

! A GENERAL HYDROGENOLYSIS PROGRAM.

!

%EXTERNALROUTINE HYD(%STRING(63)S)

%EXTERNALROUTINESPEC PROMPT(%STRING(63)S)

%EXTERNALROUTINESPEC DEFINE(%STRING(63)S)

!

! DEFINE ARRAYS FOR REFERENCE AND DATA.

!

%RECORDFORMAT HCS(%STRING(10)HC,%REAL SENSFACT,RELNO,%INTEGER CNO)

%RECORD (HCS) %ARRAY DATA(1:16)

%RECORD (HCS) %ARRAY EXPTL(1:16)

%REALARRAY TIME(1:10), PEAKS(1:10,1:16), SUM(1:10); !TIMES, PEAK HEIGHTS, AND A SUMMING ARRAY.

!

! SET UP THE DATA RECORD

!

! THIS MAY BE EXPANDED AT THE USERS WISH.

!

DATA(1)+HC=" METHANE "

DATA(2)+HC=" ETHANE "

DATA(3)+HC=" PROPANE "

DATA(4)+HC=" ISO BUT "

DATA(5)+HC=" BUTANE "

DATA(6)+HC=" NEOPENT "

DATA(7)+HC=" ISOPENT "

DATA(8)+HC=" NPENT "

DATA(9)+HC=" CYCPENT "

DATA(10)+HC=" NEOHEX "

DATA(11)+HC=" 2MP "

DATA(12)+HC=" 3MP "

DATA(13)+HC=" N-HEX "

DATA(14)+HC=" MCP "

DATA(15)+HC=" CYCHEX "

DATA(16)+HC=" BENZENE "

DATA(1)+CNO=1

DATA(2)+CNO=2

DATA(3)+CNO=3

DATA(4)+CNO=4

DATA(5)+CNO=4

DATA(6)+CNO=5

DATA(7)+CNO=5

DATA(8)+CNO=5

DATA(9)+CNO=5

DATA(10)+CNO=6

DATA(11)+CNO=6

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DATA(14)+CNO=6
DATA(15)+CNO=6
DATA(16)+CNO=6
DATA(1)+SENSFACT=.186
DATA(2)+SENSFACT=.349
DATA(3)+SENSFACT=.512
DATA(4)+SENSFACT=.674
DATA(5)+SENSFACT=.674
DATA(6)+SENSFACT=.837
DATA(7)+SENSFACT=.837
DATA(8)+SENSFACT=.837
DATA(9)+SENSFACT=.814
DATA(10)+SENSFACT=1
DATA(11)+SENSFACT=1
DATA(12)+SENSFACT=1
DATA(13)+SENSFACT=1
DATA(14)+SENSFACT=.977
DATA(15)+SENSFACT=.977
DATA(16)+SENSFACT=.907
%REAL FACTOR
%INTEGER I,J,N,SPECIES,PEAKNO,REACTANT
%CONSTSTRING(1)%ARRAY CN(1:6)="1","2","3","4","5","6"
%BYTEINTEGER YN
%STRING(63) T,SCN
!
! SET UP THE INPUT AND OUTPUT STREAMS
!
%IF S="" %THEN S=".IN,.OUT"
%IF S->T.(",").S %THENSTART
%IF S="" %THEN S=".OUT"
%IF T="" %THEN T=".IN"
%FINISHELSESTART
T=S
S=".OUT"
%FINISH
DEFINE("1",".T")
DEFINE("2",".S")
SELECTINPUT(1)
!
! SET UP THE EXPERIMENTAL RECORD USING THE PREDEFINED ONE
!
PRINTSTRING("HOW MANY SPECIES (REACT.+PRODS)")
NEWLINE
PROMPT("NO. SPECIES:")
READ(SPECIES)
%FOR J=1,1,16 %CYCLE

