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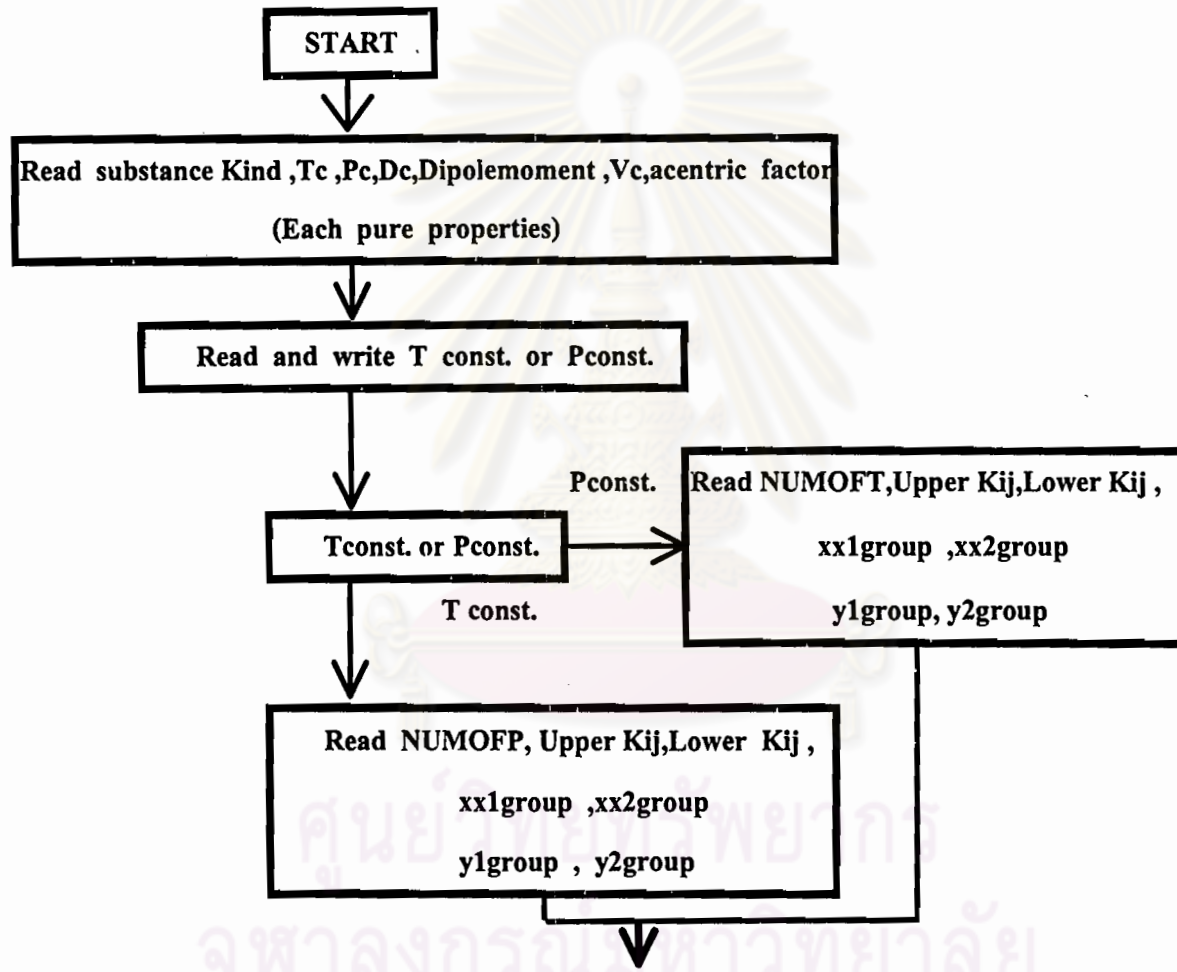
APPENDIX

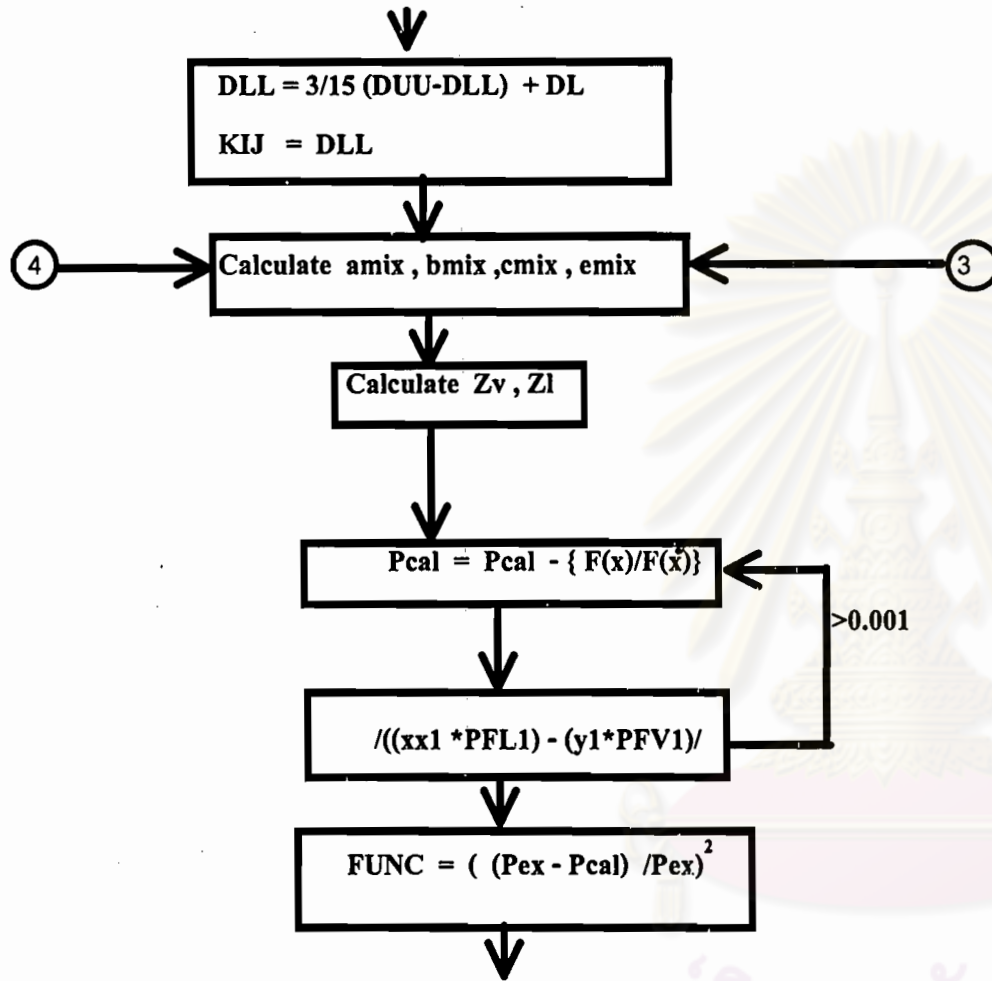


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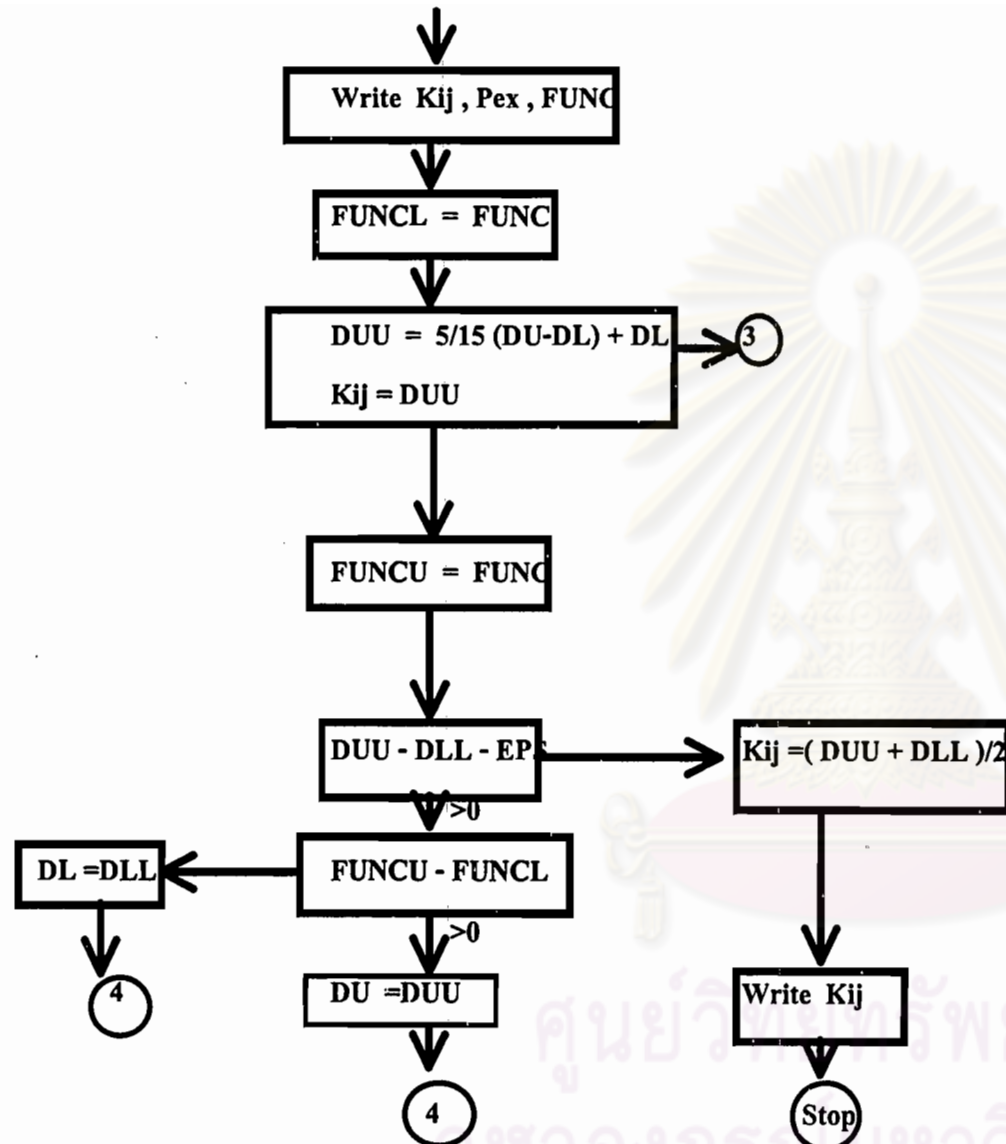
APPENDIX A

FLOW CHART FOR PROGRAM CALCULATION





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```
{PROGRAMME FOR QUARTIC EQUATION OF STATE}
```

```
Program Quartic_Equation_of_state;
```

```
Uses Strings,CRT;
```

```
VAR BC1,BC2,VC1,VC2,P1,P2,Tc1,Tc2,B1,B2,BMIX,T,P,XX1,XX2,Y1,Y2:REAL;
```

```
ER1,ER2,E1,E2,EMIX,W1,W2,DC1,DC2,pc1,pc2:REAL;
```

```
TR1,RcDipole1,Dipolemoment1,dipolemoment,redipole1,redipole2,X2,X3,X4,APLHA1,ALPHATR,
```

```
X5,X6,APLHA2,ar1,ac1,a1:REAL;
```

```
C1,C3,CR1,CC1,X7,tempdep1,tempdep11:REAL;
```

```
TR2,Dipolemoment2,Z2,Z3,Z4,APLHA3,ALPHA1,ALPHA2,ALPHA3,ALPHATR1,Z5,Z6,ALPHA4,ar2,
```

```
ac2,a2:REAL;
```

```
C2,C4,C5,C6,C7,C8,REMARK,CR2,CC2,Z7,tempdep2,tempdep22:REAL;
```

```
aMIX,cMIX,Q1,Q2,Q3,Q4,O1,O2,O3:REAL;
```

```
P1sat,P2sat,Tex,Pex,Ts,Te,ITV,Kij,min,Kanswer,Tope,SUM:REAL;
```

```
NUMOFF,NUMOFT,COUNTIT,i:INTEGER;
```

```
Pgroup:ARRAY[0..30]OF REAL;
```

```
Pexgroup:ARRAY[0..30]OF REAL;
```

```
Tgroup:ARRAY[0..30]OF REAL;
```

```
XX1group:ARRAY[0..30]OF REAL;
```

```
XX2group:ARRAY[0..30]OF REAL;
```

```
Y1group:ARRAY[0..30]OF REAL;
```

```
Y2group:ARRAY[0..30]OF REAL;
```

```
z1,zv,ANSWER,DU,DL,EPS,DUU,DLL,FUNC,FUNCL,FUNCU,FUL:REAL;
```

```
Input:text;
```

```
Fname1,Fname2,Fname3,Fname4,substance1,substance2:Array [0..29] of Char;
```

```
kind1,kind2:Array [0..9] of Char;
```

```
Found1,Found2:Integer; {strpos}
```

```
steady:Char;
```

```
{Addition Variables}
```

```
Po,Len:Integer;
```

```
{test variables}
```

```
sub1,sub2:string;
```

output:text;

Pexp:REAL;

FUNCTION J5(BMIX,AMIX,EMIX,N1,N2,M3,T,VL:REAL):REAL;

VAR J51,J52,J53:REAL;

BEGIN

J51:=(2*2.8225*0.008314*BMIX*T/(N1*N1*N1));

J52:=(AMIX*((2*VL)+EMIX-M3)/(N2*N2*N1*N1));

J53:=(3*VL*VL)+(2*EMIX*VL)-(2*M3*VL)-(M3*EMIX)
/(VL*VL*N2*N2*N1*N1);

J5:=(-0.008314*T/(N1*N1))-J51+J52+(M3*CMIX*J53);

END;

FUNCTION J9(CMIX,EMIX,M3,M4,N1,N2,T,VL:REAL):REAL;

VAR J91,J92,J93,J94:REAL;

BEGIN

J91:=(M3*CMIX/(0.008314*T));

J92:=(1/(N1*((M3*M3)+M4)));

J93:=(1/(N2*((EMIX*EMIX)+M4)));

J94:=(1/(VL*M3*EMIX));

J9:=J91*(J92+J93-J94);

END;

FUNCTION PH2(VL,M3,M4,EMIX:REAL):REAL;

VAR PH21,PH22:REAL;

BEGIN

PH21:=(4*VL*VL*VL)-(6*M3*VL*VL)+(2*M3*M3*VL);

PH22:=(3*EMIX*VL*VL)-(4*M4*VL)+(M3*M3*EMIX);

PH2:=PH21+PH22;

END;

FUNCTION S4(VL,AMIX,BMIX,CMIX,EMIX,N1,N2,M3,PH1:REAL):REAL;

VAR S41,S42,S43:REAL;

BEGIN

```

S41:=(-1.2864*CMIX*((2*VL)+EMIX)/(VL*VL*N2*N2));
S42:=(1.2864*AMIX*((2*VL)+EMIX-M3)/(N2*N2*N1*N1));
S43:=((1.2864*1.2864*BMIX*CMIX)*PH1/(VL*VL*N2*N2*N1*N1));
S4:=S41-S42-S43;
END;

```

```

FUNCTION S7(VL,AMIX,CMIX,N1,N2,M3,T:REAL):REAL;

```

```

VAR S71,S72,S73,S74:REAL;
BEGIN
S71:=(0.008314*T*(1.2864+2.8225)/(N1*N1));
S72:=(2*2.8225*M3*0.008314*T/(N1*N1*N1));
S73:=(1.2864*CMIX/(VL*N2*N1));
S74:=1.2864*((AMIX*VL)+(M3*CMIX))/(VL*N2*N1*N1);
S7:=S71+S72-S73-S74;
END;

```

