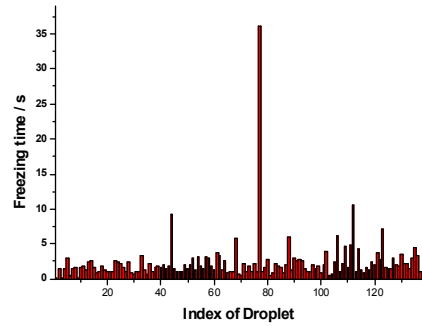
T-meas: $-36.51\text{ }^{\circ}\text{C}$, $JL = 2.62\text{ E}6$ (Trap B)



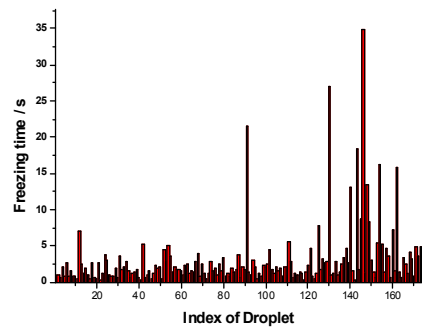
T-meas: $-36.52\text{ }^{\circ}\text{C}$ (Trap B)

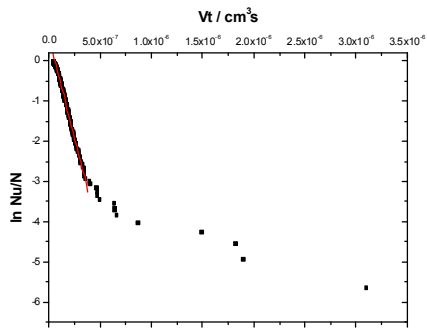


T-meas: $-36.54\text{ }^{\circ}\text{C}$, $JR = 1.07\text{ E}7$ (Trap B)

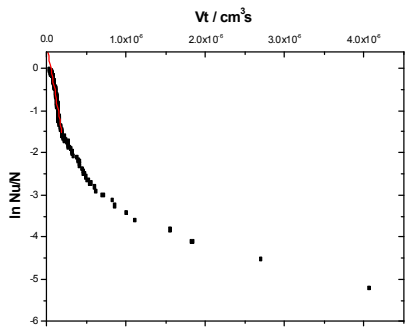
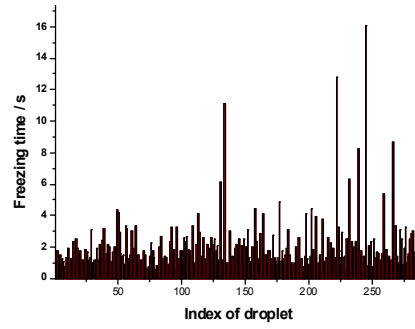


T-meas: $-36.58\text{ }^{\circ}\text{C}$, $JL = 6.19\text{ E}6$ (Trap B)

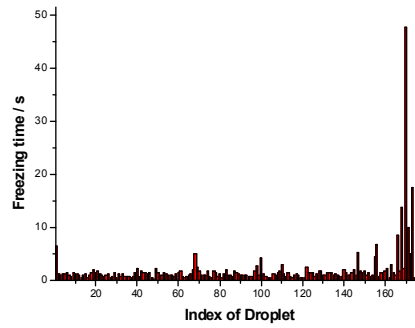




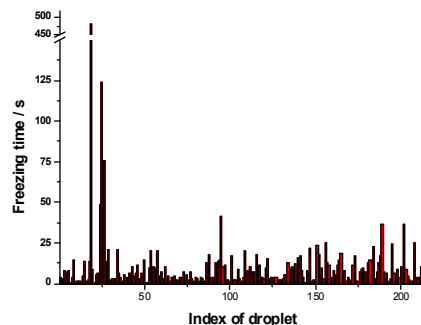
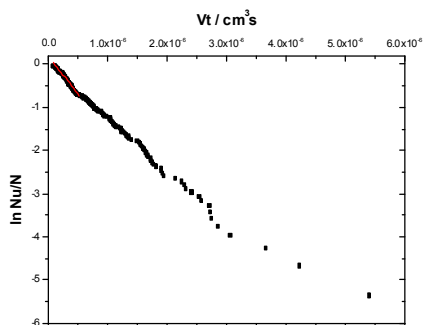
T-meas: $-36.68 \text{ }^\circ\text{C}$, JL = 1.00 E7 (Trap B)



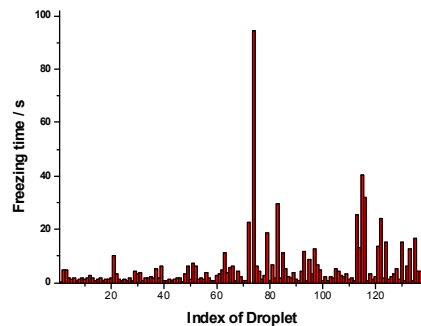
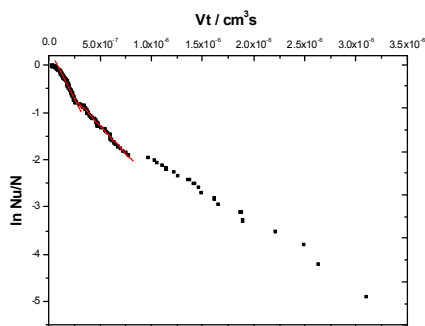
T-meas: $-36.81 \text{ }^\circ\text{C}$, JL = 1.08 E7 (Trap B)



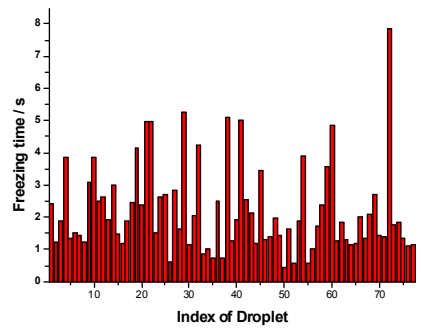
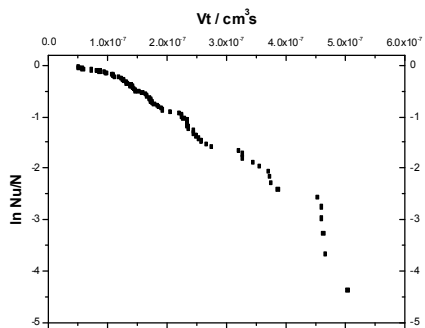
Aqueous Urea Solution – $x_{\text{urea}} = 0.01$



T-meas: $-38.29\text{ }^{\circ}\text{C}$, $JL = 1.75\text{ E}6$ (Trap B)

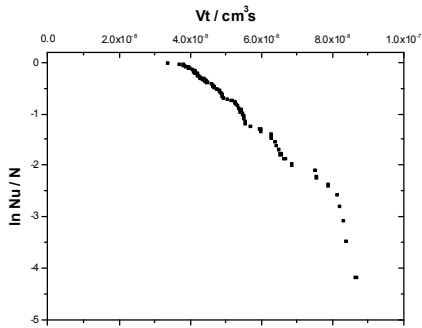


T-meas: $-38.39\text{ }^{\circ}\text{C}$, $JL = 4.16\text{ E}6$, $JR = 2.34\text{ E}6$ (Trap B)

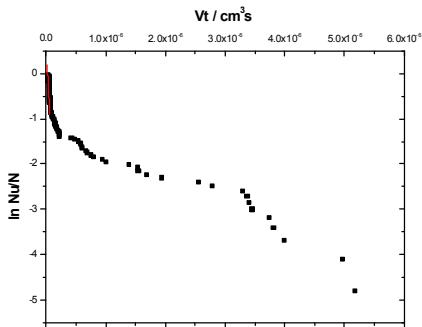
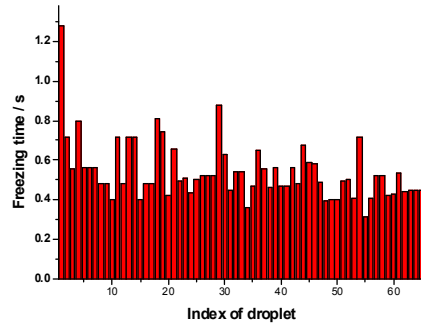


T-meas: $-38.55\text{ }^{\circ}\text{C}$, $JL = \text{N.A.}$ (Trap B)

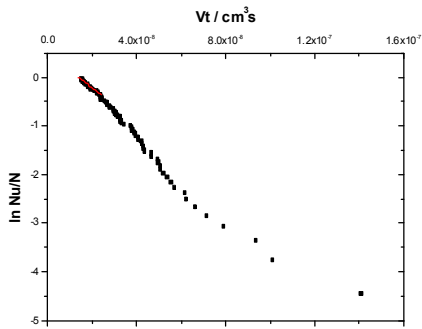
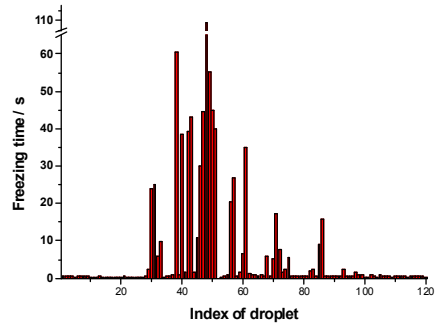
Aqueous Urea Solution – $x_{\text{urea}} = 0.02$



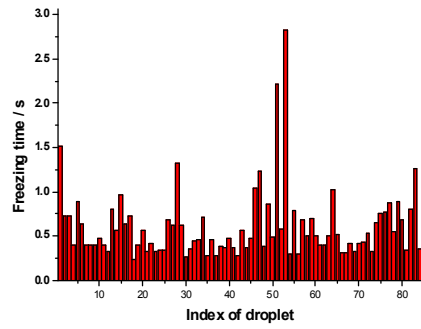
T-meas: $-41.93 \text{ }^\circ\text{C}$, $J = \text{N.A.}$ (Trap B)



T-meas: $-43.04 \text{ }^\circ\text{C}$, $J_L = 2.21 \text{ E7}$ (Trap B)

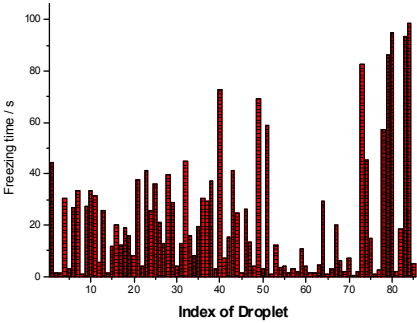
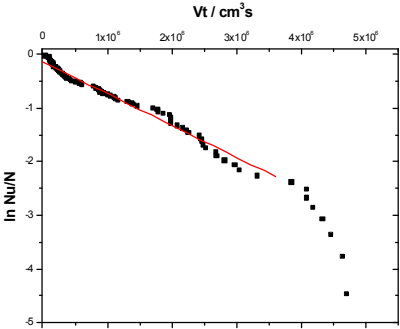


T-meas: $-43.20 \text{ }^\circ\text{C}$, $J_L = 3.55 \text{ E7}$ (Trap B)

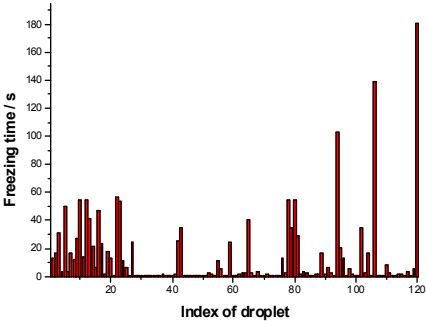
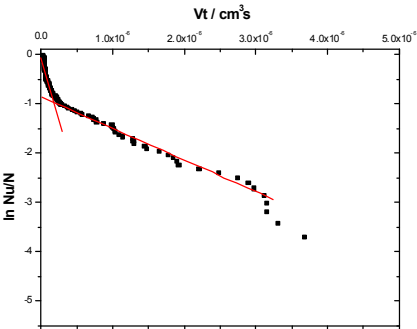


Appendix D – In N vs. V·t Diagrams for Water + 1, 4-dioxane Liquid Mixtures

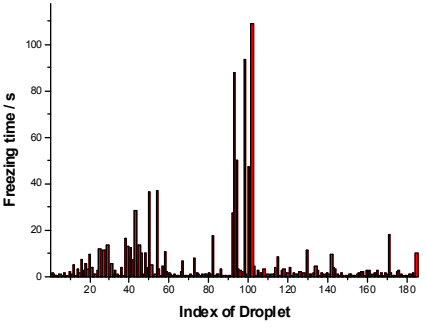
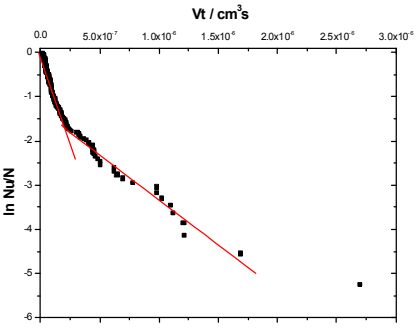
Water + 1, 4-Dioxane Binary Liquid Mixture - $x_{diox} = 0.04$



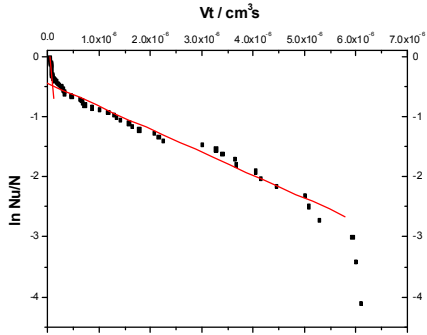
T-meas: -43.3 °C, J=5.95E5 (Trap B)



