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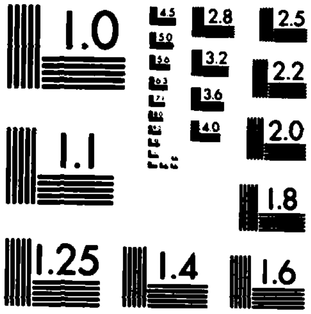

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NUMERICAL METHODS FOR THE PREPARATION OF POTENTIAL ENERGY CURVES OF DIATOMIC MOLECULES

THESIS

AFIT/GNE/PH/83M-12

Lyle L. Rutger
Capt USAF

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NUMERICAL METHODS FOR THE PREPARATION OF POTENTIAL ENERGY CURVES OF DIATOMIC MOLECULES

(with applications for lead-oxide)

THESIS

Presented to the Faculty of the School of Engineering
of the Air Force Institute of Technology
Air University
in Partial Fulfillment of the
Requirements for the Degree of
Master of Science

by
Lyle L. Rutger, B.S.
Capt USAF
Graduate Nuclear Engineering
March 1983

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Preface

This work has been prepared to provide researchers at the Air Force Institute of Technology and the Weapons Laboratory with the computer programs necessary to analyze spectroscopic data. I am grateful for the learning opportunity provided by this thesis and hope the results are helpful to those who follow me.

I am indebted to my thesis advisor, Dr. Ernest Dorko, for his guidance and encouragement throughout the development of the project. I wish to thank C. R. Vidal for his timely response in providing his program for generating potential energy curves at the start of my research. Finally and foremost, I thank my wife Vivian and children for their support in this endeavor.

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Abstract

This thesis presents the tools necessary to transform spectral data from diatomic molecules into potential energy curves which are most consistent with the experimental data and the quantum mechanical model (i.e., the Schroedinger wave equation (SWE)) for a diatomic molecule. The first of these tools, a computer program called DUNCON, generates spectroscopic constants by performing least-squares fits to spectroscopic data. The program performs fits to separate groups of data and then merges the results in a manner based upon the relative errors and correlations of the separate data sets. The second tool is a computer program provided by C. R. Vidal which contains two major routines. The first routine generates potential energy curves using the Rydberg-Klein-Rees (RKR) method. The second routine through an inverted perturbation analysis (IPA) adjusts the RKR curve so it is consistent with the SWE model. Finally, techniques are presented for extending potential energy curves to the dissociation energy, De , when the spectroscopic data alone is inadequate for the purpose.

Use of the programs is demonstrated for the diatomic molecule lead-oxide. Constants are produced for the A, B, D, a, b, and X states from previously published experimental data. A new set of assignments is made for the b state experimental data producing constants with significantly improved accuracy over those reported in literature. The b state constants are:

$$T_e = 16325.1 \pm 11.2 \text{ cm}^{-1}$$

$$W_e = 430.99 \pm 2.47 \text{ cm}^{-1}$$

$$W_eX_e = -0.757 \pm 0.441 \text{ cm}^{-1}$$

These are one standard error limits. Potential energy curves are generated for the a, A, and X states of lead-oxide. The X state potential energy curve is extended to its dissociation energy.

NUMERICAL METHODS FOR THE PREPARATION OF POTENTIAL ENERGY CURVES OF DIATOMIC MOLECULES

I Introduction

The construction of accurate potential energy curves is essential to the understanding of data gathered in pursuits ranging from the study of gas kinetics to the study of stellar structures. Potential energy curves are used to calculate Franck-Condon factors which can be used to predict the probabilities of an electronic transition. Discussed in this paper are Dunham coefficients with the corresponding model used to represent experimental data. A computer program called DUNCON is developed for generating a minimum-variance linear unbiased (MVLU) fit to independent sets of spectroscopic data. This program has a provision for merging these fits, as appropriate, to obtain weighted, correlated estimates of constants for data sets which exhibit different accuracies or are correlated. The Rydberg-Klein-Rees (RKR) method of generating potential energy versus internuclear separation curves is presented. A computer program which performs RKR calculations and then uses an inverted perturbation approach (IPA) (Ref 23) to improve the accuracy of the RKR curve is discussed in detail. The RKR-IPA program was developed by C. R. Vidal and H. Scheingraber (Ref 41). Utility of the programs is demonstrated using data reported for the diatomic molecule lead oxide (PbO).

The accuracy of any potential energy curve depends upon the analytic model used to represent experimental data and the manner in which the constants in the model are generated. The Dunham model was chosen to represent the data because of the large number of terms that can be incorporated.

The RKR method is a semi-classical WKB method which has been shown to agree quite well with quantum mechanical calculations for simple molecules (Ref 34). Because of its accuracy, it has been chosen by several researchers to ascertain the accuracy of other methods such as the Morse formula for generating potential curves (Refs 47 and 32).

A recent improvement on the RKR method, though still an approximate method, is the IPA approach which starts with an RKR curve and adjusts it to obtain an approximate but more accurate solution to the Shroedinger equation.

Methods developed by Leroy, by Tellinghuisen, and by Vidal and his coworkers are discussed. These methods can be used to extend potential energy curves when the available experimental data does not cover the entire range of the potential curve.

II Literature Background and Theory

Modeling Spectroscopic Data for Diatomic Molecules

Spectroscopic data resulting from the emission of energy by a diatomic molecule during a transition from an excited electronic state to a lower state may be represented as follows:

$$\nu\ (v',J',v'',J'') = T'(v',J') - T''(v'',J'') \qquad (1)$$

where ν is the observed line frequency in wave numbers, and the term values for the upper and lower electronic states, T' and T'' respectively, are represented by the Dunham type expression:

$$T(v,J) = \sum_{ij} A_{ij}(v + 1/2)^i\ J^j\ (J + 1)^j \qquad (2)$$

(Ref 48:1866).

Although Eq (2) has the same form as that associated with the Dunham coefficients, Y_{ij} , (Ref 18), i.e.,

$$T(v,J) = \sum_{ij} Y_{ij}(v + 1/2)^i\ J^j\ (J + 1)^j \qquad (3)$$

researchers M. M. Hessel and C. R. Vidal make the distinction that their A_{ij} values are not necessarily identical to Dunham's Y_{ij}'s (Ref 22:4443).

Dunham arrived at the expression in Eq (2) by using the Wentzel-Brillouin-Kramer method (WKB) (Refs 51; 9 and 29) to solve the Schroedinger equation for the rotating diatomic vibrator for the energy levels within one electronic state:

$$\frac{d^2\Psi}{d\xi^2} + \frac{8\pi^2\mu r_e^2}{h^2}\left[E - V(\xi) - \frac{h^2\ J(J+1)}{8\pi^2 r_e^2\mu(1+\xi)^2}\right]\Psi = 0 \tag{4}$$

where:

$\xi = (r - r_e)/r_e$

r_e = the equilibrium nuclear separation

μ = the reduced mass

V = potential of the function, with a minimum at r_e

V_r = the last term which is due to the centrifugal force of rotation.

He expressed the potential energy by expanding V about $\xi = 0$.

$$V = hca_0\xi^2(1 + a_1\ \xi + a_2\ \xi^2 + a_3\ \xi^3 + \ldots) \tag{5}$$

where $a_0 = w_e^2/4B_e$; w_e is the classical frequency of small oscillations expressed in cm-1 and $B_e = h/(8\pi^2\mu r_e\ c)$ (Ref 18:732). Finally, he obtained expressions for the Y_{ij}'s in terms of the a_k's in Eq (5).

Hessel and Vidal distinguish their constants, A_{ij} , from the Dunham constants, Y_{ij} , by pointing out that the latter are theoretically derived, while the A_{ij}'s are the results of a least-squares fit. Inherent in the least-squares fitting procedure is the fact that the A_{ij} coefficients absorb the effects of inaccuracies in the data, and are somewhat dependent upon the values of their neighboring constants and upon any missing constants (Ref 22:4447). For these reasons, the A_{ij}'s are only estimates of the theoretical Y_{ij} derived by Dunham.

Some further discussion of the A_{ij} and Y_{ij} constants is appropriate. First, a listing of the correspondence of Dunham's constants and the classical spectroscopic constants is desirable. They are given in Table I-1.