```

FUNCTION S8(VL,T,P,AMIX,BMIX,CMIX,EMIX,N1,N2,M3,PH1:REAL):REAL;

```

```

VAR S81,S82,S83,S84:REAL;
BEGIN
S81:=(-0.008314*T/(N1*N1));
S82:=(2*0.008314*2.8225*BMIX*T/(N1*N1*N1));
S83:=(AMIX*((2*VL)+EMIX-M3)/(N2*N2*N1*N1));
S84:=(M3*CMIX*PH1/(VL*VL*VL*N2*N2*N1*N1));
S8:=(-1/(P*P))*(S81-S82+S83+S84);
END;

```

```

FUNCTION S12(VL,T,M3,M4,M6,N1,N2,CMIX,EMIX:REAL):REAL;

```

```

VAR S121,S122,S123:REAL;
BEGIN
S121:=(1/(VL*M4*M4));
S122:=(1/(N1*N1*((M3*M3)+M4)));
S123:=(1/(N2*((EMIX*EMIX)+M4)*((EMIX*EMIX)+M4)));
S12:=((M6/2)*CMIX*EMIX/(0.008314*T))*(S121+S122-S123);
END;

```

```

FUNCTION S13(CMIX,T,M3,M4,M7,N1:REAL):REAL;

```

```

VAR S131,S132,S133,S134:REAL;
BEGIN
S131:=(M3*CMIX/(0.008314*T));
S132:=(2*1.2864*M3)+M7;
S133:=(M3*M3)+M4)*N1;

```

$$S134:=(((M3*M3)+M4)*S133);$$

$$S13:=S131*S132/S134;$$

END;

FUNCTION S16(VL,T,N1,N2,M3,M4,EMIX:REAL):REAL;

VAR S161,S162,S163:REAL;

BEGIN

$$S161:=(M3/(0.008314*T));$$

$$S162:=(1/(N1*((M3*M3)+M4)));$$

$$S163:=(1/(((EMIX*EMIX)+M4)*N2));$$

$$S16:=S161*(S162+S163-(1/(VL*M4)));$$

END;

FUNCTION S25(VL,T,CMIX,EMIX,N1,N2,M3,M4:REAL):REAL;

VAR S251,S252,S253,S254:REAL;

BEGIN

$$S251:=(-M3/(((M3*M3)+M4)*((M3*M3)+M4)*N1));$$

$$S252:=(1/(((EMIX*EMIX)+M4)*N2*N2));$$

$$S253:=(((2*EMIX)+M3)/(((EMIX*EMIX)+M4)*((EMIX*EMIX)+M4)*N2));$$

$$S254:=(1/(M4*EMIX*VL));$$

$$S25:=(M3*CMIX/(0.008314*T))*(S251-S252-S253+S254);$$

END;

FUNCTION T5(BMIX,AMIX,EMIX,M1,M2,M3,T,VV:REAL):REAL;

VAR T51,T52,T53:REAL;

BEGIN

$$T51:=(2*2.8225*0.008314*BMIX*T/(M1*M1*M1));$$

$$T52:=(AMIX*((2*VV)+EMIX-M3)/(M2*M2*M1*M1));$$

$$T53:=((3*VV*VV)+(2*EMIX*VV)-(2*M3*VV)-(M3*EMIX))$$

$$/(VV*VV*M2*M2*M1*M1);$$

$$T5:=((-0.008314*T/(M1*M1))-T51+T52+(M3*CMIX*T53));$$

END;

FUNCTION T9(CMIX,EMIX,M3,M4,M1,M2,T,VV:REAL):REAL;

VAR T91,T92,T93,T94:REAL;

BEGIN

$$T91:=(M3*CMIX/(0.008314*T));$$

$$T92:=(1/(M1*((M3*M3)+M4)));$$

$$T93:=(1/(M2*((EMIX*EMIX)+M4)));$$

$$T94:=(1/(VV*M3*EMIX));$$

$$T9:=T91*(T92+T93-T94);$$

```

END;
FUNCTION PH9(VV,M3,M4,EMIX:REAL):REAL;
  VAR PH91,PH92:REAL;
  BEGIN
  PH91:=(4*VV*VV*VV)-(6*M3*VV*VV)+(2*M3*M3*VV);
  PH92:=(3*EMIX*VV*VV)-(4*M4*VV)+(M3*M3*EMIX);
  PH9:=PH91+PH92;
  END;

FUNCTION U4(VV,AMIX,BMIX,CMIX,EMIX,M1,M2,M3,PH8:REAL):REAL;
  VAR U41,U42,U43:REAL;
  BEGIN
  U41:=(-1.2864*CMIX*((2*VV)+EMIX)/(VV*VV*M2*M2));
  U42:=(-1.2864*AMIX*((2*VV)+EMIX-M3)/(M2*M2*M1*M1));
  U43:=((1.2864*1.2864*BMIX*CMIX)*PH8/(VV*VV*M2*M2*M1*M1));
  U4:=U41-U42-U43;
  END;

FUNCTION U7(VV,AMIX,CMIX,M1,M2,M3,T:REAL):REAL;
  VAR U71,U72,U73,U74:REAL;
  BEGIN
  U71:=(0.008314*T*(1.2864+2.8225)/(M1*M1));
  U72:=(2*2.8225*M3*0.008314*T/(M1*M1*M1));
  U73:=(1.2864*CMIX/(VV*M2*M1));
  U74:=1.2864*((AMIX*VV)+(M3*CMIX))/(VV*M2*M1*M1);
  U7:=U71+U72-U73-U74;
  END;

FUNCTION U8(VV,T,P,AMIX,BMIX,CMIX,EMIX,M1,M2,M3,PH8:REAL):REAL;
  VAR U81,U82,U83,U84:REAL;
  BEGIN
  U81:=(-0.008314*T/(M1*M1));
  U82:=(2*0.008314*2.8225*BMIX*T/(M1*M1*M1));
  U83:=(AMIX*((2*VV)+EMIX-M3)/(M2*M2*M1*M1));
  U84:=(M3*CMIX*PH8/(VV*VV*VV*M2*M2*M1*M1));
  U8:=(-1/(P*P))*(U81-U82+U83+U84);
  END;

FUNCTION U12(VV,T,M3,M4,M6,M1,M2,CMIX,EMIX:REAL):REAL;
  VAR U121,U122,U123:REAL;

```

```

BEGIN
U121:=(1/(VV*M4*M4));
U122:=(1/(M1*M1*((M3*M3)+M4)));
U123:=(1/(M2*((EMIX*EMIX)+M4)*((EMIX*EMIX)+M4)));
U12:=(M6/2)*CMIX*EMIX/(0.008314*T))*(U121+U122-U123);
END;

```

```

FUNCTION U13(CMIX,T,M3,M4,M7,M1:REAL):REAL;

```

```

VAR U131,U132,U133,U134:REAL;
BEGIN
U131:=(M3*CMIX/(0.008314*T));
U132:=(2*1.2864*M3)+M7;
U133:=(M3*M3)+M4)*M1;
U134:=(M3*M3)+M4)*U133);
U13:=U131*U132/U134;
END;

```

```

FUNCTION U16(VV,T,M1,M2,M3,M4,EMIX:REAL):REAL;

```

```

VAR U161,U162,U163:REAL;
BEGIN
U161:=(M3/(0.008314*T));
U162:=(1/(M1*((M3*M3)+M4)));
U163:=(1/(((EMIX*EMIX)+M4)*M2));
U16:=U161*(U162+U163-(1/(VV*M4)));
END;

```

```

FUNCTION U25(VV,T,CMIX,EMIX,M1,M2,M3,M4:REAL):REAL;

```

```

VAR U251,U252,U253,U254:REAL;
BEGIN
U251:=(M3/(((M3*M3)+M4)*((M3*M3)+M4)*M1));
U252:=(1/(((EMIX*EMIX)+M4)*M2*M2));
U253:=(2*EMIX+M3)/(((EMIX*EMIX)+M4)*((EMIX*EMIX)+M4)*M2));
U254:=(1/(M4*EMIX*VV));
U25:=(M3*CMIX/(0.008314*T))*(U251-U252-U253+U254);
END;

```

```

FUNCTION J3(N1,N2,VL,EMIX,AMIX,M3,T:REAL):REAL;

```

```

VAR J31:REAL;
BEGIN
J31:=(1/(N2*N1))-(VL*((2*VL)+EMIX-M3)/(N2*N2*N1*N1));
J3:=(AMIX/(0.008314*T))*J31;

```

```

END;
FUNCTION PH7(VL,EMIX,M3,M4:REAL):REAL;
  VAR PH71:REAL;
  BEGIN
  PH71:=(4*VL*VL*VL)+(4*VL*EMIX)+(2*VL*EMIX*EMIX);
  PH7:=PH71-(3*M3*VL*VL)-(2*M4)-(M4*EMIX);
  END;
FUNCTION S5(T,CMIX,VL,N1,N2,AMIX,M3:REAL):REAL;
  VAR S51:REAL;
  BEGIN
  S51:=((1.2864*CMIX/(VL*N2)))+(AMIX*1.2864/(N1*N2))
    +(M3*1.2864*CMIX/(VL*N1*N2)));
  S5:=S51*(M3/(N1*N1*0.008314*T));
  END;
FUNCTION S11(CMIX,T,N1,N2,M3,M4,EMIX,VL:REAL):REAL;
  VAR S111:REAL;
  BEGIN
  S111:=((1/(N1*((M3*M3)+M4)))+(1/(N2*((EMIX*EMIX)+M4)))-(1/(VL*M4)));
  S11:=(1.2864*CMIX/(0.008314*T))*S111;
  END;
FUNCTION S15(M3,VL,EMIX,P,T,N1,N2:REAL):REAL;
  VAR S151:REAL;
  BEGIN
  S151:=(N2*N2*N1*N1);
  S15:=M3*((2*VL)+EMIX-M3)*((1/(P*VL))-(1/(0.008314*T)))/S151;
  END;
FUNCTION S21(AMIX,VL,M3,EMIX,CMIX,T,N1,N2:REAL):REAL;
  VAR S211:REAL;
  BEGIN
  S211:=(3*VL*VL)+(2*EMIX)+(EMIX*EMIX)-(2*M3*VL));
  S21:=(((AMIX*VL)+(M3*CMIX))/(0.008314*T*N1*N1*N2*N2*N2*N2))*S211;
  END;
FUNCTION S24(AMIX,T,M5,N1,N2,VL,M3,EMIX:REAL):REAL;
  VAR S241,S242:REAL;
  BEGIN
  S241:=(((2*VL)-M3+EMIX)/(N1*N2*N2));

```

```

S242:=(N1/(N2*N2*N2));
S24:=(AMIX/(0.008314*T*M5))*((-1/(N1*N2))+S241-S242);
END;

```

```

FUNCTION T3(M1,M2,VV,EMIX,AMIX,M3,T:REAL):REAL;
VAR T31:REAL;
BEGIN
T31:=(1/(M2*M1))-(VV*((2*VV)+EMIX-M3)/(M2*M2*M1*M1));
T3:=(AMIX/(0.008314*T))*T31;
END;

```

```

FUNCTION PH14(VV,EMIX,M3,M4:REAL):REAL;
VAR PH141:REAL;
BEGIN
PH141:=(4*VV*VV*VV)+(4*VV*EMIX)+(2*VV*EMIX*EMIX);
PH14:=PH141-(3*M3*VV*VV)-(2*M4)-(M4*EMIX);
END;

```

```

FUNCTION U5(T,CMIX,VV,M1,M2,AMIX,M3:REAL):REAL;
VAR U51:REAL;
BEGIN
U51:=(1.2864*CMIX/(VV*M2))+(AMIX*1.2864/(M1*M2))
+(M3*1.2864*CMIX/(VV*M1*M2));
U5:=U51*(M3/(M1*M1*0.008314*T));
END;

```

```

FUNCTION U11(CMIX,T,M1,M2,M3,M4,EMIX,VV:REAL):REAL;
VAR U111:REAL;
BEGIN
U111:=(1/(M1*((M3*M3)+M4)))+(1/(M2*((EMIX*EMIX)+M4)))-(1/(VV*M4));
U11:=(1.2864*CMIX/(0.008314*T))*U111;
END;

```

```

FUNCTION U15(M3,VV,EMIX,P,T,M1,M2:REAL):REAL;
VAR U151:REAL;
BEGIN
U151:=(M2*M2*M1*M1);
U15:=M3*((2*VV)+EMIX-M3)*((1/(P*VV))-(1/(0.008314*T)))/U151;
END;

```

```

FUNCTION U21(AMIX,VV,M3,EMIX,CMIX,T,M1,M2:REAL):REAL;
VAR U211:REAL;
BEGIN

```



```

U211:=(3*VV*VV)+(2*EMIX)+(EMIX*EMIX)-(2*M3*VV));
U21:=(((AMIX*VV)+(M3*CMIX))/(0.008314*T*M1*M1*M2*M2*M2*M2))*U211;
END;

```

```

FUNCTION U24(AMIX,T,M5,M1,M2,VV,M3,EMIX:REAL):REAL;

```

```

  VAR U241,U242:REAL;
  BEGIN
  U241:=(((2*VV)-M3+EMIX)/(M1*M2*M2));
  U242:=(M1/(M2*M2*M2));
  U24:=(AMIX/(0.008314*T*M5))*((-1/(M1*M2))+U241-U242);
  END;

```

```

Function COMPRESS_FACTOR(Q1,Q2,Q3,Q4,XX1,XX2,Y1,Y2:REAL):REAL;

```

```

  VAR S,E,A,B,BEGIN_VALUE,INCRE:REAL;
  RESULT:ARRAY[1..4] OF REAL;
  INDEX,COUNTER,AGAIN:INTEGER;

  M1,M2,M3,M4,M5,M6,M7,M8,N1,N2,N8,M111,N111,NN22,MN22:REAL;
  VL,VV:REAL;
  PFV1,PFL1,FV1,NIY,FL1,NIX:REAL;
  FBV,BNIV,FCV,CNIV,FAV,ANIV,FEV,ENIV:REAL;
  FBL,BNIL,FCL,CNIL,FAL,ANIL,FEL,ENIL:REAL;
  G1,G2,G3,G4,G5,G6,G7,G8,G9,G10:REAL;
  G11,G12,G13,G14,G15,G16:REAL;
  PPV,PPL:REAL;
  H1,H2,H3,H4,H5,H6,H7,H8,H9:REAL;
  H10,H11,H12,H13,H14,H15,H16,H17,H18:REAL;

  FDIF,FN,PFLP1,PFLV1,VLP1:REAL;
  DIVL1,FVVL1,DIVL2:REAL;
  J1,J2,J4,J6,J7,J8:REAL;
  FBLV1,FCLV1,FALV1,FELV1:REAL;
  S1,S2,S3,S6,S9,S10,S14:REAL;
  S17,S18,S19,S20,S22,S23,S26:REAL;
  PH1,PH3,PH4,PH5,PH6:REAL;

  PFGP1,PFGV1,VGP1,DIVG1,FVVG1,DIVG2:REAL;

```

```
T1,T2,T4,T6,T7,T8:REAL;
FBGV1,FCGV1,FAGV1,FELG1:REAL;
U1,U2,U3,U6,U9,U10,U14:REAL;
U17,U18,U19,U20,U22,U23,U26:REAL;
PH8,PH10,PH11,PH12,PH13,PH21,PH22:REAL;
PH61,PH62:REAL;
PH131,PH132:REAL;
```

```
PH91,PH92:REAL;
PH111,PH121,PH122:REAL;
S141,S181,S221:REAL;
U141,U181,U221:REAL;
DIVI:REAL;
```

```
JA5,JA9,PHA2,PHA6,SA4,SA7,SA8,SA12,SA13,SA16,SA25:REAL;
TA5,TA9,PHA9,PHA13,UA4,UA7,UA8,UA12,UA13,UA16,UA25:REAL;
JA3,PHA7,SA5,SA11,SA15,SA21,SA22,SA24:REAL;
TA3,PHA14,UA5,UA11,UA15,UA21,UA22,UA24:REAL;
```