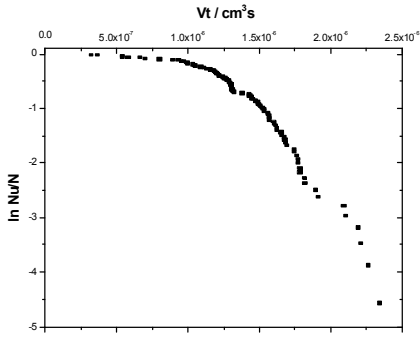
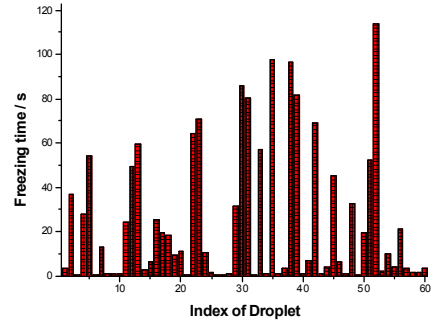
T-meas: -43.6 °C, JL=5.95E5, JR=6.43E5 (Trap B)



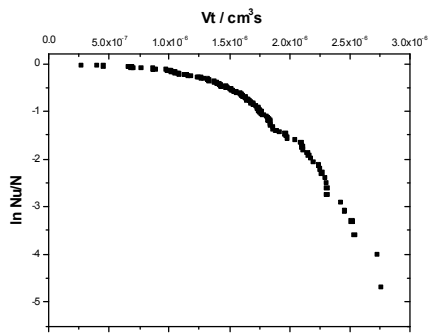
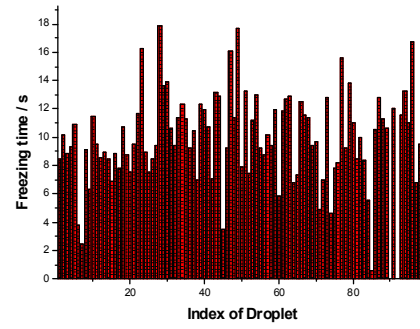
T-meas: -43.7 °C, JL=8.06E6, JR=2.03E6 (Trap B)



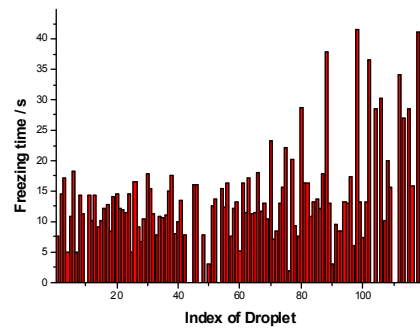
T-meas: $-43.95\text{ }^{\circ}\text{C}$, $J_L=7.04\text{E}6$, $J_R=3.80\text{E}5$ (Trap B)

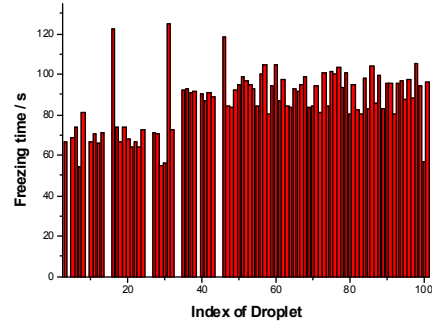
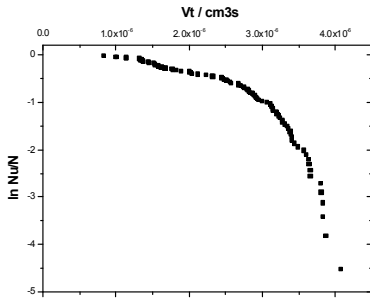


T-meas: $-43.19\text{ }^{\circ}\text{C}$, $J_L=$, $J_R=$ (Trap A)

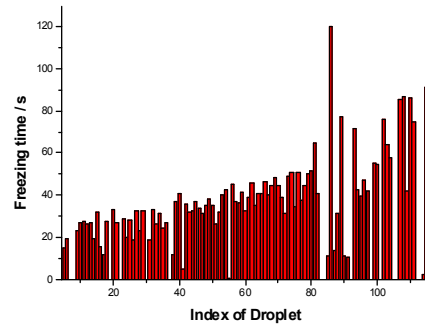
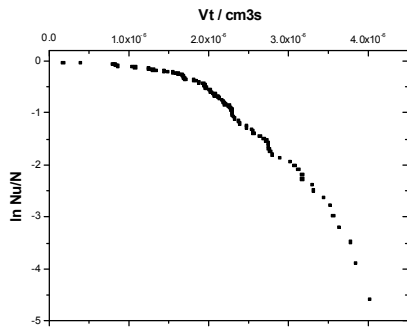


T-meas: $-43.29\text{ }^{\circ}\text{C}$, $J_L=$, $J_R=$ (Trap A)

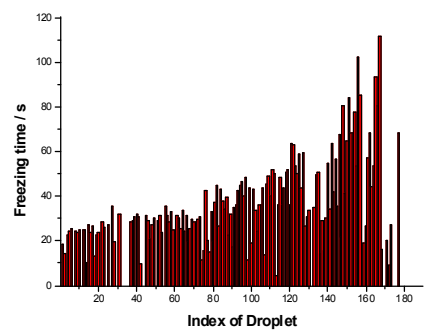
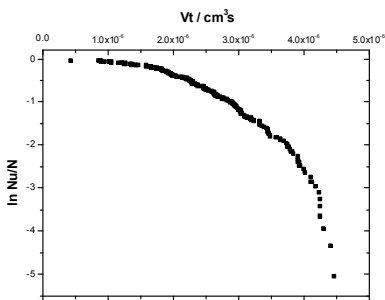




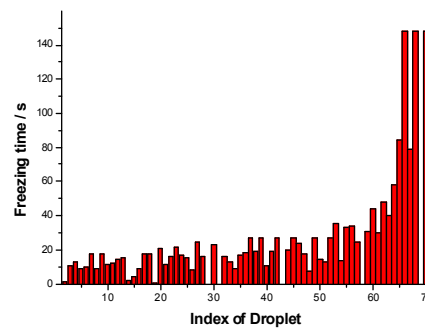
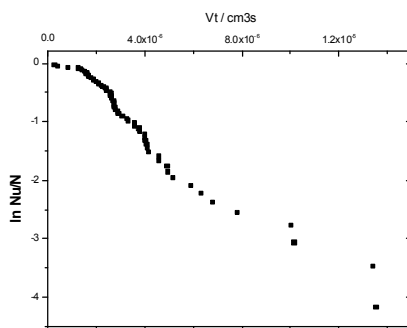
T-meas: $-43.31\text{ }^{\circ}\text{C}$, $J1=$, $JR=$ (Trap A)



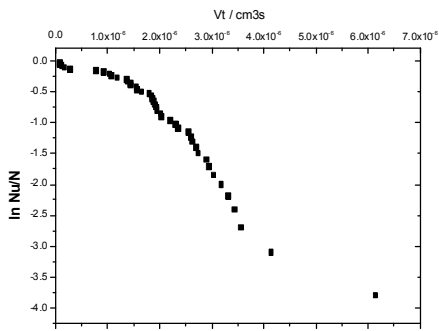
T-meas: $-43.43\text{ }^{\circ}\text{C}$, $J1=$, $JR=$ (Trap A)



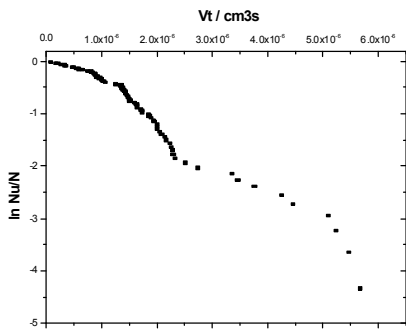
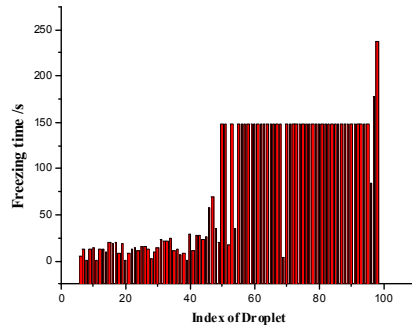
T-meas: $-43.62\text{ }^{\circ}\text{C}$, $JL=$, $JR=$ (Trap A)



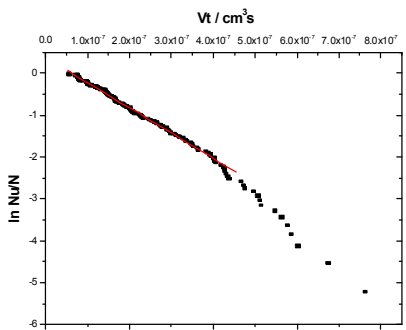
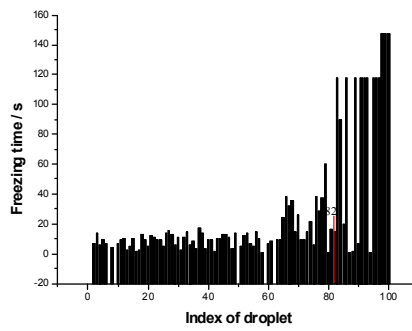
T-meas: $-44.36\text{ }^{\circ}\text{C}$, $JL=$, $JR=$ (Trap A)



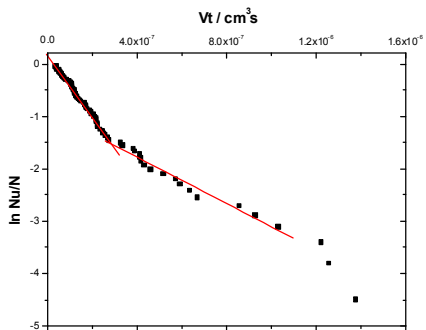
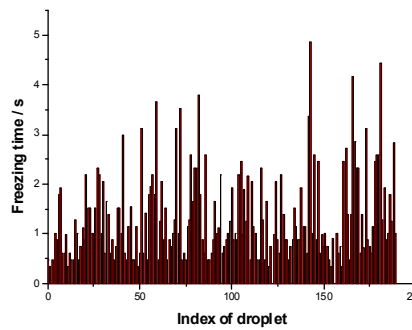
T-meas: -44.67 °C, JL= , JR= (Trap A)



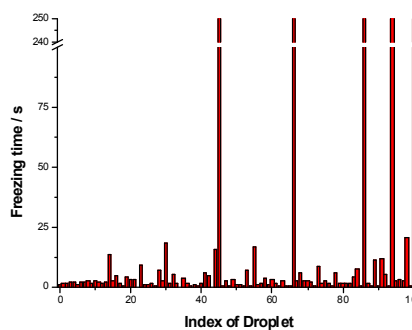
T-meas: -44.99 °C, JL= , JR= (Trap A)

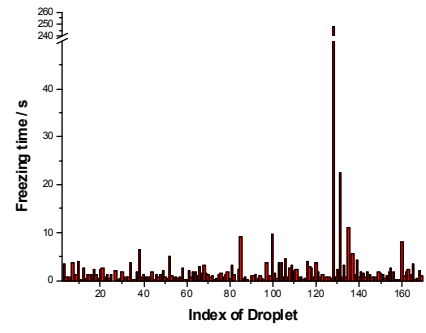
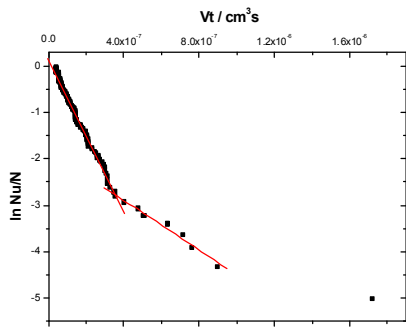


T-meas: -45.17 °C, J=6.02E6 (Trap A)



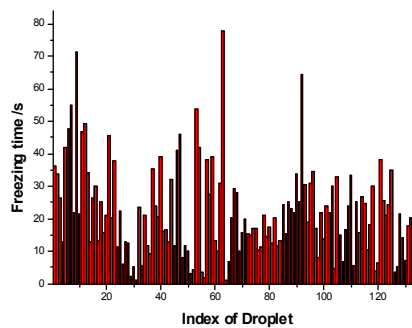
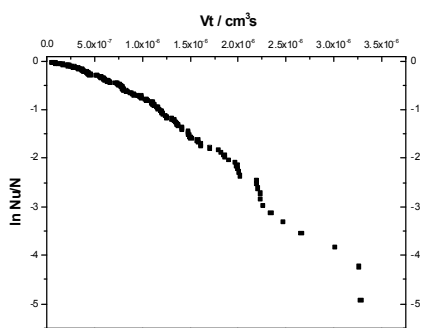
T-meas: -47.54 °C, JL=5.86E6, JR=2.21E6 (Trap A)



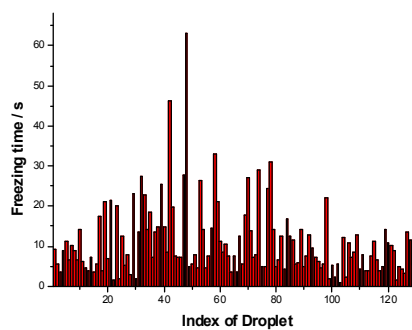
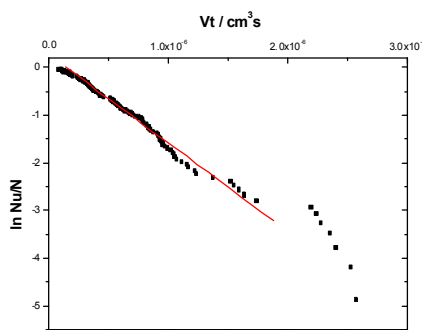