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NEWLINE
%REPEAT
PRINTSTRING("PLEASE INDICATE THESE SPECIES (INCLUDING REACTANT)")
NEWLINE
NEWLINE
PROMPT("CODE NO.:")
%FOR J=1,1,SPECIES %CYCLE
  READ(I)
  EXPTL(J)+HC=DATA(I)+HC
  EXPTL(J)+CNO=DATA(I)+CNO
  EXPTL(J)+SENSFACT=DATA(I)+SENSFACT
%REPEAT
PRINTSTRING("PLEASE NOW INDICATE WHICH IS THE REACTANT.")
NEWLINE
NEWLINE
READ(REACTANT)
SCN=CN(DATA(REACTANT)+CNO)
!
! FOR USE IN THE OUTPUT FORMAT
!
%FOR I=1,1,SPECIES %CYCLE
  EXPTL(I)+RELCNO=EXPTL(I)+CNO/DATA(REACTANT)+CNO
%REPEAT
!
! ALLOW OPTION OF RESETTING SENSITIVITY FACTORS TO EXPTL. ONES
!
PROMPT("Y/N:")
PRINTSTRING("DO YOU WISH TO SET YOU OWN SENSITIVITY FACTORS?")
NEWLINE
READSYMBOL(YN) %UNTIL YN#10 %AND YN#32
%IF YN='Y' %THENSTART
  PROMPT("SENS. FACT.:")
  %FOR I=1,1,SPECIES %CYCLE
    READ(EXPTL(I)+SENSFACT)
  %REPEAT
%FINISH
!
! TO PRINT IT OUT ALL PRETTY.
!
%ROUTINE PRINTOUT(ZSTRING(4)R)
  %INTEGER K,L
  NEWLINES(5)
  PRINTSTRING("      TIME      ")
  %FOR L=1,1,N %CYCLE
    PRINT(TIME(L),4,1)
    SPACES(4)
  %REPEAT
  NEWLINE
  PRINTSTRING("      SPECIES      ")

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%FOR K=1,1,SPECIES %CYCLE
  PRINTSTRING(R)
  PRINTSTRING(EXPTL(K)+HC)
  %FOR L=1,1,N %CYCLE
    SPACE
    PRINT(PEAKS(L,K),3,3)
    SPACES(2)
  %REPEAT
  NEWLINE
%REPEAT
%END
!
! THIS IS THE START OF THE PROPER PROGRAM
!
PROMPT("NO. DATA PTS :")
READ(N)
%FOR I=1,1,N %CYCLE
  !
  ! READ IN TIMES AND PEAK AREAS
  !
  PROMPT("TIME :")
  READ(TIME(I))
  PROMPT("PEAK AREAS :")
  %FOR J=1,1,SPECIES %CYCLE
    READ(PEAKS(I,J))
  %REPEAT
%REPEAT
!
! COMMON PEAK CORRECTION( FOR A TWO COLUMN SYSTEM)
!
PRINTSTRING("ARE THERE ANY SPECIES TO BE CORRECTED BY COMMON PEAK?")
NEWLINE
PROMPT("Y/N:")
READ SYMBOL(YN) %UNTIL YN#10 %AND YN#32
%IF YN="Y"%THENSTART
  PROMPT("HOW MANY :")
  READ(PEAKNO)
  PROMPT("FACTOR :")
  READ(FACTOR)
  %FOR J=1,1,PEAKNO %CYCLE
    %FOR I=1,1,N %CYCLE
      PEAKS(I,J)=PEAKS(I,J)*FACTOR
    %REPEAT
  %REPEAT
%FINISH
SELECTOUTPUT(2)

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! SET SUMMING ARRAY TO ZERO
!
SUM(I)=0
%FOR J=1,1,SPECIES %CYCLE
!
! CORRECT PEAKS FOR RESPONSE SENSITIVITY AND C5 CONTENT
!
PEAKS(I,J)=PEAKS(I,J)*EXPTL(J)+RELDCND/EXPTL(J)+SENSFACT
!
! SUM TOTAL C5 CONTENT FOR EACH TIME
!
SUM(I)=SUM(I)+PEAKS(I,J)
%REPEAT
%REPEAT
%FOR I=1,1,N %CYCLE
%FOR J=1,1,SPECIES %CYCLE
PEAKS(I,J)=PEAKS(I,J)*100/SUM(I)
%REPEAT
%REPEAT
PRINTOUT(" %C".SCN)
%FOR I=1,1,N %CYCLE
%FOR J=1,1,SPECIES %CYCLE
PEAKS(I,J)=PEAKS(I,J)/EXPTL(J)+RELDCND
%REPEAT
%REPEAT
PRINTOUT(" MPA")
%END
%ENDOFFILE

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Command:

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DATA INPUT:

1 NO OF SETS OF DATA
 2 NO OF CARBON ATOMS
 NO OF HYDROGEN ATOMS
 NO OF OXYGEN ATOMS
 NO OF NITROGEN ATOMS
 NO OF SULPHUR ATOMS
 NO OF FRAGMENTS
 3 LIGHT FRAGMENTATION PATTERN
 4 HEAVY FRAGMENTATION PATTERN
 5 GAMMA VALUE
 PI VALUE
 6 TIME OF SAMPLE
 7 EXPERIMENTAL PEAK HEIGHTS
 (N=NO OF CARBON+NO OF HYDROGEN+1)

INTEGER S,C,D

DATA BLANK/' '/

CALL FPRMT('NO. DATA SETS :',15)