```
{NUBER OF LOOP}
Loop_No:INTEGER;
```

```
BEGIN
```

```
BEGIN_VALUE:=0;
COUNTER:=0;
INCRE:=0.05;
WRITELN;
```

```
WHILE(BEGIN_VALUE<=1) DO
```

```
BEGIN
```

```
S:=1;
```

```
E:=0.000005;
```

```
A:=BEGIN_VALUE;
```

```
WHILE(ABS(S)>E) DO
```

```
BEGIN
```

```
B:=A;
```

```
A:=B-((B*B*B*B+Q1*B*B*B+Q2*B*B+Q3*B+Q4)/(4*B*B*B+3*Q1*B*B+2*Q2*B+Q3));
```

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```
S:=A*A*A*A+Q1*A*A*A+Q2*A*A+Q3*A+Q4;
END;
IF (COUNTER=0) THEN
BEGIN
  BEGIN_VALUE:=BEGIN_VALUE+INCRE;
  IF (A>=0)AND (A<=1) THEN
  BEGIN
    COUNTER:=COUNTER+1;
    RESULT[COUNTER]:=A;
    { WRITELN('ANSWER (',COUNTER,') IS ',RESULT[COUNTER]:10:8);}

  END;
  CONTINUE;
END;
IF (COUNTER>0) THEN
BEGIN
  IF COUNTER=4 THEN EXIT;
  IF (A<0) OR (A>1) THEN
  BEGIN
    BEGIN_VALUE:=BEGIN_VALUE+INCRE;
    CONTINUE;
  END;
  INDEX:=1;

  AGAIN:=0;
  WHILE(INDEX<=COUNTER) DO
  BEGIN
    IF( ABS(A-RESULT[INDEX]) < 0.01) THEN
    BEGIN
      INDEX:=INDEX+1;
      AGAIN:=1;
      CONTINUE;
    END;
    INDEX:=INDEX+1;
  END;
  IF(AGAIN=0) THEN
  BEGIN
```

```
COUNTER:=COUNTER+1;
```

```
RESULT[COUNTER]:=B;
```

```
END;
```

```
END;
```

```
BEGIN_VALUE:=BEGIN_VALUE+INCRE;
```

```
END;
```

```
IF (COUNTER=0) THEN
```

```
BEGIN
```

```
  WRITELN;
```

```
  WRITELN('NO ANSWER');
```

```
END;
```

```
IF (COUNTER<2) OR (COUNTER>4) THEN EXIT;
```

```
ZL:=RESULT[1];
```

```
IF (COUNTER=2) THEN
```

```
  ZV:=RESULT[2]
```

```
ELSE IF (COUNTER=3) THEN
```

```
  ZV:=RESULT[3]
```

```
ELSE
```

```
  ZV:=RESULT[4];
```

```
{ WRITELN(' ZL = ',ZL:10:8,' ZV = ',ZV:10:8);}
```

```
{PROGRAM CALCULATION PARTIAL FUGACITY COEFFICIENT  
FOR VAPOR & LIQUID PHASE IN BINARY MIXTURE}
```

```
PFV1:=5;
```

```
PFL1:=3;
```

```
P:=(XX1*P1sat)+(XX2*P2sat)/2;
```

```
ANSWER:=P;
```

```
WHILE (Abs((XX1*PFL1)-(Y1*PFV1))>0.0001) DO
```

```
  Loop_No:=0;
```

BEGIN

$$VL:=(ZL*0.008314*T/P);$$

$$VV:=(ZV*0.008314*T/P);$$

$$M1:=VV-(1.2864*BMIX);$$

$$M2:=VV+EMIX;$$

$$M3:=1.2864*BMIX;$$

$$M4:=1.2864*BMIX*EMIX;$$

$$M5:=(1.2864*BMIX)+EMIX;$$

$$M6:=3.31*BMIX;$$

$$M7:=1.2864*EMIX;$$

$$M8:=(1.2864*BMIX)-VV;$$

$$N1:=VL-(1.2864*BMIX);$$

$$N2:=VL+EMIX;$$

$$N8:=(1.2864*BMIX)-VL;$$

$$M111:=M1*M1*M1;$$

$$N111:=N1*N1*N1;$$

$$MN22:=M1*M1*N2*N2;$$

$$NN22:=N1*N1*N2*N2;$$

$$PPV:=(0.008314*T/M1)+(BMIX*0.0235*T/(M1*M1))-$$

$$(((AMIX*VV)+(1.2864*BMIX*CMIX))/(VV*M2*M1));$$

$$PPL:=(0.008314*T/N1)+(BMIX*0.0235*T/(N1*N1))-$$

$$(((AMIX*VL)+(1.2864*BMIX*CMIX))/(VL*N2*N1));$$

{VAPOR PHASE}

$$G1:=(1.2864/M1) + (2.8225/M1) + (3.631*BMIX/(M1*M1));$$

$$G2:=(((154.727*AMIX)/(T*M5))*((1/M1)+(Ln(M1/M2))/M5));$$

$$G3:=(((1.2864*CMIX)/(0.008314*T))*((Ln(M1)/((M3*M3)+M4)+(Ln(M2)/((EMIX*EMIX)+M4))-(Ln(VV)/M4)));$$

$$G4:=(((199.04*BMIX*CMIX*EMIX/T))*((Ln(VV)/(M4*M4))-(1/(M1*((M3*M3)+M4)))-$$

$$(Ln(M2)/(((EMIX*EMIX)+M4)*((EMIX*EMIX)+M4))));$$

$$G5:=(((1.2864*BMIX*CMIX)/(0.008314*T))*$$

$$(Ln(M1)*(M6+M7)/(((M3*M3)+M4)*((M3*M3)+M4)));$$

$$H1:=(VV/(M1))*((4.1089/M1)+(7.2617*BMIX/(M1*M1)));$$

$$H2:=(VV/(0.008314*T*M1))*((1.2864*CMIX/(VV*M2))+(1.2864*AMIX/(M2*M1))+$$

$$(1.6548*BMIX*CMIX/(VV*M1*M2))));$$

$$H3:=(1/PPV);$$

$$H4:=(0.0342*T/(M1*M1));$$

$$H5:=(0.0604*T*BMIX/(M111));$$

$$H6:=(1.2864*CMIX/(VV*M1*M2));$$

$$H7:=(1.2864*((AMIX*VV)+(1.2864*BMIX*CMIX))/(VV*M2*M1*M1));$$

$$FBV:=H1-H2-(H3*(H4+H5-H6-H7))+G1-G2+(G3+(G4-G5));$$

$$BNIV:=(B1-B2)*Y2);$$

$$FCV:=(-1.2864*BMIX)/(0.008314*T*M2*M1)+(1.2864*BMIX/(VV*M2*M1*PPV))+((M3/(0.008314*T))$$

*

$$((Ln(M1)/((M3*M3)+M4))+Ln(M2)/((EMIX*EMIX)+M4)-(Ln(VV)/M4));$$

$$CNIV:=(2*C1*Y1*Y2)+(2*SQRT(C1)*SQRT(C2)*((Y2*Y2)-(Y1*Y2)))-(2*C2*Y2*Y2));$$

$$FAV:=(-VV/(0.008314*T*M2*M1))+VV/(VV*M2*M1*PPV)+(Ln(M1/M2))/(0.008314*T*M5);$$

$$ANIV:=(2*A1*Y1*Y2)+(2*SQRT(A1)*SQRT(A2)*(1-Kij)*((Y2*Y2)-(Y1*Y2)))-(2*A2*Y2*Y2));$$

$$G11:=(AMIX/(0.008314*T*M5))*((M8/(M1*M2)-(Ln(M1/M2)/M5));$$

$$G12:=(-1.2864*BMIX*Ln(M1))/(((M3*M3)+M4)*((M3*M3)+M4));$$

$$G13:=(((2*EMIX)+M3)*Ln(M2))/((EMIX*EMIX)+M4)*((EMIX*EMIX)+M4));$$

$$H15:=((AMIX*VV)+(1.2864*BMIX*CMIX))/(0.008314*T*M1*M2*M2));$$

$$H16:=((AMIX*VV)+(1.2864*BMIX*CMIX))/(PPV*VV*M1*M2*M2));$$

$$FEV:=H15-H16+G11+((154.727*BMIX*CMIX/T)*(G12+(1/(M2*((EMIX*EMIX)+M4)))-G13+Ln(VV)/(M3*EMIX*EMIX))));$$

$$ENIV:=(E1-E2)*Y2);$$

{LIQUID PHASE}

$$G6:=(1.2864/N1) + (2.8225/N1) + (3.631*BMIX/(N1*N1));$$

$$G7:=(((154.727*AMIX)/(T*M5))*((1/N1)+((Ln(N1/N2))/M5)));$$

$$G8:=(((1.2864*CMIX)/(0.008314*T))*((Ln(N1)/((M3*M3)+M4))+Ln(N2)/((EMIX*EMIX)+M4)-(Ln(VV)/M4)));$$

$$G9:=((199.04*BMIX*CMIX*EMIX/T)*((Ln(VV)/(M4*M4)-(1/(N1*((M3*M3)+M4)))-$$

$$(Ln(N2)/((EMIX*EMIX)+M4)*((EMIX*EMIX)+M4))));$$

$$G10:=(((1.2864*BMIX*CMIX)/(0.008314*T))*$$

$$\begin{aligned}
& (\ln(N1)*(M6+M7)/(((M3*M3)+M4)*((M3*M3)+M4))); \\
H8: &= (VL/(N1))*((4.1089/N1)+(7.2617*BMIX/(N1*N1))); \\
H9: &= (VL/(0.008314*T*N1))*((1.2864*CMIX/(VL*N2))+(1.2864*AMIX/(N2*N1))+ \\
& (1.6548*BMIX*CMIX/(VL*N1*N2))); \\
H10: &= (1/PPL); \\
H11: &= (0.0342*T/(N1*N1)); \\
H12: &= (0.0604*T*BMIX/(N1*N1)); \\
H13: &= (1.2864*CMIX/(VL*N1*N2)); \\
H14: &= (1.2864*((AMIX*VL)+(1.2864*BMIX*CMIX))/(VL*N2*N1*N1)); \\
FBL: &= H8-H9-(H10*(H11+H12-H13-H14))+G6-G7+(G8+(G9-G10)); \\
BNIL: &= (B1-B2)*XX2); \\
FCL: &= ((-1.2864*BMIX)/(0.008314*T*N2*N1))+(1.2864*BMIX/(VL*N2*N1*PPL))+ \\
& ((M3/(0.008314*T))*((\ln(N1)/((M3*M3)+M4))+(\ln(N2)/((EMIX*EMIX)+M4))- \\
& (\ln(VL)/M4))); \\
CNIL: &= ((2*C1*XX1*XX2)+(2*SQRT(C1)*SQRT(C2)*((XX2*XX2)-(XX1*XX2)))-(2*C2* \\
& XX2*XX2)); \\
FAL: &= (-VL/(0.008314*T*N2*N1))+(VL/(VL*N2*N1*PPL))+(\ln(N1/N2))/(0.008314*T*M5); \\
ANIL: &= ((2*A1*XX1*XX2)+(2*SQRT(A1)*SQRT(A2)*(1-Kij)*((XX2*XX2)-(XX1*XX2)))-(2*A2* \\
& XX2*XX2)); \\
G14: &= ((AMIX/(0.008314*T*M5))*((N8/(N1*N2))-(\ln(N1/N2)/M5))); \\
G15: &= ((-1.2864*BMIX*\ln(N1))/(((M3*M3)+M4)*((M3*M3)+M4))); \\
G16: &= (((2*EMIX)+M3)*\ln(N2))/(((EMIX*EMIX)+M4)*((EMIX*EMIX)+M4)); \\
H17: &= (((AMIX*VL)+(1.2864*BMIX*CMIX))/(0.008314*T*N1*N2*N2)); \\
H18: &= (((AMIX*VL)+(1.2864*BMIX*CMIX))/(PPL*VL*N1*N2*N2)); \\
FEL: &= H17-H18+G14+((154.727*BMIX*CMIX/T)*(G15+(1/(N2*((EMIX*EMIX)+M4)))-G16+(\ln(VV)/(M3 \\
& *EMIX*EMIX))); \\
ENIL: &= (E1-E2)*XX2); \\
\{DIFF N(\ln FUGACITY) WITH ni When nj, tp constant\} \\
NIY: &= (FBV*BNIV)+(FCV*CNIV)+(FAV*ANIV)+(FEV*ENIV); \\
NIX: &= (FBL*BNIL)+(FCL*CNIL)+(FAL*ANIL)+(FEL*ENIL); \\
FV1: &= (ZV-1-\ln(ZV)+\ln(VV/M1)+(2.8225*BMIX/M1)+ \\
& ((AMIX/(0.008314*T*M5))*(\ln(M1/M2)))+ \\
& ((154.727*BMIX*CMIX/T)*((\ln(M1)/((M3*M3)+M4)) \\
& +(\ln(M2)/((EMIX*EMIX)+M4))-(\ln(VV)/M4))); \\
FL1: &= (ZL-1-\ln(ZL)+\ln(VL/N1)+(2.8225*BMIX/N1)+ \\
& ((AMIX/(0.008314*T*M5))*(\ln(N1/N2)))+
\end{aligned}$$

$$\begin{aligned} & ((154.727*BMIX*CMIX/T)*((Ln(N1)/((M3*M3)+M4)) \\ & + (Ln(N2)/((EMIX*EMIX)+M4)) - (Ln(VL)/M4))); \end{aligned}$$

$$PFV1:=EXP(FV1+NIY);$$

$$PFL1:=EXP(FL1+NIX);$$

{THIS PART TO SET INITIAL PRESSURE}

{PARAMETER FOR LIQUID PHASE}

{GROUP ONE}

$$J1:=(M3/(N1*N1));$$

$$J2:=(2.8225*BMIX)*((1/(N1*N1))-(2*VL/(N111)));$$

$$J4:=(M3*CMIX/(0.008314*T))*(-1)*((2*VL)-M3+EMIX)/(NN22);$$

$$J6:=M3/(VL*N1);$$

$$J7:=(2.8225*BMIX)/(N1*N1);$$

$$J8:=AMIX/(0.008314*T*N1*N2);$$

{GROUP TWO}

$$PH1:=((3*VL*VL)+(2*EMIX*VL)-(2*M3*VL)-M4);$$

$$PH3:=-2*0.008314*T*(2.8225+1.2864)/(N111);$$

$$PH4:=-6*2.8225*M3*0.008314*T/(N111*N1);$$

$$PH5:=1.2864*CMIX*PH1/(VL*VL*NN22);$$

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{GROUP THREE}

$$S1:=(VL/(N1*N1*N1))*(-(2.8225+1.2864)-(4*2.8225*1.2864*BMIX/N1));$$

$$S2:=(M3/(N1*N1*N1))*((2.8225+1.2864)+(2*2.8225*1.2864*BMIX/N1));$$

$$S3:=(VL/(0.008314*T*N1));$$

$$\text{PHA2}:=\text{PH2}(\text{VL},\text{M3},\text{M4},\text{EMIX});$$

$$\text{PH61}:=((\text{VL}*\text{N2}*\text{N1}*\text{N1}*\text{AMIX})-(((\text{AMIX}*\text{VL})+\text{M4})*\text{PHA2}));$$

$$\text{PH62}:=((\text{VL}*\text{VL}*\text{NN22}*\text{N1}*\text{N1}));$$

$$\text{PH6}:=1.2864*\text{PH61}/\text{PH62};$$

$$\text{S6}:=\text{PH3}+\text{PH4}+\text{PH5}-\text{PH6};$$

$$\text{S9}:=(-1.2864/(\text{N1}*\text{N1}))-(2.8225/(\text{N1}*\text{N1}))-(2*\text{M3}*2.8225/(\text{N111}));$$

$$\text{S10}:=((\text{AMIX}*1.2864/(0.008314*\text{T}*\text{M5}))*((-1/(\text{N1}*\text{N1}))+1/(\text{N1}*\text{N2})));$$

$$\text{SA8}:=\text{S8}(\text{VL},\text{T},\text{P},\text{AMIX},\text{BMIX},\text{CMIX},\text{EMIX},\text{N1},\text{N2},\text{M3},\text{PH1});$$

$$\text{S141}:=((\text{SA8}/(-1/(\text{P}*\text{P}))) / (\text{VL}*\text{P}*\text{P}));$$

$$\text{S14}:=((\text{M3}/(\text{N2}*\text{N1})) * (-1/(\text{P}*\text{VL}*\text{VL}))) - \text{S141};$$

$$\text{S17}:=((\text{VL}*((2*\text{VL})+\text{EMIX}-\text{M3})) - (\text{N1}*\text{N2})) / (0.008314*\text{T}*\text{NN22});$$

$$\text{S181}:=((\text{P}*\text{P}*\text{NN22}));$$

$$\text{SA8}:=\text{S8}(\text{VL},\text{T},\text{P},\text{AMIX},\text{BMIX},\text{CMIX},\text{EMIX},\text{N1},\text{N2},\text{M3},\text{PH1});$$

$$\text{S18}:=((((2*\text{VL})+\text{EMIX}-\text{M3})*\text{P}) + (\text{N1}*\text{N2}*(\text{SA8}/(-1/(\text{P}*\text{P})))) / \text{S181};$$

$$\text{S19}:=1/(0.008314*\text{T}*\text{N1}*\text{N2});$$

$$\text{S20}:=\text{AMIX}/(0.008314*\text{T}*\text{N1}*\text{N2}*\text{N2});$$

$$\text{PHA7}:=\text{PH7}(\text{VL},\text{EMIX},\text{M3},\text{M4});$$

$$\text{S221}:=((((\text{AMIX}*\text{VL})+(\text{M3}*\text{CMIX})) / (\text{VL}*\text{VL}*\text{NN22}*\text{N2}*\text{N2}))*\text{PHA7});$$

$$\text{S22}:=((\text{AMIX}/(\text{VL}*\text{N1}*\text{N2}*\text{N2})) - \text{S221});$$

$$SA8:=S8(VL,T,P,AMIX,BMIX,CMIX,EMIX,N1,N2,M3,PH1);$$

$$S23:=-SA8*((AMIX*VL)+(M3*CMIX))/(VL*N1*N2*N2);$$

{EQUATIONS TO CALCULATE FOR LIQUID PHASE}

$$SA4:=S4(VL,AMIX,BMIX,CMIX,EMIX,N1,N2,M3,PH1);$$

$$SA5:=S5(T,CMIX,VL,N1,N2,AMIX,M3);$$

$$SA7:=S7(VL,AMIX,CMIX,N1,N2,M3,T);$$

$$SA8:=S8(VL,T,P,AMIX,BMIX,CMIX,EMIX,N1,N2,M3,PH1);$$

$$SA11:=S11(CMIX,T,N1,N2,M3,M4,EMIX,VL);$$

$$SA12:=S12(VL,T,M3,M4,M6,N1,N2,CMIX,EMIX);$$

$$SA13:=S13(CMIX,T,M3,M4,M7,N1);$$

$$FBLV1:=S1-S2-(S3*SA4)+SA5-(S6/P)-(SA7*SA8)+S9-S10+SA11+SA12-SA13;$$

$$SA15:=S15(M3,VL,EMIX,P,T,N1,N2);$$

$$SA16:=S16(VL,T,N1,N2,M3,M4,EMIX);$$

$$FCLV1:=S14-SA15+SA16;$$

$$FALV1:=S17-S18+S19;$$

$$SA25:=S25(VL,T,CMIX,EMIX,N1,N2,M3,M4);$$

$$SA21:=S21(AMIX,VL,M3,EMIX,CMIX,T,N1,N2);$$

$$PHA7:=PH7(VL,EMIX,M3,M4);$$

$$SA24:=S24(AMIX,T,M5,N1,N2,VL,M3,EMIX);$$

$$FELV1:=S20-SA21-(S22/P)+S23+SA24+SA25;$$

$$DIVL2:=(BNIL*FBLV1)+(CNIL*FCLV1)+(ANIL*FALV1)+(ENIL*FELV1);$$

$$JA3:=J3(N1,N2,VL,EMIX,AMIX,M3,T);$$

$$JA5:=J5(BMIX,AMIX,EMIX,N1,N2,M3,T,VL);$$

$$JA9:=J9(CMIX,EMIX,M3,M4,N1,N2,T,VL);$$

$$FVV1:=J1+J2-JA3-J4-(JA5/P)-(1/VL)-J6-J7+J8+JA9;$$

$$DIVL1:=FVV1+DIVL2;$$

$$PFLV1:=PFL1*DIVL1;$$

$$VLP1:=(ZL*0.008314*T*(P*P));$$

$$PFLP1:=PFLV1*VLP1;$$

{PARAMETER FOR VAPOR PHASE}

{GROUP ONE}

$$T1 := -(M3 / (M1 * M1));$$

$$T2 := (2.8225 * BMIX) * ((1 / (M1 * M1)) - (2 * VV / (M111)));$$

$$T4 := (M3 * CMIX / (0.008314 * T)) * (-1) * ((2 * VV) - M3 + EMIX) / (M2 * M2 * M1 * M1);$$

$$T6 := M3 / (VV * M1);$$

$$T7 := (2.8225 * BMIX) / (M1 * M1);$$

$$T8 := AMIX / (0.008314 * T * M1 * M2);$$

{GROUP TWO}

$$PH8 := ((3 * VV * VV) + (2 * EMIX * VV) - (2 * M3 * VV) - M4);$$

$$PH10 := -2 * 0.008314 * T * (2.8225 + 1.2864) / (M111);$$

$$PH111 := (M1 * M111);$$

$$PH11 := -6 * 2.8225 * M3 * 0.008314 * T / PH111;$$

$$PH121 := M2 * M2 * M1 * M1;$$

$$PH122 := (VV * VV * PH121);$$

$$PH12 := 1.2864 * CMIX * PH8 / PH122;$$

{GROUP THREE}

$$U1 := (VV / (M111)) * (-2.8225 + 1.2864) - (4 * 2.8225 * 1.2864 * BMIX / M1);$$

$$U2 := (M3 / (M111)) * ((2.8225 + 1.2864) + (2 * 2.8225 * 1.2864 * BMIX / M1));$$

$$U3 := (VV / (0.008314 * T * M1));$$

$$PHA9 := PH9(VV, M3, M4, EMIX);$$

$$PH131 := ((VV * M2 * M1 * M1 * AMIX) - (((AMIX * VV) + M4) * PHA9));$$

$$PH132 := (VV * VV * M2 * M2 * M1 * M111);$$

$$PH13 := 1.2864 * PH131 / PH132;$$

$$U6 := PH10 + PH11 + PH12 - PH13;$$

$$U9 := (-1.2864 / (M1 * M1)) - (2.8225 / (M1 * M1)) - (2 * M3 * 2.8225 / (M111));$$

$$U10 := (AMIX * 1.2864 / (0.008314 * T * M5)) * ((-1 / (M1 * M1)) + (1 / (M1 * M2)));$$

$$UA8 := U8(VV, T, P, AMIX, BMIX, CMIX, EMIX, M1, M2, M3, PH8);$$

$$U141 := ((UA8 / (-1 / (P * P))) / (VV * P * P));$$

$$U14 := (M3 / (M2 * M1)) * ((-1 / (P * VV * VV)) - U141);$$

$$U17 := ((VV * ((2 * VV) + EMIX - M3)) - (M1 * M2))$$

$$/ (0.008314 * T * M2 * M2 * M1 * M1);$$

$$U181:=(P*P*M2*M2*M1*M1);$$

$$UA8:=U8(VV,T,P,AMIX,BMIX,CMIX,EMIX,M1,M2,M3,PH8);$$

$$U18:=((((2*VV)+EMIX-M3)*P)+(M1*M2*(UA8/(-1/(P*P)))))/U181;$$

$$U19:=1/(0.008314*T*M1*M2);$$

$$U20:=AMIX/(0.008314*T*M1*M2*M2);$$

$$PHA14:=PH14(VV,EMIX,M3,M4);$$

$$U221:=(((AMIX*VV)+(M3*CMIX))/(VV*VV*M1*M1*M2*M2*M2*M2))*PHA14);$$

$$U22:=(AMIX/(VV*M1*M2*M2))-U221;$$

$$UA8:=U8(VV,T,P,AMIX,BMIX,CMIX,EMIX,M1,M2,M3,PH8);$$

$$U23:=-UA8*((AMIX*VV)+(M3*CMIX))/(VV*M1*M2*M2);$$

{EQUATION TO CALCULATE FOR VAPOR PHASE}

$$UA4:=U4(VV,AMIX,BMIX,CMIX,EMIX,M1,M2,M3,PH8);$$

$$UA5:=U5(T,CMIX, VV,M1,M2,AMIX,M3);$$

$$UA7:=U7(VV,AMIX,CMIX,M1,M2,M3,T);$$

$$UA8:=U8(VV,T,P,AMIX,BMIX,CMIX,EMIX,M1,M2,M3,PH8);$$

$$UA11:=U11(CMIX,T,M1,M2,M3,M4,EMIX, VV);$$

$$UA12:=U12(VV,T,M3,M4,M6,M1,M2,CMIX,EMIX);$$

$$UA13:=U13(CMIX,T,M3,M4,M7,M1);$$

$$FBGV1:=U1-U2-(U3*UA4)+UA5-(U6/P)-(UA7*UA8)+U9-U10+UA11+UA12-UA13;$$

$$UA15:=U15(M3, VV,EMIX,P,T,M1,M2);$$

$$UA16:=U16(VV,T,M1,M2,M3,M4,EMIX);$$

$$FCGV1:=U14-UA15+UA16;$$

$$FAGV1:=U17-U18+U19;$$

$$UA25:=U25(VV,T,CMIX,EMIX,M1,M2,M3,M4);$$

$$UA21:=U21(AMIX, VV,M3,EMIX,CMIX,T,M1,M2);$$

$$PHA14:=PH14(VV,EMIX,M3,M4);$$

$$UA24:=U24(AMIX,T,M5,M1,M2, VV,M3,EMIX);$$

$$FELG1:=U20-UA21-(U22/P)+U23+UA24+UA25;$$

$$DIVG2:=(BNIV*FBGV1)+(CNIV*FCGV1)+(ANIV*FAGV1)+(ENIV*FELG1);$$

$$TA3:=T3(M1,M2, VV,EMIX,AMIX,M3,T);$$

$$TA5:=T5(BMIX,AMIX,EMIX,M1,M2,M3,T, VV);$$

$$TA9:=T9(CMIX,EMIX,M3,M4,M1,M2,T, VV);$$

$$FVVG1:=T1+T2-TA3-T4-(TA5/P)-(1/VV)-T6-T7+T8+TA9;$$

```

DIVG1:=FVVG1+DIVG2;
PFGV1:=PFV1*DIVG1;
VGP1:=(ZV*0.008314*T*(P*P));
PFGP1:=PFGV1*VGP1;

```

```

{FINAL PROPOSE EQUATION}
DIVI:=(Abs((XX1*PFL1)-(Y1*PFV1)));
FDIF:=(XX1*PFLP1)-(Y1*PFGP1);
FN:=(XX1*PFL1)-(Y1*PFV1);
P:=P-(FN/FDIF);

```

```

IF (P>Pex) THEN

```

```

begin

```

```

    P:=ANSWER;

```

```

    Loop_No:=30;

```

```

end

```

```

else if(P < 0) THEN

```

```

begin

```

```

    Loop_No:=30;

```

```

end

```

```

else IF (P > ANSWER ) THEN

```

```

begin

```

```

    ANSWER:=P;

```

```

end;

```

```

Loop_No:=Loop_No+1;

```

```

END;

```

```

WRITELN('PCAL = ',ANSWER:10:8,' MPa');

```

```

writeln('No. of loop = ',Loop_No);

```

```

writeln('KIJ = ',KIJ:10:8);

```

```

{ WRITELN('DIVIATION = ',DIVI:10:8);}

```

```

END;

```

```

FUNCTION ROOTofQEOS(XX1,XX2,Y1,Y2,Kij,T,P:REAL):REAL;

```

BEGIN

Pex:=P;

Bc1:=0.165 * Vc1;

P1:=(exp((-0.03125 * ln(T/Tc1)) -(0.0054*(ln(T/Tc1)*ln(T/Tc1))));

B1:=Bc1 * P1 * P1 * P1;

Bc2:=0.165 * Vc2;

P2:=(exp((-0.03125 * ln(T/Tc2)) -(0.0054*(ln(T/Tc2)*ln(T/Tc2))));

B2:=Bc2 * P2 * P2 * P2;

BMIX:=(Y1 * B1) + (Y2 * B2);

ER1:=0.63189 * (1 - (0.81660 * W1) + (3.25246 * W1 * W1));

E1:=ER1/DCi;

ER2:=0.63189 * (1 - (0.81660 * W2) + (3.25246 * W2 * W2));

E2:=ER2/(DC2);

EMIX:=(Y1 * E1) + (Y2 * E2);

{

Calculate value a of polar component!

}

IF (StrLComp(kind1,'POLAR',5)=0) THEN

BEGIN

TR1:=T/Tc1;

ReDipole1:=(0.3976 * DipoleMoment1) / (Sqrt(0.008314 * Tc1 * Vc1));

IF (TR1 <=1) THEN

BEGIN

X2:=0.14988+(0.97848 * W1)+(-0.01390*ReDipole1)+(0.02928 * ReDipole1 * ReDipole1);

X3:=-0.32379+(1.84591*W1)+(0.39338*ReDipole1)+(-0.25483*ReDipole1*ReDipole1);

X4:=(0.14833)+(-3.46693 * W1)+(-0.39170 * ReDipole1) + (-0.01597 * ReDipole1 *

ReDipole1);

ALPHA1:=(1+(X2*(1-(Sqrt(TR1)))+X3*(1-Sqrt(TR1))*(1-(Sqrt(TR1))))+(X4*(1-Sqrt(TR1))*(1-

Sqrt(TR1))*(1-Sqrt(TR1)));

ALPHATR:=ALPHA1 * ALPHA1;

END

```

ELSE
BEGIN
  X2:=0.14988+(0.97848 * W1)+(-0.01390*ReDipole1)+(0.02928 * ReDipole1 * ReDipole1);
  X5:=0.11048+(0.57743*W1)+(0.41218*ReDipole1)+(-0.10676*ReDipole1*ReDipole1);
  X6:=0.02581+(-0.027*W1)+(0.38327*ReDipole1)+(-0.09008*ReDipole1*ReDipole1);

ALPHA2:=(1+(X2*(1-(Sqrt(TR1)))+X5*(1-Sqrt(TR1)))*(1-(Sqrt(TR1))))+(X6*(1-Sqrt(TR1))*(1-Sqrt(TR1))*
(1-Sqrt(TR1)));
  ALPHATR:=ALPHA2 * ALPHA2;
END;

ar1:=1.84713*(1-(0.05218*W1)+(1.06446*W1*W1)-(0.0273*ReDipole1)+(0.02048*ReDipole1*Re
Dipole1));
ac1:=(ar1*8.314*(1/1000)*Tc1)/(Dc1);
al:=ac1*ALPHATR;

{
  Calculate value c of polar component1
}

cr1:=1.78336*(1+(-1.29690*W1)+(2.78945*W1*W1)+(0.07*ReDipole1)+(0.01188*ReDipole1*ReD
ipole1));
cc1:=(cr1*8.314*(1/1000)*Tc1)/Dc1;
X7:=(-0.77357)+(-1.45342*W1)-(0.04725 * ReDipole1) - (0.09669 * ReDipole1 * ReDipole1 );
tempdep1:=(1+ (X7 * (1 - Sqrt(TR1)))));
tempdep11:=tempdep1*tempdep1;
c1:=cc1*tempdep11;
END
{
  Calculate value a of nonpolar component1
}
ELSE
BEGIN
  TR1:=T/Tc1;
  IF(TR1<=1) THEN
  BEGIN
    X2:=0.14988+(0.97848*W1);

```

```

X3:=(-0.32379)+(1.84591*W1);
X4:=0.14833+((-3.46693)*W1);
ALPHA1:=(1+(X2*(1-Sqrt(TR1))))+(X3*(1-(Sqrt(TR1)))*(1-(Sqrt(TR1))))
+(X4*(1-SQRT(TR1)) * (1-Sqrt(TR1)) * (1-Sqrt(TR1)));
ALPHATR:=ALPHA1*ALPHA1;
END
ELSE
BEGIN
X2:=0.14988+(0.97848*W1);
X5:=0.11048+(0.57743*W1);
X6:=0.02581+(-0.027*W1);
ALPHA2:=(1+(X2*(1-Sqrt(TR1))))+(X5*(1-(Sqrt(TR1)))*(1-(Sqrt(TR1))))
+(X6*(1-SQRT(TR1)) * (1-Sqrt(TR1)) * (1-Sqrt(TR1)));
ALPHATR:=ALPHA2*ALPHA2;
END;
ar1:=1.84713*(1-(0.05218*W1))+(1.06446*W1*W1);
ac1:=(ar1*8.314*(1/1000)*Tc1)/(DC1);
a1:=ac1*ALPHATR;
{
Calculate value c of nonpolar component1
}
cr1:=1.78336*(1+(-1.29690*W1)+(2.78945*W1*W1));
cc1:=(cr1*8.314*(1/1000)*Tc1)/Dc1;
X7:=(-0.77357)+(-1.45342*W1);
tempdep1:=(1+(X7*(1-Sqrt(TR1)))));
tempdep11:=tempdep1*tempdep1;
c1:=cc1*tempdep11;
END;
{
Calculate value a of polar component2
}
IF (StrLComp(kind2,'POLAR',5)=0) THEN
BEGIN
TR2:=T/Tc2;
ReDipole2:=(0.3976 * DipoleMoment2) / (Sqrt(0.008314 * Tc2 * Vc2));
IF (TR2 <=1) THEN
BEGIN

```



```

Z2:=0.14988+(0.97848 * W2)+ (-0.01390*ReDipole2)+ (0.02928 * ReDipole2 *
ReDipole2);
Z3:=-0.32379+(1.84591*W2)+(0.39338*ReDipole2)+(-0.25483*ReDipole2*ReDipole2);
Z4:=(0.14833)+(-3.46693 * W2)+(-0.39170 * ReDipole2) + (-0.01597 * ReDipole2 *
ReDipole2);
{there are error here}

ALPHA3:=(1+(Z2*(1-(Sqrt(TR2))))+Z3*(1-Sqrt(TR2)))*(1-(Sqrt(TR2))))+(Z4*(1-Sqrt(TR2))*(1-Sqrt(TR2))*
(1-Sqrt(TR2)));
ALPHATR1:=ALPHA3 * ALPHA3;

```

```

END
ELSE
BEGIN
Z2:=0.14988+(0.97848 * W2)+(-0.01390*ReDipole2)+ (0.02928 * ReDipole2 * ReDipole2);
Z5:=0.11048+(0.57743*W2)+(0.41218*ReDipole2)+(-0.10676*ReDipole2*ReDipole2);
Z6:=0.02581+(-0.027*W2)+(0.38327*ReDipole2)+(-0.09008*ReDipole2*ReDipole2);
ALPHA4:=(1+(Z2*(1-(Sqrt(TR2))))+Z5*(1-Sqrt(TR2)))*(1-(Sqrt(TR2))))
+(Z6 * (1 - Sqrt(TR2)) * (1 - Sqrt(TR2)) * (1-Sqrt(TR2)));
ALPHATR1:=ALPHA4 * ALPHA4;
END;

```

```

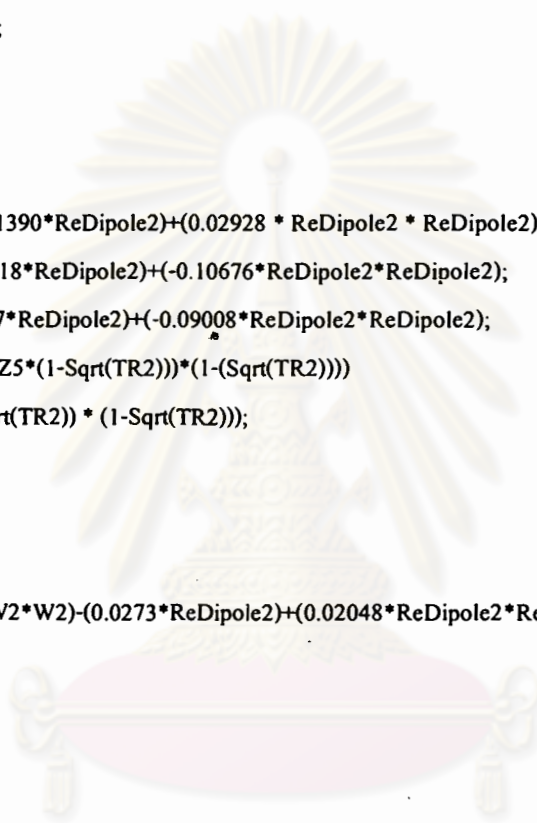
ar2:=1.84713*(1-(0.05218*W2)+(1.06446*W2*W2)-(0.0273*ReDipole2)+(0.02048*ReDipole2*ReDipole2));
ac2:=(ar2*8.314*(1/1000)*Tc2)/Dc2;
a2:=ac2*ALPHATR1;
{
Calculate value c of polar component2
}

```

```

cr2:=1.78336*(1+(-1.29690*W2)+(2.78945*W2*W2)+(0.07*ReDipole2)+(0.01188*ReDipole2*ReDipole2));
cc2:=(cr2*8.314*(1/1000)*Tc2)/Dc2;
Z7:=-(-0.77357)+(-1.453428*W2)-(0.04725 * ReDipole2) - (0.09669 * ReDipole2 * ReDipole2);
tempdep2:=(1+ (Z7 * (1 - Sqrt(TR2)))));
tempdep22:=tempdep2*tempdep2;

```



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```

c2:=cc2*tempdep22;
END
{
  Calculate value a of nonpolar component2
}
ELSE
BEGIN
  TR2:=T/Tc2;
  IF(TR2<=1) THEN
  BEGIN
    Z2:=0.14988+(0.97848*W2);
    Z3:=(-0.32379)+(1.84591*W2);
    Z4:=0.14833+((-3.46693)*W2);
    ALPHA3:=(1+(Z2*(1-Sqrt(TR2))))+(Z3*(1-Sqrt(TR2)))*(1-Sqrt(TR2))
      +(Z4*(1-SQRT(TR2)) * (1-Sqrt(TR2)) * (1-Sqrt(TR2)));
    ALPHATR1:=ALPHA3*ALPHA3;
  END
  ELSE
  BEGIN
    Z2:=0.14988+(0.97848*W2);
    Z5:=0.11048+(0.57743*W2);
    Z6:=0.02581+(-0.027*W2);
    ALPHA4:=(1+(Z2*(1-Sqrt(TR2))))+(Z5*(1-Sqrt(TR2)))*(1-Sqrt(TR2))
      +(Z6*(1-SQRT(TR2)) * (1-Sqrt(TR2)) * (1-Sqrt(TR2)));
    ALPHATR1:=ALPHA4*ALPHA4;
  END;
  ar2:=1.84713*(1-(0.05218*W2))+(1.06446*W2*W2);
  ac2:=(ar2*8.314*(1/1000)*Tc2)/DC2;
  a2:=ac2*ALPHATR1;
  {
    Calculate value c of nonpolar component2
  }
  cr2:=1.78336*(1+(-1.29690*W2)+(2.78945*W2*W2));
  cc2:=(cr2*8.314*(1/1000)*Tc2)/DC2;
  Z7:=(-0.77357)+(-1.45342*W2);
  tempdep2:=(1+(Z7 * (1 - Sqrt(TR2))));
  tempdep22:=tempdep2*tempdep2;

```

```
c2:=cc2*tempdep22;
```

```
END;
```

```
{OLD FASION
```

```
aMIX:=(Y1*Y1*a1)+(2*Y2*Y2*(Sqrt(a1*a2)))+(Y2*Y2*A2);
```

```
cMIX:=(Y1*Y1*c1)+(2*Y1*Y2*Sqrt(c1*c2))+(Y2*Y2*c2);
```

```
}
```

```
aMIX:=(Y1*Y1*a1)+(2*Y1*Y2*(Sqrt(a1*a2))*(1-Kij))+(Y2*Y2*a2);
```

```
cMIX:=(Y1*Y1*c1)+(2*Y1*Y2*(Sqrt(c1*c2)))+(Y2*Y2*c2);
```

```
{
```

```
O1:=(((P*P*EMIX*BMIX*1.2864)-(P*P*EMIX*BMIX*2.8225))/(0.008314*0.008314*T*T));
```

```
O3:=0.008314*0.008314*0.008314*T*T*T;
```

```
O2:=(((P*P)/(0.008314*0.008314*T*T))*((1.2864*1.2864*BMIX*BMIX)-(2*1.2864*BMIX*EMIX)))+(A  
MIX*P)/(0.008314*0.008314*T*T));
```

```
Q4:=(-CMIX*(1.2864)*(1.2864)*BMIX*BMIX*P*P*P)/(0.008314*0.008314*0.008314*0.008314*T*T*  
T*T);
```

```
Q3:=(((P*P*P*EMIX*1.2864*1.2864*BMIX*BMIX)+(1.2864*BMIX*CMIX*P*P)-(1.2864*BMIX*AMIX*  
P*P))/O3)+O1;
```

```
Q2:=((P/(0.008314*T))*((BMIX*1.2864)-(BMIX*2.8225)-EMIX))+O2;
```

```
Q1:=((P/(0.008314*T))*((-2*1.2864*BMIX)+EMIX))-1;
```

```
COMPRESS_FACTOR(Q1,Q2,Q3,Q4,XX1,XX2,Y1,Y2);
```

```
END;
```

```
BEGIN {Main}
```

```
clrscr;
```

```
Assign (Input,'C:\TP\data\datafile.dat');
```

```
Reset(Input);
```

```
{Temp file}
```

```
Assign (output,'c:\tp\data\temp.dat');
```

```
Rewrite(output);
```

```
Write('Enter name of the substance1: ');Readln(Fname1);
```

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```

Found1:=0;
WHILE(Found1=0) DO
BEGIN
  WHILE NOT EOF(Input) DO
  BEGIN
    Readln(Input,Fname3);
    Len:=StrLen(Fname1);
    Po:=StrLComp(StrLower(Fname1),StrLower(Fname3),Len);
    If (Po=0) then
    BEGIN
      Found1:=1;
      Break;
    END;
  END;
END;
IF (Found1=0) THEN
BEGIN
  Write('Enter New Substance1 again: ');Readln(Fname1);
  Reset(Input);
END;
END;

Reset(Input);
Write('Enter name of the substance2: ');Readln(Fname2);
Found2:=0;
WHILE(Found2=0) Do
BEGIN
  WHILE NOT EOF(Input) DO
  BEGIN
    Readln(Input,Fname4);
    Len:=StrLen(Fname2);
    Po:=StrLComp(StrLower(Fname4),StrLower(Fname2),Len);
    If (Po=0) then
    BEGIN
      Found2:=1;
      Break;
    END;
  END;
END;
END;

```

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มหาวิทยาลัย

```
IF(Found2=0)THEN
BEGIN
  Write('Enter New Substance2 again: ');Readln(Fname2);
  Reset(Input);
  END;
END;

Reset(Input);
readln(Input);
readln(Input);
WHILE NOT EOF(Input) DO
BEGIN
  Readln(Input,substance1,kind1,Tc1,Pc1,Dc1,DipoleMoment1,Vc1,W1);
  Len:=StrLen(Fname1);

  Po:=StrLComp(StrLower(substance1),StrLower(Fname1),Len);
  If (Po=0) then
    Break;
END;

Reset(Input);
Readln(Input);
Readln(Input);
WHILE NOT EOF(Input) DO
BEGIN
  readln(Input,substance2,kind2,Tc2,Pc2,Dc2,DipoleMoment2,Vc2,W2);
  Len:=StrLen(Fname2);
  Po:=StrLComp(StrLower(substance2),StrLower(Fname2),Len);
  If (Po=0) then
    Break;
END;

write('Enter Temperature(K) : ');readln(T);
Tex:=T;
Write('Enter Pressure (MPa) : ');readln(P);
Pex:=P;
write('Enter XX1 : ');readln(XX1);
write('Enter XX2 : ');readln(XX2);
```

```

write('Enter Y1 : ');readln(Y1);
write('Enter Y2 : ');readln(Y2);
write('Enter P1sat: ');readln(P1sat);
write('Enter P2sat: ');readln(P2sat);
{
ROOTofQEOS(XX1,XX2,Y1,Y2,0,T,P);
}
write('SELECT Pconst. OR Tconst. (T,P): ');
readln(steady);

```

```

IF (steady='P') OR (steady='p') THEN
BEGIN

```

```

{write('Please enter no.of Temperature data points: ');
readln(NUMOFT);
write('Please enter upper Kij value ');
readln(DU);
write('Please enter lower Kij value ');
readln(DL); }

```

```

COUNTIT:=1;
WHILE(COUNTIT<=NUMOFT)DO
BEGIN
write('please enter Tgroup['',COUNTIT,'']: ');
readln(Tgroup[COUNTIT]);
COUNTIT:=COUNTIT+1;
END;

```

```

COUNTIT:=1;
WHILE(COUNTIT<=NUMOFT)DO
BEGIN
write('please enter XX1['',COUNTIT,'']: ');
readln(XX1group[COUNTIT]);
COUNTIT:=COUNTIT+1;
END;

```

```

COUNTIT:=1;

```

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```
WHILE(COUNTIT<=NUMOFT)DO
BEGIN
  write('please enter XX2group['',COUNTIT,'']: ');
  readln(XX2group[COUNTIT]);
  COUNTIT:=COUNTIT+1;
END;
```

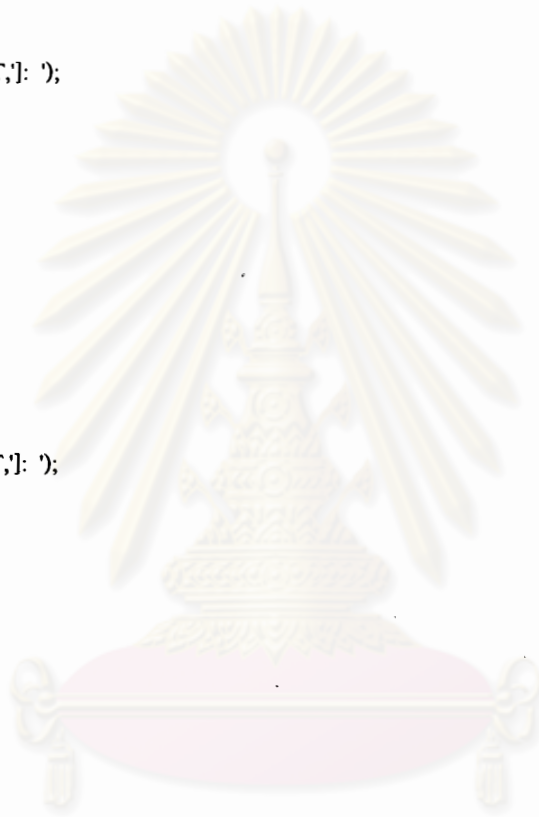
```
COUNTIT:=1;
WHILE(COUNTIT<=NUMOFT)DO
BEGIN
  write('please enter Y1group['',COUNTIT,'']: ');
  readln(Y1group[COUNTIT]);
  COUNTIT:=COUNTIT+1;
END;
```

```
COUNTIT:=1;
WHILE(COUNTIT<=NUMOFT)DO
BEGIN
  write('please enter Y2group['',COUNTIT,'']: ');
  readln(Y2group[COUNTIT]);
  COUNTIT:=COUNTIT+1;
END;}
```

```
EPS:=0.000001;
COUNTIT:=1;
```

```
WHILE (1=1) DO
BEGIN
```

```
  DLL:=(3/15)*(DU-DL)+DL;
  Kij:=DLL;
  WHILE (COUNTIT<=NUMOFT)DO
  BEGIN
    XX1:=XX1group[COUNTIT];
```



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```

XX2:=XX2group[COUNTIT];
Y1:=Y1group[COUNTIT];
Y2:=Y2group[COUNTIT];
T:=Tgroup[COUNTIT];
Pex:=0.1013;
P:=Pex;
ROOTofQEOS(XX1,XX2,Y1,Y2,Kij,T,P);

```

```

SUM:=SUM+((Pex-P)*(Pex-P)/Pex);
COUNTIT:=COUNTIT+1;
END;
FUNCL:=SUM;
WRITELN('FUNCL = ',FUNCL);

```

```

COUNTIT:=1;
DUU:=((5/15)*(DU-DL))+DL;
Kij:=DUU;
WHILE (COUNTIT<=NUMOFT)DO

```

```

BEGIN
XX1:=XX1group[COUNTIT];
XX2:=XX2group[COUNTIT];
Y1:=Y1group[COUNTIT];
Y2:=Y2group[COUNTIT];
T:=Tgroup[COUNTIT];
Pex:=0.1013;
P:=Pex;

```

```

ROOTofQEOS(XX1,XX2,Y1,Y2,Kij,T,P);
SUM:=SUM+((Pex-P)*(Pex-P)/Pex);
COUNTIT:=COUNTIT+1;
END;
FUNCU:=SUM;
WRITELN('FUNCU = ',FUNCU);

```

```

IF(DUU-DLL-EPS > 0) THEN
BEGIN
FUL:=FUNCU-FUNCL;
IF(FUL>0) THEN

```



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```

BEGIN
    DU:=DUU;
    CONTINUE;
END
ELSE
BEGIN
    DL:=DLL;
    CONTINUE;
END;
END
ELSE
BEGIN
Kij:=(DLL+DUU)/2;
WRITE('Kij Answer : ',Kij);
{This part use for show Pcal of all temperatures }

writeln(' sum = ',sum:10:8);
COUNTIT:=1;
WHILE (COUNTIT<=NUMOFT)DO
BEGIN
XX1:=XX1group[COUNTIT];
XX2:=XX2group[COUNTIT];
Y1:=Y1group[COUNTIT];
Y2:=Y2group[COUNTIT];
T:=Tgroup[COUNTIT];
Pex:=0.1013;
P:=Pex;

ROOTofQEOS(XX1,XX2,Y1,Y2,Kij,T,P);
Writeln('Pcal of temperature ',Tgroup[COUNTIT],' = ',P,'MPa');
COUNTIT:=COUNTIT+1;
END;
EXIT;
END;
END;
END;

```



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สงครภมมหาวิทาลัย

```

COUNTIT:=1;
WHILE (COUNTIT<=NUMOFT)DO
BEGIN
ROOTofQEOS(XX1group[COUNTIT],XX2group[COUNTIT],Y1group[COUNTIT],
Y2group[COUNTIT],Kij,Tgroup[COUNTIT],Pex);
WRITELN('Pcal of temperature ',Tgroup[COUNTIT],' = ',P,'MPa');
COUNTIT:=COUNTIT+1;
END;
EXIT;
END;
END;
END;

```



```

IF (steady='T') OR (steady='t') THEN

```

```

BEGIN

```

```

write('Please enter no.of pressure data points: ');
readln(NUMOFP);
write('Please enter upper Kij value ');
readln(DU);
write('Please enter lower Kij value ');
readln(DL);

```

```

COUNTIT:=1;

```

```

WHILE(COUNTIT<=NUMOFP)DO

```

```

BEGIN

```

```

write('please enter Pexgroup[',COUNTIT,']: ');
readln(Pexgroup[COUNTIT]);
COUNTIT:=COUNTIT+1;

```

```

END;

```

```

COUNTIT:=1;

```

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```
WHILE(COUNTIT<=NUMOFP)DO
BEGIN
  write('please enter XX1[,COUNTIT,]: ');
  readln(XX1group[COUNTIT]);
  COUNTIT:=COUNTIT+1;
END;
```

```
COUNTIT:=1;
WHILE(COUNTIT<=NUMOFP)DO
BEGIN
  write('please enter XX2group[,COUNTIT,]: ');
  readln(XX2group[COUNTIT]);
  COUNTIT:=COUNTIT+1;
END;
```

```
COUNTIT:=1;
WHILE(COUNTIT<=NUMOFP)DO
BEGIN
  write('please enter Y1group[,COUNTIT,]: ');
  readln(Y1group[COUNTIT]);
  COUNTIT:=COUNTIT+1;
END;
```

```
COUNTIT:=1;
WHILE(COUNTIT<=NUMOFP)DO
BEGIN
  write('please enter Y2group[,COUNTIT,]: ');
  readln(Y2group[COUNTIT]);
  COUNTIT:=COUNTIT+1;
END;
```

```
EPS:=0.000001;
COUNTIT:=1;
```

```
WHILE (1=1) DO
BEGIN
```



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```

DLL:=(3/32)*(DU-DL))+DL;
Kij:=DLL;
WHILE (COUNTIT<=NUMOFP)DO
BEGIN
XX1:=XX1group[COUNTIT];
XX2:=XX2group[COUNTIT];
Y1:=Y1group[COUNTIT];
Y2:=Y2group[COUNTIT];
P:=Pexgroup[COUNTIT];
ROOTofQEOS(XX1,XX2,Y1,Y2,Kij,T,P);

SUM:=SUM+((Pexgroup[COUNTIT]-P)*(Pexgroup[COUNTIT]-P)/Pexgroup[COUNTIT]);
COUNTIT:=COUNTIT+1;
END;
FUNCL:=SUM;
WRITELN("FUNCL = ',FUNCL);

COUNTIT:=1;
DUU:=(5/32)*(DU-DL))+DL;
Kij:=DUU;
WHILE (COUNTIT<=NUMOFP)DO
BEGIN
XX1:=XX1group[COUNTIT];
XX2:=XX2group[COUNTIT];
Y1:=Y1group[COUNTIT];
Y2:=Y2group[COUNTIT];
P:=Pexgroup[COUNTIT];
ROOTofQEOS(XX1,XX2,Y1,Y2,Kij,T,P);

SUM:=SUM+((Pexgroup[COUNTIT]-P)*(Pexgroup[COUNTIT]-P)/Pexgroup[COUNTIT]);
COUNTIT:=COUNTIT+1;
END;
FUNCU:=SUM;
WRITELN("FUNCU = ',FUNCU);

IF(DUU-DLL-EPS > 0) THEN

```

```
BEGIN
FUL:=FUNCU-FUNCL;
  IF(FUL>0) THEN
    BEGIN
      DU:=DUU;
      CONTINUE;
    END
  ELSE
    BEGIN
      DL:=DLL;
      CONTINUE;
    END;
END
ELSE
BEGIN
Kij:=(DLL+DUU)/2;
WRITE('Kij Answer : ',Kij:10:8);
writeln('sum = ',sum:10:8);
EXIT;
END;
END;
END;
END.
```



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```
{PROGRAM FOR PENG - ROBINSON EQUATION OF STATE}
```

```
Program_Peng_Robinson_Equation_of_state;
```

```
Uses Strings,CRT;
```

```
VAR BC1,BC2,VC1,VC2,P1,P2,Tc1,Tc2,B1,B2,BMIX,T,P,XX1,XX2,Y1,Y2:REAL;
```

```
W1,W2,pc1,pc2,DC1,DC2:REAL;
```

```
Dipolemoment1,Dipolemoment2:REAL;
```

```
TR1,ac1,a1:REAL;
```

```
TR2,Z1,Z2,Z3,Z4,ac2,a2:REAL;
```

```
AMIX,Q2,Q3,Q4:REAL;
```

```
P1sat,P2sat,Tex,Pex,Ts,Te,ITV,Kij,min,Kanswer,Tope,SUM:REAL;
```

```
NUMOFFP,NUMOFT,COUNTIT,i:INTEGER;
```

```
Pgroup:ARRAY[0..30]OF REAL;
```

```
Pexgroup:ARRAY[0..30]OF REAL;
```

```
Tgroup:ARRAY[0..30]OF REAL;
```

```
XX1group:ARRAY[0..30]OF REAL;
```

```
XX2group:ARRAY[0..30]OF REAL;
```

```
Y1group:ARRAY[0..30]OF REAL;
```

```
Y2group:ARRAY[0..30]OF REAL;
```

```
z1,zv,ANSWER,DU,DL,EPS,DUU,DLL,FUNC,FUNCL,FUNCU,FUL:REAL;
```

```
DPFL11,DPFJ1,PFLV1,VLP1,PFLP1,DIV!:REAL;
```

```
ALPHA11,ALPHA22,ALPHA1,ALPHA2:REAL;
```

```
AQ,BQ:REAL;
```

```
Input:text;
```

```
Fname1,Fname2,Fname3,Fname4,substance1,substance2:Array [0..29] of Char;
```

```
kind1,kind2:Array [0..9] of Char;
```

```
Found1,Found2:Integer; {strpos}
```

```
steady:Char;
```

```
{Addition Variables}
```

```
Po,Len:Integer;
```

```
{test variables}
```

```
sub1,sub2:string;
```

```
output:text;
```

```
Pexp:REAL;
```

```
Function COMPRESS_FACTOR(Q2,Q3,Q4,XX1,XX2,Y1,Y2:REAL):REAL;
```

```
VAR S,E,A,B,BEGIN_VALUE,INCRE:REAL;
```

```
RESULT:ARRAY[1..4] OF REAL;
```

```
INDEX,COUNTER,AGAIN:INTEGER;
```

```
VL,VV:REAL;
```

```
FDIF,FN,PFLP1,PFLV1,VLPI:REAL;
```

```
PFL1,PFV1,CPFV1,DPFL1:REAL;
```

```
PFGP1,PGV1:REAL;
```

```
BETA1,BETA2,BETA,DFPL1:REAL;
```

```
PHI1,PHI2,PHI,CPFV1:REAL;
```

```
VGPI:REAL;
```

```
{NUBER OF LOOP}
```

```
Loop_No:INTEGER;
```

```
BEGIN
```

```
BEGIN_VALUE:=0;
```

```
COUNTER:=0;
```

```
INCRE:=0.05;
```

```
WRITELN;
```

```
WHILE(BEGIN_VALUE<=1) AND (COUNTER<3) DO
```

```
BEGIN
```

```
S:=1;
```

```
E:=0.000005;
```

```
A:=BEGIN_VALUE;
```

```
WHILE(ABS(S)>E) DO
```

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```
BEGIN
  B:=A;
  A:=B-((B*B*B+(Q2*B*B)+(Q3*B)+Q4)/(3*B*B+2*Q2*B+Q3));
  S:=(A*A*A)+(Q2*A*A)+(Q3*A)+Q4;
END;
IF (COUNTER=0) THEN
BEGIN
  BEGIN_VALUE:=BEGIN_VALUE+INCRE;
  IF (A>=0)AND (A<=1) THEN
  BEGIN
    COUNTER:=COUNTER+1;
    RESULT[COUNTER]:=A;
    {this is a test}
    WRITELN('ANSWER (' ,COUNTER,') IS ',RESULT[COUNTER]:10:8);

  END;
  CONTINUE;
END;
IF (COUNTER>0) THEN
BEGIN
  { IF COUNTER=3 THEN EXIT;}
  IF (A<0) OR (A>1) THEN
  BEGIN
    BEGIN_VALUE:=BEGIN_VALUE+INCRE;
    CONTINUE;
  END;
  INDEX:=1;

  AGAIN:=0;
  WHILE(INDEX<=COUNTER) DO
  BEGIN
    IF( ABS(A-RESULT[INDEX]) < 0.01) THEN
    BEGIN
```



```
INDEX:=INDEX+1;
```

```
AGAIN:=1;
```

```
CONTINUE;
```

```
END;
```

```
INDEX:=INDEX+1;
```

```
END;
```

```
IF(AGAIN=0) THEN
```

```
BEGIN
```

```
COUNTER:=COUNTER+1;
```

```
RESULT[COUNTER]:=B;
```

```
END;
```

```
END;
```

```
BEGIN_VALUE:=BEGIN_VALUE+INCRE;
```

```
END;
```

```
IF (COUNTER=0) THEN
```

```
BEGIN
```

```
WRITELN;
```

```
WRITELN('NO ANSWER');
```

```
END;
```

```
IF (COUNTER<2) OR (COUNTER>3) THEN EXIT;
```

```
ZL:=RESULT[1];
```

```
IF (COUNTER=2) THEN
```

```
ZV:=RESULT[2]
```

```
ELSE
```

```
ZV:=RESULT[3];
```

```
{ WRITELN(' ZL = ',ZL:10:8,' ZV = ',ZV:10:8);}
```

```
{PROGRAM CALCULATION PARTIAL FUGACITY COEFFICIENT
```

FOR VAPOR & LIQUID PHASE IN BINARY MIXTURE}

PFV1:=5;

PFL1:=3;

P:=((XX1*P1sat)+(XX2*P2sat))/2;

ANSWER:=P;

writeln('Pex =',Pex:10:8,' P = ',P:10:8);

WHILE (Abs((XX1*PFL1)-(Y1*PFV1))>0.001) DO

Loop_No:=0;

BEGIN

VL:=(ZL*0.008314*T/P);

VV:=(ZV*0.008314*T/P);

{vapour phase}

CPFV1:=(((B1/BMIX)*(ZV-1))-(ln(ZV-BMIX)))+(AMIX/(4.828*BMIX))

*((B1/BMIX)-((2/AMIX)*Y2*(1-Kij)*sqrt(A1*A2))))

*ln((ZV+(2.41*BMIX))/(ZV-(0.414*BMIX)));

{liquid phase}

DPFL1:=(((B1/BMIX)*(ZL-1))-(ln(ZL-BMIX)))+(AMIX/(4.828*BMIX))

*((B1/BMIX)-((2/AMIX)*XX2*(1-Kij)*sqrt(A1*A2))))

*ln((ZL+(2.41*BMIX))/(ZL-(0.414*BMIX)));

PFV1:=EXP(CPFV1);

PFL1:=EXP(DPFL1);

{THIS PART TO SET INITIAL PRESSURE}

{LIQUID}

BETA1:=ZL+(2.414*BMIX);

BETA2:=ZL-(0.414*BMIX);

BETA:=(AMIX/(4.828*BMIX))*((B1/BMIX)-((2*XX2*(1-Kij)*SQRT(A1*A2))

/AMIX));

DPFL11:=((P/(0.008314*T))*((B1/BMIX)+(BETA*(BETA2-BETA1)/(BETA2*BETA1))))

```
-(1/(VL-BMIX));
```

```
PFLV1:=EXP(DPFL1)*DPFL11;
```

```
VLP1:=- (ZL*0.008314*T/(P*P));
```

```
PFLP1:=PFLV1*VLP1;
```

```
{VAPOR}
```

```
PHI1:=ZV+(2.414*BMIX);
```

```
PHI2:=ZV-(0.414*BMIX);
```

```
PHI:=(AMIX/(4.828*BMIX))*((B1/BMIX)-((2*Y2*(1-Kij)*SQRT(A1*A2))  
/AMIX));
```

```
CPFV11:=((P/(0.008314*T))*((B1/BMIX)+(PHI*(PHI2-PHI1)/(PHI2*PHI1))))  
-(1/(VV-BMIX));
```

```
PFGV1:=EXP(CPFV1)*CPFV11;
```

```
VGP1:=- (ZV*0.008314*T/(P*P));
```

```
PFGP1:=PFGV1*VGP1;
```

```
{FINAL PROPOSE EQUATION}
```

```
DIVI:=(Abs((XX1*PFL1)-(Y1*PFV1)));
```

```
FDIF:=(XX1*PFLP1)-(Y1*PFGP1);
```

```
FN:=(XX1*PFL1)-(Y1*PFV1);
```

```
P:=P-(FN/FDIF);
```

```
{ writeln('Old P = ',ANSWER:10:8,' New P = ',P:10:8);}
```

```
IF (P>Pex) THEN
```

```
begin
```

```
    P:=ANSWER;
```

```
    Loop_No:=30;
```

```
end
```

```
else if(P < 0) THEN
```

```
begin
```

```
    Loop_No:=30;
```

```
end
```

```
else IF (P > ANSWER ) THEN
```

```

begin
  ANSWER:=P;
end;
Loop_No:=Loop_No+1;

END;
WRITELN('PCAL = ',ANSWER:10:8,' MPa');
writeln('No. of loop = ',Loop_No);
writeln('KIJ = ',KIJ:10:8);

{ WRITELN('DIVIATION = ',DIVI:10:8);}

END;
FUNCTION ROOTofQEOS(XX1,XX2,Y1,Y2,Kij,T,P:REAL):REAL;
BEGIN
  Pex:=P;
  ALPHA11:=1+((0.37646+(1.54226*W1)-(0.26992*W1*W1))*(1-SQRT(TR1)));
  ALPHA22:=1+((0.37646+(1.54226*W2)-(0.26992*W2*W2))*(1-SQRT(TR2)));
  ALPHA1:=ALPHA11*ALPHA11;
  ALPHA2:=ALPHA22*ALPHA22;
  AC1:=0.457235*(0.008314*0.008314*TC1*TC1)/PC1;
  AC2:=0.457235*(0.008314*0.008314*TC2*TC2)/PC2;
  A1:=AC1*ALPHA1;
  A2:=AC2*ALPHA2;
  AMIX:=((Y1*Y1*A1)+(2*Y1*Y2*(SQRT(A1*A2))*(1-Kij))+(Y2*Y2*A2));
  B1:=0.077796*0.008314*TC1/PC1;
  B2:=0.077796*0.008314*TC2/PC2;
  BMIX:=(Y1*B1)+(Y2*B2);

  AQ:=AMIX*P/(0.008314*0.008314*T*T);
  BQ:=BMIX*P/(0.008314*T);

```

```
Q4:=-1*((AQ*BQ)-(BQ*BQ)-(BQ*BQ*BQ));
Q3:=AQ-(2*BQ)-(3*BQ*BQ);
Q2:=-1*(1-BQ);
COMPRESS_FACTOR(Q2,Q3,Q4,XX1,XX2,Y1,Y2);
END;
```

```
BEGIN {Main}
```

```
  clrscr;
```

```
  Assign (Input,'C:\TP\data\datafile.dat');
```

```
  Reset(Input);
```

```
  {Temp file}
```

```
  Assign (output,'c:\tp\data\temp.dat');
```

```
  Rewrite(output);
```

```
  Write('Enter name of the substance1: ');Readln(Fname1);
```

```
  Found1:=0;
```

```
  WHILE(Found1=0) DO
```

```
  BEGIN
```

```
    WHILE NOT EOF(Input) DO
```

```
    BEGIN
```

```
      Readln(Input,Fname3);
```

```
      Len:=StrLen(Fname1);
```

```
      Po:=StrLComp(StrLower(Fname1),StrLower(Fname3),Len);
```

```
      If (Po=0) then
```

```
      BEGIN
```

```
        Found1:=1;
```

```
        Break;
```

```
      END;
```

```
    END;
```

```
  IF (Found1=0) THEN
```

```
  BEGIN
```

```
    Write('Enter New Substance1 again: ');Readln(Fname1);
```

```
    Reset(Input);
```

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```
END;
END;

Reset(Input);
Write('Enter name of the substance2: ');Readln(Fname2);
Found2:=0;
WHILE(Found2=0) Do
BEGIN
  WHILE NOT EOF(Input) DO
  BEGIN
    Readln(Input,Fname4);
    Len:=StrLen(Fname2);
    Po:=StrLComp(StrLower(Fname4),StrLower(Fname2),Len);
    If (Po=0) then
    BEGIN
      Found2:=1;
      Break;
    END;
  END;
END;
IF(Found2=0)THEN
BEGIN
  Write('Enter New Substance2 again: ');Readln(Fname2);
  Reset(Input);
END;
END;
Reset(Input);
readln(Input);
readln(Input);
WHILE NOT EOF(Input) DO
BEGIN
  Readln(Input,substance1,kind1,Tc1,Pc1,Dc1,DipoleMoment1,Vc1,W1);
  Len:=StrLen(Fname1);
```

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```
Po:=StrLComp(StrLower(substance1),StrLower(Fname1),Len);
If (Po=0) then
    Break;
END;

Reset(Input);
Readln(Input);
Readln(Input);
WHILE NOT EOF(Input) DO
BEGIN
    readln(Input,substance2,kind2,Tc2,Pc2,Dc2,DipoleMoment2,Vc2,W2);
    Len:=StrLen(Fname2);
    Po:=StrLComp(StrLower(substance2),StrLower(Fname2),Len);
    If (Po=0) then
        Break;
END;

write('Enter Temperature(K) : ');readln(T);
Tex:=T;
Write('Enter Pressure (MPa) : ');readln(P);
Pex:=P;

write('Enter XX1 : ');readln(XX1);
write('Enter XX2 : ');readln(XX2);
write('Enter Y1 : ');readln(Y1);
write('Enter Y2 : ');readln(Y2);

write('Enter P1sat: ');readln(P1sat);
write('Enter P2sat: ');readln(P2sat);
{
ROOTofQEOS(XX1,XX2,Y1,Y2,0,T,P);
}
write('SELECT Pconst. OR Tconst. (T,P): ');
```

```
readln(steady);
IF (steady='P') OR (steady='p') THEN
BEGIN

write('Please enter no.of Temperature data points: ');
readln(NUMOFT);
write('Please enter upper Kij value ');
readln(DU);
write('Please enter lower Kij value ');
readln(DL);

COUNTIT:=1;
WHILE(COUNTIT<=NUMOFT)DO
BEGIN
write('please enter Tgroup[' ,COUNTIT,']: ');
readln(Tgroup[COUNTIT]);
COUNTIT:=COUNTIT+1;
END;

COUNTIT:=1;
WHILE(COUNTIT<=NUMOFT)DO
BEGIN
write('please enter XX1[' ,COUNTIT,']: ');
readln(XX1group[COUNTIT]);
COUNTIT:=COUNTIT+1;
END;

COUNTIT:= 1;
WHILE(COUNTIT<=NUMOFT)DO
BEGIN
write('please enter XX2group[' ,COUNTIT,']: ');
```



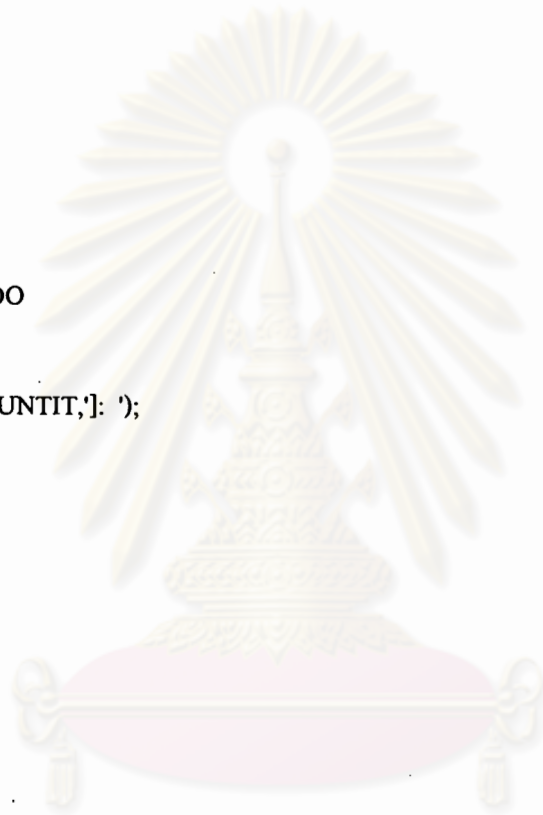
```
readln(XX2group[COUNTIT]);
COUNTIT:=COUNTIT+1;
END;
```

```
COUNTIT:=1;
WHILE(COUNTIT<=NUMOFT)DO
BEGIN
write('please enter Y1group[,COUNTIT,]: ');
readln(Y1group[COUNTIT]);
COUNTIT:=COUNTIT+1;
END;
```

```
COUNTIT:=1;
WHILE(COUNTIT<=NUMOFT)DO
BEGIN
write('please enter Y2group[,COUNTIT,]: ');
readln(Y2group[COUNTIT]);
COUNTIT:=COUNTIT+1;
END;
```

```
EPS:=0.000001;
WHILE (1=1) DO
BEGIN
```

```
DLL:=((3/15)*(DU-DL))+DL;
Kij:=DLL;
WHILE (COUNTIT<=NUMOFT)DO
BEGIN
XX1:=XX1group[COUNTIT];
XX2:=XX2group[COUNTIT];
Y1:=Y1group[COUNTIT];
Y2:=Y2group[COUNTIT];
T:=Tgroup[COUNTIT];
ROOTofQEOS(XX1,XX2,Y1,Y2,Kij,T,P);
```



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```

SUM:=SUM+((Pex-P)*(Pex-P)/Pex);
COUNTIT:=COUNTIT+1;
END;
FUNCL:=SUM;
WRITELN('FUNCL = ',FUNCL);

```

```

COUNTIT:=1;
DUU:=((5/15)*(DU-DL))+DL;
Kij:=DUU;
WHILE (COUNTIT<=NUMOFT)DO
BEGIN
XX1:=XX1group[COUNTIT];
XX2:=XX2group[COUNTIT];
Y1:=Y1group[COUNTIT];
Y2:=Y2group[COUNTIT];
T:=Tgroup[COUNTIT];
ROOTofQEOS(XX1,XX2,Y1,Y2,Kij,T,P);

```

```

SUM:=SUM+((Pex-P)*(Pex-P)/Pex);
COUNTIT:=COUNTIT+1;
END;
FUNCU:=SUM;
WRITELN('FUNCU = ',FUNCU);

```

```

IF(DUU-DLL-EPS > 0) THEN
BEGIN
FUL:=FUNCU-FUNCL;
IF(FUL>0) THEN
BEGIN
DU:=DUU;
CONTINUE;
END

```

```
ELSE
BEGIN
    DL:=DLL;
    CONTINUE;
END;

END

ELSE
BEGIN
Kij:=(DLL+DUU)/2;
WRITE('Kij Answer : ',Kij);
{This part use for show Pcal of all temperatures }

COUNTIT:=1;
WHILE (COUNTIT<=NUMOFT)DO
BEGIN
ROOTofQEOS(XX1group[COUNTIT],XX2group[COUNTIT],Y1group[COUNTIT],
Y2group[COUNTIT],Kij,Tgroup[COUNTIT],Pex);
WRITELN('Pcal of temperature ',Tgroup[COUNTIT], ' = ',P,'MPa');
COUNTIT:=COUNTIT+1;
END;

EXIT;
END;

END;
END;
```

```
IF (steady='T') OR (steady='t') THEN
```

```
BEGIN
```

```
write('Please enter no.of pressure data points: ');
```

```
readln(NUMOFP);
```

```
write('Please enter upper Kij value ');
```

```
readln(DU);
```

```
write('Please enter lower Kij value ');
```

```
readln(DL);
```

```
COUNTIT:=1;
```

```
WHILE(COUNTIT<=NUMOFP)DO
```

```
BEGIN
```

```
write('please enter Pexgroup[' ,COUNTIT,']: ');
```

```
readln(Pexgroup[COUNTIT]);
```

```
COUNTIT:=COUNTIT+1;
```

```
END;
```

```
COUNTIT:=1;
```

```
WHILE(COUNTIT<=NUMOFP)DO
```

```
BEGIN
```

```
write('please enter XX1[' ,COUNTIT,']: ');
```

```
readln(XX1group[COUNTIT]);
```

```
COUNTIT:=COUNTIT+1;
```

```
END;
```

```
COUNTIT:=1;
```

```
WHILE(COUNTIT<=NUMOFP)DO
```

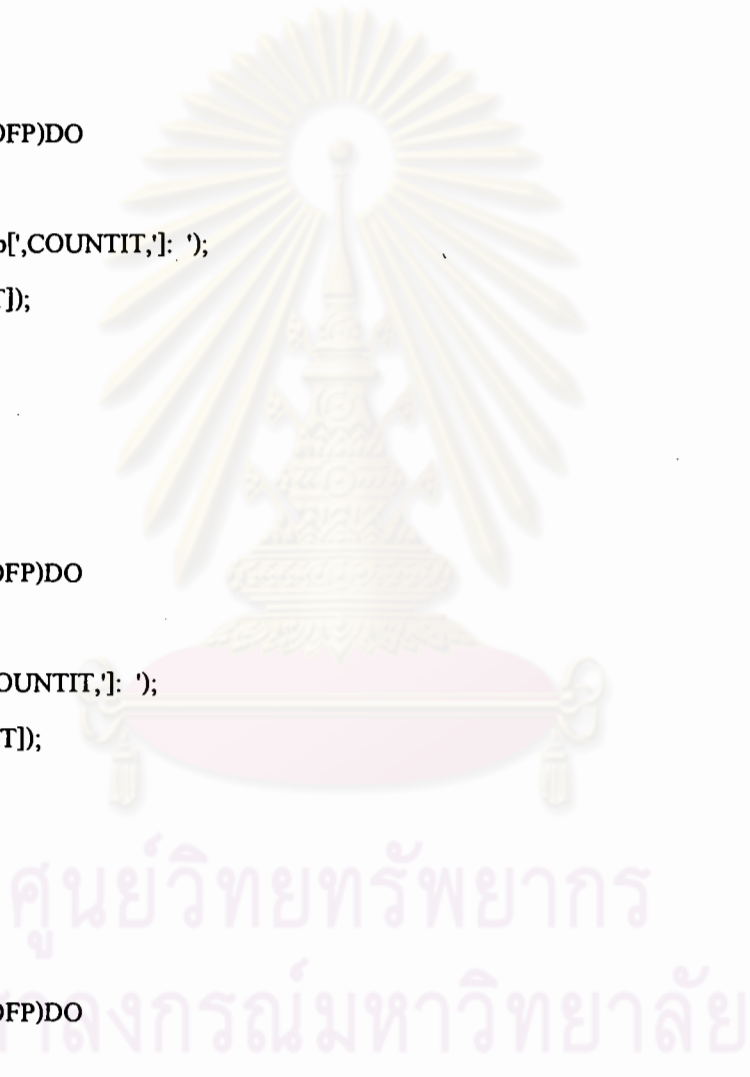
```
BEGIN
```

```
write('please enter XX2group[' ,COUNTIT,']: ');
```

```
readln(XX2group[COUNTIT]);
```

```
COUNTIT:=COUNTIT+1;
```

```
END;
```



```
COUNTIT:=1;
WHILE(COUNTIT<=NUMOFP)DO
BEGIN
  write('please enter Y1group[,COUNTIT,]: ');
  readln(Y1group[COUNTIT]);
  COUNTIT:=COUNTIT+1;
END;
```

```
COUNTIT:=1;
WHILE(COUNTIT<=NUMOFP)DO
BEGIN
  write('please enter Y2group[,COUNTIT,]: ');
  readln(Y2group[COUNTIT]);
  COUNTIT:=COUNTIT+1;
END;
```

```
EPS:=0.000001;
COUNTIT:=1;
```

```
WHILE (1=1) DO
BEGIN
```

```
  DLL:=((3/15)*(DU-DL))+DL;
```

```
  Kij:=DLL;
```

```
  WHILE (COUNTIT<=NUMOFP)DO
```

```
  BEGIN
```

```
    XX1:=XX1group[COUNTIT];
```

```
    XX2:=XX2group[COUNTIT];
```

```
    Y1:=Y1group[COUNTIT];
```

```
    Y2:=Y2group[COUNTIT];
```

```
    P:=Pexgroup[COUNTIT];
```

```
    ROOTofQEOS(XX1,XX2,Y1,Y2,Kij,T,P);
```



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```

SUM:=SUM+((Pexgroup[COUNTIT]-P)*(Pexgroup[COUNTIT]-P)/Pexgroup[COUNTIT]);
COUNTIT:=COUNTIT+1;
END;
FUNCL:=SUM;
WRITELN('FUNCL = ',FUNCL);

```

```

COUNTIT:=1;
DUU:=((5/15)*(DU-DL))+DL;
Kij:=DUU;
WHILE (COUNTIT<=NUMOFFP)DO
BEGIN
XX1:=XX1group[COUNTIT];
XX2:=XX2group[COUNTIT];
Y1:=Y1group[COUNTIT];
Y2:=Y2group[COUNTIT];
P:=Pexgroup[COUNTIT];
ROOTofQEOS(XX1,XX2,Y1,Y2,Kij,T,P);

```

```

SUM:=SUM+((Pexgroup[COUNTIT]-P)*(Pexgroup[COUNTIT]-P)/Pexgroup[COUNTIT]);
COUNTIT:=COUNTIT+1;
END;
FUNCU:=SUM;
WRITELN('FUNCU = ',FUNCU);

```

```

IF(DUU-DLL-EPS > 0) THEN

```

```

BEGIN

```

```

FUL:=FUNCU-FUNCL;

```

```

    IF(FUL>0) THEN

```

```

        BEGIN

```

```

            DU:=DUU;

```

```

            CONTINUE;

```

```

        END

```

```
ELSE
BEGIN
    DL:=DLL;
    CONTINUE;
END;

END
ELSE
BEGIN
Kij:=(DLL+DUU)/2;
WRITE('Kij Answer : ',Kij:10:8);
writeln(' sum = ',sum:10:8);

EXIT;

END;

END;
END;
END.
```



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APPENDIX B

Explanation of variables used in the computer program

ZL	=	Z^l	(see Notation)
ZV	=	Z^v	(see Notation)
VV	=	V^v	(see Notation)
VL	=	V^l	(see Notation)
BMIX	=	β_{mix}	
EMIX	=	emix	
CMIX	=	cmix	
AMIX	=	amix	
FBV	=	$\frac{\partial (\ln \phi^v)_{a,c,e}}{\partial \beta}$	
FBL	=	$\frac{\partial (\ln \phi^l)_{a,c,e}}{\partial \beta}$	
BNIV	=	$n(\partial \beta / \partial n_i)_j$	in vapor phase
BNIL	=	$n(\partial \beta / \partial n_i)_j$	in liquid phase
FCV	=	$\frac{\partial (\ln \phi^v)_{a,c,\beta}}{\partial c}$	
FCL	=	$\frac{\partial (\ln \phi^l)_{a,c,\beta}}{\partial c}$	
CNIV	=	$n(\partial c / \partial n_i)_j$	in vapor phase
CNIL	=	$n(\partial c / \partial n_i)_{jj}$	in liquid phase
FAV	=	$\frac{\partial (\ln \phi^v)_{c,e,\beta}}{\partial a}$	
FAL	=	$\frac{\partial (\ln \phi^l)_{c,e,\beta}}{\partial a}$	
ANIV	=	$n(\partial a / \partial n_i)_j$	in vapor phase
ANIL	=	$n(\partial a / \partial n_i)_{jj}$	in liquid phase
FEV	=	$\frac{\partial (\ln \phi^v)_{c,a,\beta}}{\partial e}$	

FEL	=	$\frac{\partial (\ln \phi)_{c,a,\beta}}{\partial e}$
ENIV	=	$n(\partial e / \partial n_i)_j$ in vapor phase
ENIL	=	$n(\partial e / \partial n_i)_j$ in liquid phase
NIY	=	$n(\partial \ln \phi^v / \partial n_i)_j$
NIX	=	$n(\partial \ln \phi^l / \partial n_i)_{jj}$
FV1	=	$\ln \phi^v$
FL1	=	$\ln \phi^l$
		Λ
PFV1	=	ϕ^v_i
		Λ
PFL1	=	ϕ^l_i
XX1	=	mole fraction in liquid phase of component 1
XX2	=	mole fraction in liquid phase of component 2
Y1	=	mole fraction in vapor phase of component 1
Y2	=	mole fraction in vapor phase of component 2
DU	=	Upper limit of interaction parameter
DL	=	Lower limit of interaction parameter

Function COMPRESS_FACTOR this function calculates compressibility factor in vapor phase (Z^v) and compressibility factor in liquid phase (Z^l) of the system .

Function ROOTofQEOS this function calculates the parameters of Quartic equation of state : c, e, a, β for binary fluids .

APPENDIX C

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PHYSICAL PROPERTIES OF PURE SUBSTANCE

SUBSTANCE	KIND	Tc	Pc	Dc	Dipole moment	Vc	ω
ACETALDEHYDE	polar	461	5.642	6.494	2.5	0.154	0.303
ACETIC ACID	polar	594.6	5.794	5.845	1.74	0.171	0.4624
ACETONE	polar	508	4.761	4.614	2.88	0.209	0.3064
ACETONITILE	polar	547.7	4.832	5.854	3.87	0.212	0.3498
ACETYLENE	nonpolar	309	6.281	8.885	0	0.113	0.1873
AMMONIA	polar	405.4	1.129	13.79	1.47	0.073	0.2515
ANILINE	polar	699	5.379	3.649	1.6	0.274	0.384
BENZENE	nonpolar	561.5	4.832	3.892	0	0.259	0.2108
BENZOIC ACID	polar	752	4.619	2.9333	1.7	0.341	0.62
BROMOBENZENE	polar	670	4.518	3.098	1.7	0.324	0.251
1,3 BUTADIENE	nonpolar	425	4.326	4.537	0	0.221	0.1932
n-BUTANE	nonpolar	426	3.647	3.9216	0	0.255	0.1913
1-BUTANOL	polar	563	4.417	3.649	1.66	0.274	0.593

SUBSTANCE	KIND	Tc	Pc	Dc	Dipole moment	Vc	ω
2-BUTANOL	polar	536.1	4.234	3.718	1.7	0.269	0.577
2-BUTANONE	polar	535.5	4.153	3.75	3.2	0.267	0.3241
1-BUTENE	polar	419.6	4.072	4.167	0.3	0.24	0.191
n-BUTYLACETATE	polar	579	3.181	2.5	1.8	0.4	0.417
n-BUTYL ALCOHOL	polar	560	4.903	3.649	1.66	0.274	0.3516
s-BUTYL ALCOHOL	polar	538	4.194	3.731	1.66	0.268	0.6882
CARBONDIOXIDE	nonpolar	304.1	7.395	10.45	0	0.094	0.2276
CARBONDISULFIDE	polar	552	8.003	6.25	0	0.16	0.109
CARBONMONOXIDE	nonpolar	132.9	3.487	10.741	0.11	0.093	0.0663
CARBONTETRACHLORIDE	polar	556.1	4.559	4.559	0	0.0276	0.1926
CARBONYL SULFIDE	polar	378.8	6.161	7.402	0.71	0.135	0.1041
CHLOROBENZENE	nonpolar	632	4.518	3.244	1.69	0.308	0.2505
1-CHLOROBUTANE	polar	542	3.728	3.206	2	0.312	0.218
2-CHLOROBUTANE	polar	520.6	4.001	3.279	2.1	0.305	0.3

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SUBSTANCE	KIND	Tc	Pc	Dc	Dipole moment	Vc	ω
CHLOROFORM	polar	536.4	5.454	4.184	1.01	0.239	0.2129
CHLOROTRIFLUOROMETHANE	polar	302	3.92	5.543	0.5	0.5	0.198
CYCLOHEXANE	nonpolar	554	4.093	3.214	0	0.311	0.2149
CYCLOHEXENE	polar	560.4	4.396	3.323	0.6	0.301	0.21
DICHLORODIFLUOROMETHANE	polar	384.5	4.007	4.587	0.51	0.51	0.1796
1,1 DICHLOROETHANE	polar	523	5.134	4.242	0.24	0.24	0.2477
1,2 DICHLOROETHANE	polar	561	5.369	4.444	2.06	0.225	0.299
DIETHYLAMINE	polar	496.5	3.667	3.37	0.92	0.301	0.299
DIETHYL ETHER	polar	466.7	3.626	3.571	1.15	0.28	0.2846
DIMETHYL ETHER	polar	400	5.369	5.261	1.3	0.178	0.2036
DIMETHYL SULFIDE	nonpolar	503	5.602	4.975	1.5	0.201	0.191
ETHANE	nonpolar	305.1	4.943	6.876	0	0.145	0.0989
ETHANOL	polar	516.3	6.383	5.989	1.69	0.167	0.6371
ETHYL ACETATE	polar	523.1	3.892	3.496	1.78	0.286	0.3611
ETHYLBENZENE	polar	617.2	3.647	2.674	0.4	0.374	0.302
ETHYL BUTYLATE	polar	566	3.039	2.379	1.74	0.395	0.461
ETHYL CHLORIDE	polar	460.2	5.268	5.115	2.06	0.196	0.1905

SUBSTANCE	KIND	Tc	Pc	Dc	Dipole moment	Vc	ω
ETHYLCYCLOHEXANE	nonpolar	609	3.039	2.222	0	0.45	0.243
ETHYL ETHER	polar	467.6	3.596	3.547	1.15	0.282	0.4
ETHYL FORMATE	polar	508.5	4.802	4.367	2	0.229	0.285
ETHYLENE	nonpolar	282.7	5.116	7.857	0	0.129	0.0852
ETHYLENE GLYCOL	polar	645	7.8	5.236	2.2	0.191	1.136
ETHYL METHYL ETHER	polar	437.7	4.396	4.5	1.23	0.221	0.4
n- HEPTANE	polar	539.8	2.715	2.335	0.34	0.432	0.3494
n-HEXANE	nonpolar	507.8	2.988	2.715	0	0.37	0.3047
1-HEXENE	polar	504	3.211	2.857	0.4	0.35	0.285
HYDROCHLORIC ACID	polar	324.7	8.418	12.36	1.1	0.081	0.133
HYDROGEN FLUORIDE	polar	461	6.564	14.45	1.9	0.069	0.329
HYDDROGEN SULFIDE	polar	373.2	9.056	10.14	0.9	0.099	0.081
ISOBUTANE	nonpolar	407	3.748	3.807	0.05	0.263	0.177
ISOBUTYL ACETATE	polar	561	3.14	2.422	1.87	0.414	0.455
ISOBUTYL ALCOHOL	polar	547.8	4.356	3.662	1.7	0.273	0.592
ISOPENTANE	nonpolar	460.8	3.323	0.25	0	0.306	0.227
ISOPROPYL ACETATE	polar	549.4	3.373	2.899	1.8	0.345	0.391
METHANOL	polar	513	7.972	8.498	1.7	0.119	0.5656

SUBSTANCE	KIND	Tc	Pc	Dc	Dipole moment	Vc	ω
METHYL ACETATE	polar	506.7	4.69	4.392	1.679	0.228	0.3253
METHYL CHLORIDE	polar	416.3	6.646	7.194	1.87	0.139	0.1529
METHYLCYCLOHEXANE	nonpolar	572.1	3.466	2.908	0	0.344	0.235
METHYL ETHYL ETHER	polar	437.7	4.396	4.5	1.23	0.221	0.2189
METHYL ETHYL KETONE	polar	536.8	4.265	3.745	3.3	0.267	0.32
METHYL FLUORIDE	polar	317.7	6.262	8.85	1.85	0.113	0.2037
METHYL FORMATE	polar	487.2	6.078	5.814	1.8	0.172	0.257
METHYL ISOBUTYLATE	polar	540.55	3.414	2.951	1.98	0.339	0.362
NAPHTHALENE	nonpolar	748.4	4.103	2.421	0	0.413	0.302
NITROMETHANE	polar	588	6.392	5.774	3.1	0.173	0.31
NONENE	polar	592	2.37	1.724	0.59	0.58	0.3962
n-OCTANE	nonpolar	569	2.492	2.049	0	0.492	0.587
1-OCTANOL	polar	652.5	2.897	2.041	2	0.49	0.386
1-OCTENE	polar	566.7	2.654	2.155	0.3	0.464	0.2486
n-PENTANE	nonpolar	470.2	3.343	3.222	0	0.304	0.579
1-PENTANOL	polar	588.2	3.961	3.068	1.7	0.326	0.233
1-PENTENE	polar	464.8	3.576	3.3333	0.4	0.3	0.438
PHENOL	nonpolar	694.2	6.209	4.367	1.6	0.15	0.1517

SUBSTANCE	KIND	Tc	Pc	Dc	Dipole moment	Vc	ω
PROPANE	nonpolar	369.8	4.255	4.989	0.084	0.2	0.6279
1- PROPANOL	polar	536.7	5.166	4.583	1.68	0.219	0.6279
2- PROPANOL	polar	508.3	4.761	4.55	1.66	0.219	0.5331
PROPIONIC ACID	polar	612.5	5.369	4.257	1.76	0.235	0.313
PROPIONITRILE	polar	564.2	4.234	4.367	3.7	0.229	0.3935
n- PROPYL ACETATE	polar	549.2	3.352	2.899	1.79	0.345	0.6279
PROPYL ALCOHOL	polar	536.7	5.06	4.542	1.67	0.219	0.3416
n- PROPYLBENZENE	polar	638.8	3.206	2.275	0.35	0.44	0.144
PROPYLENE	polar	364.9	4.659	5.525	0.4	0.181	1.106
PROPYLENE GLYCOL	polar	625	6.149	4.219	3.6	0.237	0.297
PYRIDINE	polar	617	6.08	3.355	2.2	0.298	0.612
TERTIALY BUTANOL	polar	506.2	4.022	3.636	1.7	0.275	0.2641
TOLUENE	polar	593.6	4.214	3.169	0.45	0.316	0.32
TRIETHYL AMINE	polar	299.2	3.039	2.485	0.39	0.402	0.205
TRIMETHYL AMINE	nonpolar	433.3	4.143	3.937	0.6	0.254	0.303
2,2,4 TRIMETHYLPENTANE	nonpolar	544	2.603	2.137	2.137	0.468	0.303
VINYL ACETATE	polar	525	4.407	3.774	1.7	0.265	0.34
VINYL CHLORIDE	polar	425	5.217	5.917	1.5	0.169	0.122

SUBSTANCE	KIND	Tc	Pc	Dc	Dipole moment	Vc	ω
WATER	polar	647.15	2.212	17.94	1.85	0.055	0.3449
m- XYLENE	polar	617	3.546	2.666	0.33	0.376	0.326
p- XYLENE	polar	616.2	3.556	2.639	0.1	0.379	0.32

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VITA

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