T-meas: $-47.64 \text{ }^\circ\text{C}$, JL= $8.51\text{E}6$, JR= $2.68\text{E}6$ (Trap A)

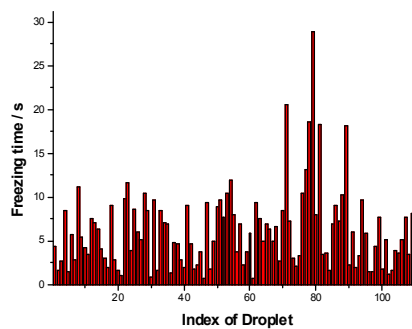
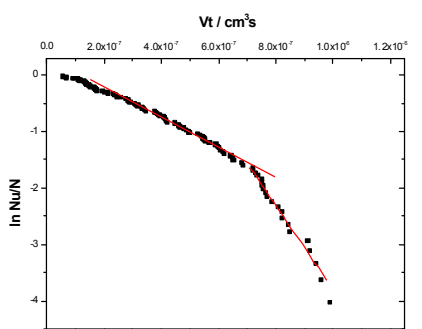
Water + 1, 4-Dioxane Binary Liquid Mixture - $x_{\text{diox}} = 0.133$



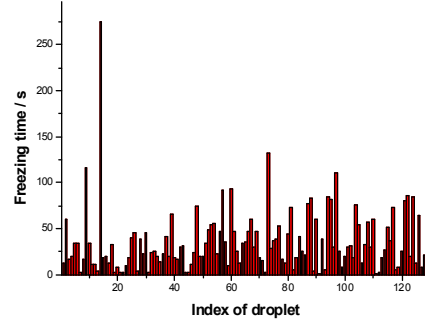
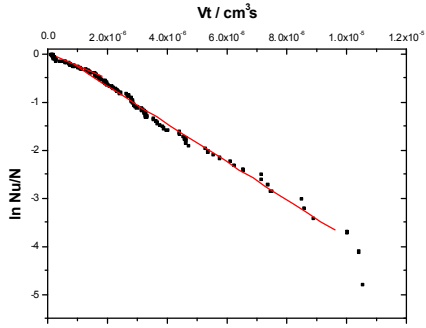
T-meas: -54.85 °C, JL= , JR= (Trap B)



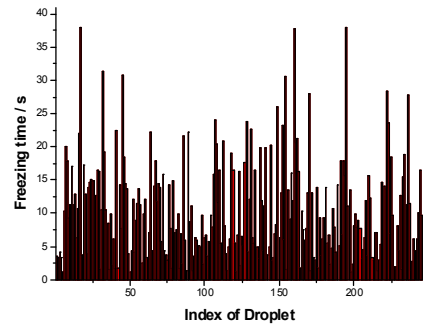
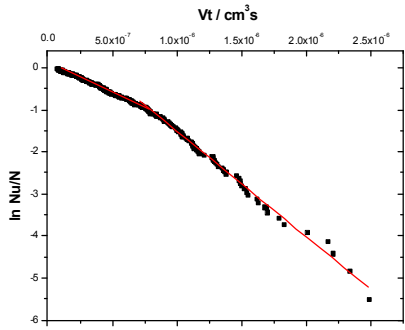
T-meas: -54.98 °C, JL= , JR=1.85 E6 (Trap B)



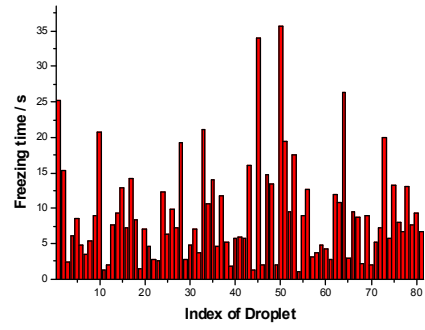
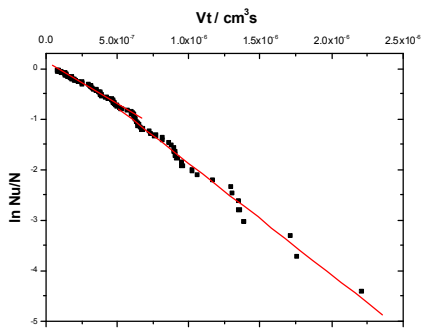
T-meas: -54.07 °C, JL= 2.71 E6, JR=7.42 E6 (Trap B)



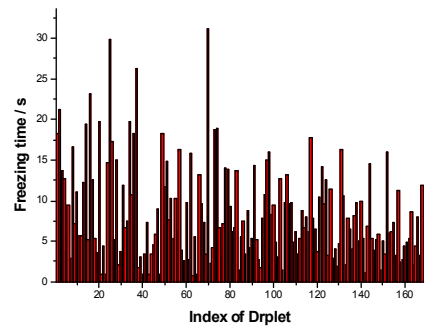
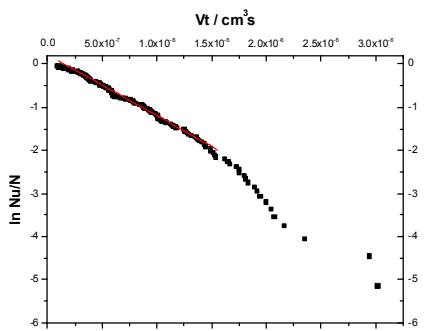
T-meas: $-54.34\text{ }^{\circ}\text{C}$, $J_L = 2.37\text{ E}5$, $J_R = 3.94\text{ E}5$ (Trap B)



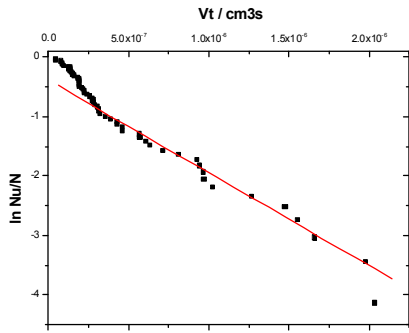
T-meas: $-54.46\text{ }^{\circ}\text{C}$, $J_L = 1.40\text{ E}6$, $J_R = 2.51\text{ E}6$ (Trap B)



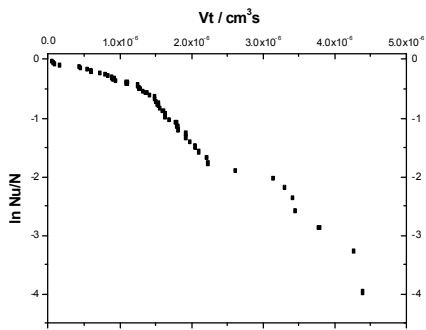
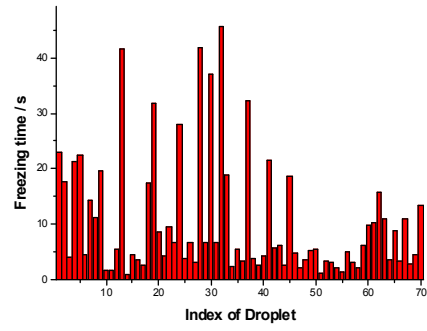
T-meas: $-54.55\text{ }^{\circ}\text{C}$, $J_L = 1.67\text{ E}6$, $J_R = 2.20\text{ E}6$ (Trap B)



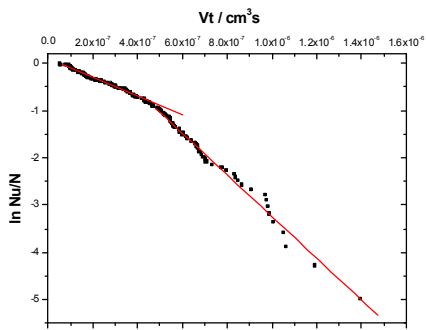
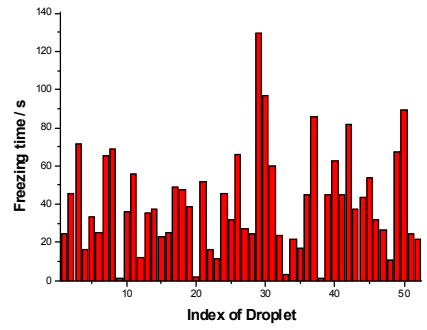
T-meas: $-54.65\text{ }^{\circ}\text{C}$, $J_L =$, $J_R = 1.42\text{ E}6$ (Trap B)



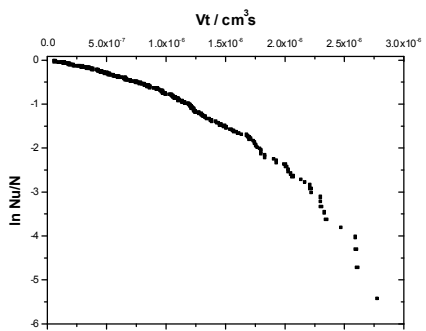
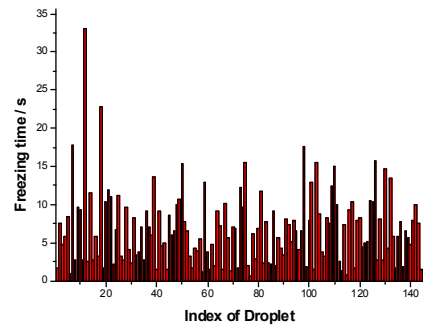
T-meas: -55.10 °C, $J_L =$, $J_R = 1.56 \text{ E6}$ (Trap B)



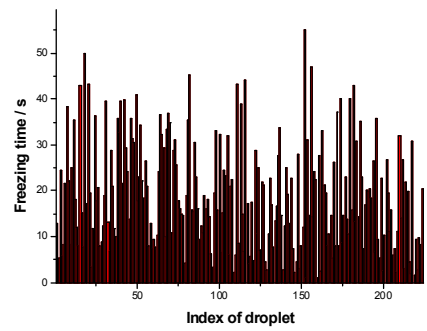
T-meas: -55.12 °C, $J_L =$, $J_R =$ (Trap B)

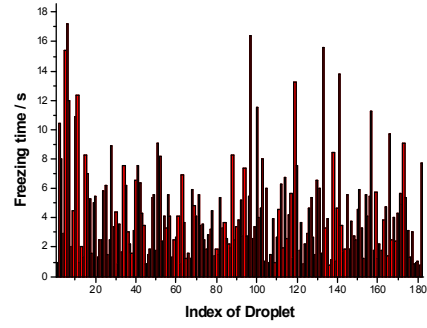
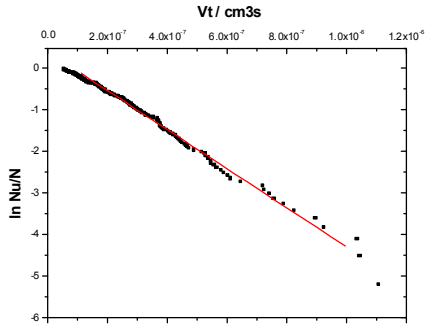


T-meas: -55.18 °C, $J_L = 2 \text{ E6}$, $J_R = 4.40 \text{ E6}$ (Trap B)

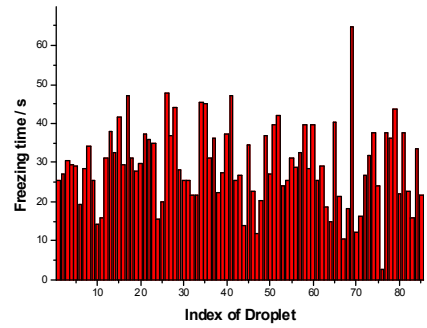
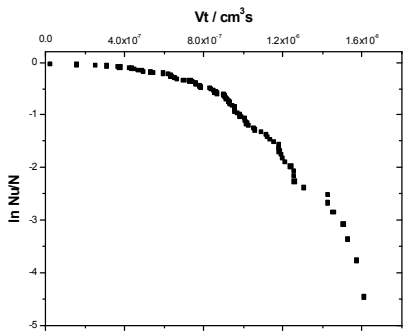


T-meas: -55.23 °C, $J_L =$, $J_R =$ (Trap B)

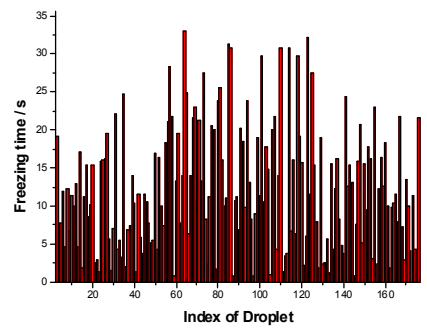
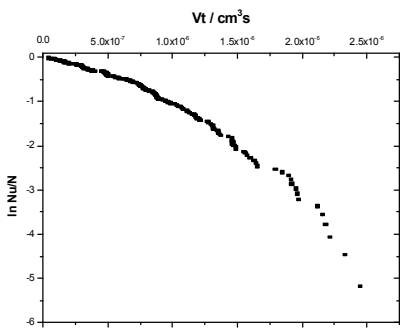




