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PROGRAMS FOR CALCULATING RELATIVE INTENSITIES IN THE VIBRATIONAL STRUCTURE OF ELECTRONIC BAND SYSTEMS

Berkeley, California

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PROGRAMS FOR CALCULATING RELATIVE INTENSITIES IN THE VIBRATIONAL STRUCTURE OF ELECTRONIC BAND SYSTEMS*

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ABSTRACT

Source-deck listings of two computer programs are given for the calculation of relative intensities in the vibrational structure of an electronic transition. The first program finds turning points of an electronic potential-energy curve by direct numerical evaluation of the Klein action integrals in the RKR procedure. The second program uses these turning points to construct an effective potential for the molecule with rotational quantum number J. The radial Schrödinger equation then is solved for this potential to yield vibrational-rotational wavefunctions from which the program calculates Franck-Condon factors, r-centroids, and relative intensities.

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† Now at Harvard University, Cambridge, Massachusetts.

INTRODUCTION

This report supplements a previous paper,[1] hereafter referred to as I, which describes the calculation of relative intensities in the vibrational structure of an electronic transition. All computer programs used in I are documented herein.

Much of the programming was done by Mr. J. V. V. Kasper or in collaboration with him. The programs presented are not in final polished form and the author assumes the responsibility for all remaining errors that have gone undetected. No systematic attempt has been made to test all possible branches in these programs. However, these programs have been running successfully for over six months.

Much of the programming logic has been mentioned before in I. Comment cards have been liberally used in the Fortran source deck listings so that a description of the methods used in each program is self-contained. Comment cards also describe fully the preparation of data cards for each program. To further aid the user, sample data decks, which were successfully tested, are included. The output from these sample decks is displayed in the Appendix.

These programs are written for an IBM 709/7090/7094 installation. All source decks shown are photographic reproductions of machine listings.

PROGRAM FOR FINDING TURNING POINTS OF A POTENTIAL BY RKR PROCEDURE

Remarks

The input may be either in the form of spectroscopic constants for the electronic state, or the actual G(v) and B_v spectroscopic data. In the former case, the program requires about 3 sec per pair of turning points, whereas in the latter case[2] it is 5 sec. It is also possible to use a combination of input modes, i. e., vibrational constants and rotational B_v data, or vice versa.

When giving G(v) data, the zero-point energy may be assigned by the user, or found from extrapolation by the program. This latter feature allows the use of zero-line measurements or tabulated $\Delta G(v)$ data.

Limitations

(a) If tabulated G(v) or B_v data are used that have anomalous behavior, it is possible for the interpolation procedures NTRPSR or NTRPDP to fail.
(b) If less than eight G(v) or B_v data points are to be read in, NUST in subroutine RKR must be modified.
(c) Since errors tend to accumulate in the calculation of the turning points for each higher vibrational level, the potential curve is less accurate as the dissociation limit is approached.

Listing

Table I lists the source decks and Table II gives a sample data deck for the RKR program.

Table I. Source-deck listing for RKR program.

```
CMAIN FINDS TURNING POINTS FOR A MOLECULE BY RYDBERG-KLEIN-REES METHOD  MAIN 000
C     ALL INPUT IS IN WAVE NUMBERS AND ANGSTROMS.                       MAIN 001
C     USER SPECIFIES CHOICE BETWEEN MASS UNITS BASED ON C12 = 12, OR    MAIN 002
C     O16 = 16.                                                         MAIN 003
C     THE FOLLOWING COMMENT CARDS DESCRIBE THE PREPARATION OF DATA CARDSMAIN 004
C                                                                       MAIN 005
      DIMENSION XI(200),YI(200),XO(3000),V(3000),S(3000),KV(200),       MAIN 006
     Z          ETRIAL(200),QIRA(2),QIEN(3),QIMS(2),ZIMS(2),ZIRA(2),    MAIN 007
     Z          ZIEN(3),ECALC(200),XPRN(5),VPRN(5),DTFRMT(10),          MAIN 008
     Z          G(200),BV(200),FMT(24), U(200),RMIN(200),RMAX(200),     MAIN 009
     Z          DUFMT(10),BVF(200)                                      MAIN 010
      COMMON XI,YI,XO,V,XH,NSTA,N,MSTA,M,XMIN,XMAX,INSC,MBEG,NUSED,S,   MAIN 011
     Z       NI,NS,MAXIT,FACM,ZMU,DE,WE,WEXE,WEYE,WEZE,WETE,BE,ALPHAE,  MAIN 012
     Z       GAMMAE,DELTAE,AS,BS,MQ,STEP,U,BV,G,ICK,H,ITR,HDES,EPSLNE   MAIN 013
C                                                                       MAIN 014
C      FIRST CARD IN DATA HAS A ONE IN COLUMN 1 IF A PROBLEM FOLLOWS.   MAIN 015
C      VERY LAST CARD IN DATA MUST BE A BLANK CARD.....                 MAIN 016
C                                                                       MAIN 017
    1 CALL TIME(BEGIN)                                                  MAIN 018
      WRITEOUTPUTTAPE6,140,BEGIN                                        MAIN 019
  140 FORMAT (9H0 TIME =   F10.5)                                       MAIN 020
      READINPUTTAPE5,100,ITEST                                          MAIN 021
  100 FORMAT (I1)                                                       MAIN 022
    2 IF (ITEST) 3,400,3                                                MAIN 023
C                                                                       MAIN 024
C      NEXT TWO CARDS IN DATA HAVE NAME OF PROBLEM IN COLUMNS 1-72,     MAIN 025
C      WHERE CARRIAGE CONTROL IS IN COLUMN 1.  NEXT CARD HAS IIMS AND   MAIN 026
C      MASSES OF THE TWO ATOMS, OR IIMS AND REDUCED MASS IN FIRST MASS  MAIN 027
C      FIELD WITH SECOND BLANK.                                         MAIN 028
C      IIMS = 1, MASS UNITS ARE BASED ON C12 = 12.                      MAIN 029
C      IIMS = 2, MASS UNITS ARE BASED ON O16 = 16.                      MAIN 030
C                                                                       MAIN 031
    3 READINPUTTAPE5,101,(FMT(I),I=1,24)                                MAIN 032
  101 FORMAT (12A6)                                                     MAIN 033
      READINPUTTAPE5,102,IIMS,ZMAS1,ZMAS2                               MAIN 034
  102 FORMAT (I4,2F10.0)                                                MAIN 035
C                                                                       MAIN 036
C      NEXT CARD IN DATA HAS IQHK, AND NUMBER OF LEVELS, EACH           MAIN 037
C      IN I4 FORMAT, AS WELL AS THE FORMAT STATEMENT WHICH CONTROLS THE MAIN 038
C      READING OF THE LEVELS (IN COLUMNS 13-72)--FOR EXAMPLE- (4E16.8). MAIN 039
C      IQHK = 0 IF THE FOLLOWING CARDS CONTAIN THE TABULATED G CURVE.   MAIN 040
C      IF A PARTICULAR VALUE IS TO BE INTERPOLATED, SET G(I) = -10.     MAIN 041
C      IF IT IS DESIRED TO USE CONSTANTS  TO GENERATE THE ENTIRE        MAIN 042
C      G CURVE, IQHK MUST NOT BE EQUAL TO ZERO.                         MAIN 043
C      A HOLLERITH TEXT MUST BE PUNCHED IN COLUMNS 13-72,               MAIN 044
C      AS IT WILL BE PRINTED, E.G.,   (1H )                             MAIN 045
C      THE NEXT CARD IN SUCH A CASE CONTAINS                            MAIN 046
C      WE,WEXE,WEYE,WEZE,AND WETE.                                      MAIN 047
C                                                                       MAIN 048
    5 READINPUTTAPE5,103,IQHK,     N,(DTFRMT(I),I=1,10)                 MAIN 049
103   FORMAT(2I4,4X,10A6)                                               MAIN 050
      IIEN = 2                                                          MAIN 051
    6 IF (IQHK) 8,7,8                                                   MAIN 052
    8 READINPUTTAPE5,114,WE,WEXE,WEYE,WEZE,WETE                         MAIN 053
  114 FORMAT (5E10.0)                                                   MAIN 054
      GO TO 9                                                           MAIN 055
    7 READINPUTTAPE5,DTFRMT,(G(I),I=1,N)                                MAIN 056
C                                                                       MAIN 057
```

Table I. (Contd.)

```
C     THE ZERO POINT ENERGY MAY BE FOUND BY EXTRAPOLATION, OR IT MAY BE MAIN 058
C     FIXED BY THE USER FROM HIS TABULATED G(V) CURVE.                  MAIN 059
C     NEXT CARD CONTAINS IOPEV.                                         MAIN 060
C     SET IOPEV = 0, IF THE ZERO POINT ENERGY IS TO BE FOUND BY         MAIN 061
C     EXTRAPOLATION, AND THE G(V) CURVE IS TO BE RAISED OR LOWERED      MAIN 062
C     ACCORDINGLY.                                                      MAIN 063
C     THIS IS PARTICULARLY USEFUL IF DELTA G(V) DATA IS TO BE USED.     MAIN 064
C     SET IOPEV = 1, IF THE TABULATED G(V) CURVE IS TO BE USED UNCHANGEDMAIN 065
C     SET IOPEV = 2, IF THE G(V) CURVE IS TO BE CONSTRUCTED FROM CONSTANMAIN 066
C                                                                       MAIN 067
9     READ INPUT TAPE 5, 100, IOPEV                                     MAIN 068
C                                                                       MAIN 069
C      THE NEXT SET OF CARDS CONTAINS THE BV CURVE WITH THE SAME        MAIN 070
C      RESTRICTIONS AS FOR G CURVE ABOVE.  NUMBER OF VALUES HERE MUST BEMAIN 071
C      EQUAL TO THE NUMBER ABOVE                                        MAIN 072
C                                                                       MAIN 073
      READINPUTTAPE5,103,IBHK,     N,(DUFMT(I),I=1,10)                  MAIN 074
      IIEB = 2                                                          MAIN 075
   30 IF (IBHK) 31,32,31                                                MAIN 076
   31 READINPUTTAPE5,114,BE,ALPHAE,GAMMAE,DELTAE,EPSLNE                 MAIN 077
      GO TO 33                                                          MAIN 078
   32 READINPUTTAPE5,DUFMT,(BV(I),I=1,N)                                MAIN 079
C                                                                       MAIN 080
C     THE ROTATIONAL CONSTANT BE MAY BE FOUND BY EXTRAPOLATION, OR IT   MAIN 081
C     MAY BE FIXED BY THE USER.                                         MAIN 082
C     NEXT CARD CONTAINS IOPA AND BEQUIL.                               MAIN 083
C     SET IOPA = 0, IF THE VALUE OF BE IS TO BE FOUND BY EXTRAPOLATION  MAIN 084
C     FROM THE BV DATA READ IN.    LEAVE BEQUIL BLANK.                  MAIN 085
C     SET IOPA = 1, IF THE VALUE OF BE IS TO BE GIVEN BY BEQUIL.        MAIN 086
C     SET IOPA = 2, IF ROTATIONAL CONSTANTS ARE USED.    LEAVE BEQUIL   MAIN 087
C     BLANK.                                                            MAIN 088
C                                                                       MAIN 089
33    READ INPUT TAPE 5,102,IOPA,BEQUIL                                 MAIN 090
C                                                                       MAIN 091
C     NEXT DATA CARD CONTAINS RE, THE INTERNUCLEAR EQUILIBRIUM DISTANCE.MAIN 092
C                                                                       MAIN 093
      READ INPUT TAPE 5,106,RE                                          MAIN 094
106   FORMAT(F10.0)                                                     MAIN 095
C                                                                       MAIN 096
C     NEXT DATA CARD CONTAINS VSTART,VFIN,AND HDED WHERE                MAIN 097
C     TURNING POINTS ARE CALCULATED FROM VIBRATIONAL LEVEL VSTART TO    MAIN 098
C     VFIN IN STEPS OF HDED     E.G. FROM 0.5 TO 20.5 IN STEPS OF 1.0.  MAIN 099
C                                                                       MAIN 100
      READ INPUT TAPE 5,114,VSTART,VFIN,HDED                            MAIN 101
C                                                                       MAIN 102
C     NEXT CARD CONTAINS IOPFG.                                         MAIN 103
C     SET IOPFG = 1, IF INTERMEDIATE STEPS IN THE EVALUATION OF THE     MAIN 104
C     KLEIN ACTION INTEGRALS ARE TO BE PRINTED.                         MAIN 105
C     SET IOPFG = 0, IF INTERMEDIATE PRINT-OUT IS TO BE SKIPPED.        MAIN 106
C     NORMALLY THE USER SHOULD SET IOPFG = 0.                           MAIN 107
C                                                                       MAIN 108
      READ INPUT TAPE 5,100,IOPFG                                       MAIN 109
C     THIS TERMINATES COMMENT CARDS ON THE PREPARATION OF DATA.         MAIN 110
C     IF NO FURTHER PROBLEMS FOLLOW, REMEMBER TO ADD A BLANK CARD TO    MAIN 111
C     THE DATA DECK.                                                    MAIN 112
C                                                                       MAIN 113
C                                                                       MAIN 114
      QIRA(2) = 6HANGST.                                                MAIN 115
```

Table I. (Contd.)

```
      QIEN(2) = 6H1/CM                                                  MAIN 116
      QIMS(1) = 6HC12=12                                                MAIN 117
      QIMS(2) = 6HO16=16                                                MAIN 118
C                                                                       MAIN 119
C      PRINT HEADING                                                    MAIN 120
C                                                                       MAIN 121
      WRITEOUTPUTTAPE6,101,(FMT(I),I=1,24)                              MAIN 122
C                                                                       MAIN 123
C      PRINT THE MASSES AND THEIR UNITS.                                MAIN 124
C                                                                       MAIN 125
   10 IF (ZMAS2) 12,12,11                                               MAIN 126
   11 WRITEOUTPUTTAPE6,121,QIMS(IIMS),ZMAS1,ZMAS2                       MAIN 127
  121 FORMAT (///40H  THE MASSES OF THE TWO ATOMS, BASED ON A6, 6H, ARE MAIN 128
     Z         F10.6, 5H AND  F10.6///)                                MAIN 129
      GO TO 20                                                          MAIN 130
   12 WRITEOUTPUTTAPE6,111,QIMS(IIMS),ZMAS1                             MAIN 131
  111 FORMAT (///46H  THE REDUCED MASS OF THE TWO ATOMS, BASED ON A6,   MAIN 132
     Z          5H, IS  F10.6///)                                      MAIN 133
C                                                                       MAIN 134
C                                                                       MAIN 135
C                                                                       MAIN 136
C      PRINT G(V) DATA, OR VIBRATIONAL CONSTANTS                        MAIN 137
C                                                                       MAIN 138
   20 IF (IQHK) 22,21,22                                                MAIN 139
   22 WRITEOUTPUTTAPE6,DTFRMT                                           MAIN 140
      WRITEOUTPUTTAPE6,116,WE,WEXE,WEYE,WEZE,WETE                       MAIN 141
  116 FORMAT (63H0 THE G(V) CURVE IS CONSTRUCTED FROM THE FOLLOWING INPUMAIN 142
     ZT DATA.  // 7H  WE = F10.3,8H, WEXE =F10.4,8H, WEYE =E10.5,8H, WEZMAIN 143
     ZE =E10.5,8H, WETE =E10.5 )                                        MAIN 144
      GO TO 40                                                          MAIN 145
   21 WRITEOUTPUTTAPE6,122,QIEN(IIEN)                                   MAIN 146
  122 FORMAT (32H  THE INPUT G VALUES, ENERGY IN A6,                    MAIN 147
     Z        18H, ARE GIVEN BELOW.  //)                                MAIN 148
      WRITEOUTPUTTAPE6,115,(G(I),I=1,N)                                 MAIN 149
  115 FORMAT (1X10F11.3)                                                MAIN 150
      WRITEOUTPUTTAPE6,128                                              MAIN 151
  128 FORMAT (20X48HVALUES OF -10. ARE TO BE FOUND BY INTERPOLATION.)   MAIN 152
C                                                                       MAIN 153
C      PRINT BV DATA, OR ROTATIONAL CONSTANTS                           MAIN 154
C                                                                       MAIN 155
   40 IF (IBHK) 41,42,41                                                MAIN 156
   41 WRITEOUTPUTTAPE6,DUFMT                                            MAIN 157
      WRITEOUTPUTTAPE6,120,BE,ALPHAE,GAMMAE,DELTAE,EPSLNE               MAIN 158
  120 FORMAT (64H0 THE BV(V) CURVE IS CONSTRUCTED FROM THE FOLLOWING INPMAIN 159
     ZUT DATA. //7H  BE = 1PE11.5,10H, ALPHAE = E11.4,10H, GAMMAE =     MAIN 160
     Z E11.4,10H, DELTAE = E11.4, 10H, EPSLNE =  E11.4)                 MAIN 161
      GO TO 43                                                          MAIN 162
   42 WRITEOUTPUTTAPE6,127,QIEN(IIEB)                                   MAIN 163
  127 FORMAT (33H  THE INPUT BV VALUES, ENERGY IN A6,                   MAIN 164
     Z  18H, ARE GIVEN BELOW.  //)                                      MAIN 165
      WRITEOUTPUTTAPE6,129,(BV(I),I=1,N)                                MAIN 166
  129 FORMAT (1X10F11.6)                                                MAIN 167
      WRITEOUTPUTTAPE6,128                                              MAIN 168
C                                                                       MAIN 169
C      PRINT HEADING                                                    MAIN 170
43    WRITEOUTPUTTAPE6,101,(FMT(I),I=1,24)                              MAIN 171
C                                                                       MAIN 172
  200 IF (ZMAS2) 201,201,202                                            MAIN 173
```

Table I. (Contd.)

```
  201 ZMU = ZMAS1                                                       MAIN 174
      GO TO 204                                                         MAIN 175
  202 ZMU = ZMAS1*ZMAS2/(ZMAS1+ZMAS2)                                   MAIN 176
  204 ZIMS(1) = 1.0                                                     MAIN 177
      ZIMS(2) = .9996784                                                MAIN 178
      ZIRA(1) = 1.0                                                     MAIN 179
      ZIRA(2) = 1.889766                                                MAIN 180
      ZMU = ZMU * ZIMS(IIMS)                                            MAIN 181
      ZIEN(1) = ZMU * 3.643668E3                                        MAIN 182
      ZIEN(2) = ZMU * 1.6610826E-2                                      MAIN 183
      ZIEN(3) = ZMU * 1.339776E2                                        MAIN 184
      FACM = 60.201702/ZMU                                              MAIN 185
  206 XI(1) = 0.5                                                       MAIN 186
  207 DO 208 I = 2,N                                                    MAIN 187
      IL = I - 1                                                        MAIN 188
      XI(I) = XI(IL) + 1.0                                              MAIN 189
  208 CONTINUE                                                          MAIN 190
      ZERO = 0.0                                                        MAIN 191
      WRITEOUTPUTTAPE7,101,(FMT(I),I=1,24)                              MAIN 192
      WRITEOUTPUTTAPE7,138,RE,ZERO                                      MAIN 193
  138 FORMAT (1XF9.7,F10.3)                                             MAIN 194
210   CALL RKR(RMIN,RMAX,VSTART,VFIN,HDED,NFIN,EV1,U,IQHK,IBHK,IOPEV,   MAIN 195
     Z         IOPA,BEQUIL,IOPFG)                                       MAIN 196
      GO TO 1                                                           MAIN 197
  400 CALL EXIT                                                         MAIN 198
      END                                                               MAIN 199
```

Table I. (Contd.)

```
CRKR    FINDS TURNING POINTS FROM G(V) AND BV DATA, OR FROM CONSTANTS     RKR  000
       SUBROUTINE RKR(RMIN,RMAX,VSTA,VFIN,HDED,M,EV1,U,IQHK,IBHK,IOPEV,   RKR  001
      Z                IOPA,BEQUIL,IOPFG)                                 RKR  002
       DIMENSION                UEV(3000),EV(3000),BV(200),BI(3000),     RKR  003
      Z           TEMP(200),U(200),RMIN(200),RMAX(200),Y(200),Z(200),    RKR  004
      Z           ZOC(9),MZ(5),IZ(5),IB(40),IG(40)                       RKR  005
D      DIMENSION V(200),G(200),BO(200),OEV(200),OV(200),XG(20),YG(20),   RKR  006
      Z           ZG(20),EPSH(1),AGAUS(5,20),XGAUS(5,20),VSTA(1),VFIN(1), RKR  007
      Z           HDED(1),DENQ(20)                                       RKR  008
       COMMON Y,TEMP,UEV,EV,Q,NST,N,MST,M,XMIN,XMAX,INSC,MBEG,NUSED,BI,  RKR  009
      Z        NI,NS,MAXIT,FACM,ZMU,DE,WE,WEXE,WEYE,WEZE,WETE,BE,ALPHAE, RKR  010
      Z        GAMMAE,DELTAE,    VNIN,BQ,MQ,SPEP,    U,BV,Z,ICK,H,  K,HDES RKR  011
      Z        ,EPSLNE                                                   RKR  012
       GFUNCF(X)= ((((((((WETE*X)+WEZE)*X)+WEYE)*X)-WEXE)*X)+WE)*X       RKR  013
       BFUNCF(X) = ((((((((EPSLNE*X)+DELTAE)*X)+GAMMAE)*X)-ALPHAE)*X)+BE RKR  014
C       FAC = (HPLANCK*NAV/8*PI**2*C)**.5*E8/ZMU**.5                     RKR  015
       FAC = 4.1057859/SQRTF(ZMU)                                        RKR  016
       NPROB = 1                                                         RKR  017
       NUST = 8                                                          RKR  018
       EV1 = 0.0                                                         RKR  019
  201  CALL TIME(BEGIN)                                                  RKR  020
C                                                                        RKR  021
C       TURNING POINTS FOUND FOR V = VSTA,VFIN,HDED.                     RKR  022
C                                                                        RKR  023
C      INTERPOLATE G(V) AND BV DATA                                      RKR  024
C                                                                        RKR  025
  202  JJ = 0                                                            RKR  026
       JK = 0                                                            RKR  027
       IJ = 0                                                            RKR  028
       IK = 0                                                            RKR  029
       HDES = .01                                                        RKR  030
       MBEG = 1                                                          RKR  031
       IF(IOPEV-1)3000,3001,3000                                         RKR  032
3001   EV1 = Z(1)                                                        RKR  033
3000   WRITEOUTPUTTAPE6,114,NUST                                         RKR  034
  114  FORMAT (20H0 NUSED IN BESRKR = I2,1H.)                            RKR  035
       DO 187 I = 1,N                                                    RKR  036
       IF (Z(I) + 10.) 182,183,182                                       RKR  037
  182  IJ = IJ + 1                                                       RKR  038
       TEMP(IJ) = Y(I)                                                   RKR  039
       U(IJ) = Z(I)                                                      RKR  040
       GO TO 184                                                         RKR  041
  183  JJ = JJ + 1                                                       RKR  042
       UEV(JJ) = Y(I)                                                    RKR  043
       IG(JJ) = I                                                        RKR  044
  184  IF (BV(I) + 10.) 185,186,185                                      RKR  045
  185  IK = IK + 1                                                       RKR  046
       RMIN(IK) = Y(I)                                                   RKR  047
       RMAX(IK) = BV(I)                                                  RKR  048
       GO TO 187                                                         RKR  049
  186  JK = JK + 1                                                       RKR  050
       EV(JK) = Y(I)                                                     RKR  051
       IB(JK) = I                                                        RKR  052
  187  CONTINUE                                                          RKR  053
       IF (JJ) 191,191,188                                               RKR  054
  188  CALL NTRPSR (TEMP,U,UEV,BI,HDES,IJ,JJ,VNIN,VN,INSC,MBEG,NUST)     RKR  055
       LOC = 8                                                           RKR  056
       IF (INSC) 288,189,288                                             RKR  057
```

Table I. (Contd.)

```
  189 DO 190 I = 1,JJ                                                   RKR  058
      IJ = IG(I)                                                        RKR  059
      Z(IJ) = BI(I)                                                     RKR  060
  190 CONTINUE                                                          RKR  061
  191 IF (JK) 196,196,192                                               RKR  062
  192 CALL NTRPSR (RMIN,RMAX,EV,BI,HDES,IK,JK,VNIN,VN,INSC,MBEG,NUST)   RKR  063
      LOC = 9                                                           RKR  064
  193 IF (INSC) 288,194,288                                             RKR  065
  194 DO 195 I = 1,JK                                                   RKR  066
      IK = IB(I)                                                        RKR  067
      BV(IK) = BI(I)                                                    RKR  068
  195 CONTINUE                                                          RKR  069
  196 IF (IQHK) 204,203,204                                             RKR  070
  204 EV1 = -GFUNCF(0.5)                                                RKR  071
      IOPEV = 0                                                         RKR  072
      DO 170 I = 1,N                                                    RKR  073
      Z(I) = GFUNCF(Y(I)) + EV1                                         RKR  074
  170 CONTINUE                                                          RKR  075
      GO TO 211                                                         RKR  076
  203 INTG = INTQ                                                       RKR  077
      MBEG = 1                                                          RKR  078
      M = 1                                                             RKR  079
      UEV(1) = 0.                                                       RKR  080
      HDES = 1.                                                         RKR  081
      EV1 = -EV1                                                        RKR  082
      IF (EV1) 211,206,206                                              RKR  083
  206 CALL NTRPSR(Y,Z,UEV,EV,HDES,N,M,VNIN,VN,INSC,MBEG,NUST)           RKR  084
      LOC = 1                                                           RKR  085
  208 IF (INSC) 288,210,288                                             RKR  086
  210 EV1 = EV(1)                                                       RKR  087
C     EV1 NOW CONTAINS THE ZERO POINT ENERGY BY EXTRAPOLATION.          RKR  088
  211 IF (IBHK) 171,207,171                                             RKR  089
  171 EV(1) = BE                                                        RKR  090
      DO 172 I = 1,N                                                    RKR  091
      BV(I) = BFUNCF(Y(I))                                              RKR  092
  172 CONTINUE                                                          RKR  093
      GO TO 205                                                         RKR  094
  207 IF (IOPA) 2071,2072,2071                                          RKR  095
 2071 EV(1) = BEQUIL                                                    RKR  096
      GO TO 205                                                         RKR  097
 2072 CALL NTRPSR (Y,BV,UEV,EV,HDES,N,M,VNIN,VN,INSC,MBEG,NUST)         RKR  098
C     EV(1) NOW CONTAINS BE BY EXTRAPOLATION                            RKR  099
      LOC = 7                                                           RKR  100
      IF (INSC) 288,205,288                                             RKR  101
  205 V(1) = 0.                                                         RKR  102
      G(1) = 0.                                                         RKR  103
      BO(1) = EV(1)                                                     RKR  104
      DO 209 I = 1,N        DO 209                                      RKR  105
      V(I+1) = Y(I)                                                     RKR  106
      G(I+1) = Z(I)                                                     RKR  107
      BO(I+1) = BV(I)                                                   RKR  108
  209 CONTINUE                                                          RKR  109
      NP = N + 1                                                        RKR  110
      IF (IOPEV) 2091,2092,2091                                         RKR  111
 2091 CONTINUE                                                          RKR  112
      EV1 = EV1 + G(2)                                                  RKR  113
 2092 DO 213 I = 2,NP                                                   RKR  114
      G(I) = G(I) - EV1                                                 RKR  115
```

Table I. (Contd.)

```
      Y(I) = V(I)                                                       RKR  116
      Z(I) = G(I)                                                       RKR  117
      BV(I) = BO(I)                                                     RKR  118
  213 CONTINUE                                                          RKR  119
      IF (IOPEV) 2131,2132,2131                                         RKR  120
 2131 EV1 = -G(2)                                                       RKR  121
 2132 IF (NPROB-17) 2133,2134,2133                                      RKR  122
 2134 M = 1                                                             RKR  123
      EV(1) = DE                                                        RKR  124
      CALL NTRPSR (Z,Y,EV,UEV,HDES,NP,M,VNIN,VN,INSC,MBEG,NUST)         RKR  125
      LOC = 2                                                           RKR  126
      IF (INSC) 288,2135,288                                            RKR  127
 2135 NP = NP + 1                                                       RKR  128
      Y(NP) = UEV                                                       RKR  129
      V(NP) = UEV                                                       RKR  130
      Z(NP) = DE                                                        RKR  131
      G(NP) = DE                                                        RKR  132
      BO(NP) = 0.                                                       RKR  133
      BV(NP) = 0.                                                       RKR  134
 2133 Y(1) = 0.                                                         RKR  135
      Z(1) = 0.                                                         RKR  136
      BV(1) = BO(1)                                                     RKR  137
      VMIN = VSTA                                                       RKR  138
      VN = VFIN                                                         RKR  139
      HDES = HDED                                                       RKR  140
      M = 0                                                             RKR  141
      WRITEOUTPUTTAPE6,113,(Y(I),Z(I),I=1,NP)                           RKR  142
  113 FORMAT (33H0 THE G(V) VALUES USED BELOW ARE / 6(4X1HV10X1HG4X) // RKR  143
     Z        6(1XF7.3,F12.4))                                          RKR  144
      WRITEOUTPUTTAPE6,108,(Y(I),BV(I),I=1,NP)                          RKR  145
  108 FORMAT (33H0 THE BV(V) VALUES USED BELOW ARE / 6(4X1HV9X2HBV4X) //RKR  146
     Z        6(1XF7.3,F12.7))                                          RKR  147
      IF (IQHK) 215,212,215                                             RKR  148
  215 M = XFIXF((VFIN-VSTA)/HDED) + 1                                   RKR  149
      DO 217 I = 1,M                                                    RKR  150
      OEV(I) = VSTA + FLOATF(I-1)*HDED                                  RKR  151
      OV(I) = GFUNCF(OEV(I))                                            RKR  152
  217 CONTINUE                                                          RKR  153
      INSC = 0                                                          RKR  154
      GO TO 218                                                         RKR  155
  212 CALL NTRPDP(V,G,OEV,OV,HDED,NP,M,VSTA,VFIN,INSC,MBEG,NUST)        RKR  156
      LOC = 2                                                           RKR  157
      WRITEOUTPUTTAPE6,106,HDES,VMIN,VN,MBEG,NUST,INSC,NP,M             RKR  158
  106 FORMAT (6H0HDES=1PE15.7,7H, VMIN=E15.7,5H, VN=E15.7,7H, MBEG=I5/  RKR  159
     Z9X7H, NUST=I5,7H, INSC=I5,4H, N=I5,4H, M=I5)                      RKR  160
  218 WRITEOUTPUTTAPE6,109                                              RKR  161
  109 FORMAT (54H0 OUTPUT V,G--LEVELS AT WHICH TURNING POINTS ARE FOUND/RKR  162
     Z        6(4X1HV10X1HG4X) //)                                      RKR  163
      WRITEOUTPUTTAPE6,107,(OEV(I),OV(I),I=1,M)                         RKR  164
  107 FORMAT (6(1XF7.3,F12.4))                                          RKR  165
  214 IF (INSC) 288,216,288                                             RKR  166
  216 DO 219 I = 1,M                                                    RKR  167
      TEMP(I) = OEV(I)                                                  RKR  168
      U(I) = OV(I)                                                      RKR  169
  219 CONTINUE                                                          RKR  170
C                                                                       RKR  171
C     INTEGRATION CONSTANTS                                             RKR  172
C                                                                       RKR  173
```

Table I. (Contd.)

```
      STEP = .9                                                         RKR  174
      MZ(1) = 101                                                       RKR  175
      MZ(2) = 81                                                        RKR  176
      MZ(3) = 61                                                        RKR  177
      IZ(1) = 8                                                         RKR  178
D     XGAUS(1,1) = .019855071751232                                     RKR  179
D     XGAUS(1,2) = .101666761293186                                     RKR  180
D     XGAUS(1,3) = .237233795041836                                     RKR  181
D     XGAUS(1,4) = .408282678752175                                     RKR  182
D     XGAUS(1,5) = 1. - XGAUS(1,4)                                      RKR  183
D     XGAUS(1,6) = 1. - XGAUS(1,3)                                      RKR  184
D     XGAUS(1,7) = 1. - XGAUS(1,2)                                      RKR  185
D     XGAUS(1,8) = 1. - XGAUS(1,1)                                      RKR  186
D     AGAUS(1,1) = .050614268145188                                     RKR  187
D     AGAUS(1,2) = .111190517226687                                     RKR  188
D     AGAUS(1,3) = .156853322938944                                     RKR  189
D     AGAUS(1,4) = .181341891689181                                     RKR  190
D     AGAUS(1,5) = AGAUS(1,4)                                           RKR  191
D     AGAUS(1,6) = AGAUS(1,3)                                           RKR  192
D     AGAUS(1,7) = AGAUS(1,2)                                           RKR  193
D     AGAUS(1,8) = AGAUS(1,1)                                           RKR  194
      IZ(2) = 6                                                         RKR  195
D     XGAUS(2,1) = .033765242898424                                     RKR  196
D     XGAUS(2,2) = .169395306766868                                     RKR  197
D     XGAUS(2,3) = .380690406958402                                     RKR  198
D     XGAUS(2,4) = 1. - XGAUS(2,3)                                      RKR  199
D     XGAUS(2,5) = 1. - XGAUS(2,2)                                      RKR  200
D     XGAUS(2,6) = 1. - XGAUS(2,1)                                      RKR  201
D     AGAUS(2,1) = .085662246189585                                     RKR  202
D     AGAUS(2,2) = .180380786524070                                     RKR  203
D     AGAUS(2,3) = .233956967286345                                     RKR  204
D     AGAUS(2,4) = AGAUS(2,3)                                           RKR  205
D     AGAUS(2,5) = AGAUS(2,2)                                           RKR  206
D     AGAUS(2,6) = AGAUS(2,1)                                           RKR  207
      IZ(3) = 4                                                         RKR  208
D     XGAUS(3,1) = .069431844202974                                     RKR  209
D     XGAUS(3,2) = .330009478207572                                     RKR  210
D     XGAUS(3,3) = 1. - XGAUS(3,2)                                      RKR  211
D     XGAUS(3,4) = 1. - XGAUS(3,1)                                      RKR  212
D     AGAUS(3,1) = .173927422568727                                     RKR  213
D     AGAUS(3,2) = .326072577431273                                     RKR  214
D     AGAUS(3,3) = AGAUS(3,2)                                           RKR  215
D     AGAUS(3,4) = AGAUS(3,1)                                           RKR  216
D     ZG(1) = ZG(3)                                                     RKR  217
      WRITEOUTPUTTAPE6,100                                              RKR  218
  100 FORMAT (1H1)                                                      RKR  219
  224 DO 280 I = 1,M                                                    RKR  220
D     TEMPI = OEV(I)                                                    RKR  221
      NUS2 = NUST/2                                                     RKR  222
      NB = NUS2 + 1                                                     RKR  223
      NF = N - NB + 1                                                   RKR  224
      DO 225 J = NB,NF                                                  RKR  225
      IF (TEMPI - V(J)) 235,235,225                                     RKR  226
  225 CONTINUE                                                          RKR  227
      ISG = NF + 1                                                      RKR  228
      GO TO 237                                                         RKR  229
  235 ISG = J                                                           RKR  230
  237 NSTA = ISG - NUS2                                                 RKR  231
```

Table I. (Contd.)

```
D       VMIN = 0.                                                       RKR  232
        FEG = 0.                                                        RKR  233
        GEG = 0.                                                        RKR  234
        LT = 1                                                          RKR  235
        IZGD = 0                                                        RKR  236
        GDO = 0.                                                        RKR  237
        FDO = 0.                                                        RKR  238
        ISG = 0                                                         RKR  239
        ISB = 0                                                         RKR  240
C                                                                       RKR  241
C       COMMENCE FINDING TURNING POINTS BY INTEGRATION                  RKR  242
C                                                                       RKR  243
        CALL TIME (BEGIA)                                               RKR  244
D 226   BS = VMIN + (TEMPI - VMIN) * STEP                               RKR  245
  227   IF (LT-3) 228,228,301                                           RKR  246
  228   MQ = MZ(LT)                                                     RKR  247
  223   KM = (MQ-1)/2                                                   RKR  248
        TMIN = VMIN                                                     RKR  249
        TS = BS                                                         RKR  250
        A = (TS-TMIN)/FLOATF(MQ-1)                                      RKR  251
        MX = 0                                                          RKR  252
        IF (IQHK) 401,229,401                                           RKR  253
  229   CALL NTRPSR(Y,Z,UEV,EV,A,NP,MX,TMIN,TS,INSC,MBEG,NUST)          RKR  254
  230   LOC = 3                                                         RKR  255
  231   IF (INSC) 288,232,288                                           RKR  256
  232   IF (GDO) 236,233,236                                            RKR  257
  233   MX = 0                                                          RKR  258
        IF (IBHK) 403,239,403                                           RKR  259
  239   CALL NTRPSR(Y,BV,UEV,BI,A,NP,MX,TMIN,TS,INSC,MBEG,NUST)         RKR  260
        LOC = 4                                                         RKR  261
  234   IF (INSC) 288,236,288                                           RKR  262
  236   DO 238 J = 1,MQ                                                 RKR  263
        DENQ = U(I) - EV(J)                                             RKR  264
        IF (DENQ) 292,292,241                                           RKR  265
  241   UEV(J) = 1./SQRTF(DENQ)                                         RKR  266
        EV(J) = BI(J) * UEV(J)                                          RKR  267
  238   CONTINUE                                                        RKR  268
        FSUM = UEV(1) + 4.*UEV(2) + UEV(MQ)                             RKR  269
        GSUM = EV(1) + 4.*EV(2) + EV(MQ)                                RKR  270
  240   DO 242 J = 2,KM                                                 RKR  271
        FSUM = FSUM + 4.*UEV(2*J) + 2.*UEV(2*J-1)                       RKR  272
        GSUM = GSUM + 4.*EV(2*J) + 2.*EV(2*J-1)                         RKR  273
  242   CONTINUE                                                        RKR  274
        FEG2 = A*FSUM/3.                                                RKR  275
        GEG2 = A*GSUM/3.                                                RKR  276
  250   IF (LT - 1) 262,262,254                                         RKR  277
  301   IZDO = (LT-1)/3                                                 RKR  278
        IF (IZDO - 3) 304,304,303                                       RKR  279
  303   IZDO = 3                                                        RKR  280
  304   NGAS = IZ(IZDO)                                                 RKR  281
        DO 306 J = 1,NGAS                                               RKR  282
D       XG(J) = (BS-VMIN) * XGAUS(IZDO,J) + VMIN                        RKR  283
        UEV(J) = XG(J)                                                  RKR  284
  306   CONTINUE                                                        RKR  285
        MST = 1                                                         RKR  286
D       EPSH = TEMPI - XG(NGAS)                                         RKR  287
        FEPS = EPSH                                                     RKR  288
        IF (EPSH(1)) 276,307,308                                        RKR  289
```

Table I. (Contd.)

```
  307 IF (EPSH(2)) 276,276,308                                          RKR  290
  308 IF (IQHK) 405,309,405                                             RKR  291
  309 CALL NTRPDP(V,G,XG,YG,EPSH,NP,NGAS,VMIN,BS,INSC,MST,NUST)         RKR  292
      LOC = 5                                                           RKR  293
  310 IF (INSC) 288,311,288                                             RKR  294
  311 IF (IZGD) 312,312,340                                             RKR  295
  312 IF (GDO)  318,314,318                                             RKR  296
  314 MST = 1                                                           RKR  297
      IF (IBHK) 407,315,407                                             RKR  298
  315 CALL NTRPSR (Y,BV,UEV,BI,FEPS,NP,NGAS,TMIN,TS,INSC,MST,NUST)      RKR  299
      LOC = 6                                                           RKR  300
  316 IF (INSC) 288,318,288                                             RKR  301
  318 FSUM = 0.0                                                        RKR  302
      GSUM = 0.0                                                        RKR  303
      DO 320 J = 1,NGAS                                                 RKR  304
      IF (IQHK) 718,317,718                                             RKR  305
D 317 DENQ(J) = OV(I) - YG(J)                                           RKR  306
  718 IF (DENQ(J)) 292,292,323                                          RKR  307
  323 XG(J) = AGAUS(IZDO,J)/SQRTF(DENQ(J))                              RKR  308
      YG(J) = BI(J) * XG(J)                                             RKR  309
      FSUM = FSUM + XG(J)                                               RKR  310
      GSUM = GSUM + YG(J)                                               RKR  311
  320 CONTINUE                                                          RKR  312
      IF (BI(NGAS)-BI(1)) 322,321,322                                   RKR  313
  321 IZGD = 1                                                          RKR  314
D 322 BSV = BS - VMIN                                                   RKR  315
      FEG2 = BSV * FSUM                                                 RKR  316
  324 GEG2 = BSV * GSUM                                                 RKR  317
      GO TO 254                                                         RKR  318
  340 FSUM = 0.0                                                        RKR  319
      DO 342 J = 1,NGAS                                                 RKR  320
D     DENQ = OV(I) - YG(J)                                              RKR  321
      IF (DENQ) 292,292,341                                             RKR  322
  341 XG(J) = AGAUS(IZDO,J)/SQRTF(DENQ)                                 RKR  323
      FSUM = FSUM + XG(J)                                               RKR  324
  342 CONTINUE                                                          RKR  325
      GSUM = BI(NGAS) * FSUM                                            RKR  326
      GO TO 322                                                         RKR  327
  254 IF (FEG2/FEG - 1.E-6) 255,255,256                                 RKR  328
  255 FDO = 1.                                                          RKR  329
  256 IF (GEG2/GEG - 1.E-6) 257,257,258                                 RKR  330
  257 GDO = 1.                                                          RKR  331
  258 IF (ABSF(FEG2/FEG1) - .9) 260,260,259                             RKR  332
  259 FDO = 1.                                                          RKR  333
  260 IF (ABSF(GEG2/GEG1) - .9) 262,262,261                             RKR  334
  261 GDO = 1.                                                          RKR  335
  262 LT = LT + 1                                                       RKR  336
      FEG1 = FEG2                                                       RKR  337
      GEG1 = GEG2                                                       RKR  338
  264 IF (FDO) 269,266,269                                              RKR  339
  266 FEG = FEG + FEG2                                                  RKR  340
  268 IF (GDO) 272,270,272                                              RKR  341
  269 IF (GDO) 276,270,276                                              RKR  342
  270 GEG = GEG + GEG2                                                  RKR  343
D 272 VMIN = BS                                                         RKR  344
      IF (IOPFG) 273,274,273                                            RKR  345
  273 CALL TIME (AFTEA)                                                 RKR  346
      XTIQ = (AFTEA-BEGIA)*60.                                          RKR  347
```

Table I. (Contd.)

```
      BEGIA = AFTEA                                                     RKR  348
      WRITEOUTPUTTAPE6,110,FEG,GEG,XTIQ                                 RKR  349
  110 FORMAT (6X6HFEG = 1PE15.7, 8H, GEG = E15.7,10X9HREQUIRED 0PF8.5,  RKR  350
     Z        9H SECONDS.)                                              RKR  351
  274 IF (LT-20) 226,226,290                                            RKR  352
  276 F = FEG * FAC                                                     RKR  353
      GF = GEG / FAC                                                    RKR  354
      RMAX(I) = SQRTF(F*F + F/GF) + F                                   RKR  355
      RMIN(I) = RMAX(I) - 2.*F                                          RKR  356
      CALL TIME(AFTER)                                                  RKR  357
      XTIQ = 60.*(AFTER-BEGIN)                                          RKR  358
      BEGIN = AFTER                                                     RKR  359
      WRITEOUTPUTTAPE6,104,TEMPI,U(I),RMIN(I),RMAX(I),XTIQ,BI(NGAS)     RKR  360
     Z                      ,F,GF                                      RKR  361
  104 FORMAT (10H0 FOR V = F7.3,6H, G = F10.3,14H 1/CM, RMIN = F10.7,   RKR  362
     Z        12H AND RMAX = F10.7,27H ANGSTROMS.  THIS REQUIRED F8.5,  RKR  363
     Z        9H SECONDS. / 20X12H ALSO, BV =  F12.7 /20X49H THE KLEIN ARKR  364
     ZCTION INTEGRALS F AND G ARE EQUAL TO   2E15.8///)                 RKR  365
      WRITEOUTPUTTAPE7,105,RMIN(I),U(I),RMAX(I),U(I)                    RKR  366
  105 FORMAT (1XF9.7,F10.3 / 1XF9.7,F10.3)                              RKR  367
  280 CONTINUE                                                          RKR  368
      DO 284 I = 1,N                                                    RKR  369
      Z(I) = Z(I+1)                                                     RKR  370
      Y(I) = Y(I+1)                                                     RKR  371
      BV(I) = BV(I+1)                                                   RKR  372
  284 CONTINUE                                                          RKR  373
      WRITEOUTPUTTAPE6,100                                              RKR  374
  286 RETURN                                                            RKR  375
  288 ZOC(1) = 6H EV1                                                   RKR  376
      ZOC(2) = 6HG(LEV)                                                 RKR  377
      ZOC(3) = 6HS.P.EV                                                 RKR  378
      ZOC(4) = 6HS.P.BV                                                 RKR  379
      ZOC(5) = 6HD.P.EV                                                 RKR  380
      ZOC(6) = 6HD.P.BV                                                 RKR  381
      ZOC(7) = 6H BV1                                                   RKR  382
      ZOC(8) = 6HG FILL                                                 RKR  383
      ZOC(9) = 6HBVFILL                                                 RKR  384
      WRITEOUTPUTTAPE6,102,ZOC(LOC),U(I)                                RKR  385
  102 FORMAT (26H0 NTRPDP UNSUCCESSFUL FOR A6, 11H, WHEN U =  E16.8)    RKR  386
      INTG = 1                                                          RKR  387
      GO TO 286                                                         RKR  388
  290 WRITEOUTPUTTAPE6,103                                              RKR  389
  103 FORMAT (20H0 TEG REACHED MAXIT    )                               RKR  390
      INTG = 1                                                          RKR  391
      GO TO 286                                                         RKR  392
  292 INTG = 1                                                          RKR  393
      WRITEOUTPUTTAPE6,111                                              RKR  394
  111 FORMAT (22H0 DENQ IS NOT POSITIVE)                                RKR  395
      GO TO 286                                                         RKR  396
  401 MX = MQ                                                           RKR  397
      DO 402 J = 1,MQ                                                   RKR  398
      UEV(J) = TMIN + FLOATF(J-1) * A                                   RKR  399
      EV(J) = GFUNCF(UEV(J))                                            RKR  400
  402 CONTINUE                                                          RKR  401
      GO TO 232                                                         RKR  402
  403 MX = MQ                                                           RKR  403
      DO 404 J = 1,MQ                                                   RKR  404
      UEV(J) = TMIN + FLOATF(J-1) * A                                   RKR  405
```

Table I. (Contd.)

```
      BI(J) = BFUNCF(UEV(J))                                    RKR  406
  404 CONTINUE                                                  RKR  407
      GO TO 236                                                 RKR  408
  405 CALL DGUNC (XG,DENQ,NGAS,TEMPI)                           RKR  409
      GO TO 311                                                 RKR  410
  407 DO 408 J = 1,NGAS                                         RKR  411
      BI(J) = BFUNCF(UEV(J))                                    RKR  412
  408 CONTINUE                                                  RKR  413
      GO TO 318                                                 RKR  414
      END                                                       RKR  415
```

Table I. (Contd.)


```
CNTRPSR  INTERPOLATION PROGRAM (BY SUCCESSIVE RANGES)  SINGLE PREC.      NTRPS000
C                                                                        NTRPS001
C       THE METHOD OF LAGRANGE IS USED.  THE INPUT POINTS NEED NOT BE    NTRPS002
C       EQUALLY SPACED.  THERE ARE TWO MODES OF INPUT AVAILABLE.  THE    NTRPS003
C       FIRST OCCURS WHEN M = 0.  THE ABSCISSAE ARE THEN GENERATED FROM  NTRPS004
C       XMIN,XMAX,AND XH.  AT EXIT M = NO. OF POINTS FOUND, AND XO       NTRPS005
C       CONTAINS THE ABSCISSAE.  M WILL BE CHECKED TO INSURE THAT THE    NTRPS006
C       DIMENSION IS NOT EXCEEDED.  MDIMM = THE DIMENSION OF THE XO, YO  NTRPS007
C       ARRAYS.  THE SECOND MODE OCCURS WHEN M IS POSITIVE.  THE M       NTRPS008
C       ABSCISSAE ARE THEN ASSUMED TO HAVE BEEN GENERATED PRIOR TO       NTRPS009
C       ENTRY.  THE STARTING INDEX FOR THE OUTPUT ARRAY MUST BE          NTRPS010
C       SPECIFIED.  THE FIRST POINT FOUND WILL BE AT XO(MBEG).  XH MUST  NTRPS011
C       BE GIVEN SINCE THE ORDINATE FOR ANY POINT CLOSER THAN .01*XH TO  NTRPS012
C       AN INPUT POINT IS TAKEN AS THAT FOR THE INPUT POINT.  -NUSED- IS NTRPS013
C       THE NUMBER OF POINTS USED FOR EACH INTERPOLATED POINT.  *NUSED*  NTRPS014
C       MUST BE EVEN AND LESS THAN OR EQUAL TO -N-.  NUSED = 8 IS        NTRPS015
C       SUGGESTED.  ANY POINT FARTHER THAN NUSED/2 POINTS FROM EITHER ENDNTRPS016
C       IS FOUND FROM THE NUSED/2 ON EACH SIDE.  NTRPSR WILL SCALE AND   NTRPS017
C       RESCALE IN ORDER TO AVOID OVERFLOW.  IF THE FIRST SCALING DOES   NTRPS018
C       NOT SUCCEED, NTRPSR WILL TRY UP TO 7 TIMES MORE BEFORE RETURNING NTRPS019
C       IN THE ERROR MODE. (INSC = 1)                                    NTRPS020
C       INPUT IS  XI,YI,(XO),XH,N,M,(XMIN),(XMAX),MBEG,NUSED.            NTRPS021
C       OUTPUT IS  (XO),YO,INSC.                                         NTRPS022
C       INSC = 0 IF PROGRAM WAS SUCCESSFUL.  IF NOT, INSC = 1.           NTRPS023
C                                                                        NTRPS024
      SUBROUTINE NTRPSR(XJ,YJ,XO,YO,XN,N,K,XNIN,XNAX,INSC,MBEG,NUSED)    NTRPS025
      DIMENSION XI(200),YI(200),XO(3000),YO(3000),XJ(200),YJ(200),       NTRPS026
     Z          NUMB(200)                                               NTRPS027
      MDIMM = 3000                                                       NTRPS028
      XMAX = XNAX                                                        NTRPS029
      XMIN = XNIN                                                        NTRPS030
      XH = ABSF(XN)                                                      NTRPS031
      M = K                                                              NTRPS032
      IREV = 0                                                           NTRPS033
      IREX = 0                                                           NTRPS034
C     M IS ZERO, IF XH, XMIN, XMAX ARE TO BE USED.  IF M IS NOT = TO     NTRPS035
C     ZERO, THEN XO(I), I = 1,M WILL BE USED AS ABSCISSA.                NTRPS036
  200 IF (M) 270,201,206                                                 NTRPS037
  201 M = XINTF(ABSF((XMAX-XMIN)/XH)) + 1                                NTRPS038
C     IF M IS MORE THAN DIMENSION OF XO, RETURN IN ERROR MODE.           NTRPS039
      IF (M+MBEG-MDIMM-2) 202,272,272                                    NTRPS040
  202 MF = MBEG + M - 1                                                  NTRPS041
      IF (XMAX - XMIN) 203,204,204                                       NTRPS042
  203 XMIN = XNAX                                                        NTRPS043
      XMAX = XNIN                                                        NTRPS044
      IREV = 1                                                           NTRPS045
  204 DO 205 I = MBEG,MF                                                 NTRPS046
      XO(I) = FLOATF(I-MBEG) * XH + XMIN                                 NTRPS047
  205 CONTINUE                                                           NTRPS048
  206 DO 207 I = 1,N                                                     NTRPS049
      XI(I) = XJ(I)                                                      NTRPS050
  207 CONTINUE                                                           NTRPS051
      MF = MBEG + M - 1                                                  NTRPS052
      MSTA = MBEG                                                        NTRPS053
      NUST = NUSED/2                                                     NTRPS054
      NS = NUST + 1                                                      NTRPS055
      NF = N - NS + 1                                                    NTRPS056
      NFP = NF + 1                                                       NTRPS057
```

Table I. (Contd.)

```
      DO 208 I = NS,NFP                                                 NTRPS058
      NUMB(I) = 0                                                       NTRPS059
  208 CONTINUE                                                          NTRPS060
      IF (XO(MF) - XO(MBEG)) 209,211,211                                NTRPS061
  209 M2 = M/2                                                          NTRPS062
      M2F = MBEG + M2 - 1                                               NTRPS063
      DO 210 I = MBEG,M2F                                               NTRPS064
      K = MF + MBEG - I                                                 NTRPS065
      TEMP = XO(I)                                                      NTRPS066
      XO(I) = XO(K)                                                     NTRPS067
      XO(K) = TEMP                                                      NTRPS068
  210 CONTINUE                                                          NTRPS069
      IREV = 1                                                          NTRPS070
  211 IF (XI(N)-XI(1)) 212,216,216                                      NTRPS071
  212 N2 = N/2                                                          NTRPS072
      DO 214 I = 1,N2                                                   NTRPS073
      K = N + 1 - I                                                     NTRPS074
      TEMP = XJ(I)                                                      NTRPS075
      TEMS = YJ(I)                                                      NTRPS076
      XJ(I) = XJ(K)                                                     NTRPS077
      YJ(I) = YJ(K)                                                     NTRPS078
      XJ(K) = TEMP                                                      NTRPS079
      YJ(K) = TEMS                                                      NTRPS080
  214 CONTINUE                                                          NTRPS081
      IREX = 1                                                          NTRPS082
  216 IF (NF-NS) 236,218,218                                            NTRPS083
  218 DO 226 J = MBEG,MF                                                NTRPS084
      DO 224 I = NS,NF                                                  NTRPS085
  220 IF (XO(J) - XI(I)) 222,222,224                                    NTRPS086
  222 NUMB(I) = NUMB(I) + 1                                             NTRPS087
      GO TO 226                                                         NTRPS088
  224 CONTINUE                                                          NTRPS089
      NUMB(NFP) = NUMB(NFP) + 1                                         NTRPS090
  226 CONTINUE                                                          NTRPS091
      GO TO 238                                                         NTRPS092
  236 NUMB(NFP) = M                                                     NTRPS093
  238 M = 0                                                             NTRPS094
  239 DO 250 L = NS,NFP                                                 NTRPS095
      IF (NUMB(L)) 250,250,242                                          NTRPS096
  242 M = NUMB(L)                                                       NTRPS097
      NSTA = L - NUST                                                   NTRPS098
      GO TO 100                                                         NTRPS099
  246 IF (INSC) 274,248,274                                             NTRPS100
  248 MSTA = MSTA + M                                                   NTRPS101
  250 CONTINUE                                                          NTRPS102
  240 K = MSTA - MBEG                                                   NTRPS103
      IF (IREV) 256,256,252                                             NTRPS104
  252 M2F = K/2 + MBEG - 1                                              NTRPS105
      DO 254 I = MBEG,M2F                                               NTRPS106
      J = MF + MBEG - I                                                 NTRPS107
      TEMP = XO(I)                                                      NTRPS108
      TEMS = YO(I)                                                      NTRPS109
      XO(I) = XO(J)                                                     NTRPS110
      YO(I) = YO(J)                                                     NTRPS111
      XO(J) = TEMP                                                      NTRPS112
      YO(J) = TEMS                                                      NTRPS113
  254 CONTINUE                                                          NTRPS114
  256 IF (IREX) 262,262,258                                             NTRPS115
```

Table I. (Contd.)

```
  258 DO 260 I = 1,N2                                                   NTRPS116
      J = N + 1 - I                                                     NTRPS117
      TEMP = XJ(I)                                                      NTRPS118
      TEMS = YJ(I)                                                      NTRPS119
      XJ(I) = XJ(J)                                                     NTRPS120
      YJ(I) = YJ(J)                                                     NTRPS121
      XJ(J) = TEMP                                                      NTRPS122
      YJ(J) = TEMS                                                      NTRPS123
  260 CONTINUE                                                          NTRPS124
  262 RETURN                                                            NTRPS125
  270 WRITEOUTPUTTAPE6,2101                                             NTRPS126
 2101 FORMAT (44H0 ERROR IN INPUT TO NTRPSR.  M IS NEGATIVE.    )       NTRPS127
      INSC = 1                                                          NTRPS128
      GO TO 240                                                         NTRPS129
  272 H = (XMAX-XMIN)/FLOATF(MDIMM-MBEG)                                NTRPS130
      WRITEOUTPUTTAPE6,2102,H                                           NTRPS131
 2102 FORMAT (58H0 ERROR IN INPUT TO NTRPSR.  MINIMUM ALLOWABLE SPACING NTRPS132
     8IS     1PE12.3)                                                   NTRPS133
      INSC = 1                                                          NTRPS134
      GO TO 240                                                         NTRPS135
  274 WRITEOUTPUTTAPE6,2103,L                                           NTRPS136
 2103 FORMAT (43H0 INTR1 WAS UNABLE TO INTERPOLATE IN RANGE    I3)      NTRPS137
      GO TO 240                                                         NTRPS138
  100 NCON = 1                                                          NTRPS139
      REFA = 1.414214                                                   NTRPS140
      NFIN = NSTA + NUSED - 1                                           NTRPS141
      DO 98 I = NSTA,NFIN                                               NTRPS142
      XI(I) = XJ(I)                                                     NTRPS143
      YI(I) = YJ(I)                                                     NTRPS144
   98 CONTINUE                                                          NTRPS145
      NSTA1 = NSTA + 1                                                  NTRPS146
      XSCALE = (XI(NFIN) - XI(NSTA))/10.                                NTRPS147
      YMAX = YI(NSTA)                                                   NTRPS148
      YMIN = YI(NSTA)                                                   NTRPS149
 1001 DO 1002 I = NSTA1,NFIN                                            NTRPS150
      YMAX = MAX1F(YMAX,YI(I))                                          NTRPS151
      YMIN = MIN1F(YMIN,YI(I))                                          NTRPS152
 1002 CONTINUE                                                          NTRPS153
   91 YSCALE = YMAX - YMIN                                              NTRPS154
 1003 DO 1004 I = NSTA,NFIN                                             NTRPS155
      XI(I) = XI(I)/XSCALE                                              NTRPS156
      YI(I) = (YI(I)-YMIN)/YSCALE + .5                                  NTRPS157
 1004 CONTINUE                                                          NTRPS158
      XH = ABSF(XN)/XSCALE                                              NTRPS159
      MFIN = MSTA + M - 1                                               NTRPS160
      MTA = MSTA                                                        NTRPS161
 1005 EPSIL = .01*XH                                                    NTRPS162
  101 DO 110 II=  MTA,MFIN                                              NTRPS163
      XO(II) = XO(II)/XSCALE                                            NTRPS164
      YO(II) = 0.0                                                      NTRPS165
      PNUM = 1.0                                                        NTRPS166
 1011 DO 107 I = NSTA,NFIN                                              NTRPS167
C     FIND XO(II)-XI(I) FOR NUMERATOR AND CHECK FOR NEARNESS.           NTRPS168
      XNUM    = XO(II) - XI(I)                                          NTRPS169
 1012 IF (ABSF(XNUM   )-EPSIL) 102,102,103                              NTRPS170
  102 YO(II) = YI(I)                                                    NTRPS171
      GO TO 109                                                         NTRPS172
C     PNUM = PRODUCT OF ALL XNUM                                        NTRPS173
```

Table I. (Contd.)

```
  103 PNUM = PNUM*XNUM                                                  NTRPS174
C     CONSTRUCT DENOMINATOR AND SUM                                     NTRPS175
      PDEN = 1.0                                                        NTRPS176
  104 DO 106 J = NSTA,NFIN                                              NTRPS177
 1043 IF (I-J) 105,106,105                                              NTRPS178
  105 PDEN =       (XI(I) - XI(J))*PDEN                                 NTRPS179
 1051 IF QUOTIENT OVERFLOW 1103,106                                     NTRPS180
  106 CONTINUE                                                          NTRPS181
      DEN = PDEN*XNUM                                                   NTRPS182
      YO(II) = YI(I)/DEN + YO(II)                                       NTRPS183
      IF ACCUMULATOR OVERFLOW  1121, 107                                NTRPS184
  107 CONTINUE                                                          NTRPS185
      YO(II) = YO(II)*PNUM                                              NTRPS186
  109 YO(II) = (YO(II)-.5)*YSCALE + YMIN                                NTRPS187
      XO(II) = XO(II) * XSCALE                                          NTRPS188
  110 CONTINUE                                                          NTRPS189
      INSC = 0                                                          NTRPS190
      GO TO 246                                                         NTRPS191
 1103 WRITEOUTPUTTAPE6,1104,NCON,XSCALE                                 NTRPS192
      WRITEOUTPUTTAPE6,1108,II,I,J                                      NTRPS193
 1104 FORMAT (8H  NCON = I3, 11H, XSCALE =   F10.7)                     NTRPS194
 1108 FORMAT (26H  OVERFLOW OCCURRED AT II= I4,4H  I= I3,4H  J= I3)     NTRPS195
      NCON = NCON + 1                                                   NTRPS196
 1105 DO 1106 I = NSTA,NFIN                                             NTRPS197
      XI(I) = XI(I)/REFA                                                NTRPS198
 1106 CONTINUE                                                          NTRPS199
      XO(II) = XO(II) * XSCALE                                          NTRPS200
      MTA = II                                                          NTRPS201
      XH   = XH  /REFA                                                  NTRPS202
      XSCALE = XSCALE*REFA                                              NTRPS203
      IF (NCON-8)  1005,1005,1107                                       NTRPS204
 1107 INSC = 1                                                          NTRPS205
      GO TO 246                                                         NTRPS206
 1121 WRITEOUTPUTTAPE6,1122                                             NTRPS207
 1122 FORMAT (48H0 ACCUMULATOR OVERFLOW.  DEN MUST BE TOO SMALL.    )   NTRPS208
      INSC = 1                                                          NTRPS209
      GO TO 246                                                         NTRPS210
      FREQUENCY 1051(1,9),1001(50),1003(50),101(500),1011(50),          NTRPS211
     1  1012(0,0,1),104(50),1043(1,0,1)                                 NTRPS212
      END                                                               NTRPS213
```

Table I. (Contd.)

```
CNTRPDP  INTERPOLATION PROGRAM(BY SUCCESSIVE RANGES) DOUBLE PRECISION.  NTRPD000
C                                                                       NTRPD001
C       THE METHOD OF LAGRANGE IS USED.  THE INPUT POINTS NEED NOT BE   NTRPD002
C       EQUALLY SPACED.  THERE ARE TWO MODES OF INPUT AVAILABLE.  THE   NTRPD003
C       FIRST OCCURS WHEN M = 0.  THE ABSCISSAE ARE THEN GENERATED FROM NTRPD004
C       XMIN,XMAX,AND XH.  AT EXIT M = NO. OF POINTS FOUND, AND XO      NTRPD005
C       CONTAINS THE ABSCISSAE.  M WILL BE CHECKED TO INSURE THAT THE   NTRPD006
C       DIMENSION IS NOT EXCEEDED.  MDIMM = THE DIMENSION OF THE XO, YO NTRPD007
C       ARRAYS.  THE SECOND MODE OCCURS WHEN M IS POSITIVE.  THE M      NTRPD008
C       ABSCISSAE ARE THEN ASSUMED TO HAVE BEEN GENERATED PRIOR TO      NTRPD009
C       ENTRY.  THE STARTING INDEX FOR THE OUTPUT ARRAY MUST BE         NTRPD010
C       SPECIFIED.  THE FIRST POINT FOUND WILL BE AT XO(MBEG).  XH MUST NTRPD011
C       BE GIVEN SINCE THE ORDINATE FOR ANY POINT CLOSER THAN .01*XH TO NTRPD012
C       AN INPUT POINT IS TAKEN AS THAT FOR THE INPUT POINT.  -NUSED- IS NTRPD013
C       THE NUMBER OF POINTS USED FOR EACH INTERPOLATED POINT.  *NUSED* NTRPD014
C       MUST BE EVEN AND LESS THAN OR EQUAL TO -N-.  NUSED = 8 IS       NTRPD015
C       SUGGESTED.  ANY POINT FARTHER THAN NUSED/2 POINTS FROM EITHER ENDNTRPD016
C       IS FOUND FROM THE NUSED/2 ON EACH SIDE.  NTRPSR WILL SCALE AND  NTRPD017
C       RESCALE IN ORDER TO AVOID OVERFLOW.  IF THE FIRST SCALING DOES  NTRPD018
C       NOT SUCCEED, NTRPSR WILL TRY UP TO 7 TIMES MORE BEFORE RETURNING NTRPD019
C       IN THE ERROR MODE. (INSC = 1)                                   NTRPD020
C       INPUT IS  XI,YI,(XO),XH,N,M,(XMIN),(XMAX),MBEG,NUSED.           NTRPD021
C       OUTPUT IS  (XO),YO,INSC.                                        NTRPD022
C       INSC = 0 IF PROGRAM WAS SUCCESSFUL.  IF NOT, INSC = 1.          NTRPD023
C                                                                       NTRPD024
      SUBROUTINE NTRPDP(XJ,YJ,XO,YO,XN,N,K,XNIN,XNAX,INSC,MBEG,NUSED)   NTRPD025
D     DIMENSION XI(200),YI(200),XJ(200),YJ(200),XO(200),YO(200),XMIN(1),NTRPD026
     Z          XMAX(1),XNUM(1),EPSIL(1)                               NTRPD027
      DIMENSION NUMB(200)                                               NTRPD028
      MDIMM = 200                                                       NTRPD029
D     XMAX = XNAX                                                       NTRPD030
D     XMIN = XNIN                                                       NTRPD031
D     XH   = XN                                                         NTRPD032
      M = K                                                             NTRPD033
C     M IS ZERO, IF XH IS TO BE USED.  IF NOT, XH=(XMAX-XMIN)/(M-1).    NTRPD034
  200 IF (M) 270,201,205                                                NTRPD035
D 201 M =  INTF((XMAX - XMIN)/XH) + 1.                                  NTRPD036
C     IF M IS MORE THAN DIMENSION OF XO, RETURN IN ERROR MODE.          NTRPD037
  202 IF (M+MBEG-MDIMM-2) 203,272,272                                   NTRPD038
  203 MF = MBEG + M - 1                                                 NTRPD039
      DO 204 I = MBEG,MF                                                NTRPD040
D     XO(I) = FLOATF(I-MBEG) * XH + XMIN                                NTRPD041
  204 CONTINUE                                                          NTRPD042
  205 DO 206 I = 1,N                                                    NTRPD043
D     XI(I) = XJ(I)                                                     NTRPD044
  206 CONTINUE                                                          NTRPD045
      MF = MBEG + M - 1                                                 NTRPD046
      MSTA = MBEG                                                       NTRPD047
      NUST = NUSED/2                                                    NTRPD048
      NS = NUST + 1                                                     NTRPD049
      NF = N - NS + 1                                                   NTRPD050
      NFP = NF + 1                                                      NTRPD051
      DO 207 I = NS,NFP                                                 NTRPD052
      NUMB(I) = 0                                                       NTRPD053
  207 CONTINUE                                                          NTRPD054
  209 IF (NF-NS) 236,210,210                                            NTRPD055
  210 DO 226 J = MBEG,MF                                                NTRPD056
      DO 224 I = NS,NF                                                  NTRPD057
```

Table I. (Contd.)

```
  214 IF (XO(J) - XI(I)) 216,215,224                                    NTRPD058
  215 IF (XO(J+20 )-XI(I+200)) 216,216,224                              NTRPD059
  216 NUMB(I) = NUMB(I) + 1                                             NTRPD060
      GO TO 226                                                         NTRPD061
  224 CONTINUE                                                          NTRPD062
      NUMB(NFP) = NUMB(NFP) + 1                                         NTRPD063
  226 CONTINUE                                                          NTRPD064
      GO TO 238                                                         NTRPD065
  236 NUMB(NFP) = M                                                     NTRPD066
  238 M = 0                                                             NTRPD067
  239 DO 250 L = NS,NFP                                                 NTRPD068
      IF (NUMB(L)) 250,250,242                                          NTRPD069
  242 M = NUMB(L)                                                       NTRPD070
      NSTA = L - NUST                                                   NTRPD071
      GO TO 100                                                         NTRPD072
  246 IF (INSC) 274,248,274                                             NTRPD073
  248 MSTA = MSTA + M                                                   NTRPD074
  250 CONTINUE                                                          NTRPD075
  240 K = MSTA - MBEG                                                   NTRPD076
      RETURN                                                            NTRPD077
  270 WRITEOUTPUTTAPE6,2101                                             NTRPD078
 2101 FORMAT (44H0 ERROR IN INPUT TO NTRPSR.  M IS NEGATIVE.    )       NTRPD079
      INSC = 1                                                          NTRPD080
      GO TO 240                                                         NTRPD081
  272 H = (XMAX-XMIN)/FLOATF(MDIMM-MBEG)                                NTRPD082
      WRITEOUTPUTTAPE6,2102,H                                           NTRPD083
 2102 FORMAT (58H0 ERROR IN INPUT TO NTRPSR.  MINIMUM ALLOWABLE SPACING NTRPD084
     8IS      1PE12.3)                                                  NTRPD085
      INSC = 1                                                          NTRPD086
      GO TO 240                                                         NTRPD087
  274 WRITEOUTPUTTAPE6,2103,L                                           NTRPD088
 2103 FORMAT (43H0 INTR1 WAS UNABLE TO INTERPOLATE IN RANGE    I3)      NTRPD089
      GO TO 240                                                         NTRPD090
  100 NCON = 1                                                          NTRPD091
      REFA = 1.414214                                                   NTRPD092
      NFIN = NSTA + NUSED - 1                                           NTRPD093
      DO 98 I = NSTA,NFIN                                               NTRPD094
D     XI(I) = XJ(I)                                                     NTRPD095
D     YI(I) = YJ(I)                                                     NTRPD096
   98 CONTINUE                                                          NTRPD097
      NSTA1 = NSTA + 1                                                  NTRPD098
      XSCALE = (XI(NFIN) - XI(NSTA))/10.                                NTRPD099
      YMAX = YI(NSTA)                                                   NTRPD100
      YMIN = YI(NSTA)                                                   NTRPD101
 1001 DO 1002 I = NSTA1,NFIN                                            NTRPD102
      YMAX = MAX1F(YMAX,YI(I))                                          NTRPD103
      YMIN = MIN1F(YMIN,YI(I))                                          NTRPD104
 1002 CONTINUE                                                          NTRPD105
D  91 YSCALE = YMAX - YMIN                                              NTRPD106
 1003 DO 1004 I = NSTA,NFIN                                             NTRPD107
D     XI(I) = XI(I)/XSCALE                                              NTRPD108
D     YI(I) = (YI(I)-YMIN)/YSCALE + .5                                  NTRPD109
 1004 CONTINUE                                                          NTRPD110
D     XH   = XN  /XSCALE                                                NTRPD111
      MFIN = MSTA + M - 1                                               NTRPD112
      MTA = MSTA                                                        NTRPD113
D1005 EPSIL = .01*XH                                                    NTRPD114
  101 DO 110 II=  MTA,MFIN                                              NTRPD115
```

Table I. (Contd.)

```
D       XO(II) = XO(II)/XSCALE                                          NTRPD116
D       YO(II) = 0.0                                                    NTRPD117
D       PNUM = 1.0                                                      NTRPD118
 1011   DO 107 I = NSTA,NFIN                                            NTRPD119
C       FIND XO(II)-XI(I) FOR NUMERATOR AND CHECK FOR NEARNESS.         NTRPD120
D       XNUM     = XO(II) - XI(I)                                       NTRPD121
 1012   IF (ABSF(XNUM    )-EPSIL) 102,1013,103                          NTRPD122
 1013   IF (ABSF(XNUM(2))-EPSIL(2)) 102,102,103                         NTRPD123
D 102   YO(II) = YI(I)                                                  NTRPD124
        GO TO 109                                                       NTRPD125
C       PNUM = PRODUCT OF ALL XNUM                                      NTRPD126
D 103   PNUM = PNUM*XNUM                                                NTRPD127
C       CONSTRUCT DENOMINATOR AND SUM                                   NTRPD128
D       PDEN = 1.0                                                      NTRPD129
  104   DO 106 J = NSTA,NFIN                                            NTRPD130
 1043   IF (I-J) 105,106,105                                            NTRPD131
D 105   PDEN =       (XI(I) - XI(J))*PDEN                               NTRPD132
 1051   IF QUOTIENT OVERFLOW 1103,106                                   NTRPD133
  106   CONTINUE                                                        NTRPD134
D       DEN = PDEN*XNUM                                                 NTRPD135
D       YO(II) = YI(I)/DEN + YO(II)                                     NTRPD136
        IF ACCUMULATOR OVERFLOW  1121, 107                              NTRPD137
  107   CONTINUE                                                        NTRPD138
D       YO(II) = YO(II)*PNUM                                            NTRPD139
D 109   YO(II) = (YO(II)-.5)*YSCALE + YMIN                              NTRPD140
D       XO(II) = XO(II) * XSCALE                                        NTRPD141
  110   CONTINUE                                                        NTRPD142
        INSC = 0                                                        NTRPD143
        GO TO 246                                                       NTRPD144
 1103   WRITEOUTPUTTAPE6,1104,NCON,XSCALE                               NTRPD145
        WRITEOUTPUTTAPE6,1108,II,I,J                                    NTRPD146
 1104   FORMAT (8H  NCON = I3, 11H, XSCALE =   F10.7)                   NTRPD147
 1108   FORMAT (26H  OVERFLOW OCCURRED AT II= I4,4H  I= I3,4H  J= I3)   NTRPD148
        NCON = NCON + 1                                                 NTRPD149
 1105   DO 1106 I = NSTA,NFIN                                           NTRPD150
D       XI(I) = XI(I)/REFA                                              NTRPD151
 1106   CONTINUE                                                        NTRPD152
D       XO(II) = XO(II) * XSCALE                                        NTRPD153
        MTA = II                                                        NTRPD154
D       XH    = XH  /REFA                                               NTRPD155
D       XSCALE = XSCALE*REFA                                            NTRPD156
        IF (NCON-8)  1005,1005,1107                                     NTRPD157
 1107   INSC = 1                                                        NTRPD158
        GO TO 246                                                       NTRPD159
 1121   WRITEOUTPUTTAPE6,1122                                           NTRPD160
 1122   FORMAT (48H0 ACCUMULATOR OVERFLOW.  DEN MUST BE TOO SMALL.    )  NTRPD161
        INSC = 1                                                        NTRPD162
        GO TO 246                                                       NTRPD163
        FREQUENCY 1051(1,9),1001(50),1003(50),101(500),1011(50),        NTRPD164
       1  1012(0,0,1),104(50),1043(1,0,1)                               NTRPD165
        END                                                             NTRPD166
```

Table I. (Contd.)


```
CDGUNC   FINDS G(V) - G(V-X)                                            DGUNC000
      SUBROUTINE DGUNC (XG,DENQ,NGAS,TEMPI)                             DGUNC001
D     DIMENSION XG(20),DENQ(20)                                         DGUNC002
      DIMENSION UEV(3000),EV(3000),BV(200),BI(3000),TEMP(200),U(200),   DGUNC003
     Z          Y(200),Z(200)                                           DGUNC004
      COMMON Y,TEMP,UEV,EV,Q,NST,N,MST,M,XMIN,XMAX,INSC,MBEG,NUST ,BI,  DGUNC005
     Z       NI,NS,MAXIT,FACM,ZMU,DE,WE,WEXE,WEYE,WEZE,WETE,BE,ALPHAE, DGUNC006
     Z       GAMMAE,DELTAE,   VNIN,BQ,MQ,SPEP,   U,BV,Z,ICK,H,  K,HDES DGUNC007
     Z       ,EPSLNE                                                   DGUNC008
      V = TEMPI                                                         DGUNC009
      VA = V*V                                                          DGUNC010
      VB = VA*V                                                         DGUNC011
      VC = VB*V                                                         DGUNC012
  205 DO 210 I = 1,NGAS                                                 DGUNC013
D     Y = TEMPI - XG(I)                                                 DGUNC014
      X = Y                                                             DGUNC015
      XA = X*X                                                          DGUNC016
      XB = XA*X                                                         DGUNC017
      XC = XB*X                                                         DGUNC018
      DENQ(I) = WE*X + (XA-2.*V*X)*WEXE + ((VA*X-V*XA)*3.+XB) * WEYE    DGUNC019
     Z          + ((VB*X+V*XB)*4.-6.*VA*XA-XC) * WEZE                   DGUNC020
     Z          + ((VC*X-V*XC)*5.+(VA*XB-VB*XA)*10.) * WETE             DGUNC021
  210 CONTINUE                                                          DGUNC022
      RETURN                                                            DGUNC023
      END                                                               DGUNC024
```

```
CTIME                                                                   TIME 000
C     DISCARD THIS SUBROUTINE IF YOUR 709/7090/7094 INSTALLATION HAS    TIME 001
C     AN ON-LINE CLOCK ADDRESSABLE BY CALL TIME(X)                      TIME 002
      SUBROUTINE TIME(X)                                                TIME 003
1     X = 0.0                                                           TIME 004
      RETURN                                                            TIME 005
      END                                                               TIME 006
```

Table II. Sample data deck for RKR program.

```
*      DATA
1
1 RKR PROCEDURE APPLIED TO THE X STATE OF SILICON NITRIDE   TEST PROGRAM
 MOLECULAR CONSTANTS ARE TAKEN FROM JENKINS AND DE LASZLO
   2 9.33526
   1  10     (42H TURNING POINTS ARE GENERATED BY CONSTANTS)
 1151.680  6.560
2
   1  10     (42H TURNING POINTS ARE GENERATED BY CONSTANTS)
 0.7310     0.00567
2
1.5718
0.5        9.5        1.0
```

PROGRAM FOR CALCULATING RELATIVE INTENSITIES

Remarks

The input to this program is extremely flexible. The potential may be generated by subroutine POTGEN or may be read in. The output is Franck-Condon factors, relative intensities (quantum/sec) scaled to ten, relative intensities (energy/sec) scaled to ten, and the off-diagonal matrix elements $\langle v'J'|r|v''J''\rangle/\langle v'J'|v''J''\rangle$ and $\langle v'J'|r^2|v''J''\rangle/\langle v'J'|v''J''\rangle$, commonly known as the r-centroid and the square of the r-centroid. The heart of this program is subroutine SCHR which solves the radial Schrödinger equation for its eigenvalues and wavefunctions. This program has been described in detail elsewhere.[3] About 0.9 min is required to calculate all the above-named quantities for ten vibrational levels of the lower state with four vibrational levels of the upper state.[2]

Limitations

Presently the program will calculate at one time the Franck-Condon factors, etc., of only four specified vibrational levels of the upper state with the vibrational levels of the lower state. Also the same (J', J") pair must be used for each transition. This is due to lack of additional space in core storage. The program may be easily modified to allow more flexible usage.

Listing

Table III lists the source decks and Table IV gives a sample data deck for the relative-intensity program.

Table III. Source-deck listing for relative-intensity program.

```
CMAIN COMPUTES INTENSITY DISTRIBUTION FOR ELECTRONIC TRANSITIONS.        MAIN 000
C     THIS PROGRAM USES D2 NU SCHR AND SIMPSONS RULE TO FIND             MAIN 001
C     THE FRANCK CONDON OVERLAP FACTORS AND CORRECTS FOR                 MAIN 002
C     FREQUENCY DEPENDENCE AND SCALES TO TEN.                            MAIN 003
C     THE POTENTIAL MAY BE GENERATED INTERNALLY.  OTHERWISE              MAIN 004
C      POINTS ON THE POTENTIAL CURVE ARE READ IN.  THEY ARE INTERPOLATEDMAIN 005
C      TO ANY DESIRED SPACING (LESS THAN 2000 POINTS).  D2 NU SCHR       MAIN 006
C      IS USED TO FIND THE ENERGY LEVELS.  NTRPSR IS USED TO INTERPOLATEMAIN 007
C      THE GIVEN POTENTIAL POINTS.  THE 2 POINTS AT SMALLEST R ARE       MAIN 008
C      FITTED EXACTLY TO A FUNCTION OF THE FORM A/X**12+ C.  SIMILARLY   MAIN 009
C      THE TWO POINTS AT GREATEST R ARE FITTED EXACTLY TO A FUNCTION OF MAIN 010
C      THE FORM A/X**B.  THESE ARE THEN USED TO EXTRAPOLATE THE          MAIN 011
C      POTENTIAL TO THE GIVEN LIMITS.  A SUBROUTINE POTGEN MUST BE       MAIN 012
C      INCLUDED.  THIS WILL COMPUTE THE POTENTIAL CURVE OR WILL BE A     MAIN 013
C      DUMMY TO SATISFY ENTRY REQUIREMENTS.                              MAIN 014
C                                                                        MAIN 015
      DIMENSION XI(200,2),YI(200,2),XO(2000),V(2000,2),S(2000)           MAIN 016
     Z          ,SU(2000,4),ETRIAL(200,2)   ,QIRA(2),QIEN(3),QIMS(2)     MAIN 017
     Z          ,ZIMS(2),ZIRA(2),ZIEN(3),ECALC(200,2),XPRN(5),VPRN(5)    MAIN 018
     Z          ,DTFRMT(10),DUFMT(10),BVF(100,2),RESULT(100,4)           MAIN 019
     Z          ,KV(100,2),N(2),NL(2),DE(2),PRFMT(10),PNFT(4)            MAIN 020
     Z          ,DIV(4),WE(2),RE(2),RCNTRD(100,4),RRCN(100,4)            MAIN 021
     Z          ,DDIV(4)                                                 MAIN 022
      COMMON XI,YI,XO,V,XH,NSTA,N,MSTA,M,XMIN,XMAX,INSC,MBEG,NUSED,S,    MAIN 023
     Z       NI,NS,MAXIT,FACM,ZMU,DE,WE,WEXE,SU                          MAIN 024
C                                                                        MAIN 025
C      THE FOLLOWING COMMENT CARDS DESCRIBE THE PREPARATION OF DATA.     MAIN 026
C                                                                        MAIN 027
C      FIRST CARD IN DATA HAS A ONE IN COLUMN 1 IF A PROBLEM FOLLOWS.    MAIN 028
C      VERY LAST CARD IN DATA MUST BE A BLANK CARD.....                  MAIN 029
C                                                                        MAIN 030
    1 CALL TIME(BEGIN)                                                   MAIN 031
      WRITEOUTPUTTAPE6,160,BEGIN                                         MAIN 032
  160 FORMAT (9H0 TIME =   F10.5)                                        MAIN 033
      READINPUTTAPE5,100,ITEST                                           MAIN 034
  100 FORMAT (I1)                                                        MAIN 035
    2 IF (ITEST) 3,400,3                                                 MAIN 036
C                                                                        MAIN 037
C      NEXT  CARD IN DATA HAS NAME OF PROBLEM IN COLUMNS 1-72, WHERE     MAIN 038
C      CARRIAGE CONTROL IS IN COLUMN 1.  SECOND CARD HAS IIMS AND        MAIN 039
C      MASSES OF THE TWO ATOMS.                                          MAIN 040
C     IF ZMAS2 = 0, ZMAS1 IS TAKEN AS THE REDUCED MASS IN THE IIMS UNITSMAIN 041
C      IIMS = 1, MASS UNITS ARE BASED ON C12 = 12.                       MAIN 042
C      IIMS = 2, MASS UNITS ARE BASED ON O16 = 16.                       MAIN 043
C                                                                        MAIN 044
    3 READINPUTTAPE5,101                                                 MAIN 045
  101 FORMAT (72H1 PROBLEM NAME DATE                                     MAIN 046
     Z                                )                                  MAIN 047
      READINPUTTAPE5,102,IIMS,ZMAS1,ZMAS2                                MAIN 048
  102 FORMAT (I4,2F10.0)                                                 MAIN 049
C                                                                        MAIN 050
C      NEXT CARD IN DATA HAS IIRA, IIEN, AND THE NUMBER OF POINTS, EACH  MAIN 051
C      IN I4 FORMAT, AS WELL AS THE FORMAT STATEMENT WHICH CONTROLS THE  MAIN 052
C      READING OF THE POINTS (IN COLUMNS 13-72)--FOR EXAMPLE- (4E16.8).  MAIN 053
C      IIEN = 1, ENERGY IS IN ATOMIC UNITS.  (1 A.U. = 27.1961 E.V.)     MAIN 054
C      IIEN = 2, ENERGY IS IN 1/CM.                                      MAIN 055
C      IIEN = 3, ENERGY IS IN ELECTRON VOLTS.  ( 1 E.V. = 8065.68 1/CM)  MAIN 056
C      IIRA = 1, DISTANCE IS IN ATOMIC UNITS.  ( 1 A.U. = .529166 ANG.)  MAIN 057
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Table III. (Contd.)

```
C       IIRA = 2, DISTANCE IS IN ANGSTROMS.                                MAIN 058
C       FOLLOWING CARDS CONTAIN THE INPUT POTENTIAL POINTS.                MAIN 059
C       IF IT IS DESIRED TO USE A FUNCTION TO GENERATE THE WHOLE           MAIN 060
C       POTENTIAL CURVE, THE FIRST 12 COLUMNS OF THE IIRA, ETC. CARD       MAIN 061
C       MUST BE BLANK.  A HOLLERITH TEXT MUST BE PUNCHED IN 13-72, AS      MAIN 062
C       IT WILL BE PRINTED.  THE NEXT CARD IN SUCH A CASE CONTAINS         MAIN 063
C       XMIN,XMAX,ETC.                                                     MAIN 064
C      FIRST TIME THROUGH IS THE GROUND STATE                              MAIN 065
C      THE SECOND TIME THROUGH IS THE UPPER STATE                          MAIN 066
C      A MAXIMUM OF FOUR LEVELS OF THE UPPER STATE CAN BE USED IN          MAIN 067
C      COMPUTING INTENSITIES AT ONE TIME.                                  MAIN 068
C      THE SAME VALUE OF IIEN,IIRA,NDE,XH,XMIN,XMAX,IIRA1,NET              MAIN 069
C      ,IIEN1 MUST BE USED FOR BOTH THE GROUND AND UPPER STATE             MAIN 070
C                                                                          MAIN 071
       IKON = 1                                                            MAIN 072
     5 READINPUTTAPE5,103,IIRA,IIEN,N(IKON),(DTFRMT(I),I=1,10)             MAIN 073
   103 FORMAT (3I4, 10A6)                                                  MAIN 074
     6 IF (IIRA) 7,8,7                                                     MAIN 075
     7 NIKON = N(IKON)                                                     MAIN 076
       READINPUTTAPE5,DTFRMT,(XI(I,IKON),YI(I,IKON),I=1,NIKON)             MAIN 077
C                                                                          MAIN 078
C       NEXT CARD CONTAINS NDE AND THE DISSOCIATION ENERGY WHERE NDE IS    MAIN 079
C       ZERO IF ZERO PT OF POTENTIAL CURVE IS AT R=INFINITY, OR ONE IF ATMAIN 080
C       R=REQUILIBRIUM.  DISSOCIATION ENERGY HAS SAME UNITS AS POTENTIAL.MAIN 081
C                                                                          MAIN 082
       READINPUTTAPE5,105,NDE,DE(IKON)                                     MAIN 083
   105 FORMAT (I4,F10.0)                                                   MAIN 084
       GO TO 17                                                            MAIN 085
C                                                                          MAIN 086
C       NEXT DATA CARD CONTAINS XMIN,XMAX,XH,IIRA, WHERE IIRA GIVES THE    MAIN 087
C       UNITS FOR THE MIN AND MAX DISTANCES AND THE SPACING XH.            MAIN 088
C                                                                          MAIN 089
     8 READINPUTTAPE5,104,DE(IKON),WE(IKON),RE(IKON)                       MAIN 090
    17 READINPUTTAPE5,104,XMIN,XMAX,XH,IIRA1                               MAIN 091
104    FORMAT(3F10.0,I4)                                                   MAIN 092
C                                                                          MAIN 093
C       NEXT CARD HAS NO. AND IIEN OF EXPECTED ENERGY LEVELS, AND NET      MAIN 094
C       WHICH HAS THE SAME INTERPRETATION FOR ETRIAL(I) AS NDE DOES FOR    MAIN 095
C       THE POTENTIAL CURVE ABOVE.                                         MAIN 096
C      IT ALSO CONTAINS THE VARIABLE FORMAT FOR READING ENERGY LEVELS      MAIN 097
C                                                                          MAIN 098
       READINPUTTAPE5,106,NL(IKON),IIEN1,NET,(DUFMT(I),I=1,10)             MAIN 099
   106 FORMAT (3I4, 10A6)                                                  MAIN 100
       IF (NL) 15,15,14                                                    MAIN 101
    14 NLIKON = NL(IKON)                                                   MAIN 102
C                                                                          MAIN 103
C      READ IN ENERGY LEVELS                                               MAIN 104
C                                                                          MAIN 105
       READINPUTTAPE5,DUFMT,(KV(I,IKON),ETRIAL(I,IKON),I=1,NLIKON)         MAIN 106
C                                                                          MAIN 107
C      GO BACK TO STATEMENT 5 AND READ IN UPPER STATE                      MAIN 108
C                                                                          MAIN 109
    15 GO TO (1501,1502), IKON                                             MAIN 110
  1501 IKON = 2                                                            MAIN 111
       GO TO 5                                                             MAIN 112
C                                                                          MAIN 113
C      AFTER BOTH THE LOWER AND UPPER STATES ARE READ IN,                  MAIN 114
C      D2 NU SCHR MODIFIED FOR THE 709/7090/7094 IS DESCRIBED  IN          MAIN 115
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Table III. (Contd.)

```
C     R. N. ZARE AND J. K. CASHION, UCRL-10881, 1963                    MAIN 116
C     FOR THIS PROGRAM THE CONSTANTS ARE USED AS FOLLOWS                MAIN 117
C     IF NI = 1, PRINTS ITERATIONS, OTHERWISE NOT                       MAIN 118
C     IF NS = 1, PRINTS WAVEFUNCTION EVERY IPSIQ POINTS, OTHERWISE NOT  MAIN 119
C     IF NS = 33, PRINTS EIGENVALUES AND NODE COUNT                     MAIN 120
C     EPS IS THE CONVERGENCE CRITERION                                  MAIN 121
C     EPS IS IN THE SAME UNITS AS THE POTENTIAL CURVE                   MAIN 122
C     MAXIT IS THE MAXIMUM NUMBER OF TIMES SCHR WILL TRY TO SATISFY THE MAIN 123
C     CONVERGENCE CRITERION                                             MAIN 124
C                                                                       MAIN 125
1502  LLIM = 100                                                        MAIN 126
      KLIM = 2                                                          MAIN 127
      READ INPUT TAPE 5,107,NI,NS,IPSIQ,MAXIT,EPS                       MAIN 128
107   FORMAT(4I4,E10.0)                                                 MAIN 129
C                                                                       MAIN 130
C     NEXT TWO CARDS ARE THE VALUES OF J FOR THE LOWER AND UPPER STATE  MAIN 131
C                                                                       MAIN 132
      READINPUTTAPE5,144,JROTL,JROTU                                    MAIN 133
144   FORMAT(I3)                                                        MAIN 134
C                                                                       MAIN 135
C     NEXT SIX CARDS ARE THE ROTATIONAL CONSTANTS, BE, ALPHAE, GAMMAE,  MAIN 136
C     FOR THE LOWER AND UPPER STATES.                                   MAIN 137
C     THE ROTATIONAL CONSTANTS ARE IN WAVE NUMBERS                      MAIN 138
C                                                                       MAIN 139
      READ INPUT TAPE 5,2000,BE1,AE1,GE1,BE2,AE2,GE2                    MAIN 140
2000  FORMAT(E20.8)                                                     MAIN 141
C                                                                       MAIN 142
C     NEXT DATA CARD CONTAINS TE, OR THE CORRESPONDING QUANTITY IF THE  MAIN 143
C     FIRST POTENTIAL IS NOT THE GROUND STATE.  TE IS IN WAVE NUMBERS   MAIN 144
C                                                                       MAIN 145
      READ INPUT TAPE 5,2000,TE                                         MAIN 146
C                                                                       MAIN 147
C     NEXT CARD CONTAINS NPOT.                                          MAIN 148
C     THE POTENTIAL IS PRINTED AT EVERY NPOT POINT.                     MAIN 149
C     NPOT = 5 IS SUGGESTED TO THE USER.                                MAIN 150
C                                                                       MAIN 151
      READ INPUT TAPE 5,144,NPOT                                        MAIN 152
C                                                                       MAIN 153
C     THIS TERMINATES COMMENT CARDS ON THE PREPARATION OF DATA.         MAIN 154
C     IF NO FURTHER PROBLEMS FOLLOW, REMEMBER TO ADD A BLANK CARD TO THEMAIN 155
C     DATA DECK                                                         MAIN 156
C                                                                       MAIN 157
C                                                                       MAIN 158
      QIRA(1) = 6HA.U.                                                  MAIN 159
      QIRA(2) = 6HANGST.                                                MAIN 160
      QIEN(1) = 6HA.U.                                                  MAIN 161
      QIEN(2) = 6H1/CM                                                  MAIN 162
      QIEN(3) = 6HE.V.                                                  MAIN 163
      QIMS(1) = 6HC12=12                                                MAIN 164
      QIMS(2) = 6HO16=16                                                MAIN 165
      PRFMT(1) = 6H(1H06X                                               MAIN 166
      PRFMT(2) = 6H3HV--4                                               MAIN 167
      PRFMT(3) = 6H(11X5H                                               MAIN 168
      PRFMT(4) = 6HV- = I                                               MAIN 169
      PRFMT(5) = 6H3,11X)                                               MAIN 170
      PRFMT(6) = 3H//)                                                  MAIN 171
      PNFT(1)  = 6H3HV--1                                               MAIN 172
      PNFT(2)  = 6H3HV--2                                               MAIN 173
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Table III. (Contd.)

```
      PNFT(3)  = 6H3HV--3                                               MAIN 174
      PNFT(4)  = 6H3HV--4                                               MAIN 175
C                                                                       MAIN 176
C     OUTPUT IS IN WAVE NUMBERS AND ANGSTROMS                           MAIN 177
C      PRINT HEADING                                                    MAIN 178
C                                                                       MAIN 179
      WRITEOUTPUTTAPE6,101                                              MAIN 180
C                                                                       MAIN 181
C      PRINT THE MASSES AND THEIR UNITS.                                MAIN 182
C                                                                       MAIN 183
   10 IF (ZMAS2) 12,12,11                                               MAIN 184
   11 WRITEOUTPUTTAPE6,121,QIMS(IIMS),ZMAS1,ZMAS2                       MAIN 185
  121 FORMAT (///40H  THE MASSES OF THE TWO ATOMS, BASED ON A6, 6H, ARE MAIN 186
     Z        F10.6, 5H AND  F10.6///)                                  MAIN 187
      GO TO 20                                                          MAIN 188
   12 WRITEOUTPUTTAPE6,111,QIMS(IIMS),ZMAS1                             MAIN 189
  111 FORMAT (///46H  THE REDUCED MASS OF THE TWO ATOMS, BASED ON A6,   MAIN 190
     Z         5H, IS  F10.6///)                                        MAIN 191
C                                                                       MAIN 192
C      PRINT THE INPUT POTENTIAL, THE DISSOCIATION ENERGY, AND UNITS,   MAIN 193
C      IF READ IN.                                                      MAIN 194
C                                                                       MAIN 195
      IKON = 1                                                          MAIN 196
   20 IF (IIRA) 21,22,21                                                MAIN 197
   21 WRITEOUTPUTTAPE6,122,QIRA(IIRA),QIEN(IIEN)                        MAIN 198
  122 FORMAT (35H  THE INPUT POTENTIAL POINTS, R IN A6, 15H AND ENERGY IMAIN 199
     ZN  A6, 18H, ARE GIVEN BELOW.  // 1X 5(6X1HR10X1HV4X) //)          MAIN 200
      NIKON = N(IKON)                                                   MAIN 201
      WRITEOUTPUTTAPE6,114,(XI(I,IKON),YI(I,IKON),I=1,NIKON)            MAIN 202
  114 FORMAT (1X F10.6,F12.4,F10.6,F12.4,F10.6,F12.4,F10.6,F12.4,       MAIN 203
     Z        F10.6,F12.4)                                              MAIN 204
      WRITEOUTPUTTAPE6,123,DE(IKON)                                     MAIN 205
  123 FORMAT (47H0 DISSOCIATION ENERGY IN SAME UNITS AS ABOVE IS  E20.8)MAIN 206
      GO TO 23                                                          MAIN 207
   22 WRITEOUTPUTTAPE6,127                                              MAIN 208
  127 FORMAT (50H  THE POTENTIAL FUNTION IS GENERATED INTERNALLY.   )   MAIN 209
      WRITEOUTPUTTAPE6,DTFRMT                                           MAIN 210
C                                                                       MAIN 211
C      PRINT RMIN, RMAX, THE SPACING, AND THE UNITS.                    MAIN 212
C                                                                       MAIN 213
   23 WRITEOUTPUTTAPE6,124,XMIN,XMAX,XH,QIRA(IIRA1)                     MAIN 214
  124 FORMAT (//// 9H  RMIN = F10.7, 9H, RMAX = F10.7, 12H, SPACING =   MAIN 215
     Z         F10.7,  9H, ALL IN  A6)                                  MAIN 216
C                                                                       MAIN 217
C      PRINT THE TRIAL ENERGY LEVELS AND THEIR UNITS.                   MAIN 218
C                                                                       MAIN 219
      IF (NL) 25,25,24                                                  MAIN 220
   24 NLIKON = NL(IKON)                                                 MAIN 221
      WRITEOUTPUTTAPE6,125,QIEN(IIEN1),(KV(I,IKON),ETRIAL(I,IKON),I=1,NLMAIN 222
     1IKON)                                                             MAIN 223
  125 FORMAT (////29H  THE TRIAL ENERGY LEVELS IN A6,16HARE GIVEN BELOW.MAIN 224
     Z        //1X 5(5HLEVEL3X6HENERGY6X)//  (1H  I4,1PE16.7,I4,E16.7,  MAIN 225
     Z        I4,E16.7,I4,E16.7,I4,E16.7))                              MAIN 226
      GO TO 18                                                          MAIN 227
25    WRITEOUTPUTTAPE6,161,DE(IKON),WE(IKON),RE(IKON)                   MAIN 228
  161 FORMAT (7H  DE = F10.2,7H, WE = F10.3,11H, AND RE = F10.6)        MAIN 229
C                                                                       MAIN 230
C      PRINT THE CONVERGENCE CRITERION.                                 MAIN 231
```

Table III. (Contd.)

```
C                                                                       MAIN 232
   18 GO TO (1801,1802),IKON                                            MAIN 233
 1801 IKON = 2                                                          MAIN 234
      GO TO 20                                                          MAIN 235
 1802 WRITEOUTPUTTAPE6,126,EPS,QIEN(IIEN)                               MAIN 236
  126 FORMAT (////43H  CONVERGENCE CRITERION IS ERROR LESS THAN  E9.2,  MAIN 237
     Z        2XA6)                                                     MAIN 238
C                                                                       MAIN 239
C      PRINT HEADING                                                    MAIN 240
      WRITEOUTPUTTAPE6,101                                              MAIN 241
C                                                                       MAIN 242
  200 IF (ZMAS2) 201,201,202                                            MAIN 243
  201 ZMU = ZMAS1                                                       MAIN 244
      GO TO 204                                                         MAIN 245
  202 ZMU = ZMAS1*ZMAS2/(ZMAS1+ZMAS2)                                   MAIN 246
  204 ZIMS(1) = 1.0                                                     MAIN 247
      ZIMS(2) = .9996784                                                MAIN 248
      ZIRA(1) = 1.0                                                     MAIN 249
      ZIRA(2) = 1.889766                                                MAIN 250
      ZMU = ZMU * ZIMS(IIMS)                                            MAIN 251
      ZIEN(1) = ZMU * 3.643668E3                                        MAIN 252
      ZIEN(2) = ZMU * 1.6610826E-2                                      MAIN 253
      ZIEN(3) = ZMU * 1.339776E2                                        MAIN 254
      FACM = 60.201702/ZMU                                              MAIN 255
      IPOTGN = 0                                                        MAIN 256
      N2 = N(2)                                                         MAIN 257
      NL2 = NL(2)                                                       MAIN 258
  210 IF (IIRA) 214,212,214                                             MAIN 259
C      POTGEN MUST GENERATE THE ENTIRE POTENTIAL CURVE.  IN ADDITION,   MAIN 260
C      IT MUST SET THE VALUES OF IIRA,IIEN,M,NDE, AND DE.  NDE WILL BE  MAIN 261
C      USED TO SET THE HEIGHT OF THE POTENTIAL CURVE.                   MAIN 262
  212 CALL POTGEN (IPOTGN,DE,NDE,IIRA,IIEN,RE,ETRIAL,KV,NL,IIEN1,NET,WE,MAIN 263
     1ZMU,XMAX,XMIN,XH,FACM,XO,V,M)                                     MAIN 264
      IF(IPOTGN-10)213,213,1                                            MAIN 265
213   CALL POTGEN(IPOTGN,DE(2),NDE,IIRA,IIEN,RE(2),ETRIAL(1,2),KV(1,2), MAIN 266
     1NL(2),IIEN1,NET,WE(2),ZMU,XMAX,XMIN,XH,FACM,XO,V(1,2),M)          MAIN 267
      IF (IPOTGN - 10) 226,226,1                                        MAIN 268
  214 DO 216 I = 1,N                                                    MAIN 269
      YI(I) = YI(I)*ZIEN(IIEN)                                          MAIN 270
      XI(I) = XI(I)*ZIRA(IIRA)                                          MAIN 271
  216 CONTINUE                                                          MAIN 272
      DE = DE*ZIEN(IIEN)                                                MAIN 273
      DE(2) = DE(2)*ZIEN(IIEN)                                          MAIN 274
  220 DO 222 I = 1,N2                                                   MAIN 275
      YI(I,2) = YI(I,2) *ZIEN(IIEN)                                     MAIN 276
      XI(I,2) = XI(I,2)*ZIRA(IIRA)                                      MAIN 277
  222 CONTINUE                                                          MAIN 278
  226 XMIN = XMIN*ZIRA(IIRA1)                                           MAIN 279
      XMAX = XMAX*ZIRA(IIRA1)                                           MAIN 280
      XH   = XH  *ZIRA(IIRA1)                                           MAIN 281
      EPS = EPS * ZIEN(IIEN)                                            MAIN 282
      NL2 = NL(2)                                                       MAIN 283
      DO 235 I = 1,NL2                                                  MAIN 284
      ETRIAL(I,2) = ETRIAL(I,2)*ZIEN(IIEN1)                             MAIN 285
  235 CONTINUE                                                          MAIN 286
  236 DO 238 I = 1,NL                                                   MAIN 287
      ETRIAL(I) = ETRIAL(I)*ZIEN(IIEN1)                                 MAIN 288
  238 CONTINUE                                                          MAIN 289
```

Table III. (Contd.)

```
C       CHECK FOR RESCALING OF POTENTIAL TO ZERO AT R=INFINITY
  239 IF (NDE) 308,244,240
  240 IF (IPOTGN) 244,241,244
  241 DO 242 I = 1,N
      YI(I) = YI(I) - DE
  242 CONTINUE
      DO 243 I = 1,N2
      YI(I,2) = YI(I,2) - DE(2)
  243 CONTINUE
  244 IF (NET) 300,247,245
  245 DO 246 I = 1,NL
      ETRIAL(I) = ETRIAL(I)-DE+(BE1-AE1*(FLOATF(I-1)+.5)+GE1*(FLOATF(I-1
     1)+.5)**2)*FLOATF(JROTL*(JROTL+1))/FACM
  246 CONTINUE
      DO 2461 I = 1,NL2
      ETRIAL(I,2) = ETRIAL(I,2)-DE(2)+(BE2-AE2*(FLOATF(I-1)+.5)+GE2*(FLO
     1ATF(I-1)+.5)**2)*FLOATF(JROTU*(JROTU+1))/FACM
 2461 CONTINUE
  247 DO 248 I = 1,NL
      ECALC(I) = ETRIAL(I)
  248 CONTINUE
      DO 2481 I = 1,NL2
      ECALC(I,2) = ETRIAL(I,2)
 2481 CONTINUE
      IF(IPOTGN) 250,249,250
  249 NUSED = 8
      CALL TIME(AFTER)
      XTIQ = 60. * (AFTER-BEGIN)
      BEGIN = AFTER
      WRITEOUTPUTTAPE6,131,XTIQ
  131 FORMAT (23H0 TIME BEFORE POTFIT =   F10.5)
      IKON = 1
 2490 CALL POTFIT(XI(1,IKON),YI(1,IKON),N(IKON),XO,V(1,IKON),M,XH,
     Z              XMIN,XMAX,INSC,NUSED,FACM)
      IF (INSC) 1,2491,1
 2491 CALL TIME(AFTER)
      XTIQ = 60. * (AFTER-BEGIN)
      BEGIN = AFTER
      WRITEOUTPUTTAPE6,132,XTIQ
  132 FORMAT (20H0 TIME FOR POTFIT =  F10.5)
C
C       PRINT THE POTENTIAL CURVE GENERATED (ANGSTROMS AND 1/CM)
  250 WRITEOUTPUTTAPE6,108
  108 FORMAT (37H0 THE POTENTIAL FUNCTION GENERATED IS ///
     Z         1X 5(3X 4HR(A) 6X 7HV(1/CM) 2X))
  252 NPOT4 = NPOT*4
      NPOT5 = NPOT*5
  254 DO 270 I = 1,M,NPOT5
  256 IF (M-I-NPOT4) 258,262,262
  258 JFIN = (M-I)/NPOT
  260 IF (JFIN) 272,272,264
  262 JFIN = 5
  264 DO 266 J = 1,JFIN
      IPRN = I + NPOT*(J-1)
      XPRN(J) = XO(IPRN)*.529166
      VPRN(J) = (V(IPRN,IKON)+DE(IKON))*FACM
  266 CONTINUE
      IF (VPRN(1) - 1.E6) 268,269,269
```

Table III. (Contd.)

```
  269 WRITEOUTPUTTAPE6,141,(XPRN(J),VPRN(J),J=1,JFIN),IPRN                MAIN 348
  141 FORMAT (1X0PF10.6,1PE12.5,4(0PF10.6,1PE12.5),4XI5)                  MAIN 349
      GO TO 270                                                           MAIN 350
  268 WRITEOUTPUTTAPE6,109,(XPRN(J),VPRN(J),J=1,JFIN),IPRN                MAIN 351
  109 FORMAT (1X F10.6,F12.4,F10.6,F12.4,F10.6,F12.4,F10.6,F12.4,         MAIN 352
     Z        F10.6,F12.4,4XI5)                                           MAIN 353
  270 CONTINUE                                                            MAIN 354
  272 CALL TIME(AFTER)                                                    MAIN 355
      XTIQ = 60. * (AFTER-BEGIN)                                          MAIN 356
      BEGIN = AFTER                                                       MAIN 357
      WRITEOUTPUTTAPE6,135,XTIQ                                           MAIN 358
  135 FORMAT (32H0 TIME FOR PRINT OF POTENTIAL = F9.4,9H SECONDS.)        MAIN 359
      GO TO (2721,2729), IKON                                             MAIN 360
 2721 IKON = 2                                                            MAIN 361
      WRITEOUTPUTTAPE6,101                                                MAIN 362
      GO TO 2490                                                          MAIN 363
2729  DO 2728 J = 1,M                                                     MAIN 364
      V(J,1) = FLOATF(JROTL*(JROTL+1))/XO(J)**2+V(J,1)                    MAIN 365
      IF ACCUMULATOR OVERFLOW 2724,2725                                   MAIN 366
2724  V(J,1) = 1.0E+30                                                    MAIN 367
2725  V(J,2) = FLOATF(JROTU*(JROTU+1))/XO(J)**2+V(J,2)                    MAIN 368
      IF ACCUMULATOR OVERFLOW 2727,2728                                   MAIN 369
2727  V(J,2) = 1.0E+30                                                    MAIN 370
2728  CONTINUE                                                            MAIN 371
 2722 MTEMQ = M                                                           MAIN 372
      LLK = 0                                                             MAIN 373
      KLK = 0                                                             MAIN 374
C      FIND THE ENERGY LEVELS THROUGH USE OF SCHR.                        MAIN 375
  274 NLIKON = NL(IKON)                                                   MAIN 376
      DO 285 I = 1,NLIKON                                                 MAIN 377
  276 IF (SCHR(NI,NS,MAXIT,EPS,IPSIQ,V(1,IKON),XO,S ,M       ,XMIN,       MAIN 378
     Z        XMAX,KV(I,IKON),ECALC(I,IKON),FACM)-1.) 284,278,300        MAIN 379
  278 LLK = LLK + 1                                                       MAIN 380
  280 IF (LLK-LLIM) 284,284,304                                           MAIN 381
  284 M = MTEMQ                                                           MAIN 382
      DO 281 J = 1,M                                                      MAIN 383
      XO(J) = FLOATF(J-1)*XH + XMIN                                       MAIN 384
  281 CONTINUE                                                            MAIN 385
      BVSUM = S(1)**2/XO(1)**2 + 4.*S(2)**2/XO(2)**2 + S(M)**2/XO(M)**2 MAIN 386
      KSIMP = M - 1                                                       MAIN 387
      DO 287 J = 3,KSIMP,2                                                MAIN 388
      BVSUM = 2.*S(J)**2/XO(J)**2 + 4.*S(J+1)**2/XO(J+1)**2 + BVSUM       MAIN 389
  287 CONTINUE                                                            MAIN 390
      GO TO (2875,2871), IKON                                             MAIN 391
 2871 DO 2872 J = 1,M                                                     MAIN 392
      SU(J,I) = S(J)                                                      MAIN 393
 2872 CONTINUE                                                            MAIN 394
      GO TO 2878                                                          MAIN 395
 2875 DO 2877 IK = 1,NL2                                                  MAIN 396
      DO 2876 J = 1,M                                                     MAIN 397
      XO(J) = (FLOATF(J-1)*XH+XMIN)*SU(J,IK)                              MAIN 398
 2876 CONTINUE                                                            MAIN 399
 2879 CONTINUE                                                            MAIN 400
      CALL SIMP(S,SU(1,IK),M,XH,RESULT(I,IK))                             MAIN 401
      CALL SIMP(S,XO,M,XH,RCNTRD(I,IK))                                   MAIN 402
 2877 CONTINUE                                                            MAIN 403
      DO 2882 IK = 1,NL2                                                  MAIN 404
      DO 2881 J = 1,M                                                     MAIN 405
```

Table III. (Contd.)

```
      XO(J) = (FLOATF(J-1)*XH+XMIN)**2*SU(J,IK)                         MAIN 406
 2881 CONTINUE                                                          MAIN 407
      CALL SIMP(S,XO,M,XH,RRCN(I,IK))                                   MAIN 408
 2882 CONTINUE                                                          MAIN 409
 2878 BVF(I,IKON) = FACM * BVSUM * XH / 3.                              MAIN 410
      ECALC(I,IKON) = DE(IKON) * FACM + ECALC(I,IKON)                   MAIN 411
      CALL TIME(AFTER)                                                  MAIN 412
      XTIQ = 60. * (AFTER-BEGIN)                                        MAIN 413
      BEGIN = AFTER                                                     MAIN 414
      WRITEOUTPUTTAPE6,162,ECALC(I,IKON),BVF(I,IKON),XTIQ               MAIN 415
  162 FORMAT (30H0 SCHR FINDS ENERGY LEVEL G = F11.5,15H 1/CM AND BV =  MAIN 416
     Z        F11.7,9H 1/CM IN F7.4,9H SECONDS. )                      MAIN 417
  285 CONTINUE                                                          MAIN 418
      GO TO (2852,2851),IKON                                            MAIN 419
 2851 IKON = 1                                                          MAIN 420
      GO TO 2722                                                        MAIN 421
 2852 WRITEOUTPUTTAPE6,101                                              MAIN 422
      WRITEOUTPUTTAPE6,110,LLK                                          MAIN 423
  110 FORMAT (38H0 PROGRAM SUCCESSFUL.  (MAXIT REACHED  I2, 7H TIMES)  )MAIN 424
      WRITEOUTPUTTAPE6,128                                              MAIN 425
  128 FORMAT (35H0 THE BELOW IS FOR THE LOWER STATE. )                  MAIN 426
      WRITEOUTPUTTAPE6,133                                              MAIN 427
  133 FORMAT (54H0VIB. NO.   GIVEN ENERGY  CALC. ENERGY      DIFFERENCE MAIN 428
     Z        13X43HGIVEN DELTA G  CALC. DELTA G     DIFFERENCE /44X    MAIN 429
     Z        26HDIFFERENCE = CALC. - GIVEN //)                         MAIN 430
  286 DO 288 I = 1,NL                                                   MAIN 431
      ETRIAL(I) = (ETRIAL(I) + DE) * FACM                               MAIN 432
      DIFF = ECALC(I) - ETRIAL(I)                                       MAIN 433
      IF (I-1) 290,290,292                                              MAIN 434
  292 DGT = ETRIAL(I) - ETRIAL(I-1)                                     MAIN 435
      DGC = ECALC(I) - ECALC(I-1)                                       MAIN 436
      DIFDE = DGC - DGT                                                 MAIN 437
      WRITEOUTPUTTAPE6,136,DGT,DGC,DIFDE                                MAIN 438
  136 FORMAT (   64X3F15.5)                                             MAIN 439
  290 WRITEOUTPUTTAPE6,134,KV(I),ETRIAL(I),ECALC(I),DIFF                MAIN 440
  134 FORMAT (I8, 3F15.5)                                               MAIN 441
  288 CONTINUE                                                          MAIN 442
      WRITEOUTPUTTAPE6,130                                              MAIN 443
  130 FORMAT (1H128X8HVIB. NO.3X9HCALC.  BV //)                         MAIN 444
      DO 294 I = 1,NL                                                   MAIN 445
      WRITEOUTPUTTAPE6,129,KV(I),BVF(I)                                 MAIN 446
  129 FORMAT (28XI7,3F15.8)                                             MAIN 447
  294 CONTINUE                                                          MAIN 448
      WRITEOUTPUTTAPE6,101                                              MAIN 449
      WRITEOUTPUTTAPE6,137                                              MAIN 450
  137 FORMAT (35H0 THE BELOW IS FOR THE UPPER STATE. )                  MAIN 451
      WRITEOUTPUTTAPE6,138                                              MAIN 452
  138 FORMAT (54H0VIB. NO.   GIVEN ENERGY  CALC. ENERGY      DIFFERENCE MAIN 453
     Z        /44X26HDIFFERENCE = CALC. - GIVEN //)                     MAIN 454
      DO 388 I = 1,NL2                                                  MAIN 455
      ETRIAL(I,2) = (ETRIAL(I,2) + DE(2)) * FACM                        MAIN 456
      DIFF = ECALC(I,2)-ETRIAL(I,2)                                     MAIN 457
      WRITEOUTPUTTAPE6,134,KV(I,2),ETRIAL(I,2),ECALC(I,2),DIFF          MAIN 458
  388 CONTINUE                                                          MAIN 459
      WRITEOUTPUTTAPE6,130                                              MAIN 460
      DO 394 I = 1,NL2                                                  MAIN 461
      WRITEOUTPUTTAPE6,129,KV(I,2),BVF(I,2)                             MAIN 462
  394 CONTINUE                                                          MAIN 463
```

Table III. (Contd.)

```
      DO 510 J = 1,NL                                                   MAIN 464
      DO 510 IK = 1,NL2                                                 MAIN 465
      RCNTRD(J,IK) = RCNTRD(J,IK)*0.529166/RESULT(J,IK)                 MAIN 466
      RRCN(J,IK) = RRCN(J,IK)*0.529166**2/RESULT(J,IK)                  MAIN 467
      RESULT(J,IK) = RESULT(J,IK)**2                                    MAIN 468
510   CONTINUE                                                          MAIN 469
      WRITE OUTPUT TAPE 6,500                                           MAIN 470
500   FORMAT(24H1 FRANCK-CONDON FACTORS       )                         MAIN 471
      PRFMT(2) = PNFT(NL2)                                              MAIN 472
      WRITE OUTPUT TAPE 6,PRFMT,(KV(J,2),J = 1,NL2)                     MAIN 473
      DO 520 J = 1,NL                                                   MAIN 474
      WRITE OUTPUT TAPE 6,508,KV(J),(RESULT(J,ILK),ILK = 1,NL2)         MAIN 475
508   FORMAT(6X,I4,4(10X,E10.4,10X))                                    MAIN 476
520   CONTINUE                                                          MAIN 477
      WRITE OUTPUT TAPE 6,514                                           MAIN 478
514   FORMAT(32H1 R-CENTROID FACTORS (ANGSTROMS)  )                     MAIN 479
      WRITE OUTPUT TAPE 6,PRFMT,(KV(J,2),J = 1,NL2)                     MAIN 480
      DO 516 J = 1,NL                                                   MAIN 481
      WRITE OUTPUT TAPE 6,508,KV(J),(RCNTRD(J,ILK),ILK = 1,NL2)         MAIN 482
516   CONTINUE                                                          MAIN 483
      WRITE OUTPUT TAPE 6,517                                           MAIN 484
517   FORMAT(17H1 R**2-CENTROIDS   )                                    MAIN 485
      WRITE OUTPUT TAPE 6,PRFMT,(KV(J,2),J = 1,NL2)                     MAIN 486
      DO 518 J = 1,NL                                                   MAIN 487
      WRITE OUTPUT TAPE 6,508,KV(J),(RRCN(J,ILK),ILK = 1,NL2)           MAIN 488
518   CONTINUE                                                          MAIN 489
C                                                                       MAIN 490
C     CORRECT FOR FREQUENCY DEPENDENCE                                  MAIN 491
C     AND SCALE TO TEN                                                  MAIN 492
C                                                                       MAIN 493
      DO 5121 IK = 1,NL2                                                MAIN 494
      DIV(IK) = 0.0                                                     MAIN 495
      DDIV(IK) = 0.0                                                    MAIN 496
      DO 5121 J = 1,NL                                                  MAIN 497
      RESULT(J,IK) = RESULT(J,IK)   *(TE+ECALC(IK,2)-ECALC(J,1))**3     MAIN 498
      RCNTRD(J,IK) = RESULT(J,IK)*(TE+ECALC(IK,2)-ECALC(J,1))           MAIN 499
5121  CONTINUE                                                          MAIN 500
      DO 5022 IK = 1,NL2                                                MAIN 501
      DO 5022 J = 1,NL                                                  MAIN 502
      DIV(IK) = MAX1F(DIV(IK),RESULT(J,IK))                             MAIN 503
      DDIV(IK) = MAX1F(DDIV(IK),RCNTRD(J,IK))                           MAIN 504
5022  CONTINUE                                                          MAIN 505
      DO 5023 IK = 1,NL2                                                MAIN 506
      DO 5023 J = 1,NL                                                  MAIN 507
      RESULT(J,IK) = RESULT(J,IK)/DIV(IK)*10.0                          MAIN 508
      RCNTRD(J,IK) = RCNTRD(J,IK)/DDIV(IK)*10.0                         MAIN 509
5023  CONTINUE                                                          MAIN 510
      WRITE OUTPUT TAPE 6,5024                                          MAIN 511
5024  FORMAT(48H1 RELATIVE INTENSITY(QUANTUM/SEC) SCALED TO TEN  )      MAIN 512
      WRITE OUTPUT TAPE 6,PRFMT,(KV(J,2),J = 1,NL2)                     MAIN 513
      DO 5026 J = 1,NL                                                  MAIN 514
      WRITE OUTPUT TAPE 6,509,KV(J),(RESULT(J,ILK),ILK = 1,NL2)         MAIN 515
509   FORMAT(6X,I4,4(12X,F6.3,12X))                                     MAIN 516
5026  CONTINUE                                                          MAIN 517
      WRITE OUTPUT TAPE 6,5030                                          MAIN 518
5030  FORMAT(47H1 RELATIVE INTENSITY(ENERGY/SEC) SCALED TO TEN  )       MAIN 519
      WRITE OUTPUT TAPE 6,PRFMT,(KV(J,2),J = 1,NL2)                     MAIN 520
      DO 5027 J = 1,NL                                                  MAIN 521
```

Table III. (Contd.)

```
      WRITE OUTPUT TAPE 6,509,KV(J),(RCNTRD(J,ILK),ILK = 1,NL2)          MAIN 522
5027  CONTINUE                                                           MAIN 523
      WRITE OUTPUT TAPE 6,5031                                           MAIN 524
5031  FORMAT(12H1 CONSTANTS )                                            MAIN 525
      WRITE OUTPUT TAPE 6,144,JROTL,JROTU                                MAIN 526
      WRITE OUTPUT TAPE 6,2000,TE,BE1,BE2,AE1,AE2,GE1,GE2                MAIN 527
      GO TO 1                                                            MAIN 528
  300 KLK = KLK + 1                                                      MAIN 529
  301 IF (KLK-KLIM) 284,302,302                                          MAIN 530
  302 WRITEOUTPUTTAPE6,112,KLIM                                          MAIN 531
  112 FORMAT (26H0 SCHR NOT SUCCESSFUL FOR I2, 28HTH TIME, GO TO NEXT PRMAIN 532
     ZOBLEM.  )                                                          MAIN 533
      GO TO 1                                                            MAIN 534
  304 WRITEOUTPUTTAPE6,113,LLIM,I                                        MAIN 535
  113 FORMAT (28H0 SCHR DID NOT CONVERGE FOR I2,17HTH TIME WHEN I = I3) MAIN 536
  306 GO TO 1                                                            MAIN 537
  308 WRITEOUTPUTTAPE6,120,NDE                                           MAIN 538
  120 FORMAT (25H0 ERROR IN INPUT.  NDE =    I10)                        MAIN 539
      GO TO 1                                                            MAIN 540
  400 CALL EXIT                                                          MAIN 541
      END                                                                MAIN 542
```

```
CPOTFIT  USING NTRPSR,MINFIT,MAXFIT                                      POTFT000
      SUBROUTINE POTFIT (XI,YI,N,XO,V,M,XH,XMIN,XMAX,INSC,NUSED,FACM)    POTFT001
      DIMENSION XI(400),YI(400),XO(2000),V(2000)                         POTFT002
  248 MBEG = 1                                                           POTFT003
      XMAXT = XMAX                                                       POTFT004
      XMINT = XMIN                                                       POTFT005
C      CHECK FOR EXTRAPOLATION AT SMALL R.                               POTFT006
  250 IF (XMIN - XI(1)) 252,254,254                                      POTFT007
  252 XMAX  = XI(1)                                                      POTFT008
      CALL MINFIT (XI,YI,N,XO,V,M,XH,XMIN,XMAX,INSC,FACM)                POTFT009
      IF (INSC) 712,253,712                                              POTFT010
  253 MT = M                                                             POTFT011
      XMIN = XO(MT) + XH                                                 POTFT012
      MBEG = M + 1                                                       POTFT013
C      PREPARE TO INTERPOLATE.                                           POTFT014
  254 M = 0                                                              POTFT015
      XMAX = XMAXT                                                       POTFT016
      NL = N-1                                                           POTFT017
  256 IF ( XMAX-XI(NL))260,260,258                                       POTFT018
  258 XMAX = XI(NL)                                                      POTFT019
  260 CALL NTRPSR(XI,YI,XO,V,XH,N,M,XMIN,XMAX,INSC,MBEG,NUSED)           POTFT020
C      CHECK FOR EXTRAPOLATION AT LARGE R.                               POTFT021
      IF (INSC) 712,262,712                                              POTFT022
  262 IF (XMAXT-XMAX) 267,267,264                                        POTFT023
  264 MBEG = M + MBEG                                                    POTFT024
      XMIN = XO(MBEG-1) + XH                                             POTFT025
      XMAX = XMAXT                                                       POTFT026
  266 CALL MAXFIT (XI,YI,N,XO,V,M,XH,XMIN,XMAX,INSC,FACM,MBEG)           POTFT027
  267 XMIN = XMINT                                                       POTFT028
      M = M + MBEG - 1                                                   POTFT029
  712 RETURN                                                             POTFT030
      END                                                                POTFT031
```

Table III. (Contd.)

```
CMINFIT          Y = A/X**12+ C                                          MINFT000
      SUBROUTINE MINFIT (X,Y,N,XO,V,M,XH,XMIN,XMAX,INSC,FACM)            MINFT001
      DIMENSION X (400),Y (400),XO(2000),V(2000)                         MINFT002
      R12FUF(X) = A/X**12 + C                                            MINFT003
      M = XFIXF((XMAX-XMIN)/XH) + 1                                      MINFT004
      A = (Y(1)-Y(2))/(1./X(1)**12 - 1./X(2)**12)                        MINFT005
      C = Y(1) - A/X(1)**12                                              MINFT006
  212 DO 214 I = 1,M                                                     MINFT007
      XO(I) = FLOATF(I-1)*XH + XMIN                                      MINFT008
      V (I) = R12FUF(XO(I))                                              MINFT009
  214 CONTINUE                                                           MINFT010
      A = A*FACM*.529166**12                                             MINFT011
      C = C*FACM                                                         MINFT012
      WRITEOUTPUTTAPE6,101,A,C                                           MINFT013
  101 FORMAT (70H0 LEFT END OF POTENTIAL FUNCTION IS FOUND FROM Y=A/X**1MINFT014
     Z2+C, WHERE A =  1PE14.7, 9H AND C = E14.7  )                       MINFT015
      RETURN                                                             MINFT016
      END                                                                MINFT017
```

```
CMAXFIT          Y = A/X**B                                              MAXFT000
      SUBROUTINE MAXFIT (X,Y,N,XO,V,M,XH,XMIN,XMAX,INSC,FACM,MBEG)       MAXFT001
      DIMENSION X (400),Y (400),XO(2000),V(2000)                         MAXFT002
      R6FUNF(X) = A/X**B                                                 MAXFT003
      L = N - 1                                                          MAXFT004
      B = LOGF(Y(L)/Y(N))/LOGF(X(N)/X(L))                                MAXFT005
      A = Y(N) * X(N)**B                                                 MAXFT006
      M = XFIXF((XMAX-XMIN)/XH) + 1                                      MAXFT007
      MFIN = MBEG + M - 1                                                MAXFT008
  202 DO 204 I = MBEG,MFIN                                               MAXFT009
      XO(I) = FLOATF(I-MBEG)*XH + XMIN                                   MAXFT010
      V(I) = R6FUNF(XO(I))                                               MAXFT011
  204 CONTINUE                                                           MAXFT012
      A = A*FACM*.529166**B                                              MAXFT013
      WRITEOUTPUTTAPE6,206,A,B                                           MAXFT014
  206 FORMAT (68H0 RIGHT END OF POTENTIAL FUNCTION IS FOUND FROM Y=A/X**MAXFT015
     ZB, WHERE A = E14.7,  9H AND B =  E14.7)                            MAXFT016
      RETURN                                                             MAXFT017
      END                                                                MAXFT018
```

Table III. (Contd.)

```
CNTRPSR  INTERPOLATION PROGRAM (BY SUCCESSIVE RANGES)  SINGLE PREC.     NTRPS000
C                                                                       NTRPS001
C       THE METHOD OF LAGRANGE IS USED.  THE INPUT POINTS NEED NOT BE   NTRPS002
C       EQUALLY SPACED.  THERE ARE TWO MODES OF INPUT AVAILABLE.  THE   NTRPS003
C       FIRST OCCURS WHEN M = 0.  THE ABSCISSAE ARE THEN GENERATED FROM NTRPS004
C       XMIN,XMAX,AND XH.  AT EXIT M = NO. OF POINTS FOUND, AND XO      NTRPS005
C       CONTAINS THE ABSCISSAE.  M WILL BE CHECKED TO INSURE THAT THE   NTRPS006
C       DIMENSION IS NOT EXCEEDED.  MDIMM = THE DIMENSION OF THE XO, YO NTRPS007
C       ARRAYS.  THE SECOND MODE OCCURS WHEN M IS POSITIVE.  THE M      NTRPS008
C       ABSCISSAE ARE THEN ASSUMED TO HAVE BEEN GENERATED PRIOR TO      NTRPS009
C       ENTRY.  THE STARTING INDEX FOR THE OUTPUT ARRAY MUST BE         NTRPS010
C       SPECIFIED.  THE FIRST POINT FOUND WILL BE AT XO(MBEG).  XH MUST NTRPS011
C       BE GIVEN SINCE THE ORDINATE FOR ANY POINT CLOSER THAN .01*XH TO NTRPS012
C       AN INPUT POINT IS TAKEN AS THAT FOR THE INPUT POINT.  -NUSED- IS NTRPS013
C       THE NUMBER OF POINTS USED FOR EACH INTERPOLATED POINT.  *NUSED* NTRPS014
C       MUST BE EVEN AND LESS THAN OR EQUAL TO -N-.  NUSED = 8 IS       NTRPS015
C       SUGGESTED.  ANY POINT FARTHER THAN NUSED/2 POINTS FROM EITHER ENDNTRPS016
C       IS FOUND FROM THE NUSED/2 ON EACH SIDE.  NTRPSR WILL SCALE AND  NTRPS017
C       RESCALE IN ORDER TO AVOID OVERFLOW.  IF THE FIRST SCALING DOES  NTRPS018
C       NOT SUCCEED, NTRPSR WILL TRY UP TO 7 TIMES MORE BEFORE RETURNING NTRPS019
C       IN THE ERROR MODE. (INSC = 1)                                   NTRPS020
C       INPUT IS  XI,YI,(XO),XH,N,M,(XMIN),(XMAX),MBEG,NUSED.           NTRPS021
C       OUTPUT IS  (XO),YO,INSC.                                        NTRPS022
C       INSC = 0 IF PROGRAM WAS SUCCESSFUL.  IF NOT, INSC = 1.          NTRPS023
C                                                                       NTRPS024
      SUBROUTINE NTRPSR(XJ,YJ,XO,YO,XN,N,K,XNIN,XNAX,INSC,MBEG,NUSED)   NTRPS025
      DIMENSION XI(400),YI(400),XO(2000),YO(2000),XJ(400),YJ(400),NUMB(4NTRPS026
     100)                                                               NTRPS027
      MDIMM = 2000                                                      NTRPS028
      XMAX = XNAX                                                       NTRPS029
      XMIN = XNIN                                                       NTRPS030
      XH = ABSF(XN)                                                     NTRPS031
      M = K                                                             NTRPS032
      IREV = 0                                                          NTRPS033
      IREX = 0                                                          NTRPS034
C     M IS ZERO, IF XH, XMIN, XMAX ARE TO BE USED.  IF M IS NOT = TO    NTRPS035
C     ZERO, THEN XO(I), I = 1,M WILL BE USED AS ABSCISSA.               NTRPS036
  200 IF (M) 270,201,206                                                NTRPS037
  201 M = XINTF(ABSF((XMAX-XMIN)/XH)) + 1                               NTRPS038
C     IF M IS MORE THAN DIMENSION OF XO, RETURN IN ERROR MODE.          NTRPS039
      IF (M+MBEG-MDIMM-2) 202,272,272                                   NTRPS040
  202 MF = MBEG + M - 1                                                 NTRPS041
      IF (XMAX - XMIN) 203,204,204                                      NTRPS042
  203 XMIN = XNAX                                                       NTRPS043
      XMAX = XNIN                                                       NTRPS044
      IREV = 1                                                          NTRPS045
  204 DO 205 I = MBEG,MF                                                NTRPS046
      XO(I) = FLOATF(I-MBEG) * XH + XMIN                                NTRPS047
  205 CONTINUE                                                          NTRPS048
  206 DO 207 I = 1,N                                                    NTRPS049
      XI(I) = XJ(I)                                                     NTRPS050
  207 CONTINUE                                                          NTRPS051
      MF = MBEG + M - 1                                                 NTRPS052
      MSTA = MBEG                                                       NTRPS053
      NUST = NUSED/2                                                    NTRPS054
      NS = NUST + 1                                                     NTRPS055
      NF = N - NS + 1                                                   NTRPS056
      NFP = NF + 1                                                      NTRPS057
```

Table III. (Contd.)

```
      DO 208 I = NS,NFP                                          NTRPS058
      NUMB(I) = 0                                                NTRPS059
  208 CONTINUE                                                   NTRPS060
      IF (XO(MF) - XO(MBEG)) 209,211,211                         NTRPS061
  209 M2 = M/2                                                   NTRPS062
      M2F = MBEG + M2 - 1                                        NTRPS063
      DO 210 I = MBEG,M2F                                        NTRPS064
      K = MF + MBEG - I                                          NTRPS065
      TEMP = XO(I)                                               NTRPS066
      XO(I) = XO(K)                                              NTRPS067
      XO(K) = TEMP                                               NTRPS068
  210 CONTINUE                                                   NTRPS069
      IREV = 1                                                   NTRPS070
  211 IF (XI(N)-XI(1)) 212,216,216                               NTRPS071
  212 N2 = N/2                                                   NTRPS072
      DO 214 I = 1,N2                                            NTRPS073
      K = N + 1 - I                                              NTRPS074
      TEMP = XJ(I)                                               NTRPS075
      TEMS = YJ(I)                                               NTRPS076
      XJ(I) = XJ(K)                                              NTRPS077
      YJ(I) = YJ(K)                                              NTRPS078
      XJ(K) = TEMP                                               NTRPS079
      YJ(K) = TEMS                                               NTRPS080
  214 CONTINUE                                                   NTRPS081
      IREX = 1                                                   NTRPS082
  216 IF (NF-NS) 236,218,218                                     NTRPS083
  218 DO 226 J = MBEG,MF                                         NTRPS084
      DO 224 I = NS,NF                                           NTRPS085
  220 IF(XO(J)-XJ(I))222,222,224                                 NTRPS086
  222 NUMB(I) = NUMB(I) + 1                                      NTRPS087
      GO TO 226                                                  NTRPS088
  224 CONTINUE                                                   NTRPS089
      NUMB(NFP) = NUMB(NFP) + 1                                  NTRPS090
  226 CONTINUE                                                   NTRPS091
      GO TO 238                                                  NTRPS092
  236 NUMB(NFP) = M                                              NTRPS093
  238 M = 0                                                      NTRPS094
  239 DO 250 L = NS,NFP                                          NTRPS095
      IF (NUMB(L)) 250,250,242                                   NTRPS096
  242 M = NUMB(L)                                                NTRPS097
      NSTA = L - NUST                                            NTRPS098
      GO TO 100                                                  NTRPS099
  246 IF (INSC) 274,248,274                                      NTRPS100
  248 MSTA = MSTA + M                                            NTRPS101
  250 CONTINUE                                                   NTRPS102
  240 K = MSTA - MBEG                                            NTRPS103
      IF (IREV) 256,256,252                                      NTRPS104
  252 M2F = K/2 + MBEG - 1                                       NTRPS105
      DO 254 I = MBEG,M2F                                        NTRPS106
      J = MF + MBEG - I                                          NTRPS107
      TEMP = XO(I)                                               NTRPS108
      TEMS = YO(I)                                               NTRPS109
      XO(I) = XO(J)                                              NTRPS110
      YO(I) = YO(J)                                              NTRPS111
      XO(J) = TEMP                                               NTRPS112
      YO(J) = TEMS                                               NTRPS113
  254 CONTINUE                                                   NTRPS114
  256 IF (IREX) 262,262,258                                      NTRPS115
```

Table III. (Contd.)

```
  258 DO 260 I = 1,N2                                                   NTRPS116
      J = N + 1 - I                                                     NTRPS117
      TEMP = XJ(I)                                                      NTRPS118
      TEMS = YJ(I)                                                      NTRPS119
      XJ(I) = XJ(J)                                                     NTRPS120
      YJ(I) = YJ(J)                                                     NTRPS121
      XJ(J) = TEMP                                                      NTRPS122
      YJ(J) = TEMS                                                      NTRPS123
  260 CONTINUE                                                          NTRPS124
  262 RETURN                                                            NTRPS125
  270 WRITEOUTPUTTAPE6,2101                                             NTRPS126
 2101 FORMAT (44H0 ERROR IN INPUT TO NTRPSR.  M IS NEGATIVE.    )       NTRPS127
      INSC = 1                                                          NTRPS128
      GO TO 240                                                         NTRPS129
  272 H = (XMAX-XMIN)/FLOATF(MDIMM-MBEG)                                NTRPS130
      WRITEOUTPUTTAPE6,2102,H                                           NTRPS131
 2102 FORMAT (58H0 ERROR IN INPUT TO NTRPSR.  MINIMUM ALLOWABLE SPACING NTRPS132
     8IS     1PE12.3)                                                   NTRPS133
      INSC = 1                                                          NTRPS134
      GO TO 240                                                         NTRPS135
  274 WRITEOUTPUTTAPE6,2103,L                                           NTRPS136
 2103 FORMAT (43H0 INTR1 WAS UNABLE TO INTERPOLATE IN RANGE    I3)      NTRPS137
      GO TO 240                                                         NTRPS138
  100 NCON = 1                                                          NTRPS139
      REFA = 1.414214                                                   NTRPS140
      NFIN = NSTA + NUSED - 1                                           NTRPS141
      DO 98 I = NSTA,NFIN                                               NTRPS142
      XI(I) = XJ(I)                                                     NTRPS143
      YI(I) = YJ(I)                                                     NTRPS144
   98 CONTINUE                                                          NTRPS145
      NSTA1 = NSTA + 1                                                  NTRPS146
      XSCALE = (XI(NFIN) - XI(NSTA))/10.                                NTRPS147
      IF (XSCALE) 995,991,995                                           NTRPS148
  991 XSCALE = 1.                                                       NTRPS149
  995 YMAX = YI(NSTA)                                                   NTRPS150
      YMIN = YI(NSTA)                                                   NTRPS151
 1001 DO 1002 I = NSTA1,NFIN                                            NTRPS152
      YMAX = MAX1F(YMAX,YI(I))                                          NTRPS153
      YMIN = MIN1F(YMIN,YI(I))                                          NTRPS154
 1002 CONTINUE                                                          NTRPS155
   91 YSCALE = YMAX - YMIN                                              NTRPS156
      IF (YSCALE) 915,915,1003                                          NTRPS157
  915 YSCALE = 1.                                                       NTRPS158
 1003 DO 1004 I = NSTA,NFIN                                             NTRPS159
      XI(I) = XI(I)/XSCALE                                              NTRPS160
      YI(I) = (YI(I)-YMIN)/YSCALE + .5                                  NTRPS161
 1004 CONTINUE                                                          NTRPS162
      XH = ABSF(XN)/XSCALE                                              NTRPS163
      MFIN = MSTA + M - 1                                               NTRPS164
      MTA = MSTA                                                        NTRPS165
 1005 EPSIL = .01*XH                                                    NTRPS166
  101 DO 110 II=  MTA,MFIN                                              NTRPS167
      XO(II) = XO(II)/XSCALE                                            NTRPS168
      YO(II) = 0.0                                                      NTRPS169
      PNUM = 1.0                                                        NTRPS170
 1011 DO 107 I = NSTA,NFIN                                              NTRPS171
C     FIND XO(II)-XI(I) FOR NUMERATOR AND CHECK FOR NEARNESS.           NTRPS172
      XNUM    = XO(II) - XI(I)                                          NTRPS173
```

Table III. (Contd.)

```
 1012 IF (ABSF(XNUM    )-EPSIL) 102,102,103                          NTRPS174
  102 YO(II) = YI(I)                                                 NTRPS175
      GO TO 109                                                      NTRPS176
C     PNUM = PRODUCT OF ALL XNUM                                     NTRPS177
  103 PNUM = PNUM*XNUM                                               NTRPS178
C     CONSTRUCT DENOMINATOR AND SUM                                  NTRPS179
      PDEN = 1.0                                                     NTRPS180
  104 DO 106 J = NSTA,NFIN                                           NTRPS181
 1043 IF (I-J) 105,106,105                                           NTRPS182
  105 PDEN =       (XI(I) - XI(J))*PDEN                              NTRPS183
 1051 IF QUOTIENT OVERFLOW 1103,106                                  NTRPS184
  106 CONTINUE                                                       NTRPS185
      DEN = PDEN*XNUM                                                NTRPS186
      YO(II) = YI(I)/DEN + YO(II)                                    NTRPS187
      IF ACCUMULATOR OVERFLOW  1121, 107                             NTRPS188
  107 CONTINUE                                                       NTRPS189
      YO(II) = YO(II)*PNUM                                           NTRPS190
  109 YO(II) = (YO(II)-.5)*YSCALE + YMIN                             NTRPS191
      XO(II) = XO(II) * XSCALE                                       NTRPS192
  110 CONTINUE                                                       NTRPS193
      INSC = 0                                                       NTRPS194
      GO TO 246                                                      NTRPS195
 1103 WRITEOUTPUTTAPE6,1104,NCON,XSCALE                              NTRPS196
      WRITEOUTPUTTAPE6,1108,II,I,J                                   NTRPS197
 1104 FORMAT (8H  NCON = I3, 11H, XSCALE =   F10.7)                  NTRPS198
 1108 FORMAT (26H  OVERFLOW OCCURRED AT II= I4,4H  I= I3,4H  J= I3)  NTRPS199
      NCON = NCON + 1                                                NTRPS200
 1105 DO 1106 I = NSTA,NFIN                                          NTRPS201
      XI(I) = XI(I)/REFA                                             NTRPS202
 1106 CONTINUE                                                       NTRPS203
      XO(II) = XO(II) * XSCALE                                       NTRPS204
      MTA = II                                                       NTRPS205
      XH    = XH  /REFA                                              NTRPS206
      XSCALE = XSCALE*REFA                                           NTRPS207
      IF (NCON-8)  1005,1005,1107                                    NTRPS208
 1107 INSC = 1                                                       NTRPS209
      GO TO 246                                                      NTRPS210
 1121 WRITEOUTPUTTAPE6,1122                                          NTRPS211
 1122 FORMAT (48H0 ACCUMULATOR OVERFLOW.  DEN MUST BE TOO SMALL.    )NTRPS212
      INSC = 1                                                       NTRPS213
      GO TO 246                                                      NTRPS214
      FREQUENCY 1051(1,9),1001(50),1003(50),101(500),1011(50),       NTRPS215
     1  1012(0,0,1),104(50),1043(1,0,1)                              NTRPS216
      END                                                            NTRPS217
```

Table III. (Contd.)

```
CSIMP                                                                   SIMPS000
C     INTEGRATION OF A PRODUCT S*SS BY SIMPSONS RULE.                   SIMPS001
      SUBROUTINE SIMP(S,SS,N,H,RESULT)                                  SIMPS002
      DIMENSION S(2000),SS(2000)                                        SIMPS003
      SUM = 0.0                                                         SIMPS004
      DO 1 J = 2,N,2                                                    SIMPS005
1     SUM = SUM + 2.0*S(J)*SS(J) + 4.0*S(J-1)*SS(J-1)                   SIMPS006
      RESULT = SUM*H/3.0                                                SIMPS007
      RETURN                                                            SIMPS008
      END                                                               SIMPS009
```

```
CTIME                                                                   TIME 000
C     DISCARD THIS SUBROUTINE IF YOUR 709/7090/7094 INSTALLATION HAS    TIME 001
C     AN ON-LINE CLOCK ADDRESSABLE BY CALL TIME(X)                      TIME 002
      SUBROUTINE TIME(X)                                                TIME 003
1     X = 0.0                                                           TIME 004
      RETURN                                                            TIME 005
      END                                                               TIME 006
```

```
CPOTGEN     THIS IS A DUMMY SUBROUTINE                                  POTGN000
C     POTGEN GENERATES THE POTENTIAL.                                   POTGN001
      SUBROUTINE POTGEN(IPOTGN,DE,NDE,IIRA,IIEN,RE,ETRIAL,KV,NL,IIEN1,  POTGN002
     Z                  NET,WE,ZMU,XMAX,XMIN,XH,FACM,XO,V,M)            POTGN003
1     IPOTGN = 10                                                       POTGN004
      RETURN                                                            POTGN005
      END                                                               POTGN006
```

Table III. (Contd.)

```
CSCHRV   PRINTS EVERY -IPSIQ-TH POINT OF THE WAVE FUNCTIONS.
C      RADIAL SOLUTION TO SCHRODINGER EQUATION SUBROUTINE
       FUNCTION SCHR (NI,NS,MAXIT,EPS,IPSIQ,V,P,S,N,RMIN,RMAX,KV,E0,FACM)
       DIMENSION V(2000,2),S(2000),P(2000),Y(3)
C       USE UNITS SUCH THAT SCHR EQN IS-PSI2 + (E-V)PSI = 0
C      NI=1, PRINT ITERATIONS
C      NI=OTHERWISE, DONT PRINT
C      NS=1, PRINT SOLUTIONS WITH EACH ENERGY LEVEL
C      NS=33, PRINT ENERGY LEVELS ONLY
C      NS=OTHERWISE, DONT PRINT
       IF(NI-1)6,4,6
   4   EPRIN = E0*FACM
       WRITEOUTPUTTAPE6,5,KV,EPRIN
   5   FORMAT (47H1SCHR- SOLUTION OF RADIAL SCHR. EQUATION FOR V= I3, 5X
      Z          7HETRIAL= 1PE15.7,  9H   (1/CM)   )
       WRITEOUTPUTTAPE6,3
   3   FORMAT(70H0 ITER          E                F(E)              DF(E)
      X      D(E)      )
   6   CALL EFMT(K)
       H = (RMAX-RMIN)/FLOATF(N-1)
       H2=H**2
   8   HV=H2/12.
       E=E0
       TEST = -1.
       DE=0.
C
C      START ITER LOOP
C
  12   DO 171 IT=1,MAXIT
C      .....START INWARD INTEGRATION
  30   P(N)=1.E-30
  32   GN=V(N)-E
  34   GI=V(N-1)-E
C      .....TEST IF E TOO HIGH
       IF(GI) 35, 36, 36
  35   WRITEOUTPUTTAPE6,899
 899   FORMAT(50H DIFFERENCE EQUATION SOLUTION TECHNIQUE FAILS          )
       SCHR = 2.
       GO TO 250
  36   P(N-1)=P(N)*EXPF(RMAX*SQRTF(GN)-(RMAX-H)*SQRTF(GI))
  38   Y=(1.-HV*GN)*P(N)
  40   Y(2)=(1.-HV*GI)*P(N-1)
C      .....INTEGRATE
       K=0
  44   M=N-2
  46   Y(3)=Y(2)+((Y(2)-Y)+H2*GI*P(M+1))
  48   GI=V(M)-E
  50   P(M)=Y(3)/(1.-HV*GI)
C      .....TEST FOR OVERFLOW
  52   IF(K)54,70,54
C      .....OVERFLOW
  54   K=0
       M1=M+1
       PM=P(M1)
  55   DO 56 J=M1,N
  56   P(J)=P(J)/PM
  58   Y=Y/PM
  60   Y(2)=Y(2)/PM
```

Table III. (Contd.)

```
 62    Y(3)=Y(3)/PM                                                    SCHRV058
       GI= V(M+1) - E                                                  SCHRV059
       GO TO 46                                                        SCHRV060
C      .....TEST FOR CROSSING PT.                                      SCHRV061
 70    IF(ABSF(P(M))-ABSF(P(M+1))    ) 90, 90, 72                      SCHRV062
72     IF(M-2)      90,90,81                                           SCHRV063
 81    Y= Y(2)                                                         SCHRV064
 82    Y(2)=Y(3)                                                       SCHRV065
 84    M=M-1                                                           SCHRV066
 86    GO TO 46                                                        SCHRV067
C                                                                      SCHRV068
 90    PM=P(M)                                                         SCHRV069
       MSAVE = M                                                       SCHRV070
 92    YIN=Y(2)/PM                                                     SCHRV071
 94    DO 96 J=M,N                                                     SCHRV072
 96    P(J)=P(J)/PM                                                    SCHRV073
C                                                                      SCHRV074
C      .....START OUTWARD INTEGRATION                                  SCHRV075
C                                                                      SCHRV076
 100   P(1)=1.E-20                                                     SCHRV077
 102   Y=0.                                                            SCHRV078
 104   GI=V-E                                                          SCHRV079
 106   Y(2)=(1.-HV*GI)*P                                               SCHRV080
       K = 0                                                           SCHRV081
 108   DO 132 I=2,M                                                    SCHRV082
 110   Y(3)=Y(2)+((Y(2)-Y)+H2*GI*P(I-1))                               SCHRV083
 112   GI=V(I)-E                                                       SCHRV084
 114   P(I)=Y(3)/(1.-HV*GI)                                            SCHRV085
C      .....TEST FOR OVERFLOW                                          SCHRV086
 116   IF(K)118,130,118                                                SCHRV087
 118   K=0                                                             SCHRV088
       I1=I-1                                                          SCHRV089
       PM=P(I1)                                                        SCHRV090
       DO 120 J=1,I1                                                   SCHRV091
 120   P(J)=P(J)/PM                                                    SCHRV092
 122   Y=Y/PM                                                          SCHRV093
 124   Y(2)=Y(2)/PM                                                    SCHRV094
 126   Y(3)=Y(3)/PM                                                    SCHRV095
       GI=V(I1)-E                                                      SCHRV096
       GO TO 110                                                       SCHRV097
C                                                                      SCHRV098
 130   Y=Y(2)                                                          SCHRV099
 132   Y(2)=Y(3)                                                       SCHRV100
C                                                                      SCHRV101
C      .....FINISHED OUTWARD INTEGRATION                               SCHRV102
 134   PM=P(M)                                                         SCHRV103
       IF(PM)135,149,135                                               SCHRV104
 135   YOUT=Y/PM                                                       SCHRV105
 136   YM=Y(3)/PM                                                      SCHRV106
 138   DO 140 J=1,M                                                    SCHRV107
 140   P(J)=P(J)/PM                                                    SCHRV108
C                                                                      SCHRV109
C      .....CORRECTION                                                 SCHRV110
C                                                                      SCHRV111
 142   DF=0.                                                           SCHRV112
 144   DO 146 J=1,N                                                    SCHRV113
 146   DF=DF-P(J)**2                                                   SCHRV114
 148   F=(-YOUT-YIN+2.*YM)/H2+(V(M)-E)                                 SCHRV115
```

Table III. (Contd.)

```
      DOLD=DE                                                           SCHRV116
      IF(K)149,150,149                                                  SCHRV117
 149  F=9.999999E+29                                                    SCHRV118
      DF=-F                                                             SCHRV119
      DE=ABSF(.0001*E)                                                  SCHRV120
      GO TO 152                                                         SCHRV121
 150  DE=-F/DF                                                          SCHRV122
 152  IF(NI-1)164,162,164                                               SCHRV123
 156  FORMAT( 1H0      I4, 2X,  1P4E16.7,5X,29H THE CROSSING PT. OCCURS ASCHRV124
     1T        I4)                                                      SCHRV125
  162 EPRIN  = E*FACM                                                   SCHRV126
      DEPRIN = DE*FACM                                                  SCHRV127
      WRITEOUTPUTTAPE6,156,IT,EPRIN,F,DF,DEPRIN,MSAVE                   SCHRV128
 164  EOLD = E                                                          SCHRV129
      E=E+DE                                                            SCHRV130
 166  TEST=MAX1F(ABSF(DOLD)-ABSF(DE),TEST)                              SCHRV131
 168  IF(TEST)171,170,170                                               SCHRV132
 170  IF( ABSF( E-EOLD) - ABSF(EPS))  172,172,171                       SCHRV133
 171  CONTINUE                                                          SCHRV134
      SCHR=1.                                                           SCHRV135
      GO TO 173                                                         SCHRV136
C     .....CONVERGED-COUNT NODES                                        SCHRV137
 172  SCHR=0.                                                           SCHRV138
 173  KV=0                                                              SCHRV139
      NL=N-2                                                            SCHRV140
 174  DO 192 J=3,NL                                                     SCHRV141
 176  IF(P(J))178,177,177                                               SCHRV142
 177  IF(P(J-1))180,192,192                                             SCHRV143
178   IF(P(J-1))192,270,184                                             SCHRV144
C     POS. NODE                                                         SCHRV145
 180  IF(P(J+1))192,182,182                                             SCHRV146
 182  IF(P(J-2))190,192,192                                             SCHRV147
C     NEG. NODE                                                         SCHRV148
 184  IF(P(J+1))186,192,192                                             SCHRV149
 186  IF(P(J-2))192,190,190                                             SCHRV150
C     FALSE NODE DUE TO UNDERFLOW                                       SCHRV151
270   IF(P(J+1))280,192,192                                             SCHRV152
280   IF(P(J-2))192,192,190                                             SCHRV153
 190  KV=KV+1                                                           SCHRV154
 192  CONTINUE                                                          SCHRV155
C     .....NORMALIZE                                                    SCHRV156
 200  SN=SQRTF(-H*DF)                                                   SCHRV157
 202  DO 204 J=1,N                                                      SCHRV158
 204  S(J)=P(J)/SN                                                      SCHRV159
C     .....PRINT SOLUTION                                               SCHRV160
 208  E = E*FACM                                                        SCHRV161
      IF(NS-1)236,210,236                                               SCHRV162
  210 IPSIA = IPSIQ * 300                                               SCHRV163
      IPSIB = IPSIQ *  49                                               SCHRV164
      IPSIC = IPSIQ * 250                                               SCHRV165
      IPSID = IPSIQ *  50                                               SCHRV166
      DO 234 JF=1,N,IPSIA                                               SCHRV167
 214  FORMAT(47H1SCHR- SOLUTION OF RADIAL SCHR. EQUATION FOR V= I3, 7H  SCHRV168
     X   E= 1PE15.7 /20H0   I        S(I)    5(20H    I        S(I)     ))SCHRV169
 218  WRITEOUTPUTTAPE6,214,KV,E                                         SCHRV170
 220  JL=XMINOF(JF+IPSIB,N)                                             SCHRV171
 222  DO 234 J=JF,JL,IPSIQ                                              SCHRV172
 224  IL=XMINOF(J+IPSIC,N)                                              SCHRV173
```

Table III. (Contd.)

```
 228  FORMAT(6(I5,1PE15.7))                                          SCHRV174
 232  WRITEOUTPUTTAPE6,228,(I,S(I),I=J,IL,IPSID)                     SCHRV175
 234  CONTINUE                                                       SCHRV176
 236  E0=E                                                           SCHRV177
      IF(NS-33) 874,875,874                                          SCHRV178
 875  WRITEOUTPUTTAPE6,876,KV,E                                      SCHRV179
876   FORMAT(50H0 SOLUTION OF RADIAL SCHRODINGER EQUATION FOR V = I3,  SCHRV180
     1 7H   E =  1PE15.7 )                                           SCHRV181
874   CONTINUE                                                       SCHRV182
 250  RETURN                                                         SCHRV183
      FREQUENCY 52(0,1,0),70(0,0,1),72(0,0,1),94(100),55(50),108(100),11SCHRV184
     16(0,1,0),138(100),144(200),152(1,0,0),          202(200)        SCHRV185
      END                                                            SCHRV186
```

Table III. (Contd.)

```
        COUNT   80                                                      EFMT 000
        LBL     EFMT                                                    EFMT 001
        REM NU EFM,EFM AND LFM FOR FORTRAN 2                            EFMT 002
        REM                                                             EFMT 003
        ENTRY EFM                                                       EFMT 004
        ENTRY EFMT                                                      EFMT 005
LFM     OCT 476000000004                                                EFMT 006
        TTR 1,4                                                         EFMT 007
EFMT    CLA 1,4                                                         EFMT 008
        STA SETN+1                                                      EFMT 009
        CLA TTR                                                         EFMT 010
        TXI EFM+1,4,-1                                                  EFMT 011
EFM     CLA HPR                                                         EFMT 012
        STO OVER+2                                                      EFMT 013
        OCT 476000000002                                                EFMT 014
SET .   CLA X                          TTR  ANALY                       EFMT 015
        STO 8                                                           EFMT 016
        TTR 1,4                                                         EFMT 017
X       TTR ANALY                                                       EFMT 018
ANALY   SXD SAVEX,1                                                     EFMT 019
        LXD 0,1                                                         EFMT 020
        TTR *+14,1                                                      EFMT 021
        TTR MQO                        MQ OVER                          EFMT 022
SAVEX   PZE                              SAVE  XA IN DEC.,THEN  ACC.    EFMT 023
        TTR ACMQ                         11                             EFMT 024
        TTR AC                            10                            EFMT 025
        TTR MQ                            9                             EFMT 026
ZERO    PZE                                                             EFMT 027
        TTR ACMQO                      AC AND MQ OVER                   EFMT 028
        TTR ACO                                                         EFMT 029
AC      CLA ZERO                                                        EFMT 030
        TTR RETRN                                                       EFMT 031
ACMQ    CLA ZERO                         3                              EFMT 032
        TTR MQ                                                          EFMT 033
MQ      LDQ ZERO                         1, MQ UNDER                    EFMT 034
RETRN   LXD SAVEX,1                                                     EFMT 035
        STO SAVEX                                                       EFMT 036
        CLA 0                                                           EFMT 037
        STA *+2                                                         EFMT 038
        CLA SAVEX                                                       EFMT 039
        TTR **                                                          EFMT 040
ACMQO   ORA MAX                                                         EFMT 041
MQO     STO SAVEA                                                       EFMT 042
        LLS 0                                                           EFMT 043
        LDQ MAX                                                         EFMT 044
        LRS 0                                                           EFMT 045
        TTR OVER+1                                                      EFMT 046
ACO     ORA MAX                                                         EFMT 047
OVER    STO SAVEA                                                       EFMT 048
        CLA 0                                                           EFMT 049
        HPR 63                         PAUSE OVERFLOW                   EFMT 050
        CLA SAVEA                      PRESS START TO CONTINUE          EFMT 051
        TTR RETRN                                                       EFMT 052
SAVEA   PZE                                                             EFMT 053
THREE   PZE 0,0,3                                                       EFMT 054
TTR     TTR SETN                                                        EFMT 055
HPR     HPR 63                                                          EFMT 056
SETN    ANA THREE                                                       EFMT 057
        STO -                                                           EFMT 058
        TTR OVER+3                                                      EFMT 059
MAX     OCT 377777777777                                                EFMT 060
        END                                                             EFMT 061
```

Table IV. Sample data deck for relative-intensity program.

```
*      DATA
1
1 SILICON NITRIDE INTENSITY DISTRIBUTION          TEST PROGRAM
   2  9.33526
   2   2  25     (2F10.0)
 1.3613170 12376.760
 1.3686189 11369.400
 1.3764643 10348.920
 1.3849046  9315.320
 1.3941121  8268.600
 1.4041987  7208.760
 1.4154399  6135.800
 1.4281304  5049.720
 1.4428560  3950.520
 1.4605683  2838.200
 1.4834289  1712.760
 1.5188710   574.200
 1.5718000     0.
 1.6311431   574.200
 1.6788244  1712.760
 1.7140474  2838.200
 1.7442476  3950.520
 1.7715936  5049.720
 1.7970281  6135.800
 1.8211572  7208.760
 1.8442578  8268.600
 1.8666328  9315.320
 1.8883695 10348.920
 1.9096753 11369.400
 1.9305798 12376.760
   1 50488.0
1.100      2.100      0.001          2
  10    2    1     (8XI2,F10.0)
          0   574.200
          1  1712.760
          2  2838.200
          3  3950.520
          4  5049.720
          5  6135.800
          6  7208.760
          7  8268.600
          8  9315.320
          9 10348.920
   2   2  25     (2F10.0)
 1.3841050 10068.404
 1.3882994  9287.577
 1.3935768  8499.421
 1.3999376  7699.832
 1.4074129  6885.047
 1.4160805  6051.643
 1.4261043  5196.535
 1.4377249  4316.981
 1.4514711  3410.577
 1.4682963  2475.260
 1.4903674  1509.307
 1.5254273   511.333
 1.5800000     0.
 1.6445856   511.333
```

Table IV. (Contd.)

```
 1.6996278   1509.307
 1.7421381   2475.260
 1.7798702   3410.577
 1.8149804   4316.981
 1.8484052   5196.535
 1.8806691   6051.643
 1.9119547   6885.047
 1.9423804   7699.832
 1.9719579   8499.421
 2.0006375   9287.577
 2.0283271  10068.404
   1  15872.0
1.100      2.100      0.001          2
   4    2    1     (8XI2,F10.0)
           0    511.333
           1   1509.307
           2   2475.260
           3   3410.577
   6    6   10   10 0.001


0.7310
0.00567

0.7235
0.01037

24300.0
  5
```

APPENDIX: COMPUTER OUTPUT OF SAMPLE DATA DECKS

Table V shows the computer output when the sample data deck given in Table II is run with the RKR program compiled from Table I; Table VI shows the computer output when the sample data deck given in Table IV is run with the relative-intensity program compiled from Table III.

Table V. RKR program output.

```
 RKR PROCEDURE APPLIED TO THE X STATE OF SILICON NITRIDE   TEST PROGRAM
MOLECULAR CONSTANTS ARE TAKEN FROM JENKINS AND DE LASZLO


 THE REDUCED MASS OF THE TWO ATOMS, BASED ON O16=16, IS   9.335260


TURNING POINTS ARE GENERATED BY CONSTANTS

 THE G(V) CURVE IS CONSTRUCTED FROM THE FOLLOWING INPUT DATA.

 WE =   1151.6800, WEXE =    6.5600, WEYE =.          , WEZE =.          , WETE =.
TURNING POINTS ARE GENERATED BY CONSTANTS

 THE BV(V) CURVE IS CONSTRUCTED FROM THE FOLLOWING INPUT DATA.

 BE = 7.31000E-01, ALPHAE = 5.6700E-03, GAMMAE =-0.        , DELTAE =-0.        , EPSLNE =-0.


 RKR PROCEDURE APPLIED TO THE X STATE OF SILICON NITRIDE   TEST PROGRAM
MOLECULAR CONSTANTS ARE TAKEN FROM JENKINS AND DE LASZLO

 NUSBC IN BESRKR =  8.

 THE G(V) VALUES USED BELOW ARE
  V          G          V          G          V          G          V          G          V          G          V          G

  0.         0.        0.500    574.2000    1.500    1712.7599    2.500    2838.1999    3.500    3950.5199    4.500    5049.7198
  5.500   6135.7999    6.500   7208.7599    7.500    8268.5997    8.500    9315.3197    9.500   10348.9197

 THE BV(V) VALUES USED BELOW ARE
  V         BV          V         BV          V         BV          V         BV          V         BV          V         BV

  0.      0.7310000    0.500   0.7281650    1.500   0.7224950    2.500   0.7168250    3.500   0.7111550    4.500   0.7054850
  5.500   0.6998150    6.500   0.6941450    7.500   0.6884750    8.500   0.6828050    9.500   0.6771350

 OUTPUT V,G--LEVELS AT WHICH TURNING POINTS ARE FOUND
  V          G          V          G          V          G          V          G          V          G          V          G

  0.500    574.2000    1.500   1712.7600    2.500   2838.2000    3.500   3950.5199    4.500   5049.7199    5.500   6135.7999
  6.500   7208.7599    7.500   8268.5999    8.500   9315.3198    9.500  10348.9198
```

Table V. (Contd.)

```
FOR V =   0.500, G =    574.200 1/CM, RMIN =  1.5188710 AND RMAX =  1.6311431 ANGSTROMS.  THIS REQUIRED  0.      SECONDS.
                ALSO, BV =    0.7281650
                THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.56136035E-01 0.22658374E-01

FOR V =   1.500, G =   1712.760 1/CM, RMIN =  1.4834289 AND RMAX =  1.6788244 ANGSTROMS.  THIS REQUIRED  0.      SECONDS.
                ALSO, BV =    0.7224950
                THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.97697736E-01 0.39229474E-01

FOR V =   2.500, G =   2838.200 1/CM, RMIN =  1.4605683 AND RMAX =  1.7140474 ANGSTROMS.  THIS REQUIRED  0.      SECONDS.
                ALSO, BV =    0.7168250
                THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.12673954E-00 0.50625280E-01

FOR V =   3.500, G =   3950.520 1/CM, RMIN =  1.4428560 AND RMAX =  1.7442476 ANGSTROMS.  THIS REQUIRED  0.      SECONDS.
                ALSO, BV =    0.7111550
                THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.15069580E-00 0.59878376E-01

FOR V =   4.500, G =   5049.720 1/CM, RMIN =  1.4281304 AND RMAX =  1.7715936 ANGSTROMS.  THIS REQUIRED  0.      SECONDS.
                ALSO, BV =    0.7054850
                THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.17173158E-00 0.67876304E-01

FOR V =   5.500, G =   6135.800 1/CM, RMIN =  1.4154399 AND RMAX =  1.7970281 ANGSTROMS.  THIS REQUIRED  0.      SECONDS.
                ALSO, BV =    0.6998150
                THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.19079412E-00 0.75009913E-01

FOR V =   6.500, G =   7208.760 1/CM, RMIN =  1.4041987 AND RMAX =  1.8211572 ANGSTROMS.  THIS REQUIRED  0.      SECONDS.
                ALSO, BV =    0.6941450
                THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.20847923E-00 0.81524249E-01

FOR V =   7.500, G =   8268.600 1/CM, RMIN =  1.3941121 AND RMAX =  1.8442578 ANGSTROMS.  THIS REQUIRED  0.      SECONDS.
                ALSO, BV =    0.6884750
                THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.22507283E-00 0.87539440E-01

FOR V =   8.500, G =   9315.320 1/CM, RMIN =  1.3849045 AND RMAX =  1.8666328 ANGSTROMS.  THIS REQUIRED  0.      SECONDS.
                ALSO, BV =    0.6828050
                THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.24086412E-00 0.93173706E-01

FOR V =   9.500, G =  10348.920 1/CM, RMIN =  1.3764643 AND RMAX =  1.8883695 ANGSTROMS.  THIS REQUIRED  0.      SECONDS.
                ALSO, BV =    0.6771350
                THE KLEIN ACTION INTEGRALS F AND G ARE EQUAL TO  0.25595257E-00 0.98470822E-01
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Table VI. Relative-intensity program output.

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SILICON NITRIDE INTENSITY DISTRIBUTION          TEST PROGRAM


THE REDUCED MASS OF THE TWO ATOMS, BASED ON O16=16, IS    9.335260


THE INPUT POTENTIAL POINTS, R IN ANGST. AND ENERGY IN 1/CM  , ARE GIVEN BELOW.

     R          V          R          V          R          V          R          V          R          V

 1.361317  12376.7599  1.368619  11369.3999  1.376464  10348.9199  1.384905   9315.3199  1.394112   8268.6000
 1.404199   7208.7599  1.415440   6135.8000  1.428130   5049.7200  1.442856   3950.5200  1.460568   2838.2000
 1.483429   1712.7600  1.518871    574.2000  1.571800      0.      1.631143    574.2000  1.678824   1712.7600
 1.714047   2838.2000  1.744248   3950.5200  1.771594   5049.7200  1.797028   6135.8000  1.821157   7208.7599
 1.844258   8268.6000  1.866633   9315.3199  1.888369  10348.9199  1.909675  11369.3999  1.930580  12376.7599

DISSOCIATION ENERGY IN SAME UNITS AS ABOVE IS       0.50488000E 05


RMIN =  1.1000000, RMAX =  2.1000000, SPACING =  0.0010000, ALL IN ANGST.


THE TRIAL ENERGY LEVELS IN 1/CM  ARE GIVEN BELOW.

LEVEL   ENERGY       LEVEL   ENERGY       LEVEL   ENERGY       LEVEL   ENERGY       LEVEL   ENERGY

  0   5.7419999E 02   1   1.7127600E 03   2   2.8382000E 03   3   3.9505200E 03   4   5.0497200E 03
  5   6.1358000E 03   6   7.2087600E 03   7   8.2686000E 03   8   9.3153199E 03   9   1.0348920E 04
THE INPUT POTENTIAL POINTS, R IN ANGST. AND ENERGY IN 1/CM  , ARE GIVEN BELOW.

     R          V          R          V          R          V          R          V          R          V

 1.384105  10068.4039  1.388299   9287.5769  1.393577   8499.4209  1.399938   7699.8320  1.407413   6885.0470
 1.416090   6051.6429  1.426104   5196.5350  1.437725   4316.9810  1.451471   3410.5770  1.468296   2475.2600
 1.490367   1509.3070  1.525427    511.3330  1.580000      0.      1.644586    511.3330  1.699628   1509.3070
 1.742138   2475.2600  1.779870   3410.5770  1.814980   4316.9810  1.848405   5196.5350  1.880669   6051.6429
 1.911955   6885.0470  1.942380   7699.8320  1.971958   8499.4209  2.000637   9287.5769  2.028327  10068.4039

DISSOCIATION ENERGY IN SAME UNITS AS ABOVE IS       0.15871999E 05


RMIN =  1.1000000, RMAX =  2.1000000, SPACING =  0.0010000, ALL IN ANGST.


THE TRIAL ENERGY LEVELS IN 1/CM  ARE GIVEN BELOW.

LEVEL   ENERGY       LEVEL   ENERGY       LEVEL   ENERGY       LEVEL   ENERGY       LEVEL   ENERGY

  0   5.1133299E 02   1   1.5093070E 03   2   2.4752600E 03   3   3.4105770E 03

CONVERGENCE CRITERION IS ERROR LESS THAN  1.00E-03  1/CM
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Table VI. (Contd.)

SILICON NITRIDE INTENSITY DISTRIBUTION TEST PROGRAM

TIME BEFORE POTFIT = 0.

LEFT END OF POTENTIAL FUNCTION IS FOUND FROM Y=A/X**12+C, WHERE A = 6.5624240E 05 AND C = -5.4312680E 04

RIGHT END OF POTENTIAL FUNCTION IS FOUND FROM Y=A/X**B, WHERE A = -0.1843505E 06 AND B = 0.2396292E 01

TIME FOR POTFIT = 0.

THE POTENTIAL FUNCTION GENERATED IS

R(A)	V(1/CM)	R(A)	V(1/CM)	R(A)	V(1/CM)	R(A)	V(1/CM)	R(A)	V(1/CM)	
1.100000	205274.6602	1.105000	194199.1992	1.110000	183756.4551	1.115000	173907.6738	1.120000	164616.6484	21
1.125000	155849.4902	1.130000	147574.5371	1.135000	139762.1484	1.140000	132384.6191	1.145000	125415.9453	46
1.150000	118831.8906	1.155000	112609.6572	1.160000	106727.9414	1.165000	101166.7441	1.170000	95907.3340	71
1.175000	90932.1533	1.180000	86224.7275	1.185000	81769.5977	1.190000	77552.2588	1.195000	73559.1143	96
1.200000	69777.3779	1.205000	66195.0381	1.210000	62800.8188	1.215000	59584.1284	1.220000	56535.0068	121
1.225000	53644.0840	1.230000	50902.5591	1.235000	48302.1587	1.240000	45835.0869	1.245000	43494.0078	146
1.250000	41272.0205	1.255000	39162.6240	1.260000	37159.6997	1.265000	35257.4858	1.270000	33450.5459	171
1.275000	31733.7578	1.280000	30102.3035	1.285000	28551.6296	1.290000	27077.4470	1.295000	25675.7041	196
1.300000	24342.5852	1.305000	23074.4841	1.310000	21867.9983	1.315000	20719.9128	1.320000	19627.2021	221
1.325000	18586.9966	1.330000	17596.5886	1.335000	16653.4219	1.340000	15755.0769	1.345000	14899.2701	246
1.350000	14083.8391	1.355000	13306.7396	1.360000	12566.0364	1.365000	11859.6443	1.370000	11185.7922	271
1.375000	10535.2366	1.380000	9907.3490	1.385000	9304.0481	1.390000	8725.9846	1.395000	8171.7239	296
1.400000	7639.0359	1.405000	7128.5466	1.410000	6641.1568	1.415000	6175.7377	1.420000	5730.6632	321
1.425000	5305.6486	1.430000	4900.7443	1.435000	4515.9811	1.440000	4150.6864	1.445000	3804.0929	346
1.450000	3475.4547	1.455000	3164.4078	1.460000	2870.5324	1.465000	2593.6631	1.470000	2333.3247	371
1.475000	2089.1022	1.480000	1860.5940	1.485000	1647.3567	1.490000	1448.9069	1.495000	1264.9209	396
1.500000	1095.0128	1.505000	938.8093	1.510000	795.9440	1.515000	666.0608	1.520000	548.8205	421
1.525000	443.9079	1.530000	350.9660	1.535000	269.6675	1.540000	199.6944	1.545000	140.7352	446
1.550000	92.4844	1.555000	54.6443	1.560000	26.9235	1.565000	9.0385	1.570000	0.7111	471
1.575000	1.6714	1.580000	11.6533	1.585000	30.3970	1.590000	57.6488	1.595000	93.1608	496
1.600000	136.6916	1.605000	188.0049	1.610000	246.8704	1.615000	313.0620	1.620000	386.3606	521
1.625000	466.5507	1.630000	553.4224	1.635000	646.7746	1.640000	746.4041	1.645000	852.1140	546
1.650000	963.7133	1.655000	1081.0151	1.660000	1203.8379	1.665000	1332.0043	1.670000	1465.3398	571
1.675000	1603.6760	1.680000	1746.8437	1.685000	1894.6728	1.690000	2047.0255	1.695000	2203.7491	596
1.700000	2364.6935	1.705000	2529.7126	1.710000	2698.6600	1.715000	2871.4026	1.720000	3047.8218	621
1.725000	3227.7375	1.730000	3411.0101	1.735000	3597.5085	1.740000	3787.1060	1.745000	3979.6739	646
1.750000	4175.0609	1.755000	4373.2339	1.760000	4574.1024	1.765000	4777.5763	1.770000	4983.5575	671
1.775000	5192.0093	1.780000	5402.7653	1.785000	5615.6592	1.790000	5830.5624	1.795000	6047.3519	696
1.800000	6265.8502	1.805000	6486.0188	1.810000	6707.8674	1.815000	6931.3579	1.820000	7156.4438	721
1.825000	7383.1766	1.830000	7611.3573	1.835000	7840.8148	1.840000	8071.4157	1.845000	8303.0166	746
1.850000	8535.4229	1.855000	8768.7688	1.860000	9003.0602	1.865000	9238.2977	1.870000	9474.4625	771
1.875000	9711.5092	1.880000	9949.3544	1.885000	10187.8752	1.890000	10426.9159	1.895000	10666.2990	796
1.900000	10905.8463	1.905000	11145.4172	1.910000	11385.3303	1.915000	11629.5367	1.920000	11871.5869	821
1.925000	12111.5048	1.930000	12349.3149	1.935000	12585.0442	1.940000	12818.7108	1.945000	13050.3424	846
1.950000	13279.9598	1.955000	13507.5880	1.960000	13733.2465	1.965000	13956.9574	1.970000	14178.7441	871
1.975000	14398.6281	1.980000	14616.6288	1.985000	14832.7671	1.990000	15047.0646	1.995000	15259.5416	896
2.000000	15470.2192	2.005000	15679.1121	2.010000	15886.2465	2.015000	16091.6366	2.020000	16295.3030	921
2.025000	16497.2644	2.030000	16697.5393	2.035000	16896.1458	2.040000	17093.1035	2.045000	17288.4270	946
2.050000	17482.1350	2.055000	17674.2454	2.060000	17864.7749	2.065000	18053.7412	2.070000	18241.1592	971
2.075000	18427.0457	2.080000	18611.4172	2.085000	18794.2893	2.090000	18975.6775	2.095000	19155.5991	996

TIME FOR PRINT OF POTENTIAL = 0. SECONDS.

Table VI. (Contd.)

SILICON NITRIDE INTENSITY DISTRIBUTION TEST PROGRAM

LEFT END OF POTENTIAL FUNCTION IS FOUND FROM Y=A/X**12+C, WHERE A = 1.0824779E 06 AND C = -2.7700926E 04

RIGHT END OF POTENTIAL FUNCTION IS FOUND FROM Y=A/X**B, WHERE A = -0.3839180E 07 AND B = 0.9183305E 01

TIME FOR POTFIT = 0.

THE POTENTIAL FUNCTION GENERATED IS

R(A)	V(1/CM)	R(A)	V(1/CM)	R(A)	V(1/CM)	R(A)	V(1/CM)	R(A)	V(1/CM)	
1.100000	333082.3633	1.105000	314813.2891	1.110000	297587.8828	1.115000	281342.2344	1.120000	266016.6016	21
1.125000	251555.0938	1.130000	237905.4766	1.135000	225018.8730	1.140000	212849.5664	1.145000	201354.6758	46
1.150000	190494.2188	1.155000	180230.5879	1.160000	170528.6445	1.165000	161355.3965	1.170000	152679.9531	71
1.175000	144473.3438	1.180000	136708.4023	1.185000	129359.6260	1.190000	122403.0869	1.195000	115816.3584	96
1.200000	109578.3477	1.205000	103669.2451	1.210000	98070.4512	1.215000	92764.4902	1.220000	87734.9346	121
1.225000	82966.3320	1.230000	78444.1611	1.235000	74154.7754	1.240000	70085.3184	1.245000	66223.6875	146
1.250000	62550.4990	1.255000	59079.0308	1.260000	55775.1885	1.265000	52637.4688	1.270000	49656.9048	171
1.275000	46825.0479	1.280000	44133.9478	1.285000	41576.0977	1.290000	39144.4199	1.295000	36832.2319	196
1.300000	34633.2397	1.305000	32541.4956	1.310000	30551.3860	1.315000	28657.6079	1.320000	26855.1719	221
1.325000	25139.3435	1.330000	22505.6565	1.335000	21949.8940	1.340000	20468.0662	1.345000	19056.4048	246
1.350000	17711.3440	1.355000	16429.5110	1.360000	15207.7144	1.365000	14042.9445	1.370000	12932.3400	271
1.375000	11873.1987	1.380000	10862.9611	1.385000	9884.9602	1.390000	9016.0759	1.395000	8309.4109	296
1.400000	7692.5469	1.405000	7136.3415	1.410000	6625.4777	1.415000	6150.2122	1.420000	5705.0557	321
1.425000	5285.9261	1.430000	4889.3934	1.435000	4513.5172	1.440000	4157.3465	1.445000	3820.1700	346
1.450000	3501.1172	1.455000	3199.1960	1.460000	2913.7604	1.465000	2644.3413	1.470000	2390.4904	371
1.475000	2151.8147	1.480000	1927.9307	1.485000	1718.4811	1.490000	1523.1176	1.495000	1341.4402	396
1.500000	1173.1340	1.505000	1017.8584	1.510000	875.2619	1.515000	744.9872	1.520000	626.6684	421
1.525000	519.9307	1.530000	424.1486	1.535000	339.1136	1.540000	264.4832	1.545000	199.8984	446
1.550000	145.0051	1.555000	99.4539	1.560000	62.9005	1.565000	35.0074	1.570000	15.4422	471
1.575000	3.8795	1.580000	-0.	1.585000	3.4838	1.590000	14.0346	1.595000	31.3561	496
1.600000	55.1595	1.605000	85.1637	1.610000	121.0958	1.615000	162.6906	1.620000	209.6907	521
1.625000	261.8468	1.630000	318.9180	1.635000	380.6708	1.640000	446.8798	1.645000	517.3263	546
1.650000	591.7890	1.655000	670.0799	1.660000	752.0042	1.665000	837.3752	1.670000	926.0130	571
1.675000	1017.7440	1.680000	1112.4018	1.685000	1209.8268	1.690000	1309.8631	1.695000	1412.3639	596
1.700000	1517.1881	1.705000	1624.2155	1.710000	1733.2920	1.715000	1844.2899	1.720000	1957.0878	621
1.725000	2071.5687	1.730000	2187.6226	1.735000	2305.1423	1.740000	2424.0285	1.745000	2544.1825	646
1.750000	2665.5164	1.755000	2787.9460	1.760000	2911.3916	1.765000	3035.7765	1.770000	3161.0305	671
1.775000	3287.0844	1.780000	3413.8755	1.785000	3541.3351	1.790000	3669.4180	1.795000	3798.0745	696
1.800000	3927.2545	1.805000	4056.9131	1.810000	4187.0065	1.815000	4317.4925	1.820000	4448.3563	721
1.825000	4579.5283	1.830000	4710.9673	1.835000	4842.6364	1.840000	4974.5016	1.845000	5106.5333	746
1.850000	5238.6945	1.855000	5370.9554	1.860000	5503.3289	1.865000	5635.8088	1.870000	5768.3916	771
1.875000	5901.0767	1.880000	6033.8647	1.885000	6166.7785	1.890000	6299.7972	1.895000	6432.9152	796
1.900000	6566.1324	1.905000	6699.4464	1.910000	6832.8605	1.915000	6966.3719	1.920000	7099.9904	821
1.925000	7233.7340	1.930000	7367.6164	1.935000	7501.6541	1.940000	7635.8669	1.945000	7770.2760	846
1.950000	7904.9041	1.955000	8039.7776	1.960000	8174.9232	1.965000	8310.3715	1.970000	8446.1519	871
1.975000	8582.2997	1.980000	8718.8488	1.985000	8855.8389	1.990000	8993.3083	1.995000	9131.3016	896
2.000000	9269.8649	2.005000	9417.9734	2.010000	9563.9174	2.015000	9706.2119	2.020000	9844.9547	921
2.025000	9980.2441	2.030000	10112.1746	2.035000	10240.8367	2.040000	10366.3202	2.045000	10488.7103	946
2.050000	10608.0906	2.055000	10724.5422	2.060000	10838.1436	2.065000	10948.9719	2.070000	11057.1008	971
2.075000	11162.6027	2.080000	11265.5474	2.085000	11366.0016	2.090000	11464.0341	2.095000	11559.7064	996

TIME FOR PRINT OF POTENTIAL = 0. SECONDS.

SCHR FINDS ENERGY LEVEL G = 510.74768 1/CM AND BV = 0.7183588 1/CM IN 0. SECONDS.

SCHR FINDS ENERGY LEVEL G = 1508.87561 1/CM AND BV = 0.7079762 1/CM IN 0. SECONDS.

SCHR FINDS ENERGY LEVEL G = 2475.04663 1/CM AND BV = 0.6975725 1/CM IN 0. SECONDS.

Table VI. (Contd.)

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SCHR FINDS ENERGY LEVEL G =  3410.83838 1/CM AND BV =  0.6871293 1/CM IN  0.    SECONDS.
SCHR FIND  ENERGY LEVEL G =   574.28906 1/CM AND BV =  0.7281663 1/CM IN  0.    SECONDS.
SCHR FINDS ENERGY LEVEL G =  1712.95313 1/CM AND BV =  0.7224968 1/CM IN  0.    SECONDS.
SCHR FINDS ENERGY LEVEL G =  2838.48242 1/CM AND BV =  0.7168278 1/CM IN  0.    SECONDS.
SCHR FINDS ENERGY LEVEL G =  3950.87549 1/CM AND BV =  0.7111584 1/CM IN  0.    SECONDS.
SCHR FINDS ENERGY LEVEL G =  5050.12109 1/CM AND BV =  0.7054850 1/CM IN  0.    SECONDS.
SCHR FINDS ENERGY LEVEL G =  6136.20654 1/CM AND BV =  0.6998171 1/CM IN  0.    SECONDS.
SCHR FINDS ENERGY LEVEL G =  7209.21094 1/CM AND BV =  0.6941557 1/CM IN  0.    SECONDS.
SCHR FINDS ENERGY LEVEL G =  8269.12012 1/CM AND BV =  0.6884710 1/CM IN  0.    SECONDS.
SCHR FINDS ENERGY LEVEL G =  9315.89746 1/CM AND BV =  0.6827840 1/CM IN  0.    SECONDS.
SCHR FINDS ENERGY LEVEL G = 10349.67578 1/CM AND BV =  0.6770849 1/CM IN  0.    SECONDS.
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SILICON NITRIDE INTENSITY DISTRIBUTION        TEST PROGRAM

PROGRAM SUCCESSFUL.  (MAXIT REACHED  0 TIMES)

THE BELOW IS FOR THE LOWER STATE.
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VIB. NO.	GIVEN ENERGY	CALC. ENERGY	DIFFERENCE DIFFERENCE = CALC. - GIVEN	GIVEN DELTA G	CALC. DELTA G	DIFFERENCE
0	574.20011	574.28906	0.08895			
				1138.56004	1138.66406	0.10402
1	1712.76016	1712.95313	0.19296			
				1125.44006	1125.52930	0.08923
2	2838.20023	2838.48242	0.28220			
				1112.31970	1112.39307	0.07336
3	3950.51993	3950.87549	0.35556			
				1099.20010	1099.24561	0.04550
4	5049.72003	5050.12109	0.40106			
				1086.07971	1086.08545	0.00574
5	6135.79974	6136.20654	0.40680			
				1072.96014	1073.00439	0.04425
6	7208.75989	7209.21094	0.45105			
				1059.83972	1059.90918	0.06946
7	8268.59961	8269.12012	0.52051			
				1046.72021	1046.77734	0.05713
8	9315.31982	9315.89746	0.57764			
				1033.59985	1033.77832	0.17847
9	10348.91968	10349.67578	0.75610			

Table VI. (Contd.) **UCRL-10925**

VIB. NO.	CALC. BV
0	0.72816626
1	0.72249678
2	0.71682784
3	0.71115841
4	0.70548503
5	0.69981708
6	0.69415566
7	0.68847096
8	0.68278404
9	0.67708492

SILICON NITRIDE INTENSITY DISTRIBUTION TEST PROGRAM

THE BELOW IS FOR THE UPPER STATE.

VIB. NO.	GIVEN ENERGY	CALC. ENERGY	DIFFERENCE DIFFERENCE = CALC. - GIVEN
0	511.33312	510.74768	-0.58544
1	1509.30696	1508.87561	-0.43135
2	2475.26004	2475.04663	-0.21341
3	3410.57684	3410.83838	0.26154

VIB. NO.	CALC. BV
0	0.71835880
1	0.70797616
2	0.69757245
3	0.68712933

Table VI. (Contd.)

FRANCK-CONDON FACTORS

V''	V' = 0	V' = 1	V' = 2	V' = 3
0	0.9812E 00	0.1862E-01	0.9118E-04	0.4651E-04
1	0.1691E-01	0.9232E 00	0.5966E-01	0.2385E-07
2	0.1769E-02	0.5015E-01	0.8193E 00	0.1274E-00
3	0.8185E-04	0.7427E-02	0.9868E-01	0.6680E 00
4	0.4064E-05	0.5441E-03	0.1995E-01	0.1549E-00
5	0.1551E-06	0.3818E-04	0.2149E-02	0.4233E-01
6	0.1278E-07	0.2180E-05	0.2003E-03	0.6418E-02
7	0.3751E-09	0.1336E-06	0.1611E-04	0.7658E-03
8	0.1501E-09	0.1471E-07	0.8705E-06	0.8276E-04
9	0.4100E-09	0.3401E-08	0.1801E-06	0.4551E-05

R-CENTROID FACTORS (ANGSTROMS)

V''	V' = 0	V' = 1	V' = 2	V' = 3
0	0.1582E 01	0.1300E 01	0.2791E 01	0.1710E 01
1	0.1906E 01	0.1593E 01	0.1383E 01	0.1489E 03
2	0.1733E 01	0.1864E 01	0.1603E 01	0.1442E 01
3	0.1911E 01	0.1763E 01	0.1842E 01	0.1611E 01
4	0.1894E 01	0.1898E 01	0.1786E 01	0.1830E 01
5	0.2009E 01	0.1904E 01	0.1892E 01	0.1804E 01
6	0.1888E 01	0.1980E 01	0.1915E 01	0.1890E 01
7	0.2056E 01	0.1994E 01	0.1962E 01	0.1927E 01
8	0.1321E 01	0.1838E 01	0.2078E 01	0.1953E 01
9	0.1439E 01	0.1261E 01	0.1788E 01	0.2129E 01

R**2-CENTROIDS

V''	V' = 0	V' = 1	V' = 2	V' = 3
0	0.2503E 01	0.1611E 01	0.6121E 01	0.2761E 01
1	0.3532E 01	0.2542E 01	0.1872E 01	0.4512E 03
2	0.3044E 01	0.3406E 01	0.2579E 01	0.2059E 01
3	0.3587E 01	0.3137E 01	0.3341E 01	0.2609E 01
4	0.3615E 01	0.3560E 01	0.3209E 01	0.3311E 01
5	0.3977E 01	0.3640E 01	0.3550E 01	0.3268E 01
6	0.3616E 01	0.3890E 01	0.3673E 01	0.3552E 01
7	0.4176E 01	0.3977E 01	0.3838E 01	0.3711E 01
8	0.1626E 01	0.3451E 01	0.4265E 01	0.3812E 01
9	0.2080E 01	0.1449E 01	0.3291E 01	0.4440E 01

Table VI. (Contd.)

RELATIVE INTENSITY(QUANTUM/SEC) SCALED TO TEN

V''	V' = 0	V' = 1	V' = 2	V' = 3
0	10.000	0.232	0.001	0.001
1	0.149	10.000	0.836	0.000
2	0.013	0.471	10.000	2.188
3	0.001	0.060	1.044	10.000
4	0.000	0.004	0.182	2.011
5	0.000	0.000	0.017	0.474
6	0.000	0.000	0.001	0.062
7	0.000	0.000	0.000	0.006
8	0.000	0.000	0.000	0.001
9	0.000	0.000	0.000	0.000

RELATIVE INTENSITY(ENERGY/SEC) SCALED TO TEN

V''	V' = 0	V' = 1	V' = 2	V' = 3
0	10.000	0.243	0.002	0.001
1	0.142	10.000	0.875	0.000
2	0.012	0.449	10.000	2.291
3	0.000	0.054	0.996	10.000
4	0.000	0.003	0.165	1.918
5	0.000	0.000	0.014	0.431
6	0.000	0.000	0.001	0.053
7	0.000	0.000	0.000	0.005
8	0.000	0.000	0.000	0.000
9	0.000	0.000	0.000	0.000

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CONSTANTS
0
0
    0.24299999E 05
    0.73100000E 00
    0.72350000E 00
    0.56699999E-02
    0.10370000E-01
   -0.
   -0.

TIME =     0.
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REFERENCES

1. R. N. Zare, Lawrence Radiation Laboratory Report UCRL-11110, November 1963, J. Chem. Phys. (to be published).

2. All timing information refers to IBM 7094.

3. R. N. Zare and J. K. Cashion, Lawrence Radiation Laboratory Report UCRL-10881, July 1963 (unpublished).

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