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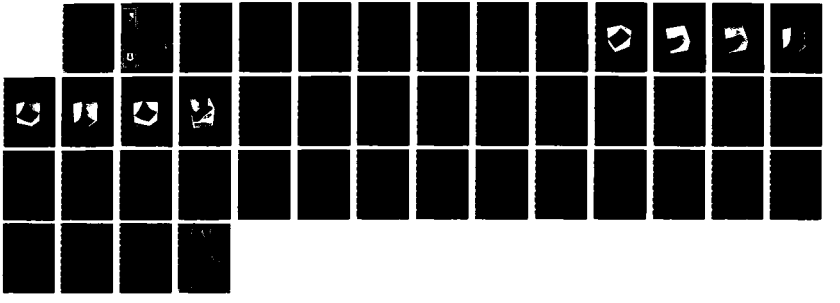

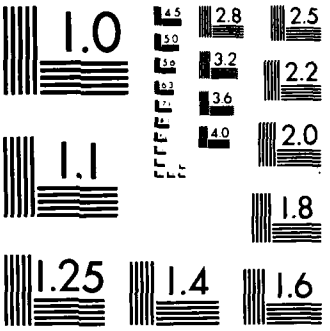

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FRANK J. SEILER RESEARCH LABORATORY

TEMPERATURE-COMPOSITION SURFACES FOR PHYSICAL PROPERTIES OF ALUMINUM CHLORIDE - 1-METHYL-3-ETHYLIMIDAZOLIUM CHLORIDE ROOM TEMPERATURE MOLTEN SALTS

LT COL ARMAND A. FANNIN, JR.

DR. JOHN S. WILKES

July 1986

AIR FORCE SYSTEMS COMMAND
UNITED STATES AIR FORCE

FJSRL-TR-86-0004

This document was prepared by the Electrochemistry Division, Directorate of Chemical Sciences, Frank J. Seiler Research Laboratory, United States Air Force Academy, CO. The research was conducted under Project Work Unit number 2303-F2-10. Dr. John S. Wilkes was the project scientist.

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This report has been reviewed by the Commander and is releasable to the National Technical Information Service (NTIS). At NTIS it will be available to the general public, including foreign nations.

This technical report has been reviewed and is approved for publication.

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Project Scientist

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Director, Chemical Sciences

KENNETH E. SIEGENTHALER, Lt Col, USAF
Chief Scientist

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Density, specific conductivity, equivalent conductivity, absolute viscosity, kinematic viscosity and the Walden product for molten salts composed of aluminum chloride and 1-methyl-3-ethylimidazolium chloride were plotted in three dimensions. The properties were dependent on temperature and composition.

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TEMPERATURE - COMPOSITION SURFACES FOR PHYSICAL PROPERTIES OF ALUMINUM CHLORIDE - 1-METHYL-3-ETHYLIMIDAZOLIUM CHLORIDE ROOM TEMPERATURE MOLTEN SALTS

Lt Col Armand A. Fannin, Jr.
Dr John S. Wilkes

July 1986

Directorate of Chemical Sciences
The Frank J. Seiler Research Laboratory
Air Force Systems Command
United States Air Force Academy
Colorado Springs, Colorado 80840

LIST OF ILLUSTRATIONS

INTRODUCTION

Molten salts composed of aluminum chloride and 1-methyl-3-ethylimidazolium chloride are interesting and useful as electrolytes in electrochemical cells and as solvents for a variety of applications. We have reported that the physical properties (density, electric conductivity and viscosity) depend strongly on temperature and melt composition (1). In our original report we plotted the physical properties as conventional two-dimensional graphs, showing the dependence of temperature and compositions separately. In this report we show the properties plotted as three-dimensional surfaces. This treatment of the data make certain trends much easier to visualize. The plots were made possible by the acquisition of the graphics program DISSPLA™.

PLOTTING METHOD

DISSPLA™ is a set of FORTRAN calls that provides for the plotting of data or functional surfaces generated in user provided programs. Details about the use and content of DISSPLA™ are contained in the software documentation. The FORTRAN programs written to plot figures 1 - 8 are listed in Appendix A. The essential feature of each is a function that calculates the desired physical property as a function of temperature and composition.

PHYSICAL PROPERTY SURFACES

The functions for the temperature and composition dependencies of the properties used were as reported in reference 1. In summary, the temperature behavior was fitted to a V-T-F model for conductivity and viscosity and to a linear model for density. The composition behavior for all properties was fitted to a complex structural model that is discussed in detail in reference 1. This model allows for the marked change that occurs in some properties at equimolar composition. The equations and fitted parameters are collected in Appendix B. In all plots the temperature is plotted in degrees Celsius and the composition is plotted as mole fraction of aluminum chloride. Superimposed on each surface is a polygon that encloses the area where actual measurements were made.

Density

The density surface is shown in figure 1. The density decreases linearly with temperature at all compositions, however the strength of the dependence varies with composition. The density increases with increasing $AlCl_3$ mole fraction, as expected.

Electric Conductivity

Both specific and equivalent conductivities were plotted. Specific conductivity is shown in figure 2 and equivalent conductivity is shown in figure 3. The cusp occurring at all temperatures at 0.5 mole fraction is much sharper in specific conductivity as a consequence of the large partial molar volume of $AlCl_3$.

Viscosity

Kinematic and absolute viscosity are presented in figures 4-7. For figures 4 and 6 the units are centistokes and centipoise respectively. It may be easily seen that the melt viscosity extends to both higher and lower values than typical values for water. The region of steep increase in viscosity corresponds to the highly structured basic region at low temperatures. To show more detail in the region of lower viscosities, figures 5 and 7 show unitless representations where both viscosities are drawn on a $\log_{10}$ scale.

Walden product

For solutions where the Walden product (equivalent conductivity times the absolute viscosity) is a constant, changes in conductivity may be attributed to only changes in the viscosity. While the theory holds exactly only for infinitely dilute solutions in solvents of differing viscosity, the melts may at least qualitatively be considered a solvent with viscosity a function of the composition. Since concentration of the transporting species changes smoothly and monotonically on each half of the mole fraction diagram, one would expect two monotonically varying Walden product surfaces intersecting at 0.5 mole fraction. The variation from such surfaces drawn in figure 8 gives strong indication of some strong specific interactions or structure in the melts.

REFERENCE

1. Armand A. Fannin, Jr., Danilo A. Floreani, Lowell A. King, John S. Landers, Bernard J. Piersma, Daniel J. Stech, Robert L. Vaughn, John S. Wilkes, and John L. Williams, J. Phys. Chem., 88, 2614 (1984).