TABLE I-1

Correspondence Between Dunham Coefficients and Classical Spectroscopic Constants

Y^{*}_{00}	$Y_{01} \sim B_e$	$Y_{02} \sim D_e Y_{03} \sim F\ Y_{04} \sim H$
$Y_{10} \sim w_e$	$Y_{11} \sim -\alpha_e$	$Y_{12} \sim \beta_e$
$Y_{20} \sim -w_e x_e$	$Y_{21} \sim \gamma_e$	
$Y_{30} \sim w_e y_e$		
$Y_{40} \sim w_e z_e$		

$^*Y_{00}$ is defined as:

$$Y_{00} = 1/4\ Y_{20} + 1/4\ Y_{01}\ ((Y_{11}Y_{10}/(6\ Y_{01}^2)) - 1)^2 \qquad (6)$$

This is the expression normally reported in the literature based upon the work of Dunham (Ref 18), although the expression for Y_{00} is not explicity stated in Dunham's work. Sandeman

(Ref 40) and Jarmain (Ref 25) expand on Dunham's work. Using this material, the expression given in Eq (6) can be verified. In addition to this derivation, the expression for Y_{00} was found in the following works: (Refs 49; 28:325; 35:117; and 41:4450). The expression for Y_{00} was found to be in error in two publications. First, Herzberg's Y_{00} is larger than that in Eq (6) by $+3/4\ Y_{20}$ (Ref 21:109). Second, in McKeever's work, due to a typographical error, "$+1/4\ Y_{20}$" was omitted (Ref 3:47). The works of Sandeman and Jarmain compliment Dunham's work, making easier the understanding of Dunham's work.

Returning to Eq (1), it should be noted that when a least-squares fit is performed using Eq (2), the bottom of the potential energy curve of the lower state is typically assigned a value of "0." This is done by omitting the A''_{00} term from the fit. When A'_{00} is found from the least-squares fit, it is not equivalent to Dunham's Y'_{00} for the upper state. For this reason, Vidal assigns an asterisk to A'_{00} and calls it $\overset{*}{A}_{00}$. This term is made up of three components as shown (Ref 44):

$$\overset{*}{A}_{00} = A'_{00} + Te - A''_{00} \qquad (7)$$

A'_{00} and A''_{00} are estimated from Eq (6). These A'_{00} and A''_{00} are then the best estimates of Dunham's Y'_{00} and Y''_{00} . Eq (7) can be solved for Te' , the electronic term energy of the upper state:

$$Te = A^{*}_{00} - A'_{00} + A''_{00} \qquad (8)$$

In applying Dunham's expression, one should be aware of its inadequacies. Expressions such as the Morse potential (Ref 21:57):

$$U(r-r_e) = D_e\ (1 - \exp(-B(r-r_e))^2 \qquad (9)$$

are constructed to guarantee that as $r \rightarrow r_e$, $U \rightarrow 0$ and as $r \rightarrow \infty$, U approaches the dissociation energy, D_e. Eq (5) on the other hand does not necessarily satisfy these two criteria. Sandeman showed that if Morse's equation is expanded about $(r-r_e) = 0$, it takes on a form similar to Dunham's Eq (5), but is expressed in terms of two constants and additional numerical coefficients as follows:

$$U = a_0(1 - a + 0.583a^2\xi - 0.250a^3\xi + 0.086a^4\xi - \ldots) \qquad (10)$$

A comparison of Eqs (5) and (10) shows that Dunham's expression is a more general form of Morse's equation. Sandeman also applies a similar expansion to an equation for potential energy developed by Kratzner (Ref 30) and obtained a similar correspondence with Dunham's expression. Because of the increased number of variables and, in turn, the increased flexibility, Dunham's expression has the potential for being more accurate. But, because of this freedom, obtaining constants which satisfy the convergence criterion is more difficult and is not guaranteed for large values of r or v .

Jarmain made a term-by-term comparison of similar expressions developed from Dunham's work and by the RKR method and showed that, upon neglecting Dunham's small corrections, the potentials produced by the two are mathematically identical (Ref 25:217). Based upon this, the use of Dunham's expression (Eq (3)) to represent spectroscopic data for input to an RKR program for generating potential curves is justified and appropriate.

In applying Dunham's expression, one should remember that his equations are developed for small oscillations about r_e. At energy levels approaching the dissociation limit, Eq (2) may no longer be appropriate. Eqs (1) and (2) are for simple cases. In cases where Λ-type doubling occurs, or where isotopic effects are being considered, more complex models must be substituted for Eqs (1) and (2). Works cited in the bibliography by Vidal and his coworkers present variations of Eq (2).

Spectroscopic Constants by Merging Least-Squares Fit Data

The large quantities of data obtained in a spectroscopic analysis requires that the data be reduced to a more manageable form. For example, Eqs (1) and (2) in the previous section are used to calculate reportable constants. To make these models usable, the A_{ij} coefficients must be determined. The most widely used method of generating these coefficients is to perform a linear least-squares fit to the experimental data. For spectroscopic data, a model is created, typically involving a power series expansion based upon the rotational and vibrational quantum numbers as expressed in Eqs (1) and (2). If only band head data is being analyzed, the model takes the following form:

$$\nu = \sum_{i0} A'_{i0} (v' + 1/2) - \sum_{i0} A''_{i0} (v'' + 1/2)^i \qquad (11)$$

If several different transitions are involved, different values of the A''_i ground state constants may be obtained. In addition, the accuracy of the A''_i's may be different. It is desirable to merge these constants and obtain a best estimate of the ground state constants. This can be done by accomplishing a weighted least-squares fit of the data. Such a merging can produce more accurate estimates of the constants and reduce the error limits associated with them. The merged fit may also improve the upper state constants.

Merging may also be desirable for the case when two groups of data are available with significantly different standard errors. For example, if infrared data for vibration-rotation band transitions and microwave data for transitions between adjacent rotational levels are available, the greater accuracy of the microwave data can improve the accuracy of the other constants if a weighted merged fit is performed.

There are other methods of data fitting available. These methods include least absolute deviation, least-squares deviation, maximum likelihood, and minimum chi-squared. All have different fit criteria (Ref 2:3). Also, nonlinear least-squares fits are possible (Refs 4 and 15). The present report deals only with the least-squares fit techniques.

The least-squares method or "regression" method minimizes the sum of the squared deviations between observed values and values calculated using the constants obtained from the fit. The least-squares method provides the minimum-variance linear unbiased (MVLU) estimates of the constants; that is, the least-squares method introduces no bias. The fits produced are linear functions of the data. When the fit is used to reproduce data, the generated data exhibits the smallest possible variance from the original data that can be achieved with the model and data used (Ref 2).

In performing a least-squares fit, the following assumptions are made:

1. The model (equation) chosen to represent the data is a perfect description of the physical event.

2. The model is linear in the constants to be estimated.

3. The mean error of the experimental data is zero. Any systematic error present must be small compared to the variances and random errors of the data.

4. The variance-covariance elements must be finite and their relative values known if different groups of data are to be merged (Ref 2:7).

In reducing spectroscopic data, three methods are available:

1. The reduction of each band, i.e., each a group of transitions from one electronic state to another, separately.

2. The reduction of a number of bands simultaneously.

3. The reduction of the bands separately and then merging the resulting data.

The first and third techniques are developed in this paper. The method of approach is now described. Least-squares fitting techniques are based upon the following matrix equation:

$$\nu = X\beta + \varepsilon \qquad (12)$$

where ν is a column matrix containing the experimentally observed line frequencies expressed in wavenumbers, X is a matrix made up of the $(v + 1/2)$ and the $J(J + 1)$ terms as dictated by the model in Eqs (1), (2), or (11) as chosen. β is a column matrix made up of the A_{ij} constants which are to be calculated. The ε column matrix contains the unknown errors associated with each observed experimental data point. These matrices are written out explicity in Appendix A to aid the user in understanding the program DUNCON.

Eq (12) is then solved for β as:

$$\beta = (X^T X)^{-1} X^T \nu \qquad (13)$$

The estimated variance of the fit is expressed as follows:

$$\sigma^2 = (\nu - X\beta)^T \; (\nu - X\beta)/f_m \tag{14}$$

where f_m is the degree of freedom of the calculation. The degrees of freedom, f_m , is equal to the number of experimental values ν used in the fit minus the number of constants to be obtained in the β matrix. The variance-covariance matrix for the constants obtained in Eq (13) is calculated by the following relation:

$$\theta = \sigma^2 \; (X^T X)^{-1} \tag{15}$$

The diagonal elements of the ϑ matrix are the variances of the constants and the off diagonal elements are their covariances. The correlation between the calculated constants is expressed by the correlation *coefficients* which are obtained using the variances and covariances in the following manner:

$$C_{ij} = \theta_{ij}/(\theta_{ii}\theta_{jj})^2 \tag{16}$$

The subscripts refer to the two constants for which the coefficient expresses the correlation.

As mentioned earlier, the performance of separate fits to each band will yield several values for the constants associated with the lower electronic state. The variances for different bands may also differ significantly. If the variances of the bands are the same, the data can be combined in one large data group and reduced simultaneously. If estimates of the errors are available, a weighted fit based upon the error may and should be performed.