READ *,ISETS

DIMENSION P(40),FH(10),FD(10),PER(20),D(20),KK(7),NH(20),NH(8),
 WND(8),STOKE(200,13),PPhi(200),TIM(200),PH(200),
 WPLOG(200),PERK(200),PCOUNT(200),PCCOUNT(200),PBLOG(200)

DO 7777 INOS=1,ISETS

DO 7777 J=1,13

7777 STORE(INOS,J)=0.0

ONEC=0.0111

ONED=0.00015

ONES3=0.0076

ONE07=0.00037

ONEN5=0.0037

TWDC=0.00006

TWOS3=0.0000289

TWON5=0.0000068

ONE08=0.000204

ONES4=0.0422

TWOS4=0.00049

TW008=0.0000021

ONES6=0.00014

CA0=0.00000175

CAS3=0.000836

CA07=0.0000041

CAN5=0.00004107

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S3ANS=0.000028
CAS4=0.0004684
DAS4=0.00000633
S3AS4=0.0016036
D7AS4=0.00001561
NSAS4=0.00015614
CA08=0.00000988
S3A08=0.00000676
NSA08=0.000003293
S4A08=0.00008609
CAS6=0.00000155
S3AS6=0.00000053
CA2S4=0.00000988
S3A2S4=0.00000112
NSA2S4=0.00000329
THRES4=0.00000104
S4AS6=0.00000295
CALL FPRMPT('NO. CARBONS :',13)
READ *,C
CALL FPRMPT('NO. HYDROGENS :',15)
READ *,N
CALL FPRMPT('NO. OXYGENS :',13)
READ *,O
CALL FPRMPT('NO. NITROGENS :',15)
READ *,NON
CALL FPRMPT('NO. SULPHURS :',14)
READ *,NOS
CALL FPRMPT('NO. FRAGMENTS :',15)
READ *,M
PMAX=100*N
CALL FPRMPT('O2/REACTANT :',13)
READ *,RAT
PINF=((RAT*2)/((RAT*2)+N))*PMAX
DINF=((1.0-(PINF/(100.0*FLOAT(N))))**N)*100.0
K=N+M+1
IPEAK=N+M+2
S=M+1
NN(1)=N
DO 47 I=2,N
47 NN(I)=NN(I-1)*(N-I+1)
CALL FPRMPT('LIGHT F. P. :',13)
READ *,(FH(IFRAG),IFRAG=1,S)
CALL FPRMPT('HEAVY F. P. :',13)
READ *,(FD(IFRAG),IFRAG=1,S)
CALL FPRMPT('GAMMA AND PI :',14)
READ *,(GAMMA,PI)

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WRITE(6,1003) (BLANK,LULU=1,N)
1003 FORMAT('0',2X,6HPARENT,2X,A1,'-1H',4X,A1,'-2H',4X,A1,'-3H',4X,A1,'
0-4H',4X,A1,'-5H',4X,A1,'-6H',4X,A1,'-7H',4X)
WRITE(6,102) (FH(IFRAG),IFRAG=1,S)
102 FORMAT('0',8F8.4)
WRITE(6,38)
38 FURMAT('0',3X,'HEAVY HYDROCARBON FRAGMENTATION PATTERN')
WRITE(6,1003) (BLANK,LULU=1,N)
WRITE(6,102) (FD(IFRAG),IFRAG=1,S)
DO 56 INOS=1,ISETS
CALL FPRMPT('TIME :',6)
READ *,TIME
TIM(INOS)=TIME
CALL FPRMPT('PEAK HEIGHTS :',14)
READ *,(P(J),J=1,K)
PCOUNT(INOS)=0
DO 77 J=1,M
77 PCOUNT(INOS)=PCOUNT(INOS)+P(J)
WRITE (6,33)
33 FORMAT ('0',10X,25HEXPERIMENTAL PEAK HEIGHTS)
DO 123 KZ=1,7
123 KK(KZ)=8-KZ
NHIGH=8-M
WRITE(6,1002) (BLANK,KK(KZ),KZ=NHIGH,7)
1002 FORMAT('0',2X,A1,'D-',11,4X,A1,'D-',11,4X,A1,'D-',11,4X,A1,'D-',
W11,4X,A1,'D-',11,4X,A1,'D-',11,4X,A1,'D-',11,4X)
WRITE(6,25) (P(J),J=1,M)
25 FORMAT('0',13F8.2)
WRITE(6,1001) (BLANK,LULU=1,N)
1001 FORMAT('0',4X,'D0',5X,A1,'D1',5X,A1,'D2',5X,A1,'D3',5X,A1,'D4',5X,
WA1,'D5',5X,A1,'D6',5X,A1,'D7',5X,A1,'D8',5X,A1,'D9',5X,A1,'D10',5X
U,A1,'D11',5X,A1,'D12')
WRITE (6,25)(P(J),J=5,K)
DO 3 J=1,K
IF (P(J).LT.0.0) GO TO 31
L=1ABS(J-5)
IF(L.EQ.N) GO TO 3
SIC = ONEC*C+ ONED*(N-L)+ ONES3*NOS + ONE07*0+ ONENS*NON
P(J+1)=P(J+1)-SIC*P(J)
IF (L.GT.N-2) GO TO 3
DIC=TWOC*C*(C-1) +TWUS3*NOS*(NOS-1)+TWNOS*NON*(NON-1)+ ONES4*NOS+
WONE0B*0+CAU*C*(N-L)+ CAS3*C*NOS+ CA07*0*C+ CAN5*C*NON+
WDAS3*(N-L)*NOS+ S3A07*NOS*0+ S3AN5*NOS*NON
P(J+2)=P(J+2)-DIC*P(J)
IF (L.GT.N-3) GO TO 3
TIC=CAS4*C*NOS+ DAS4*(N-L)*NOS+ S3AS4*NOS*(NOS-1)

