APPENDIX- B

MATLAB PROGRAMMES USED TO CALCULATE ACTIVITY AND OSMOTIC COEFFICIENTS (PITZER MODEL)

```
%%%%%%
clc
clearall
closeall
m=[0.1:0.05:1.4];
Api=[0.4453, 0.4675,0.4917,0.5080, 0.5251,0.5370,
0.5493,0.5595,0.5700,0.5825,0.5954,0.6054,0.6149,0.6234,0.6329,0.6400,0
.6481,0.6522,0.6563,...
    0.6630,0.6766,0.6805,0.6844,0.6921,0.6999,0.7018,0.7037];
I=[0.4:0.2:5.6];
beta0=0.2358;
beta1=2.485;
beta2=-47.35;
sigma=0.003;
b=1.2;
alpha1=1.4;
alpha2=12.0;
Cpi=-0.0012;
%%%%%%%%%
fori=1:27
fpi(1,i)=-Api(1,i)*[sqrt(I(1,i))/[1+(b*sqrt(I(1,i)))]];%eq.6
Bpi(1,i)=beta0+(beta1*exp(-alpha1*sqrt(I(1,i))))+(beta2*exp(-
alpha2*sqrt(I(1,i))));%eq.7
end
%%%%%%%
fori=1:27
pi(1,i)=1+4*fpi(1,i)+m(1,i)*Bpi(1,i)+(m(1,i).^2)*Cpi;%%%%eq.5
end
%%%%%
Cgamma=(3/2)*Cpi;%%%%%%%eq.11
%%%%%%%%%%
fori=1:27
a(1,i)=1+b*sqrt(I(1,i));
end
fori=1:27
fgamma(1,i)=-Api(1,i)*((sqrt(I(1,i))/a(1,i))+((2/b)*log(a(1,i))));%eq 9

Bgamma(1,i)=2*beta0+((2*beta1)/((alpha1.^2)*I(1,i)))*(1-
(1+(alpha1*sqrt(I(1,i)))...
    -(0.5*(alpha1.^2)*I(1,i)))*exp(-
alpha1*sqrt(I(1,i))))+((2*beta2)/((alpha2.^2)*I(1,i)))*(1-
(1+(alpha2*sqrt(I(1,i)))...
-(0.5*(alpha2.^2)*I(1,i)))*exp(-alpha2*sqrt(I(1,i))));%eq.10
end
fori=1:27
loggamma(1,i)=4*fgamma(1,i)+m(1,i)*Bgamma(1,i)+m(1,i).^2*Cgamma;%eq.8
end
fori=1:27
gamma(1,i)=exp(loggamma(1,i));
```

```
end
```

MATLAB PROGRAMMES USED TO CALCULATE ACTIVITY AND OSMOTIC COEFFICIENTS (BROMLEY MODEL)

```
clear all;
B=0.1016;
I=[.000400,.000600,.000800,.00100,.001200,.001400,.001600,.001800,.0020
0,.002200,.002400,.002600,.002800,.00300,.003200,.003400,.003600,.00380
0,.00400,.004200,.004400,.004600,.004800,.00500,.005200,.005400,.005600
];
for i=1:27
    loggammapow(1,i)=-
0.511*sqrt(I(1,i))/(1+sqrt(I(1,i)))+((0.06+0.6*B)*I(1,i))/((1+0.375*I(1
,i))^2)+B*I(1,i)/4;
    gammapow(1,i)=10^(loggammapow(1,i));
    gamma(1,i)=gammapow(1,i)^4;
end
```

MATLAB PROGRAMMES USED TO CALCULATE EXCESS GIBBS ENERGY VALUES

```
m=0.1:0.05:1.40;
M=400.15;
R=8.3143;
T=298;
fi=[0.7856,0.7641,0.7426,0.7214,0.7003,0.6860,0.6718,0.6622,0.6526,0.65
03,0.6480,0.6493,0.6507,0.6533,0.6559,0.6630,0.6701,0.6720,...
    0.6740,0.6885,0.7030,0.7057,0.7085,0.7029,0.6973,0.6713,0.6454];
lng=[1.1464,1.3394,1.5325,1.7096,1.8867,2.0363,2.186,2.3188,2.4517,2.55
72,2.6627,2.7536,2.8446,2.9315,3.0185,3.0849,3.1514,3.2198,3.2882,3.342
6,3.3971,3.4801,...
    3.5631,3.6850,3.8070,4.0232,4.2395];
for i=1:27;
    k(1,i)=R*T*m(1,i)*((10^4-(m(1,i)*M))./1800)*(1-fi(1,i)-lng(1,i));
end
```