Melt Density

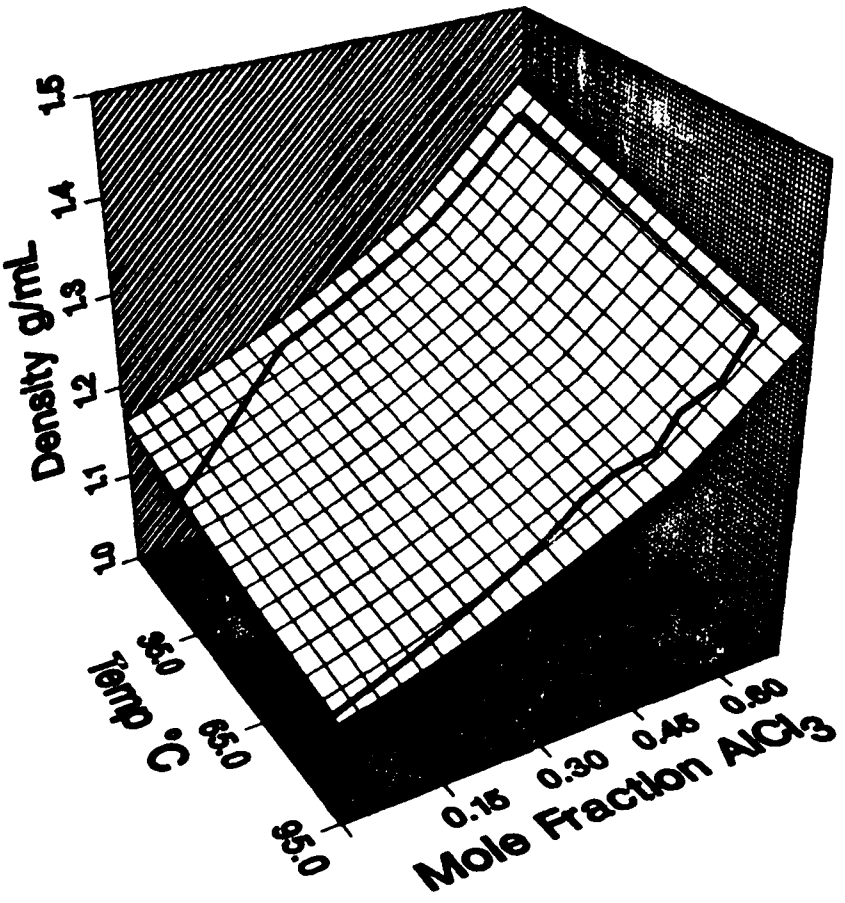

Figure 1

Melt Specific Conductivity

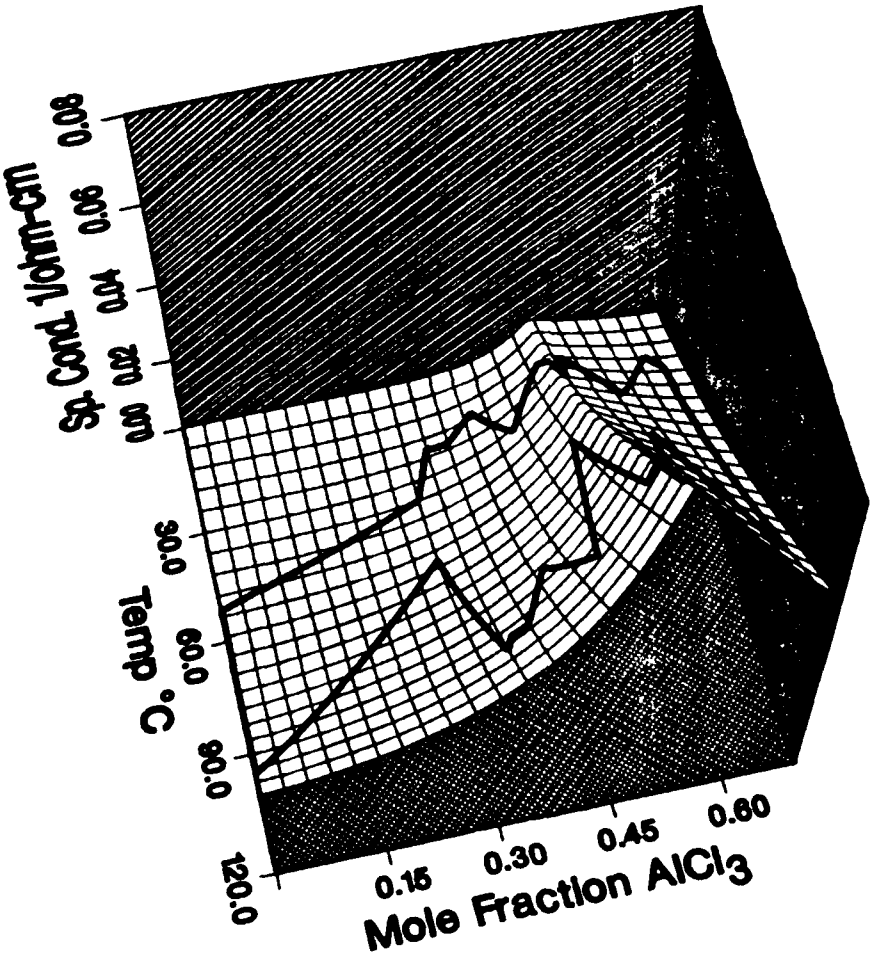

Figure 2

Melt Equiv. Conductivity

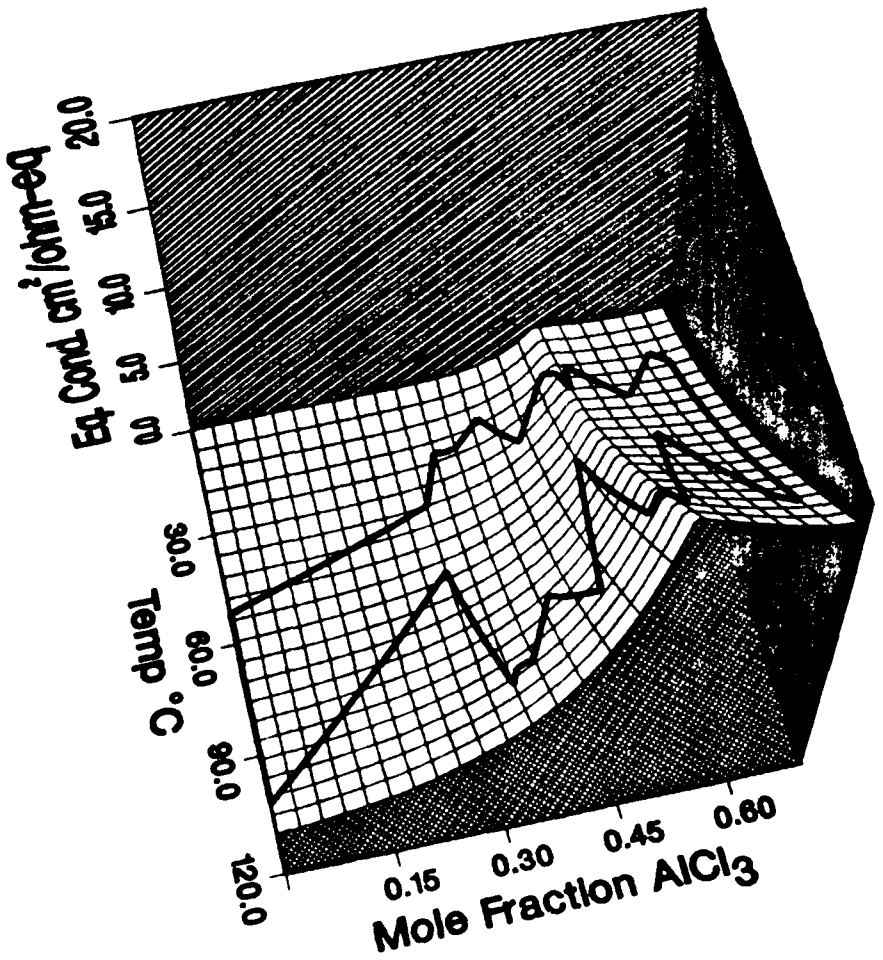

Figure 3

Melt Kinematic Viscosity

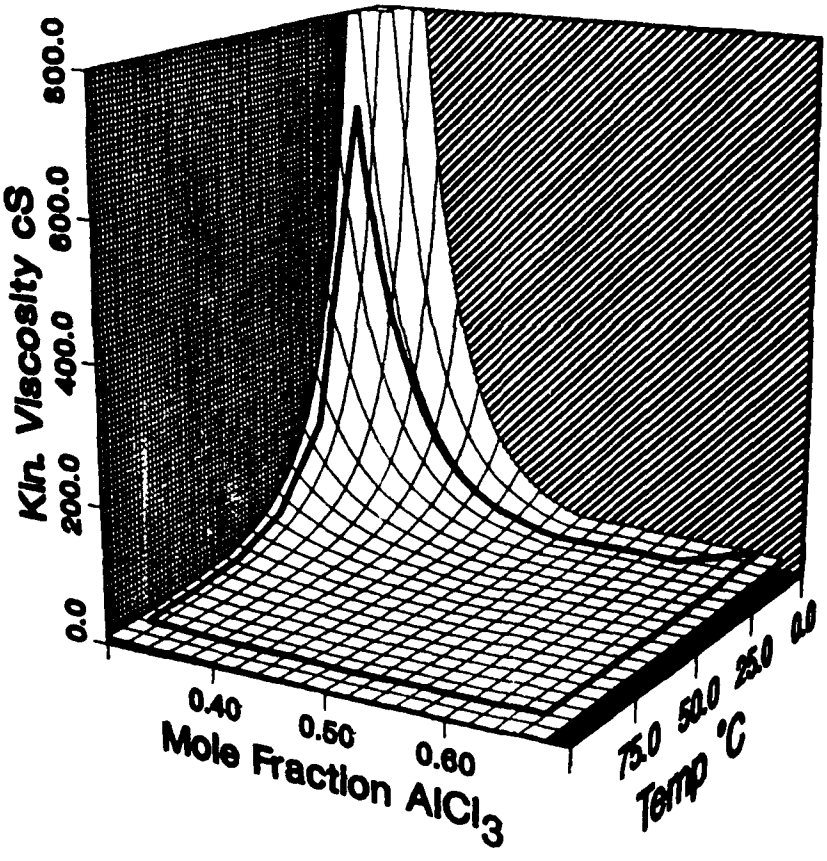

Figure 4

Melt Kinematic Viscosity

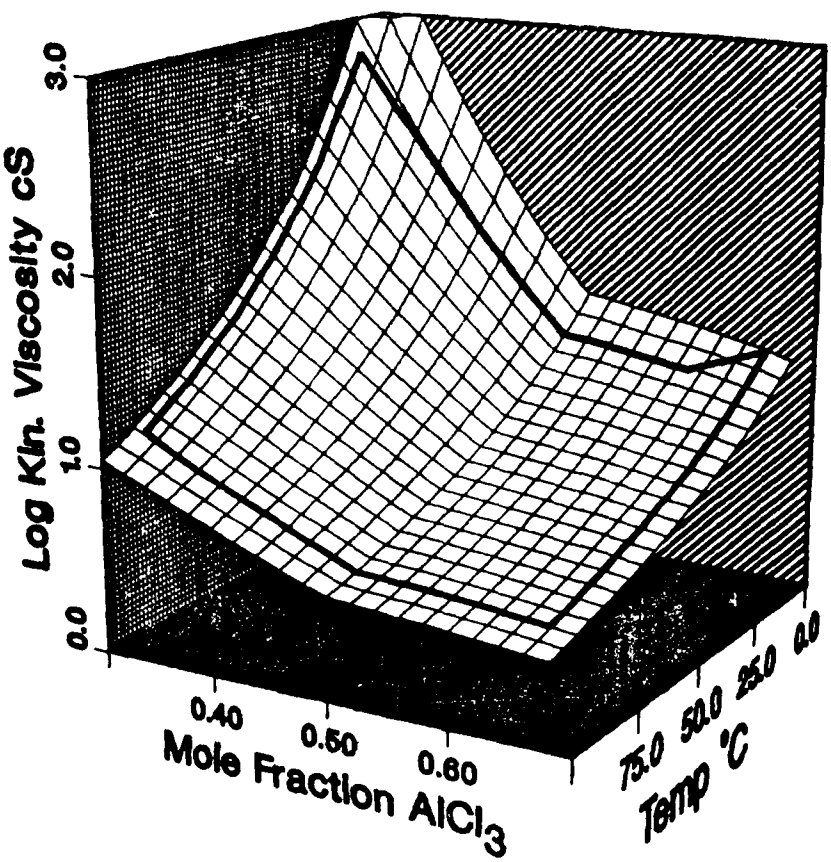

Figure 5

Melt Absolute Viscosity

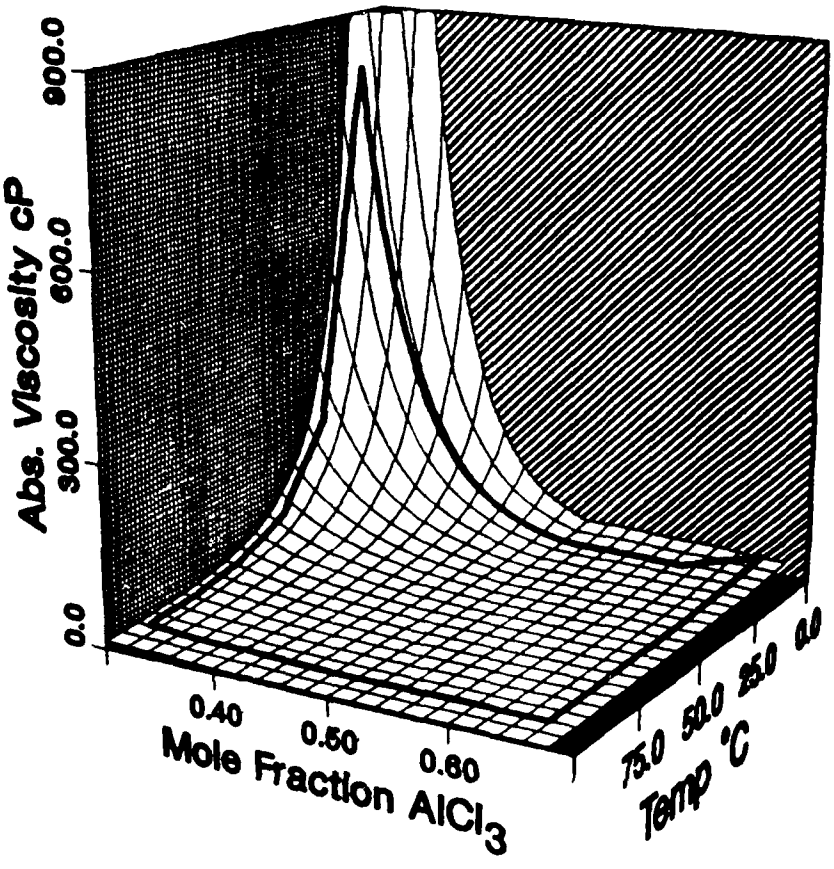

Figure 6

Melt Absolute Viscosity

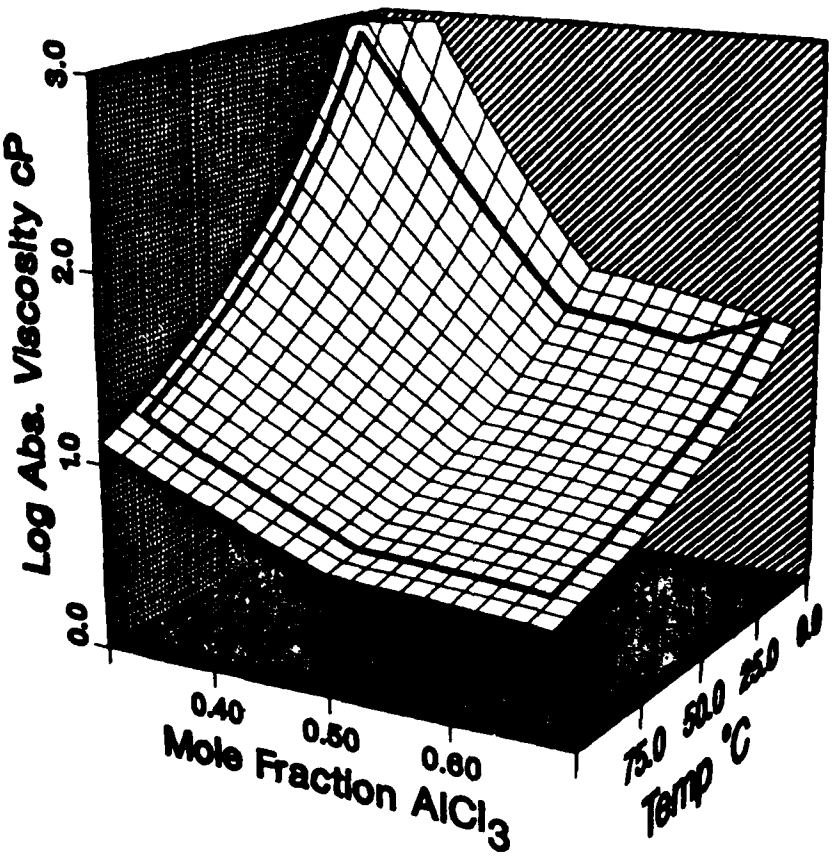

Figure 7

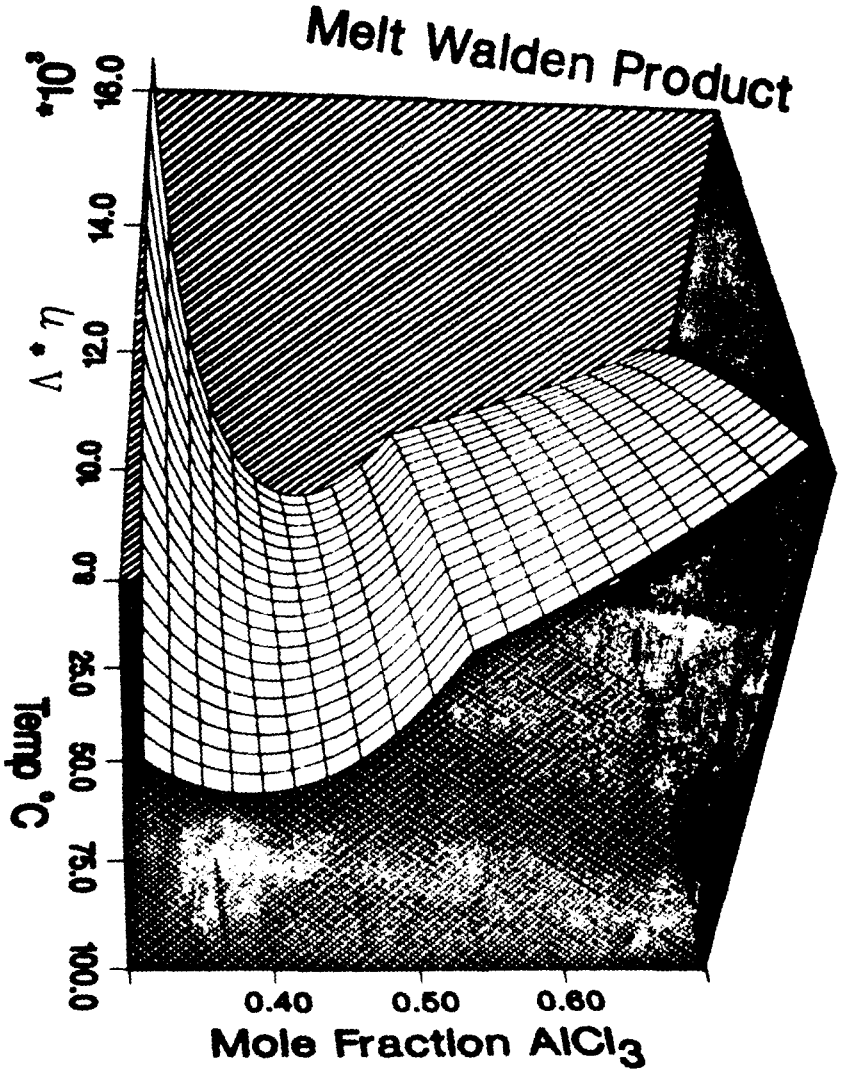
Melt Walden Product
*10³
16.0
14.0
12.0
10.0
Λ • η
0.0
25.0
50.0
75.0
100.0
Temp °C
0.40
0.50
0.60
Mole Fraction AlCl3

Figure 8

APPENDIX A

The FORTRAN programs for the different three-dimensional plots are largely the same. The principal differences are the function that generates the surface, the name of the data file containing the vertices of the polygon superimposed on the surface, the axes names and ranges and the view point.

A few comments about the programs are included here to simplify future use or modification for similar plots.