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P(J+3) = P(J+3) - TIC*P(J)
IF (L.GT.N-4) GO TO 3
FRIC= TWDS4*NDS*(NDS-1)+ TWOOB*O*(O-1)+S4AOB*NUS*U+UNES6*NOS
P(J+4) = P(J+4) - FRIC*P(J)
IF (L.GT.N-5) GO TO 3
FFIC= CAS6*C*NDS+ S3AS6*NDS*(NDS-1)+ CAZS4*C*NDS*(NDS-1)
U+S3A2S4*NDS*(NDS-1)*(NDS-2)+ N5A2S4*NGN*NDS*(NDS-1)
P(J+5) = P(J+5) - FFIC*P(J)
IF (L.GT.N-6) GO TO 3
SXIC= THRES4*NDS*(NDS-1)*(NDS-2)+ S4AS6*NDS*(NDS-1)
P(J+6) = P(J+6) - SXIC*P(J)
GO TO 3
31 P(J) = 0.0
3 CONTINUE
WRITE(6,35)
35 FORMAT('0',10X,34HPEAK HEIGHTS CORRECTED FOR ISOTOPE,2X)
DO 124 KZ=1,7
124 KK(KZ)=8-KZ
NHIGH=8-M
WRITE (6,1002) (BLANK, KK(KZ), KZ=NHIGH, 7)
WRITE(6,25) (P(J), J=1, M)
WRITE(6,1001) (BLANK, LULU=1, N)
WRITE (6,25) (P(J), J=S, K)
WRITE (6,2121) GAMMA, PI
2121 FORMAT('0', 6X, 6HGAMMA=, F7.4, 8X, 3HPI=, F7.4, 2X)
IFRAG=1
799 FH(IFRAG)=FH(IFRAG+1)
FD(IFRAG)=FD(IFRAG+1)
IF(IFRAG.EQ.M) GO TO 79
IFRAG=IFRAG+1
GO TO 799
79 CONTINUE
DO 4 I=1, IPEAK
J=IPEAK-I
IF(J.EQ.M) GO TO 45
L=J-S
IF (P(J).LT.0.0) GO TO 4
NH(1)=1
ND(1)=1
NH(2)=N-L
ND(2)=L
IF(S.LY.3) GO TO 901
DO 46 IVY=3, S
NH(IVY)=NH(IVY-1)*(NH(2)-IVY+2)
46 ND(IVY)=ND(IVY-1)*(L-IVY+2)
901 CONTINUE

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DO 4 NPL=1,N
NB=NPL+1
DO 4 NA=1,NB
NHL=NA-1
NDL=NPL-NHL
NWAYS=NPL
IF(NHL.EQ.0) NWAYS=1
IF(NHL.LT.2) GO TO 902
DO 48 IRIS=2,NHL
48 NWAYS=NWAYS*(NPL-IRIS+1)/IRIS
902 CONTINUE
CORR=NWAYS*(NHL*FH(NPL)+NDL*FD(NPL))*ND(NDL+1)*NH(NHL+1)/
W(NN(NPL)*NPL)*ZD**NDL*ZH**NHL
KEY=J-NHL-2*NDL
IF(KEY.LE.0) GO TO 4
207 P(KEY)=P(KEY)-CORR*P(J)
4 CONTINUE
45 WRITE (6,300)
300 FORMAT ('0',10X,22HCORRECTED PEAK HEIGHTS)
PCCOUNT(INOS)=0
DO 776 J=1,M
776 PCCOUNT(INOS)=PCCOUNT(INOS)+P(J)
PERR(INOS)=PCCOUNT(INOS)/PCOUNT(INOS)
DO 125 KZ=1,7
125 KK(KZ)=8-KZ
NHIGH=8-M
WRITE(6,1002) (BLANK, KK(KZ), KZ=NHIGH,7)
WRITE(6,25) (P(J), J=1, M)
WRITE(6,1001) (BLANK, LULU=1, N)
WRITE (6,25) (P(J), J=S, K)
DO 82 NHIGH=1, M
IFRAG=S-NHIGH
FD(IFRAG+1)=FD(IFRAG)
82 FH(IFRAG+1)=FH(IFRAG)
FD(1)=1.0000
FH(1)=1.0000
TOTAL=0.0
DO 60 J=S, K
IF (P(J).LT.0.0) GO TO 60
TOTAL=TOTAL+P(J)
60 CONTINUE
WRITE (6,400)
400 FORMAT ('0',10X, 30HPERCENTAGE OF ISOTOPIC SPECIES)
WRITE(6,1001) (BLANK, LULU=1, N)
DO 810 J=S, K
LLL=J-S+1