Matlab program used to calculate adiabatic compressibility (β), acoustic impedance (Z), surface tension (σ) and intermolecular free length (L_f)

```
At 298K and 0.1M
k=2.055*10^-6;
u=[1656.96,1682.03,1701.18,1710.5,1708.56,1697.20,1673.91,1642.2,1602.6
5,1556.94,1506.0];
p=[1109.825,1103.881,1098.368,1090.749,1081.98,1072.837,1061.966,1050.9
12,1039.109,1026.831,1013.166];
for i=1:11;
    beta(1,i)=1/(u(1,i)^2*p(1,i));
    Z(1,i)=u(1,i)*p(1,i);
    sigma(1,i)=6.3*10^-4*p(1,i)*u(1,i)^(3/2);
end
for i=1:11;
    lf(1,i)=k*sqrt(beta(1,i));
```

```
end
```

At 303 and 0.1M

```
k=2.075*10^-6;
u=[1645.43,1671.04,1619.79,1700.90,1700.48,1691.29,1670.71,1642.15,1606
.21,1564.54,1517.54];
p=[1106.333,1100.425,1094.948,1087.43,1078.807,1069.87,1059.271,1048.49
9,1037.025,1025.059,1011.664];
for i=1:11;
    beta(1,i)=1/(u(1,i)^2*p(1,i));
    Z(1,i)=u(1,i)*p(1,i);
    sigma(1,i)=6.3*10^-4*p(1,i)*u(1,i)^(3/2);
end
for i=1:11;
    lf(1,i)=k*sqrt(beta(1,i));
end
```

At 308K and 0.1M

```
k=2.095*10^-6;
u=[1633.63,1659.6,1680.06,1691.11,1692.18,1684.88,1668.89,1641.31,1608.
8,1570.78,1527.44];
p=[1102.814,1096.921,1091.492,1084.068,1075.579,1066.826,1056.469,1045.
967,1034.785,1023.102,1009.951];
for i=1:11;
    beta(1,i)=1/(u(1,i)^2*p(1,i));
    Z(1,i)=u(1,i)*p(1,i);
    sigma(1,i)=6.3*10^-4*p(1,i)*u(1,i)^(3/2);
end
for i=1:11;
    lf(1,i)=k*sqrt(beta(1,i));
end
```

At 318K and 0.1M

```
k=2.115*10^-6;
u=[1621.83,1648.07,1669.24,1681.11,1683.46,1678.02,1662.53,1639.74,1610
.44,1575.77,1535.80];
p=[1099.277,1093.391,1088.001,1080.662,1072.292,1063.706,1053.571,1043.
318,1033.297,1020.974,1008.043];
for i=1:11;
    beta(1,i)=1/(u(1,i)^2*p(1,i));
    Z(1,i)=u(1,i)*p(1,i);
    sigma(1,i)=6.3*10^-4*p(1,i)*u(1,i)^(3/2);
end
for i=1:11;
    lf(1,i)=k*sqrt(beta(1,i));
end
```

At 318K and 0.1M

```
k=2.135*10^-6;
u=[1609.99,1636.46,1658.28,1670.91,1674.50,1670.8,1657.57,1637.45,1611.
16,1579.53,1542.86];
p=[1095.722,1089.838,1084.475,1077.208,1068.949,1060.514,1050.583,1040.
551,1029.872,1018.681,1005.946];
for i=1:11;
    beta(1,i)=1/(u(1,i)^2*p(1,i));
    Z(1,i)=u(1,i)*p(1,i);
    sigma(1,i)=6.3*10^-4*p(1,i)*u(1,i)^(3/2);
end
for i=1:11;
    lf(1,i)=k*sqrt(beta(1,i));
end
```

Matlab program used to calculate relative association (R_A), apparent molal volume (ϕ_V) and apparent molal compressibility (ϕ_K)

At 298K and 0.6 M

```
m=0.6;
uo=[1656.96,1682.9,1700.79,1710.11,1707.28,1694.97,1668.52,1629.82,1599
.91,1545.6,1497.08];
po=[1109.558,1102.542,1095.158,1085.094,1075.316,1064.974,1051.506,1036
.523,1027.143,1010.938,997.241];
u=[1656.96,1684.95,1703.87,1712.58,1713.38,1704.52,1683.96,1656.29,1617
.04,1580.69,1537.35];
p=[1109.558,1111.57,1113.092,1112.892,1111.574,1109.212,1106.091,1103.2
45,1098.62,1094.796,1090.656];
M=249.69;
for i=1:11
    beta(1,i)=1/(u(1,i)^2*p(1,i));
    betao(1,i)=1/(uo(1,i)^2*po(1,i));
end
for i=1:11
    R(1,i)=(p(1,i)/po(1,i)).*(uo(1,i)/u(1,i)).^(1/3);
    fiv(1,i)=((1000/(m.*po(1,i))).*(po(1,i)-p(1,i)))+(M/po(1,i));
    fik(1,i)=((1000/(m.*po(1,i))).*((po(1,i).*beta(1,i))-
(p(1,i).*betao(1,i))))+(betao(1,i)*M/po(1,i));
end
```

At 303K and 0.6M

```
m=0.6;
```

```
uo=[1645.43,1671.80,1690.35,1700.72,1699.45,1689.22,1657.78,1630.77,160
3.61,1553.89,1409.33];
po=[1106.066,1099.079,1091.757,1081.811,1072.180,1062.035,1048.863,1034
.231,1025.103,1009.281,995.844];
u=[1645.43,1673.63,1693.28,1702.76,1705.35,1698.08,1679.99,1655.29,1619
.79,1586.65,1546.82];
p=[1106.066,1108.079,1109.638,1109.505,1108.35,1106.142,1103.245,1100.6
51,1096.318,1092.703,1088.753];
M=249.69;
for i=1:11
    beta(1,i)=1/(u(1,i)^2*p(1,i));
    betao(1,i)=1/(uo(1,i)^2*po(1,i));
end
for i=1:11
    R(1,i)=(p(1,i)/po(1,i)).*(uo(1,i)/u(1,i)).^(1/3);
    fiv(1,i)=((1000/(m.*po(1,i))).*(po(1,i)-p(1,i)))+(M/po(1,i));
    fik(1,i)=((1000/(m.*po(1,i))).*((po(1,i).*beta(1,i))-
(p(1,i).*betao(1,i))))+(betao(1,i)*M/po(1,i));
end
```

At 308K and 0.6M

```
m=0.6;
uo=[1633.63,1660.41,1679.59,1691.14,1691.31,1683.01,1662.53,1630.89,160
6.35,1560.94,1519.74];
po=[1102.551,1095.588,1088.318,1078.479,1068.982,1059.024,1046.133,1031
.803,1022.903,1007.425,994.236];
u=[1633.63,1662.45,1682.4,1692.63,1696.72,1691.16,1675.48,1653.54,1621.
48,1591.27,1554.74];
p=[1102.551,1104.563,1106.145,1106.067,1105.043,1102.987,1100.302,1097.
933,1093.879,1090.459,1086.668];
M=249.69;
for i=1:11
    beta(1,i)=1/(u(1,i)^2*p(1,i));
    betao(1,i)=1/(uo(1,i)^2*po(1,i));
end
for i=1:11
    R(1,i)=(p(1,i)/po(1,i)).*(uo(1,i)/u(1,i)).^(1/3);
    fiv(1,i)=((1000/(m.*po(1,i))).*(po(1,i)-p(1,i)))+(M/po(1,i));
    fik(1,i)=((1000/(m.*po(1,i))).*((po(1,i).*beta(1,i))-
(p(1,i).*betao(1,i))))+(betao(1,i)*M/po(1,i));
end
```

At 313K and 0.6M

```
m=0.6;
uo=[1621.83,1648.97,1668.7,1681.32,1682.86,1676.39,1658.58,1630.21,1608
.1,1566.68,1528.75];
po=[1099.014,1092.068,1084.84,1075.1,1065.725,1055.938,1043.294,1029.24
8,1020.556,1005.387,992.42];
u=[1621.83,1651.01,1671.42,1682.32,1687.74,1683.84,1670.46,1651.06,1622
.23,1594.76,1561.21];
```

```
p=[1099.014,1101.013,1102.613,1102.58,1101.675,1099.751,1097.266,1095.0
98,1091.292,1088.051,1084.414];
M=249.69;
for i=1:11
    beta(1,i)=1/(u(1,i)^2*p(1,i));
    betao(1,i)=1/(uo(1,i)^2*po(1,i));
end
for i=1:11
    R(1,i)=(p(1,i)/po(1,i)).*(uo(1,i)/u(1,i)).^(1/3);
    fiv(1,i)=((1000/(m.*po(1,i))).*(po(1,i)-p(1,i)))+(M/po(1,i));
    fik(1,i)=((1000/(m.*po(1,i))).*((po(1,i).*beta(1,i))-
(p(1,i).*betao(1,i))))+(betao(1,i)*M/po(1,i));
end
```

At 318K and 0.6M

```
m=0.6;
uo=[1609.99,1637.51,1657.67,1671.3,1674.09,1669.35,1654.08,1628.73,1608
.88,1571.17,1536.3];
po=[1095.459,1088.521,1081.328,1071.674,1062.409,1052.777,1040.361,1026
.573,1018.069,1003.183,990.417];
u=[1609.99,1639.45,1660.33,1671.88,1678.67,1676.13,1664.94,1647.88,1622
.04,1597.12,1566.32];
p=[1095.459,1097.439,1099.045,1099.049,1098.242,1096.434,1094.134,1092.
153,1088.569,1054.494,1082.0];
M=249.69;
for i=1:11
    beta(1,i)=1/(u(1,i)^2*p(1,i));
    betao(1,i)=1/(uo(1,i)^2*po(1,i));
end
for i=1:11
    R(1,i)=(p(1,i)/po(1,i)).*(uo(1,i)/u(1,i)).^(1/3);
    fiv(1,i)=((1000/(m.*po(1,i))).*(po(1,i)-p(1,i)))+(M/po(1,i));
    fik(1,i)=((1000/(m.*po(1,i))).*((po(1,i).*beta(1,i))-
(p(1,i).*betao(1,i))))+(betao(1,i)*M/po(1,i));
end
```