xx(min) etc.:	the minimum and maximum axes values
call ptekal:	Tektronix 4014 terminal as output device. The figures for this report were copied from a TEK 4014 screen, which has the highest resolution available at FJSRL and is much faster than a digital plotter.
call ptk41:	Tektronix 4107 as output device. Used for all but final copies. One or the other of these two calls is commented out.
call x3name etc.:	the axes labels
call vuangl:	establishes the viewpoint. The arguments are with respect to the center of the box containing the surface. The first argument is the angle (in the x-y or temperature-composition surface) from a line through the center of the box containing the surface parallel to the x (temperature) axis. The second argument is the angle up from the base plane (x,y). The third argument is the distance from the center.
call messag:	Early versions had messages printed on the box walls. These were commented out for the final copy.
call bshift:	moves the whole figure in x and y directions in order to get complete figure on screen.

```
ABSOLUTE VISCOSITY
      external avis
      integer tic
      logical ok
      dimension a(4),b(4),x(2),y(2),iabove(1)
      dimension xx(3),yy(3),zz(3)
      dimension xpoly(50),ypoly(50),xcrv(10),ycrv(10),zcrv(10)
      data iabove/4HABOV/
      min=1
      max=2
      tic=3
      xx(min)=0.0
      xx(max)=100.0
      xx(tic)=25.0
      yy(min)=0.301
      yy(max)=0.70
      yy(tic)=0.1
      zz(max)=900.
      zz(min)=0.0
      zz(tic)=300.
      call idpoly(xpoly,ypoly,npoly)
c     call ptk41
      call ptekal
c     call prpdev(ok)
c     if(.not. ok) stop
c     call hp7470
      call hwrot('AUTO')
      call swissm
      call shdchr(90.,1,.002,1)
      call height(.325)
      call physor(.5,0.5)
      call bshift(0.4,0.)
      call nobrdr
      call area2d(7.5,9.75)
      xl=xmess('Melt Absolute Viscosity$',100)
      call messag('Melt Absolute Viscosity$',100,4.0-xl/2.,9.25)
      call volm3d(8.,8.,9.)
      call mixalf ('INSTRU')
      call x3name('Temp (eh.5)o(exhx)C$',100)
      call y3name('Mole Fraction AlCl(1.5)3(lx)$',100)
      call z3name('Abs. Viscosity cP$',100)
      call vuangl(30.,15.,40.)
      call graf3d(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max),
     1 zz(min),zz(tic),zz(max))
      call thkcrv(.05)
      do 25 ii=1,npoly
      call ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
25    call curv3d(xcrv,ycrv,zcrv,ncrv,0)
      call blsur
      call surfun(avis,5,xx(tic)*.2,5,yy(tic)*.2,0)
      call grfiti(0.,0.,0.,0.,8.,0.,0.,0.,9.)
      call area2d(8.,9.)
      call cross
      call graf(yy(min),yy(tic),yy(max),zz(min),zz(tic),zz(max))
      call height(.525)
```

```
c    xl=xmess('AlCl3$',100)
c    xpos=4.0-xl/2.
c    call messag('AlCl3$',100,xpos,7.)
c    call blrec(xpos-.1,6.9,xl+.2,.725,.02)
     a(1)=yy(min)
     a(2)=yy(max)
     a(3)=yy(max)
     a(4)=yy(min)
     b(1)=zz(min)
     b(2)=zz(min)
     b(3)=zz(max)
     b(4)=zz(max)
     x(1)=yy(min)
     x(2)=yy(max)
     y(1)=zz(min)
     y(2)=zz(min)
     call curve(a,b,4,0)
     call shdpat(19)
c    shadpat was 17
     call shdcrv(x,y,2,0,0,iabove)
     call end3gr(0)
     call grfiti(0.,0.,0.,8.,0.,0.,8.,0.,9.)
     call area2d(8.,9.)
     call cross
     call graf(xx(min),xx(tic),xx(max),zz(min),zz(tic),zz(max))
c    next 4 lines put msg on x-z wall
c    xl=xmess('deg C$',100)
c    xpos=4.0-xl/2.
c    call messag('deg C$',100,xpos,7.)
c    call blrec(xpos-.1,6.9,xl+.2,.725,.02)
     a(1)=xx(min)
     a(2)=xx(max)
     a(3)=xx(max)
     a(4)=xx(min)
     b(1)=zz(min)
     b(2)=zz(min)
     b(3)=zz(max)
     b(4)=zz(max)
     x(1)=xx(min)
     x(2)=xx(max)
     y(1)=zz(min)
     y(2)=zz(min)
     call curve(a,b,4,0)
     call shdpat(10)
c    shadpat was 18
     call shdcrv(x,y,2,0,0,iabove)
     call end3gr(0)
     call grfiti(0.,0.,0.,8.,0.,0.,0.,8.,0.)
     call area2d(8.,8.)
     call cross
     call graf(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max))
     a(1)=xx(min)
     a(2)=xx(max)
     a(3)=xx(max)
     a(4)=xx(min)
```

```
b(1)=yy(min)
b(2)=yy(min)
b(3)=yy(max)
b(4)=yy(max)
x(1)=xx(min)
x(2)=xx(max)
y(1)=yy(min)
y(2)=yy(min)
call curve(a,b,4,0)
call shdpat(5)
call shdcrv(x,y,2,0,0,iabove)
call end3gr(0)
call endpl(0)
call donepl
stop
end
function avis(t,x)
f=1.0-abs((2*x-1)/(1-x))
x8=f*f
if(x.lt.0.5) then
     x2=(1.0-f)*(1.0-f)
     x5=2.0*f*(1.0-f)
     x11=0.0
     x14=0.0
else
     x2=0.0
     x5=0.0
     x14=(1.0-f)*(1.0-f)
     x11=2.0*f*(1.0-f)
endif
a2=252.3
a5=189.9
a8=142.2
a11=137.2
a14=132.2
b2=732.5
b5=0.
b8=0.
b11=0.
b14=0.
c2=-4.669
c5=0.
c8=0.
c11=0.
c14=0.
T0=x2*a2+x5*a5+a8*x8+a11*x11+a14*x14
ck=x2*b2+x5*b5+b8*x8+b11*x11+b14*x14
aln=x2*c2+x5*c5+c8*x8+c11*x11+c14*x14
ta=t+273.15
ck=732.5
aln=-4.669
z=ck/(ta-T0)+0.5*alog(ta)+aln
elamda=exp(z)
tb=(t-60.0)*1.0e-4
z=1.1279*x2+1.2208*x5+1.2662*x8+1.3263*x11+1.3567*x14
```

```
      dense=z-tb*(6.1096*x2+6.6170*x5+8.0153*x8+8.7004*x11+9.6190*x14)
      em=146.64+133.34*(x/(1.0-x))
      if (elamda.gt.900.) elamda=900.
      avis=(elamda)
      end
      subroutine ldpoly(xpoly,ypoly,npoly)
      dimension xpoly(*),ypoly(*)
      open(unit=8,name='3dvis.dat',status='OLD',err=99)
      do 10 i=1,100
      read(8,'(2f12.0)',err=99,end=20) xpoly(i),ypoly(i)
      write(5,'(2x,2f12.4)') xpoly(i),ypoly(i)
10    npoly=i
20    write(5,'(2x,i4,'' vertex polygon from 3dvis.dat '')') npoly
      close(8)
      return
99    write(5,'('' Error in reading 3Dvis.DAT file'')')
      stop
      end
      subroutine ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
      dimension xpoly(*),ypoly(*),xcrv(*),ycrv(*),zcrv(*)
      nsegs=5
      delta=1.0/nsegs
      if(ii .ne. 1) then
           x1=xpoly(ii-1)
           y1=ypoly(ii-1)
      else
           x1=xpoly(npoly)
           y1=ypoly(npoly)
      end if
      x2=xpoly(ii)
      y2=ypoly(ii)
      xx=x1
      deltax=(x2-x1)*delta
      yy=y1
      deltay=(y2-y1)*delta
      do 30 i=1,nsegs+1
      xcrv(i)=xx
      ycrv(i)=yy
      zcrv(i)=avis(xx,yy)
      xx=xx+deltax
30    yy=yy+deltay
      ncrv=nsegs+1
      return
      end
```

```
SPECIFIC CONDUCTIVITY
      external cond
      integer tic
      logical ok
      dimension a(4),b(4),x(2),y(2),iabove(1)
      dimension xx(3),yy(3),zz(3)
      dimension xpoly(50),ypoly(50),xcrv(10),ycrv(10),zcrv(10)
      data iabove/4HABOV/
      min=1
      max=2
      tic=3
      xx(min)=0.0
      xx(max)=120.0
      xx(tic)=30.0
      yy(min)=0.0
      yy(max)=0.70
      yy(tic)=0.15
      zz(max)=0.08
      zz(min)=0.0
      zz(tic)=.02
      call ldpoly(xpoly,ypoly,npoly)
c     call ptk41
      call ptekal
c     call prpdev(ok)
c     if(.not. ok) stop
c     call hp7470
      call hwrot('AUTO')
      call swissm
      call shdchr(90.,1,.002,1)
      call height(.325)
      call physor(.5,0.5)
      call bshift(0.3,0.)
      call nobrdr
      call area2d(7.5,9.75)
      xl=xmess('Melt Specific Conductivity$',100)
      call messag('Melt Specific Conductivity$',100,4.0-xl/2.,9.25)
      call volm3d(8.,8.,9.)
      call mixalf ('INSTRU')
      call x3name('Temp (eh.5)o(exhx)C$',100)
      call y3name('Mole Fraction AlCl(1.5)3(1x)$',100)
      call z3name('Sp. Cond. 1/ohm-cm$',100)
      call vuangl(-13.,62.,40.)
      call graf3d(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max),
     1 zz(min),zz(tic),zz(max))
      call thkcrv(.05)
      do 25 ii=1,npoly
      call ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
25    call curv3d(xcrv,ycrv,zcrv,ncrv,0)
      call blsur
      call surfun(cond,5,xx(tic)*.2,5,yy(tic)*.2,0)
      call grfiti(0.,0.,0.,0.,8.,0.,0.,0.,9.)
      call area2d(8.,9.)
      call cross
      call graf(yy(min),yy(tic),yy(max),zz(min),zz(tic),zz(max))
      call height(.525)
c     xl=xmess('AlCl3$',100)
```

```
c    xpos=4.0-xl/2.
c    call messag('AlCl3$',100,xpos,7.)
c    call blrec(xpos-.1,6.9,xl+.2,.725,.02)
     a(1)=yy(min)
     a(2)=yy(max)
     a(3)=yy(max)
     a(4)=yy(min)
     b(1)=zz(min)
     b(2)=zz(min)
     b(3)=zz(max)
     b(4)=zz(max)
     x(1)=yy(min)
     x(2)=yy(max)
     y(1)=zz(min)
     y(2)=zz(min)
     call curve(a,b,4,0)
     call shdpat(19)
c    shadpat was 17
     call shdcrv(x,y,2,0,0,iabove)
     call end3gr(0)
     call grfiti(0.,8.,0.,8.,8.,0.,0.,8.,9.)
     call area2d(8.,9.)
     call cross
     call graf(xx(min),xx(tic),xx(max),zz(min),zz(tic),zz(max))
c    next 4 lines put msg on x-z wall
c    xl=xmess('deg C$',100)
c    xpos=4.0-xl/2.
c    call messag('deg C$',100,xpos,7.)
c    call blrec(xpos-.1,6.9,xl+.2,.725,.02)
     a(1)=xx(min)
     a(2)=xx(max)
     a(3)=xx(max)
     a(4)=xx(min)
     b(1)=zz(min)
     b(2)=zz(min)
     b(3)=zz(max)
     b(4)=zz(max)
     x(1)=xx(min)
     x(2)=xx(max)
     y(1)=zz(min)
     y(2)=zz(min)
     call curve(a,b,4,0)
     call shdpat(10)
c    shadpat was 18
     call shdcrv(x,y,2,0,0,iabove)
     call end3gr(0)
     call grfiti(0.,0.,0.,8.,0.,0.,0.,8.,0.)
     call area2d(8.,8.)
     call cross
     call graf(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max))
     a(1)=xx(min)
     a(2)=xx(max)
     a(3)=xx(max)
     a(4)=xx(min)
     b(1)=yy(min)
```

```
b(2)=yy(min)
b(3)=yy(max)
b(4)=yy(max)
x(1)=xx(min)
x(2)=xx(max)
y(1)=yy(min)
y(2)=yy(min)
call curve(a,b,4,0)
call shdpat(5)
call shdcrv(x,y,2,0,0,1above)
call end3gr(0)
call endpl(0)
call donepl
stop
end
function cond(t,x)
f=1.0-abs((2*x-1)/(1-x))
x8=f*f
if(x.lt.0.5) then
     x2=(1.0-f)*(1.0-f)
     x5=2.0*f*(1.0-f)
     x11=0.0
     x14=0.0
else
     x2=0.0
     x5=0.0
     x14=(1.0-f)*(1.0-f)
     x11=2.0*f*(1.0-f)
endif
a2=259.9
a5=189.1
a8=123.4
a11=126.5
a14=121.9
b2=493.4
b5=763.0
b8=790.9
b11=802.1
b14=813.3
c2=8.0711
c5=8.7437
c8=8.9753
c11=8.9519
c14=8.9253
T0=x2*a2+x5*a5+a8*x8+a11*x11+a14*x14
ck=x2*b2+x5*b5+b8*x8+b11*x11+b14*x14
aln=x2*c2+x5*c5+c8*x8+c11*x11+c14*x14
ta=t+273.15
z=-ck/(ta-T0)-0.5*alog(ta)+aln
elamda=exp(z)
tb=(t-60.0)*1.0e-4
z=1.1279*x2+1.2208*x5+1.2662*x8+1.3263*x11+1.3567*x14
dense=z-tb*(6.1096*x2+6.6170*x5+8.0153*x8+8.7004*x11+9.6190*x14)
em=146.64+133.34*(x/(1.0-x))
cond=elamda*dense/em
end
```

```
      subroutine ldpoly(xpoly,ypoly,npoly)
      dimension xpoly(*),ypoly(*)
      open(unit=8,name='3dCON.dat',status='OLD',err=99)
      do 10 i=1,100
      read(8,'(2f12.0)',err=99,end=20) xpoly(i),ypoly(i)
      write(5,'(2x,2f12.4)') xpoly(i),ypoly(i)
10    npoly=i
20    write(5,'(2x,i4,'' vertex polygon from 3dCON.dat '')') npoly
      close(8)
      return
99    write(5,'('' Error in reading 3DCON.DAT file'')')
      stop
      end
      subroutine ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
      dimension xpoly(*),ypoly(*),xcrv(*),ycrv(*),zcrv(*)
      nsegs=5
      delta=1.0/nsegs
      if(ii .ne. 1) then
           x1=xpoly(ii-1)
           y1=ypoly(ii-1)
      else
           x1=xpoly(npoly)
           y1=ypoly(npoly)
      end if
      x2=xpoly(ii)
      y2=ypoly(ii)
      xx=x1
      deltax=(x2-x1)*delta
      yy=y1
      deltay=(y2-y1)*delta
      do 30 i=1,nsegs+1
      xcrv(i)=xx
      ycrv(i)=yy
      zcrv(i)=cond(xx,yy)
      xx=xx+deltax
30    yy=yy+deltay
      ncrv=nsegs+1
      return
      end
```

```
DENSITY
      external dense
      integer tic
      logical ok
      dimension a(4),b(4),x(2),y(2),iabove(1)
      dimension xx(3),yy(3),zz(3)
      dimension xpoly(50),ypoly(50),xcrv(10),ycrv(10),zcrv(10)
      data iabove/4HABOV/
      min=1
      max=2
      tic=3
      xx(min)=5.0
      xx(max)=95.0
      xx(tic)=30.0
      yy(min)=0.0
      yy(max)=0.70
      yy(tic)=0.15
      zz(max)=1.50
      zz(min)=1.00
      zz(tic)=.1
      call ldpoly(xpoly,ypoly,npoly)
C     call ptk41
      call ptekal
c     call prpdev(ok)
c     if(.not. ok) stop
c     call hp7470
      call hwrot('AUTO')
      call swissm
      call shdchr(90.,1,.002,1)
      call height(.325)
      call physor(.5,.625)
      call area2d(7.5,9.75)
      xl=xmess('Melt Density$',100)
      call messag('Melt Density$',100,4.0-xl/2.,9.25)
      call volm3d(8.,8.,9.)
      call mixalf ('INSTRU')
      call x3name('Temp (eh.5)o(exhx)C$',100)
      call y3name('Mole Fraction AlCl(1.5)3(1x)$',100)
      call z3name('Density g/mL',12)
      call vuangl(-30.,30.,30.)
      call graf3d(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max),
     1 zz(min),zz(tic),zz(max))
      call thkcrv(.05)
      do 25 ii=1,npoly
      call ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
25    call curv3d(xcrv,ycrv,zcrv,ncrv,0)
      call blsur
      call surfun(dense,5,xx(tic)*.2,5,yy(tic)*.2,0)
      call grfiti(0.,0.,0.,0.,8.,0.,0.,0.,9.)
      call area2d(8.,9.)
      call cross
      call graf(yy(min),yy(tic),yy(max),zz(min),zz(tic),zz(max))
      call height(.525)
      xl=xmess('AlCl3$',100)
      xpos=4.0-xl/2.
```

```
c    call messag('AlCl3$',100,xpos,7.)
c    call blrec(xpos-.1,6.9,xl+.2,.725,.02)
     a(1)=yy(min)
     a(2)=yy(max)
     a(3)=yy(max)
     a(4)=yy(min)
     b(1)=zz(min)
     b(2)=zz(min)
     b(3)=zz(max)
     b(4)=zz(max)
     x(1)=yy(min)
     x(2)=yy(max)
     y(1)=zz(min)
     y(2)=zz(min)
     call curve(a,b,4,0)
     call shdpat(19)
c    shadpat was 17
     call shdcrv(x,y,2,0,0,iabove)
     call end3gr(0)
     call grfiti(0.,8.,0.,8.,8.,0.,0.,8.,9.)
     call area2d(8.,9.)
     call cross
     call graf(xx(min),xx(tic),xx(max),zz(min),zz(tic),zz(max))
c    next 4 lines put msg on x-z wall
c    xl=xmess('deg C$',100)
c    xpos=4.0-xl/2.
c    call messag('deg C$',100,xpos,7.)
c    call blrec(xpos-.1,6.9,xl+.2,.725,.02)
     a(1)=xx(min)
     a(2)=xx(max)
     a(3)=xx(max)
     a(4)=xx(min)
     b(1)=zz(min)
     b(2)=zz(min)
     b(3)=zz(max)
     b(4)=zz(max)
     x(1)=xx(min)
     x(2)=xx(max)
     y(1)=zz(min)
     y(2)=zz(min)
     call curve(a,b,4,0)
     call shdpat(10)
c    shadpat was 18
     call shdcrv(x,y,2,0,0,iabove)
     call end3gr(0)
     call grfiti(0.,0.,0.,8.,0.,0.,0.,8.,0.)
     call area2d(8.,8.)
     call cross
     call graf(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max))
     a(1)=xx(min)
     a(2)=xx(max)
     a(3)=xx(max)
     a(4)=xx(min)
     b(1)=yy(min)
     b(2)=yy(min)
```

```
      b(3)=yy(max)
      b(4)=yy(max)
      x(1)=xx(min)
      x(2)=xx(max)
      y(1)=yy(min)
      y(2)=yy(min)
      call curve(a,b,4,0)
      call shdpat(5)
      call shdcrv(x,y,2,0,0,iabove)
      call end3gr(0)
      call endpl(0)
      call donepl
      stop
      end
      function dense(t,x)
      f=1.0-abs((2*x-1)/(1-x))
      tb=(t-60.0)*1.0e-4
      x8=f*f
      if(x.lt.0.5) then
           x2=(1.0-f)*(1.0-f)
           x5=2.0*f*(1.0-f)
           x11=0.0
           x14=0.0
      else
           x2=0.0
           x5=0.0
           x14=(1.0-f)*(1.0-f)
           x11=2.0*f*(1.0-f)
      endif
      z=1.1279*x2+1.2208*x5+1.2662*x8+1.3263*x11+1.3567*x14
      dense=z-tb*(6.1096*x2+6.6170*x5+8.0153*x8+8.7004*x11+9.6190*x14)
      end
      subroutine ldpoly(xpoly,ypoly,npoly)
      dimension xpoly(*),ypoly(*)
      open(unit=8,name='3dpoly.dat',status='OLD',err=99)
      do 10 i=1,100
      read(8,'(2f12.0)',err=99,end=20) xpoly(i),ypoly(i)
      write(5,'(2x,2f12.4)') xpoly(i),ypoly(i)
10    npoly=i
20    write(5,'(2x,i4,'' vertex polygon from 3dpoly.dat '')') npoly
      close(8)
      return
99    write(5,'('' Error in reading 3DPOLY.DAT file'')')
      stop
      end
      subroutine ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
      dimension xpoly(*),ypoly(*),xcrv(*),ycrv(*),zcrv(*)
      nsegs=5
      delta=1.0/nsegs
      if(ii .ne. 1) then
           x1=xpoly(ii-1)
```

```
          y1=ypoly(ii-1)
      else
          x1=xpoly(npoly)
          y1=ypoly(npoly)
      end if
      x2=xpoly(ii)
      y2=ypoly(ii)
      xx=x1
      deltax=(x2-x1)*delta