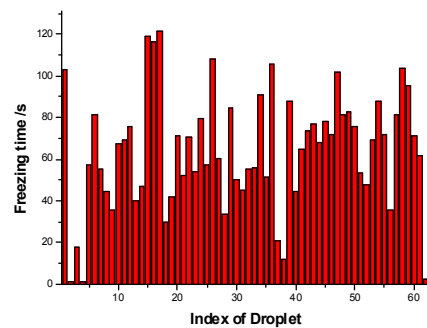
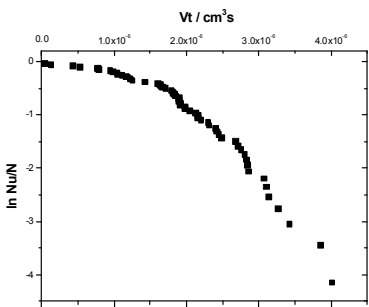
T-meas: $-55.28\text{ }^{\circ}\text{C}$, $J_L =$, $J_R = 4.73\text{ E}6$ (Trap B)



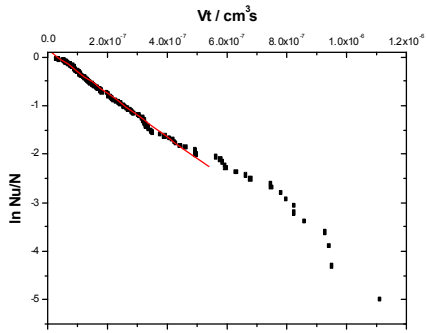
T-meas: $-55.36\text{ }^{\circ}\text{C}$, $J_L =$, $J_R =$ (Trap B)



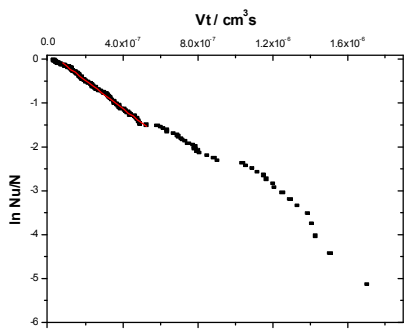
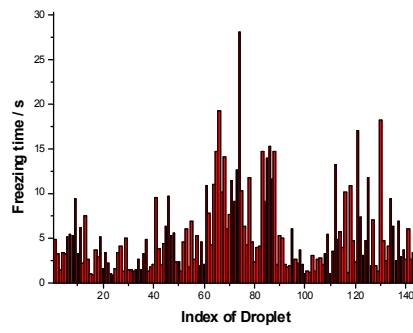
T-meas: $-55.39\text{ }^{\circ}\text{C}$, $J_L =$, $J_R =$ (Trap B)



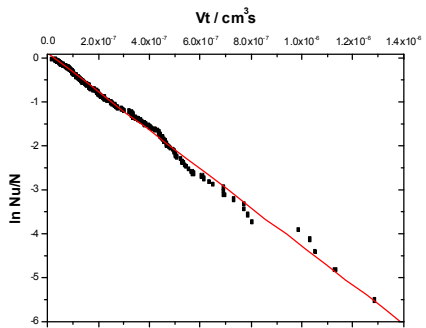
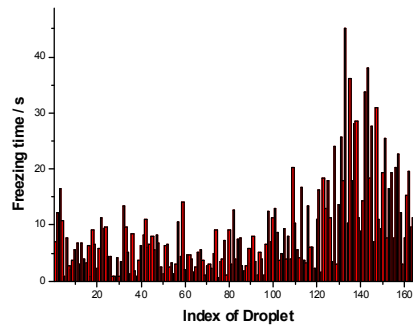
T-meas: $-55.47\text{ }^{\circ}\text{C}$, $J_L =$, $J_R =$ (Trap B)



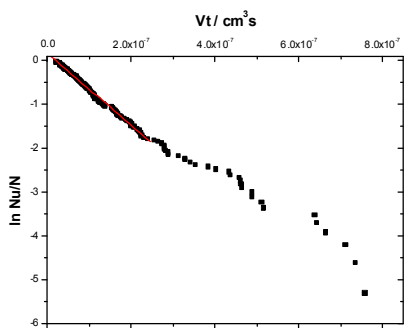
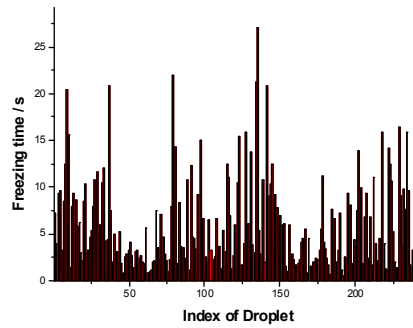
T-meas: -55.51 °C, JL= , JR=4.49 E6 (Trap B)



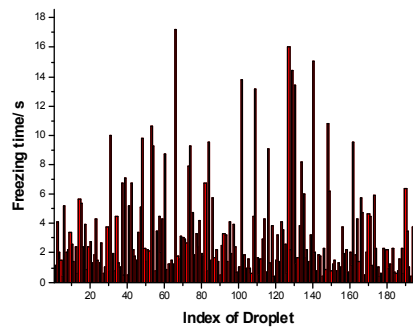
T-meas: -55.64 °C, JL= , JR=3.25 E6 (Trap B)

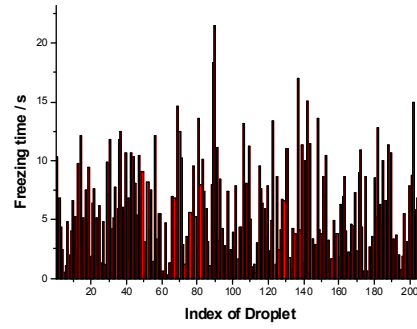
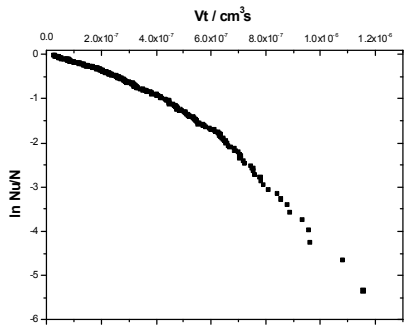


T-meas: -55.77 °C, JL= 4.41 E6 (Trap B)

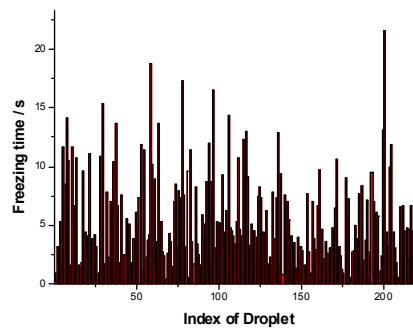
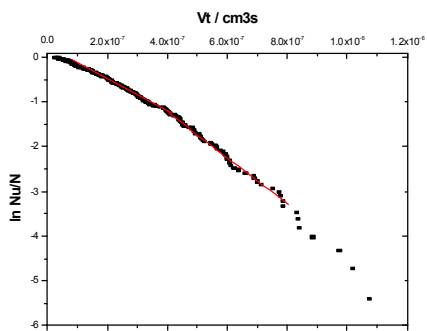


T-meas: -55.86 °C, JL= 8.23 E6 (Trap B)

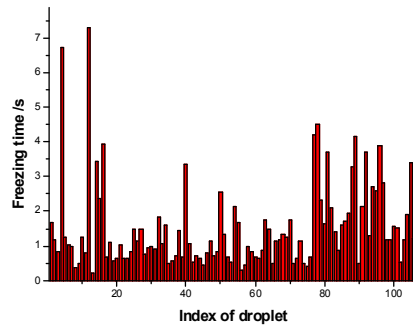
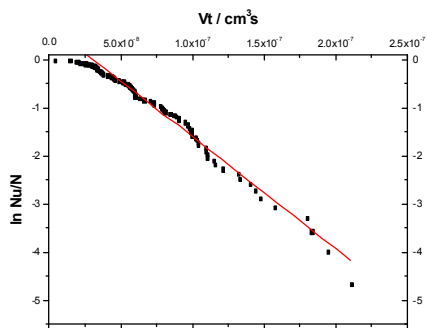




T-meas: -55.87 °C, J = (Trap B)

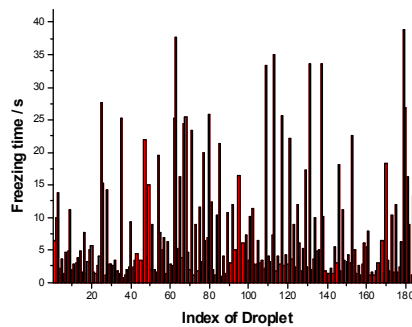
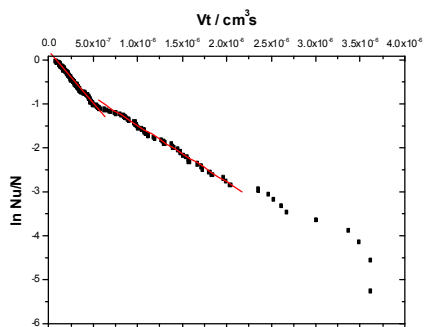


T-meas: -55.97 °C, JL= 3.58 E6, JR= 5.13 E6 (Trap B)

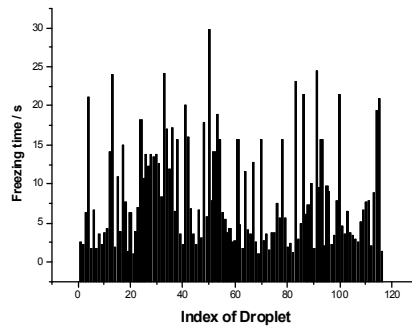
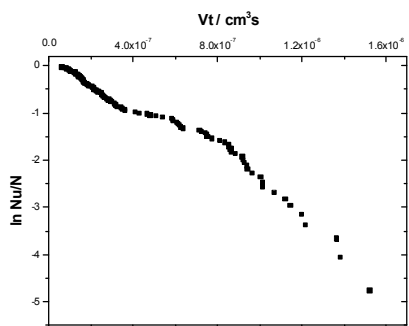


T-meas: -56.16 °C, JR= 2.32 E7 (Trap B)

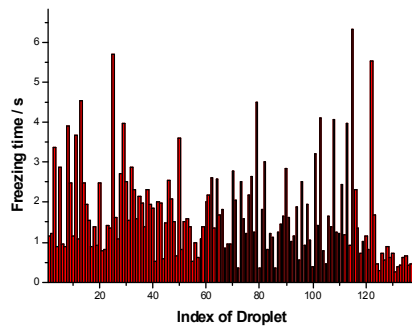
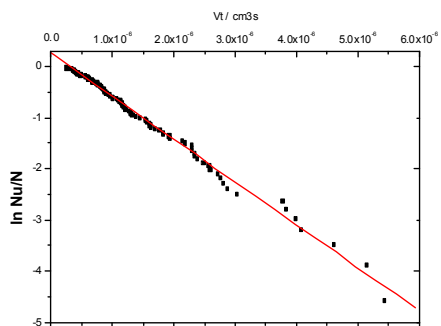
Water + 1, 4-Dioxane Binary Liquid Mixture - $x_{\text{diox}} = 0.136$



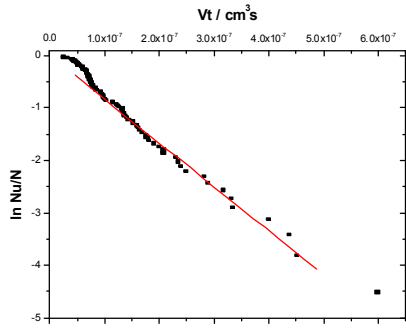
T-meas: $-55.66\text{ }^{\circ}\text{C}$, JL= 2.39 E6, JR= 1.28 E6 (Trap B)



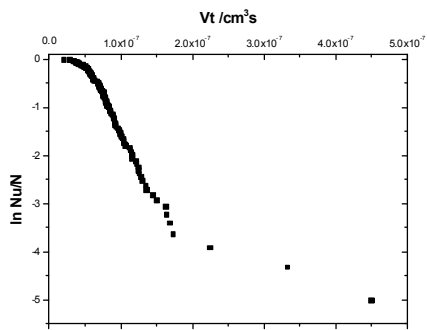
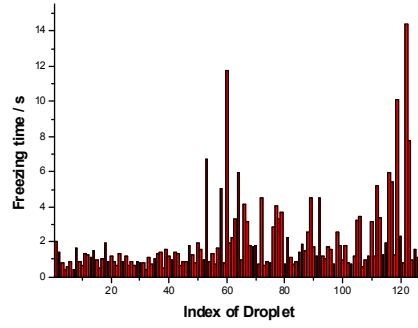
T-meas: $-55.66\text{ }^{\circ}\text{C}$ (Trap B)



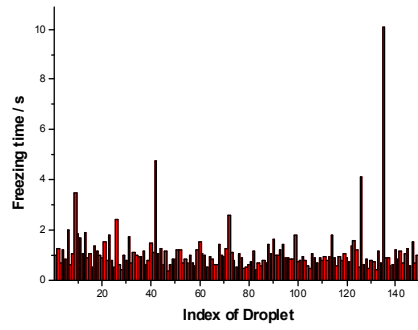
T-meas: $-55.89\text{ }^{\circ}\text{C}$, JR= 8.37 E6 (Trap B)



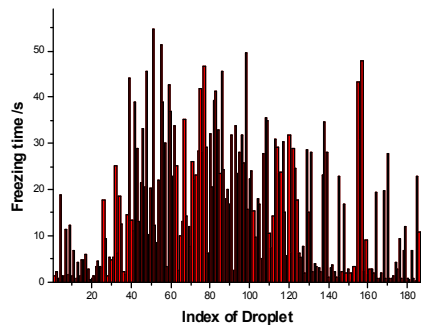
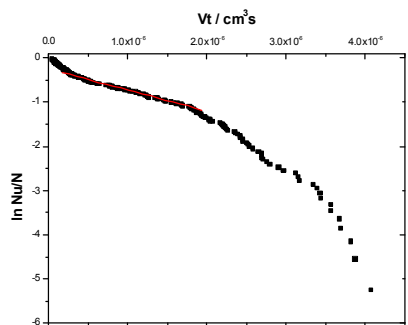
T-meas: -55.94 °C, JR= 8.36 E6 (Trap B)



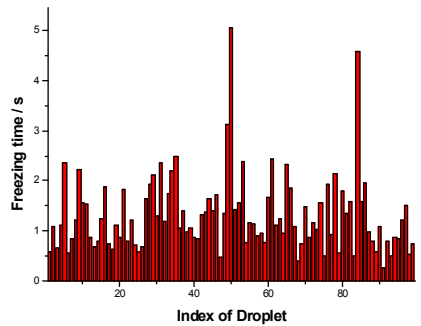
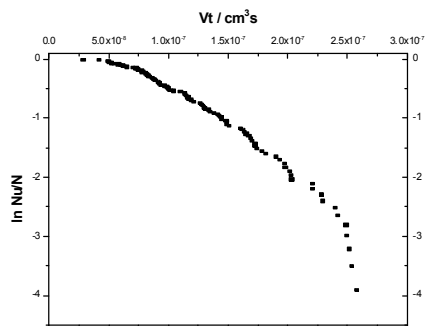
T-meas: -56.11 °C (Trap B)



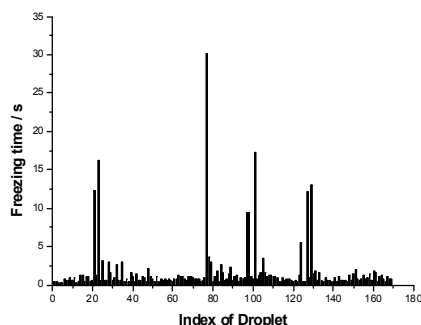
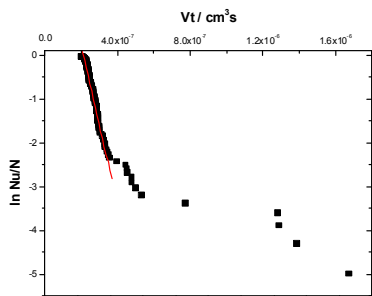
Water + 1, 4-Dioxane Binary Liquid Mixture - $x_{\text{diox}} = 0.143$



T-meas: -56.18 °C, JL= 4.79 E5 (Trap B)

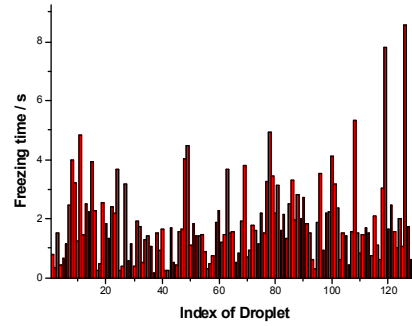
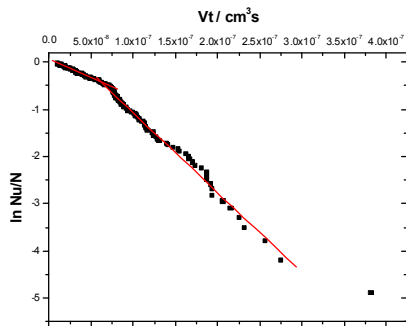


T-meas: -56.22 °C, JL= (Trap B)

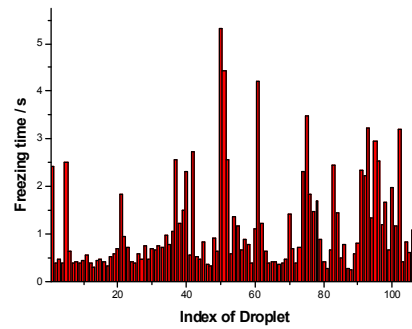
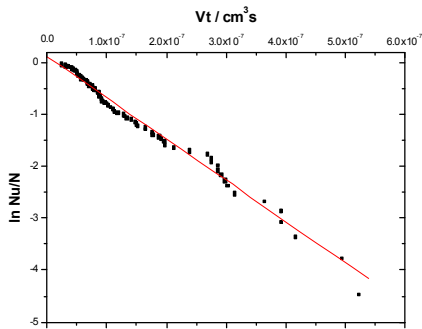


T-meas: -56.30 °C, JL= 1.63 E7 (Trap B)

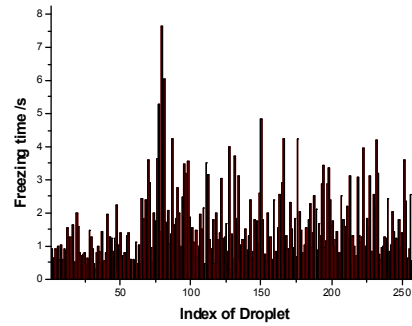
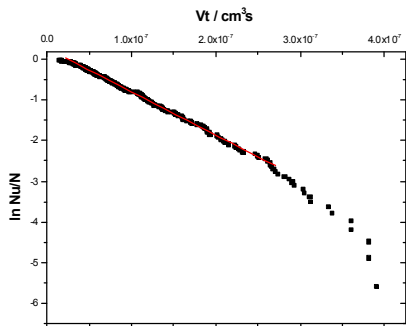
Water + 1, 4-Dioxane Binary Liquid Mixture - $x_{\text{diox}} = 0.163$



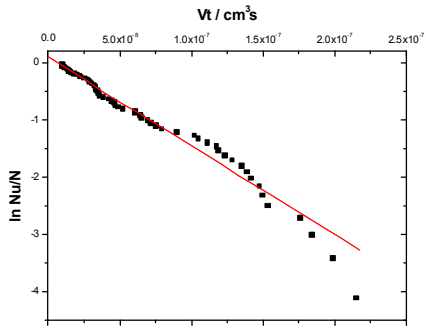
T-meas: -56.24 °C, JL=7.68 E6, JR=1.69 E7 (Trap B)



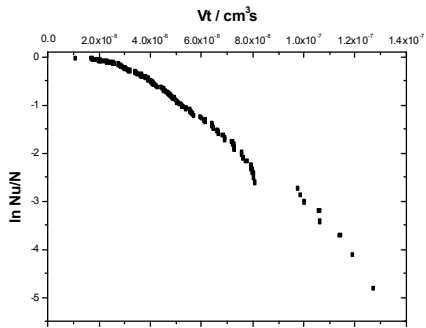
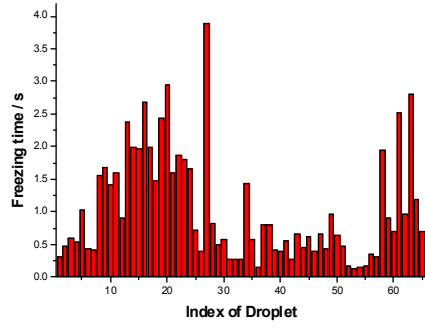
T-meas.: -56.35 °C, J = 7.95 E6 (Trap B)



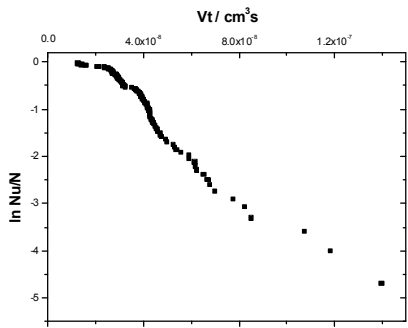
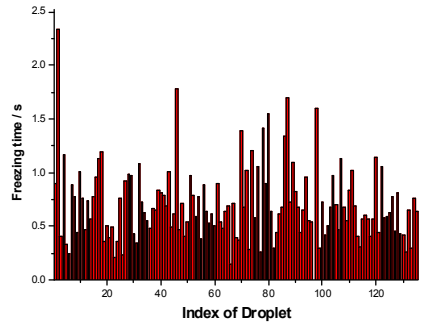
T-meas.: -56.36 °C, J = 1.07 E7 (Trap B)



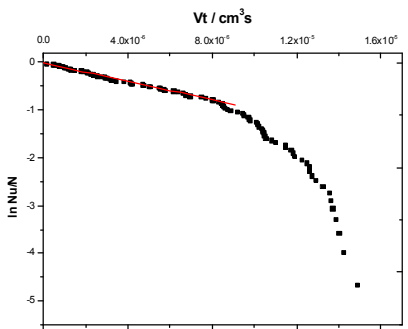
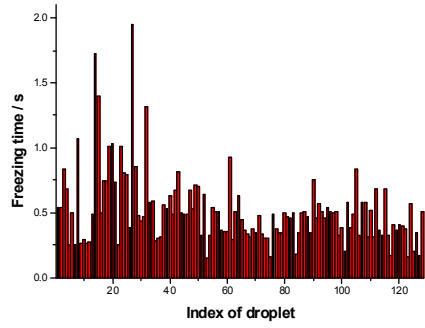
T-meas.: -56.85 °C, J = 1.54 E7 (Trap B)



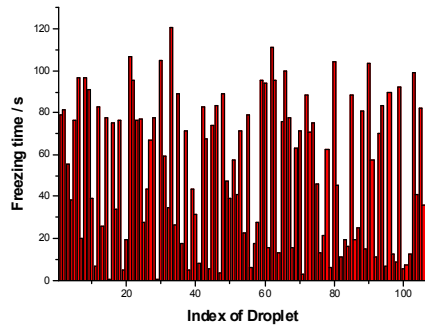
T-meas.: -56.97 (Trap B)

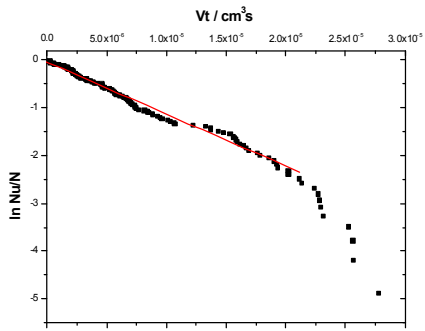


T-meas.: -57.11 (Trap B)

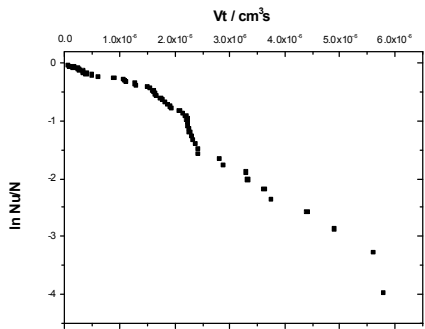
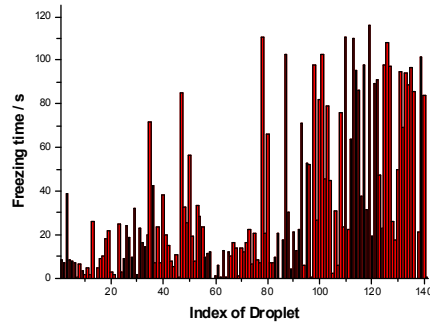


T-meas.: -56.10 °C, J = 9.67 E4 (Trap A)

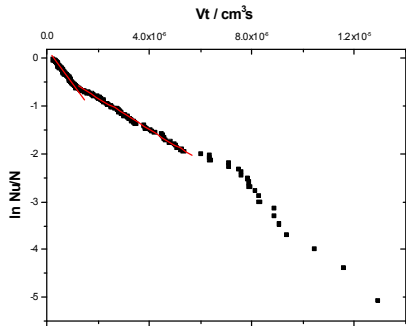
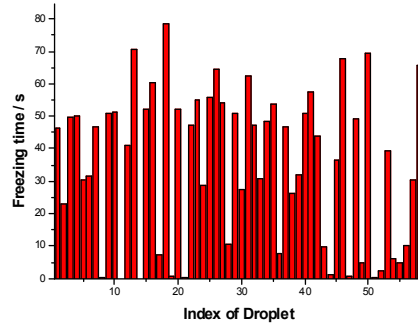




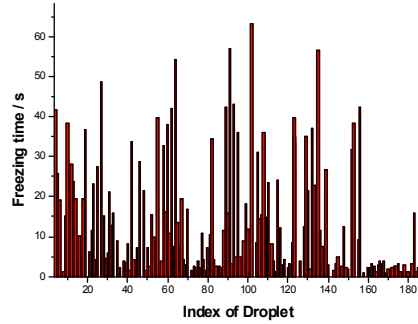
T-meas.: -56.11 °C, J = 1.09 E5 (Trap A)

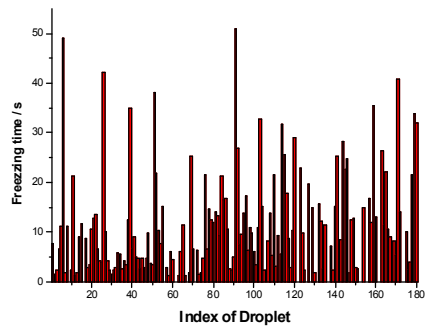
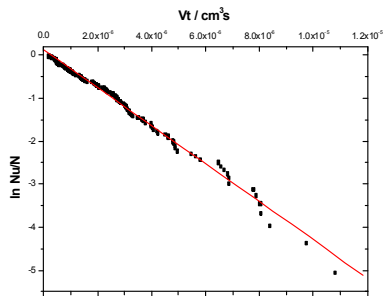


T-meas.: -56.14 °C (Trap A)

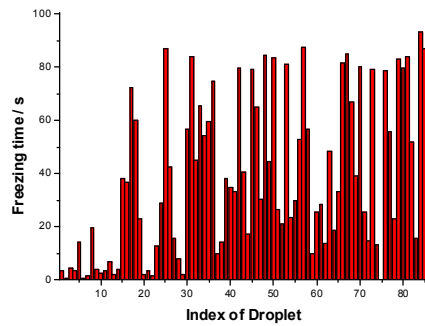
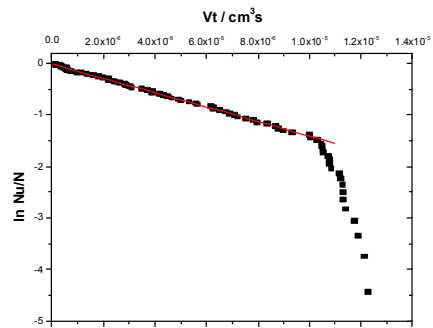


T-meas: -56.23 °C, JL=6.8 E5, JR=3.3 E5 (Trap A)

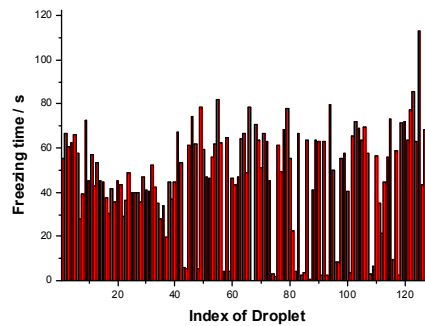
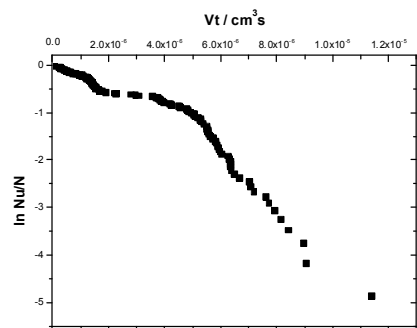




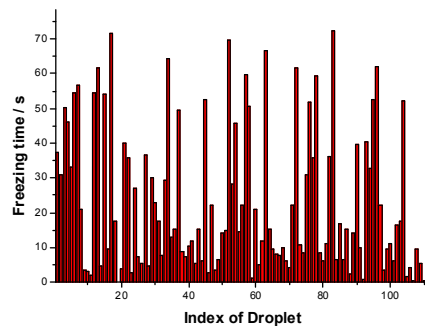
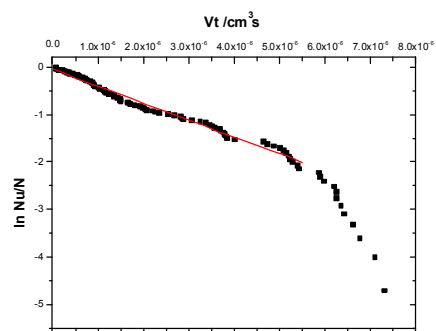
T-meas.: $-56.34\text{ }^{\circ}\text{C}$, $J = 4.42\text{ E}5$ (Trap A)



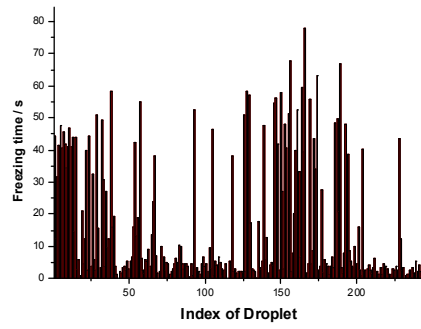
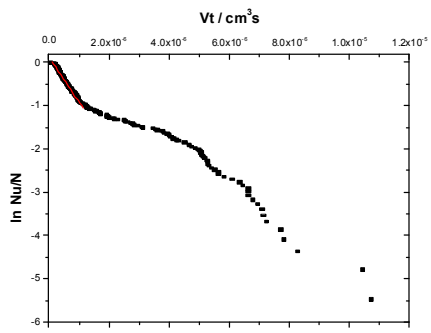
T-meas.: $-56.51\text{ }^{\circ}\text{C}$, $J = 1.39\text{ E}5$ (Trap A)



T-meas.: $-56.54\text{ }^{\circ}\text{C}$ (Trap A)

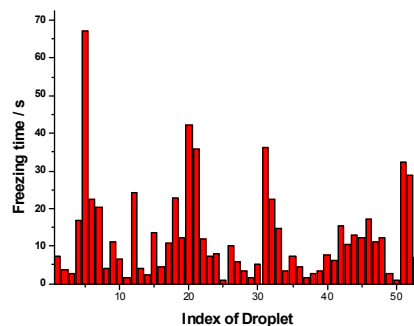
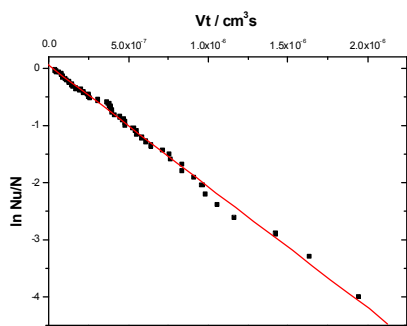


T-meas.: $-56.70\text{ }^{\circ}\text{C}$, $J = 3.57\text{ E}5$ (Trap A)

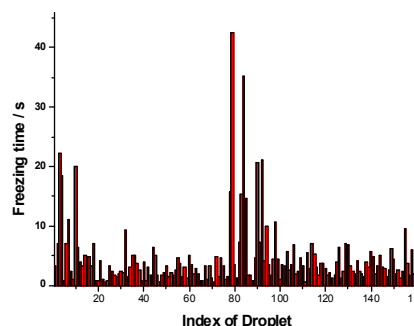
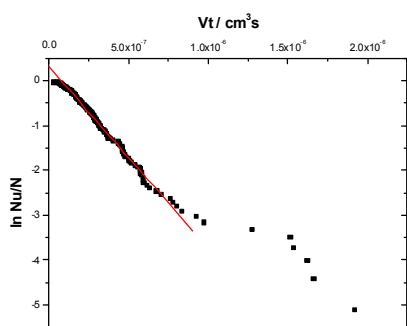


T-meas.: -56.96 °C, J = 1.04 E6 (Trap A)

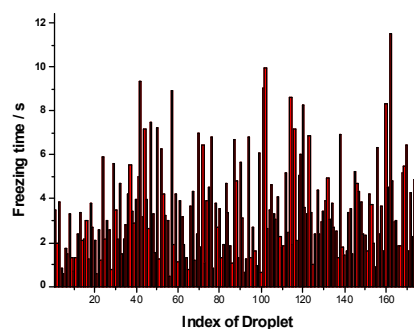
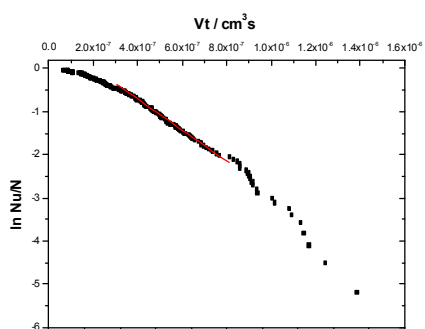
Water + 1, 4-Dioxane Binary Liquid Mixture - $x_{\text{diox}} = 0.207$



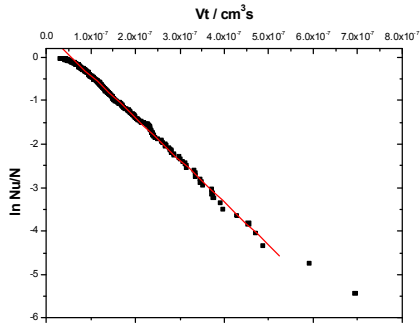
T-meas: -55.16 °C, $J = 2.12 \text{ E}6$ (Trap B)



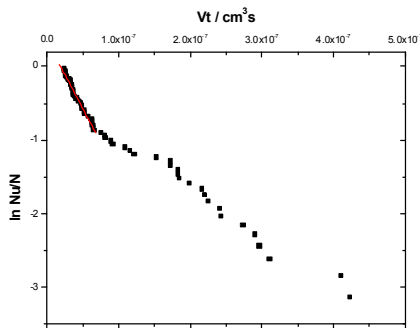
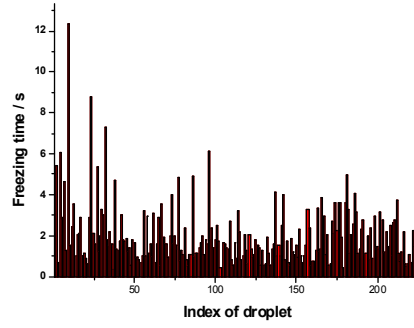
T-meas: -55.31 °C, $J = 4.05 \text{ E}6$ (Trap B)



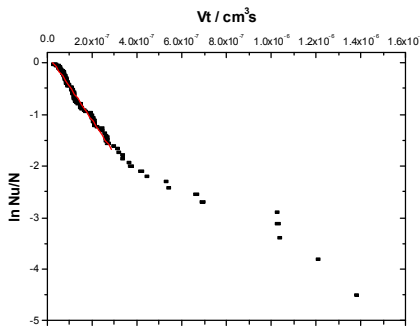
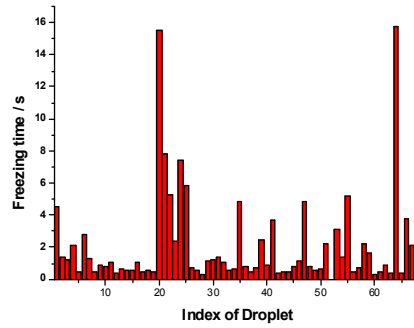
T-meas: -55.51 °C, $J_R = 5.76 \text{ E}6$ (Trap B)



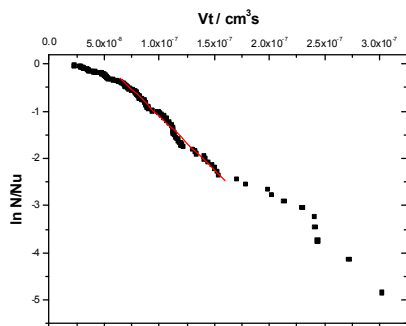
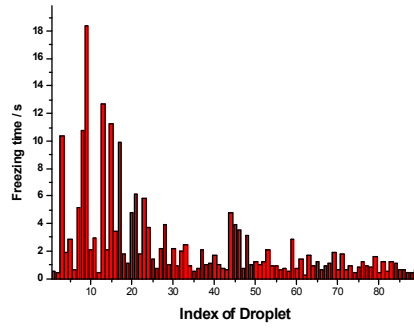
T-meas: $-55.81\text{ }^{\circ}\text{C}$, JR = $9.72\text{ E}6$ (Trap B)



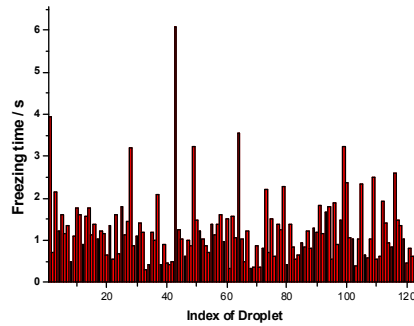
T-meas: $-55.88\text{ }^{\circ}\text{C}$, JL = $1.85\text{ E}7$ (Trap B)

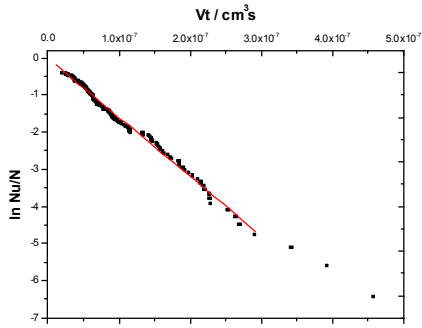


T-meas: $-56.08\text{ }^{\circ}\text{C}$, JL = $6.45\text{ E}6$ (Trap B)

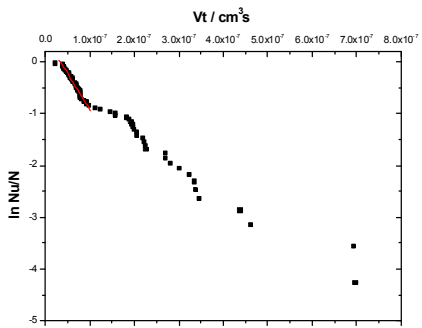
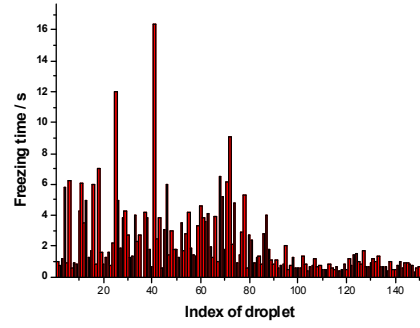


T-meas: $-56.22\text{ }^{\circ}\text{C}$, JR = $2.27\text{ E}7$ (Trap B)

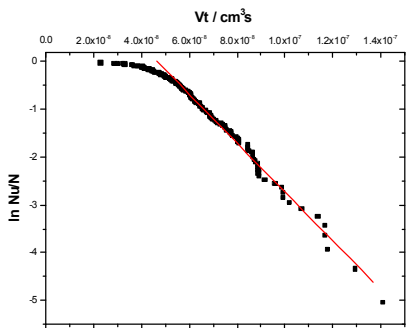
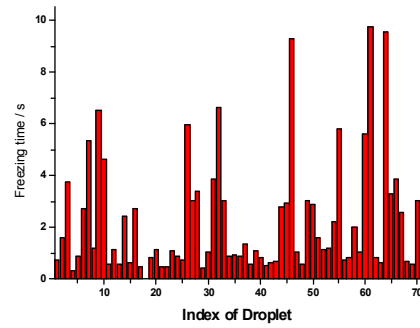




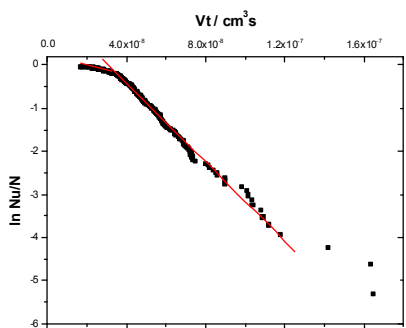
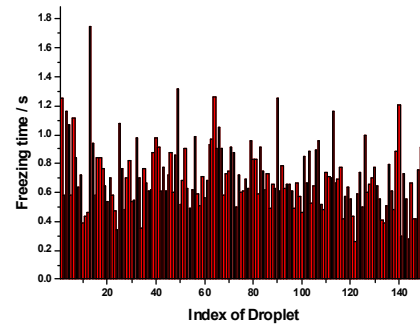
T-meas: -56.29 °C, JL = 1.33 E7 (Trap B)



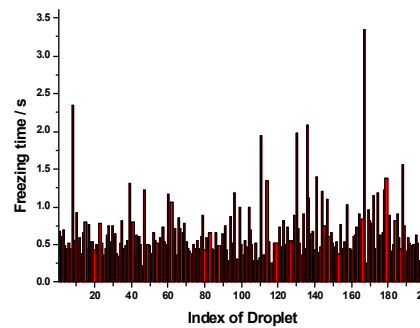
T-meas: -56.31 °C, JL = 1.4 E7 (Trap B)



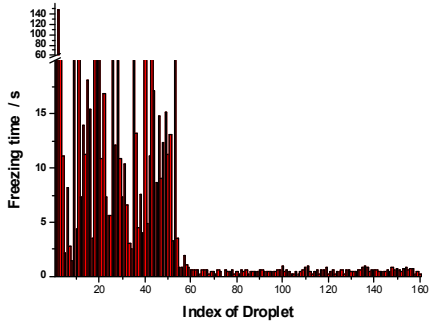
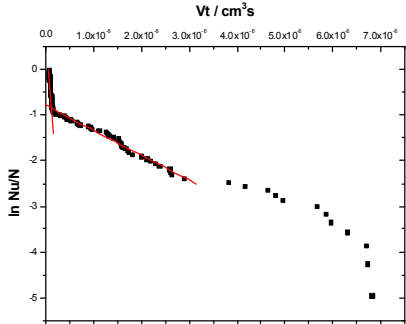
T-meas: -56.63 °C, JR = 5.14 E7 (Trap B)



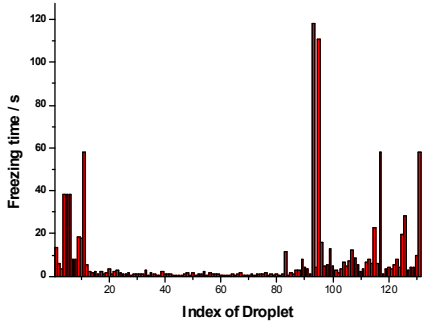
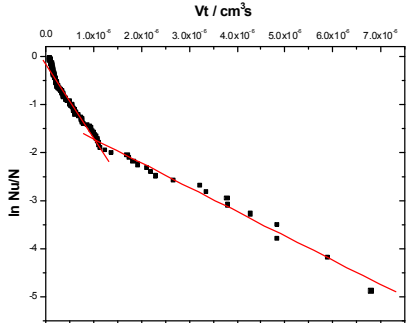
T-meas: -56.88 °C, JL= 1.06 E7, JR = 4.56 E7 (Trap B)



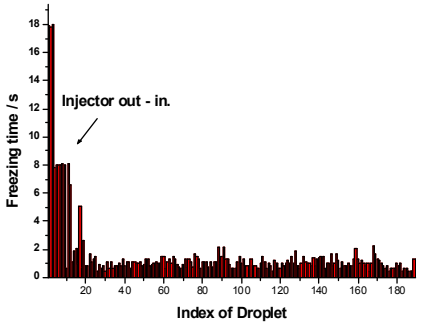
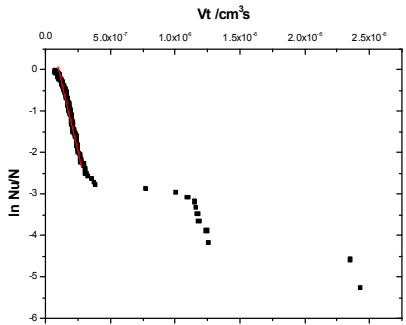
Water + 1, 4-Dioxane Binary Liquid Mixture - $x_{diox} = 0.3$



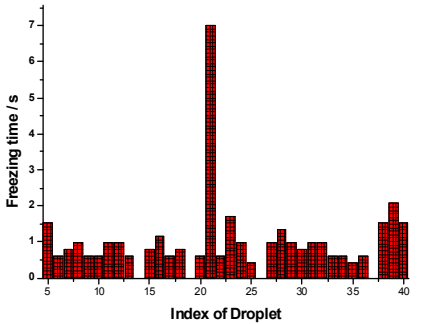
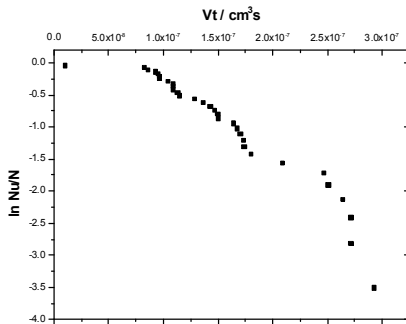
T-meas: -51.14 °C, $J_L = 1.27 \text{ E}7$, $J_R = 5.45 \text{ E}5$ (Trap A)



T-meas: -51.44 °C, $J_L = 1.56 \text{ E}6$, $J_R = 5.05 \text{ E}5$ (Trap A)

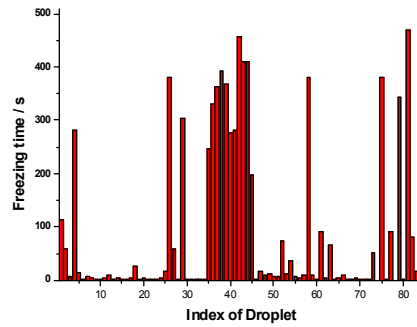
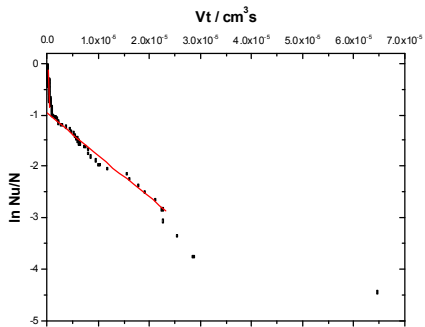


T-meas: -51.84 °C, $J_R = 1.33 \text{ E}7$ (Trap A)

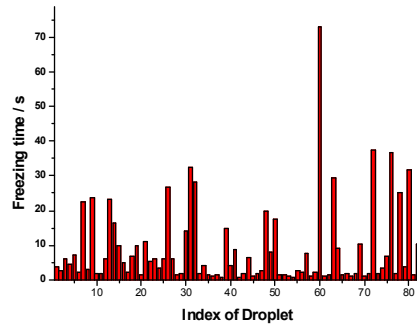
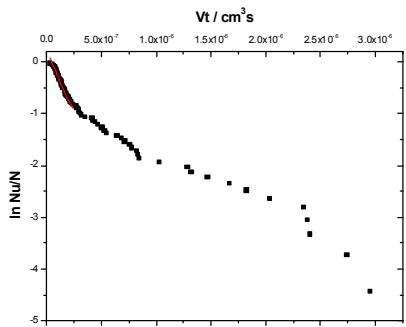


T-meas: -53.65 °C (Trap A)

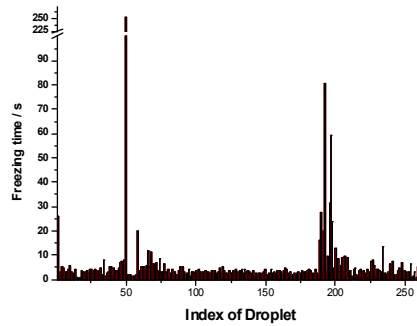
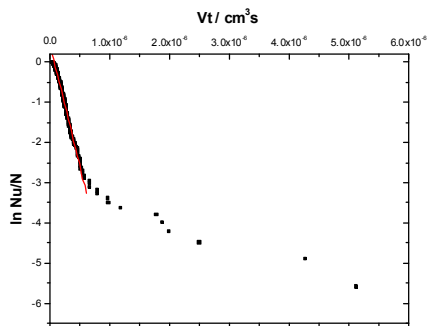
Water + 1, 4-Dioxane Binary Liquid Mixture - $x_{\text{diox}} = 0.363$



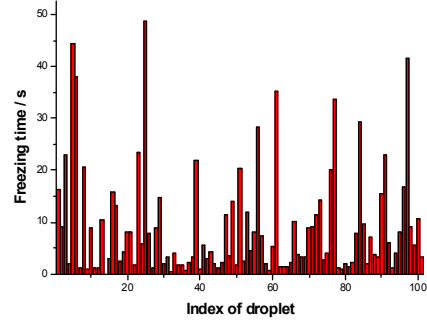
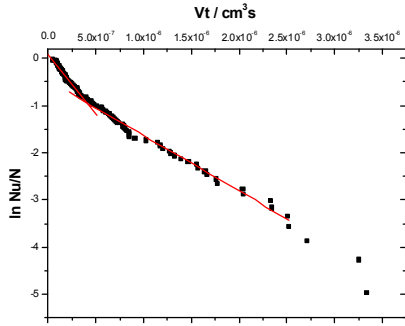
T-meas: $-51.61\text{ }^{\circ}\text{C}$, $J_L = 1.90\text{ E}6$, $J_R = 8.18\text{ E}4$ (Trap B)



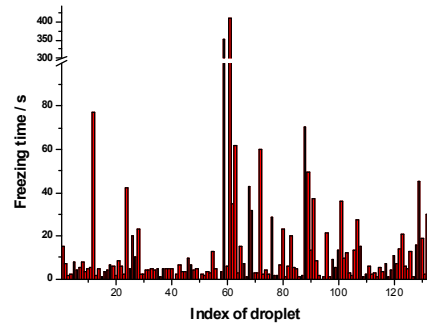
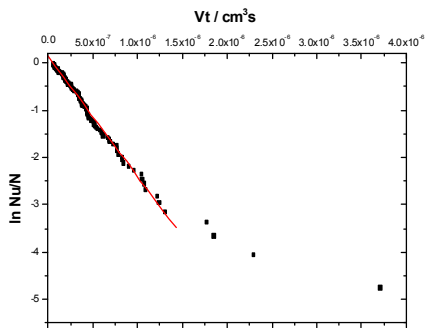
T-meas: $-51.68\text{ }^{\circ}\text{C}$, $J_L = 4.64\text{ E}6$ (Trap B)



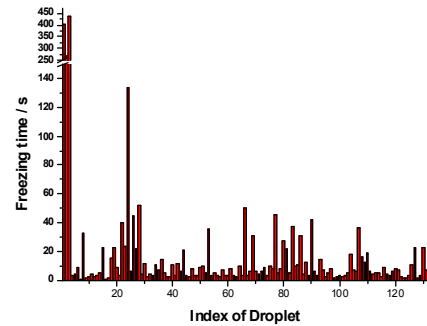
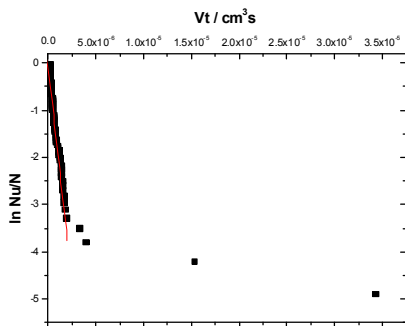
T-meas: $-51.70\text{ }^{\circ}\text{C}$, $J_L = 6.03\text{ E}6$ (Trap B)



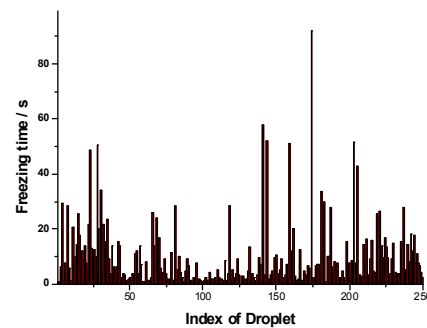
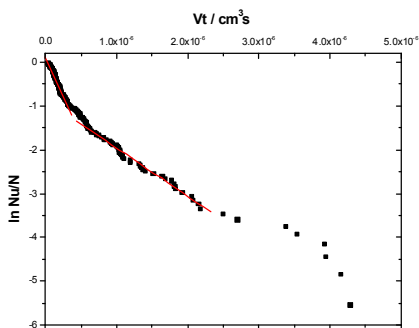
T-meas: $-51.72\text{ }^{\circ}\text{C}$, $J_L = 2.70\text{ E}6$, $J_R = 1.17\text{ E}6$ (Trap B)