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810 STORE(INOS,LLL) = PER(J)
WRITE(6,25) (PER(J),J=S,K)
PHI=0.0
DO 80 J=S,K
L=J-S
IF(PER(J).LT.0.0) GO TO 80
PHI=PHI+L*PER(J)
80 CONTINUE
PPhi(INOS) = PHI
PH(INOS)=PINF-PHI
WRITE(6,410) TIME,TOTAL,PHI
410 FORMAT('0',9X,4H1IME,9X,5HTOTAL,9X,3HPHI/F14.1,F15.2,F13.2)
WRITE(6,34) PHI
34 FORMAT('0',10X,31HBINOMIAL DISTRIBUTION WITH PHI=,F9.2,2X)
YY=PHI/(100*N)
XX=1.0000-YY
D(1)=100*XX*N
JEAN=N+1
DO 59 JIM=2,JEAN
59 D(JIM)=D(JIM-1)*(JEAN-JIM+1)*YY/(XX*(JIM-1))
WRITE(6,1001) (BLANK,LULU=1,N)
WRITE(6,25) (D(JIM),JIM=1,JEAN)
56 CONTINUE
DO 111 INOS=1,15ETS
PDLOG(INOS)=ALOG10(STORE(INOS,1)-DINF)
PLOG(INOS)=ALOG10(PH(INOS))
111 CONTINUE
WRITE(6,9999) C,N,O,NON,NUS,PMAX,PINF
9999 FORMAT('1',4X,'COMPOUND IS C ',I2,' H ',I2,' O ',I2,' N ',I2,
W' S ',I2,10X,'PHI MAX =',F7.2,2X,'PHI INFINITY =',
WF7.2)
9998 FORMAT(' ',4X,113(1H*))
9997 FORMAT(' ',4X,'*', ' TIME ', ' ', ' ',3X,'D0',2X,'*',3X,'D1',2X,'*',
W3X,'D2',2X,'*',3X,'D3',2X,'*',3X,'D4',2X,'*',3X,'D5',2X,'*',3X
W,'D6',2X,'*',3X,'D7',2X,'*',3X,'D8',2X,'*',3X,'D9',2X,'*',2X,
W'D10',2X,'*',2X,'D11',2X,'*',2X,'D12',2X,'*')
9996 FORMAT(' ',4X,'*',F5.1,2X,'*',13(1X,F5.2,1X,'*'))
WRITE(6,9998)
WRITE(6,9997)
WRITE(6,9998)
DO 8888 INOS=i,15ETS
8888 WRITE(6,9996) TIM(INOS),(STORE(INOS,J),J=1,13)
WRITE(6,9991)
9991 FORMAT(' ',4X,113(1H*))
666 FORMAT(' ',24X,76(1H*))
667 FORMAT(' ',24X,'*', ' TIME ', ' ', ' ',LG D0-DI ' , ' ', ' ',LG.PINF- P',
W' ',6X,'PHI',4X,'*',1X,'PHI INF - PHI', ' ', ' ', ' PEAK FACTOR *')

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WRITE(6,666)
DO 777 INDS=1,ISETS
777 WRITE(6,9992) TIM(INDS),PDLOG(INDS),PLOG(INDS),PPhi(INDS),
WPH(INDS),PERR(INDS)
9992 FORMAT(' ',24X,'*',1X,F5.1,2X,'*',2X,F6.4,1X,'*',2X,
WPH6.4,2X,'*',F10.2,3X,'*',F10.2,5X,'*',4X,F6.3,4X,'*')
WRITE(6,665)
665 FORMAT(' ',24X,76(1H*))
3000 STOP
END
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Command:

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ZEXTERNALROUTINE PROFILE(ZSTRING(63)S)
ZINTEGER I,N
ZLONGREAL SITES,RATENP,RATEIB,RATEPR,SRATENP,SRATEIB,SRATEPR,RATIO1, ZC
RATIO2,M1B,M1PR,M2PR,M1ET,M2ET,M1HE,M2HE,M1P,M1NB,M2NB,M3ET,M3HE,F
ZLONGREALARRAY NONP(0:140),NOIB(0:140),NOPR(0:140),NOET(0:140),ZC
NOME(0:140),SUM(0:140),NONB(0:140),NOIP(0:140)
PRINTSTRING("
NORMAL RATES OF NEOPENTANE , ISOBUTANE AND PROPANE HYDROGENOLYSIS PLEASE.")
NEWLINE
READ(SRATENP)
READ(SRATEIB)
READ(SRATEPR)
PRINTSTRING("H FROM NEUPENTANE , ISOBUTANE AND PROPANE PLEASE")
NEWLINE
READ(M1P)
READ(M1NB)
READ(M1B)
READ(M1PR)
READ(M1ET)
READ(M1HE)
READ(M2NB)
READ(M2PR)
READ(M2ET)
READ(M2HE)
READ(M3ET)
READ(M3HE)
PRINTSTRING("NO. OF SITES / 10**17")
NEWLINE
READ(SITES)
PRINTSTRING("TIME LIMIT DIVISABLE BY 10")
NEWLINE
READ(N)
ZCYCLE
  READ(RATIO1);READ(RATIO2)
  ZIF RATIO1<0 ZTHENEXIT
  NOIP(0)=0
  NONB(0)=0
  NOIB(0)=0
  NOPR(0)=0
  NOET(0)=0
  NOME(0)=0
  NONP(0)=193
  RATENP=SRATENP
  RATEIB=0
  RATEPR=0
  ZFOR I=1,1,N ZCYCLE
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NOIP(I)=NOIP(I-1)+RATENP*MIP*60*SITES
NONB(I)=NONB(I-1)+(RATENP*M1NB+RATEIB*M2NB)*60*SITES
NOPR(I)=NOPR(I-1)+(RATENP*M1PR+RATEIB*M2PR-RATEPR)*60*SITES
NOET(I)=NOET(I-1)+(RATENP*M1ET+RATEIB*M2ET+RSET*RATEPR)*60*SITES
NOME(I)=NOME(I-1)+(RATENP*M1ME+RATEIB*M2ME+RATEPR*M3ME)*60*SITES
KATENP=SKATENP*(NONP(I)/(NONP(I)+NOIB(I)*RATIO1+NOPR(I)*RATIO2))
RATEIB=SRATEIB*(NOIB(I)/(NOIB(I)+((NONP(I)+NOPR(I)*RATIO2)/RATIO1)))
RATEPR=SKATEPR*(NOPR(I)/(NOPR(I)+((NONP(I)+NOIB(I)*RATIO1)/RATIO2)))
ZREPEAT
ZFOR I=0,1,N ZCYCLE
SUM(I)=NONP(I)+NOIP(I)+(NONB(I)*4+NOIB(I)*4+NOPR(I)*3+NOET(I)*2+NOME(I))/5
NONP(I)=NONP(I)*100/SUM(I)
NOIP(I)=NOIP(I)*100/SUM(I)
NONB(I)=NONB(I)*100*.8/SUM(I)
NOIB(I)=NOIB(I)*100*.8/SUM(I)
NOPR(I)=NOPR(I)*100*.6/SUM(I)
NOET(I)=NOET(I)*100*.4/SUM(I)
NOME(I)=NOME(I)*100*.2/SUM(I)
ZREPEAT
ZFOR I=0,10,N ZCYCLE
SPACES(5)
PRINT(NONP(I),4,4);SPACES(5)
PRINT(NOIP(I),4,4);SPACES(5)
PRINT(NONB(I),4,4);SPACES(5)
PRINT(NOIB(I),4,4);SPACES(5)
PRINT(NOPR(I),4,4);SPACES(5)
PRINT(NOET(I),4,4);SPACES(5)
PRINT(NOME(I),4,4)
NEWLINES(2)
ZREPEAT
ZREPEAT
ZEND
ZENDOFFILE

```

Command:

```

%EXTERNALROUTINE PROFILE2(%STRING(63)S)
%INTEGER I,N
%LONGREAL SITES,RATENP,RATEIB,RATEPR,SRATENP,SRATEIB,SRATEPR,RATIO1, %C
RATIO2,H1B,H1PR,H2PR,H1ET,H2ET,H1HE,H2HE,H1P,H1NB,H2NB,H3ET,H3HE,F
%LONGREALARRAY NONP(0:140),NOIB(0:140),NOPR(0:140),NOET(0:140),%C
NOHE(0:140),SUM(0:140),NONB(0:140),NOIP(0:140)
PRINTSTRING("
NORMAL RATES OF NEOPENTANE , ISOBUTANE AND PROPANE HYDROGENOLYSIS PLEASE.")
NEWLINE
READ(SRATENP)
READ(SRATEIB)
READ(SRATEPR)
PRINTSTRING("LIMITING RATE OF METHANE FORMATION")
NEWLINE
READ(F)
PRINTSTRING("M FROM NEOPENTANE , ISOBUTANE AND PROPANE PLEASE")
NEWLINE
READ(H1P)
READ(H1NB)
READ(H1B)
READ(H1PR)
READ(H1ET)
READ(H1HE)
READ(H2NB)
READ(H2PR)
READ(H2ET)
READ(H2HE)
READ(H3ET)
READ(H3HE)
PRINTSTRING("NO. OF SITES / 10**17")
NEWLINE
READ(SITES)
F=F*60*SITES
PRINTSTRING("TIME LIMIT DIVISABLE BY 10")
NEWLINE
READ(N)
%CYCLE
  READ(RATIO1);READ(RATIO2)
  %IF RATIO1<0 %THENEXIT
  NOIP(0)=0
  NONB(0)=0
  NOIB(0)=0
  NOPR(0)=0
  NOET(0)=0
  NOHE(0)=0
  NONP(0)=193

```

4

```

RATEPR=0
%FOR I=1,1,N ZCYCLE
  NOME(I)=NOME(I-1)+(RATENP*M1ME+RATEIB*M2ME+RATEPR*M3ME)*60*SITES
  RATENP=RATENP*F/(NOME(I)-NOME(I-1))
  RATEIB=RATEIB*F/(NOME(I)-NOME(I-1))
  RATEPR=RATEPR*F/(NOME(I)-NOME(I-1))
  NONP(I)=NONP(I-1) - RATENP*60*SITES
  NOIB(I)=NOIB(I-1)+RATENP*60*M1B*SITES-RATEIB*60*SITES
  NOIP(I)=NOIP(I-1)+RATENP*M1P*60*SITES
  NONB(I)=NONB(I-1)+(RATENP*M1NB+RATEIB*M2NB)*60*SITES
  NOPR(I)=NOPR(I-1)+(RATENP*M1PR+RATEIB*M2PR-RATEPR)*60*SITES
  NOET(I)=NOET(I-1)+(RATENP*M1ET+RATEIB*M2ET+M3ET*RATEPR)*60*SITES
  NOME(I)=NOME(I-1)+(RATENP*M1ME+RATEIB*M2ME+RATEPR*M3ME)*60*SITES
  RATENP=SRATENP*(NONP(I)/(NONP(I)+NOIB(I)*RATIO1+NOPR(I)*RATIO2))
  RATEIB=SRATEIB*(NOIB(I)/(NOIB(I)+((NONP(I)+NOPR(I)*RATIO2)/RATIO1)))
  RATEPR=SRATEPR*(NOPR(I)/(NOPR(I)+((NONP(I)+NOIB(I)*RATIO1)/RATIO2)))
%REPEAT
%FOR I=0,1,N ZCYCLE
  SUM(I)=NONP(I)+NOIP(I)+(NONB(I)*4+NOIB(I)*4+NOPR(I)*3+NOET(I)*2+NOME(I))/5
  NONP(I)=NONP(I)*100/SUM(I)
  NOIP(I)=NOIP(I)*100/SUM(I)
  NONB(I)=NONB(I)*100*.8/SUM(I)
  NOIB(I)=NOIB(I)*100*.8/SUM(I)
  NOPR(I)=NOPR(I)*100*.6/SUM(I)
  NOET(I)=NOET(I)*100*.4/SUM(I)
  NOME(I)=NOME(I)*100*.2/SUM(I)
%REPEAT
%FOR I=0,10,N ZCYCLE
  SPACES(5)
  PRINT(NONP(I),4,4);SPACES(5)
  PRINT(NOIP(I),4,4);SPACES(5)
  PRINT(NONB(I),4,4);SPACES(5)
  PRINT(NOIB(I),4,4);SPACES(5)
  PRINT(NOPR(I),4,4);SPACES(5)
  PRINT(NOET(I),4,4);SPACES(5)
  PRINT(NOME(I),4,4)
  NEWLINES(2)
%REPEAT
%REPEAT
%END
%ENDOFFILE

```

Command:

5