      yy=y1
      deltay=(y2-y1)*delta
      do 30 i=1,nsegs+1
      xcrv(i)=xx
      ycrv(i)=yy
      zcrv(i)=dense(xx,yy)
      xx=xx+deltax
30    yy=yy+deltay
      ncrv=nsegs+1
      return
      end
```

```
 EQUIVALENT CONDUCTIVITY
      external cond
      integer tic
      logical ok
      dimension a(4),b(4),x(2),y(2),iabove(1)
      dimension xx(3),yy(3),zz(3)
      dimension xpoly(50),ypoly(50),xcrv(10),ycrv(10),zcrv(10)
      data iabove/4HABOV/
      min=1
      max=2
      tic=3
      xx(min)=0.0
      xx(max)=120.0
      xx(tic)=30.0
      yy(min)=0.0
      yy(max)=0.70
      yy(tic)=0.15
      zz(max)=20.
      zz(min)=0.0
      zz(tic)=5.
      call ldpoly(xpoly,ypoly,npoly)
c     call ptk41
      call ptekal
c     call prpdev(ok)
c     if(.not. ok) stop
c     call hp7470
      call hwrot('AUTO')
      call swissm
      call shdchr(90.,1,.002,1)
      call height(.325)
      call physor(.5,0.5)
      call bshift(0.3,0.)
      call nobrdr
      call area2d(7.5,9.75)
      xl=xmess('Melt Equiv. Conductivity$',100)
      call messag('Melt Equiv. Conductivity$',100,4.0-xl/2.,9.25)
      call volm3d(8.,8.,9.)
      call mixalf ('INSTRU')
      call x3name('Temp (eh.5)o(exhx)C$',100)
      call y3name('Mole Fraction AlCl(1.5)3(1x)$',100)
      call z3name('Eq. Cond. cm(eh.5)2(hxex)/ohm-eq$',100)
      call vuangl(-13.,62.,40.)
      call graf3d(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max),
     1 zz(min),zz(tic),zz(max))
      call thkcrv(.05)
      do 25 ii=1,npoly
      call ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
25    call curv3d(xcrv,ycrv,zcrv,ncrv,0)
      call blsur
      call surfun(cond,5,xx(tic)*.2,5,yy(tic)*.2,0)
      call grfiti(0.,0.,0.,0.,8.,0.,0.,0.,9.)
      call area2d(8.,9.)
      call cross
      call graf(yy(min),yy(tic),yy(max),zz(min),zz(tic),zz(max))
      call height(.525)
```

```
c    xl=xmess('AlCl3$',100)
c    xpos=4.0-xl/2.
c    call messag('AlCl3$',100,xpos,7.)
c    call blrec(xpos-.1,6.9,xl+.2,.725,.02)
     a(1)=yy(min)
     a(2)=yy(max)
     a(3)=yy(max)
     a(4)=yy(min)
     b(1)=zz(min)
     b(2)=zz(min)
     b(3)=zz(max)
     b(4)=zz(max)
     x(1)=yy(min)
     x(2)=yy(max)
     y(1)=zz(min)
     y(2)=zz(min)
     call curve(a,b,4,0)
     call shdpat(19)
c    shadpat was 17
     call shdcrv(x,y,2,0,0,iabove)
     call end3gr(0)
     call grfiti(0.,8.,0.,8.,8.,0.,0.,8.,9.)
     call area2d(8.,9.)
     call cross
     call graf(xx(min),xx(tic),xx(max),zz(min),zz(tic),zz(max))
c    next 4 lines put msg on x-z wall
c    xl=xmess('deg C$',100)
c    xpos=4.0-xl/2.
c    call messag('deg C$',100,xpos,7.)
c    call blrec(xpos-.1,6.9,xl+.2,.725,.02)
     a(1)=xx(min)
     a(2)=xx(max)
     a(3)=xx(max)
     a(4)=xx(min)
     b(1)=zz(min)
     b(2)=zz(min)
     b(3)=zz(max)
     b(4)=zz(max)
     x(1)=xx(min)
     x(2)=xx(max)
     y(1)=zz(min)
     y(2)=zz(min)
     call curve(a,b,4,0)
     call shdpat(10)
c    shadpat was 18
     call shdcrv(x,y,2,0,0,iabove)
     call end3gr(0)
     call grfiti(0.,0.,0.,8.,0.,0.,0.,8.,0.)
     call area2d(8.,8.)
     call cross
     call graf(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max))
     a(1)=xx(min)
     a(2)=xx(max)
     a(3)=xx(max)
     a(4)=xx(min)
```

```
b(1)=yy(min)
b(2)=yy(min)
b(3)=yy(max)
b(4)=yy(max)
x(1)=xx(min)
x(2)=xx(max)
y(1)=yy(min)
y(2)=yy(min)
call curve(a,b,4,0)
call shdpat(5)
call shdcrv(x,y,2,0,0,1above)
call end3gr(0)
call endpl(0)
call donepl
stop
end
function cond(t,x)
f=1.0-abs((2*x-1)/(1-x))
x8=f*f
if(x.lt.0.5) then
     x2=(1.0-f)*(1.0-f)
     x5=2.0*f*(1.0-f)
     x11=0.0
     x14=0.0
else
     x2=0.0
     x5=0.0
     x14=(1.0-f)*(1.0-f)
     x11=2.0*f*(1.0-f)
endif
a2=259.9
a5=189.1
a8=123.4
a11=126.5
a14=121.9
b2=493.4
b5=763.0
b8=790.9
b11=802.1
b14=813.3
c2=8.0711
c5=8.7437
c8=8.9753
c11=8.9519
c14=8.9253
T0=x2*a2+x5*a5+a8*x8+a11*x11+a14*x14
ck=x2*b2+x5*b5+b8*x8+b11*x11+b14*x14
aln=x2*c2+x5*c5+c8*x8+c11*x11+c14*x14
ta=t+273.15
z=-ck/(ta-T0)-0.5*alog(ta)+aln
elamda=exp(z)
tb=(t-60.0)*1.0e-4
z=1.1279*x2+1.2208*x5+1.2662*x8+1.3263*x11+1.3567*x14
dense=z-tb*(6.1096*x2+6.6170*x5+8.0153*x8+8.7004*x11+9.6190*x14)
em=146.64+133.34*(x/(1.0-x))
```

```
      cond=elamda
      end
      subroutine ldpoly(xpoly,ypoly,npoly)
      dimension xpoly(*),ypoly(*)
      open(unit=8,name='3dCON.dat',status='OLD',err=99)
      do 10 i=1,100
      read(8,'(2f12.0)',err=99,end=20) xpoly(i),ypoly(i)
      write(5,'(2x,2f12.4)') xpoly(i),ypoly(i)
 10   npoly=i
 20   write(5,'(2x,i4,'' vertex polygon from 3dCON.dat '')') npoly
      close(8)
      return
 99   write(5,'('' Error in reading 3DCON.DAT file'')')
      stop
      end
      subroutine ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
      dimension xpoly(*),ypoly(*),xcrv(*),ycrv(*),zcrv(*)
      nsegs=5
      delta=1.0/nsegs
      if(ii .ne. 1) then
           x1=xpoly(ii-1)
           y1=ypoly(ii-1)
      else
           x1=xpoly(npoly)
           y1=ypoly(npoly)
      end if
      x2=xpoly(ii)
      y2=ypoly(ii)
      xx=x1
      deltax=(x2-x1)*delta
      yy=y1
      deltay=(y2-y1)*delta
      do 30 i=1,nsegs+1
      xcrv(i)=xx
      ycrv(i)=yy
      zcrv(i)=cond(xx,yy)
      xx=xx+deltax
 30   yy=yy+deltay
      ncrv=nsegs+1
      return
      end
```

```
KINEMATIC VISCOSITY
      external avis
      integer tic
      logical ok
      dimension a(4),b(4),x(2),y(2),iabove(1)
      dimension xx(3),yy(3),zz(3)
      dimension xpoly(50),ypoly(50),xcrv(10),ycrv(10),zcrv(10)
      data iabove/4HABOV/
      min=1
      max=2
      tic=3
      xx(min)=0.0
      xx(max)=100.0
      xx(tic)=25.0
      yy(min)=0.301
      yy(max)=0.70
      yy(tic)=0.1
      zz(max)=3.
      zz(min)=0.0
      zz(tic)=1.
      call ldpoly(xpoly,ypoly,npoly)
c     call ptk41
      call ptekal
c     call prpdev(ok)
c     if(.not. ok) stop
c     call hp7470
      call hwrot('AUTO')
      call swissm
      call shdchr(90.,1,.002,1)
      call height(.325)
      call physor(.5,0.5)
      call bshift(0.4,0.)
      call nobrdr
      call area2d(7.5,9.75)
      xl=xmess('Melt Kinematic Viscosity$',100)
      call messag('Melt Kinematic Viscosity$',100,4.0-xl/2.,9.25)
      call volm3d(8.,8.,9.)
      call mixalf ('INSTRU')
      call x3name('Temp (eh.5)o(exhx)C$',100)
      call y3name('Mole Fraction AlCl(1.5)3(1x)$',100)
      call z3name('Log Kin. Viscosity cS$',100)
      call vuangl(30.,15.,40.)
      call graf3d(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max),
     1 zz(min),zz(tic),zz(max))
      call thkcrv(.05)
      do 25 ii=1,npoly
      call ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
25    call curv3d(xcrv,ycrv,zcrv,ncrv,0)
      call blsur
      call surfun(avis,5,xx(tic)*.2,5,yy(tic)*.2,0)
      call grfiti(0.,0.,0.,0.,8.,0.,0.,0.,9.)
      call area2d(8.,9.)
      call cross
      call graf(yy(min),yy(tic),yy(max),zz(min),zz(tic),zz(max))
      call height(.525)
```

```
c     xl=xmess('AlCl3$',100)
c     xpos=4.0-xl/2.
c     call messag('AlCl3$',100,xpos,7.)
c     call blrec(xpos-.1,6.9,xl+.2,.725,.02)
      a(1)=yy(min)
      a(2)=yy(max)
      a(3)=yy(max)
      a(4)=yy(min)
      b(1)=zz(min)
      b(2)=zz(min)
      b(3)=zz(max)
      b(4)=zz(max)
      x(1)=yy(min)
      x(2)=yy(max)
      y(1)=zz(min)
      y(2)=zz(min)
      call curve(a,b,4,0)
      call shdpat(19)
c     shadpat was 17
      call shdcrv(x,y,2,0,0,iabove)
      call end3gr(0)
      call grfiti(0.,0.,0.,8.,0.,0.,8.,0.,9.)
      call area2d(8.,9.)
      call cross
      call graf(xx(min),xx(tic),xx(max),zz(min),zz(tic),zz(max))
c     next 4 lines put msg on x-z wall
c     xl=xmess('deg C$',100)
c     xpos=4.0-xl/2.
c     call messag('deg C$',100,xpos,7.)
c     call blrec(xpos-.1,6.9,xl+.2,.725,.02)
      a(1)=xx(min)
      a(2)=xx(max)
      a(3)=xx(max)
      a(4)=xx(min)
      b(1)=zz(min)
      b(2)=zz(min)
      b(3)=zz(max)
      b(4)=zz(max)
      x(1)=xx(min)
      x(2)=xx(max)
      y(1)=zz(min)
      y(2)=zz(min)
      call curve(a,b,4,0)
      call shdpat(10)
c     shadpat was 18
      call shdcrv(x,y,2,0,0,iabove)
      call end3gr(0)
      call grfiti(0.,0.,0.,8.,0.,0.,0.,8.,0.)
      call area2d(8.,8.)
      call cross
      call graf(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max))
      a(1)=xx(min)
      a(2)=xx(max)
      a(3)=xx(max)
      a(4)=xx(min)
```

```
b(1)=yy(min)
b(2)=yy(min)
b(3)=yy(max)
b(4)=yy(max)
x(1)=xx(min)
x(2)=xx(max)
y(1)=yy(min)
y(2)=yy(min)
call curve(a,b,4,0)
call shdpat(5)
call shdcrv(x,y,2,0,0,iabove)
call end3gr(0)
call endpl(0)
call donepl
stop
end
function avis(t,x)
f=1.0-abs((2*x-1)/(1-x))
x8=f*f
if(x.lt.0.5) then
     x2=(1.0-f)*(1.0-f)
     x5=2.0*f*(1.0-f)
     x11=0.0
     x14=0.0
else
     x2=0.0
     x5=0.0
     x14=(1.0-f)*(1.0-f)
     x11=2.0*f*(1.0-f)
endif
a2=252.3
a5=189.9
a8=142.2
a11=137.2
a14=132.2
b2=732.5
b5=0.
b8=0.
b11=0.
b14=0.
c2=-4.669
c5=0.
c8=0.
c11=0.
c14=0.
T0=x2*a2+x5*a5+a8*x8+a11*x11+a14*x14
ck=x2*b2+x5*b5+b8*x8+b11*x11+b14*x14
aln=x2*c2+x5*c5+c8*x8+c11*x11+c14*x14
ta=t+273.15
ck=732.5
aln=-4.669
z=ck/(ta-T0)+0.5*alog(ta)+aln
elamda=exp(z)
tb=(t-60.0)*1.0e-4
de=1.1279*x2+1.2208*x5+1.2662*x8+1.3263*x11+1.3567*x14
```

```
      dense=de-tb*(6.1096*x2+6.6170*x5+8.0153*x8+8.7004*x11+9.6190*x14)
      em=146.64+133.34*(x/(1.0-x))
      elamda=elamda/dense
      if (elamda.gt.1000.) elamda=1000.
      avis=alog10(elamda)
      end
      subroutine ldpoly(xpoly,ypoly,npoly)
      dimension xpoly(*),ypoly(*)
      open(unit=8,name='3dvis.dat',status='OLD',err=99)
      do 10 i=1,100
      read(8,'(2f12.0)',err=99,end=20) xpoly(i),ypoly(i)
      write(5,'(2x,2f12.4)') xpoly(i),ypoly(i)
10    npoly=i
20    write(5,'(2x,i4,'' vertex polygon from 3dvis.dat '')') npoly
      close(8)
      return
99    write(5,'('' Error in reading 3Dvis.DAT file'')')
      stop
      end
      subroutine ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
      dimension xpoly(*),ypoly(*),xcrv(*),ycrv(*),zcrv(*)
      nsegs=5
      delta=1.0/nsegs
      if(ii .ne. 1) then
           x1=xpoly(ii-1)
           y1=ypoly(ii-1)
      else
           x1=xpoly(npoly)
           y1=ypoly(npoly)
      end if
      x2=xpoly(ii)
      y2=ypoly(ii)
      xx=x1
      deltax=(x2-x1)*delta
      yy=y1
      deltay=(y2-y1)*delta
      do 30 i=1,nsegs+1
      xcrv(i)=xx
      ycrv(i)=yy
      zcrv(i)=avis(xx,yy)
      xx=xx+deltax
30    yy=yy+deltay
      ncrv=nsegs+1
      return
      end
```

```
WALDEN PRODUCT
      external wald
      integer tic
      logical ok
      dimension a(4),b(4),x(2),y(2),iabove(1)
      dimension xx(3),yy(3),zz(3)
      dimension xpoly(50),ypoly(50),xcrv(10),ycrv(10),zcrv(10)
      data iabove/4HABOV/
      min=1
      max=2
      tic=3
      xx(min)=0.0
      xx(max)=100.0
      xx(tic)=25.0
      yy(min)=0.301
      yy(max)=0.70
      yy(tic)=0.1
      zz(max)=16000.
      zz(min)=8000.0
      zz(tic)=2000.
c     call ldpoly(xpoly,ypoly,npoly)
c     call ptk41
      call ptekal
c     call prpdev(ok)
c     if(.not. ok) stop
c     call hp7470
      call hwrot('AUTO')
      call swissm
      call shdchr(90.,1,.002,1)
      call height(.325)
      call physor(.5,0.5)
      call bshift(0.3,0.)
      call nobrdr
      call area2d(7.5,9.75)
      xl=xmess('Melt Walden Product$',100)
      call messag('Melt Walden Product$',100,4.0-xl/2.,9.25)
      call volm3d(8.,8.,9.)
      call mixalf ('INSTRU')
      call x3name('Temp (eh.5)o(exhx)C$',100)
      call y3name('Mole Fraction AlCl(1.5)3(lx)$',100)
      call z3name('(m6)L(mx) * (m7)c(mx)$',100)
      call vuangl(-11.,40.,40.)
      call graf3d(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max),
     1 zz(min),zz(tic),zz(max))
      call thkcrv(.05)
      do 25 ii=1,npoly
c     call ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
25    call curv3d(xcrv,ycrv,zcrv,ncrv,0)
      call blsur
      call surfun(wald,5,xx(tic)*.2,5,yy(tic)*.2,0)
      call grfiti(0.,0.,0.,0.,8.,0.,0.,0.,9.)
      call area2d(8.,9.)
      call cross
      call graf(yy(min),yy(tic),yy(max),zz(min),zz(tic),zz(max))
      call height(.525)
```

```
c     xl=xmess('AlCl3$',100)
c     xpos=4.0-xl/2.
c     call messag('AlCl3$',100,xpos,7.)
c     call blrec(xpos-.1,6.9,xl+.2,.725,.02)
      a(1)=yy(min)
      a(2)=yy(max)
      a(3)=yy(max)
      a(4)=yy(min)
      b(1)=zz(min)
      b(2)=zz(min)
      b(3)=zz(max)
      b(4)=zz(max)
      x(1)=yy(min)
      x(2)=yy(max)
      y(1)=zz(min)
      y(2)=zz(min)
      call curve(a,b,4,0)
      call shdpat(19)
c     shadpat was 17
      call shdcrv(x,y,2,0,0,iabove)
      call end3gr(0)
      call grfiti(0.,8.,0.,8.,8.,0.,0.,8.,9.)
      call area2d(8.,9.)
      call cross
      call graf(xx(min),xx(tic),xx(max),zz(min),zz(tic),zz(max))
c     next 4 lines put msg on x-z wall
c     xl=xmess('deg C$',100)
c     xpos=4.0-xl/2.
c     call messag('deg C$',100,xpos,7.)
c     call blrec(xpos-.1,6.9,xl+.2,.725,.02)
      a(1)=xx(min)
      a(2)=xx(max)
      a(3)=xx(max)
      a(4)=xx(min)
      b(1)=zz(min)
      b(2)=zz(min)
      b(3)=zz(max)
      b(4)=zz(max)
      x(1)=xx(min)
      x(2)=xx(max)
      y(1)=zz(min)
      y(2)=zz(min)
      call curve(a,b,4,0)
      call shdpat(10)
c     shadpat was 18
      call shdcrv(x,y,2,0,0,iabove)
      call end3gr(0)
      call grfiti(0.,0.,0.,8.,0.,0.,0.,8.,0.)
      call area2d(8.,8.)
      call cross
      call graf(xx(min),xx(tic),xx(max),yy(min),yy(tic),yy(max))
      a(1)=xx(min)
      a(2)=xx(max)
      a(3)=xx(max)
      a(4)=xx(min)
```

```
b(1)=yy(min)
b(2)=yy(min)
b(3)=yy(max)
b(4)=yy(max)
x(1)=xx(min)
x(2)=xx(max)
y(1)=yy(min)
y(2)=yy(min)
call curve(a,b,4,0)
call shdpat(5)
call shdcrv(x,y,2,0,0,1above)
call end3gr(0)
call endpl(0)
call donepl
stop
end
function wald(t,x)
f=1.0-abs((2*x-1)/(1-x))
x8=f*f
if(x.lt.0.5) then
     x2=(1.0-f)*(1.0-f)
     x5=2.0*f*(1.0-f)
     x11=0.0
     x14=0.0
else
     x2=0.0
     x5=0.0
     x14=(1.0-f)*(1.0-f)
     x11=2.0*f*(1.0-f)
endif
a2=259.9
a5=189.1
a8=123.4
a11=126.5
a14=121.9
b2=493.4
b5=763.0
b8=790.9
b11=802.1
b14=813.3
c2=8.0711
c5=8.7437
c8=8.9753
c11=8.9519
c14=8.9253
T0=x2*a2+x5*a5+a8*x8+a11*x11+a14*x14
ck=x2*b2+x5*b5+b8*x8+b11*x11+b14*x14
aln=x2*c2+x5*c5+c8*x8+c11*x11+c14*x14
ta=t+273.15
z=-ck/(ta-T0)-0.5*alog(ta)+aln
elamda=exp(z)
tb=(t-60.0)*1.0e-4
z=1.1279*x2+1.2208*x5+1.2662*x8+1.3263*x11+1.3567*x14
dense=z-tb*(6.1096*x2+6.6170*x5+8.0153*x8+8.7004*x11+9.6190*x14)
em=146.64+133.34*(x/(1.0-x))
```

```
      elamda=elamda*em/dense
      av2=252.3
      av5=189.9
      av8=142.2
      av11=137.2
      av14=132.2
      etak=732.5
      etaaln=-4.669
      etaT0=x2*av2+x5*av5+av8*x8+av11*x11+av14*x14
      avis=exp(etak/(ta-T0)+0.5*alog(ta)+etaaln)
      wald=min(elamda*avis,20000.)
      end
      subroutine ldpoly(xpoly,ypoly,npoly)
      dimension xpoly(*),ypoly(*)
      open(unit=8,name='3dCON.dat',status='OLD',err=99)
      do 10 i=1,100
      read(8,'(2f12.0)',err=99,end=20) xpoly(i),ypoly(i)
      write(5,'(2x,2f12.4)') xpoly(i),ypoly(i)
10    npoly=i
20    write(5,'(2x,i4,'' vertex polygon from 3dCON.dat '')') npoly
      close(8)
      return
99    write(5,'('' Error in reading 3DCON.DAT file'')')
      stop
      end
      subroutine ntrpol(xpoly,ypoly,npoly,ii,xcrv,ycrv,zcrv,ncrv)
      dimension xpoly(*),ypoly(*),xcrv(*),ycrv(*),zcrv(*)
      nsegs=5
      delta=1.0/nsegs
      if (ii .ne. 1) then
           x1=xpoly(ii-1)
           y1=ypoly(ii-1)
      else
           x1=xpoly(npoly)
           y1=ypoly(npoly)
      end if
      x2=xpoly(ii)
      y2=ypoly(ii)
      xx=x1
      deltax=(x2-x1)*delta
      yy=y1
      deltay=(y2-y1)*delta
      do 30 i=1,nsegs+1
      xcrv(i)=xx
      ycrv(i)=yy
      zcrv(i)=wald(xx,yy)
      xx=xx+deltax
30    yy=yy+deltay
      ncrv=nsegs+1
      return
      end
```

APPENDIX B

THREE-DIMENSIONAL EQUATIONS FOR MeEtImCl-$AlCl_3$ BINARY MELTS

DENSITY: g/cm3 [Valid for $0.25 \leq N \leq 0.6666$ and $10\ °C \leq t \leq 90\ °C$]

$$\rho = \underline{X}_2\underline{a}_2 + \underline{X}_5\underline{a}_5 + \underline{X}_8\underline{a}_8 + \underline{X}_{11}\underline{a}_{11} + \underline{X}_{14}\underline{a}_{14} + (\underline{X}_2\underline{b}_2 + \underline{X}_5\underline{b}_5 + \underline{X}_8\underline{b}_8 + \underline{X}_{11}\underline{b}_{11} + \underline{X}_{14}\underline{b}_{14})(\underline{t} - 60) \quad (1)$$

where the $\underline{a}_i$'s and $\underline{b}_i$'s represent the parameters in the equation below for the individual "complexes" with 2, 5, 8, 11, and 14 chlorides.

$$\rho = \underline{a} + \underline{b}(\underline{t} - 60) \quad (2)$$

The $\underline{X}_i$'s may be calculated most conveniently as follows: Let $\underline{f}$ be the anion fraction of $AlCl_4^-$. Then $\underline{f} = 1 - |(2\underline{N} - 1)/(1 - \underline{N})|$. For $0 < \underline{N} < 0.5$, $\underline{X}_2 = (1 - \underline{f})^2$, $\underline{X}_5 = 2\underline{f}(1 - \underline{f})$, and $\underline{X}_{11}$ and $\underline{X}_{14} = 0$. For $0.5 < \underline{N} \leq 0.667$, $\underline{X}_2$ and $\underline{X}_5 = 0$, $\underline{X}_{11} = 2\underline{f}(1 - \underline{f})$, and $\underline{X}_{14} = (1 - \underline{f})^2$. At all compositions $\underline{X}_8 = \underline{f}^2$.

TABLE I. Least Squares Fitted Parameters for Equation 1 Densities.[a]

i	$\underline{a}_i$	$-\underline{b}_i \times 10^4$
2	1.1279	6.1096
5	1.2208	6.6170
8	1.2662	8.0153
11	1.3263	8.7004
14	1.3567	9.1690

[a] The parameters yield $\sigma = 0.0004$ in ρ, where $\sigma = [\Sigma(\rho_{calc} - \rho_{exp})^2/(\text{number of points} - \text{number of fitted parameters})]^{1/2}$.

CONDUCTIVITY: $cm^2/eq/L$ [Valid for $0.30 \leq N \leq 0.6666$ and $20\ °C \leq t \leq 100\ °C$]

VISCOSITY: cP [Valid for $0.31 \leq N \leq 0.6666$ and $10\ °C \leq t \leq 90\ °C$]

$$\ln \Lambda = -\underline{k}_\Lambda / (\underline{T} - \underline{T}_o) - 1/2 \ln \underline{T} + \ln \underline{A}_\Lambda \quad (3)$$

and

$$\ln \eta = \underline{k}_\eta / (\underline{T} - \underline{T}_o) + 1/2 \ln \underline{T} + \ln \underline{A}_\eta \quad (4)$$

where

$$\underline{T}_o = \underline{X}_2\underline{a}_2 + \underline{X}_5\underline{a}_5 + \underline{X}_8\underline{a}_8 + \underline{X}_{11}\underline{a}_{11} + \underline{X}_{14}\underline{a}_{14} \quad (5)$$

$$\underline{k} = \underline{X}_2\underline{b}_2 + \underline{X}_5\underline{b}_5 + \underline{X}_8\underline{b}_8 + \underline{X}_{11}\underline{b}_{11} + \underline{X}_{14}\underline{b}_{14} \quad (6)$$

$$\ln \underline{A} = \underline{X}_2\underline{c}_2 + \underline{X}_5\underline{c}_5 + \underline{X}_8\underline{c}_8 + \underline{X}_{11}\underline{c}_{11} + \underline{X}_{14}\underline{c}_{14} \quad (7)$$

where the $\underline{a}$'s, $\underline{b}$'s, and $\underline{c}$'s represent the $\underline{T}_o$, $\underline{k}_\Lambda$ and $\ln \underline{A}_\Lambda$, respectively, for each of the individual "complexes" with 2, 5, 8, 11, and 14 chlorides.

The $\underline{X}_i$'s are calculated as given for densities.

TABLE II. Least Squares Fitted Parameters for Equations 3, 4 and 5-7 Equivalent Conductivities and Absolute Viscosities of 1-Methyl-3-ethylimidazolium Chloride - Aluminum Chloride Binary Mixtures

Eq 3 or 4 Parameters	Equations 5-7 "complex" species parameter				
	2	5	8	11	14
Eq 3 and 5-7 Parameters for Equivalent Conductivity[a]					
$\underline{T}_o$, K	259.5	189.1	123.4	126.5	121.9
$\underline{k}_\Lambda$, K	493.4	763.0	790.9	802.1	813.3
$\ln \underline{A}_\Lambda$	8.0711	8.7437	8.9753	8.9519	8.9253
Eq 4 and 5-7 Parameters for Absolute Viscosity[b]					
$\underline{T}_o$, K	252.3	189.9	142.2	137.2	132.2
$\underline{k}_\eta$, K	732.5[c]				
$\ln \underline{A}_\eta$	-4.669[c]				

[a] The parameters yield $\sigma = 0.02$ in $\ln \Lambda$, where $\sigma = [\Sigma(\ln \Lambda_{calc} - \ln \Lambda_{exp})^2 / (\text{number of points} - \text{number of fitted parameters})]^{1/2}$.

[b] The parameters yield $\sigma = 0.03$ in $\ln \eta$, where $\sigma = [\Sigma(\ln \eta_{calc} - \ln \eta_{exp})^2 / (\text{number of points} - \text{number of fitted parameters})]^{1/2}$.

[c] These values are not parameters but averaged values of $\underline{k}_\eta$ and $\ln \underline{A}_\eta$ to be used for absolute viscosity calculations at all compositions.

END

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