Albritton describes an approach, the correlated least-squares fit, which is more general than the weighted least-square fit (Refs 2 and 3). Albritton showed that one need not use all raw data at one time to obtain a merged fit. He showed that a weighted simultaneous multiband fit and a merged band-by-band fit are equivalent. The merged fit is presented in this paper.

The bands or other groups of data are first reduced in a least-squares manner as previously discussed.

Then the data obtained in the initial least-squares fit may be expressed in the following manner:

$$y = X\beta^M + S \tag{17}$$

where y is a column matrix made up of the constants obtained from the separate least-squares fits and β^M is a column matrix which will hold the desired merged constants. The y matrix will often contain several values for the same constant. Each constant will be represented only one time in the β^M matrix. The X matrix relates the redundant values in the y matrix to the corresponding constants in the β^M matrix. Explicit examples of these matrices are given in Appendix A.

To perform a weighted, correlated least-squares fit, a matrix composed of the variance-covariance matrices from a separate least-squares fit is required. This matrix is given the symbol "θI." It is structured as follows:

$$\theta I = \begin{bmatrix} \theta_1 & 0 & 0 \\ 0 & \theta_2 & 0 \\ 0 & 0 & \theta_3 \end{bmatrix} \tag{18}$$

where θ_1 , θ_2 and θ_3 are the variance-covariance matrices of Eq (15). The formula required to obtain the merged constants is as follows:

$$\beta^M = (X^T \theta I^{-1} X)^{-1} X^T \theta I^{-1} y \tag{19}$$

The estimated variance of the new merged fit is given by:

$$\sigma^2 = (y - X\beta^M)^T \theta I^{-1} (y - X\beta^M)/f_m \tag{20}$$

where f_m is the degree of freedom. The variance-covariance matrix of the merged constants is obtained by the following calculation:

$$\theta^M = \sigma^2 (X^T \theta I^{-1} X)^{-1} \tag{21}$$

The formulas are discussed in future detail in the appendices.

As in all analysis, the data should be checked to insure that the errors predicted by the least-squares fit follow a normal distribution pattern. Albritton provides a fairly complete discussion of the checks commonly used (Ref 2:14-31).

Having established that the errors of the data are normally distributed, one should then construct confidence limits for the constants based upon the degrees of freedom and the confidence one wishes to have that the true value is within the assigned limits. The placing of too much reliance upon error limits specified by one standard deviation, $1 \times \theta_{ii}^{1/2}$, should be avoided. Even if a large sample of data is taken, one can only be about 68% certain that the "true value" lies within a range of $\pm 1 \times \theta_{ii}^{1/2}$. If a 95% confidence level is desired and the degrees of freedom, f_m, is greater than 30, one must assign limits of $\pm 2 \times \theta_{ii}^{1/2}$. The multiplier of $\theta_{ii}^{1/2}$ is student's t-factor. It is named after its originator, W. S. Gosset (1876-1937). It is a function of the degrees of freedom of the calculation and the desired confidence level, "$1-\alpha$." Dixon and Massey (Ref 17) give a tabulation of student's t-factor as a function of the degrees of freedom and the degree of confidence. The confidence limits for the constant are then expressed as follows:

$$\beta_i + t(f_m, 1-\alpha)\theta_{ii}^{1/2} \tag{22}$$

Having established the limits, one can assume that the probability of the true value of falling within the limit $\pm t\theta_{ii}^{1/2}$ is "$1-\alpha$" where α may vary between 0 and 1.

With the confidence limits for the estimated constants properly established, one can then determine if the constants are significant (Ref 27). For example, if a constant has a value of 3 and an assigned error limit of ±5, the range in which the true value of the constant might be found is -2 to +8. This range includes 0; hence, the constant is not significant. If the assigned confidence limits, $\beta_i \pm t\theta_\alpha^{1/2}$ includes zero, then the constant is insignificant and may normally be discarded. Two exceptions to this rule may be encountered.

The first exception concerns the case where a non-zero correlation between two molecular constants exists. If non-zero correlation coefficients are involved, standard errors must be calculated using the most general formulation involving both variances and covariances. If large correlations exist, the rounding of a constant to the number of significant digits dictated by the standard error of the constant, may result in loss of information, i.e., rounding may introduce unnecessary inaccuracies into the calculated data (Ref 2:2).

Albritton suggests that one digit beyond the "one standard error digit" should suffice for most fits. A simple check is to use the rounded constants and see that they reproduce to some desired accuracy the values calculated using the unrounded constants obtained from the fit.

The second exception occurs, where it may prove necessary to retain a constant when not justified by the standard error, in the extension of the potential curve to its dissociation limits (Ref 10:83).

Before merging data from separate least-squares fits, a check should be made for systematic errors. A simple check is to verify that for a given set of confidence limits, say 95%, the error limits for the common constants obtained in two independent fits overlap each other. If they do not, then it is probable that one set contains a systematic error. A second more sophisticated test involves the computation of the confidence limits for the differences for pairs of corresponding constants checking to see if they include zero (Ref 2:45). Calculation of the confidence limits of differences involves student's t-factor and methods are given by Bennet and Franklin (Ref 5); and Dixon and Massey (Ref 17). A more extensive discussion of the covariance-variance data and how it may be used is presented by Albritton (Refs 2 and 3).

Finally, Albritton provides a recommendation as to what data should be provided in a report on the results of a spectroscopic study. He lists the following as essential data:

1. The observed line numbers (with assignments).
2. If room permits, the variance-covariance matrix used to merge the data.
3. The model used to represent the experimental data.

4. The estimated molecular constants.

5. The standard error of the constants and the degrees of freedom involved in the calculations. This data will enable the reader to establish his own confidence limits.

6. The estimated variance of the variance, σ_σ , may be helpful. An estimate of this value for large samples of normally distributed data may be obtained by the formula (Ref 16):

$$\sigma_\sigma = \sigma/[2f_m]^{\frac{1}{2}} \tag{23}$$

Other data which may be appropriate include the variance-covariance matrix of the final merged constants and the results of the testing to determine the normality of the data sample.

Rydberg-Klein-Rees Potential Energy Curves

Potential energy curves for diatomic molecules are plots of potential energy versus the internuclear distance between atoms. Figure II-1 shows a typical curve. From this plot of energy versus internuclear distance, it can be seen that as the nuclei approach each other the potential becomes infinite; and as their separation increases, the curve asymptotically approaches the dissociation energy, D_e . The equilibrium internuclear distance, r_e , is the distance at which the potential energy of the molecule is at a minimum.

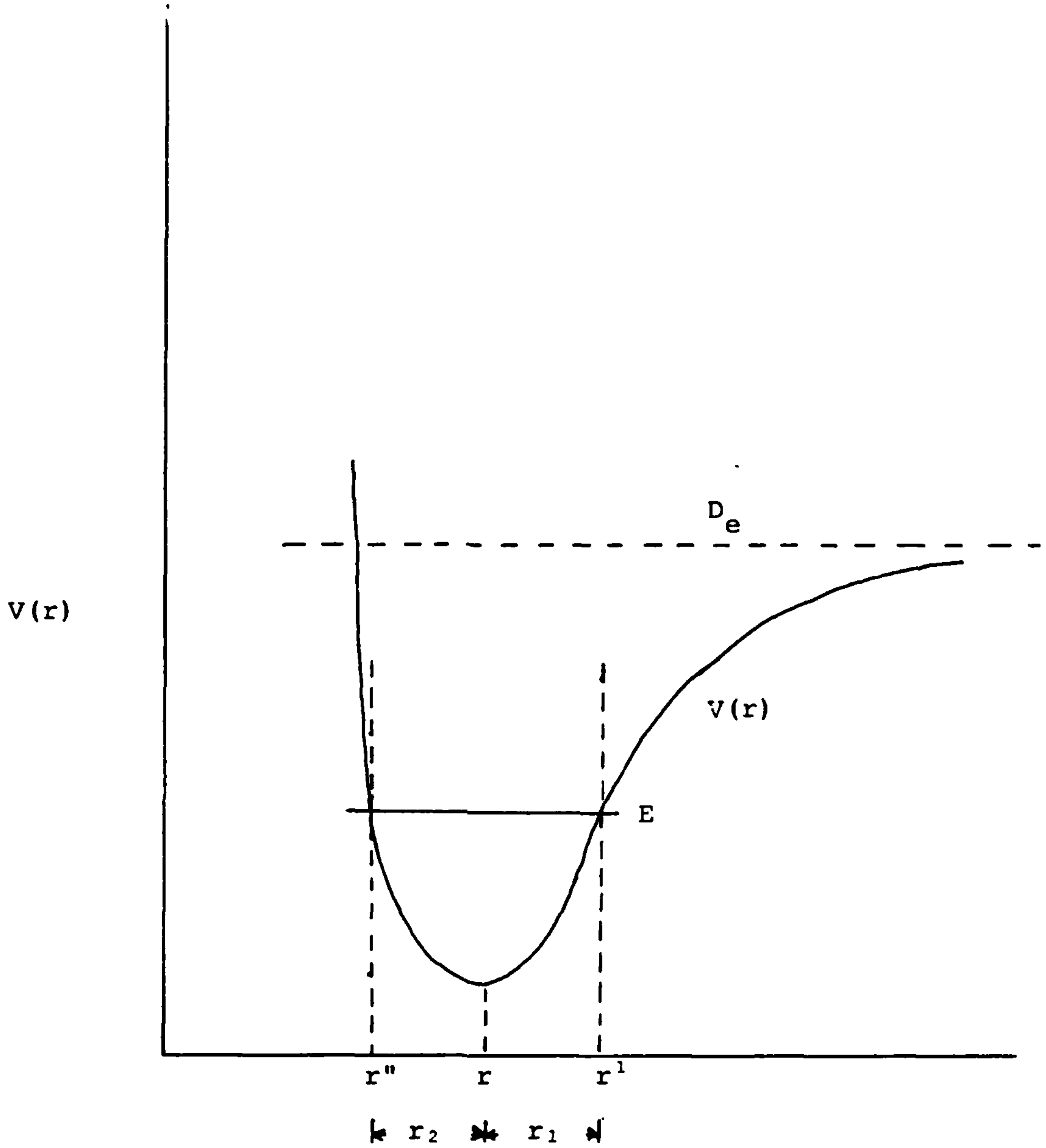

Fig II-1. Potential Energy Versus Internuclear Distance for a Diatomic Molecule

The Rydberg-Klein-Rees (RKR) model for the potential energy curve is developed in this section. Rydberg started with the expression for the total energy, E , for a rotating-vibrating diatomic molecule:

$$E = p^2/2\mu + V(r) \tag{24}$$

The $p^2/2\mu$ term in Eq (24) is the kinetic energy of the system, p in turn, is the linear momentum. The second term, $V(r)$ is defined as follows:

$$V(r) = U(r) + \kappa/r^2 = U(r) + P^2/2\mu r^2 \tag{25}$$

where $U(r)$ is the potential energy of the system, P is the angular momentum of the system, and μ is the reduced mass.

Based on this energy expression, Rydberg developed a procedure for graphically determining the classical turning points for a diatomic molecule (Ref 39). Klein modified Rydberg's derivation so that the turning point could be calculated numerically (Ref 52). Reese obtained quadratic and cubic analytic solutions approximating Klein's formulas (Ref 38).

Klein's mathematical development is given here. Terms used in the development are shown in Fig II-1 as an aid in following the presentation. The classical turning points are deisnged r' and r''. Klein defined the turning points in terms of the quantities r_1 and r_2 . For his analysis,

r_1 and r_2 are measured from r_e , r_1 being positive and r_2 negative. Then r' and r'' are defined as follows:

$$r' = r_1 + r_e \qquad (26)$$

$$r'' = r_e + r_2 \qquad (27)$$

Then

$$dr' = dr_1 \qquad (28)$$

$$dr'' = dr_2 \qquad (29)$$

$$dr = dr_1 \text{ or } dr_2 \qquad (30)$$

Klein designated the width of the potential curve as $2f$ and from Eqs (26) and (27), it follows that:

$$2f = (r_1 + r_e) - (r_2 + r_e) = r_1 - r_2 \qquad (31)$$

The energy in Eq (24) may be expressed as a function of "I," the action integral for a rotating vibrator and "κ." These terms are defined as follows:

$$I = \oint P dr \qquad (32)$$

$$\kappa = P^2/(2\mu) \qquad (33)$$

The following relationships which involve the period, τ , and the average position of a harmonic oscillator, $\overline{1/r}$, are known:

$$1/\tau = \partial E/\partial I \qquad (34)$$

$$\overline{1/r^2} = (\partial E/\partial \kappa) \tag{35}$$

$$\rho = \tau(\partial E/\partial \kappa) \tag{35'}$$

Using Eqs (32) and (34) and solving for the differential of E and adding the results, the following is obtained:

$$\delta E = (1/\tau)\delta I + (\rho/\tau)\delta\kappa \tag{36}$$

Inverting Eq (32), the following is obtained:

$$\tau = \partial E/\partial I \tag{37}$$

Setting Eq (36) equal to zero and solving for ρ, the following is obtained:

$$\rho = -\partial I/\partial \kappa \tag{38}$$

From the equation for the momentum, $p = \mu v = \mu(dr/dt)$, one can, by integrating over one cycle, obtain an expression for the period of vibration for a harmonic oscillator:

$$\tau = \oint \mu(dr/p) \tag{39}$$

Solving Eq (24) for p and substituting into Eq (39), the period of oscillation may be expressed as:

$$\tau = (\mu/2) \oint (E-V(r))^{-\frac{1}{2}}dr \tag{40}$$

The integral in Eq (40) can be broken into two parts, one to be integrated from r_e to r_1, and the other from r_2 to r_e (as depicted in Fig II-1). This operation yields:

$$\tau = 2(\mu)^{\frac{1}{2}} \left[\int_{r_e}^{r_1} dr/(E-V(r))^{\frac{1}{2}} - \int_{r_2}^{r_e} dr/(E-V(r))^{\frac{1}{2}} \right] \quad (41)$$

The factor of two is introduced to account for one vibration cycle from r_e through r_1 and r_2 and back to r_e again. Rearranging Eq (41) and recombining the integrals, one obtains:

$$\tau = (2\mu)^{\frac{1}{2}} \int_{r_2}^{r_1} (dr_1-dr_2)/(E-V(r))^{\frac{1}{2}} \quad (42)$$

Now to change the variables of integration, Klein defined the following terms:

$$y = V(r) - V(r_e) \quad (43)$$

and

$$x = E - V(r_e) \quad (44)$$

where x is constant for a given E. Then r may be expressed as a function of y as follows:

$$r = r_1(y),\ r > r_e \quad (45)$$

$$r = r_2(y),\ r < r_e \quad (46)$$

and when at r_e, $r_1(0) = r_2(0) = r_e$. Subtracting Eq (43) from Eq (44):

$$x - y = E - V(r) \quad (47)$$

and if the "f" of Eq (31) is function of y, then as defined

$$r_1(y) - r_2(y) = 2f(y) \tag{48}$$

then

$$dr_1/dy - dr_2/dy = 2df(y)dy \tag{49}$$

or

$$dr_1 - dr_2 = 2f'(y)dy \tag{50}$$

Using Eqs (45), (46), (47), and (50) to change the variable of integration and integration limits in Eq (42), Klein obtained:

$$\tau = 2\ (2\mu)^{\frac{1}{2}} \int_{y_2}^{y_1} 2\ f'(y)\ dy/(x-y)^{\frac{1}{2}} \tag{51}$$

From Eq (43) when $r = r_e$, then $V(r) = V(r_e)$ and $y = 0$. Thus, the integral in Eq (51) may be evaluated from 0 (defined as the bottom of the potential well) to some value X.

$$\tau = 2\ (2\mu)^{\frac{1}{2}} \int_{0}^{x} f'(y)\ dy/(x-y)^{\frac{1}{2}} \tag{52}$$

This is the first of two integral equations central to Klein's derivation.

Combining Eqs (28), (35), (35'), and (40) yields:

$$\rho = \tau\ \overline{(1/r^2)} = (\mu/2)^{\frac{1}{2}} \oint (1/r^2)\ [dr/E-V(r))^{\frac{1}{2}}] \tag{53}$$

By definition:

$$dr/r^2 = -(1/r) \tag{54}$$

Then Eq (53) becomes:

$$\rho = -(\mu/2) \oint d(1/r)/(x-y)^{\frac{1}{2}} \tag{55}$$

Again, the integral in Eq (55) may be broken into two parts. Then for $r > r_e$:

$$r'' = r_2 + r_e \tag{56}$$

$$1/r'' = 1/(r_2 + r_e) \tag{57}$$

and if r_e is set equal to "0" then:

$$1/r'' = 1/r_2 \tag{58}$$

Similarily for $r < 0$:

$$1/r' = 1/r_1 \tag{59}$$

Then for small oscillations about r_e , Eq (53) may be written as the difference between the integrals:

$$\rho = 2\ (\mu/2)^{\frac{1}{2}} \left[\int_{1/r_e}^{1/r_1} -d(1/r_1)/(x-y)^{\frac{1}{2}} - \int_{1/r_2}^{1/r_e} -d(1/r)/(x-y)^{\frac{1}{2}} \right] \tag{60}$$

$$\rho = (2\mu) \int_{1/r_2}^{1/r_1} d(1/r_2 - 1/r_1)/(x-y)^{\frac{1}{2}} \qquad (61)$$

Klein established the following definition:

$$2g(y) = 1/r_2 - 1/r_1 \qquad (62)$$

Differentiating with respect to y yields:

$$2dg(y) = (d/dy)\ (1/r_2) - (d/dy)\ (1/r_1) \qquad (63)$$

Changing the notation yields:

$$2g'dy = d(1/r_2) - d(1/r_1) \qquad (64)$$

Substituting Eq (64) into Eq (61) yields:

$$\rho = 2\ (2\mu)^{\frac{1}{2}} \int_0^y [g'(y)dy/(x-y)^{\frac{1}{2}}] \qquad (65)$$

with the limits of integration assigned in the same manner as for Eq (52). This is the second integral which is central to Klein's derivation.

