

Supplementary Material for

The structure and size of some hydrated ions and the ions channels selectivity

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Instructions:

MATLAB 7.11 R2010b was used to finish all numerical calculations and fits.

Consulting the structural parameters ¹ of the coordination shell of ions, the radii of coordinated ions, Na⁺, K⁺, Rb⁺, Cs⁺, Cl⁻, Br⁻ and I⁻ are successively taken as 0.24, 0.27, 0.29, 0.295, 0.32, 0.34 and 0.35nm. According to the spatial constraints,² when

fit the data of $\frac{P_w}{P_w^*}$ and the molarities c with equation (8), the critical volume

concentration c_{cr} of NaCl, KCl, NaBr, KBr, RbCl, RbBr, CsCl, CsBr, RbI and CsI in aqueous solution are taken as 4.73, 4.04, 4.26, 3.49, 3.66, 3.32, 3.57, 3.24, 3.17 and 3.10 M (molarity) respectively.

● The $(v_s - Hv_w)$ and v_s in aqueous solution of NaCl

Run the following program to obtain NWMS, VMS, MSMW and VMW, where dd1 and dd2, and m1 and m2 are the relative densities 1000*(d-d0), and molalities for aqueous solutions ³⁻⁴ of NaCl at 25°C respectively, d0 (0.997047) is the density (g/cm³) of pure water ⁵ used by the literatures, and 58.4428 and 18.0153 are the molar mass of NaCl and water respectively.

```
d0=0.997047;
dd1=[0.415 1.650 2.380 3.261 3.905 4.611 5.089 6.508 8.094 10.205 12.132 13.333 14.580
16.965 20.126 27.378 34.436 39.432 53.636 73.625 88.787 109.459];
m1=[0.01000 0.03994 0.05773 0.07924 0.09500 0.11233 0.12410 0.15909 0.19837 0.25093
0.29918 0.32936 0.36079 0.42120 0.5018 0.6889 0.8741 1.0069 1.3923 1.9546 2.3971 3.0234];
dd2=[38.933 48.796 57.540 67.528 73.894 75.235 83.760 91.243 100.841 106.970 108.045
124.038 138.134 153.162 167.162 180.036 195.522];
m2=[0.99472 1.26102 1.50179 1.78243 1.96500 2.00338 2.25174 2.47333 2.76245 2.95143
2.98355 3.48710 3.94470 4.44730 4.93030 5.38590 5.95180];
dd=[dd1 dd2];
d=(dd+1000*d0)/1000;
m=[m1 m2];
mw=1000;
ms=58.4428*m;
NWMS=mw./ms*58.4428/18.0153;
MSMW=18.0153*ms./(mw*58.4428);
VMW=18.0153*(ms+mw)/(d.*mw);
VMS=58.4428*(ms+mw)/(d.*ms);
```

Fit the data of VMS and NWMS, VMW and MSMW with equation (4) and (5) respectively, where confidence level: 99% and custom equation: $y=a*x+b$. The results are as follow respectively.

For equation (4):

General model:

$$f(x) = a*x+b$$

Coefficients (with 99% confidence bounds):

$$a = 18.07 \quad (18.07, 18.07)$$

$$b = 18.97 \quad (18.42, 19.53)$$

Goodness of fit:

SSE: 54.35

R-square: 1

Adjusted R-square: 1

RMSE: 1.212

For equation (5):

General model:

$$f(x) = a*x+b$$

Coefficients (with 99% confidence bounds):

$$a = 20.8 \quad (20.43, 21.17)$$

$$b = 18.04 \quad (18.03, 18.06)$$

Goodness of fit:

SSE: 0.01802

R-square: 0.9985

Adjusted R-square: 0.9984

RMSE: 0.02237

Further run the following program to obtain the c corresponding to $\frac{P_w}{P_w^*}(a)^6$ for

aqueous solution of NaCl at molalities (mp), where c is the volume concentration ($mol \cdot dm^{-3}$) and 3.1686kPa is the vapor pressure of pure water⁵ at 25°C.

```
cor=spline(m,d);
```

```
mp=[0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8 3.0 3.2 3.4 3.6 3.8 4.0 4.2 4.4 4.6 4.8 5.0 5.2];
```

```
dp=ppval(cor,mp);
```

```
a=[3.1476 3.1268 3.1058 3.0846 3.0631 3.0413 3.0192 2.9968 2.9740 2.9509 2.9274 2.9035 2.8793 2.8547 2.8298 2.8044 2.7786 2.7525 2.7259 2.6989 2.6716 2.6438 2.6156 2.5871 2.5581 2.5287]/3.1686;
```

```
c=mp.*dp./(mp*58.4428+1000)*1000;
```

Fit the data of a and c with equation (8), where confidence level: 99%, custom equation: $y = (1-vs*x)^{(2/3)}+b1*(1-\exp(-b2*x))*x^{(2/3)}$ and start: $b1=0.1$, $b2=1$, $vs=0.1$. The result is as follow.

General model:

$$f(x) = (1-vs*x)^{(2/3)}+b1*(1-\exp(-b2*x))*x^{(2/3)}$$

Coefficients (with 99% confidence bounds):

$b_1 = 0.02852$ (0.02449, 0.03255)
 $b_2 = 1.532$ (1.257, 1.807)
 $v_s = 0.08327$ (0.07994, 0.08661)

Goodness of fit:

SSE: 2.024e-005

R-square: 0.9998

Adjusted R-square: 0.9998

RMSE: 0.000938

(Here the highest c is 4.6735M)

● **The $(v_s - Hv_w)$ and v_s in aqueous solution of KCl**

Run the following program to obtain NWMS, VMS, MSMW and VMW, where dd1 and dd2, and m1 and m2 are the relative densities ($1000*(d-d_0)$), and molalities for aqueous solutions⁷⁻⁸ of KCl respectively, 0.997045 (d_0) is the density (g/cm^3) of pure water⁵ at 25°C used by the literatures, and 74.5513 and 18.0153 are the molar mass of KCl and water respectively.

```

d0=0.997045;
dd1=[4.681 9.270 14.008 18.392 23.004 27.894 32.693 36.996 41.401 44.656];
m1=[0.09974 0.19910 0.30304 0.40037 0.50389 0.61488 0.72503 0.82477 0.92801 1.00491];
dd2=[2.387 2.644 4.086 4.514 20.064 20.678 39.660 40.133 59.700 59.925 78.205 97.981 98.280
116.628 117.065 134.965 135.138 152.558 153.399 167.300 167.566];
m2=[0.05103 0.05581 0.08769 0.09635 0.43865 0.45498 0.89356 0.90321 1.37765 1.38366
1.84381 2.36692 2.37450 2.88083 2.89358 3.41002 3.41230 3.93177 3.95785 4.40004 4.40058];
dd=[dd1 dd2];
d=(dd+1000*d0)/1000;
m=[m1 m2];
mw=1000
ms=74.5513*m
NWMS=mw./ms*74.5513/18.0153
VMS=74.5513*(ms+mw)/(d.*ms)
MSMW=18.0153*ms/(mw*74.5513)
VMW=18.0153*(ms+mw)/(d.*mw)
  