```
ZEXTERNALROUTINE ENSEMBLE3(%STRING(63)S)
ZEXTERNALROUTINESPEC PROMPT(%STRING(63)S,ZINTEGER I)
ZINTEGER I,N
%REAL ACT1,ACT2,ACT
%REALARRAY ACTS(1:9)
PROMPT("METAL 1 ACT:",12)
READ(ACT1)
PROMPT("METAL 2 ACT:",12)
READ(ACT2)
PROMPT("ENSEMBLE SIZE:",14)
%CYCLE
READ(N)
%IF N<1%THENEXIT
%FOR I=9,-1,1 %CYCLE
    ACTS(I)=(ACT1*(I/10)**N)+(ACT2*((10-I)/10)**N)
%REPEAT
NEWLINES(3)
PRINTSTRING("
Activities for ensemble size ")
WRITE(N,1)
NEWLINES(2)
%FOR I=9,-1,1 %CYCLE
    ACT=ACTS(I)
    PRINTFL(ACT,3)
    SPACES(3)
%REPEAT
NEWLINE
%REPEAT
%END
%ENDOFFILE
```

Command:

Q

```
%EXTERNALROUTINE ENSEMBLE (ZSTRING(63)S)
%EXTERNALROUTINESPEC PROMPT(ZSTRING(16)S,ZINTEGER I)
%ROUTINESPEC DISTRIBUTION(ZINTEGER N,ZREALARRAYNAME NO,ZREAL APM1,APM2)
%REALFNSPEC ACTIVITY(ZINTEGER I,ZREALARRAYNAME NO,ZREAL M1ACT,M2ACT)
%REALARRAY NO(0:20)
%INTEGER I,N
%REAL APM1,APM2,M1ACT,M2ACT,ACT
PROMPT("METAL ACT. :",12)
NEWLINES(2)
PRINTSTRING("The data required is as follows:")
NEWLINE
PRINTSTRING("The activities of the two pure metals, (prompt 'METAL ACT. :')")
NEWLINE
PRINTSTRING("This will be followed by a request for an ensemble size, which")
NEWLINE
PRINTSTRING("should be in the range 1-20 inclusive. An ensemble size less than")
NEWLINE
PRINTSTRING("zero will terminate the program.")
NEWLINES(2)
PRINTSTRING("Results are displayed as absolute rates for various mole")
NEWLINE
PRINTSTRING("fractions of the metals (in the metal phase), from 0.9 metal one")
NEWLINE
PRINTSTRING("to 0.1 metal one, in steps of 0.1")
NEWLINES(4)
READ(M1ACT)
READ(M2ACT)
PROMPT("ENSEMBLE SIZE :",15)
NEWLINES(4)
%CYCLE
  READ(N) %UNTIL N<=20
  %IF N<=0 %THENEXIT
  PRINTSTRING("Activities for ensemble size")
  WRITE(N,3)
  NEWLINES(2)
  %FOR I=1,1,9 %CYCLE
    APM1=(10-I)/10
    APM2=I/10
    DISTRIBUTION(N,NO,APM1,APM2)
    ACT = ACTIVITY(N,NO,M1ACT,M2ACT)
    PRINTFL(ACT,3)
    SPACES(3)
  %REPEAT
  NEWLINES(5)
%REPEAT
%ROUTINE DISTRIBUTION(ZINTEGER N,ZREALARRAYNAME NO,ZREAL APM1,APM2)
```

```

%INTEGER I
PT(0)=1
PT(1)=1
%IF N>1%THEN BUILD(PT,2,N)
%FOR I=0,1,N %CYCLE
    NO(I)=((APM1**(N-I))*(APM2**I))*PT(I)
%REPEAT
%RETURN
%ROUTINE BUILD(%INTEGERARRAYNAME X,%INTEGER N,ESIZE)
    X(N)=X(N-1)
    %FOR I=N-1,-1,1 %CYCLE
        X(I)=X(I)+X(I-1)
    %REPEAT
    %UNLESS N=ESIZE %THEN BUILD(X,N+1,ESIZE)
    %RETURN
%END
%END
%REALFN ACTIVITY (%INTEGER N,%REALARRAYNAME NO,%REAL M1ACT,M2ACT)
%INTEGER I
%REALARRAY ACTS(0:N)
%REAL SUM
SUM=0
ACTS(0)=M1ACT*NO(0)
ACTS(N)=M2ACT*NO(N)
%IF N>1 %THENSTART
    %FOR I=1,1,N-1 %CYCLE
        ACTS(I)=NO(I)*(EXP(LOG(M1ACT)*((N-I)/N))*EXP(LOG(M2ACT)*(I/N)))
    %REPEAT
%FINISH
%FOR I=0,1,N %CYCLE
    SUM=SUM+ACTS(I)
%REPEAT
%RESULT = SUM
%END
%END
%ENDOFFILE

```

Command: