

MASTER

Beam experiments on KrF, XeF, KrBr and XeBr excimer formation

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COMPUTER PROGRAMS FOR THE SIMULATION
OF BOUND-FREE EMISSION SPECTRA

Marc Vrakking

VDF/NO 87-19

Appendix belonging to EUT Internal Report VDF/NO 87-17

INHOUDSOPGAVE

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COMPUTER PROGRAMS FOR THE SIMULATION OF BOUND-FREE EMISSION SPECTRA

In order to analyse experimental bound-free rare gas halide emission spectra a number of computer-programs have been written on the central Burroughs 7900 mainframe at the Eindhoven University of Technology. In this report a summary will be given of the purpose of the major source-programs.

The total program structure is shown in Figure 1. Names starting with an 'S' are source-files containing programs written in FORTRAN (except programs S/CONVERTER and S/CONVERTER/MAT). Names starting with a 'D' are data-files. All files are stored under user TNNDW20, where the programs are stored as MINIB2/'S' or 'D'/GEBONDENVRIJ/FILENAME.

Program S/POTCALC

Program S/POTCALC is largely based on a program which was already written at IMS¹. In this program the emission-spectra of individual vibrational levels are determined by calculating the overlap-integral $\langle v | \mu_{eg} | E_g \rangle$ of the radial wave-functions of the bound vibrational upper states $|v\rangle$ and the free lower states $|E_g\rangle$.

For the calculation of the vibrational states $|v\rangle$ a method is applied, which was introduced by Cooley^{2,3}. This is essentially the application of 6th order Numerov-integration in a predictor-corrector method. The free lower state wave-functions are calculated by a simple outward integration. According to the WKB-method these wave-functions are normalized, from conservation of particles ($|\psi|^2 \sim E^{-1/2}$), by the condition that the amplitude of the sinusoidal wave varies like $E^{-1/4}$ at infinity, where E is the kinetic energy of the free ground state rare gas and halogen atoms.

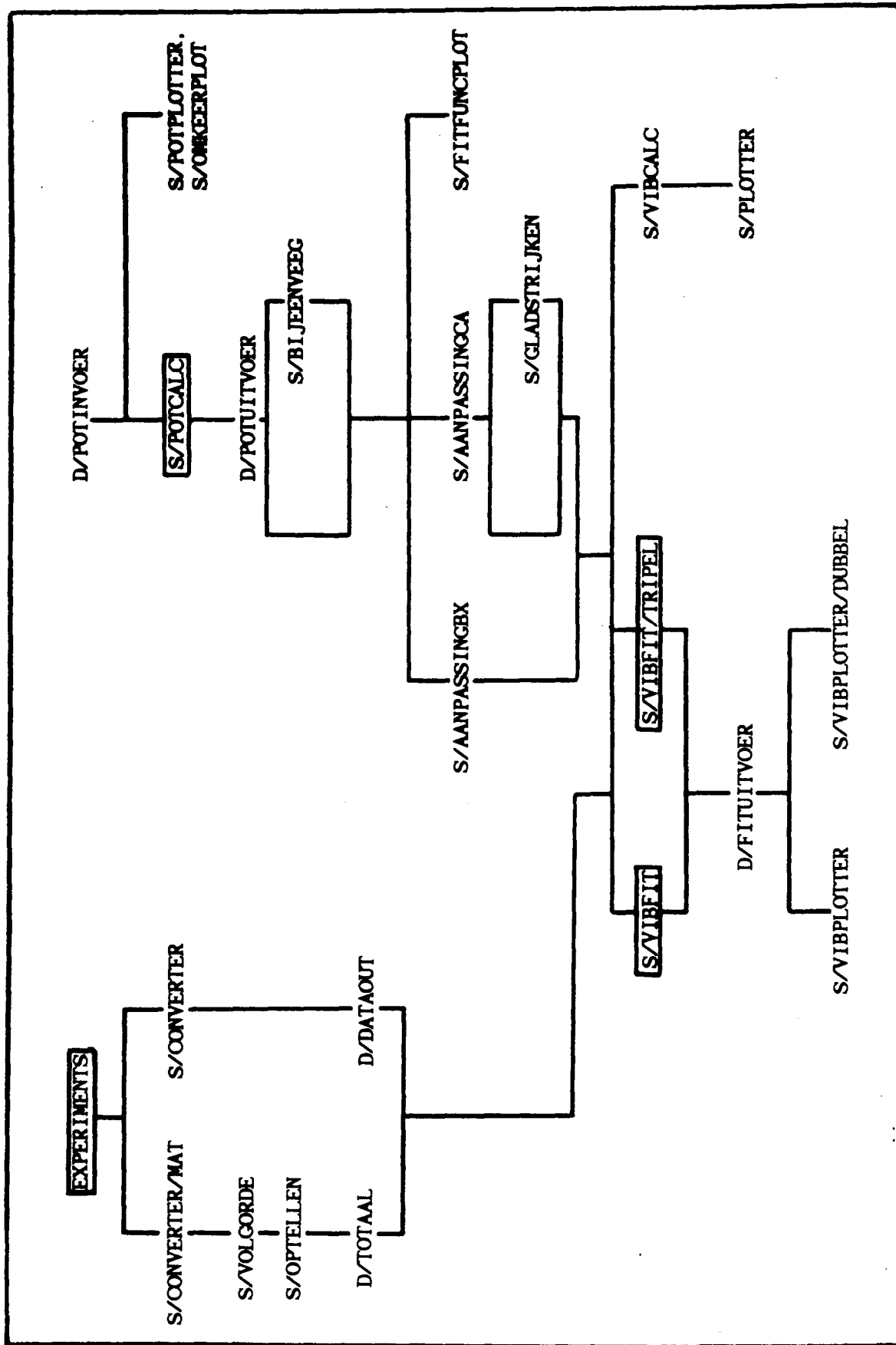


Figure 1: The relation between the available programs for the simulation of bound-free rare gas halide emission spectra.

As input program **S/POTCALC** requires variables giving the potential curves of the upper and lower states and the transition moments, and variables which determine the precision and the size of the calculation which is to be done. Drawing on the comparison between excited state rare gas atoms $(np)^5(n+1)s$ and ground state alkali atoms $(np)^6(n+1)s$, the potential curves are represented by a Rittner-type potential⁴, which is given as

$$V(R) = U_1 + U_2 + U_3 \exp(-U_4 R) + U_5 \exp(-U_6 R) - U_7/R - U_8/R^4 - U_9/R^6 \quad (1)$$

For an explanation of the meaning of the terms in this expression the reader is referred to Ref. 1.

In the present version of **S/POTCALC** the electronic transition moment is represented as

$$TM(R) = \exp(-\gamma(R-R_e)) / (C(1) + C(2)R + C(3)R^2 + C(4)R^3 + C(5)R^4) \quad (2)$$

However, there are also other representations in use.

All input is usually stored in a file **D/POTINVOER**. An example of a listing of this file along with an explanation of the meaning of all the variables is given below.

FILE **D/POTINVOER**

100 1 If this parameter equals 1, a printer backupfile is made with information about the current program-run.

200 1 If this parameter equals 1, detailed information
is written on the before-mentioned printer
backupfile about the determination of the bound
upper states.

300 2.0,8.0 RMIN, RMAX. These variables determine the interval
where wave-functions and contributions to the
overlap-integrals have to be calculated.

400 1000 N. The amount of integration-intervals between
RMIN and RMAX.

500 0.5,50 EPS, ITMAX. Stopcriterium in cm^{-1} and maximum
amount of iterations in the calculation of bound
wave-functions.

600 150,1 VMU, STEP. Vibrational quantum number up to which
the calculation has to be done and integer
interval between vibrational quantum numbers
where the calculation has to be done.

700 1500,10 NAC, STEP2. Amount of lower states to be
calculated and energy interval in cm^{-1} between
consecutive free lower states.

800 130,230 LMIN, LMAX. These variables determine the
wavelength interval in nm where the spectra have to
be calculated.

900 .2 STEP3. The intervalsize in nm for the calculated
spectra.

1000 UPPARR(1)...UPPARR(9) Parameters to express the
upper state potential (see Eq. 1)

1100 LOWARR(1)...LOWARR(9) Parameters to express the
lower state potential (see Eq. 1)

1200 0 If this parameter equals 1, a flat electronic

calculation is carried out, and NAC, the amount of free lower states used. In our calculations we adopted the following values:

N=1000

VIB=180

NAC=1300-1500

With this input one complete calculation requires about 3000 secs of processing time on the Burroughs-79 (6000 PT-units).

Program S/BIJEENVEEG

In a number of applications it is undesirable to treat all the spectra of individual vibrational levels separately, but rather one wants to group the vibrational states into regular entities. In this case a lot of I/O time is saved if the operation of collecting the vibrational states is done immediately after the calculations in program S/POTCALC. The present program transforms a datafile containing calculations done for given values of VIB and STEP, into a new datafile with newly defined values VIB2 and STEP2. Spectra of individual vibrational states are summed to give a new spectrum, which is assigned a vibrational energy which is the average of the vibrational energies of all states included in the summation.

Programs S/AANPASSINGBX and S/AANPASSINGCA

It is desirable to be able to change the relative shape of the potential curves and the shape of the electronic transition moment without having to resort to a completely new, expensive calculation

through program S/POTCALC. Using simple semi-classical arguments this is indeed possible^{5,6}.

Following the classical Franck-Condon principle the electronic transition from an upper state to a lower state happens so fast that both the position and the velocities of the particles involved remain unchanged in the transition. This means, in quantum-mechanical terms, that contributions to the overlap-integral will arise mainly from areas where there is a stationary phase-difference between the upper and lower state wave-functions⁷. Thus the position along the internuclear axis and the wavelength of the emitted photon are strongly related. This implies that a change of the electronic transition moment can be directly related to an intensity change at a corresponding wavelength. And in the case of a change of the relative shape of the potential curves the intensity at a certain wavelength which was calculated for the old set of potential curves can directly be related to the intensity at a corresponding wavelength for the new set of potential curves.

A complication can occur, if there is the possibility of more than one point of stationary phase along the internuclear axis and thus contributions at one wavelength from more than one position along the internuclear axis (see Figure 2), as is the case for rare gas halide B(1/2)-X(1/2) transitions. In this case a classical expression is used to differentiate between the relative probabilities for the emission at a certain wavelength to originate from either of the point of stationary phase as

$$\rho_i(\nu) \sim 1/\left[\sqrt{2m(E_\nu - V_u(r))} \frac{d}{dR}(V_u(R) - V_l(R)) \right]_{R=R_{\nu_i}} \quad (3)$$

According to this expression the relative emission probability $\rho_i(\nu)$

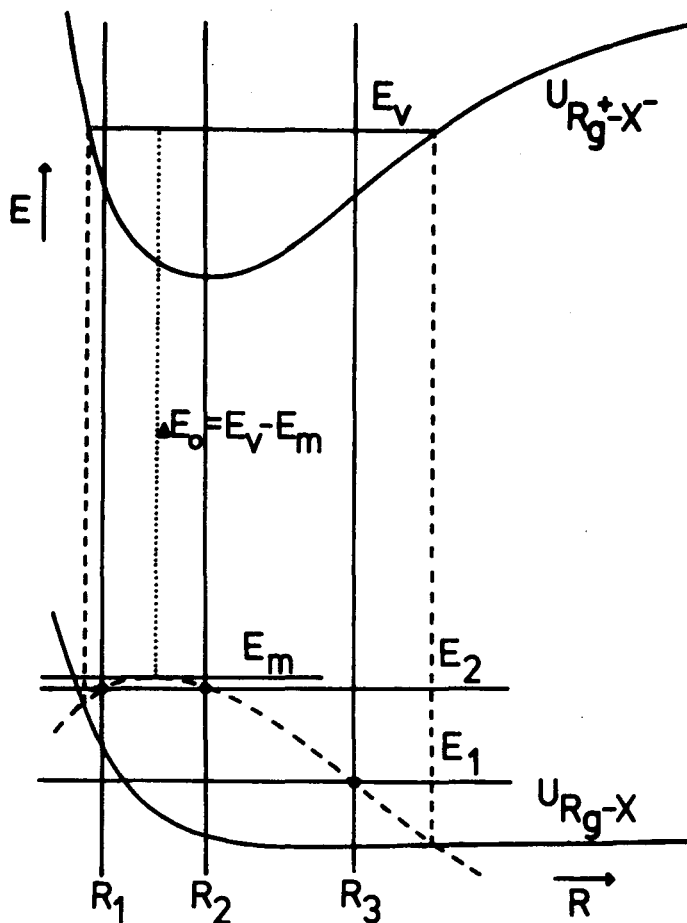


Figure 2: Schematic view of the transition from a vibrational state $|v\rangle$ of a bound $Rg^{+}X^{-}$ ion-pair state to a free $Rg-X$ state. The dashed line is Mulliken's difference potential¹⁰ given as $U_M = U_{Rg-X} - U_{Rg^{+}X^{-}} + E_v$, which gives the location of the points of stationary phase along the internuclear axis. At these points the kinetic energy is conserved during a vertical transition. From this figure it follows that at a free lower state energy E_1 (and a corresponding wavelength $hc/(E_v - E_1)$) there is only one point of stationary phase along the internuclear axis, whereas for a free lower state energy E_2 (and a corresponding wavelength $hc/(E_v - E_2)$) there are two such points. The long wavelength limit of the emission spectrum is determined by the emission to the maximum of Mulliken's difference potential ($\lambda_{\max} = hc/(E_v - E_M)$).

is inversely proportional to the velocity of the particles at an internuclear distance R_{v_i} (and thus proportional to the time-interval spent in the neighbourhood of R_{v_i}) and further, inversely proportional to the difference between the gradients of the upper and lower state potential at R_{v_i} , which means proportional to the width of the interval of stationary phase around R_{v_i} .

Programs **S/AANPASSINGBX** and **S/AANPASSINGCA** have been written to satisfy needs as they arose in the simulations carried out so far. Therefore, whereas **S/AANPASSINGCA** has the option of changing both the relative shape of the potential curves and the shape of the electronic transition moment, **S/AANPASSINGBX** has so far been restricted to the latter. The option of changing the relative shapes of the potential curves can easily be incorporated into the program in the future, when necessary.

Programs **S/AANPASSINGBX** and **S/AANPASSINGCA** require as input a file **D/POTINVOER**, which contains among other things the parameters of the new electronic transition moment and, inside the program, the parameters of the old electronic transition moment. With this information a specified file **D/POTUITVOER** can be transformed into a new D-file.

Program **S/GIADSTRIJKEN**

With this program calculated C(3/2)-A(3/2) emission spectra from individual vibrational states can be given an envelope which goes down exponentially towards shorter wavelengths. This is achieved by fitting the calculated secondary maxima of the emission spectrum to an exponential function.

Program S/CONVERTER

Within the Atomic Collisions and Spectroscopy Group there are standard procedures to transport experimental data to the Burroughs 7900 central EUT-computer, where historically these data are analysed with programs written in Algol. Program **S/CONVERTER** is a small Algol-program which converts a transported data-file to a file **D/DATAOUT**, which is suitable for use in Fortran-programs such as **S/VIBFIT** and **S/VIBFIT/TRIPEL**.

Programs S/CONVERTER/MAT, S/VOLGORDE and S/OPTELLEN

Program **S/CONVERTER/MAT** is very similar to program **S/CONVERTER**. However, where **S/CONVERTER** involves the transportation of merely one data-file, **S/CONVERTER/MAT** is used when a measurement has been repeated several times, as is often done during an experiment. In program **S/CONVERTER/MAT** all the measurements at a certain wavelength (from different scans of the spectrum) are collected and stored together on a file **D/DATAOUT**. The program **S/VOLGORDE** puts all measurements at a certain wavelength in order of magnitude and stores them on a file **D/DATAOUT/2**. Finally program **S/OPTELLEN** generates an experimental emission spectrum, by adding up the individual measurements at each wavelength, with the option of leaving out several values (highest and/or lowest) at each wavelength, to be rid of noise peaks and measurements where the beam source did not function as desired. This final spectrum is stored on a file **D/TOTAAL**.

Programs S/VIBFIT and S/VIBFIT/TRIPEL

The programs S/VIBFIT and S/VIBFIT/TRIPEL are two programs which are used to derive vibrational state distributions from experimental emission spectra. The only difference between the two programs is the fact that S/VIBFIT/TRIPEL offers the possibility to determine the vibrational state distribution simultaneously in several different electronic excimer states, whereas S/VIBFIT is applicable in the case of only one electronic excimer state. Thus S/VIBFIT can be used to get a rough idea of the vibrational state distributions, whereas S/VIBFIT/TRIPEL offers the opportunity to eliminate errors due to overlapping emissions from more than one electronic transition. In the present form of S/VIBFIT/TRIPEL an experimental spectrum can be fitted to three different electronic transitions, with the restriction that these originate from two different upper states. This obviously arises from the fact that this program has been written in order to do simultaneous simulations of B(1/2)-X(1/2), C(3/2)-A(3/2) and B(1/2)-A(1/2) continua. It goes without saying that in the near future this program can and should be further extended in order to include yet more bound-free excimer transitions, and a number of atomic and molecular emissions due to competing inelastic reaction channels (cf. the fairly large Br₂^{*} emission which is encountered in the reactions of Kr (³P_{0,2})+Br₂ and Xe (³P_{0,2})+Br₂).

The vibrational state distributions are determined through a linear least squares analysis. This least squares method is based on the following matrix-equation^{8,9}

$$\bar{D} = \bar{S} \cdot \bar{P} \quad (4)$$

where $\bar{D}(0:NMEETP-1)$ is an array which contains the experimental spectrum, $\bar{P}(0:NPAR-1)$ is an array which contains the vibrational state distribution to be determined and $\bar{S}(0:NPAR-1, 0:NMEETP-1)$ is a matrix in which the spectra of the individual vibrational levels are stored, which serve as basis functions in the least squares analysis.

The least squares solution $\bar{P}(0:NPAR-1)$ is determined by the condition that

$$R = \sum_{i=0}^{NMEETP-1} \left[\bar{D}(i) - \sum_{j=0}^{NPAR-1} \bar{S}(i,j) \bar{P}(j) \right]^2 \quad (5)$$

be minimal. This condition requires that

$$\frac{\delta R}{\delta P(k)} = -2 \sum_{i=0}^{NMEETP-1} \bar{S}(i,k) \left[\bar{D}(i) - \sum_{j=0}^{NPAR-1} \bar{S}(i,j) \bar{P}(j) \right] = 0$$

(6)

These are the Gaussian normal equations, which can be solved using standard matrix algebra.

When using the programs **S/VIBFIT** and **S/VIBFIT/TRIPEL** it is important to limit to some extent the number of basis functions and thus the number of fit-parameters. In our experiments vibrational levels up to $v=180$ may be occupied, but because of experimental errors in the data and uncertainties in the validity of the calculated spectra from single vibrational levels, a fit with 180 fit-parameters and basis functions will yield a completely unphysical vibrational distribution. Rather, a number of vibrational levels should be taken together in the calculation (within **S/VIBFIT** and **S/VIBFIT/TRIPEL** or beforehand, using **S/BIJEENVEEG**), the average of their spectra being used as one basis function.

In Figure 3 the relation between the uncertainties in the experimental data and the amount of vibrational levels which are taken together is shown. In the calculations leading to this figure experimental data were generated by mapping a flat vibrational distribution on a given set of 150 spectra from single vibrational levels from the XeBr B(1/2)-X(1/2) transition. These exact data, normalized to a maximum value of 10000 'counts', were perturbed in the

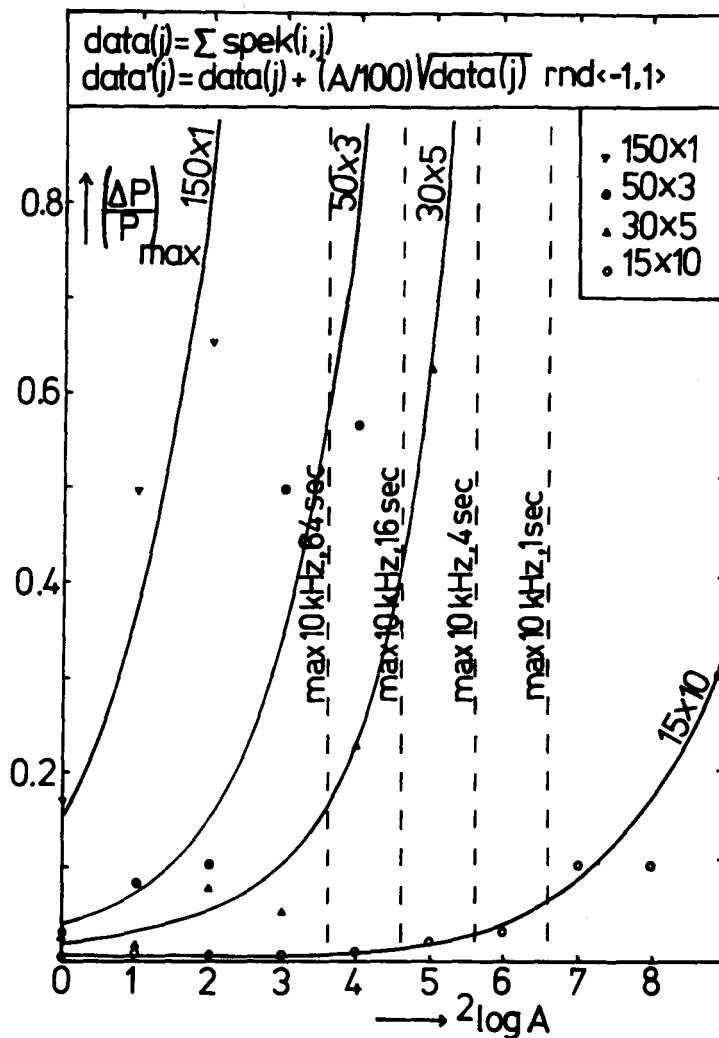


Figure 3: The relationship between the uncertainties in the experimental data and the amount of vibrational levels which are taken together in a least squares fit of an emission spectrum. See text for detailed explanation.

following way,

$$\bar{D}(i)' = \bar{D}(i) [1 + A \sqrt{D(i)} \text{RND}/100] \quad (7)$$

where RND is a random number between -1 and 1. Thus, for example, A=100 would correspond to an uncertainty of approximately one standard deviation for an experiment where the maximum amount of counts at a certain wavelength is equal to 10000. Figure 3 shows the maximum relative deviation from a flat vibrational state distribution as a function of A and the amount of vibrational levels taken together in the calculation. Thus, since we can calculate the value of the parameter A from our experimental conditions, we have a recipe to determine how many vibrational levels should produce one basis function in the least squares fit. It should be stressed that the use of this recipe is conditional on the correctness of the available potential curves and electronic transition moment, which often turns out to be a major problem.

Finally, the structure of the programs S/VIBFIT and S/VIBFIT/TRIPEL is such that when a data-file D/DATAOUT and one (or more) data-files D/POTUITVOER are available, the program proceeds through an interactive input of the amount of vibrational states to be used and the amount of vibrational levels to be taken together in the calculation.

Both programs create a previewfile which contains a comparison of the experimental and the simulated spectrum and a file D/FITUITVOER where the vibrational state distributions which were determined are stored.

Programs S/VIBPLOTTER and S/VIBPLOTTER/DUBBEL

These programs give a graphical representation of the vibrational state distributions determined in the programs S/VIBFIT and S/VIBFIT/TRIPEL, using the information which was stored on file D/FITUITVOER. As an example, Figure 4 shows some typical output of S/VIBFIT/DUBBEL.

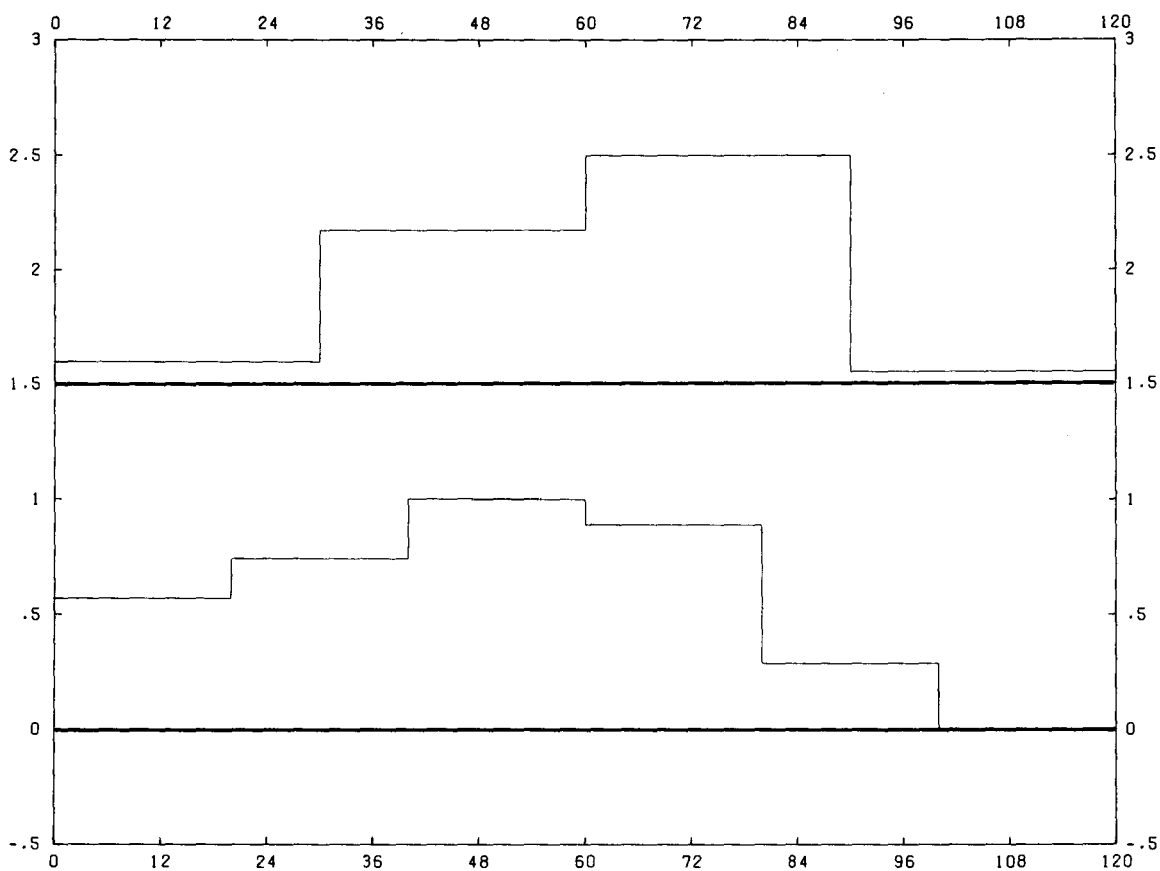


Figure 4: Some typical output of program S/VIBPLOTTER/DUBBEL: the XeBr B(1/2) state (lower curve) and C(3/2) state (upper curve) vibrational distributions determined from the emission spectrum from the reaction of $\text{Xe}^* + \text{CF}_2\text{Br}_2$. For detailed information on the potential curves and transition moment used see ref. 6.

Programs S/VIBCALC and S/PLOTTER

Program S/VIBCALC can be used to generate a total emission-spectrum starting from given spectra for the individual vibrational levels, calculated in program S/POTCALC. The program offers the possibility of applying a number of different vibrational state distributions, including linear surprisal distributions, Boltzmann-distributions and a flat distribution.

As input S/VIBCALC requires a file D/POTUITVOER and a file D/VIBINVOER. A typical listing of D/VIBINVOER along with an explanation of the variables is given below.

FILE D/VIBINVOER

- 100 1 If this parameter equals 1, a printer backupfile is made with information about the current program-run.
- 200 1 KEUS. Integer to choose the type of vibrational state distribution:
- 1) Linear surprisal distribution.
 - 2) Flat distribution
 - 3) Linear distribution: $P(I)=1+C1*EU(I)/EMAX$
 - 4) Boltzmann distribution
- 300 -8 Depending on the value of KEUS this variable represents the linear surprisal parameter λ_V , a dummy, the parameter C1 or the Boltzmann-temperature.
- 400 45.8 Bonding energy of the halide atom in the target gas molecule (kcal/mol).
- 500 8.81 Rare gas metastable state energy (eV).

Program **S/VIBCALC** generates a spectrum which is stored on a file **D/VIBUITVOER**. A graphical representation of this spectrum is directly available with the plotprogram **S/PLOTTER**. This program is also often used to plot experimental spectra, stored on **D/DATAOUT** or **D/TOTAAL**. As an example Figure 5 shows the spectrum of $\text{Xe}^* + \text{CBr}_4$ plotted with **S/PLOTTER**.

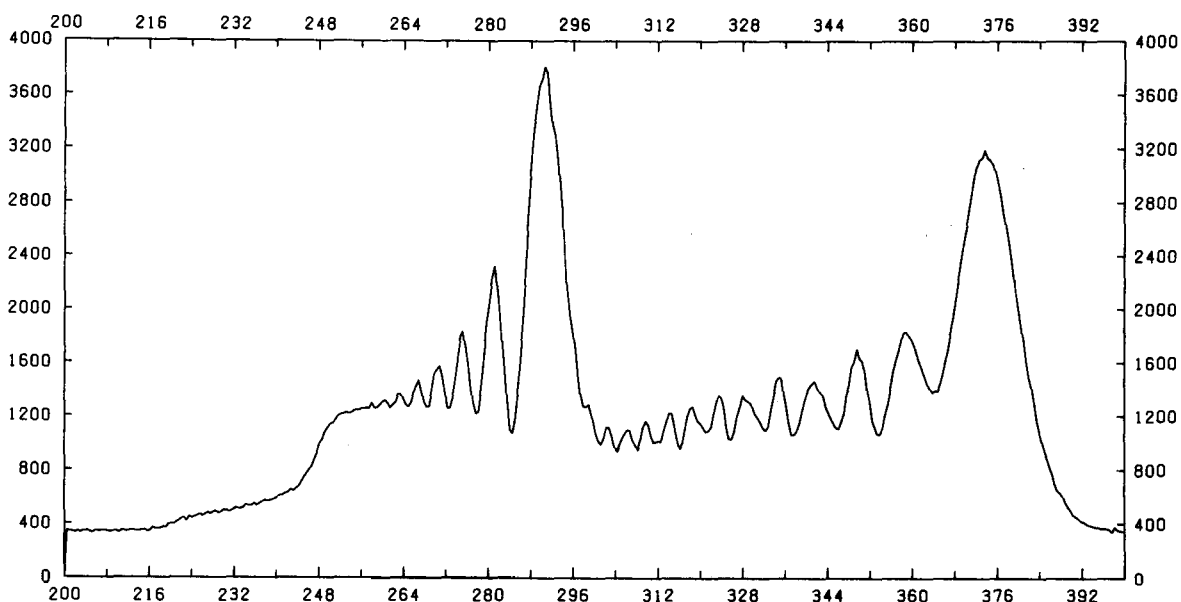


Figure 5: The XeBr emission spectrum from the reaction of $\text{Xe}^* + \text{CBr}_4$, plotted using program **S/PLOTTER**.

Program S/POTPLOTTER

This program, using a file **D/POTINVOER**, gives a graphical representation of a set of potential curves, including Mulliken's difference potential¹⁰ at a specified energy. As an example Figure 6 shows the potential curves of the XeBr B(1/2)-X(1/2) transition, with Mulliken's difference potential for $E=55000 \text{ cm}^{-1}$.

Figure 6: The potential curves for the XeBr B(1/2)-X(1/2) transition⁵, with Mulliken's difference potential¹⁰ for $E=55000 \text{ cm}^{-1}$, plotted using program S/POTPLOTTER.

Program S/OMKEERPLOT

This program, using a file D/POTINVOER can be used to give a graphical representation of the energy-dependence of the wavelengths of the emission at the classical turning points for a number of specified lower state potentials. As an example Figure 7 shows the emission from the turning points in the XeBr C(3/2)-A(3/2) transition, using the ab-initio C(3/2) state potential curve and a number of trial A(3/2) state potential curves.

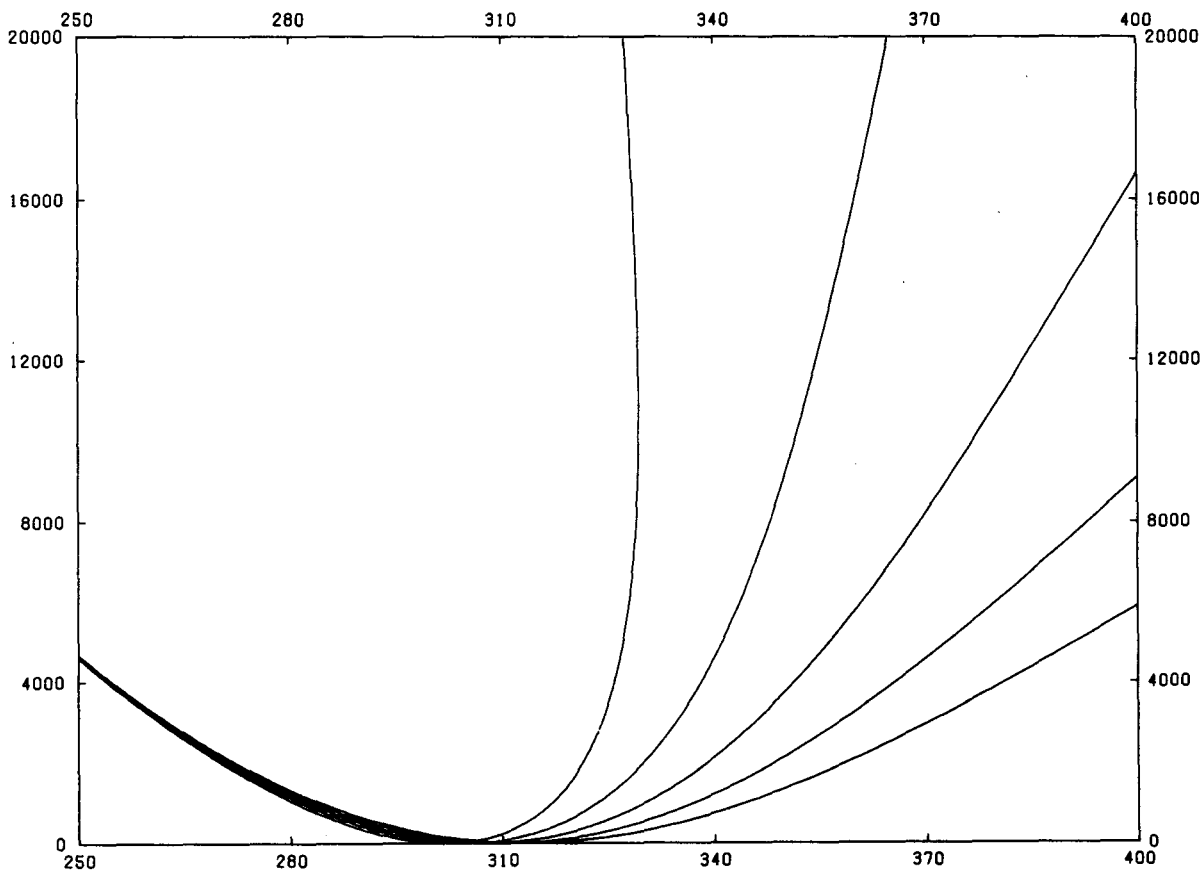


Figure 7: Emission from the turning points in the XeBr C(3/2)-A(3/2) transition, using the ab-initio C(3/2) state potential curve given in ref. 3, and an A(3/2) state potential represented as $V_{A(3/2)}(r) = A \exp(- 2.9464 R) + 600 [\text{cm}^{-1}]$, where A takes on the values 6.0E7, 5.5E7, 5.0E7, 4.5E7 and 4.0E7, respectively. In the final A(3/2) state potential which was determined from computer simulations of several XeBr emission spectra a value of A of 4.8536E7 was adopted (see ref. 6).

Program S/FITFUNC PLOT

This program can be used to get a graphical representation of the fit-functions used in programs S/VIBFIT and S/VIBFIT/TRIPEL. As an example Figure 8 shows the fit-functions used in the simulations of XeBr C(3/2)-A(3/2) continua.

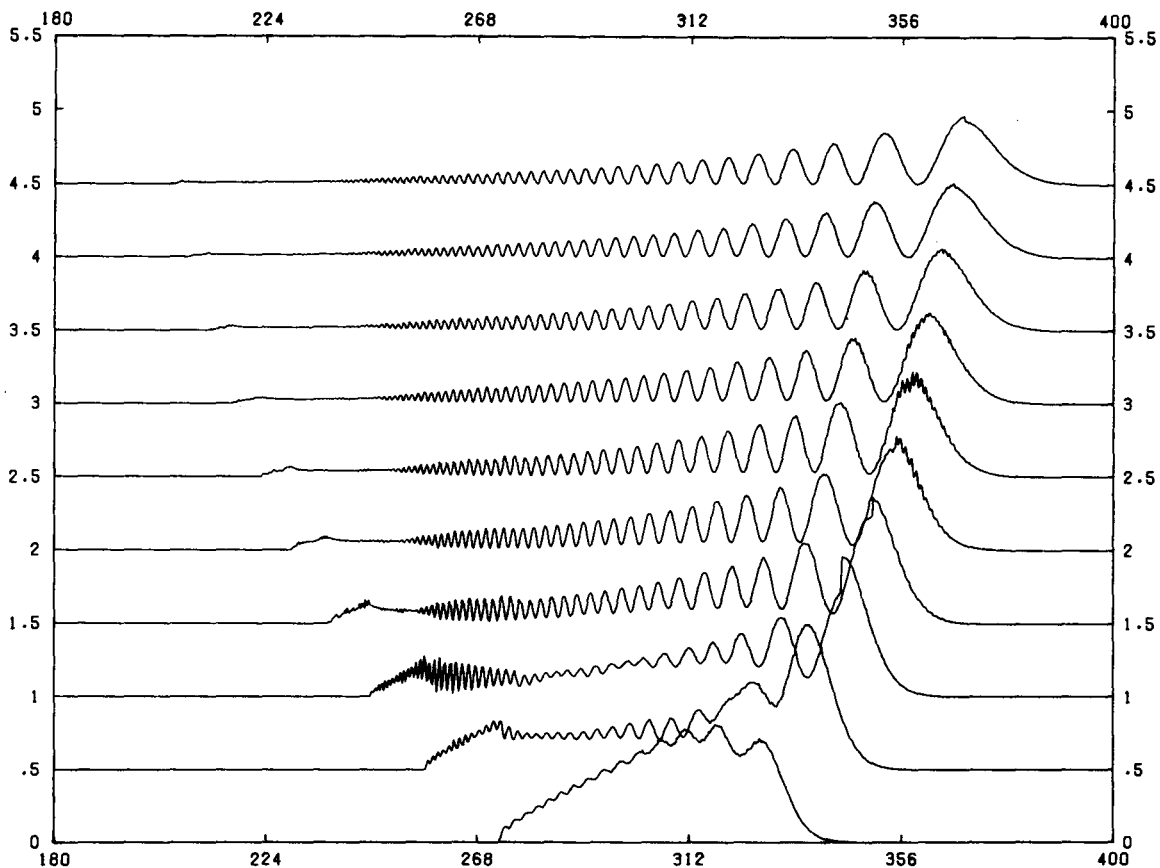


Figure 8: Fit-functions used in the simulations of XeBr C(3/2)-A(3/2) continua, plotted using program S/FITFUNC PLOT. See ref. 6 for the parameters used to represent the potential curves and the electronic transition moment.

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10000 C MINIB2/S/GEBONDENVRIJ/POTCALC
10010 C
10020 C This program is part of a series of programs to simulate
10030 C bound-free rare gas halide emission spectra.
10040 C In this program the emission spectra of individual vibrational
10050 C upper states are determined by calculating the overlap
10060 C integrals of the radial parts of the bound upper state wave-
10070 C functions and the free lower state wave-functions.
10080 C The input variables, describing the potential curves
10090 C and the electronic transition moment, and the precision
10100 C and the size of the calculation, are usually stored on
10110 C a specified FILE 4. The spectra are stored on a specified
10120 C FILE 5.
10130 C
10140 C*****
10150 C
10160 C DECLARATIONS
10170 C *****
10180 C
10190 FILE 1(KIND=REMOTE) % WRITE TO TERMINAL
10200 FILE 2(KIND=REMOTE) % READ FROM TERMINAL
10210 FILE 3(KIND=PRINTER)
10220 FILE 4(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/POTINVOER")
10230 FILE 5(KIND=DISK, MAXRECSIZE=30, BLOCKSIZE=480, AREASIZE=30,
10240 * TITLE="MINIB2/D/GEBONDENVRIJ/POTUITVOER",
10250 * PROTECTION=SAVE, NEWFILE=TRUE)
10260 REAL*4 RMIN, RMAX, EPS, STEP2, UPPARR, LOWARR, DUMMY, GAMMA, C1,
10270 * C2, C3, C4, C5, M1, M2, MURED, H, UMINUP, UMINLO, R, UUP, ULO, REUP, TM, E,
10280 * E1, FAC, AMP, Y, EE, FCF, STEP3, REALJB, HULP, SPEK, NU, OMEUUP, PSU, EU
10290 INTEGER*4 INTACT, TERM, N, ITMAX, VMU, STEP, NAC, SQUEST, SEDEL, SHALO,
10300 * I, J, K, TERM2, VIB, JMIN, JMAX, INTJB, LMIN, LMAX, KMAX, TRANS
10310 DIMENSION UPPARR(9), LOWARR(9), R(0:1001), UUP(0:1001), ULO(0:1001),
10320 * TM(0:1001), PSU(1:180, 0:1001), EU(180), FCF(1:180, 1:1500),
10330 * Y(0:1001), SPEK(1:180, 0:1019)
10340 C
10350 C INPUT VARIABLES
10360 C *****
10370 C
10380 SQUEST=0
10390 INTACT=4
10400 WRITE(1,1)
10410 READ(2,/) SQUEST
10420 1 FORMAT(' INVOER INTERACTIEF VANAF TERMINAL (JA=1)?')
10430 C 1 FORMAT(' INPUT INTERACTIVE FROM TERMINAL (YES=1)?')
10440 IF(SQUEST.EQ.1) INTACT=2
10450 C
10460 SQUEST=0
10470 TERM=0
10480 IF(INTACT.EQ.2) WRITE(1,2)
10490 READ(INTACT,/) SQUEST
10500 2 FORMAT(' AANMAAK PRINTERFILE MET PROGRAMMAGEGEVENS (JA=1)?')
10510 C 2 FORMAT(' CREATE A PRINTERFILE WITH PROGRAM INFO (YES=1)?')
10520 IF(SQUEST.EQ.1) TERM=1
10530 SQUEST=0
10540 TERM2=0
10550 IF(TERM.EQ.0) READ(INTACT,/) DUMMY
10560 IF(TERM.EQ.0) GOTO 22
10570 IF(INTACT.EQ.2) WRITE(1,21)

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10580      21  FORMAT(' UITVOERIGE GEGEVENS OVER GEBONDEN TOESTANDEN (JA=1)?')
10590      C 21  FORMAT(' EXTENSIVE INFO ON BOUND UPPER STATES (YES=1)?')
10600          READ(INTACT,/) SQUEST
10610          IF(SQUEST.EQ.1) TERM2=1
10620      22  CONTINUE
10630      C
10640          IF(INTACT.EQ.2) WRITE(1,3)
10650          READ(INTACT,/) RMIN,RMAX
10660      3    FORMAT(' INVOER RMIN, RMAX IN ANGSTROEM: ')
10670      C 3    FORMAT(' INPUT OF RMIN, RMAX IN ANGSTROEM: ')
10680          IF(INTACT.EQ.2) WRITE(1,4)
10690          READ(INTACT,/) N
10700      4    FORMAT(' INVOER AANTAL INTEGRATIE STAPPEN N: ')
10710      C 4    FORMAT(' INPUT AMOUNT OF INTEGRATION STEPS N: ')
10720          IF(INTACT.EQ.2) WRITE(1,5)
10730          READ(INTACT,/) EPS,ITMAX
10740      5    FORMAT(' INVOER BEEINDIGINGSKRITERIA EPS, ITMAX: ')
10750      C 5    FORMAT(' INPUT STOPCRITERIA EPS, ITMAX: ')
10760          IF(INTACT.EQ.2) WRITE(1,6)
10770          READ(INTACT,/) VMU,STEP
10780      6    FORMAT(' INVOER AANTAL BOVENNIVEAUS EN STAPGROOTTE: ')
10790      C 6    FORMAT(' INPUT AMOUNT OF UPPER STATES AND INTERVALSIZE: ')
10800          IF(INTACT.EQ.2) WRITE(1,7)
10810          READ(INTACT,/) NAC,STEP2
10820      7    FORMAT(' INVOER AANTAL BENEDENNIVEAUS EN STAPGROOTTE: ')
10830      C 7    FORMAT(' INPUT AMOUNT OF LOWER STATES AND INTERVALSIZE: ')
10840          IF(INTACT.EQ.2) WRITE(1,71)
10850          READ(INTACT,/) LMIN,LMAX
10860      71   FORMAT(' INVOER GOLFLENGTE INTERVALGRENZEN LMIN,LMAX: ')
10870      C 71   FORMAT(' INPUT BOUNDARIES WAVELENGTH INTERVAL LMIN, LMAX: ')
10880          IF(INTACT.EQ.2) WRITE(1,72)
10890          READ(INTACT,/) STEP3
10900      72   FORMAT(' INVOER STAPGROOTTE IN GOLFLENGTEINTERVAL: ')
10910      C 72   FORMAT(' INPUT STEPSIZE IN WAVELENGTH INTERVAL: ')
10920          IF(INTACT.EQ.2) WRITE(1,8)
10930          READ(INTACT,/) UPPARR(1),
10940          *   UPPARR(2),UPPARR(3),UPPARR(4),UPPARR(5),UPPARR(6),
10950          *   UPPARR(7),UPPARR(8),UPPARR(9)
10960      8    FORMAT(' INVOER POTENTIAALGEGEVENS UPPARR(1)...UPPARR(9): ')
10970      C 8    FORMAT(' INPUT POTENTIAL PARAMETERS UPPARR(1)...UPPARR(9): ')
10980          IF(INTACT.EQ.2) WRITE(1,9)
10990          READ(INTACT,/) LOWARR(1),
11000          *   LOWARR(2),LOWARR(3),LOWARR(4),LOWARR(5),LOWARR(6),
11010          *   LOWARR(7),LOWARR(8),LOWARR(9)
11020      9    FORMAT(' INVOER POTENTIAALGEGEVENS LOWARR(1)...LOWARR(9): ')
11030      C 9    FORMAT(' INPUT POTENTIAL PARAMETERS LOWARR(1)...LOWARR(9): ')
11040      C
11050          SQUEST=0
11060          TRANS=0
11070          IF(INTACT.EQ.2) WRITE(1,10)
11080          READ(INTACT,/) SQUEST
11090      10   FORMAT(' CONSTANT OVERGANGSMOMENT (JA=1)?')
11100      C 10   FORMAT(' FLAT TRANSITION MOMENT (YES=1)?')
11110          IF(SQUEST.EQ.0) TRANS=1
11120          IF(TRANS.EQ.0.AND.INTACT.EQ.4) READ(INTACT,/) DUMMY,DUMMY,
11130          *   DUMMY,DUMMY
11140          IF(TRANS.EQ.1.AND.INTACT.EQ.2) WRITE(1,11)
11150      11   FORMAT(' INVOER OVERGANGSMOMENT GAMMA,C1,C2,C3,C4,C5: ')
11160      C 11   FORMAT(' INPUT TRANSITION MOMENT GAMMA,C1,C2,C3,C4,C5: ')
11170          IF(TRANS.EQ.1) READ(INTACT,/) GAMMA,C1,C2,C3,C4,C5
11180      C
11190          IF(INTACT.EQ.2) WRITE(1,12)

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11200      READ(INTACT,/) SEDEL
11210      12  FORMAT( ' INVOER EDELGAS NE=1, AR=2, KR=3, XE=4: ' )
11220      C 12  FORMAT( ' INPUT RARE GAS NE=1, AR=2, KR=3, XE=4: ' )
11230      IF(INTACT.EQ.2) WRITE(1,13)
11240      READ(INTACT,/) SHALO
11250      13  FORMAT( ' INVOER HALOGEEN F=1, CL=2, BR=3, I=4: ' )
11260      C 13  FORMAT( ' INPUT HALOGEN F=1, CL=2, BR=3, I=4: ' )
11270      C
11280      IF(SEDEL.EQ.1) M1=20.183
11290      IF(SEDEL.EQ.2) M1=39.948
11300      IF(SEDEL.EQ.3) M1=83.80
11310      IF(SEDEL.EQ.4) M1=131.30
11320      IF(SHALO.EQ.1) M2=18.998
11330      IF(SHALO.EQ.2) M2=35.453
11340      IF(SHALO.EQ.3) M2=79.909
11350      IF(SHALO.EQ.4) M2=126.9044
11360      MURED=M1*M2/(M1+M2)
11370      C
11380      IF(TERM.EQ.1) CALL VARCOM(RMIN,RMAX,N,VMU,STEP,NAC,STEP2,
11390      *      UPPARR,LOWARR,GAMMA,C1,C2,C3,C4,C5,MURED)
11400      C
11410      C      CALCULATION OF POTENTIAL CURVES AND TRANSITION MOMENTS
11420      C      *****
11430      C
11440      H=(RMAX-RMIN)/(N+1)
11450      UMINUP=10**10
11460      UMINLO=10**10
11470      C
11480      DO 30 I=0,N+1,1
11490      R(I)=RMIN+I*H
11500      C      R(I)=R(I)*1.09      Note: for XeBr B-X(1/2) calculation!
11510      UUP(I)=UPPARR(1)+UPPARR(2)
11520      *      +UPPARR(3)*EXP(-UPPARR(4)*R(I))
11530      *      +UPPARR(5)*EXP(-UPPARR(6)*R(I))
11540      *      -UPPARR(7)/R(I)
11550      *      -UPPARR(8)/(R(I)**4)
11560      *      -UPPARR(9)/(R(I)**6)
11570      ULO(I)=LOWARR(1)+LOWARR(2)
11580      *      +LOWARR(3)*EXP(-LOWARR(4)*R(I))
11590      *      +LOWARR(5)*EXP(-LOWARR(6)*R(I))
11600      *      -LOWARR(7)/R(I)
11610      *      -LOWARR(8)/(R(I)**4)
11620      *      -LOWARR(9)/(R(I)**6)
11630      IF(UUP(I).GT.UMINUP) GOTO 20
11640      UMINUP=UUP(I)
11650      REUP=R(I)
11660      20  IF(ULO(I).GT.UMINLO) GOTO 25
11670      UMINLO=ULO(I)
11680      25  CONTINUE
11690      C      R(I)=R(I)/1.09      Note: for XeBr B-X(1/2) calculation!
11700      30  CONTINUE
11710      C
11720      DO 40 I=0,N+1,1
11730      TM(I)=1.
11740      IF(TRANS.EQ.1) TM(I)=EXP(GAMMA*(R(I)-REUP))/
11750      C      *      ((R(I)-C1)**2+C2) + C3
11760      *      (C1+C2*R(I)+C3*(R(I)**2)+C4*(R(I)**3)+C5*(R(I)**4))
11770      40  CONTINUE
11780      C
11790      C
11800      C      CALCULATION OF BOUND UPPER STATES
11810      C      *****

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11820 C
11830 OMEUUP=150.
11840 E=UMINUP+OMEUUP/2
11850 IF(VMU.NE.1) GOTO 50
11860 IF(INTACT.EQ.2) WRITE(3,14)
11870 14 FORMAT(' TRIAL-ENERGIEWAARDE VOOR DE BOVENTOESTAND: ')
11880 C 14 FORMAT(' TRIAL ENERGY VALUE FOR UPPER STATE')
11890 C
11900 C If VMU equals 1 the spectrum of only one vibrational level
11910 C will be calculated. In this case the calculation does not
11920 C start from the well of the upper state potential curve, but
11930 C a vibrational energy can be specified by the user.
11940 C
11950 45 READ(INTACT,/)E1
11960 IF(E1.LT.E) WRITE(3,15)
11970 15 FORMAT(' TRIAL-ENERGIEWAARDE LIGT BENEDEN POTENTIAALMINIMUM',/,
11980 * ' VOER EEN HOGERE WAARDE IN!')
11990 C 15 FORMAT(' TRIAL ENERGY VALUE LIES BELOW THE MINIMUM OF THE',/,
12000 C * ' UPPER STATE POTENTIAL CURVE',/,
12010 C * ' PLEASE ENTER A HIGHER VALUE!')
12020 IF(E1.LT.E) GOTO 45
12030 E=E1
12040 50 CONTINUE
12050 C
12060 IF(TERM.EQ.1) WRITE(3,16) UMINUP,REUP
12070 16 FORMAT(/,' UMINUP= ',E14.7,/,', REUP= ',F9.4,/)
12080 WRITE(1,/) TIME(2)/60.
12090 CALL BWAVE(1,DUMMY,VMU,STEP,UUP,R,N,E,OMEUUP,MURED,EPS,
12100 * ITMAX,VIB,EU,PSU,TERM2)
12110 C
12120 C Subroutine BWAVE is the subroutine where the actual calculation
12130 C of the upper state wave-functions takes place. An explanation of
12140 C the parameters in the heading of BWAVE is included in the
12150 C source text of BWAVE.
12160 C
12170 WRITE(1,/) TIME(2)/60.
12180 IF(TERM.EQ.1.AND.VMU.NE.1) WRITE(3,17) (EU(2)-EU(1))/STEP
12190 17 FORMAT(/,' BEREKENDE OMEGA IN BOVENTOESTAND: ',F9.2,/)
12200 C 17 FORMAT(/,' CALCULATED OMEGA IN UPPER STATE: ',F9.2,/)
12210 C
12220 C CALCULATION OF FREE LOWER STATES AND FRANCK-CONDON FACTORS
12230 C *****
12240 C
12250 C Initialization
12260 C
12270 FAC=MURED/16.86
12280 DO 120 I=1,NAC,1
12290 E=LOWARR(1)+LOWARR(2)+(I-.5)*STEP2
12300 EE=E**.25*N**.5
12310 C
12320 JMAX=N
12330 JMIN=1
12340 DO 60 J=1,N-5,1
12350 IF(JMIN.EQ.1.AND.ULO(J+5).LE.E) JMIN=J
12360 60 CONTINUE
12370 C
12380 DO 70 J=1,N,1
12390 Y(J)=0
12400 70 CONTINUE
12410 C
12420 C Integration
12430 C

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12440      Y(JMIN+1)=1.
12450      DO 80 J=JMIN+2,N,1
12460      Y(J)=Y(J-1)*(2+FAC*H*H*(ULO(J-1)-E)/
12470      * (1-FAC*H*H*(ULO(J-1)-E)/12))-Y(J-2)
12480      80 CONTINUE
12490      C
12500      C      Determination of wave-function amplitudo 'at infinity'
12510      C
12520      K=JMAX-1
12530      AMP=0.
12540      90 IF(ABS(Y(K-1)).LE.ABS(Y(K)).AND.ABS(Y(K)).GT.ABS(Y(K+1))) AMP=
12550      * ABS(Y(K))
12560      IF(AMP.NE.0) GOTO 95
12570      K=K-1
12580      IF(K.GT.1) GOTO 90
12590      WRITE(1,18)
12600      18 FORMAT(' ERROR: PROGRAMMA WORDT GESTAAKT OMDAT HET INTEGRATIE',
12610      * 'INTERVAL TE KLEIN IS VOOR HET BEREKENEN VAN BETROUWBARE',
12620      * 'VRIJ GOLFFUNCTIES. DE WAARDE VAN RMAX DIENT TE WORDEN',
12630      * 'VERHOOGD.')
12640      C 18 FORMAT(' ERROR: PROGRAM STOPPED BECAUSE THE INTEGRATION',
12650      C * 'INTERVAL IS TOO SMALL FOR A CALCULATION OF RELIABLE FREE',
12660      C * 'LOWER STATE WAVE-FUNCTIONS. THE VALUE OF RMAX HAS TO',
12670      C * 'BE ENLARGED.')
12680      GOTO 999
12690      C
12700      C      Normalization
12710      C
12720      95 DO 100 J=2,N+1,1
12730      Y(J)=Y(J)/AMP/EE
12740      100 CONTINUE
12750      C
12760      C      Calculation of Franck-Condon factors
12770      C
12780      DO 110 J=1,VIB,1
12790      FCF(J,I)=0.
12800      DO 105 K=2,N,1
12810      FCF(J,I)=FCF(J,I)+PSU(J,K)*TM(K)*Y(K)
12820      105 CONTINUE
12830      FCF(J,I)=FCF(J,I)**2
12840      110 CONTINUE
12850      C
12860      120 CONTINUE
12870      WRITE(1,/) TIME(2)/60.
12880      C
12890      C      DETERMINATION OF THE EMISSION SPECTRA OF INDIVIDUAL
12900      C      VIBRATIONAL STATES
12910      C      *****
12920      C
12930      C
12940      KMAX=INT((LMAX-LMIN)/STEP3)
12950      DO 140 I=1,VIB,1
12960      DO 130 K=0,KMAX,1
12970      NU=(10**7)/(LMIN+K*STEP3)
12980      REALJB=.5+(EU(I)-LOWARR(1)-LOWARR(2)-NU)/STEP2
12990      INTJB=INT(REALJB)
13000      IF(INTJB.GT.NAC-1) GOTO 130
13010      IF(INTJB.LE.0) GOTO 130
13020      HULP=REALJB-INTJB
13030      SPEK(I,K)=(NU*5.)*((1-HULP)*FCF(I,INTJB)+HULP*FCF(I,INTJB+1))
13040      130 CONTINUE
13050      140 CONTINUE

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13060 C
13070 C Output to a file D/POTUITVOER
13080 C
13090 WRITE(5,/) LMIN,LMAX,STEP3
13100 WRITE(5,/) VIB,STEP
13110 WRITE(5,/) UMINUP
13120 WRITE(5,/) EU
13130 C
13140 DO 161 I=1,180
13150 DO 151 J=1,34
13160 WRITE(5) (SPEK(I,30*(J-1)+K),K=0,29)
13170 151 CONTINUE
13180 161 CONTINUE
13190 C
13200 999 CONTINUE
13210 CLOSE(5,DISP=CRUNCH)
13220 C Crunching of outputfile D/POTUITVOER
13230 C
13240 END
13250 C
13260 SUBROUTINE BWAVE(MODE,EMAX,VMU,STEP,U,R,N,E,OMEU,MURED,EPS,ITMAX,
13270 * VIBC,EU,PSI,TERM)
13280 C
13290 C In this subroutine the radial parts of the upper state wave-
13300 C functions are calculated, using an algorithm developed by
13310 C Cooley (Math. Computation XV, 363 (1961)).
13320 C If the parameter MODE equals 1 then vibrational states are
13330 C determined up to  $v=VMU$ , at an interval STEP. If the parameter
13340 C MODE equals 2, then vibrational states are determined up to
13350 C an energy EMAX.
13360 C The array U gives the potential energy at an internuclear
13370 C distance specified by array R, the parameter E is a trial
13380 C energy value for the first vibrational state to be determined,
13390 C and OMEU is an estimate of the OMEGA-value of the potential
13400 C curve. The parameters N, EPS, ITMAX and MURED have the meaning
13410 C introduced in the main source program.
13420 C As output an integer VIBC, representing the amount of vibra-
13430 C tional states determined, an array EU, containing the energy
13440 C eigenvalues, and a matrix PSI, containing the radial wave-
13450 C functions are given.
13460 C If the parameter TERM is given the value 1, then a printerfile
13470 C is created with extensive information on the calculation of
13480 C the radial wave-functions.
13490 C
13500 C DECLARATIONS
13510 C *****
13520 C
13530 REAL*4 FAC,MURED,U,E,H,R,Y,SOM,DE,EPS,EU,OMEU,EMAX,PSI
13540 INTEGER*4 VIB,VIBC,STEP,IT,JMIN,JMAX,N,M,NO,INO,MODE,VMU,
13550 * ITMAX,TERM,J,JINV
13560 DIMENSION U(0:1001),R(0:1001),Y(0:1001),EU(180),PSI(1:180,0:1001)
13570 C
13580 C INITIALIZATION
13590 C *****
13600 C
13610 IF(TERM.EQ.1) WRITE(3,2)
13620 2 FORMAT(//,' *** CALCULATIE VAN GEBONDEN GOLFFUNCTIES ***')
13630 C 2 FORMAT(//,' *** CALCULATION OF BOUND WAVE-FUNCTIONS ***')
13640 FAC=MURED/16.86
13650 VIB=0
13660 VIBC=0
13670 IT=0

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13680      H=R(2)-R(1)
13690      5  IF (TERM.EQ.1) WRITE(3,8) E
13700      8  FORMAT(/, ' TRIAL-ENERGIE= ',E14.7, '//,
13710      *  ' IT      M      R(M)      E      DE')
13720      C 8  FORMAT(/, ' TRIAL ENERGY VALUE= ',E14.7, '//,
13730      C  *  ' IT      M      R(M)      E      DE')
13740      25  JMIN=1
13750          JMAX=N+1
13760          DO 10 J=1, N-24, 1
13770          IF(JMIN.EQ.1.AND.U(J+25).LE.E) JMIN=J
13780      10  CONTINUE
13790          DO 20 JINV=26, N+1, 1
13800          J=N+27-JINV
13810          IF(JMAX.EQ.N+1.AND.U(J-25).LE.E) JMAX=J
13820      20  CONTINUE
13830      C
13840          Y(JMIN)=0
13850          Y(JMIN+1)=(1-FAC*H*H*(U(JMIN+1)-E))
13860          Y(JMAX)=(1-FAC*H*H*(U(JMAX)-E))
13870          Y(JMAX-1)=(1-FAC*H*H*(U(JMAX-1)-E))*EXP(SQRT(FAC)*
13880      *      (R(JMAX)*SQRT(U(JMAX)-E)-R(JMAX-1)*SQRT(U(JMAX-1)-E)))
13890      C
13900      C  INWARD INTEGRATION
13910      C *****
13920      C
13930          M=0
13940          Y(JMAX-2)=H*H*Y(JMAX-1)*(1/H/H+FAC*(U(JMAX-1)-E)/
13950      *      (1-FAC*H*H*(U(JMAX-1)-E)/12))
13960      C
13970          DO 40 JINV=JMIN+1, JMAX-3, 1
13980          J=JMIN+JMAX-2-JINV
13990          IF(M.NE.0) GOTO 40
14000          Y(J)=Y(J+1)*(2+FAC*H*H*(U(J+1)-E)/
14010      *      (1-FAC*H*H*(U(J+1)-E)/12))-Y(J+2)
14020          IF(ABS(Y(J)).LE.ABS(Y(J+1))) M=J
14030      40  CONTINUE
14040      C
14050          IF(Y(M).EQ.0) M=M+1
14060          DO 50 JINV=M, JMAX, 1
14070          J=M+JMAX-JINV
14080          Y(J)=Y(J)/Y(M)
14090      50  CONTINUE
14100      C
14110      C  OUTWARD INTEGRATION
14120      C *****
14130      C
14140          DO 60 J=JMIN+2, M, 1
14150          Y(J)=Y(J-1)*(2+FAC*H*H*(U(J-1)-E)/
14160      *      (1-FAC*H*H*(U(J-1)-E)/12))-Y(J-2)
14170      60  CONTINUE
14180      C
14190          DO 70 J=JMIN+1, M, 1
14200          Y(J)=Y(J)/Y(M)
14210      70  CONTINUE
14220      C
14230      C  CALCULATON OF NEW ENERGY EIGENVALUE
14240      C *****
14250      C
14260          SOM=0
14270          DO 80 J=JMIN+1, JMAX-1, 1
14280          SOM=SOM+(Y(J)/(1-FAC*H*H*(U(J)-E)/12))**2
14290      80  CONTINUE

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14300      DE=(( -Y(M-1)+2*Y(M)-Y(M+1) )/H/H/FAC+U(M)-E)/SOM
14310      E=E+DE
14320      IT=IT+1
14330      IF (TERM.EQ.1) WRITE(3,18) IT,M,R(M),E,DE
14340  18  FORMAT(' ',I3,' ',I4,' ',E14.7,' ',E14.7,' ',E14.7)
14350  C
14360      IF(ABS(DE).GT.EPS) GOTO 130
14370  C
14380  C      DETERMINATION OF VIBRATIONAL QUANTUM NUMBER
14390  C      *****
14400  C
14410      NO=0
14420      INO=0
14430      DO 90 IO=JMIN+1,JMAX
14440      IF(ABS(Y(IO)).LE.ABS(Y(IO-1)).AND.INO.EQ.0) NO=NO+1
14450      IF(ABS(Y(IO)).LE.ABS(Y(IO-1)).AND.INO.EQ.0) INO=1
14460      IF(ABS(Y(IO)).GT.ABS(Y(IO-1)).AND.INO.EQ.1) INO=0
14470  90  CONTINUE
14480      IF(TERM.EQ.1) WRITE(3,19) NO
14490  19  FORMAT(/,' STOPCRITERIUM BEREIKT, VIBR. QUANTUMGETAL= ',I4,/)
14500  C 19  FORMAT(/,' STOPCRITERIUM REACHED, VIBR. QUANTUM NUMBER= ',I4,/)
14510      IF(VMU.EQ.1) GOTO 95
14520  C
14530      IF(NO.EQ.VIB+1) GOTO 95
14540      IF(NO.GT.VIB+1.AND.VIB.GT.0) E=E+EU(VIBC)/2
14550      IF(NO.GT.VIB+1.AND.VIB.EQ.0) E=E-OMEU/4
14560      IF(NO.LT.VIB+1) E=E+OMEU
14570      IF(E.GT.EMAX.AND.MODE.EQ.2) GOTO 140
14580  C
14590  C      NORMALIZATION AND STORAGE OF CALCULATED WAVE-FUNCTION
14600  C      *****
14610  C
14620  95  IF(VIBC.GT.0) OMEU=(E-EU(VIBC))/STEP
14630      VIB=VIB+STEP
14640      VIBC=VIBC+1
14650      EU(VIBC)=E
14660  C
14670      DO 125 I=1,200
14680      IF(I.NE.VIBC) GOTO 125
14690      DO 100 J=1,JMIN,1
14700      PSI(I,J)=0.0
14710  100 CONTINUE
14720  C
14730      DO 110 J=JMIN+1,JMAX,1
14740      PSI(I,J)=Y(J)/(1-FAC*H*H*(U(J)-E)/12)/SQRT(SOM)*SQRT((N+1)*H)
14750  110 CONTINUE
14760  C
14770      DO 120 J=JMAX+1,N+1,1
14780      PSI(I,J)=0.0
14790  120 CONTINUE
14800  125 CONTINUE
14810  C
14820      IF(VMU.EQ.1) GOTO 140
14830      E=E+OMEU*STEP
14840      IF(VIB.GE.VMU.AND.MODE.EQ.1) GOTO 140
14850      IF(E.GT.EMAX.AND.MODE.EQ.2) GOTO 140
14860  C
14870      IT=0
14880      GOTO 5
14890  C
14900  130 IF(IT.LT.ITMAX) GOTO 25
14910  C

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14920      140 RETURN
14930      END
14940      C
14950      C
14960      C
14970      SUBROUTINE VARCOM(RMIN,RMAX,N,VMU,STEP,NAC,STEP2,
14980      *      UPPARR,LOWARR,GAMMA,C1,C2,C3,C4,C5,MURED)
14990      C
15000      C      This subroutine is used to create a printerfile containing
15010      C      information on the parameters used in the calculation.
15020      C      All parameters have the meaning introduced in the main source
15030      C      program
15040      C
15050      REAL*4 RMIN,RMAX,GAMMA,MURED,UPPARR,LOWARR,C1,C2,C3,C4,C5
15060      INTEGER N,VMU,STEP,NAC,STEP2
15070      DIMENSION UPPARR(9),LOWARR(9)
15080      C
15090      WRITE(3,1) RMIN,RMAX,N,VMU,STEP,NAC,STEP2
15100      1  FORMAT(/, ' A) OPERATIE-VARIABLEN',//, ' RMIN= ',F9.2, ' RMAX= ',
15110      *      F9.2,/, ' AANTAL PUNTEN= ',I4,/,
15120      *      ' AANTAL GEBONDEN TOESTANDEN= ',I4,/,
15130      *      ' INTERVAL VIBRATIONEEL QUANTUMGETAL= ',I4,/,
15140      *      ' AANTAL VRIJE TOESTANDEN= ',I4,/,
15150      *      ' ENERGIE-INCREMENT VRIJE TOESTANDEN= ',I4, ' CM-1',///)
15160      C 1  FORMAT(/, ' A) OPERATION-VARIABLES',//, ' RMIN= ',F9.2, ' RMAX= ',
15170      C      *      F9.2,/, ' AMOUNT OF STEPS= ',I4,/,
15180      C      *      ' AMOUNT OF BOUND STATES= ',I4,/,
15190      C      *      ' INTERVAL VIBRATIONAL QUANTUM NUMBER= ',I4,/,
15200      C      *      ' AMOUNT OF FREE STATES= ',I4,/,
15210      C      *      ' ENERGY INCREMENT OF FREE STATES= ',I4, ' CM-1',///)
15220      C
15230      WRITE(3,2)
15240      2  FORMAT(' B) SYSTEEM-VARIABLEN',//,
15250      *      ' PARAMETERS VOOR GEBONDEN EN VRIJE TOESTANDEN:',/)
15260      C 2  FORMAT(' B) SYSTEM VARIABLES',//,
15270      C      *      ' PARAMETERS FOR BOUND AND FREE STATES:',/)
15280      DO 10 I=1,9
15290      WRITE(3,3) I,UPPARR(I),LOWARR(I)
15300      3  FORMAT(' I= ',I2, ' UPPARR(I)= ',E14.7, ' LOWARR(I)= ',E14.7)
15310      10  CONTINUE
15320      WRITE(3,4)
15330      4  FORMAT(/, ' PARAMETERS VOOR HET ELECTRONISCH OVERGANGSMOMENT',/)
15340      C 4  FORMAT(/, ' PARAMETERS FOR THE ELECTRONIC TRANSITION MOMENT',/)
15350      WRITE(3,5) GAMMA,C1,C2,C3,C4,C5
15360      5  FORMAT(' GAMMA= ',E14.7,/, ' C1= ',E14.7,/, ' C2= ',E14.7,/,
15370      *      ' C3= ',E14.7,/, ' C4= ',E14.7,/, ' C5= ',E14.7,/)
15380      C*
15390      RETURN
15400      END

```

```

10000 C MINIB2/S/GEBONDENVRIJ/BIJEENVEEG
10010 C
10020 C This program is part of a series of programs to simulate
10030 C bound-free rare gas halide emission spectra.
10040 C This program uses spectra stored on a specified FILE 1, and
10050 C copies them to a specified FILE 2, where however spectra from
10060 C a number of vibrational states are collected into one function.
10070 C This is a very useful, I/O time-saving preparation for later
10080 C use of the calculated spectra in programs MINIB2/S/GEBONDENVRIJ/
10090 C TRANSAANPASSING and MINIB2/S/GEBONDENVRIJ/AANPASSINGCA, where
10100 C a procedure of this kind would have to be followed anyway.
10110 C
10120 C*****
10130 C
10140 FILE 1(KIND=DISK,TITLE="MINIB2/D/GEBONDENVRIJ/XEBRCA/2")
10150 FILE 2(KIND=DISK,TITLE="MINIB2/D/GEBONDENVRIJ/XEBRCA/3",
10160 * NEWFILE=TRUE,PROTECTION=SAVE)
10170 FILE 3(KIND=REMOTE)
10180 INTEGER LMIN,LMAX,VIB,STEP,VIB2,STEP2
10190 REAL STEP3,UMINUP,EU,EU2,SPEK,SPEK2
10200 DIMENSION SPEK(0:179,0:1019),SPEK2(0:14,0:1019),EU(0:179),
10210 * EU2(0:179)
10220 C
10230 READ(1,/) LMIN,LMAX,STEP3
10240 READ(1,/) VIB,STEP
10250 READ(1,/) UMINUP
10260 READ(1,/) EU
10270 C
10280 VIB2=10
10290 STEP2=15
10300 IF(VIB2*STEP2.GT.VIB) WRITE(3,5)
10310 IF(VIB2*STEP2.GT.VIB) GOTO 50
10320 5 FORMAT(' OP FILE 1 STAAN ONVOLDOENDE BEREKENDE SPECTRA.')
10330 C 5 FORMAT(' INSUFFICIENT AMOUNT OF SPECTRA ON FILE 1.')
10340 C
10350 C The parameter STEP2 determines the amount of spectra of
10360 C individual vibrational states which have to be collected into
10370 C one fitfunction. The parameter VIB2 determines the amount of
10380 C fitfunction which are to be formed in this way.
10390 C
10400 WRITE(2,/) LMIN,LMAX,STEP3
10410 WRITE(2,/) VIB2,1
10420 WRITE(2,/) UMINUP
10430 DO 20 I=0,VIB-1
10440 DO 10 J=1,34
10450 READ(1) (SPEK(I,30*(J-1)+K),K=0,29)
10460 10 CONTINUE
10470 20 CONTINUE
10480 C
10490 DO 25 I=0,VIB2-1
10500 DO 22 K=0,STEP2-1
10510 EU2(I)=EU2(I)+EU(STEP2*I+K)/STEP2
10520 DO 30 J=0,1019
10530 30 SPEK2(I,J)=SPEK2(I,J)+SPEK(STEP2*I+K,J)
10540 22 CONTINUE
10550 25 CONTINUE
10560 C
10570 WRITE(2,/) EU2

```

```
10580      DO 40 I=0,VIB2-1
10590      DO 35 J=1,34
10600      WRITE(2) (SPEK2(I,30*(J-1)+K),K=0,29)
10610      35 CONTINUE
10620      40 CONTINUE
10630      C
10640      50 CLOSE(2,DISP=CRUNCH)
10650      END
```

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10000 C MINIB2/S/GEBONDENVRIJ/AANPASSINGBX
10010 C
10020 C This program is part of a series of programs to simulate
10030 C bound-free rare gas halide emission spectra.
10040 C When doing simulations of experimental emission spectra it
10050 C often occurs that, having calculated the emission spectra of
10060 C individual vibrational states for a given set of potential
10070 C curves and a given transition moment, one wants to modify
10080 C either of these. For this purpose there are two programs,
10090 C the present one, to be used for transitions where there may
10100 C be more than one point of stationary phase for a given combi-
10110 C nation of upper state and lower state energies (for example
10120 C B-X(1/2) transitions), and MINIB2/S/GEBONDENVRIJ/AANPASSINGCA,
10130 C when there is only one point of stationary phase (for example
10140 C C-A(3/2) transitions). Since there has as yet never been the
10150 C necessity of transforming B-X(1/2) potential curves, the present
10160 C program only has the option of changing the transition moment.
10170 C The structure of the program is such that spectra on a
10180 C specified FILE 1 are transformed and copied to a specified
10190 C FILE 2.
10200 C
10210 C*****
10220 C
10230 C DECLARATIONS
10240 C *****
10250 C
10260 FILE 1(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/XEBRBX/4")
10270 FILE 2(KIND=DISK, TITLE="MINIB2/D/GEBONDENVRIJ/XEBRBX/5",
10280 * PROTECTION=SAVE, NEWFILE=TRUE)
10290 FILE 3(KIND=REMOTE)
10300 FILE 4(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/POTINVOER")
10310 FILE 5(KIND=PRINTER)
10320 REAL STEP3, UMINUP, EU, SPEK, DUMMY, RMIN, RMAX, UPPARR,
10330 * LOWARR, H, UDIF, R, UUP, ULO, UMUL, REUP, GAMMA, GAMMA2,
10340 * D1, D2, D3, D4, D5, C1, C2, C3, C4, C5, TM, TM2, RBI, LABBI1, LABBI2,
10350 * LABMIN, RBU, LABMAX, G, LAB, NU, R1,
10360 * R2
10370 INTEGER STEP, LMIN, LMAX, VIB, N, IREUP, IBI, IBU, I1, I2
10380 DIMENSION EU(0:179), SPEK(0:179, 0:1019), UPPARR(1:9),
10390 * LOWARR(1:9), UUP(0:1001), ULO(0:1001), UMUL(0:1001),
10400 * TM(0:1001), TM2(0:1001), G(0:1001), R(0:1001),
10410 * IR1(0:1001), IR2(0:1001), IBI(0:179), IBU(0:179)
10420 C
10430 C INPUT VARIABLES
10440 C *****
10450 C
10460 READ(1,/) LMIN, LMAX, STEP3
10470 READ(1,/) VIB, STEP
10480 READ(1,/) UMINUP
10490 READ(1,/) EU
10500 WRITE(2,/) LMIN, LMAX, STEP3
10510 WRITE(2,/) VIB, STEP
10520 WRITE(2,/) UMINUP
10530 WRITE(2,/) EU
10540 C
10550 DO 40 I=0, VIB-1
10560 DO 30 J=1, 34
10570 READ(1) (SPEK(I, 30*(J-1)+K), K=0, 29)

```

```

10580      30 CONTINUE
10590      40 CONTINUE
10600      C
10610          READ(4,/) DUMMY
10620          READ(4,/) DUMMY
10630          READ(4,/) RMIN,RMAX
10640          READ(4,/) N
10650          READ(4,/) DUMMY,DUMMY
10660          READ(4,/) DUMMY,DUMMY
10670          READ(4,/) DUMMY,DUMMY
10680          READ(4,/) DUMMY,DUMMY
10690          READ(4,/) DUMMY
10700          READ(4,/) UPPARR(1),
10710          * UPPARR(2),UPPARR(3),UPPARR(4),UPPARR(5),UPPARR(6),
10720          * UPPARR(7),UPPARR(8),UPPARR(9)
10730          READ(4,/) LOWARR(1),
10740          * LOWARR(2),LOWARR(3),LOWARR(4),LOWARR(5),LOWARR(6),
10750          * LOWARR(7),LOWARR(8),LOWARR(9)
10760      C
10770      C      CALCULATION OF POTENTIAL CURVES
10780      C      *****
10790      C
10800          H=(RMAX-RMIN)/(N+1)
10810          UMINUP=10**10
10820          UDIF=10**10
10830      C
10840          DO 31 I=0,N+1,1
10850          R(I)=RMIN+I*H
10860      C      R(I)=R(I)*1.09          Note: for XeBr B-X(1/2_ calculation!
10870          UUP(I)=UPPARR(1)+UPPARR(2)
10880          * +UPPARR(3)*EXP(-UPPARR(4)*R(I))
10890          * +UPPARR(5)*EXP(-UPPARR(6)*R(I))
10900          * -UPPARR(7)/R(I)
10910          * -UPPARR(8)/(R(I)**4)
10920          * -UPPARR(9)/(R(I)**6)
10930          ULO(I)=LOWARR(1)+LOWARR(2)
10940          * +LOWARR(3)*EXP(-LOWARR(4)*R(I))
10950          * +LOWARR(5)*EXP(-LOWARR(6)*R(I))
10960          * -LOWARR(7)/R(I)
10970          * -LOWARR(8)/(R(I)**4)
10980          * -LOWARR(9)/(R(I)**6)
10990          UMUL(I)=UUP(I)-ULO(I)
11000          IF(UMUL(I).LE.UDIF) IMUL=I
11010          IF(UMUL(I).LE.UDIF) UDIF=UMUL(I)
11020          IF(UUP(I).GE.UMINUP) GOTO 37
11030          UMINUP=UUP(I)
11040          IREUP=I
11050          REUP=R(I)
11060      37 CONTINUE
11070      C      R(I)=R(I)/1.09          Note: for XeBr B-X(1/2) calculation!
11080      31 CONTINUE
11090      C
11100      C      PARAMETERS FOR THE OLD TRANSITION MOMENT
11110      C      *****
11120      C
11130          GAMMA2=0.3
11140          D1=33.50
11150          D2=-36.25
11160          D3=14.70
11170          D4=-2.648
11180          D5=0.182
11190      C

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```

11200      READ(4,/) DUMMY
11210      READ(4,/) GAMMA, C1, C2, C3, C4, C5
11220      C
11230      C      Parameters for the new transition moment are stored on
11240      C      FILE 4, the inputfile for MINIB2/S/GEBONDENVRIJ/POTCALC.
11250      C
11260      C      CALCULATION OF THE OLD AND NEW TRANSITION MOMENTS
11270      C      *****
11280      C
11290      DO 41 I=0, N+1
11300      C      R(I)=R(I)*1.09      Note: for XeBr B-X(1/2) calculation!
11310      TM(I)=EXP(0.6*(R(I)-REUP))/
11320      *      (C1+C2*R(I)+C3*R(I)**2+C4*R(I)**3+C5*R(I)**4)
11330      C      *      EXP(0.2*((R(I)-REUP)**2))
11340      C      R(I)=R(I)/1.09      Note: for XeBr B-X(1/2) calculation!
11350      TM2(I)=EXP(GAMMA2*(R(I)-REUP))/
11360      *      (D1+D2*R(I)+D3*R(I)**2+D4*R(I)**3+D5*R(I)**4)
11370      C
11380      C      The arrays TM and TM2 are used to store the new and the old
11390      C      transition moment, respectively.
11400      C
11410      41 CONTINUE
11420      C
11430      C      DETERMINATION OF INNER AND OUTER TURNING POINTS OF THE BOUND
11440      C      UPPER STATES
11450      C      *****
11460      C
11470      DO 100 I=0, VIB-1
11480      IREUP2=IREUP
11490      CALL SNIJPU(UUP, 0, IREUP2, EU(I), RBI)
11500      C
11510      C      Subroutine SNIJPU is a subroutine which calculates, within
11520      C      an interval determined by array-indices I1 and I2, the
11530      C      location where a function F takes on a specified value E.
11540      C      See source text of SNIJPU.
11550      C
11560      IBI(I)=INT(RBI)+1
11570      IREUP2=IREUP
11580      N2=N
11590      CALL SNIJPU(UUP, IREUP2, N2, EU(I), RBU)
11600      IBU(I)=INT(RBU)
11610      100 CONTINUE
11620      C
11630      DO 80 J=0, N
11640      G(J)=ABS(1/(UUP(J+1)-UUP(J)-ULO(J+1)+ULO(J)))
11650      C
11660      C      Array G is used to store the inverse of the difference
11670      C      between the gradient of the upper and lower state potential
11680      C      curves. G(J) is a measure for the width of the stationary
11690      C      phase contributions around R(J).
11700      C
11710      80 CONTINUE
11720      C
11730      C      TRANSFORMATION OF CALCULATED EMISSION SPECTRA
11740      C      *****
11750      C
11760      LABMIN=10**7/(EU(VIB-1)-LOWARR(1))
11770      LABMAX=10**7/UDIF
11780      JMIN=INT((LABMIN-LMIN)/STEP3)+1
11790      JMAX=INT((LABMAX-LMIN)/STEP3)
11800      C
11810      C      Determination of the location of the points of stationary

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11820 C phase as a function of the wavelength of the emitted photon.
11830 C
11840 DO 90 J=JMIN,JMAX
11850 LAB=LMIN+J*STEP3
11860 NU=10**7/LAB
11870 IMUL2=IMUL
11880 CALL SNIJPU(UMUL,0,IMUL2,NU,R1)
11890 IR1(J)=INT(R1)
11900 IMUL2=IMUL
11910 N2=N
11920 CALL SNIJPU(UMUL,IMUL2,N2,NU,R2)
11930 IR2(J)=INT(R2)
11940 90 CONTINUE
11950 C
11960 DO 95 I=0,VIB-1
11970 C
11980 C Selection of points of stationary phase which are classically
11990 C attainable, followed by transformation of the calculated
12000 C emission spectra
12010 C
12020 DO 94 J=JMIN,JMAX
12030 IF(IR1(J).LT.IBI(I).AND.IR2(J).GT.IBU(I)) GOTO 94
12040 IF(IR1(J).GE.IBI(I).AND.IR2(J).LE.IBU(I)) GOTO 92
12050 IF(IR1(J).GE.IBI(I).AND.IR2(J).GT.IBU(I)) GOTO 91
12060 SPEK(I,J)=SPEK(I,J)+(TM(IR2(J))/TM2(IR2(J)))**2
12070 GOTO 94
12080 91 SPEK(I,J)=SPEK(I,J)*(TM(IR1(J))/TM2(IR1(J)))**2
12090 GOTO 94
12100 92 F1=1/SQRT(EU(I)-UUP(IR1(J)))*G(IR1(J))
12110 F2=1/SQRT(EU(I)-UUP(IR2(J)))*G(IR2(J))
12120 SPEK(I,J)=SPEK(I,J)*
12130 * (F1*TM(IR1(J))**2+F2*TM(IR2(J))**2)/
12140 * (F1*TM2(IR1(J))**2+F2*TM2(IR2(J))**2)
12150 94 CONTINUE
12160 95 CONTINUE
12170 C
12180 DO 140 I=0,VIB-1
12190 DO 130 J=1,34
12200 WRITE(2) (SPEK(I,30*(J-1)+K),K=0,29)
12210 130 CONTINUE
12220 140 CONTINUE
12230 C
12240 CLOSE(6,DISP=CRUNCH)
12250 END
12260 C
12270 C
12280 SUBROUTINE SNIJPU(F,I1,I2,E,R3)
12290 C
12300 C Subroutine SNIJPU is a subroutine which calculates, within
12310 C boundaries determined by the array-indices I1 and I2, the
12320 C location where a function F takes on a specified value E.
12330 C As output the subroutine gives a parameter R3 which
12340 C is an optimal real approximation of the array-index where
12350 C the function F takes on the value E. If there is no point
12360 C between I1 and I2 where F takes on the value E, then R3 is
12370 C given the value -1.
12380 C
12390 REAL F,E,R3
12400 INTEGER I1,I2,I3
12410 DIMENSION F(0:4001)
12420 C*
12430 IF((I2-I1).LE.1) GOTO 30

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```

12440      IF(F(I1).LT.E.AND.F(I2).LT.E) R3=-1
12450      IF(F(I1).GE.E.AND.F(I2).GE.E) R3=-1
12460      IF(R3.LT.0) GOTO 40
12470      C*
12480      IF(F(I2).GE.F(I1)) GOTO 20
12490      10  I3=INT((I2+I1)/2)
12500      IF(F(I3).LT.E) I2=I3
12510      IF(F(I3).GT.E) I1=I3
12520      IF((I2-I1).LE.1) GOTO 30
12530      GOTO 10
12540      C*
12550      20  I3=INT((I2+I1)/2)
12560      IF(F(I3).LT.E) I1=I3
12570      IF(F(I3).GE.E) I2=I3
12580      IF((I2-I1).LE.1) GOTO 30
12590      GOTO 20
12600      C
12610      30  R3=I1+(F(I1)-E)/(F(I1)-F(I2))
12620      40  CONTINUE
12630      C
12640      RETURN
12650      END

```



```

10000 C MINIB2/S/GEBONDENVRIJ/AANPASSINGCA
10010 C
10020 C This program is part of a series of programs to simulate
10030 C bound-free rare gas halide emission spectra
10040 C When doing simulations of experimental emission spectra it
10050 C often occurs that, having calculated the emission spectra of
10060 C individual vibrational states for a given set of potential
10070 C curves and a given transition moment, one wants to modify
10080 C either of these. For this purpose there are two programs,
10090 C MINIB2/S/GEBONDENVRIJ/AANPASSINGBX, to be used for transtions
10100 C where there may be more than one point of stationary phase
10110 C for a given combination of upper state and lower state
10120 C energies (for example B-X(1/2) transitions), and the present
10130 C one, to be used when there is only one point of stationary
10140 C phase (for example C-A(3/2) transitions).
10150 C
10160 C*****
10170 C
10180 C DECLARATIONS
10190 C *****
10200 C
10210 FILE 1(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/XEBRCA/3")
10220 FILE 2(KIND=DISK, TITLE="MINIB2/D/GEBONDENVRIJ/XEBRCA/4",
10230 * PROTECTION=SAVE, NEWFILE=TRUE)
10240 FILE 3(KIND=REMOTE)
10250 FILE 4(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/POTINVOERCA")
10260 FILE 5(KIND=PRINTER)
10270 REAL STEP3, UMINUP, EU, SPEK, DUMMY, RMIN, RMAX, UPPARR,
10280 * LOWARR, H, UDIF, R, UUP, ULO, ULO2, UMUL, UMUL2, REUP, GAMMA, GAMMA2,
10290 * D1, D2, D3, D4, D5, C1, C2, C3, C4, C5, TM, TM2, RBI, LABBI1, LABBI2,
10300 * LABMIN, RBU, LABMAX, G, LAB, NU, R1, LABIAC, LABUAC, RKOUD,
10310 * R2, DELTTE, CORR, LABBI, LABBU, LABOUD, ROUD, RNU, NUOUD, LOUD
10320 INTEGER LMIN, LMAX, KMAX, VIB, N, IREUP, IBI, IBU, I1, I2, JBIN,
10330 * JBUI, IOUD, SPEK2, INU, IKOUD, STEP
10340 DIMENSION EU(0:179), SPEK(0:29, 0:1019), UPPARR(1:9),
10350 * LOWARR(1:9), UUP(0:1001), ULO(0:1001), UMUL(0:1001),
10360 * TM(0:1001), TM2(0:1001), G(0:1001), R(0:1001),
10370 * IR1(0:1001), IR2(0:1001), IBI(0:179), IBU(0:179),
10380 * SPEK2(0:29, 0:1019), UMUL2(0:1001), ULO2(0:1001),
10390 * RULO(0:9), UULO(0:9)
10400 C
10410 C INPUT VARIABLES
10420 C *****
10430 C
10440 READ(1,/) LMIN, LMAX, STEP3
10450 READ(1,/) VIB, STEP
10460 READ(1,/) UMINUP
10470 READ(1,/) EU
10480 C
10490 WRITE(2,/) LMIN, LMAX, STEP3
10500 WRITE(2,/) VIB, STEP
10510 WRITE(2,/) UMINUP
10520 WRITE(2,/) EU
10530 C
10540 DO 40 I=0, VIB-1
10550 DO 30 J=1, 34
10560 READ(1) (SPEK(I, 30*(J-1)+K), K=0, 29)
10570 30 CONTINUE

```

```

10580      40 CONTINUE
10590      C
10600      READ(4,/) DUMMY
10610      READ(4,/) DUMMY
10620      READ(4,/) RMIN,RMAX
10630      READ(4,/) N
10640      READ(4,/) DUMMY,DUMMY
10650      READ(4,/) DUMMY,DUMMY
10660      READ(4,/) DUMMY,DUMMY
10670      READ(4,/) DUMMY,DUMMY
10680      READ(4,/) DUMMY
10690      READ(4,/) UPPARR(1),
10700      * UPPARR(2),UPPARR(3),UPPARR(4),UPPARR(5),UPPARR(6),
10710      * UPPARR(7),UPPARR(8),UPPARR(9)
10720      READ(4,/) LOWARR(1),
10730      * LOWARR(2),LOWARR(3),LOWARR(4),LOWARR(5),LOWARR(6),
10740      * LOWARR(7),LOWARR(8),LOWARR(9)
10750      C
10760      C CALCULATION OF POTENTIAL CURVES
10770      C *****
10780      C
10790      H=(RMAX-RMIN)/(N+1)
10800      UMINUP=10**10
10810      UDIF=10**10
10820      C
10830      DO 31 I=0,N+1,1
10840      R(I)=RMIN+I*H
10850      UUP(I)=UPPARR(1)+UPPARR(2)
10860      * +UPPARR(3)*EXP(-UPPARR(4)*R(I))
10870      * +UPPARR(5)*EXP(-UPPARR(6)*R(I))
10880      * -UPPARR(7)/R(I)
10890      * -UPPARR(8)/(R(I)**4)
10900      * -UPPARR(9)/(R(I)**6)
10910      ULO(I)=LOWARR(1)+LOWARR(2)
10920      * +LOWARR(3)*EXP(-LOWARR(4)*R(I))
10930      * +LOWARR(5)*EXP(-LOWARR(6)*R(I))
10940      * -LOWARR(7)/R(I)
10950      * -LOWARR(8)/(R(I)**4)
10960      * -LOWARR(9)/(R(I)**6)
10970      ULO2(I)=4.8536E7*EXP(-2.9464*R(I))+600
10980      C
10990      C A modification of the potential curves is achieved by
11000      C introducing a new lower state potential curve ULO2.
11010      C
11020      UMUL(I)=UUP(I)-ULO(I)
11030      UMUL2(I)=UUP(I)-ULO2(I)
11040      IF(10*(INT(I/10)).EQ.I) WRITE(5,/) R(I),UUP(I),ULO(I),ULO2(I),
11050      * UMUL2(I)
11060      IF(UMUL(I).LE.UDIF) IMUL=I
11070      IF(UMUL(I).LE.UDIF) UDIF=UMUL(I)
11080      IF(UUP(I).GE.UMINUP) GOTO 37
11090      UMINUP=UUP(I)
11100      IREUP=I
11110      REUP=R(I)
11120      37 CONTINUE
11130      31 CONTINUE
11140      C
11150      C PARAMETERS FOR THE OLD TRANSITION MOMENT
11160      C *****
11170      C
11180      GAMMA2=0.0
11190      DI=19.96

```

```

11200          D2=-25.62
11210          D3=12.57
11220          D4=-2.799
11230          D5=0.248
11240      C
11250          READ(4,/) DUMMY
11260          READ(4,/) GAMMA,C1,C2,C3,C4,C5
11270      C
11280      C      Parameters for the new transition moment are stored on
11290      C      FILE 4, the inputfile for MINIB2/S/GEBONDENVRIJ/POTCALC
11300      C
11310      C      CALCULATION OF THE OLD AND NEW TRANSITION MOMENTS
11320      C      *****
11330      C
11340          DO 41 I=0,N+1
11350      C      GAMMA=0.4      For quick changes FILE 4 may be overruled.
11360          TM(I)=EXP(GAMMA*(R(I)-REUP))/
11370          *      (C1+C2*R(I)+C3*R(I)**2+C4*R(I)**3+C5*R(I)**4)
11380          TM2(I)=EXP(GAMMA2*(R(I)-REUP))/
11390          *      (D1+D2*R(I)+D3*R(I)**2+D4*R(I)**3+D5*R(I)**4)
11400      C
11410      C      The arrays TM and TM2 are used to store the new and the old
11420      C      transition moment, respectively.
11430      C
11440      41  CONTINUE
11450      C
11460      C      TRANSFORMATION OF THE TRANSITION MOMENT OF CALCULATED EMISSION
11470      C      SPECTRA
11480      C      *****
11490      C
11500          LABMIN=10**7/(EU(VIB-1)-LOWARR(1))
11510          LABMAX=LMAX
11520          JMIN=INT((LABMIN-LMIN)/STEP3)+1
11530          JMAX=INT((LABMAX-LMIN)/STEP3)
11540      C
11550      C      Determination of the location of the points of stationary
11560      C      phase as a function of the wavelength of the emitted photon.
11570      C
11580          DO 90 J=JMIN,JMAX
11590          LAB=LMIN+J*STEP3
11600          NU=10**7/LAB
11610          IMUL2=IMUL
11620          N2=N
11630          CALL SNIJPU(UMUL,0,N2,NU,R1)
11640          IR1(J)=INT(R1)
11650      90  CONTINUE
11660      C
11670      C      Transformation of the calculated emission spectra.
11680      C
11690          DO 95 I=0,VIB-1
11700          DO 94 J=JMIN,JMAX
11710          IF(IR1(J).EQ.-1) GOTO 94
11720      91  SPEK(I,J)=SPEK(I,J)*(TM(IR1(J))/TM2(IR1(J)))**2
11730      94  CONTINUE
11740      95  CONTINUE
11750      C
11760      C      TRANSFORMATION OF THE POTENTIAL CURVES OF CALCULATED EMISSION
11770      C      SPECTRA
11780      C      *****
11790      C
11800      C      Determination of internuclear distance for the new potential
11810      C      curves where an emitted photon will have wavelength LAB.

```

```

11820      C
11830      KMAX=INT((LMAX-LMIN)/STEP3)
11840      DO 200 K=0,KMAX
11850      LAB=LMIN+K*STEP3
11860      NU=1E7/LAB
11870      RNU=-1
11880      IF(RNU.NE.-1) GOTO 210
11890      DO 210 J=0,N
11900      IF(UMUL2(J).LE.NU.AND.UMUL2(J+1).GT.NU) RNU=(NU-
11910      *   UMUL2(J))/(UMUL2(J+1)-UMUL2(J))+J
11920      210 CONTINUE
11930      INU=INT(RNU)
11940      C
11950      C   Calculation of the wavelength of an emitted photon for the
11960      C   old potential curves, at the previously determined internuclear
11970      C   distance.
11980      C
11990      IF(INU.EQ.-1) GOTO 200
12000      NUOUD=UMUL(INU)*(1-RNU+INU)+UMUL(INU+1)*(RNU-INU)
12010      LOUD=1E7/NUOUD
12020      C
12030      C   Transformation of the calculated emission spectrum.
12040      C
12050      RKOUD=(LOUD-LMIN)/STEP3
12060      IKOUD=INT(RKOUD)
12070      IF(IKOUD.LT.0.OR.IKOUD.GT.1018) GOTO 220
12080      DO 220 I=0,VIB-1
12090      SPEK2(I,K)=SPEK(I,IKOUD)*(1-RKOUD+IKOUD)+
12100      *   SPEK(I,IKOUD+1)*(RKOUD-IKOUD)
12110      220 CONTINUE
12120      C
12130      200 CONTINUE
12140      C
12150      DO 140 I=0,VIB-1
12160      DO 130 J=1,34
12170      WRITE(2) (SPEK2(I,30*(J-1)+K),K=0,29)
12180      130 CONTINUE
12190      140 CONTINUE
12200      C
12210      CLOSE(2,DISP=CRUNCH)
12220      END
12230      C
12240      C
12250      SUBROUTINE SNIJPU(F,I1,I2,E,R3)
12260      C
12270      C   For explanation see MINIB2/S/GEBONDENVRIJ/AANPASSINGBX.
12280      C
12290      REAL F,E,R3
12300      INTEGER I1,I2,I3
12310      DIMENSION F(0:4001)
12320      C
12330      IF((I2-I1).LE.1) GOTO 30
12340      IF(F(I1).LT.E.AND.F(I2).LT.E) R3=-1
12350      IF(F(I1).GE.E.AND.F(I2).GE.E) R3=-1
12360      IF(R3.LT.0) GOTO 40
12370      C
12380      IF(F(I2).GE.F(I1)) GOTO 20
12390      10 I3=INT((I2+I1)/2)
12400      IF(F(I3).LT.E) I2=I3
12410      IF(F(I3).GT.E) I1=I3
12420      IF((I2-I1).LE.1) GOTO 30
12430      GOTO 10

```

```
12440 C*
12450 20 I3=INT((I2+I1)/2)
12460 IF(F(I3).LT.E) I1=I3
12470 IF(F(I3).GE.E) I2=I3
12480 IF((I2-I1).LE.1) GOTO 30
12490 GOTO 20
12500 C
12510 30 R3=I1+(F(I1)-E)/(F(I1)-F(I2))
12520 40 CONTINUE
12530 C
12540 RETURN
12550 END
```

```

10000 C MINIB2/S/GEBONDENVRIJ/GLADSTRIJKEN
10010 C
10020 C This program is part of a series of programs to simulate
10030 C bound-free rare gas halide emission spectra.
10040 C With this program calculated C-A(3/2) emission spectra from
10050 C individual vibrational states can be given an envelope which
10060 C goes down exponentially towards shorter wavelengths. This is
10070 C achieved by fitting the calculated secondary maxima to an
10080 C exponential function.
10090 C
10100 C*****
10110 C
10120 FILE 1(KIND=DISK, TITLE="MINIB2/D/GEBONDENVRIJ/XEBRCA/4")
10130 FILE 3(KIND=PRINTER)
10140 FILE 2(KIND=DISK, TITLE="MINIB2/D/GEBONDENVRIJ/XEBRCA/5",
10150 * NEWFILE=TRUE, PROTECTION=SAVE)
10160 REAL EU, SPEK, SPEK2, STEP3, UMINUP, LAB, INTENS, INTL, INTI,
10170 * INTLI, INTLKW, B, A, CORR1, CORR2, LNA, K1, K2
10180 INTEGER LMIN, LMAX, VIB, STEP, INDEX, LABJ
10190 DIMENSION SPEK(0:9, 0:1019), SPEK2(0:9, 0:1019), EU(0:179),
10200 * LABJ(1:100), LAB(1:100), INTENS(1:100)
10210 C
10220 READ(1,/) LMIN, LMAX, STEP3
10230 READ(1,/) VIB, STEP
10240 READ(1,/) UMINUP
10250 READ(1,/) EU
10260 C
10270 WRITE(2,/) LMIN, LMAX, STEP3
10280 WRITE(2,/) VIB, STEP
10290 WRITE(2,/) UMINUP
10300 WRITE(2,/) EU
10310 C
10320 DO 20 I=0,9
10330 DO 10 J=1,34
10340 READ(1) (SPEK(I, 30*(J-1)+K), K=0, 29)
10350 10 CONTINUE
10360 20 CONTINUE
10370 C
10380 DO 50 I=2, VIB-1
10390 C
10400 SPEKMA=0
10410 DO 51 J=0, 1019
10420 IF(SPEK(I, J).GT.SPEKMA) JMAX=J
10430 IF(SPEK(I, J).GT.SPEKMA) SPEKMA=SPEK(I, J)
10440 51 CONTINUE
10450 C
10460 C Determination of the location of the secondary maxima
10470 C
10480 INDEX=0
10490 DO 40 J=400, JMAX
10500 IF(SPEK(I, J-3).GT.SPEK(I, J)) GOTO 40
10510 IF(SPEK(I, J-2).GT.SPEK(I, J)) GOTO 40
10520 IF(SPEK(I, J-1).GT.SPEK(I, J)) GOTO 40
10530 IF(SPEK(I, J+1).GE.SPEK(I, J)) GOTO 40
10540 IF(SPEK(I, J+2).GE.SPEK(I, J)) GOTO 40
10550 IF(SPEK(I, J+3).GE.SPEK(I, J)) GOTO 40
10560 INDEX=INDEX+1
10570 LABJ(INDEX)=J

```

```

10580      LAB(INDEX)=LMIN+J*STEP3
10590      INTENS(INDEX)=SPEK(I,J)
10600      C      WRITE(3,/) I, INDEX, LABJ(INDEX), LAB(INDEX), INTENS(INDEX)
10610      C 40    CONTINUE
10620      C
10630      C      Fit to an exponential function
10640      C
10650      INTL=0
10660      INTI=0
10670      INTLI=0
10680      INTLKW=0
10690      IF(INDEX.LE.1) GOTO 50
10700      C
10710      DO 60 J=1, INDEX
10720      INTL=INTL+LAB(J)
10730      INTI=INTI+ALOG(INTENS(J))
10740      INTLI=INTLI+LAB(J)*ALOG(INTENS(J))
10750      INTLKW=INTLKW+LAB(J)**2
10760      C 60    CONTINUE
10770      B=(-INTL*INTI+INDEX*INTLI)/(INDEX*INTLKW-INTL**2)
10780      LNA=((INTLKW*INTI-INTL*INTLI)/(INDEX*INTLKW-INTL**2))
10790      A=EXP(LNA)
10800      C
10810      C      Modification of the emission spectra
10820      C
10830      DO 80 J=1, INDEX-1
10840      K1=LABJ(J)
10850      K2=LABJ(J+1)
10860      CORR1=INTENS(J)/A/EXP(B*LAB(J))
10870      CORR2=INTENS(J+1)/A/EXP(B*LAB(J+1))
10880      DO 70 K=K1, K2-1
10890      SPEK(I,K)=SPEK(I,K)*((K-K1)/(K2-K1)/CORR2+(K2-K)/(K2-K1)/CORR1)
10900      C 70    CONTINUE
10910      C 80    CONTINUE
10920      DO 65 K=0, LABJ(1)-1
10930      SPEK(I,K)=SPEK(I,K)*A*EXP(B*LAB(1))/SPEK(I, LABJ(1))
10940      C 65    CONTINUE
10950      DO 66 K=LABJ(INDEX), 1019
10960      SPEK(I,K)=SPEK(I,K)*A*EXP(B*LAB(INDEX))/SPEK(I, LABJ(INDEX))
10970      C 66    CONTINUE
10980      C      WRITE(3,110)
10990      C 110   FORMAT(/)
11000      C 50    CONTINUE
11010      C
11020      DO 100 I=0, 9
11030      DO 90 J=1, 34
11040      WRITE(2) (SPEK(I, 30*(J-1)+K), K=0, 29)
11050      C 90    CONTINUE
11060      C 100   CONTINUE
11070      C
11080      CLOSE(2, DISP=CRUNCH)
11090      END

```

```

10000 C MINIB2/S/GEBONDENVRIJ/VIBFIT
10010 C
10020 C This program is part of a series of programs to simulate
10030 C bound-free rare gas halide emission spectra.
10040 C In this program an experimental emission spectrum from a
10050 C single bound-free electronic transition, stored on a specified
10060 C FILE 2, is simulated using calculated emission spectra of
10070 C individual vibrational states (or collections of emission
10080 C spectra of individual vibrational states) stored on a specified
10090 C FILE 1. Using a least squares method a vibrational distribution
10100 C of the bound upper state is determined, and stored on a
10110 C file MINIB2/D/GEBONDENVRIJ/FITUITVOER (FILE 6).
10120 C The program also creates a previewfile which contains a graphical
10130 C representation of the experimental emission spectrum and the
10140 C simulated spectrum.
10150 C
10160 C*****
10170 C
10180 C DECLARATIONS
10190 C *****
10200 C
10210 FILE 1(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/XEBRCA/5")
10220 FILE 2(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/DATAOUT")
10230 FILE 3(KIND=REMOTE) % WRITE TO TERMINAL
10240 FILE 4(KIND=REMOTE) % READ FROM TERMINAL
10250 FILE 5(KIND=PRINTER)
10260 FILE 6(KIND=DISK, TITLE="MINIB2/D/GEBONDENVRIJ/FITUITVOER",
10270 * PROTECTION=SAVE, NEWFILE=TRUE)
10280 FILE 7(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/POTINVOER")
10290 BLOCK GLOBALS
10300 $ INCLUDE "PLOTTER/FORTRAN/DECLARATION ON APPL"
10310 END
10320 $ INCLUDE "PLOTTER/FORTRAN/POLYDZ ON APPL"
10330 REAL*4 STEP3, UMINUP, EU, SPEK, STEP2, DATA, STEPFI, LABDAI,
10340 * SPRES, DATA2, RSPKLB, RDATLB, SPEKM, DATAM, UIT, RES, SPEKMA, DATAMA,
10350 * CORR, HOR, HOR2, DATAM2, SPEK2, UUP, ULO, R, UPPARR, LOWARR, DUMMY,
10360 * RMIN, RMAX, LAB, RBI, LIBI1, LIBI2, LIBI, F, L, FL, LL, LNF, LNA, A,
10370 * B, H, DATAR, AGEM, CGEM, LABSP, GEW, SIGMA, LMIN2, LMAX2, UIT3, DATAM3
10380 INTEGER*4 LMIN, LMAX, VIB, VIBF, STEP, LMIN3, LMAX3, LMINFI, LMAXFI,
10390 * NFIT, I, J, ISPKLB, IDATLB, IKAN, NKAN, SBER, NBER, LGRENS, NDATA,
10400 * JGRENS
10410 DIMENSION EU(0:179), SPEK(0:50, 0:1019), SPEKM(0:50, 0:1019),
10420 * DATA(0:1019), DATAM2(0:1019), DATAM(0:1019), UIT(0:180),
10430 * SPRES(0:180), HOR(0:1019), UPPARR(1:9), LOWARR(1:9),
10440 * HOR2(0:1019), SPEK2(0:50, 0:1019), UUP(0:4001), ULO(0:4001),
10450 * R(0:4001), LAB(0:1019), DATAR(0:1019), GEW(0:1019),
10460 * UIT3(0:180), DATAM3(0:1019)
10470 C
10480 C INPUT VARIABLES AND INITIALIZATION
10490 C *****
10500 C
10510 READ(1,/) LMIN, LMAX, STEP3
10520 READ(1,/) VIBF, STEP
10530 READ(1,/) UMINUP
10540 READ(1,/) EU
10550 WRITE(3,1) VIBF, STEP
10560 1 FORMAT(' VIBR. NIVEAUS BEREKEND TOT V=^, I4, /,
10570 * ^ STAPGROOTTE=^, I3, /,

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10580      *   ^ GEEF VBER EN STAPGROOTTE SBER: ^)
10590      C 1  FORMAT(^ VIBR. STATES DETERMINED UP TO V=^,I4,/,
10600      C      *   ^ INTERVALSIZE=^,I3,/,
10610      C      *   ^ ENTER VBER AND INTERVALSIZE SBER: ^)
10620      2  READ(4,/) VIB,SBER
10630          NBER=INT(VIB/SBER)
10640          IF(VIB/SBER-INT(VIB/SBER).NE.0) GOTO 2
10650          WRITE(6,/) VIB,SBER
10660      C
10670          DO 40 I=0,VIB-1
10680          DO 30 J=1,34
10690          READ(1) (SPEK(I,30*(J-1)+K),K=0,29)
10700      30  CONTINUE
10710      40  CONTINUE
10720      C
10730          READ(2,/) LMIN3,LMAX3,STEP2
10740      C      LMAX3=310
10750      C
10760      C      If not overruled, the program will try to fit the experimental
10770      C      emission spectrum in the entire wavelength interval determined
10780      C      by LMIN3 and LMAX3.
10790      C
10800          LMIN2=LMIN3
10810          LMAX2=LMAX3
10820      C
10830      C      LMIN3 and LMAX3, and LMIN2 and LMAX2, are the integer and real
10840      C      real versions of the wavelength boundaries, respectively.
10850      C
10860          READ(2,/) DATA
10870          CORR=-11.9
10880          LMIN2=LMIN2+CORR
10890          LMAX2=LMAX2+CORR
10900      C
10910      C      CORR is a correction variable to match the wavelength scales
10920      C      of the experimental and calculated emission spectra.
10930      C
10940      C      Optional: in simulations of B-X(1/2) continua, the influence
10950      C      of overlapping C-A(3/2) (and B-A(1/2)) emission may be
10960      C      accounted for by subtracting a straight line contribution.
10970      C
10980          NDATA=INT((LMAX2-LMIN2)/STEP2)
10990      C      DO 39 J=1,10
11000      C      AGEM=AGEM+DATA(J)/10
11010      C 39  CONTINUE
11020      C      DO 37 J=NDATA-9,NDATA
11030      C      CGEM=CGEM+DATA(J)/10
11040      C 37  CONTINUE
11050      C      LGRENS=225
11060      C      JGRENS=INT((LGRENS-LMIN2)/STEP2)
11070      C      DO 42 J=JGRENS,1019
11080      C      DATA(J)=DATA(J)-(CGEM-AGEM)*(J-JGRENS)/(NDATA-JGRENS)
11090      C 42  CONTINUE
11100      C
11110      C      NORMALIZATION OF CALCULATED AND EXPERIMENTAL EMISSION SPECTRA
11120      C      *****
11130      C
11140          SPEKMA=0
11150          DO 61 I=0,VIB-1
11160          DO 60 J=0,1019
11170          IF(SPEK(I,J).GT.SPEKMA) SPEKMA=SPEK(I,J)
11180      60  CONTINUE
11190      61  CONTINUE

```

```

11200 C
11210 DO 63 I=0,VIB-1
11220 DO 62 J=0,1019
11230 SPEK(I,J)=SPEK(I,J)/SPEKMA
11240 62 CONTINUE
11250 63 CONTINUE
11260 C
11270 DATAMA=0
11280 DO 64 J=0,1019
11290 IF(DATA(J).GT.DATAMA) DATAMA=DATA(J)
11300 64 CONTINUE
11310 C
11320 DO 65 J=0,1019
11330 DATA(J)=DATA(J)/DATAMA*10000
11340 65 CONTINUE
11350 C
11360 C DETERMINATION OF WAVELENGTH INTERVAL AND STEPSIZE FOR LEAST
11370 C SQUARES FIT
11380 C *****
11390 C
11400 LMINFI=LMIN
11410 LMAXFI=LMAX
11420 IF(LMIN2.GT.LMIN) LMINFI=INT(LMIN2+.99)
11430 IF(LMAX2.LT.LMAX) LMAXFI=LMAX2
11440 LMINFI=250
11450 C
11460 STEPMI=STEP3
11470 IF(STEP2.GT.STEP3) STEPMI=STEP2
11480 NFIT=INT((LMAXFI-LMINFI)/STEMPI)
11490 C
11500 C CREATION OF FIT-FUNCTIONS FOR LEAST SQUARES FIT
11510 C *****
11520 C
11530 C a) Joining of SBER emission spectra of individual vibrational
11540 C states into a single fit-function.
11550 C
11560 IF(SBER.EQ.1) GOTO 17
11570 DO 17 I=0,1019
11580 DO 15 J=0,NBER-1
11590 SPEK(J,I)=SPEK(SBER*J,I)
11600 DO 16 K=1,SBER-1
11610 SPEK(J,I)=SPEK(J,I)+SPEK(SBER*J+K,I)
11620 16 CONTINUE
11630 SPEK(J,I)=SPEK(J,I)/SBER
11640 15 CONTINUE
11650 17 CONTINUE
11660 DO 14 I=0,1019
11670 SPEK(NBER,I)=1
11680 14 CONTINUE
11690 C
11700 C b) The introduction of a spectral resolution into the fit-
11710 C functions
11720 C
11730 NKAN=0
11740 DO 35 IKAN=-NKAN,NKAN
11750 DO 34 J=0,NBER
11760 DO 33 I=0,1019
11770 IF(I+IKAN.GE.0.AND.I+IKAN.LE.1019) GOTO 41
11780 SPEK2(J,I)=SPEK2(J,I)+SPEK(J,I)
11790 GOTO 32
11800 41 CONTINUE
11810 SPEK2(J,I)=SPEK2(J,I)+SPEK(J,I+IKAN)

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11820      32 CONTINUE
11830      33 CONTINUE
11840      34 CONTINUE
11850      35 CONTINUE
11860      C
11870      C   CONVERSION OF CALCULATED AND EXPERIMENTAL EMISSION SPECTRA
11880      C   TO SPECTRA MATCHING THE REQUIRED WAVELENGTH INTERVAL AND
11890      C   HAVING THE CORRECT STEPSIZE.
11900      C   *****
11910      C
11920      DO 20 I=0,NFIT
11930      LABDAI=LMINFI+I*STEPFI
11940      C
11950      RSPKLB=((LABDAI-LMIN)/STEP3)
11960      ISPKLB=INT(RSPKLB)
11970      DO 10 J=0,NBER
11980      SPEKM(J,I)=(RSPKLB-ISPKLB)*SPEK2(J,ISPKLB)+
11990      * (1+ISPKLB-RSPKLB)*SPEK2(J,ISPKLB+1)
12000      10 CONTINUE
12010      C
12020      RDATAI=((LABDAI-LMIN2)/STEP2)
12030      IDATLB=INT(RDATAI)
12040      DATAM(I)=(RDATAI-IDATLB)*DATA(IDATLB)+
12050      * (1+IDATLB-RDATAI)*DATA(IDATLB+1)
12060      C
12070      20 CONTINUE
12080      C
12090      C   LEAST SQUARES FIT OF THE EXPERIMENTAL SPECTRA
12100      C   *****
12110      C
12120      DO 38 J=0,NFIT
12130      DO 36 I=0,NBER
12140      SPEK2(I,J)=SPEKM(I,J)
12150      36 CONTINUE
12160      DATAR(J)=DATAM(J)
12170      38 CONTINUE
12180      CALL FIT(NFIT+1,NBER,DATAR,SPEK2,UIT,RES)
12190      C
12200      C   Subroutine FIT determines a least squares fit of a function
12210      C   DATA by a number of fit-functions stored in a matrix MATRIX. An
12220      C   explanation of the heading of FIT is included in the source
12230      C   text of FIT.
12240      C
12250      C   GRAPHICAL REPRESENTATION OF THE EXPERIMENTAL AND SIMULATED
12260      C   EMISSION SPECTRA
12270      C   *****
12280      C
12290      DO 26 J=0,1019
12300      HOR(J)=LMIN2+STEP2*J
12310      26 CONTINUE
12320      C
12330      DO 28 J=0,NFIT-1
12340      DATAM2(J)=0
12350      DO 27 I=0,NBER
12360      DATAM2(J)=DATAM2(J)+UIT(I)*SPEKM(I,J)
12370      HOR2(J)=LMINFI+J*STEPFI
12380      27 CONTINUE
12390      28 CONTINUE
12400      C
12410      CALL POLYDZ(90,0,0,25,20,1,NDATA,HOR,DATA,10,LMINFI,LMAXFI,
12420      * 12,0,12000,.FALSE.,.FALSE.)
12430      CALL POLYDZ(90,0,0,25,20,1,NFIT,HOR2,DATAM2,10,LMINFI,LMAXFI,

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12440      *      12,0,12000,.FALSE.,.FALSE.)
12450      C
12460      29  CONTINUE
12470      C
12480      CLOSE(6,DISP=CRUNCH)
12490      END
12500      C
12510      C
12520      SUBROUTINE FIT(NMEETP,NPAR,DATA,MATRIX,UIT,RES)
12530      C
12540      C      In this subroutine a function, which is known in NMEETP
12550      C      points and stored in array DATA, is least squares fitted
12560      C      to a set of NPAR fit-functions, stored in a matrix MATRIX.
12570      C      The resultant contributions of all individual fit-functions
12580      C      are stored in an array UIT. After the fit the variable RES
12590      C      contains the normalized residu.
12600      C
12610      REAL*4 BETA,RES,DD,DATA,UIT,MATRIX,SOM,DATARE,A
12620      INTEGER NMEETP,NPAR,INDEX,I,J,K,M
12630      DIMENSION DATA(0:1019),DD(0:180),UIT(0:180),
12640      *      MATRIX(0:50,0:1019),DATARE(0:1019)
12650      C
12660      DO 150 K=0,NPAR-1
12670      SOM=0
12680      C
12690      DO 110 I=K,NMEETP-1
12700      SOM=SOM+MATRIX(K,I)**2
12710      110 CONTINUE
12720      C
12730      IF(MATRIX(K,K).GT.0) DD(K)=-SQRT(SOM)
12740      IF(MATRIX(K,K).LE.0) DD(K)=SQRT(SOM)
12750      MATRIX(K,K)=MATRIX(K,K)-DD(K)
12760      BETA=-DD(K)*MATRIX(K,K)
12770      IF(K.EQ.NPAR-1) GOTO 145
12780      C
12790      DO 140 J=K+1,NPAR-1
12800      SOM=0
12810      DO 120 I=K,NMEETP-1
12820      SOM=SOM+MATRIX(K,I)*MATRIX(J,I)
12830      120 CONTINUE
12840      SOM=SOM/BETA
12850      MATRIX(J,I)=MATRIX(J,I)-SOM*MATRIX(K,I)
12860      130 CONTINUE
12870      140 CONTINUE
12880      C
12890      145 CONTINUE
12900      150 CONTINUE
12910      C
12920      DO 151 I=0,NMEETP-1
12930      DATARE(I)=DATA(I)
12940      151 CONTINUE
12950      C
12960      DO 180 K=0,NPAR-1
12970      SOM=0
12980      DO 160 I=K,NMEETP-1
12990      SOM=SOM+MATRIX(K,I)*DATA(I)/(-DD(K)*MATRIX(K,K))
13000      160 CONTINUE
13010      DO 170 I=K,NMEETP-1
13020      DATA(I)=DATA(I)-SOM*MATRIX(K,I)
13030      170 CONTINUE
13040      180 CONTINUE
13050      C

```

```

13060      UIT(NPAR-1)=DATA(NPAR-1)/DD(NPAR-1)
13070      DO 200 K=1,NPAR-1
13080      INDEX=NPAR-1-K
13090      UIT(INDEX)=DATA(INDEX)/DD(INDEX)
13100      DO 190 J=INDEX+1,NPAR-1
13110      UIT(INDEX)=UIT(INDEX)-MATRIX(J,INDEX)*UIT(J)/DD(INDEX)
13120      190 CONTINUE
13130      200 CONTINUE
13140      C
13150      RES=0
13160      DO 210 I=NPAR,NMEETP-1
13170      RES=RES+DATA(I)**2
13180      210 CONTINUE
13190      C
13200      WRITE(3,/) RES
13210      WRITE(6,/) VIB,NBER
13220      WRITE(6,/) UIT
13230      220 CONTINUE
13240      RETURN
13250      END
13260      C
13270      C
13280      SUBROUTINE SNLJPU(F,I1,I2,E,R3)
13290      C
13300      C For explanation see MINIB2/S/GEBONDENVRIJ/AANPASSINGBX
13310      C
13320      REAL F,E,R3
13330      INTEGER I1,I2,I3
13340      DIMENSION F(0:4001)
13350      C
13360      IF((I2-I1).LE.1) GOTO 30
13370      IF(F(I1).LT.E.AND.F(I2).LT.E) R3=-1
13380      IF(F(I1).GE.E.AND.F(I2).GE.E) R3=-1
13390      IF(R3.LT.0) GOTO 40
13400      C
13410      IF(F(I2).GE.F(I1)) GOTO 20
13420      10 I3=INT((I2+I1)/2)
13430      IF(F(I3).LT.E) I2=I3
13440      IF(F(I3).GT.E) I1=I3
13450      IF((I2-I1).LE.1) GOTO 30
13460      GOTO 10
13470      C
13480      20 I3=INT((I2+I1)/2)
13490      IF(F(I3).LT.E) I1=I3
13500      IF(F(I3).GE.E) I2=I3
13510      IF((I2-I1).LE.1) GOTO 30
13520      GOTO 20
13530      C
13540      30 R3=I1+(F(I1)-E)/(F(I1)-F(I2))
13550      40 CONTINUE
13560      C
13570      RETURN
13580      END

```

```

10000 C MINIB2/S/GEBONDENVRIJ/VIBFIT/TRIPEL
10010 C
10020 C This program is part of a series of programs to simulate
10030 C bound-free rare gas halide emission spectra.
10040 C In this program an experimental emission spectrum from two
10050 C or three bound-free electronic transitions, stored on FILE 2,
10060 C is simulated using calculated emission spectra from
10070 C individual emission spectra (or collections of emission
10080 C spectra from individual vibrational states) stored on
10090 C specified FILES 1, 8 (and 7). Using a least squares method
10100 C vibrational distributions of the upper states are determined,
10110 C and stored on a file MINIB2/S/GEBONDENVRIJ/FITUITVOER (FILE 6).
10120 C The program also creates a previewfile which contains a
10130 C graphical representation of the experimental emission spectrum
10140 C and the simulated spectrum, also divided into contributions
10150 C from separate electronic transitions. It should be noted that
10160 C in the present form, it is assumed that the calculated
10170 C spectra on FILES 1 and 7 correspond to the same upper state,
10180 C this program being written for a simultaneous treatment of
10190 C B-X(1/2) (FILE 1), C-A(3/2) (FILE 8) and B-A(1/2) spectra
10200 C (FILE 7).
10210 C
10220 C *****
10230 C
10240 C DECLARATIONS
10250 C *****
10260 C
10270 FILE 1(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/XEBRBX/5")
10280 FILE 2(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/DATAOUT")
10290 FILE 3(KIND=REMOTE)
10300 FILE 4(KIND=REMOTE)
10310 FILE 5(KIND=PRINTER)
10320 FILE 6(KIND=DISK, TITLE="MINIB2/D/GEBONDENVRIJ/FITUITVOER",
10330 * PROTECTION=SAVE, NEWFILE=TRUE)
10340 C FILE 7(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/XEBRBA/2")
10350 FILE 8(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/XEBCA/5")
10360 BLOCK GLOBALS
10370 $ INCLUDE "PLOTTER/FORTRAN/DECLARATION ON APPL"
10380 END
10390 $ INCLUDE "PLOTTER/FORTRAN/POLYDZ ON APPL"
10400 $ INCLUDE "PLOTTER/FORTRAN/MPOLYD ON APPL"
10410 REAL*4 STEP3, UMINUP, EU, SPEK, STEP2, DATA, STEPF1, LABDAI,
10420 * STEP3C, UMINUC, EUC, SPEKC, RSPKLC, SPEKMC, SPEK2C,
10430 * STEP3B, UMINUB, SPEKB, SPEK2B, HULP1, HULP2, FV, FITF, MAT,
10440 * RSPKLB, RDATLB, SPEKM, DATAM, UIT, RES, SPEKMA, DATAMA,
10450 * CORR, HOR, HOR2, DATAM2, SPEK2, LAB, DATAR, SP, DATAB, DATAC, GEM,
10460 * LMIN2, LMAX2, LMINC, LMAXC
10470 INTEGER*4 LMIN, LMAX, VIB, VIBF, STEP, LMINFI, LMAXFI,
10480 * NFIT, NDATA, I, J, ISPKLB, IDATLB, IKAN, NKAN, SBER, NBER,
10490 * VIBC, VIBFC, ISPKLC, SBERC, NBERC, LMINB, LMAXB
10500 DIMENSION EU(0:179), SPEK(0:90, 0:1019), SPEKM(0:50, 0:1019),
10510 * DATA(0:1019), DATAM2(0:1019), DATAM(0:1019), UIT(0:180),
10520 * HOR(0:1019), SPEKC(0:90, 0:1019), SPEK2C(0:20, 0:1019),
10530 * SPEKB(0:90, 0:1019), SPEK2B(0:20, 0:1019),
10540 * HOR2(0:1019), SPEK2(0:50, 0:1019), EUC(0:179),
10550 * LAB(0:1019), DATAR(0:1019), SP(0:20000), DATAB(0:1019),
10560 * DATAC(0:1019), HULP1(0:1019), HULP2(0:1019), RESIDU(0:1019),
10570 * FV(0:20), FITF(0:20), MAT(0:1, 0:20)

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```

10580 C
10590 C INPUT VARIABLES AND INITIALIZATION
10600 C *****
10610 C
10620 READ(1,/) LMIN,LMAX,STEP3
10630 READ(1,/) VIBF,STEP
10640 READ(1,/) UMINUP
10650 READ(1,/) EU
10660 C
10670 READ(8,/) LMINC,LMAXC,STEP3C
10680 READ(8,/) VIBFC,STEP3C
10690 READ(8,/) UMINUC
10700 READ(8,/) EUC
10710 C
10720 C READ(7,/) LMINB,LMAXB,STEP3B
10730 C READ(7,/) VIBF,STEP
10740 C READ(7,/) UMINUB
10750 C READ(7,/) EU
10760 C
10770 WRITE(3,1) VIBF,STEP
10780 1 FORMAT(' VIBR. NIVEAUS B-X BEREKEND TOT V=',I4,/,
10790 * ' STAPGROOTTE=',I3,/)
10800 C 1 FORMAT(' VIBR. STATES B-X DETERMINED UP TO V=',I4,/,
10810 C * ' INTERVALS IZE=',I3,/)
10820 C
10830 WRITE(3,3) VIBFC,STEP3C
10840 3 FORMAT(' VIBR. NIVEAUS C-A BEREKEND TOT V=',I4,/,
10850 * ' STAPGROOTTE=',I3,/)
10860 C 3 FORMAT(' VIBR. STATES C-A DETERMINED UP TO V=',I4,/,
10870 C * ' INTERVALS IZE=',I3,/)
10880 C
10890 WRITE(3,4)
10900 4 FORMAT(' GEEF VBER EN SBER, RESP. VBERC EN SBERC:')
10910 C 4 FORMAT(' ENTER VBER AND SBER, AND VBERC AND SBERC, RESPECTIVELY:')
10920 2 READ(4,/) VIB, SBER, VIBC, SBERC
10930 C
10940 NBER=INT(VIB/SBER)
10950 NBERC=INT(VIBC/SBERC)
10960 WRITE(6,/) VIB,SBER
10970 WRITE(6,/)VIBC,SBERC
10980 C
10990 DO 40 I=0,VIB-1
11000 DO 30 J=1,34
11010 30 READ(1) (HULP1(30*(J-1)+K),K=0,29)
11020 DO 133 J=0,1019
11030 133 SPEK(I,J)=HULP1(J)
11040 40 CONTINUE
11050 C
11060 DO 140 I=0,VIBC-1
11070 DO 130 J=1,34
11080 130 READ(8) (HULP1(30*(J-1)+K),K=0,29)
11090 DO 132 J=0,1019
11100 132 SPEKC(I,J)=HULP1(J)
11110 140 CONTINUE
11120 C
11130 C DO 240 I=0,VIB-1
11140 C DO 230 J=1,34
11150 C 230 READ(7) (HULP1(30*(J-1)+K),K=0,29)
11160 C DO 232 J=0,1019
11170 C 232 SPEKB(I,J)=HULP1(J)
11180 C 240 CONTINUE
11190 C

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11200      READ(2,/) LMIN2, LMAX2, STEP2
11210      READ(2,/) DATA
11220      NDATA=INT((LMAX2-LMIN2)/STEP2)
11230      C
11240      DO 400 I=1, 5
11250      GEM=GEM+DATA(I)/10.
11260      400 CONTINUE
11270      C
11280      DO 401 I=NDATA-5, NDATA-1
11290      GEM=GEM+DATA(I)/10.
11300      401 CONTINUE
11310      C
11320      DO 402 I=1, NDATA-1
11330      DATA(I)=DATA(I)-GEM
11340      402 CONTINUE
11350      C
11360      CORR=-11.9
11370      LMIN2=LMIN2+CORR
11380      LMAX2=LMAX2+CORR
11390      C
11400      C      NORMALIZATION OF CALCULATED AND EXPERIMENTAL EMISSION SPECTRA
11410      C      *****
11420      C
11430      SPEKMA=0
11440      DO 61 I=0, VIB-1
11450      DO 60 J=0, 1019
11460      IF(SPEK(I, J).GT.SPEKMA) SPEKMA=SPEK(I, J)
11470      60 CONTINUE
11480      61 CONTINUE
11490      C
11500      DO 63 I=0, VIB-1
11510      DO 62 J=0, 1019
11520      SPEK(I, J)=SPEK(I, J)/SPEKMA
11530      62 CONTINUE
11540      63 CONTINUE
11550      C
11560      SPEKMC=0
11570      DO 69 I=0, VIBC-1
11580      DO 68 J=0, 1019
11590      IF(SPEKC(I, J).GT.SPEKMC) SPEKMC=SPEKC(I, J)
11600      68 CONTINUE
11610      69 CONTINUE
11620      C
11630      DO 71 I=0, VIBC-1
11640      DO 70 J=0, 1019
11650      SPEKC(I, J)=SPEKC(I, J)/SPEKMC
11660      70 CONTINUE
11670      71 CONTINUE
11680      C
11690      SPEKMB=0
11700      DO 89 I=0, VIB-1
11710      DO 88 J=0, 1019
11720      IF(SPEKB(I, J).GT.SPEKMB) SPEKMB=SPEKB(I, J)
11730      88 CONTINUE
11740      89 CONTINUE
11750      C
11760      DO 87 I=0, VIB-1
11770      DO 86 J=0, 1019
11780      SPEKB(I, J)=SPEKB(I, J)/SPEKMA
11790      86 CONTINUE
11800      87 CONTINUE
11810      C      WRITE(3,/) SPEKMA, SPEKMC, SPEKMB

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11820 C
11830 DATAMA=0
11840 DO 64 J=0,1019
11850 IF(DATA(J).GT.DATAMA) DATAMA=DATA(J)
11860 64 CONTINUE
11870 C
11880 DO 65 J=0,1019
11890 DATA(J)=DATA(J)/DATAMA*10000
11900 65 CONTINUE
11910 66 CONTINUE
11920 C
11930 C DETERMINATION OF WAVELENGTH INTERVAL AND STEPSIZE FOR LEAST
11940 C SQUARES FIT
11950 C *****
11960 C
11970 LMINFI=LMIN
11980 LMAXFI=LMAXC
11990 IF(LMIN2.GT.LMINFI) LMINFI=LMIN2
12000 IF(LMAX2.LT.LMAXFI) LMAXFI=LMAX2
12010 C
12020 STEPFI=STEP3
12030 IF(STEP3C.GT.STEPFI) STEPFI=STEP3C
12040 IF(STEP2.GT.STEPFI) STEPFI=STEP2
12050 NFIT=INT((LMAXFI-LMINFI)/STEPFI)
12060 C
12070 C CREATION OF FIT-FUNCTIONS FOR LEAST SQUARES FIT
12080 C *****
12090 C
12100 C a) Joining of SBER/SBERC emission spectra of individual
12110 C vibrational states into a single fit-function.
12120 C
12130 IF(SBER.EQ.1) GOTO 17
12140 DO 17 I=0,1019
12150 DO 15 J=0,NBER-1
12160 SPEK(J,I)=SPEK(SBER*J,I)
12170 DO 16 K=1,SBER-1
12180 SPEK(J,I)=SPEK(J,I)+SPEK(SBER*J+K,I)
12190 16 CONTINUE
12200 SPEK(J,I)=SPEK(J,I)/SBER
12210 15 CONTINUE
12220 17 CONTINUE
12230 C
12240 IF(SBERC.EQ.1) GOTO 77
12250 DO 77 I=0,1019
12260 DO 75 J=0,NBERC-1
12270 SPEKC(J,I)=SPEKC(SBERC*J,I)
12280 DO 76 K=1,SBERC-1
12290 SPEKC(J,I)=SPEKC(J,I)+SPEKC(SBERC*J+K,I)
12300 76 CONTINUE
12310 SPEKC(J,I)=SPEKC(J,I)/SBERC
12320 75 CONTINUE
12330 77 CONTINUE
12340 C
12350 IF(SBER.EQ.1) GOTO 97
12360 DO 97 I=0,1019
12370 DO 95 J=0,NBER-1
12380 SPEKB(J,I)=SPEKB(SBER*J,I)
12390 DO 96 K=1,SBER-1
12400 SPEKB(J,I)=SPEKB(J,I)+SPEKB(SBER*J+K,I)
12410 96 CONTINUE
12420 SPEKB(J,I)=SPEKB(J,I)/SBER
12430 95 CONTINUE

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12440 97 CONTINUE
12450 C
12460 C b) The introduction of a spectral resolution into the fit-
12470 C functions
12480 C
12490 NKAN=3
12500 DO 35 IKAN=-NKAN,NKAN
12510 C
12520 DO 34 J=0,NBER-1
12530 DO 33 I=0,1019
12540 IF(I+IKAN.GE.0.AND.I+IKAN.LE.1019) GOTO 41
12550 SPEK2(J,I)=SPEK2(J,I)+SPEK(J,I)
12560 GOTO 32
12570 41 CONTINUE
12580 SPEK2(J,I)=SPEK2(J,I)+SPEK(J,I+IKAN)
12590 32 CONTINUE
12600 33 CONTINUE
12610 34 CONTINUE
12620 C
12630 DO 345 J=0,NBERC-1
12640 DO 344 I=0,1019
12650 IF(I+IKAN.GE.0.AND.I+IKAN.LE.1019) GOTO 342
12660 SPEK2C(J,I)=SPEK2C(J,I)+SPEKC(J,I)
12670 GOTO 343
12680 342 CONTINUE
12690 SPEK2C(J,I)=SPEK2C(J,I)+SPEKC(J,I+IKAN)
12700 343 CONTINUE
12710 344 CONTINUE
12720 345 CONTINUE
12730 C
12740 DO 434 J=0,NBER-1
12750 DO 433 I=0,1019
12760 IF(I+IKAN.GE.0.AND.I+IKAN.LE.1019) GOTO 441
12770 SPEK2B(J,I)=SPEK2B(J,I)+SPEKB(J,I)
12780 GOTO 432
12790 441 CONTINUE
12800 SPEK2B(J,I)=SPEK2B(J,I)+SPEKB(J,I+IKAN)
12810 432 CONTINUE
12820 433 CONTINUE
12830 434 CONTINUE
12840 C
12850 35 CONTINUE
12860 C
12870 C CONVERSION OF CALCULATED AND EXPERIMENTAL EMISSION SPECTRA
12880 C TO SPECTRA MATCHING THE REQUIRED WAVELENGTH INTERVAL AND
12890 C HAVING THE CORRECT STEPSIZE
12900 C *****
12910 C
12920 DO 20 I=0,NFIT
12930 LABDAI=LMINFI+I*STEPFI
12940 C
12950 IF(LABDAI.GT.LMAX) GOTO 11
12960 RSPKLB=((LABDAI-LMIN)/STEP3)
12970 ISPKLB=INT(RSPKLB)
12980 DO 10 J=0,NBER-1
12990 SPEKM(J,I)=(RSPKLB-ISPKLB)*SPEK2(J,ISPKLB)+
13000 * (1+ISPKLB-RSPKLB)*SPEK2(J,ISPKLB+1)
13010 10 CONTINUE
13020 11 CONTINUE
13030 C
13040 IF(LABDAI.LT.LMINC) GOTO 12
13050 RSPKLC=((LABDAI-LMINC)/STEP3C)

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13060      ISPKLC=INT(RSPKLC)
13070      DO 13 J=0, NBERC-1
13080      SPEKM(J+NBER, I)=(RSPKLC-ISPKLC)*SPEK2C(J, ISPKLC)+
13090      * (1+ISPKLC-RSPKLC)*SPEK2C(J, ISPKLC+1)
13100      13 CONTINUE
13110      12 CONTINUE
13120      C
13130      SPEKM(NBER+NBERC, I)=1
13140      C
13150      C IF(LABDAI.LT.LMINB) GOTO 14
13160      C RSPKLB=((LABDAI-LMINB)/STEP3B)
13170      C ISPKLB=INT(RSPKLB)
13180      C DO 18 J=0, NBER-1
13190      C SPEKM(J, I)=SPEKM(J, I)+(RSPKLB-ISPKLB)*SPEK2B(J, ISPKLB)+
13200      C * (1+ISPKLB-RSPKLB)*SPEK2B(J, ISPKLB+1)
13210      C 18 CONTINUE
13220      C 14 CONTINUE
13230      C
13240      RDATLB=((LABDAI-LMIN2)/STEP2)
13250      IDATLB=INT(RDATLB)
13260      IF(I.LE.0) GOTO 20
13270      DATAM(I)=(RDATLB-IDATLB)*DATA(IDATLB)+
13280      * (1+IDATLB-RDATLB)*DATA(IDATLB+1)
13290      20 CONTINUE
13300      C
13310      C LEAST SQUARES FIT OF THE EXPERIMENTAL SPECTRUM
13320      C *****
13330      C
13340      DO 38 J=0, NFIT
13350      DO 36 I=0, NBER+NBERC-1
13360      SPEK2(I, J)=SPEKM(I, J)
13370      36 CONTINUE
13380      DATAR(J)=DATAM(J)
13390      38 CONTINUE
13400      CALL FIT(NFIT+1, NBER+NBERC, DATAR, SPEK2, UIT, RES)
13410      C
13420      C Subroutine FIT determines a least squares fit of a function
13430      C DATA by a number of fit-functions in stored in a matrix MATRIX.
13440      C An explanation of the heading of FIT is included in the source
13450      C text of FIT.
13460      C
13470      C GRAPHICAL REPRESENTATION OF THE EXPERIMENTAL AND SIMULATED
13480      C EMISSION SPECTRA
13490      C *****
13500      C
13510      DO 26 J=0, 1019
13520      HOR(J)=LMIN2+STEP2*J
13530      26 CONTINUE
13540      C
13550      DO 28 J=0, NFIT-1
13560      DATAB(J)=0
13570      DATAC(J)=0
13580      DATAM2(J)=0
13590      C
13600      DO 27 I=0, NBER-1
13610      C IF(UIT(I).LT.0) GOTO 27
13620      DATAB(J)=DATAB(J)+UIT(I)*SPEKM(I, J)
13630      27 CONTINUE
13640      C
13650      DO 39 I=NBER, NBER+NBERC-1
13660      C IF(UIT(I).LT.0) GOTO 39
13670      DATAC(J)=DATAC(J)+UIT(I)*SPEKM(I, J)

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13680      39 CONTINUE
13690      C
13700          HOR2(J)=LMINFI+J*STEPFI
13710          DATAB(J)=DATAB(J)+UIT(NBER+NBERC)
13720          DATAM2(J)=DATAB(J)+DATAC(J)
13730          DATAC(J)=DATAC(J)+UIT(NBER+NBERC)
13740          RESIDU(J)=DATAM(J)-DATAM2(J)+11000
13750      C
13760      28 CONTINUE
13770      C      GOTO 29
13780          CALL POLYDZ(90,0,0,25,20,1,NFIT,HOR2,DATAM,10,LMIN,LMAXC,
13790      *      12,0,12000,.FALSE.,.FALSE.)
13800          CALL POLYDZ(90,0,0,25,20,1,NFIT,HOR2,DATAM2,10,LMIN,LMAXC,
13810      *      12,0,12000,.FALSE.,.FALSE.)
13820          CALL POLYDZ(90,0,0,25,20,1,NFIT,HOR2,DATAB,10,LMIN,LMAXC,
13830      *      12,0,12000,.FALSE.,.FALSE.)
13840          CALL POLYDZ(90,0,0,25,20,1,NFIT,HOR2,DATAAC,10,LMIN,LMAXC,
13850      *      12,0,12000,.FALSE.,.FALSE.)
13860          CALL POLYDZ(90,0,0,25,20,1,NFIT,HOR2,RESIDU,10,LMIN,LMAXC,
13870      *      12,0,12000,.FALSE.,.FALSE.)
13880      C
13890      C      DETERMINATION OF THE SURPRISAL PARAMETERS, IF THE VIBRATIONAL
13900      C      DISTRIBUTIONS DETERMINED ARE SUPPOSED TO BE LINEAR SURPRISAL
13910      C      DISTRIBUTIONS
13920      C      *****
13930      C
13940      C      Note: this calculation can only be successful if all UIT(I)
13950      C      are > 0.
13960      C
13970          EBIND=52.7
13980          EMAX=8065*8.315-349.83*EBIND
13990      C
14000          DO 410 I=0,NBER-1
14010          DO 411 J=0,SBER-1
14020          FV(I)=FV(I)+(EU(I*SBER+J)-UMINUP)/(EMAX-UMINUP)/SBER
14030      411 CONTINUE
14040      C
14050          IF(FV(I).GE.1) GOTO 410
14060          FITF(I)=ALOG(ABS(UIT(I)))-1.5*ALOG(1-FV(I))
14070          SPEK2(0,I)=FV(I)
14080          SPEK2(1,I)=1.
14090          NMEET=I+1
14100      410 CONTINUE
14110      C
14120          CALL FIT(NMEET,2,FITF,SPEK2,UIT,RES)
14130          WRITE(3,/) UIT(0),UIT(1)
14140      C
14150          DO 412 I=0,NBERC-1
14160          DO 413 J=0,SBERC-1
14170          FV(I)=FV(I)+(EUC(I*SBERC+J)-UMINUC)/(EMAX-UMINUC)/SBERC
14180      413 CONTINUE
14190      C
14200          IF(FV(I).GE.1) GOTO 412
14210          FITF(I)=ALOG(ABS(UIT(I+NBER)))-1.5*ALOG(1-FV(I))
14220          SPEK2(0,I)=FV(I)
14230          SPEK2(1,I)=1.
14240          NMEET=I+1
14250      412 CONTINUE
14260      C
14270          CALL FIT(NMEET,2,FITF,SPEK2,UIT,RES)
14280          WRITE(3,/) UIT(0),UIT(1)
14290      C

```

```

14300      29  CONTINUE
14310      C
14320          CLOSE(6,DISP=CRUNCH)
14330          END
14340      C
14350          SUBROUTINE FIT(NMEETP,NPAR,DATA,MATRIX,UIT,RES)
14360      C
14370      C      In this subroutine a function, which is known in NMEETP
14380      C      points and stored in array DATA, is least squares fitted
14390      C      to a set of NPAR fit-functions, stored in a matrix MATRIX.
14400      C      The resultant contributions of all individual fit-functions
14410      C      are stored in an array UIT. After the fit the variable RES
14420      C      contains the normalized residu.
14430      C
14440          REAL*4 BETA,RES,DD,DATA,UIT,MATRIX,SOM,DATARE,A
14450          INTEGER NMEETP,NPAR,INDEX,I,J,K,M
14460          DIMENSION DATA(0:1019),DD(0:180),UIT(0:180),
14470          *   MATRIX(0:50,0:1019),DATARE(0:1019)
14480      C
14490          DO 150 K=0,NPAR-1
14500              SOM=0
14510      C
14520              DO 110 I=K,NMEETP-1
14530                  SOM=SOM+MATRIX(K,I)**2
14540          110  CONTINUE
14550      C
14560              IF(MATRIX(K,K).GT.0) DD(K)=-SQRT(SOM)
14570              IF(MATRIX(K,K).LE.0) DD(K)=SQRT(SOM)
14580              MATRIX(K,K)=MATRIX(K,K)-DD(K)
14590              BETA=-DD(K)*MATRIX(K,K)
14600              IF(K.EQ.NPAR-1) GOTO 145
14610      C
14620              DO 140 J=K+1,NPAR-1
14630                  SOM=0
14640                  DO 120 I=K,NMEETP-1
14650                      SOM=SOM+MATRIX(K,I)*MATRIX(J,I)
14660          120  CONTINUE
14670                  SOM=SOM/BETA
14680                  DO 130 I=K,NMEETP-1
14690                      MATRIX(J,I)=MATRIX(J,I)-SOM*MATRIX(K,I)
14700          130  CONTINUE
14710          140  CONTINUE
14720      C
14730          145  CONTINUE
14740          150  CONTINUE
14750      C
14760              DO 151 I=0,NMEETP-1
14770                  DATARE(I)=DATA(I)
14780          151  CONTINUE
14790      C
14800              DO 180 K=0,NPAR-1
14810                  SOM=0
14820                  DO 160 I=K,NMEETP-1
14830                      SOM=SOM+MATRIX(K,I)*DATA(I)/(-DD(K)*MATRIX(K,K))
14840          160  CONTINUE
14850                  DO 170 I=K,NMEETP-1
14860                      DATA(I)=DATA(I)-SOM*MATRIX(K,I)
14870          170  CONTINUE
14880          180  CONTINUE
14890      C
14900              UIT(NPAR-1)=DATA(NPAR-1)/DD(NPAR-1)
14910              DO 200 K=1,NPAR-1

```

```

14920      INDEX=NPARG-1-K
14930      UIT(INDEX)=DATA(INDEX)/DD(INDEX)
14940      DO 190 J=INDEX+1, NPAR-1
14950      UIT(INDEX)=UIT(INDEX)-MATRIX(J, INDEX)*UIT(J)/DD(INDEX)
14960      190 CONTINUE
14970      200 CONTINUE
14980      C
14990      RES=0
15000      DO 210 I=NPARG, NMEETP-1
15010      RES=RES+DATA(I)**2
15020      210 CONTINUE
15030      C
15040      WRITE(3,/) RES
15050      C WRITE(3,/) UIT
15060      WRITE(6,/) UIT
15070      220 CONTINUE
15080      RETURN
15090      END
15100      C
15110      C
15120      SUBROUTINE SNLJPU(F, I1, I2, E, R3)
15130      C
15140      C For an explanation see MINIB2/S/GEBONDENVRIJ/AANPASSINGBX
15150      C
15160      REAL F, E, R3
15170      INTEGER I1, I2, I3
15180      DIMENSION F(0:4001)
15190      C
15200      IF((I2-I1).LE.1) GOTO 30
15210      IF(F(I1).LT.E.AND.F(I2).LT.E) R3=-1
15220      IF(F(I1).GE.E.AND.F(I2).GE.E) R3=-1
15230      IF(R3.LT.0) GOTO 40
15240      C
15250      IF(F(I2).GE.F(I1)) GOTO 20
15260      10 I3=INT((I2+I1)/2)
15270      IF(F(I3).LT.E) I2=I3
15280      IF(F(I3).GT.E) I1=I3
15290      IF((I2-I1).LE.1) GOTO 30
15300      GOTO 10
15310      C
15320      20 I3=INT((I2+I1)/2)
15330      IF(F(I3).LT.E) I1=I3
15340      IF(F(I3).GE.E) I2=I3
15350      IF((I2-I1).LE.1) GOTO 30
15360      GOTO 20
15370      C
15380      30 R3=I1+(F(I1)-E)/(F(I1)-F(I2))
15390      40 CONTINUE
15400
15410      RETURN
15420      END

```

```

10000 C MINIB2/S/GEBONDENVRIJ/VIBPLOTTER
10010 C
10020 C This program is part of a series of programs to simulate
10030 C bound-free rare gas halide emission spectra.
10040 C With this program a graphical representation can be given of
10050 C a vibrational distribution determined in MINIB2/S/GEBONDENVRIJ/
10060 C VIBFIT.
10070 C
10080 C*****
10090 C
10100 FILE 1(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/FITUITVOER")
10110 BLOCK GLOBALS
10120 $ INCLUDE "PLOTTER/FORTRAN/DECLARATION ON APPL"
10130 END
10140 $ INCLUDE "PLOTTER/FORTRAN/POLYDZ ON APPL"
10150 REAL UIT,UIT2,UITMAX,HOR
10160 INTEGER M, INC, VIB, N
10170 DIMENSION UIT(0:180),HOR(0:180),UIT2(0:180)
10180 C
10190 READ(1,/) VIB, INC
10200 N=VIB/INC-1
10210 C
10220 UITMAX=0
10230 READ(1,/) UIT
10240 DO 10 I=0, N
10250 IF(UIT(I).GT.UITMAX) UITMAX=UIT(I)
10260 10 CONTINUE
10270 C
10280 DO 30 I=0, N
10290 HOR(2*I)=I*INC
10300 HOR(2*I+1)=(I+1)*INC-.01
10310 UIT2(2*I)=UIT(I)/UITMAX
10320 UIT2(2*I+1)=UIT(I)/UITMAX
10330 30 CONTINUE
10340 HOR(2*N+2)=(N+1)*INC
10350 UIT2(2*N+2)=0
10360 C
10370 CALL POLYDZ(90, 0, 0, 25, 20, 1, 2*N+3, HOR, UIT2, 10, 0, VIB, 7, -.2, 1.2,
10380 * .FALSE., .FALSE.)
10390 STOP
10400 END

```

```

10000 C MINIB2/S/GEBONDENVRIJ/VIBPLOTTER/DUBBEL
10010 C
10020 C This program is part of a series of programs to simulate
10030 C bound-free rare gas halide emission spectra.
10040 C With this program a graphical representation can be given of
10050 C the vibrational distributions determined in MINIB2/S/
10060 C GEBONDENVRIJ/VIBFIT/TRIPEL.
10070 C
10080 C*****
10090 C
10100 FILE 1(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/FITUITVOER")
10110 BLOCK GLOBALS
10120 $ INCLUDE "PLOTTER/FORTRAN/DECLARATION ON APPL"
10130 END
10140 $ INCLUDE "PLOTTER/FORTRAN/POLYDZ ON APPL"
10150 REAL UIT,UIT2,UIT3,UITMA2,UITMAX,HOR,HOR2
10160 INTEGER M,INC,INC2,VIB,VIB2,N,N2
10170 DIMENSION UIT(0:180),HOR(0:180),UIT2(0:180),UIT3(0:180),
10180 * HOR2(0:180)
10190 C
10200 READ(1,/) VIB,INC
10210 READ(1,/) VIB2,INC2
10220 VIB=10*VIB
10230 INC=10*INC
10240 VIB2=15*VIB2
10250 INC2=15*INC2
10260 N=VIB/INC-1
10270 N2=VIB2/INC2-1
10280
10290 UITMAX=0
10300 UITMA2=0
10310 READ(1,/) UIT
10320 DO 10 I=0,N
10330 IF(UIT(I).GT.UITMAX) UITMAX=UIT(I)
10340 10 CONTINUE
10350 DO 11 I=0,N2
10360 IF(UIT(I+N+1).GT.UITMA2) UITMA2=UIT(I+N+1)
10370 11 CONTINUE
10380 C
10390 DO 30 I=0,N
10400 HOR(2*I)=I*INC
10410 HOR(2*I+1)=(I+1)*INC-.01
10420 UIT2(2*I)=UIT(I)/UITMAX
10430 UIT2(2*I+1)=UIT(I)/UITMAX
10440 30 CONTINUE
10450 C
10460 DO 31 I=0,N2
10470 HOR2(2*I)=I*INC2
10480 HOR2(2*I+1)=(I+1)*INC2-.01
10490 UIT3(2*I)=UIT(I+N+1)/UITMA2+1.5
10500 UIT3(2*I+1)=UIT(I+N+1)/UITMA2+1.5
10510 31 CONTINUE
10520 C
10530 HOR(2*N+2)=(N+1)*INC
10540 UIT2(2*N+2)=0
10550 HOR2(2*N2+2)=(N2+1)*INC2
10560 UIT3(2*N2+2)=1.5
10570 C

```



```
10575      NVIB=VIB
10576      IF(VIB2.GE.NVIB) NVIB=VIB2
10580      CALL POLYDZ(90,0,0,25,20,1,2*N+3,HOR,UIT2,10,0,NVIB,7,-.5,3.0,
10590      *   .FALSE.,.FALSE.)
10600      CALL POLYDZ(90,0,0,25,20,1,2*N2+3,HOR2,UIT3,10,0,NVIB,7,-.5,
10610      *   3.0,.FALSE.,.FALSE.)
10620
10630      STOP
10640      END
```

```

10000 C MINIB2/S/GEBONDENVRIJ/VIBCALC
10010 C
10020 C This program is part of a series of programs to simulate
10030 C bound-free rare gas halide emission spectra.
10040 C In this program a bound-free emission spectrum is calculated,
10050 C assuming a vibrational distribution specified either on a FILE 3
10060 C or on the terminal, and using calculated emission spectra of
10070 C individual vibrational states stored on a specified FILE 4.
10080 C
10090 C*****
10100 C
10110 C DECLARATIONS
10120 C *****
10130 C
10140 FILE 1(KIND=REMOTE) % WRITE TO TERMINAL
10150 FILE 2(KIND=REMOTE) % READ FROM TERMINAL
10160 FILE 3(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/VIB INVOER")
10170 FILE 4(KIND=DISK, TITLE="MINIB2/D/GEBONDENVRIJ/XEBRBX/5")
10180 FILE 5(KIND=DISK, TITLE="MINIB2/D/GEBONDENVRIJ/VIBUITVOER",
10190 * PROTECTION=SAVE, NEWFILE=TRUE)
10200 FILE 6(KIND=PRINTER)
10210 REAL*4 STEP3, UMINUP, EU, SPEK, LV, DUMMY, C1, TBOLTZ, EBIND,
10220 * EMETA, KBOLTZ, SPUIT
10230 INTEGER*4 SQUEST, INTACT, LMIN, LMAX, VIB, STEP, KEUS, I, J, KMAX
10240 DIMENSION SPEK(1:180, 0:1019), EU(180), P(180), SPUIT(0:1019)
10250 C
10260 C INPUT VARIABLES
10270 C *****
10280 C
10290 SQUEST=0
10300 INTACT=3
10310 WRITE(1,1)
10320 READ(2,/) SQUEST
10330 1 FORMAT(' INVOER INTERACTIEF VANAF TERMINAL (JA=1)?' )
10340 C 1 FORMAT(' INPUT FROM TERMINAL (YES=1)?' )
10350 IF(SQUEST.EQ.1) INTACT=2
10360 C
10370 SQUEST=0
10380 TERM=0
10390 IF(INTACT.EQ.2) WRITE(1,2)
10400 READ(INTACT,/) SQUEST
10410 2 FORMAT(' AANMAAK PRINTERFILE MET PROGRAMMAGEGEVENS (JA=1)?' ,/)
10420 C 2 FORMAT(' CREATE A PRINTERFILE WITH PROGRAM-INFO (YES=1)?' ,/)
10430 IF(SQUEST.EQ.1) TERM=1
10440 C
10450 READ(4,/) LMIN, LMAX, STEP3
10460 READ(4,/) VIB, STEP
10470 READ(4,/) UMINUP
10480 READ(4,/) EU
10490 C
10500 DO 161 I=1, VIB
10510 DO 151 J=1, 34
10520 READ(4) (SPEK(I, 30*(J-1)+K), K=0, 29)
10530 151 CONTINUE
10540 161 CONTINUE
10550 C
10560 C SELECTION OF VIBRATIONAL DISTRIBUTION
10570 C *****

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```

10580 C
10590 IF(INTACT.EQ.2) WRITE(1,3) LMIN,LMAX,STEP3,VIB,STEP
10600 IF(TERM.EQ.1) WRITE(6,3) LMIN,LMAX,STEP3,VIB,STEP
10610 3 FORMAT(' OP DE UITVOERFILE VAN PROGRAMMA MINIB2/S/GEBONDENVRIJ',
10620 * /,' POTCALC STAAN BEREKENDE EMISSIE-SPEKTRA IN EEN INTERVAL',
10630 * /,' VAN ',I3,' TOT ',I3,' NM (STAPGROOTTE ',F6.2,' NM), VOOR',
10640 * /,' I4,' VIBRATIONELE NIVEAUS (STAPGROOTTE VIBRATIONEEL',
10650 * /,' QUANTUMGETAL= ',I2,').',/)
10660 C 3 FORMAT(' ON THE OUTPUTFILE OF PROGRAM MINIB2/S/GEBONDENVRIJ',
10670 C * /,' POTCALC CALCULATED EMISSION SPECTRA ARE STORED IN A',
10680 C * /,' WAVELENGTHINTERVAL BETWEEN ',I3,' AND ',I3,' NM ',
10690 C * /,' (STEPSIZE ',F6.2,' NM), FOR ',I4,' VIBRATIONAL STATES ',
10700 C * /,' (STEPSIZE VIBRATIONAL QUANTUMNUMBER= ',I2,').',/)
10710 C
10720 IF(INTACT.EQ.2) WRITE(1,4)
10730 4 FORMAT(' KIES EEN VIBRATIONELE VERDELING (1-4):',/,
10740 * '(NB. FV=EVIB/EVIBMX)',/)
10750 C 4 FORMAT(' CHOOSE A VIBRATIONAL DISTRIBUTION (1-4):',/,
10760 C * '(NOTE. FV=EVIB/EVIBMX)',/)
10770 C
10780 IF(INTACT.EQ.2) WRITE(1,5)
10790 IF(TERM.EQ.1) WRITE(6,5)
10800 5 FORMAT(' 1) P(FV)=((1-FV)**3/2)*EXP(-LV*FV)',/,
10810 * ' 2) P(FV)=C',/,
10820 * ' 3) P(FV)=(1+C1*FV)',/,
10830 * ' 4) P(FV)=EXP(-EVIB/EBOLTZ)',/)
10840 READ(INTACT,/) KEUS
10850 IF(TERM.EQ.1) WRITE(6,6) KEUS
10860 6 FORMAT(' GEMAAKTE KEUS= ',I2)
10870 C 6 FORMAT(' YOUR CHOICE= ',I2)
10880 C
10890 IF(INTACT.EQ.2.AND.KEUS.EQ.1) WRITE(1,7)
10900 7 FORMAT(' INVOER SURPRISAL PARAMETER LV= ',/)
10910 C 7 FORMAT(' INPUT SURPRISAL PARAMETER LV= ',/)
10920 IF(KEUS.EQ.1) READ(INTACT,/) LV
10930 C
10940 IF(INTACT.EQ.3.AND.KEUS.EQ.2) READ(INTACT,/) DUMMY
10950 C
10960 IF(INTACT.EQ.2.AND.KEUS.EQ.3) WRITE(1,8)
10970 8 FORMAT(' INVOER CONSTANTE C1= ')
10980 C 8 FORMAT(' INPUT CONSTANT C1= ')
10990 IF(KEUS.EQ.3) READ(INTACT,/) C1
11000 C
11010 IF(INTACT.EQ.2.AND.KEUS.EQ.4) WRITE(1,9)
11020 9 FORMAT(' INVOER BOLTZMANNTEMPERATUUR= ')
11030 C 9 FORMAT(' INPUT BOLTZMANNTEMPERATURE= ')
11040 IF(KEUS.EQ.4) READ(INTACT,/) TBOLTZ
11050 C
11060 IF(TERM.EQ.1.AND.KEUS.EQ.1) WRITE(6,10) LV
11070 IF(TERM.EQ.1.AND.KEUS.EQ.3) WRITE(6,11) C1
11080 IF(TERM.EQ.1.AND.KEUS.EQ.4) WRITE(6,12) TBOLTZ
11090 10 FORMAT(' SURPRISAL PARAMETER LV= ',F6.2,/)
11100 11 FORMAT(' CONSTANTE C1= ',F6.2,/)
11110 12 FORMAT(' BOLTZMANNTEMPERATUUR= ',F7.1,' KELVIN',/)
11120 C
11130 IF(INTACT.EQ.2) WRITE(1,13)
11140 READ(INTACT,/) EBIND
11150 IF(INTACT.EQ.2) WRITE(1,14)
11160 READ(INTACT,/) EMETA
11170 EBIND=EBIND*349.83 % CONVERSION TO,CM-1
11180 EMETA=EMETA*349.83*23.06 % CONVERSION TO CM-1
11190 13 FORMAT(' INVOER BINDINGSENERGIE (KCAL/MOL)',/)

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```

11200 C 13 FORMAT(' INPUT BONDING ENERGY (KCAL/MOL)',/)
11210 14 FORMAT(' INVOER METASTABIELENERGIE (EV)',/)
11220 C 14 FORMAT(' INPUT METASTABLES ENERGY (EV)',/)
11230 KBOLTZ=1.38E-23
11240 C
11250 C CALCULATION OF THE VIBRATIONAL DISTRIBUTION
11260 C *****
11270 C
11280 DO 100 I=1,VIB
11290 FV=(EU(I)-UMINUP)/(EMETA-EBIND-UMINUP)
11300 IF(FV.GE.1.AND.KEUS.EQ.1) GOTO 100
11310 IF(FV.GE.1.AND.KEUS.EQ.3) GOTO 100
11320 IF(KEUS.EQ.1) P(I)=(SQRT((1-FV)**3))*EXP(-LV*FV)
11330 IF(KEUS.EQ.2) P(I)=1.
11340 IF(KEUS.EQ.3) P(I)=1+C1*FV
11350 IF(KEUS.EQ.4) P(I)=EXP(-(EU(I)-UMINUP)/(KBOLTZ*TBOLTZ))
11360 C WRITE(1,/) I,FV,P(I)
11370 100 CONTINUE
11380 C
11390 C CALCULATION OF THE TOTAL EMISSION SPECTRUM
11400 C *****
11410 C
11420 KMAX=INT((LMAX-LMIN)/STEP3)
11430 DO 120 K=0,KMAX,1
11440 DO 110 I=1,VIB,1
11450 SPUIT(K)=SPUIT(K)+P(I)*SPEK(I,K)
11460 110 CONTINUE
11470 120 CONTINUE
11480 C
11490 WRITE(5,/) LMIN,LMAX,STEP3
11500 WRITE(5,/) SPUIT
11510 C
11520 CLOSE(5,DISP=CRUNCH)
11530 END

```

```

10000 C MINIB2/S/GEBONDENVRIJ/PLOTTER
10010 C
10020 C This program is part of a series of programs to simulate
10030 C bound-free rare gas halide emission spectra.
10040 C With this program a previewfile is created which gives a
10050 C graphical representation of an emission spectrum stored
10060 C on a specified FILE 1.
10070 C
10080 C*****
10090 C
10100 FILE 1(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/POTUITVOER")
10110 BLOCK GLOBALS
10120 $ INCLUDE "PLOTTER/FORTRAN/DECLARATION ON APPL"
10130 END
10140 $ INCLUDE "PLOTTER/FORTRAN/POLYD ON APPL"
10150 REAL SPUIT, HOR, STEP3
10160 INTEGER LMIN, LMAX, I
10170 DIMENSION HOR(0:1019), SPUIT(0:1019)
10180 C
10190 READ(1,/) LMIN, LMAX, STEP3
10200 READ(1,/) SPUIT
10210 C
10220 KMAX=INT((LMAX-LMIN)/STEP3)
10230 DO 10 I=0, KMAX
10240 HOR(I)=LMIN+STEP3*I
10250 10 CONTINUE
10260 C
10270 CALL POLYD(90, 0, 0, 25, 15, 1, KMAX+1, HOR, SPUIT, .FALSE., .FALSE.)
10280
10290 STOP
10300 END

```

MINIB2/S/GEBONDENVRIJ/CONVERTER

DATE & TIME PRINTED: MONDAY, JULY 20, 1987 @ 10:50:29.

```

10000 %      MINIB2/S/GEBONDENVRIJ/CONVERTER
10010 %
10020 %      This program is part of a series of programs to simulate
10030 %      bound-free rare gas halide emission spectra.
10040 %      With this program a data-file which has been transported
10050 %      to the Burroughs 7900 system, can be converted to a file
10060 %      D/DATAOUT, which is suitable for use in Fortran-programs.
10070 %
10080 %*****
10090 %
10100 BEGIN
10110 %
10120 $INCLUDE "(TNNDAW20)LIBRARY/TOF/PREFIX ON USER4."
10130 $INCLUDE "(TNNDAW20)MINIB2/S/EDGAR/ROTATIE/PROCS ON USER4."
10140 INTEGER IDNR, IEERST, ILAATST, LMIN, LMAX;
10150 REAL METING, STEP2;
10160 ARRAY DATA[0:1019];
10170 %
10180 FILE LINEOUT(KIND=DISK, UNITS=CHARACTERS, MAXRECSIZE=132, PROTECTION=SAVE,
10190      NEWFILE=TRUE, TITLE="MINIB2/D/GEBONDENVRIJ/OUT ON POOL."),
10200 OUT(KIND=DISK, UNITS=CHARACTERS, MAXRECSIZE=132, PROTECTION=SAVE,
10210      NEWFILE=TRUE, TITLE="MINIB2/D/GEBONDENVRIJ/DATAOUT ON USER4."),
10220 DUMP(KIND=DISK, PACKNAME="POOL.", NEWFILE=TRUE, PROTECTION=SAVE,
10230      TITLE="DUMP.");
10240 %
10250 IDNR:=86721141;
10260 METINGOPHALEN(IDNR, IEERST, ILAATST, DATA, LMIN, STEP2, DUMP);
10270 LMAX:=(LMIN+(ILAATST-IEERST)*STEP2+.01);
10280 WRITE(OUT, /, LMIN, LMAX, STEP2);
10290 WRITE(OUT, /, DATA);
10300 %
10310 CLOSE(OUT, CRUNCH);
10320 END.

```

```

10000 %      MINIB2/S/GEBONDENVRIJ/CONVERTER/MAT
10010 %
10020 %      This program is part of a series of programs to simulate
10030 %      bound-free rare gas halide emission spectra.
10040 %      With this program a number of data-files which have been
10050 %      transported to the Burroughs 7900 system, can be converted
10060 %      into one file D/DATAOUT, which is suitable for use in Fortran
10070 %      programs. The structure of the program is such that all the
10080 %      the measurements at one wavelength are stored together.
10090 %      This program should be used together with the programs
10100 %      MINIB2/S/GEBONDENVRIJ/VOLGORDE and MINIB2/S/GEBONDENVRIJ/
10110 %      OPTELLEN
10120 %
10130 BEGIN
10140 %
10150 $INCLUDE "(TNNDAW20)LIBRARY/TOF/PREFIX ON USER4."
10160 $INCLUDE "(TNNDAW20)MINIB2/S/EDGAR/ROTATIE/PROCS ON USER4."
10170 INTEGER I, J, K, IDNR, IEERST, ILAATST, LMIN, LMAX;
10180 REAL METING, STEP2;
10190 ARRAY DATA[0:450], IDN[1:50], MATRIX[1:50, 0:450], DATA2[1:50];
10200 %
10210 FILE LINEOUT(KIND=DISK, UNITS=CHARACTERS, MAXRECSIZE=132, PROTECTION=SAVE,
10220     NEWFILE=TRUE, TITLE="MINIB2/D/GEBONDENVRIJ/OUT ON POOL."),
10230     OUT(KIND=DISK, UNITS=CHARACTERS, MAXRECSIZE=132, PROTECTION=SAVE,
10240     NEWFILE=TRUE, TITLE="MINIB2/D/GEBONDENVRIJ/DATAOUT ON USER4."),
10250     DUMP(KIND=DISK, PACKNAME="POOL.", NEWFILE=TRUE, PROTECTION=SAVE,
10260     TITLE="DUMP.");
10270 FOR I:=1 STEP 1 UNTIL 25 DO IDN[I]:=87651509+I;
10280 %
10290 FOR I:=1 STEP 1 UNTIL 25 DO BEGIN
10300     IDNR:=IDN[I];
10310     METINGOPHALEN(IDNR, IEERST, ILAATST, DATA, LMIN, STEP2, DUMP);
10320     LMAX:=(LMIN+(ILAATST-IEERST)*STEP2+.01);
10330     FOR J:=1 STEP 1 UNTIL 450 DO MATRIX[I, J]:=DATA[J];
10340 END;
10350 %
10360 WRITE(OUT, /, LMIN, LMAX, STEP2);
10370 FOR I:=1 STEP 1 UNTIL 450 DO
10380     BEGIN FOR J:=1 STEP 1 UNTIL 25 DO DATA2[J]:=MATRIX[J, I];
10390     WRITE(OUT, /, DATA2);
10400 END;
10410 %
10420 CLOSE(OUT, CRUNCH);
10430 END.

```

```

10000 C MINIB2/S/GEBONDENVRIJ/VOLGORDE
10010 C
10020 C This program is part of a series of programs to simulate
10030 C bound-free rare gas halide emission spectra.
10040 C This program takes measurements at one wavelength, which
10050 C have been stored by program MINIB2/S/GEBONDENVRIJ/CONVERTER/MAT,
10060 C and puts them in order of magnitude, so they are suitable for
10070 C program MINIB2/S/GEBONDENVRIJ/OPTELLEN.
10080 C
10090 C*****
10100 C
10110 FILE 1(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/DATAOUT")
10120 FILE 2(KIND=DISK, TITLE="MINIB2/D/GEBONDENVRIJ/DATAOUT/2",
10130 * NEWFILE=TRUE, PROTECTION=SAVE)
10140 REAL STEP3
10150 INTEGER LMIN, LMAX, I, J
10160 DIMENSION DATA(1:50), DATA2(1:50)
10170 C
10180 READ(1,/) LMIN, LMAX, STEP3
10190 WRITE(2,/) LMIN, LMAX, STEP3
10200 C
10210 DO 100 L=1, 450
10220 C
10230 READ(1,/) DATA
10240 DATA2(1)=DATA(1)
10250 DO 50 I=2, 25
10260 DO 40 J=1, I-1
10270 JAC=I-J
10280 IF(DATA(I).LE.DATA2(JAC)) GOTO 30
10290 DATA2(JAC+1)=DATA(I)
10300 GOTO 50
10310 30 DATA2(JAC+1)=DATA2(JAC)
10320 IF(JAC.EQ.1) DATA2(1)=DATA(I)
10330 40 CONTINUE
10340 50 CONTINUE
10350 WRITE(2,/) DATA2
10360 C
10370 100 CONTINUE
10380 C
10390 CLOSE(2, DISP=CRUNCH)
10400 STOP
10410 END

```



```

10000 C MINIB2/S/GEBONDENVRIJ/OPTELLEN
10010 C
10020 C This program is part of a series of programs to simulate
10030 C bound-free rare gas halide emission spectra.
10040 C In this program data stored by MINIB2/S/GEBONDENVRIJ/VOLGORDE
10050 C on a FILE 1, are added up. Because at each wavelength all
10060 C measurements have been stored in order of magnitude, noise
10070 C peaks can easily be removed.
10080 C
10090 C*****
10100
10110 FILE 1(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/DATAOUT/2")
10120 FILE 2(KIND=DISK, TITLE="MINIB2/D/GEBONDENVRIJ/TOTAAL",
10130 * NEWFILE=TRUE, PROTECTION=SAVE)
10140 REAL SPUIT, HOR, STEP3
10150 INTEGER LMIN, LMAX, I
10160 DIMENSION DATA2(1:50), MATRIX(1:50, 0:500), TOTAAL(0:1019)
10170 C
10180 READ(1,/) LMIN, LMAX, STEP3
10190 WRITE(2,/) LMIN, LMAX, STEP3
10200 C
10210 DO 10 I=0, 449
10220 READ(1,/) DATA2
10230 DO 5 J=1, 22
10240 TOTAAL(I)=TOTAAL(I)+DATA2(J)
10250 5 CONTINUE
10260 10 CONTINUE
10270 WRITE(2,/) TOTAAL
10280 C
10290 CLOSE(2, DISP=CRUNCH)
10300 C
10310 STOP
10320 END

```

```

10000 C MINIB2/S/GEBONDENVRIJ/POTPLOTTER
10010 C
10020 C This program is part of a series of programs to simulate
10030 C bound-free rare gas halide emission spectra.
10040 C With this program a graphical representation can be given of
10050 C a set of potential curves and Mulliken's difference potential,
10060 C according to specifications on a FILE 1.
10070 C
10080 C*****
10090 C
10100 FILE 1(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/POTINVOERCA")
10110 BLOCK GLOBALS
10120 $ INCLUDE "PLOTTER/FORTRAN/DECLARATION ON APPL"
10130 END
10140 $ INCLUDE "PLOTTER/FORTRAN/POLYDZ ON APPL"
10150 REAL H, RMIN, RMAX, UPPARR, LOWARR, R, UUP, ULO, E, UMUL
10160 INTEGER I, N
10170 DIMENSION UPPARR(9), LOWARR(9), R(0:4001), UUP(0:4001), ULO(0:4001),
10180 * UMUL(0:4001)
10190 C
10200 READ(1,/) DUMMY
10210 READ(1,/) DUMMY
10220 READ(1,/) RMIN, RMAX
10230 READ(1,/) N
10240 READ(1,/) DUMMY, DUMMY
10250 READ(1,/) DUMMY, DUMMY
10260 READ(1,/) DUMMY, DUMMY
10270 READ(1,/) DUMMY, DUMMY
10280 READ(1,/) DUMMY
10290 READ(1,/) UPPARR(1),
10300 * UPPARR(2), UPPARR(3), UPPARR(4), UPPARR(5), UPPARR(6),
10310 * UPPARR(7), UPPARR(8), UPPARR(9)
10320 READ(1,/) LOWARR(1),
10330 * LOWARR(2), LOWARR(3), LOWARR(4), LOWARR(5), LOWARR(6),
10340 * LOWARR(7), LOWARR(8), LOWARR(9)
10350 READ(1,/) DUMMY
10360 READ(1,/) DUMMY, DUMMY, DUMMY, DUMMY
10370 READ(1,/) DUMMY
10380 READ(1,/) DUMMY
10390 READ(1,/) E
10400 C
10410 H=(RMAX-RMIN)/N
10420 DO 30 I=0, N+1, 1
10430 R(I)=RMIN+I*H
10440 UUP(I)=UPPARR(1)+UPPARR(2)
10450 * +UPPARR(3)*EXP(-UPPARR(4)*R(I))
10460 * +UPPARR(5)*EXP(-UPPARR(6)*R(I))
10470 * -UPPARR(7)/R(I)
10480 * -UPPARR(8)/(R(I)**4)
10490 * -UPPARR(9)/(R(I)**6)
10500 ULO(I)=LOWARR(1)+LOWARR(2)
10510 * +LOWARR(3)*EXP(-LOWARR(4)*R(I))
10520 * +LOWARR(5)*EXP(-LOWARR(6)*R(I))
10530 * -LOWARR(7)/R(I)
10540 * -LOWARR(8)/(R(I)**4)
10550 * -LOWARR(9)/(R(I)**6)
10560 UMUL(I)=ULO(I)+E-UUP(I)
10570 30 CONTINUE

```

```
10580      C
10590      CALL POLYDZ(90,0,0,20,25,1,N+2,R,UUP,10,1.5,6.5,12,0,60000,
10600      *   .FALSE.,.FALSE.)
10610      CALL POLYDZ(90,0,0,20,25,1,N+2,R,ULO,10,1.5,6.5,12,0,60000,
10620      *   .FALSE.,.FALSE.)
10630      CALL POLYDZ(90,0,0,20,25,1,N+2,R,UMUL,10,1.5,6.5,12,0,60000,
10640      *   .FALSE.,.FALSE.)
10650      C
10660      STOP
10670      END
```

```

10000 C MINIB2/S/GEBONDENVRIJ/OMKEERPLOT
10010 C
10020 C This program is part of a series of program to simulate
10030 C bound-free rare gas halide emission spectra.
10040 C In this program, for a number of sets of potential curves
10050 C specified, a figure is plotted giving the wavelengths of
10060 C emissions from the classical turning points as a function
10070 C of vibrational energy.
10080 C
10090 C*****
10100 C
10110 C DECLARATIONS
10120 C *****
10130 C
10140 FILE 2(KIND=REMOTE)
10150 FILE 3(KIND=PRINTER)
10160 FILE 4(KIND=DISK, FILETYPE=7, TITLE="MINIB2/D/GEBONDENVRIJ/POTINVOERCA")
10170 BLOCK GLOBALS
10180 $ INCLUDE "PLOTTER/FORTRAN/DECLARATION ON APPL"
10190 END
10200 $ INCLUDE "PLOTTER/FORTRAN/POLYDZ ON APPL"
10210 REAL STEP3, STEP, UMINUP, EU, SPEK, DUMMY, RMIN, RMAX, UPPARR,
10220 * LOWARR, H, UDIF, R, UUP, ULO, ULO2, UMUL, UMUL2, REUP, GAMMA, GAMMA2,
10230 * D1, D2, D3, D4, D5, C1, C2, C3, C4, C5, TM, TM2, RBI, LABB11, LABB12,
10240 * LABMIN, RBU, LABMAX, G, LAB, NU, R1, LABIAC, LABUAC, RKOUD,
10250 * R2, DELTTE, CORR, LABB1, LABBU, LABOUD, ROUD, RNU, NUOUD, LOUD
10260 INTEGER LMIN, LMAX, KMAX, VIB, N, IREUP, IBI, IBU, I1, I2, JBIN,
10270 * JBUI, IOUD, SPEK2, INU, IKOUD
10280 DIMENSION EU(0:179), SPEK(0:29, 0:1019), UPPARR(1:9),
10290 * LOWARR(1:9), UUP(0:1001), ULO(0:1001), UMUL(0:1001),
10300 * TM(0:1001), TM2(0:1001), G(0:1001), R(0:1001),
10310 * IR1(0:1001), IR2(0:1001), IBI(0:179), IBU(0:179),
10320 * SPEK2(0:29, 0:1019), UMUL2(0:1001), ULO2(0:1001),
10330 * RULO(0:9), UULO(0:9)
10340 C
10350 C INPUT VARIABLES
10360 C *****
10370 C
10380 READ(4,/) DUMMY
10390 READ(4,/) DUMMY
10400 READ(4,/) RMIN, RMAX
10410 READ(4,/) N
10420 READ(4,/) DUMMY, DUMMY
10430 READ(4,/) DUMMY, DUMMY
10440 READ(4,/) DUMMY, DUMMY
10450 READ(4,/) DUMMY, DUMMY
10460 READ(4,/) DUMMY
10470 READ(4,/) UPPARR(1),
10480 * UPPARR(2), UPPARR(3), UPPARR(4), UPPARR(5), UPPARR(6),
10490 * UPPARR(7), UPPARR(8), UPPARR(9)
10500 READ(4,/) LOWARR(1),
10510 * LOWARR(2), LOWARR(3), LOWARR(4), LOWARR(5), LOWARR(6),
10520 * LOWARR(7), LOWARR(8), LOWARR(9)
10530 C
10540 C CALCULATION THE VIBRATIONAL ENERGY DEPENDENCE OF THE WAVELENGTHS
10550 C OF THE TURNING POINT EMISSION FOR A SPECIFIED NUMBER OF
10560 C POTENTIAL CURVES
10570 C *****

```

```

10580      C
10590      H=(RMAX-RMIN)/(N+1)
10600      DO 32 K=1,8
10610
10620      UMINUP=10**10
10630      UDIF=10**10
10640      DO 31 I=0,N+1,1
10650      R(I)=RMIN+I*H
10660      UUP(I)=UPPARR(1)+UPPARR(2)
10670      * +UPPARR(3)*EXP(-UPPARR(4)*R(I))
10680      * +UPPARR(5)*EXP(-UPPARR(6)*R(I))
10690      * -UPPARR(7)/R(I)
10700      * -UPPARR(8)/(R(I)**4)
10710      * -UPPARR(9)/(R(I)**6)
10720      ULO(I)=LOWARR(1)+LOWARR(2)
10730      * +LOWARR(3)*EXP(-LOWARR(4)*R(I))
10740      * +LOWARR(5)*EXP(-LOWARR(6)*R(I))
10750      * -LOWARR(7)/R(I)
10760      * -LOWARR(8)/(R(I)**4)
10770      * -LOWARR(9)/(R(I)**6)
10780      C
10790      IF(K.EQ.1) ULO2(I)=ULO(I)
10800      IF(K.EQ.2) ULO2(I)=4.4433E7*EXP(-2.92*R(I))+700
10810      IF(K.EQ.3) ULO2(I)=5.6438E7*EXP(-3.02*R(I))
10820      IF(K.EQ.4) ULO2(I)=3.7985E7*EXP(-2.85*R(I))
10830      IF(K.EQ.5) ULO2(I)=2.6877E7*EXP(-2.7*R(I))
10840      IF(K.EQ.6) ULO2(I)=6.2258E7*EXP(-3.0*R(I))
10850      IF(K.EQ.7) ULO2(I)=8.2376E7*EXP(-3.1*R(I))
10860      IF(K.EQ.8) ULO2(I)=1.0900E8*EXP(-3.2*R(I))
10870      C
10880      UMUL2(I)=1E7/(UUP(I)-ULO2(I))
10890      UUP(I)=UUP(I)-UPPARR(1)
10900      31 CONTINUE
10910      C
10920      CALL POLYDZ(90,0,0,25,20,1,N+1,UMUL2,UUP,5,250,400,5,0,20000,
10930      * .FALSE.,.FALSE.)
10940      C
10950      32 CONTINUE
10960      C
10970      CLOSE(6,DISP=CRUNCH)
10980      END

```

```

10000 C MINIB2/S/GEBONDENVRIJ/FITFUNCPL0T
10010 C
10020 C This program is part of a series of programs to simulate
10030 C bound-free rare gas halide emission spectra.
10040 C With this program a graphical representation can be given of
10050 C the fit-functions used in MINIB2/S/GEBONDENVRIJ/VIBFIT and
10060 C MINIB2/S/GEBONDENVRIJ/VIBFIT/TRIPEL.
10070 C
10080 C*****
10090 C
10100 FILE 1(KIND=DISK,TITLE="MINIB2/D/GEBONDENVRIJ/XEBRCA/5")
10110 BLOCK GLOBALS
10120 $ INCLUDE "PLOTTER/FORTRAN/DECLARATION ON APPL"
10130 END
10140 $ INCLUDE "PLOTTER/FORTRAN/POLYDZ ON APPL"
10150 INTEGER LMIN,LMAX,VIB,STEP
10160 REAL STEP3,UMINUP,EU,EU2,SPEK,SPEK2,DATA,HOR
10170 DIMENSION SPEK(0:9,0:1019),EU(0:179),DATA(0:1019),HOR(0:1019)
10180 C
10190 READ(1,/) LMIN,LMAX,STEP3
10200 READ(1,/) VIB,STEP
10210 READ(1,/) UMINUP
10220 READ(1,/) EU
10230 C
10240 DO 20 I=0,VIB-1
10250 DO 10 J=1,34
10260 READ(1) (SPEK(I,30*(J-1)+K),K=0,29)
10270 10 CONTINUE
10280 20 CONTINUE
10290 C
10300 DO 22 I=0,VIB-1
10310 DO 21 J=0,1019
10320 21 IF(SPEK(I,J).GT.SPEKMA) SPEKMA=SPEK(I,J)
10330 22 CONTINUE
10340 C
10350 KMAX=INT((LMAX-LMIN)/STEP3)
10360 DO 30 I=0,VIB-1
10370 DO 25 J=0,KMAX
10380 HOR(J)=LMIN+J*STEP3
10390 25 DATA(J)=SPEK(I,J)/SPEKMA+.5*I
10400 CALL POLYDZ(90,0,0,25,20,1,KMAX+1,HOR,DATA,5,LMIN,LMAX,
10410 * VIB,0,.5*VIB+.5,.FALSE.,.FALSE.)
10420 30 CONTINUE
10430 C
10440 END

```