```

Fit the data of VMS and NWMS, VMW and MSMW with equation (4) and (5) respectively, where confidence level: 99%, and custom equation: $y=a*x+b$. The results are as follow respectively.

For equation (4):

General model:

$$f(x) = a*x+b$$

Coefficients (with 99% confidence bounds):

a = 18.07 (18.06, 18.07)
b = 29.66 (29.08, 30.24)

Goodness of fit:

SSE: 28.2

R-square: 1

Adjusted R-square: 1

RMSE: 0.986

For equation (5):

General model:

$$f(x) = a \cdot x + b$$

Coefficients (with 99% confidence bounds):

a = 31.23 (30.92, 31.54)

b = 18.04 (18.03, 18.05)

Goodness of fit:

SSE: 0.007596

R-square: 0.9996

Adjusted R-square: 0.9996

RMSE: 0.01618

Further run the following program to obtain the c corresponding to $\frac{P_w}{P_w^*}(a)^6$ for

aqueous solution of KCl at molalities (mp), where c is the volume concentration ($mol \cdot dm^{-3}$) and 3.1686kPa is the vapor pressure of pure water⁵ at 25°C.

cor=spline(m,d);

mp=[0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8 3.0 3.2 3.4 3.6 3.8 4.0 4.4];

dp=ppval(cor,mp)

a=[3.1478 3.1275 3.1074 3.0873 3.0672 3.0471 3.0270 3.0068 2.9865 2.9662 2.9458 2.9253
2.9048 2.8841 2.8634 2.8425 2.8215 2.8004 2.7792 2.7579 2.7148]/3.1686;

c=mp.*dp./(mp*74.5513+1000)*1000

Fit the data of a and c with equation (8), where confidence level: 99%, custom

equation: $y = (1-vs \cdot x)^{2/3} + b1 \cdot (1 - \exp(-b2 \cdot x)) \cdot x^{2/3}$ and start: b1=0.1, b2=1,

vs=0.1. The result is as follow.

General model:

$$f(x) = (1 - vs \cdot x)^{2/3} + b1 \cdot (1 - \exp(-b2 \cdot x)) \cdot x^{2/3}$$

Coefficients (with 99% confidence bounds):

b1 = 0.01368 (0.0107, 0.01666)

b2 = 1.713 (1.356, 2.07)

vs = 0.06534 (0.06256, 0.06811)

Goodness of fit:

SSE: 3.19e-006

R-square: 0.9999

Adjusted R-square: 0.9999

RMSE: 0.000421

(Here the highest c is 3.8576M)

● **The ($v_s - Hv_w$) and v_s in aqueous solution of NaBr**

Run the following program to obtain NWMS, VMS, MSMW and VMW, where dd1 and dd2, and m1 and m2 are the relative densities ($1000*(d-d_0)$), and molalities for aqueous solutions ^{3,9} of NaBr respectively, 0.997047 (d_0) is the density (g/cm^3) of pure water ⁵ at 25°C used by the literatures, and 102.8938 and 18.0153 are the molar mass of NaBr and water respectively.

d0=0.997047

dd1=[2.222 3.260 5.452 7.653 9.764 12.601 15.422 19.729 25.807 28.677 32.596 7.939 15.676 30.900 45.975 60.687 75.967];

m1=[0.02800 0.04117 0.06911 0.09728 0.12439 0.16096 0.19744 0.25335 0.33265 0.37026 0.42177 0.10095 0.20072 0.39946 0.59905 0.7967 1.0054];

dd2=[75.07 116.68 144.25 171.34 209.64 239.99 271.51 342.50];

m2=[1.0000 1.5797 1.9972 2.4066 3.001 3.4833 3.9955 5.1927];

dd=[dd1 dd2];

m=[m1 m2];

d=(dd+1000*d0)/1000;

ms= 102.8938*m

mw=1000

NWMS=ms./m1* 102.8938/18.0153

MSMW=18.0153*ms./(mw* 102.8938)

VMW=18.0153*(ms+mw)/(d.*mw)

VMS= 102.8938*(ms+mw)/(d.*ms)

Fit the data of VMS and NWMS, VMW and MSMW with equation (4) and (5) respectively, where confidence level: 99% and custom equation: $y=a*x+b$. The results are as follow respectively.

For equation (4):

General model:

$$f(x) = a*x+b$$

Coefficients (with 99% confidence bounds):

$$a = 18.07 \quad (18.07, 18.07)$$

$$b = 25.68 \quad (24.97, 26.39)$$

Goodness of fit:

SSE: 24.84

R-square: 1

Adjusted R-square: 1

RMSE: 1.039

For equation (5):

General model:

$$f(x) = a*x+b$$

Coefficients (with 99% confidence bounds):

a = 27.48 (27.2, 27.75)

b = 18.05 (18.04, 18.06)

Goodness of fit:

SSE: 0.003526

R-square: 0.9997

Adjusted R-square: 0.9997

RMSE: 0.01238

Further run the following program to obtain the c corresponding to $\frac{p_w}{p_w^*} (a)^{10}$ for aqueous solution of NaBr at molalities (mp), where c is the volume concentration ($mol \cdot dm^{-3}$) and 3.1686kPa is the vapor pressure of pure water⁵ at 25°C.

```
cor=spline(m,d);
```

```
mp=[0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.2 1.4 1.6 1.8 2.0 2.5 3.0 3.5 4.0 4.5];
```

```
dp=ppval(cor,mp);
```

```
a=[3.1579 3.1474 3.1369 3.1263 3.1156 3.1049 3.0940 3.0830 3.0718 3.0606 3.0378 3.0146  
2.9908 2.9666 2.9419 2.8780 2.8110 2.7409 2.6678 2.5917]/3.1686;
```

```
c=mp.*dp./(mp*102.8938+1000)*1000;
```

Fit the data of a and c with equation (8), where confidence level: 99%, custom equation: $y = (1-vs*x)^{(2/3)}+b1*(1-\exp(-b2*x))*x^{(2/3)}$ and start: $b1=0.1$, $b2=1$, $vs=0.1$. The result is as follow.

General model:

$$f(x) = (1-vs*x)^{(2/3)}+b1*(1-\exp(-b2*x))*x^{(2/3)}$$

Coefficients (with 99% confidence bounds):

b1 = 0.02914 (0.02399, 0.03429)

b2 = 2.218 (1.719, 2.716)

vs = 0.08892 (0.08422, 0.09361)

Goodness of fit:

SSE: 1.764e-005

R-square: 0.9997

Adjusted R-square: 0.9996
 RMSE: 0.001019
 (Here the highest c is 3.9954M)

● **The $(v_s - Hv_w)$ and v_s in aqueous solution of KBr**

Run the following program to obtain NWMS, VMS, MSMW and VMW, where dd1 and d2, and c1 and c2 are the relative densities ($1000*(d-d_0)$) and the densities (d), and molarities for aqueous solutions ^{3, 11} of KBr respectively, 0.997047 (d_0) is the density (g/cm^3) of pure water ⁵ at 25°C used by the literature³, and 119.0023 and 18.0153 are the molar mass of KBr and water respectively.

```
d0=0.997047
dd1=[5.076 9.203 16.320 20.892 26.630 33.139 49.256 65.092 79.316];
d1=(dd1+1000*d0)/1000;
c1=[0.05975 0.10855 0.19289 0.24722 0.31552 0.39315 0.5859 0.7760 0.9472];
d2=[1.000089 1.000160 1.000417 1.000841 1.001695 1.004256 1.008492 1.016955 1.042194
1.080449 1.083718 1.166031 1.166167 1.249592 1.307264];
c2=[0.001000 0.002000 0.005000 0.010005 0.020001 0.050001 0.099899 0.199882 0.499927
0.959172 0.998357 1.999826 2.003090 3.030933 3.749274];
c=[c1 c2];
d=[d1 d2*d0];
ms= 119.0023*c
mw=d*1000-ms
m=ms./mw*1000/119.0023
NWMS=mw./ms*119.0023/18.0153
MSMW=18.0153*ms./(mw*119.0023)
VMW=18.0153*(ms+mw)/(d.*mw)
VMS=119.0023*(ms+mw)/(d.*ms)
```

Fit the data of VMS and NWMS, VMW and MSMW with equation (4) and (5) respectively, where confidence level: 99%, and custom equation: $y=a*x+b$. The results are as follow respectively.

For equation (4):

General model:

$$f(x) = a*x+b$$

Coefficients (with 99% confidence bounds):

$$a = 18.07 \quad (18.07, 18.07)$$

$$b = 35.37 \quad (34.43, 36.32)$$

Goodness of fit:

SSE: 51.78

R-square: 1

Adjusted R-square: 1

RMSE: 1.534

For equation (5):

General model:

$$f(x) = a \cdot x + b$$

Coefficients (with 99% confidence bounds):

$$a = 37.14 \quad (36.75, 37.53)$$

$$b = 18.06 \quad (18.05, 18.07)$$

Goodness of fit:

SSE: 0.004191

R-square: 0.9997

Adjusted R-square: 0.9997

RMSE: 0.0138

Further run the following program to obtain the c corresponding to $\frac{P_w}{P_w^*} (a)^{10}$ for aqueous solution of KBr at molalities (mp), where c is the volume concentration ($mol \cdot dm^{-3}$) and 3.1686kPa is the vapor pressure of pure water⁵ at 25°C.

```
m=c./mw*1000
```

```
cor=spline(m,c);
```

```
mp=[0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.2 1.4 1.6 1.8 2.0 2.5 3.0 3.5 4.0];
```

```
c=ppval(cor,mp);
```

```
a=[3.1580 3.1477 3.1375 3.1273 3.1172 3.1070 3.0969 3.0867 3.0766 3.0664 3.0460 3.0256  
3.0051 2.9846 2.9639 2.9120 2.8595 2.8065 2.7527]/3.1686;
```

Fit the data of a and c with equation (8), where confidence level: 99%, custom equation: $y = (1 - vs \cdot x)^{2/3} + b1 \cdot (1 - \exp(-b2 \cdot x)) \cdot x^{2/3}$ and start: $b1=0.1$, $b2=1$, $vs=0.1$. The result is as follow.

General model:

$$f(x) = (1 - vs \cdot x)^{2/3} + b1 \cdot (1 - \exp(-b2 \cdot x)) \cdot x^{2/3}$$

Coefficients (with 99% confidence bounds):

$$b1 = 0.01288 \quad (0.01038, 0.01537)$$

$$b2 = 2.272 \quad (1.828, 2.716)$$

$$vs = 0.06627 \quad (0.0638, 0.06875)$$

Goodness of fit:

SSE: 2.091e-006

R-square: 0.9999

Adjusted R-square: 0.9999

RMSE: 0.0003615

(Here the highest c is 3.4813M)

● **The fitted values of $(v_s - Hv_w)$ and v_s in aqueous solution of RbCl**

Run the following program to obtain NWMS, VMS, MSMW and VMW, where dd1 and d2, and m1 and ws are the relative densities ($1000*(d-d_0)$) and the densities (d), and molarities and Wt.% for aqueous solutions ^{3, 12} of RbCl respectively, 0.997047 (d0) is the density (g/cm³) of pure water ⁵ at 25°C used by the literatures, and 120.9205 and 18.0153 are the molar mass of RbCl and water respectively.

```
d0=0.997047
dd1=[1.789 2.685 3.533 4.410 5.268 7.072 7.977 14.014 21.793 34.555 50.162 67.822 83.580];
d1=(dd1+1000*d0)/1000;
m1=[0.02023 0.03039 0.04002 0.04999 0.05975 0.08034 0.09068 0.16000 0.25011 0.39774
0.5857 0.8001 0.9949];
ws=[4 6 8 10 12 14 16 18 20 22 24 26 28 35 40 45];
ww=100-ws
m2=ws./(120.9205*ww).*1000
d2=[1.02693 1.04239 1.05823 1.07448 1.09117 1.10832 1.12595 1.14408 1.16273 1.18192
1.20167 1.22201 1.24296 1.32151 1.38318 1.45018];
m=[m1 m2];
d=[d1 d2];
ms=120.9205*m
mw=1000
NWMS=mw./ms*120.9205/18.0153
MSMW=18.0153*ms./(mw*120.9205)
VMW=18.0153*(ms+mw)/(d.*mw)
VMS=120.9205*(ms+mw)/(d.*ms)
```

Fit the data of VMS and NWMS, VMW and MSMW with equation (4) and (5) respectively, where confidence level: 99%, and custom equation: $y=a*x+b$. The results are as follow respectively.

For equation (4):

General model:

$$f(x) = a*x+b$$

Coefficients (with 99% confidence bounds):

$$\begin{aligned} a &= 18.07 \quad (18.07, 18.07) \\ b &= 34.41 \quad (33.74, 35.08) \end{aligned}$$

Goodness of fit:

SSE: 34.08

R-square: 1

Adjusted R-square: 1

RMSE: 1.123

For equation (5):

General model:

$$f(x) = a*x+b$$

Coefficients (with 99% confidence bounds):

$$a = 36.68 \quad (36.19, 37.17)$$

$$b = 18.04 \quad (18.02, 18.06)$$

Goodness of fit:

SSE: 0.02312

R-square: 0.9994

Adjusted R-square: 0.9993

RMSE: 0.02927

Further run the following program to obtain the c corresponding to $\frac{P_w}{P_w^*} (a)^{13}$ for aqueous solution of RbCl at molalities (mp), where c is the volume concentration ($mol \cdot dm^{-3}$) and 3.1686kPa is the vapor pressure of pure water⁵ at 25°C.

cor=spline(m,d);

mp=[0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.2 1.4 1.6 1.8 2.0 2.5 3.0 3.5 4.0];

dp=ppval(cor,mp);

a=[3.1581 3.1480 3.1380 3.1281 3.1182 3.1083 3.0985 3.0886 3.0788 3.0689 3.0492 3.0294 3.0096 2.9897 2.9698 2.9199 2.8699 2.8197 2.7694]/3.1686;

c=mp.*dp./(mp*120.9205+1000)*1000;

Fit the data of a and c with equation (8), where confidence level: 99%, custom equation: $y = (1-v_s*x)^{2/3}+b_1*(1-\exp(-b_2*x))*x^{2/3}$, and start: $b_1=0.1$, $b_2=1$, $v_s=0.1$. The result is as follow.

General model:

$$f(x) = (1-v_s*x)^{2/3}+b_1*(1-\exp(-b_2*x))*x^{2/3}$$

Coefficients (with 99% confidence bounds):

$$b_1 = 0.01028 \quad (0.008225, 0.01233)$$

$$b_2 = 2.196 \quad (1.778, 2.614)$$

$$v_s = 0.06168 \quad (0.05964, 0.06372)$$

Goodness of fit:

SSE: 1.303e-006

R-square: 0.9999

Adjusted R-square: 0.9999

RMSE: 0.0002854

(Here the highest c is 3.4876M)

- **The fitted values of $(v_s - Hv_w)$ and v_s in aqueous solution of CsCl**

Run the following program to obtain NWMS, VMS, MSMW and VMW, where

dd1 and d2, and m1 and ws are the relative densities ($1000*(d-d_0)$) and the densities, and molarities and Wt.% for aqueous solutions^{3,12} of CsCl respectively, 0.997047 (d_0) is the density (g/cm^3) of pure water⁵ at 25°C used by the literatures, and 168.3581 and 18.0153 are the molar mass of CsCl and water respectively.

```

d0=0.997047
dd1=[1.289 5.135 7.677 10.233 31.667 50.148 74.637 98.545];
d1=(dd1+1000*d0)/1000;
m1=[0.01003 0.04002 0.05991 0.07996 0.24992 0.39896 0.5998 0.7999];
ws=[4 6 8 10 12 14 16 18 20 22 24 26 28 35 40 45 50];
ww=100-ws
m2=ws./(168.3581*ww).*1000
d2=[1.02839 1.04472 1.06153 1.07884 1.09668 1.11507 1.13404 1.15362 1.17385 1.19476
1.21638 1.23874 1.26187 1.34960 1.41964 1.49688 1.58245];
m=[m1 m2];
d=[d1 d2];
ms=168.3581*m
mw=1000
NWMS=mw./ms*168.3581/18.0153
MSMW=18.0153*ms./(mw*168.3581)
VMW=18.0153*(ms+mw)/(d.*mw)
VMS=168.3581*(ms+mw)/(d.*ms)

```

Fit the data of VMS and NWMS, VMW and MSMW with equation (4) and (5) respectively, where confidence level: 99%, and custom equation: $y=a*x+b$. The results are as follow respectively.

For equation (4):

General model:

$$f(x) = a*x+b$$

Coefficients (with 99% confidence bounds):

$$\begin{aligned}
 a &= 18.07 \quad (18.07, 18.07) \\
 b &= 41.45 \quad (40.77, 42.13)
 \end{aligned}$$

Goodness of fit:

SSE: 29.85
R-square: 1
Adjusted R-square: 1
RMSE: 1.139

For equation (5):

General model:

$$f(x) = a*x+b$$

Coefficients (with 99% confidence bounds):

$$\begin{aligned}
 a &= 43.72 \quad (43.26, 44.18) \\
 b &= 18.04 \quad (18.02, 18.05)
 \end{aligned}$$

Goodness of fit:

SSE: 0.01177

R-square: 0.9997

Adjusted R-square: 0.9997

RMSE: 0.02262

Further run the following program to obtain the c corresponding to $\frac{P_w}{P_w^*} (a)^{13}$ for aqueous solution of CsCl at molalities (mp), where c is the volume concentration ($mol \cdot dm^{-3}$) and 3.1686kPa is the vapor pressure of pure water⁵ at 25°C.

```
cor=spline(m,d);
```

```
mp=[0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.2 1.4 1.6 1.8 2.0 2.5 3.0 3.5 4.0];
```

```
dp=ppval(cor,mp);
```

```
a=[3.1582 3.1482 3.1384 3.1288 3.1192 3.1096 3.1001 3.0905 3.0810 3.0715 3.0524 3.0334  
3.0143 2.9951 2.9760 2.9278 2.8793 2.8304 2.7813]/3.1686;
```

```
c=mp.*dp./(mp*168.3581+1000)*1000;
```

Fit the data of a and c with equation (8), where confidence level: 99%, custom equation: $y = (1-vs*x)^{(2/3)} + b1*(1-\exp(-b2*x))*x^{(2/3)}$, start: $b1=0.1$, $b2=1$, $vs=0.1$, and the result is as follow.

General model:

$$f(x) = (1-vs*x)^{(2/3)} + b1*(1-\exp(-b2*x))*x^{(2/3)}$$

Coefficients (with 99% confidence bounds):

$b1 =$ 0.01297 (0.01011, 0.01583)

$b2 =$ 2.09 (1.692, 2.488)

$vs =$ 0.06395 (0.06111, 0.06679)

Goodness of fit:

SSE: 2.141e-006

R-square: 0.9999

Adjusted R-square: 0.9999

RMSE: 0.0003658

(Here the highest c is 3.4019M)

● The fitted values of $(v_s - Hv_w)$ and v_s in aqueous solution of RbBr

Run the following program to obtain NWMS, VMS, MSMW and VMW, where $dd1$ and $d2$, and $m1$ and ws are the relative densities ($1000*(d-d_0)$) and the densities (d), and molarities and Wt.% for aqueous solutions^{3,12} of RbBr respectively, 0.997047 (d_0) is the density (g/cm^3) of pure water⁵ at 25°C used by the literatures, and 165.3718 and 18.0153 are the molar mass of RbBr and water respectively.

d0=0.997047

```
dd1=[5.060 6.328 8.756 11.268 12.532 15.012 17.489 27.367 39.548 58.919 87.364 115.211];
d1=(dd1+1000*d0)/1000;
m1=[0.04026 0.05038 0.06979 0.08992 0.09999 0.12000 0.13996 0.21998 0.31961 0.47998
0.7199 0.9600];
ws=[4 6 8 10 12 14 16 18 20 22 24 26 28 35 40 45 50];
ww=100-ws
m2=ws./(165.3718*ww).*1000
d2=[1.02833 1.04464 1.06143 1.07872 1.09653 1.11489 1.13383 1.15338 1.17357 1.19443
1.21600 1.23832 1.26143 1.34917 1.41924 1.49654 1.58222];
m=[m1 m2];
d=[d1 d2];
ms=165.3718*m
mw=1000
NWMS=mw./ms*165.3718/18.0153
MSMW=18.0153*ms./(mw*165.3718)
VMW=18.0153*(ms+mw)/(d.*mw)
VMS=165.3718*(ms+mw)/(d.*ms)
```

Fit the data of VMS and NWMS, VMW and MSMW with equation (4) and (5) respectively, where confidence level: 99%, and custom equation: $y=a*x+b$. The results are as follow respectively.

For equation (4):

General model:

$$f(x) = a*x+b$$

Coefficients (with 99% confidence bounds):

$$\begin{aligned} a &= 18.07 \quad (18.07, 18.07) \\ b &= 41.07 \quad (40.52, 41.63) \end{aligned}$$

Goodness of fit:

SSE: 20.95

R-square: 1

Adjusted R-square: 1

RMSE: 0.8809

For equation (5):

General model:

$$f(x) = a*x+b$$

Coefficients (with 99% confidence bounds):

$$\begin{aligned} a &= 42.93 \quad (42.54, 43.32) \\ b &= 18.04 \quad (18.03, 18.06) \end{aligned}$$

Goodness of fit:

SSE: 0.01145

R-square: 0.9997

Adjusted R-square: 0.9997

RMSE: 0.02059

Further run the following program to obtain the c corresponding to $\frac{p_w}{p_w^*}(a)^{10}$ for aqueous solution of RbBr at molalities (mp), where c is the volume concentration ($mol \cdot dm^{-3}$) and 3.1686kPa is the vapor pressure of pure water⁵ at 25°C.

```
cor=spline(m,d);
```

```
mp=[0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.2 1.4 1.6 1.8 2.0 2.5 3.0 3.5 4.0];
```

```
dp=ppval(cor,mp);
```

```
a=[3.1581 3.1479 3.1379 3.1279 3.1180 3.1081 3.0983 3.0884 3.0786 3.0688 3.0493 3.0297  
3.0102 2.9907 2.9713 2.9226 2.8739 2.8252 2.7762]/3.1686;
```

```
c=mp.*dp./(mp*165.3718+1000)*1000;
```

Fit the data of a and c with equation (8), where confidence level: 99%, custom equation: $y = (1-vs*x)^{(2/3)}+b1*(1-\exp(-b2*x))*x^{(2/3)}$, and start: $b1=0.1$, $b2=1$, $vs=0.1$. The result is as follow.

General model:

$$f(x) = (1-vs*x)^{(2/3)}+b1*(1-\exp(-b2*x))*x^{(2/3)}$$

Coefficients (with 99% confidence bounds):

$$b1 = 0.01051 \quad (0.008076, 0.01295)$$

$$b2 = 2.155 \quad (1.705, 2.605)$$

$$vs = 0.06224 \quad (0.05981, 0.06467)$$

Goodness of fit:

SSE: 1.646e-006

R-square: 0.9999

Adjusted R-square: 0.9999

RMSE: 0.0003207

(Here the highest c is 3.4102M)

● The fitted values of $(v_s - Hv_w)$ and v_s in aqueous solution of CsBr

Run the following program to obtain NWMS, VMS, MSMW and VMW, where $dd1$ and $d2$, and $m1$ and ws are the relative densities ($1000*(d-d0)$) and the densities (d), and molarities and Wt.% for aqueous solutions^{3, 12} of CsBr respectively, 0.997047 ($d0$) is the density (g/cm^3) of pure water⁵ at 25°C used by the literatures, and 212.8094 and 18.0153 are the molar mass of CsBr and water respectively.

```
d0=0.997047
```

```
dd1=[6.596 8.418 9.918 11.339 13.207 16.503 23.077 52.110 77.445 114.690 148.404];
```

```
d1=(dd1+1000*d0)/1000;
```

```
m1=[0.03981 0.05084 0.05994 0.06856 0.07991 0.09998 0.14015 0.31991 0.47968 0.7197  
0.9424];
```

15

```

ws=[4 6 8 10 12 14 16 18 20 22 24 26 28 35 40 45 50];
ww=100-ws
m2=ws./(212.8094*ww).*1000
d2=[1.02918 1.04597 1.06328 1.08114 1.09958 1.11863 1.13832 1.15869 1.17978 1.20162
1.22425 1.24772 1.27208 1.36503 1.43986 1.52305 1.61610];
m=[m1 m2];
d=[d1 d2];
ms= 212.8094*m
mw=1000
NWMS=mw./ms* 212.8094/18.0153
MSMW=18.0153*ms./(mw* 212.8094)
VMW=18.0153*(ms+mw)./(d.*mw)
VMS= 212.8094*(ms+mw)./(d.*ms)

```

Fit the data of VMS and NWMS, VMW and MSMW with equation (4) and (5) respectively, where confidence level: 99%, and custom equation: $y=a*x+b$. The results are as follow respectively.

For equation (4):

General model:

$$f(x) = a*x+b$$

Coefficients (with 99% confidence bounds):

$$a = 18.07 \quad (18.07, 18.07)$$

$$b = 48.21 \quad (47.74, 48.68)$$

Goodness of fit:

SSE: 13.29

R-square: 1

Adjusted R-square: 1

RMSE: 0.7151

For equation (5):

General model:

$$f(x) = a*x+b$$

Coefficients (with 99% confidence bounds):

$$a = 49.73 \quad (49.38, 50.08)$$

$$b = 18.05 \quad (18.04, 18.06)$$

Goodness of fit:

SSE: 0.005129

R-square: 0.9998

Adjusted R-square: 0.9998

RMSE: 0.01404

Further run the following program to obtain the c corresponding to $\frac{p_w}{p_w^*} (a)^{10}$ for

aqueous solution of CsBr at molalities (mp), where c is the volume concentration ($\text{mol} \cdot \text{dm}^{-3}$) and 3.1686kPa is the vapor pressure of pure water⁵ at 25°C.

```
cor=spline(m,d);
mp=[0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.2 1.4 1.6 1.8 2.0 2.5 3.0 3.5 4.0];
dp=ppval(cor,mp);
a=[3.1582 3.1482 3.1384 3.1288 3.1193 3.1098 3.1004 3.0910 3.0816 3.0723 3.0537 3.0351
3.0166 2.9980 2.9795 2.9328 2.8855 2.8375 2.7884]/3.1686;
c=mp.*dp./(mp*212.8094+1000)*1000;
```

Fit the data of a and c with equation (8), where confidence level: 99%, custom equation: $y = (1-v_s*x)^{2/3}+b_1*(1-\exp(-b_2*x))*x^{2/3}$, and start: $b_1=0.1$, $b_2=1$, $v_s=0.1$. The result is as follow.

General model:

$$f(x) = (1-v_s*x)^{2/3}+b_1*(1-\exp(-b_2*x))*x^{2/3}$$

Coefficients (with 99% confidence bounds):

```
b1 =      0.01517  (0.01104, 0.01931)
b2 =          1.95  (1.545, 2.355)
vs =      0.06617  (0.06209, 0.07025)
```

Goodness of fit:

SSE: 3.692e-006

R-square: 0.9998

Adjusted R-square: 0.9998

RMSE: 0.0004804

(Here the highest c is 3.3286M)

● The fitted values of $(v_s - Hv_w)$ and v_s in aqueous solution of RbI

Run the following program to obtain NWMS, VMS, MSMW and VMW, where dd1 and d2, m1 and ws are the relative densities ($1000*(d-d_0)$) and the densities (d), and molalities and Wt.% for aqueous solutions^{3, 12} of RbI respectively, 0.997047 (d_0) is the density (g/cm^3) of pure water⁵ at 25°C used by the literatures, and 212.3723 and 18.0153 are the molar mass of RbI and water respectively.

[d0=0.997047](#)

```
dd1=[1.615 3.227 4.712 6.442 9.654 12.843 16.048 34.893 75.257 111.258];
d1=(dd1+1000*d0)/1000;
m1=[0.01000 0.01999 0.02921 0.03997 0.05998 0.07991 0.09999 0.21914 0.48002 0.71911];
ws=[4 6 8 10 12 14 16 18 20 22 24 26 28 35 40 45 50];
ww=100-ws
m2=ws./(212.3723*ww).*1000
d2=[1.02831 1.04464 1.06147 1.07883 1.09675 1.11525 1.13436 1.15411 1.17453 1.19566
```

1.21754 1.24020 1.26368 1.35307 1.42481 1.50428 1.59281];

m=[m1 m2];

d=[d1 d2];

ms= 212.3723*m

mw=1000

NWMS=mw./ms* 212.3723/18.0153

MSMW=18.0153*ms./(mw*212.3723)

VMW=18.0153*(ms+mw)./(d.*mw)

VMS= 212.3723*(ms+mw)./(d.*ms)

Fit the data of VMS and NWMS, VMW and MSMW with equation (4) and (5) respectively, where confidence level: 99%, and custom equation: $y=a*x+b$. The results are as follow respectively.

For equation (4):

General model:

$$f(x) = a*x+b$$

Coefficients (with 99% confidence bounds):

$$a = 18.07 \quad (18.07, 18.07)$$

$$b = 51.92 \quad (51.45, 52.38)$$

Goodness of fit:

SSE: 15.1

R-square: 1

Adjusted R-square: 1

RMSE: 0.7772

For equation (5):

General model:

$$f(x) = a*x+b$$

Coefficients (with 99% confidence bounds):

$$a = 53.46 \quad (53.13, 53.78)$$

$$b = 18.05 \quad (18.04, 18.06)$$

Goodness of fit:

SSE: 0.004313

R-square: 0.9999

Adjusted R-square: 0.9999

RMSE: 0.01313

Further run the following program to obtain the c corresponding to $\frac{P_w}{P_w^*} (a)^{14}$ for aqueous solution of RbI at molalities (mp), where c is the volume concentration ($mol \cdot dm^{-3}$) and 3.1686kPa is the vapor pressure of pure water¹⁶ at 25°C.

cor=spline(m,d);

```

mp=[0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.2 1.4 1.6 1.8 2.0 2.5 3.0 3.5];
dp=ppval(cor,mp);
a=[3.1581 3.1480 3.1380 3.1281 3.1184 3.1086 3.0989 3.0893 3.0796 3.0700 3.0509 3.0308
3.0115 2.9922 2.9729 2.9247 2.8763 2.8278]/3.1686;
c=mp.*dp./(mp*212.3723+1000)*1000;

```

Fit the data of a and c with equation (8), where confidence level: 99%, custom equation: $y = (1-vs*x)^{(2/3)}+b1*(1-\exp(-b2*x))*x^{(2/3)}$, and start: b1=0.1, b2=1, vs=0.1. The result is as follow.

General model:

$$f(x) = (1-vs*x)^{(2/3)}+b1*(1-\exp(-b2*x))*x^{(2/3)}$$

Coefficients (with 99% confidence bounds):

```

b1 =      0.01198  (0.009357, 0.01461)
b2 =         2.482  (1.993, 2.97)
vs =      0.06484  (0.06206, 0.06761)

```

Goodness of fit:

SSE: 1.35e-006

R-square: 0.9999

Adjusted R-square: 0.9999

RMSE: 0.0003001

(Here the highest c is 3.0835M)

- **The fitted values of $(v_s - Hv_w)$ and v_s in aqueous solution of CsI**

Run the following program to obtain NWMS, VMS, MSMW and VMW, where dd1 and d2, and m1 and ws are the relative densities ($1000*(d-d_0)$) and the densities (d), and molarities and Wt.% for aqueous solutions ^{3, 12} of CsI respectively, 0.997047 (d_0) is the density (g/cm^3) of pure water ⁵ at 25°C used by the literature, and 259.8099 and 18.0153 are the molar mass of CsI and water respectively.

d0=0.997047

```

dd1=[4.032 6.057 10.044 12.047 15.704 18.024 20.013 27.938 43.661 63.077 93.685 138.370];
d1=(dd1+1000*d0)/1000;
m1=[0.02001 0.03009 0.04998 0.05999 0.07831 0.08996 0.09996 0.13994 0.21989 0.31978
0.47988 0.7195];
ws=[4 6 8 10 12 14 16 18 20 22 24 26 28 35 40 45];
ww=100-ws
m2=ws./(259.8099*ww).*1000
d2=[1.02899 1.04570 1.06294 1.08074 1.09912 1.11811 1.13775 1.15808 1.17915 1.20099
1.22364 1.24715 1.27157 1.36497 1.44044 1.52460];
m=[m1 m2];
d=[d1 d2];

```

```

ms= 259.8099*m
mw=1000
NWMS=mw./ms* 259.8099/18.0153
MSMW=18.0153*ms./(mw* 259.8099)
VMW=18.0153*(ms+mw)./(d.*mw)
VMS= 259.8099*(ms+mw)./(d.*ms)

```

Fit the data of VMS and NWMS, VMW and MSMW with equation (4) and (5) respectively, where confidence level: 99%, and custom equation: $y=a*x+b$. The results are as follow respectively.

For equation (4):

General model:

$$f(x) = a*x+b$$

Coefficients (with 99% confidence bounds):

$$\begin{array}{ll}
 a = & 18.07 \quad (18.07, 18.07) \\
 b = & 59.12 \quad (58.77, 59.46)
 \end{array}$$

Goodness of fit:

SSE: 7.836

R-square: 1

Adjusted R-square: 1

RMSE: 0.549

For equation (5):

General model:

$$f(x) = a*x+b$$

Coefficients (with 99% confidence bounds):

$$\begin{array}{ll}
 a = & 60.12 \quad (59.93, 60.32) \\
 b = & 18.06 \quad (18.06, 18.06)
 \end{array}$$

Goodness of fit:

SSE: 0.0007065

R-square: 1

Adjusted R-square: 1

RMSE: 0.005213

Further run the following program to obtain the cs corresponding to $\frac{P_w}{P_w^*} (a)^{14}$ for aqueous solution of CsI at molalities (mp), where c is the volume concentration ($mol \cdot dm^{-3}$) and 3.1686kPa is the vapor pressure of pure water⁵ at 25°C.

```

cor=spline(m,d);
mp=[0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.2 1.4 1.6 1.8 2.0 2.5 3.0];
dp=ppval(cor,mp);
a=[3.1582 3.1483 3.1386 3.1290 3.1196 3.1102 3.1009 3.0917 3.0825 3.0734 3.0553 3.0373

```

3.0195 3.0018 2.9843 2.9411 2.8986]/3.1686;

$c = mp \cdot dp / (mp \cdot 259.8099 + 1000) \cdot 1000$;

Fit the data of a and c with equation (8), where confidence level: 99%, custom equation: $y = (1 - v_s \cdot x)^{2/3} + b_1 \cdot (1 - \exp(-b_2 \cdot x)) \cdot x^{2/3}$, and start: $b_1 = 0.1$, $b_2 = 1$, $v_s = 0.1$. The result is as follow.

General model:

$$f(x) = (1 - v_s \cdot x)^{2/3} + b_1 \cdot (1 - \exp(-b_2 \cdot x)) \cdot x^{2/3}$$

Coefficients (with 99% confidence bounds):

$$b_1 = 0.004519 \quad (0.002604, 0.006434)$$

$$b_2 = 2.69 \quad (1.791, 3.588)$$

$$v_s = 0.05381 \quad (0.05165, 0.05597)$$

Goodness of fit:

SSE: 4.133e-007

R-square: 1

Adjusted R-square: 0.9999

RMSE: 0.0001718

However, the calculated values of H by using v_s 0.05381 (0.05165, 0.05597)

and the intercepts ($v_s - N_{cw} v_w$) (59.12 (58.77, 59.46)) are negative. Considering that the real highest c is only 2.5349M but the highest valid concentration is 3.10M, in order to make the distribution of the data points symmetry and uniform, disregarding some data, again fit the data of a and c with equation (8). The results are as follows.

Example 1

$cor = \text{spline}(m, d)$;

$mp = [0.1 \ 0.5 \ 1.0 \ 1.2 \ 1.4 \ 1.6 \ 1.8 \ 2.0 \ 2.5 \ 3.0]$;

$dp = \text{ppval}(cor, mp)$;

$a = [3.1582 \ 3.1196 \ 3.0734 \ 3.0553 \ 3.0373 \ 3.0195 \ 3.0018 \ 2.9843 \ 2.9411 \ 2.8986]/3.1686$;

$c = mp \cdot dp / (mp \cdot 259.8099 + 1000) \cdot 1000$;

Fit the data of aw and c with equation (8), where confidence level: 99%, custom equation: $y = (1 - v_s \cdot x)^{2/3} + b_1 \cdot (1 - \exp(-b_2 \cdot x)) \cdot x^{2/3}$, and start: $b_1 = 0.1$, $b_2 = 1$, $v_s = 0.1$.

General model:

$$f(x) = (1 - v_s \cdot x)^{2/3} + b_1 \cdot (1 - \exp(-b_2 \cdot x)) \cdot x^{2/3}$$

Coefficients (with 99% confidence bounds):

$$b_1 = 0.007194 \quad (0.004702, 0.009685)$$

$$b_2 = 2.15 \quad (1.575, 2.725)$$

$$v_s = 0.05677 \quad (0.05409, 0.05944)$$

Goodness of fit:

SSE: 9.434e-008

R-square: 1
Adjusted R-square: 1
RMSE: 0.0001161

Example 2

```
cor=spline(m,d);  
mp=[0.2 0.6 1.0 1.2 1.4 1.6 1.8 2.0 2.5 3.0];  
dp=ppval(cor,mp);  
a=[3.1483 3.1102 3.0734 3.0553 3.0373 3.0195 3.0018 2.9843 2.9411 2.8986]/3.1686;  
c=mp.*dp./(mp*259.8099+1000)*1000;
```

Fit the data of a and c with equation (8), where confidence level: 99%, custom equation: $y = (1-vs*x)^{(2/3)}+b1*(1-\exp(-b2*x))*x^{(2/3)}$, and start: b1=0.1, b2=1, vs=0.1.

General model:

$$f(x) = (1-vs*x)^{(2/3)}+b1*(1-\exp(-b2*x))*x^{(2/3)}$$

Coefficients (with 99% confidence bounds):

b1 =	0.0071	(0.004557, 0.009643)
b2 =	2.166	(1.576, 2.755)
vs =	0.05667	(0.05393, 0.0594)

Goodness of fit:

SSE: 1.073e-007
R-square: 1
Adjusted R-square: 1
RMSE: 0.0001238

Example 3

```
cor=spline(m,d);  
mp=[0.3 0.7 1.0 1.2 1.4 1.6 1.8 2.0 2.5 3.0];  
dp=ppval(cor,mp);  
a=[3.1386 3.1009 3.0734 3.0553 3.0373 3.0195 3.0018 2.9843 2.9411 2.8986]/3.1686;  
c=mp.*dp./(mp*259.8099+1000)*1000;
```

Fit the data of a and c with equation (8), where confidence level: 99%, custom equation: $y = (1-vs*x)^{(2/3)}+b1*(1-\exp(-b2*x))*x^{(2/3)}$, and start: b1=0.1, b2=1, vs=0.1.

General model:

$$f(x) = (1-vs*x)^{(2/3)}+b1*(1-\exp(-b2*x))*x^{(2/3)}$$

Coefficients (with 99% confidence bounds):

b1 =	0.007182	(0.004742, 0.009622)
b2 =	2.147	(1.616, 2.678)
vs =	0.05675	(0.05413, 0.05938)

Goodness of fit:

SSE: 9.741e-008
R-square: 1

Adjusted R-square: 1

RMSE: 0.000118

To sum up, the v_s of CsI in water is taken as $0.05944 \text{ dm}^3 \cdot \text{mol}^{-1}$.

On application of equation (4) and (8) to aqueous solutions of CaCl_2

Run the following program to obtain NWMS and VMS,, where dd and m are the relative densities ⁴ ($1000 \cdot (d-d_0)$) and molarities for aqueous solution of CaCl_2 respectively, 0.997047 (d_0)⁵ is the density (g/cm^3) of pure water ⁵ at 25°C used by the literature, and 110.9940 and 18.0153 are the molar mass of CaCl_2 and water respectively (the green data are the arithmetic mean value).

```
d0=0.997047;
dd=[4.568 8.700 44.042 81.498 125.468 162.196 181.401 251.240 263.800 285.686 341.557
372.586 390.022 413.788];
m=[0.05001 0.09583 0.50190 0.95590 1.52060 2.02090 2.29340 3.35450 3.55790 3.92350
4.93050 5.54980 5.92220 6.46440];
d=(dd+1000*d0)/1000;
mw=1000;
ms= 110.9940*m;
NWMS=mw./ms* 110.9940/18.0153;
VMS= 110.9940*(ms+mw)./(d.*ms);
```

Fit the data of VMS and NWMS equation (4), where confidence level: 99%, and custom equation: $y=a*x+b$. The results are as follow.

General model:

$$f(x) = a*x+b$$

Coefficients (with 99% confidence bounds):

a =	18.06	(18.05, 18.07)
b =	28.57	(25.56, 31.58)

Goodness of fit:

SSE: 132.9

R-square: 1

Adjusted R-square: 1

RMSE: 3.328

Further run the following program to obtain the c corresponding to water activity a at 25°C for aqueous solution ¹⁵ of CaCl_2 at molalities (mp), where c is the volume concentration ($\text{mol} \cdot \text{dm}^{-3}$).

```
cor=spline(m,d);
```

```

mp=[0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.2 1.4 1.6 1.8 2.0 2.5 3.0 3.5 4.0 4.5];
dp=ppval(cor,mp);
phi=[0.854 0.862 0.876 0.894 0.917 0.940 0.963 0.988 1.017 1.046 1.107 1.171 1.237 1.305 1.376
1.568 1.779 1.981 2.182 2.383];
a=exp(-3*mp.*phi/55.51);
c=mp.*dp./(mp*102.8938+1000)*1000;

```

Fit the data of a and c with equation (8), where confidence level: 99%, custom equation: $y = (1-vs*x)^{(2/3)}+b1*(1-\exp(-b2*x))*x^{(2/3)}$ and start: b1=0.1, b2=1, vs=0.1. The result is as follow.

General model:

$$f(x) = (1-vs*x)^{(2/3)}+b1*(1-\exp(-b2*x))*x^{(2/3)}$$

Coefficients (with 99% confidence bounds):

b1 =	0.08584	(0.08, 0.09167)
b2 =	3.161	(2.469, 3.853)
vs =	0.1985	(0.1943, 0.2027)

Goodness of fit:

SSE: 0.0001208

R-square: 0.9996

Adjusted R-square: 0.9996

RMSE: 0.002666

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