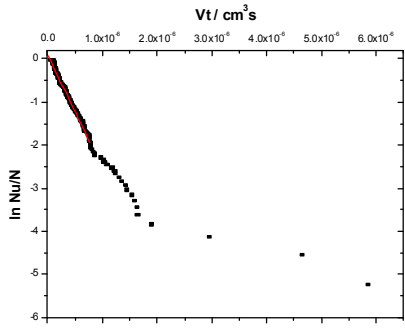
T-meas: $-51.84\text{ }^{\circ}\text{C}$, $J = 2.54\text{ E}6$ (Trap B)



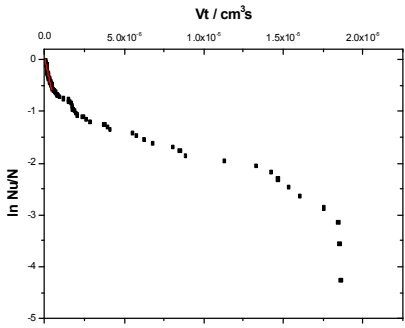
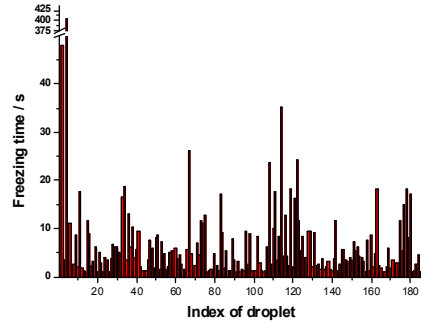
T-meas: -51.87°C , $J_L = 1.79\text{ E}6$ (Trap B)



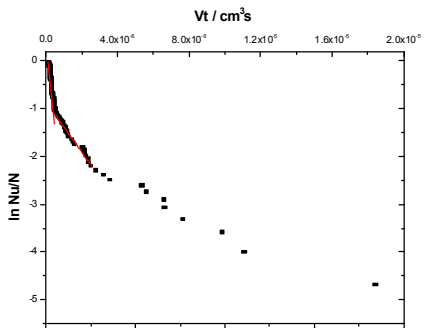
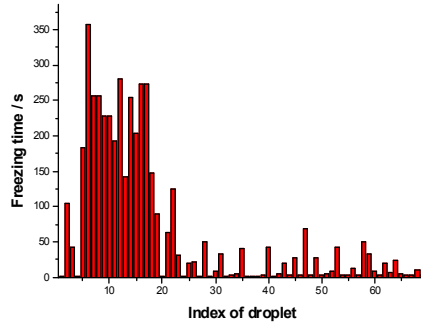
T-meas: $-52.03\text{ }^{\circ}\text{C}$, $J_L = 3.65\text{ E}6$, $J_R = 1.10\text{ E}6$ (Trap B)



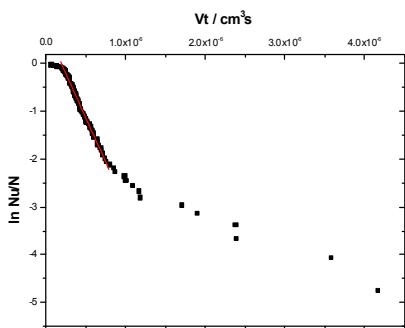
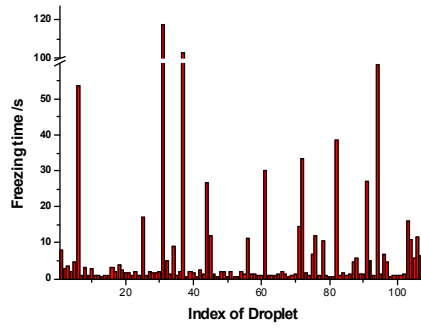
T-meas: -52.04 °C, $J_L = 2.63 \text{ E6}$ (Trap B)



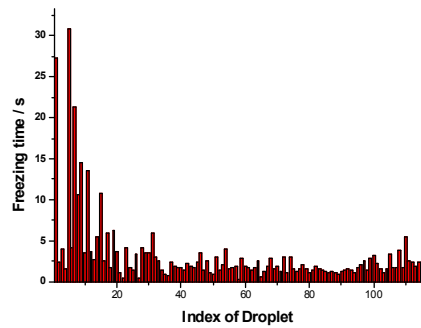
T-meas: -52.11 °C, $J_L = 1.41 \text{ E6}$ (Trap B)

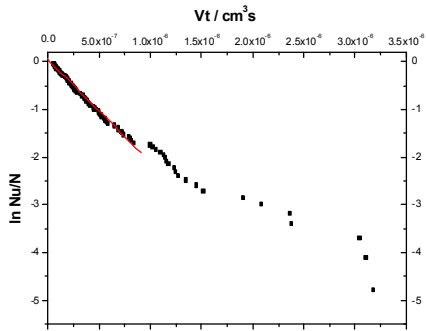


T-meas: -52.12 °C, $J_L = 3.03 \text{ E6}$, $J_R = 5.22 \text{ E5}$ (Trap B)

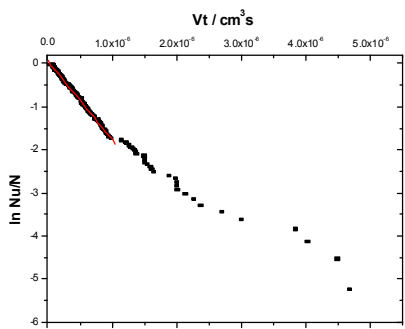
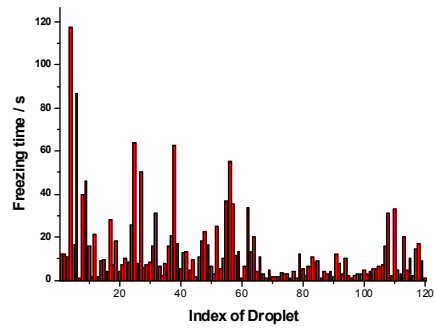


T-meas: -52.14 °C, $J_R = 3.73 \text{ E6}$ (Trap B)

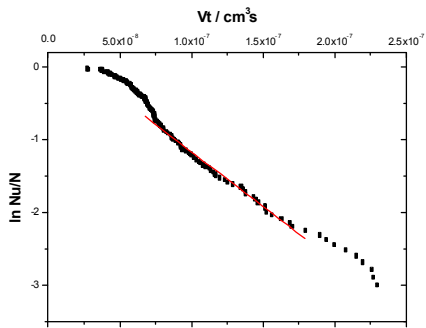
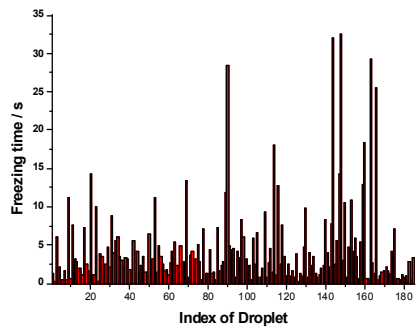




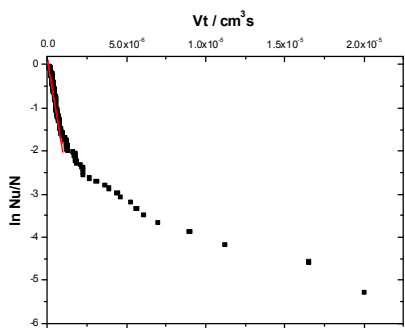
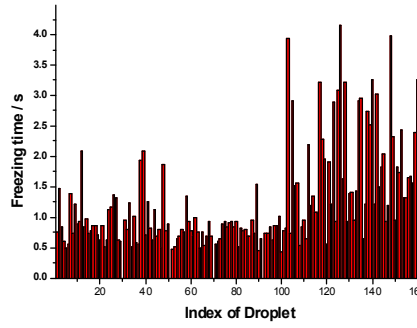
T-meas: -52.24 °C, $J_L = 2.15 \text{ E6}$ (Trap B)



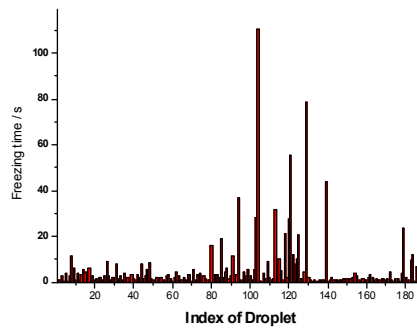
T-meas: -52.26 °C, $J_L = 1.85 \text{ E6}$ (Trap B)

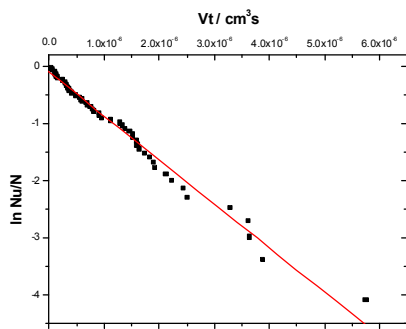


T-meas: -52.27 °C, $J_L = 1.50 \text{ E7}$ (Trap B)

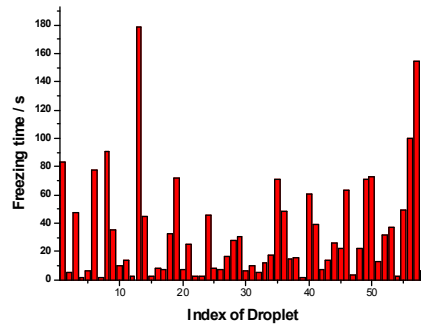


T-meas: -52.41 °C, $J_L = 2.25 \text{ E6}$ (Trap B)

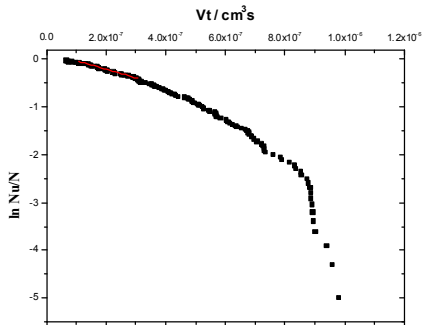




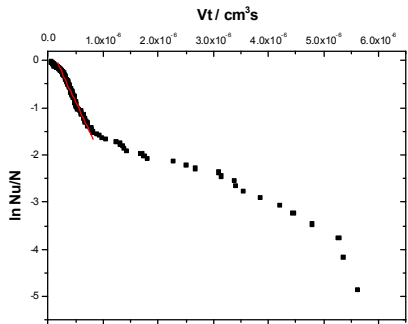
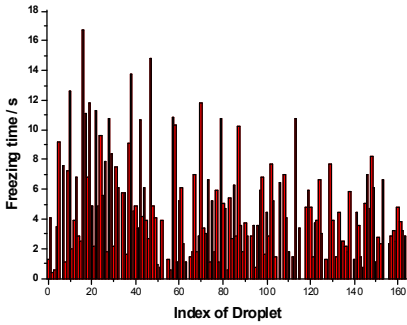
T-meas: -52.75 °C, J = 7.68 E5 (Trap B)



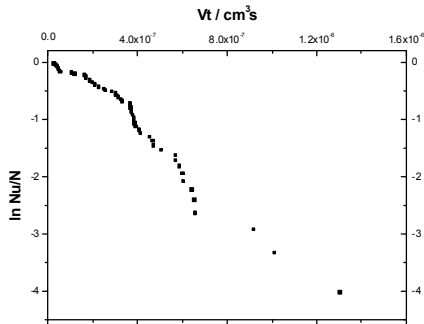
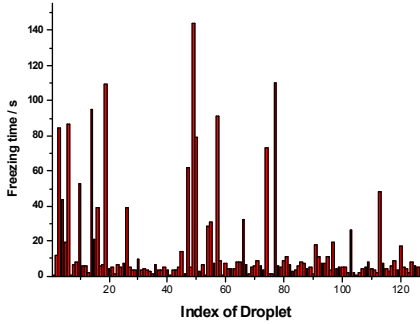
Water + 1, 4-Dioxane Binary Liquid Mixture - $x_{\text{diox}} = 0.477$



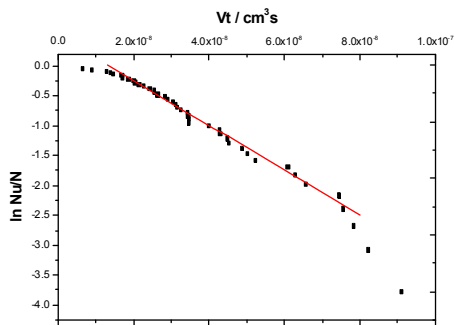
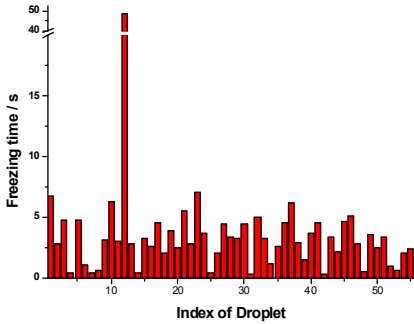
T-meas: -36.92 °C, $J_L=1.73 \text{ E}6$ (Trap A)



T-meas: -47.06 °C, $J_2=2.51 \text{ E}6$ (Trap B)



T-meas: -47.33 °C (Trap B)



T-meas: -47.69 °C, $J_R=3.73 \text{ E}7$ (Trap B)