In the next step of his development, Klein derives expression for r_{max} and r_{min}, the classical turning points for a harmonic oscillator. Klein recognized that the integrals for τ and ρ (Eqs (52) and (65)) were of the Abelian type. He multiplied both sides by $dx/(\alpha-x)^{\frac{1}{2}}$ and integrated both sides from $x = 0$ to $x = \alpha$, where $\alpha = E - (V(r)$ (Ref 35:25), i.e.,

$$ {}_{0}^{\alpha}\,\tau\; dx/(\alpha-x)^{\frac{1}{2}} = 2\ (2\mu)^{\frac{1}{2}} \int_{y=0}^{y=\alpha} f'dy \int_{x=y}^{x=\alpha} dx/[\alpha-x)(x-y)]^{\frac{1}{2}} \qquad (66) $$

In Eq (66)

$$ f'(y) = f(\alpha) \qquad (67) $$

and

$$ \int_{y}^{\alpha} dx/[(\alpha-x)(x-y)] = dx/(-x^2+y+\alpha-\alpha y)^{\frac{1}{2}} \qquad (68) $$

Eq (68) may be integrated as follows (Ref 6:300):

$$ \int dx/(uv)^{\frac{1}{2}} = 2/(bd)^{\frac{1}{2}} \tan^{-1} [(-bduv)^{\frac{1}{2}}/bv], $$

for bd>0 (69)

where $u = a+bx$, and $v = a'+dx$ and for the present integral:

$a = \alpha$ $a' = -y$

$b = -1$ $d = 1$

$bd = -1$

then the integral can be evaluated to be π . Finally, the left side of Eq (68) is evaluated as:

$$ \int_{0}^{\alpha} dx/(\alpha-x)^{\frac{1}{2}} = 2\ (2\mu)^{\frac{1}{2}}_{\pi}\ f(\alpha) \qquad (71) $$

or solving Eq (71) for $f(\alpha)$:

$$f(\alpha) = 1/(2\pi(2\mu)^{\frac{1}{2}}) \int_0^{\alpha} dx/(\alpha-x)^{\frac{1}{2}} \qquad (72)$$

and for $\alpha = y$:

$$f(y) = 1/(2\pi(2\mu)^{\frac{1}{2}}) \int_0^{y} dx/(y-x)^{\frac{1}{2}} \qquad (73)$$

Similarily, Eq (65) for "g" may be transformed into the following:

$$g(y) = \frac{1}{2\pi(2\mu)^{\frac{1}{2}}} \int_0^{y} \frac{\rho dx}{(y-x)^{\frac{1}{2}}} \qquad (74)$$

From the definitions for x given in Eq (43):

$$dx = dE \qquad (74')$$

Substituting Eq (74′) into Eq (34) yields:

$$\tau\ dx = dI \qquad (75)$$

Recalling that E is a function of I and κ, and using Eq (47), Eq (73) becomes:

$$f(V) = 1/(2\pi(2\mu)) \int_0^{I} dI/(V-E(I,\kappa))^{\frac{1}{2}} \qquad (76)$$

From Eqs (34), (35′), and (74′):

$$\rho\ dx = \rho\ dE = (\partial E/\partial\kappa)\ dE = \tau(\partial E/\partial\kappa)\ (\partial I/\tau)$$

$$= (\partial E/\partial\kappa)\partial I \qquad (77)$$

and Eq (74) becomes:

$$g(V) = 1/(2\pi(2\mu)^{1/2}) \int_0^{I'} \partial[E(I,\kappa)/\partial\kappa)\ dI]/(V-E(I,\kappa))^{1/2} \qquad (78)$$

As $E(I,\kappa)$ approaches V in Eqs (76) and (78), the integrals become infinite. To avoid these singularities, Klein instead evaluated the following expression:

$$S(V,\kappa) = 1/(\pi(2\mu)^{1/2})\ (V-E(I,\kappa))^{1/2} dI \qquad (79)$$

This expression has the following relation to the f and g of Eqs (76) and (78):

$$f = \partial S/\partial V \qquad g = -\partial S/\partial\kappa \qquad (80)$$

As shown in Eq (2), spectroscopic energy levels can be represented as power series of $(v+1/2)$ and $J(J+1)$. It is convenient then to express the integrals for f and g in terms of the quantum numbers v and J .

The expression for the radial action variable in quantum mechanical terms is

$$I = (v+1/2)h \qquad (81)$$

Then

$$d(I) = d(v+1/2)h \qquad (82)$$

The quantum mechanical expression for κ is:

$$\kappa = P^2/2\mu = J(J+1)\hbar^2/2\mu \qquad (83)$$

Then

$$\partial/\partial\kappa = 2\mu/\hbar^2 (\partial/\partial J(J+1)) \tag{84}$$

Finally, the expressions for f and g become:

$$f(V,J(J+1)) = \hbar/(2\mu)^{\frac{1}{2}} \int_0^{v'+\frac{1}{2}} \frac{d(v+\frac{1}{2})}{[V-E(v+\frac{1}{2},J(J+1)]^{\frac{1}{2}}} \tag{85}$$

$$g(V,J(J+1) = (2\mu)^{\frac{1}{2}}/\hbar \int_0^{v'+\frac{1}{2}} \frac{\partial E/\partial(J(J+1)\big|_{v+\frac{1}{2}}\, d(v+\frac{1}{2})}{[V-E(v+\frac{1}{2},J(J+1))]^{\frac{1}{2}}} \tag{86}$$

where the upper limit of integration v' is selected such that $V = E(v'+1/2,J(J+1))$ for the fixed value of $J(J+1)$ used in the integrals (Ref 35:27,28).

If the RKR calculations are evaluated for $J=0$ then Eq (2) reduces to:

$$T = \sum_{i=1} Y_{i0} (v+1/2)^i = G(v) \tag{87}$$

more commonly referred to as G_v .

Eq (85) becomes:

$$f = \int_{v_0}^{v'} (G(v) - G(v'))^{-\frac{1}{2}} dv' \tag{88}$$

(Ref 24:2), where Kaiser (Ref 26:1686) defined the lower limit of integration by the following:

$$G(v_0) = -Y_{00} \tag{89}$$

where Y_{00} is the Dunham constant previously defined in Eq (6). The variable v_0 in $G(v_0)$ may be expressed in terms of Dunham coefficients as:

$$v_0 = -1/2 - \Delta = -1/2 - (Y_{00}/Y_{10})(1 + Y_{00}Y_{20}/Y_{10}^2 + \ldots) \qquad (90)$$

For $J = 0$

$$\partial E/\partial J(J+1) = \sum_{n=0} Y_{ni}(v+1/2)^n = B(v) \qquad (91)$$

(Ref 24:2), where $B(v)$ is the spectroscopic term defined as follows:

$$B_v = B_e - \alpha(v+1/2) + \gamma(v+1/2)^2 \ldots \qquad (93)$$

(Ref 21:108).

Using these definitions, Eq (86) for g becomes:

$$g(v) = \int_{v_0}^{v} B(v')(G(v)-G(v'))^{\frac{1}{2}}\, dv' \qquad (94)$$

(Ref 24:2).

From the definitions in Eqs (22) and (62) for f and g the following expressions for inner and outer turning points may be obtained:

$$r = (f^2 + f/g)^{\frac{1}{2}} + f \qquad (95)$$

Solutions of the equations for f and g are discussed in the section on the RKR Program by C. R. Vidal.

This completes the theoretical background required for the RKR calculations. Second order semiclassical RKR formulations are not presented in this work. Several articles on the RKR method which were not referenced in this work are listed in Appendix C.

Methods for Extending RKR Curves

In many cases, because of the lack of experimental data, the constants necessary to construct an RKR curve may not be obtainable from straightforward least-square fits or their quality may be insufficient to construct accurate curves. Two techniques for improving existing constants which may, in turn, be used to produce improved RKR curves are presented here (Refs 10; 53).

As depicted in Fig II-1, the potential energy curve of a diatomic molecule should have a minimum at some intermediate distance, approach the dissociation limit for large internuclear separations and increase rapidly as the atoms approach each other. Ideally, curves generated using the RKR method should satisfy these criteria.

For many diatomic molecules, only two and, at most, three vibrational constants are available. The available rotational constants are even more limited. Attempts to generate curves based upon these constants using the RKR method can be expected to produce curves which do not meet the dissociation criteria or which do not exhibit an increasing potential for small internuclear distances. These results occur because the experimental data upon which the constants are based may represent only a fraction of the vibrational levels which exist between the bottom of the potential well and the dissociation limit.

To develop potential energy curves which obey the known constraints, Leroy and Burns have reported on a new technique which shows promising results. While they start with constants obtained from experimentally observed transitions, they then adjust these constants slightly until the new RKR potential energy curve is most consistent with all of the known constraints.

Leroy and Burns used their knowledge of the desired shape to adjust the constants. They worked with the G_v and B_v quantities as expressed in Eqs (87) and (91). Expressed in terms of these two quantities, their criteria for adjusting the molecular constants are:

1. $V(\alpha)$ assymptotically approaches the dissociation energy (De) and the difference between energy levels, $\Delta G_{v+\frac{1}{2}}$, becomes 0 for the same value of v. $\Delta G_{v+\frac{1}{2}}$ is defined as:

$$\Delta G_{v+\frac{1}{2}} = G(v + 1) - G(v) \tag{95}$$

2. The slope of the inner portion of the RKR curve must be negative. Hence:

$$dV(r)/dr < 0 \qquad (96)$$

3. The slope of the inner portion of the curve must become increasingly steeper; that is, the second derivative with respect to the internuclear separation must be positive:

$$d^2V(r)/dr^2 > 0 \qquad (97)$$

A study of Eq (88) reveals that as $\Delta G_{v+\frac{1}{2}}$ becomes smaller, the quantity f becomes larger. In turn, Eq (94) shows that f determines the width of the RKR curve. Examination of Eq (94) further reveals that the value g determines the center of the potential curve for a given energy level. In turn, Eq (93) shows that having determined the constants necessary to generate the $G(v)$´s, the other factor affecting the value of g is $B(v)$, a quantity whose value is determined by the rotational constants, Y_{ni}. From Eqs (88), (93), and (94), it follows that the width of the curve, as determined by the RKR method, and the value at which $\Delta G_{v+\frac{1}{2}} = 0$ depends only upon the vibrational constants which make up Gv. On the other hand, having selected suitable constants for Gv, the behavior of g, the rate at which the outer portion of the curve approaches D_e, and the behavior of the slope of the inner portion of the curve depends solely upon the constants which constitute B_v.

Following this logic, Leroy applied the criteria in 1 above first. If the constants obtained from experimental data do not satisfy this criteria, the value of the last experimental constant is adjusted or a value is selected for the next constant, Y_{n0}, in the series given by expression (8). The contribution from that constant, $Y_{n0}(v+1/2)^n$, is then subtracted from the $G(v)$ values calculated from the original experimentally based constants. A least-squares fit is then performed on the adjusted experimental data, $G\overset{*}{v}_j$:

$$G\overset{*}{v}_j = \sum_{i=1}^{n-1} Y_{i0}(v_j+1/2)^i - \left[Y_{n0}\ (v_j+1/2)^n\right] \qquad (98)$$

For a given Y_{n0} the experimental data fixes the values of the other constants. This new set of constants is tested to determine if Gv approaches a maximum value of D_e. Leroy and Burns say that if this value approaches D_e within $< 2\ \text{cm}^{-1}$ then the criteria in 1 is satisfied. If 1 is not satisfied, then a new trial value for Y_{n0} is chosen and the process repeated until 1 is satisfied.

At this point, a new RKR curve is generated using the new vibrational constants, Y_{i0}, and the experimental rotational constants, Y_{i1}. The curve is then evaluated according to criteria (2) and (3). If the inner portion of the curve diverges, the process followed for adjusting the constants for Gv is repeated for the constants making up Bv. The value for the last experimental constant is adjusted or a value for the next rotational constant in the

Y_{i1} series is selected. Then the B_v values given by the experimental constants are adjusted as follows:

$$B^{*}v_j = \sum_{i=0}^{n-1} Y_{i1}(v_j+1/2)^i - \left[Y_{n1}(v_j+1/2)^n\right] \qquad (99)$$

Then a least-squares fit is performed to obtain a new set of rotational constants Y_{01} through Y_{n1} . The new constants are then used to produce a new RKR curve. If the curve does not satisfy the criteria in 2 and 3, then the Y_{n1} constant is adjusted and the process repeated until 2 and 3 are satisfied.

In this manner, Leroy and Burns obtained a set of constants consistent with the experimental data and with criteria 1-3.

Tellinghuisen and Henderson describe a technique for constructing RKR based curves when experimental data does not permit the direct calculation of the rotation constants (Ref 20). Their technique is based upon a combination of the Morse and RKR potentials; hence, Morse-RKR curves.

As explained, vibrational constants provide all the information necessary to calculate f , Eq (88) and, thus, the width of the potential curve, 2f , as defined by Klein for a given vibrational energy level. Having established the width of a potential, the remaining piece of information required to construct a potential curve is the location of either the inner or outer branches of the potential curve, or the center of the potential well, i.e., g as obtained from the RKR calculations.

Tellinghuisen and Henderson point out that inner turning points on a potential curve might be approximated by the Morse potential (Ref 21:101).

$$U(r) = D_e \left(1 - e^{-\beta(r-r_e)}\right)^2 \tag{100}$$

where:

D_e = dissociation energy, cm^{-1}
r_e = equilibrium internuclear distance, A
$\beta = 0.12777\ w_e(\mu/D_e)^{\frac{1}{2}}$ (101)

where

w_e = the vibration frequency, cm^{-1}
μ = reduced mass, amu

Or because of the relation

$$D = w_e^2/4(w_e x_e) \tag{102}$$

β may be expressed as follows:

$$\beta = 0.243555\ (\mu w_e x_e)^{\frac{1}{2}} \tag{103}$$

Using these relations, Tellinghuisen investigated 25 different well-known potentials and found errors at the dissociation limit for the inner portion of the curve to be typically less than 0.02 Å and r_e to be in error by seldom more than 1%.

Further, Tellinghuisen states that a potential curve in error by Δr_{min} has identifical classical and almost identical quantum eigenvalues for $J = 0$. The wavefunctions derived from a shifted curve would be skewed with respect to a proper wavefunction.

If possible, Tellinghuisen recommends the construction of curves by formulas (102) and (103) using the experimental w_e and $w_e x_e$. If only w_e and D_e are known, then a value of D_e 40% larger than the experimental D_e should be used.

Tellinghuisen also speculates that α_e might be calculated using an expression derived by Pekeris from the Morse function:

$$\alpha_e = \frac{6B_e}{w_e}\left[\left(\frac{w_e x_e}{e}\right)^{\frac{1}{2}} - 1\right] \qquad (104)$$

(Ref 21:109). Tellinghuisen found that for 23 of the 25 cases he investigated, the α_e calculated per formula (104) had an average absolute error of 13% and an average signed error of 6%.

If one is seeking the rotational constant D_e (Y_{02}), the following relation might be used:

$$D_e = \frac{4B_e^2}{w_e^2} \qquad (104')$$

(Ref 21:10).

Tellinghuisen cautions against using Bv values made up of only two terms, i.e.,

$$Bv = B_e - \alpha\ (v+1/2) \tag{105}$$

because the Morse expression for Bv does not terminate with two terms as does Gv . Further, for high values of v , the Morse Bv will differ from the Morse-RKR Bv. The Morse-RKR Bv value must be determined by numerical methods.

Inverted Perturbation Analysis

Having constructed a semiclassical RKR curve, the next step is to determine if that curve is consistent with the Schroedinger wave equation; or, even better, to adjust the curve so it agrees with the SWE. This leads to the use of the inverted perturbation approach. The goal of the inverted perturbation approach (IPA) is to adjust the potential energy curve of rotationless molecules, $V_0(r)$, so that the quantum mechanical eigenvalues, E_{vJ} , obtained from a solution of the Schroendinger wave equation agree in a least-squares sense with the measured term values, $T(v,J)$.

The IPA technique was first demonstrated by Kosman and Hinze (Ref 23). Vidal and Scheingraber expanded the use of the IPA method. Vidal, in conjunction with several authors, has applied the IPA method to a number of molecules.

The Schroedinger wave equation (SWE) for a vibrating rotator (Eq (4)) is the basis of the IPA method. To develop the IPA method, the SWE can be expressed as follows (Ref 41):

$$(H_0^0 + H_{rot})\ \psi_{vJ}^0(r) = E_{vJ}^0 \psi_{vJ}^0(r) \qquad (106)$$

E_{vJ}^0 is the energy eigenvalue specified by the vibration and rotation quantum numbers. H_0 is the Hamiltonian of the non-rotating molecules and is made up of the terms:

$$H_0 = -\left(\frac{\hbar}{4\pi\mu c}\right)\frac{d}{dr^2} + V_0(r) \qquad (107)$$

where $V_0(r)$ is the potential energy of the rotationless molecule.

This formulation has been simplified by neglecting terms describing electronic coupling contributions (Ref 46).

The rotational motion of the molecule is described by:

$$H_{rot} = \left(\frac{\hbar}{4\pi\mu c}\right)\frac{J(J+1)}{r^2} \qquad (108)$$

In the inverted perturbation approach, one starts with an approximate potential $V_0(r)$, for example an RKR potential. Eq (106) is solved numerically for the zeroth order eigenvalues E_{vJ}^0 and the radial wavefunction $\psi_{vJ}^0(r)$. Then an energy correction ΔE_{vJ} is calculated according to the following formula:

$$\Delta E_{vJ} = E_{vJ} - E_{vJ}^0 \qquad (109)$$

where E_{vJ} is the measured term value as calculated from the spectroscopic constants and quantum numbers v and J . If the difference between the experimentally determined term values and the eigenvalues obtained from the SWE is sufficiently small, the calculation is stopped.

If the difference exceeds a specified limit, then one proceeds. As stated, the goal is to obtain some correction to $V_0^0(r)$, i.e., $\Delta V(r)$, such that the calculated and experimental E_{vJ}'s agree. Following this reasoning, then the true potential, $V_0(r)$, being sought may be expressed as a sum of the approximate potential and some delta potential:

$$V_0(r) = V_0^0(r) + \Delta V_0(r) \tag{110}$$

In turn, it follows that the true Hamiltonian differs from the approximate zero order Hamiltonian "$H_0^0 + H_{rot}$" by $\Delta V_0(r)$:

$$H_0 + H_{rot} = H_0^0 + H_{rot} + \Delta V_0(r) \tag{111}$$

First order perturbation theory gives the following relationship between the perturbation to the Hamilitonian $\Delta V_0(r)$ and and the energy change ΔE_{vJ} :

$$\Delta E_{vJ} = \left\langle \psi_{vJ}^0 \middle| \Delta V_0(r) \middle| \psi_{vJ}^0 \right\rangle \tag{112}$$

To obtain a correction to $V\ (r)$, a mathematical expression of the following form is assumed to represent $\Delta V_0(r)$:

$$\Delta V_0(r) = \sum_i c_i f_i(r) \tag{113}$$

The selection of the specific form of the function $f_i(r)$ is critical to the convergence and solution of the SWE. Discussion of the form of $f_i(r)$ will be postponed until the section describing Vidal's IPA program.

Using the $f_i(r)$ and the radial wavefunctions, ψ_{vJ}, obtained from the numerical solution of Eq (106), the expectation values for f(r) are calculated:

$$\left\langle \psi^0_{vJ} \middle| f_i(r) \middle| \psi^0_{vJ} \right\rangle \quad \begin{array}{l} v = 0,1,2,3... \\ J = 0,1,2,3... \end{array} \tag{114}$$

From Eqs (112) and (113), it follows that:

$$\Delta E_{vJ} = \sum_i c_i \left\langle \psi^0_{vJ} \middle| f_i(r) \middle| \psi^0_{vJ} \right\rangle \tag{115}$$

Having obtained ΔE_{vJ} from Eq (109), Eq (115) can be solved for the c_i coefficients. Using these coefficients in Eq (113), $\Delta V_0(r)$ may be calculated. From this, a new $V^0_0(r)$ is obtained.

$$v^0_0(r)(\text{new}) = V^0_0(r)\ (\text{old}) + \Delta V_0(r) \tag{116}$$

Then using the new $V^0_0(r)$, the calculation is repeated to obtain new energy eigenvalues. Again, the calculated E^0_{vJ} are compared with the experimental term values T(v,J) for agreement. If the agreement is not acceptable, the process is repeated.

Elaboration upon the specific numerical calculations to solve Eqs (106) through (116) is postponed until the discussion of Vidal's routine for performing the IPA calculations.

III Computer Programs

A computer program called DUNCON has been developed to generate spectroscopic constants. DUNCON is presented in Appendix A. The program generates the constants by separate least-squares fits and provides for the merging of the separate fits in a weighted manner as previously described. A description of the program, a listing with a sample fit and instruction on how to use it are contained in Appendix A.

A second program, provided by C. R. Vidal of the Max-Planck Institute for Exterrestriche Physik, West Germany, has provisions for the generation of potential energy curves by the Rydberg-Klein-Reese (RKR) method and adjustments of those curves by the inverted perturbation approach (IPA). The IPA routine adjusts the potential energy curve so it is consistent with the Shroendinger wave equation. A copy of the program with a sample problem, a description of the program, and instructions on using the program are included in Appendix B.

The DUNCON program and the RKR-IPA program may be used in a variety of combinations to generate constants and potential energy curves. Presented in Fig III-1 is a flow diagram describing the logic used in applying these programs in this work.

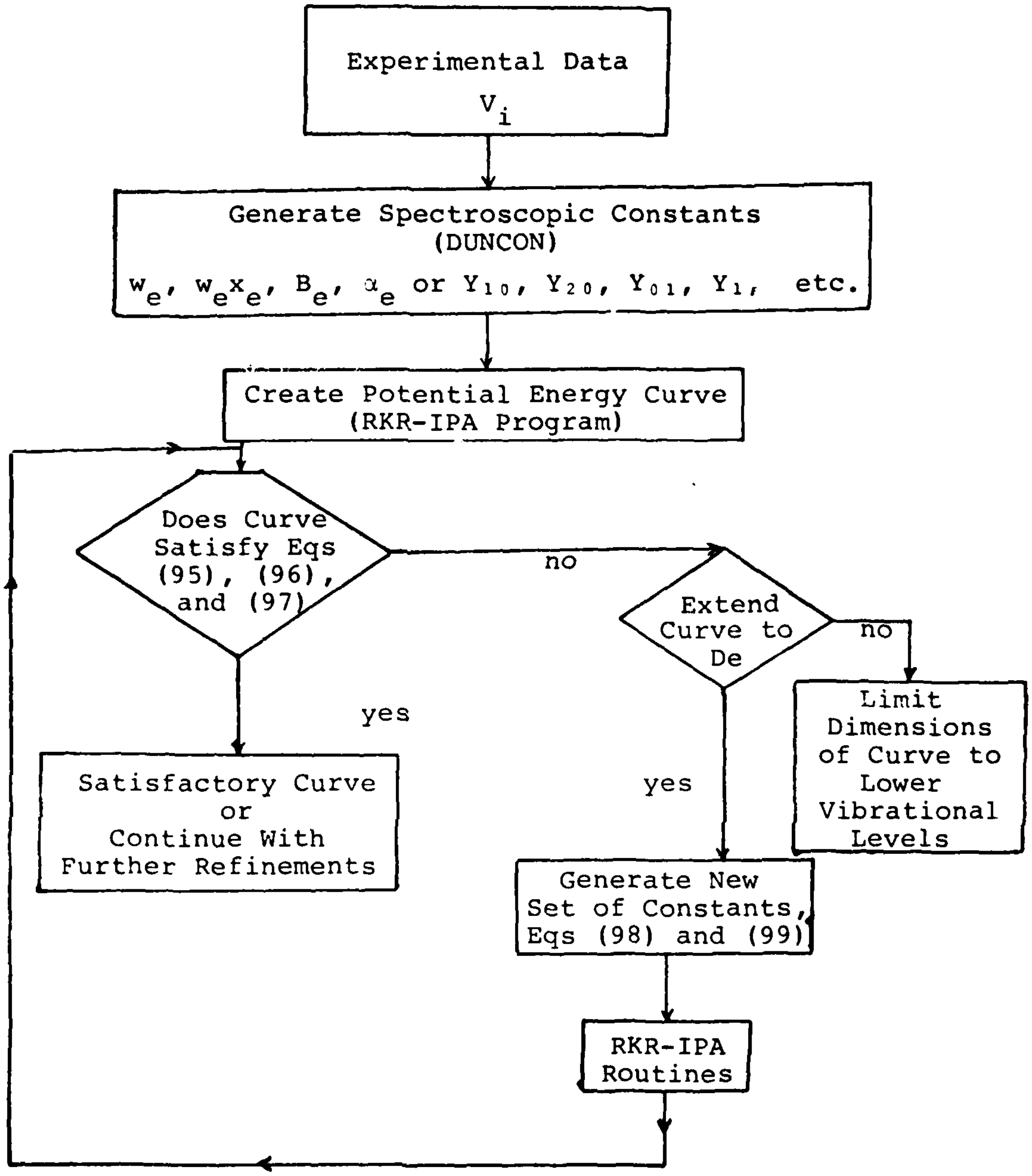

Fig III-1. Flow Diagram for Creation of Potential Energy Curves

DUNCON is used to generate spectroscopic constants by performing least-squares fits to the experimental data. These constants are then used as inputs to the RKR-IPA program. This program produces an RKR curve which is then adjusted by the IPA portion of the program.

Several options are available in the use of the RKR-IPA routines. The RKR routine can be used independently of the IPA routine. The range over which the curve is generated can be restricted to low vibrational energy levels or extended to the dissociation energy. If limited to small vibrational numbers initially, the RKR-IPA routine may be used iteratively to generate new constants and extend the curve to the dissociation limit.

In this paper, after initially generating an RKR-IPA curve, the curve is evaluated according to the criteria of Leroy and Burns, Eqs (95), (96), and (97). If a satisfactory curve is obtained, the calculation is complete. If not satisfactory, then the constants are adjusted as previously described. A modified version of the program DUNCON is used to perform the least-squares fit necessary to produce these constants. The constants are then again input into the RKR-IPA routine. The process is repeated until a satisfactory curve is obtained.

Programs demonstrating the use of DUNCON and the RKR-IPA programs are presented in Appendices A and B. Results of applying the program to the lead-oxide molecule are presented in the following chapter.

IV. Analysis of Spectroscopic Data for Lead-Oxide

This chapter contains the results of an analysis of spectroscopic data for lead-oxide (PbO). The program DUNCON was used to obtain spectroscopic constants for the X, a, b, A, B, and D electronic states of PbO. Constants from published literature were used to generate potential energy curves using the IPA-RKR routine. The potential energy curve for the ground state of lead-oxide was extended almost to the dissociation limit using the extension techniques and the RKR-IPA routine.

The experimental data of three investigations was reduced using DUNCON to yield spectroscopic constants. The data from these investigations is presented in Table IV-5. Two of the investigators, Glessner and Synder (Refs 19; 42), obtained least-squares fits, but did not have the computer routines necessary to generate error estimates and merge the data in a weighted-correlated manner. Their data is reduced, error estimates obtained, and merged using DUNCON. Lead-oxide data produced by Linton and Broida (Ref 33) is reduced using DUNCON and the A-X and a-X data is merged. Also, the results of all three investigations is merged using DUNCON. The results of reducing the data of each investigator for each transition separately is presented in Table IV-1. This data is then merged in several combinations. The constants resulting from these mergings are presented in Table IV-2. Presented in Table IV-3 are the unmerged and merged estimates for the D-X transitions. The D-X data is merged with other data in a separate fit to prevent its large variance from degrading the constants for the other transitions. Finally, the merged results of Glessner and Snyder's data, are compared in Table IV-4 with the best previous published values available.

The constants presented in columns I and II of Table IV-1 are not identical to those reported by the original investigators. When transforming their experimental data from angstroms to wavenumbers, they did not make corrections for the index of refraction of air as previously discussed. The constants listed in column III of Table IV-1 are also different from the values reported by Linton and Broida. For the A-X transition, they listed only their new band head data. They used data of other researchers to generate their constants. Their published constants are included in Table IV-4. The constants for the a-X transition of column III, Table IV-2 are also slightly different from those reported by Linton and Broida. Presumably, the slight difference arises from the difference in weighting schemes used in this report and that used by Linton and Broida.

TABLE IV-1

Constants from Separate Least-Squares Fits for Each Electronic Transition (cm^{-1})

Electronic Transition	Constant	Source of Experimental Data		
		I Glessner	II Snyder	III Linton and Broida
		[10.03]	[9.875]	[6.310]
a-x	Te	16021.54(2.81)	16021.68(2.59)	16023.12(1.38)
	We'	482.93(1.26)	484.51(1.09)	481.831(0.438)
	We'Xe	2.814(0.170)	2.970(0.146)	2.4590(0.0432)
	We"	719.36(2.19)	722.785(0.961)	720.166(0.469)
	We"Xe"	3.067(0.455)	3.712(0.105)	3.4600(0.0462)
		[2.035]		
b-x	Te	16336.43(6.08)[2]		
	We"	428.98(1.46)		
	We'Xe	-0.944(0.114)		
	We"	722.00(1.92)		
	WeXe	3.554(0.193)		
		[41.70]	[33.07]	[4.817]
A-X	Te	19846.0(25.8)	19858.52(6.88)	19864.79(2.38)
	We'	453.5(18.5)	446.30(4.92)	443.31(1.12)

TABLE IV-1--Continued

Electronic Transition	Constant	Source of Experimental Data		
		I Glessner	II Snyder	III Linton and Broida
	We'Xe'	2.04(2.74)	0.479(0.8632)	0.443(0.146)
	We"	715.7(11.3)	724.69(2.93)	720.933(0.374)
	We"Xe"	2.80(1.58)	4.012(0.390)	3.5334(0.0239)
		[52.02]	[64.63]	
B-X	Te	22290.9(10.3)	22286.22(9.06)	
	We'	495.70(4.34)	483.00(8.13)	
	We'Xe'	2.22(1.39)	-1.07(1.71)	
	We"	731.52(6.99)	721.11(3.85)	
	We"Xe"	5.06(1.11)	3.532(0.477)	

[1] The quantities in brackets are the variances of the least-squares fits (Eq (14)). Errors reported in parenthesis re one standard deviation. Column I contains least-squares fit to data produced by Glessner (Ref 19). Column II constants are based upon data produced by Snyder (Ref 42). Column III constants are the results of performing least-squares to data published by Linton and Broida (Ref 33).

[2] The constants for b-x were obtained by combining the data observed by Glessner and Synder.

TABLE IV-2

Merged PbO Constants (cm-1)[1]

Electronic State	Constant	Source of Experimental Data		
		I Merging of Glessner and Snyder Data	II Merging of Linton and Broida Data	III Merging of Glessner, Snyder, Linton, and Broida Data
a	Te	16021.51(1.69)	16024.06(1.16)	16023.16(1.80)
	We'	484.239(0.808)	481.800(0.439)	481.488(0.769)
	We'Xe'	2.949(0.109)	2.4595(0.0434)	2.4339(0.0818)
b	Te	16335.44(2.89)		16331.83(4.77)
	We'	428.43(1.21)		428.34(2.27)
	We'Xe	-0.99552(0.0983)		-1.014(0.186)
A	Te	19856.22(3.31)	19864.11(2.14)	19860.04(3.13)
	We'	447.88(3.50)	443.39(1.12)	445.32(1.83)
	We'Xe'	1.013(0.6007)	0.446(0.145)	0.655(0.249)
B	Te	22282.80(3.67)		22280.52(7.08)
	We'	489.50(2.63)		489.79(5.25)
	We'Xe'	0.149(0.363)		0.225(0.720)
X	We"	721.905(0.620)	720.736(0.244)	720.890(0.395)
	We"Xe"	3.5900(0.0683)	3.5201(0.0171)	3.5316(0.0292)

TABLE IV-2--Continued

Electronic State	Constant	Source of Experimental Data		
		I Merging of Glessner and Snyder Data	II Merging of Linton and Broida Data	III Merging of Glessner, Snyder, Linton, and Broida Data
Variance of Fit		1.0248	1.008	4.076

[1] Column I is the result of merging with DUNCON the separate fits in Columns I and II of Table IV-1.

Column II is the result of merging the separate fits in Column III of Table IV-1.

Column III is the result of merging all separate fits in Table IV-1 with DUNCON.

Errors reported in parenthesis are one standard error.

TABLE IV-3

Spectroscopic Constants for D-X Transition of PbO (cm^{-1})

Electronic State	Constant	Unmerged	Merged
		[322.3]	[4.19]
D	Te	29897.8(67.4)	30115.8(46.1)
	We'	490.0(30.8)	542.2(54.9)
	We'Xe'	-16.53(7.72)	-1.99(13.1)
X	We"	606.1(33.3)	720.989(0.401)
	We"Xe"	-8.32(3.53)	3.5312(0.0296)

Errors Reported in Parenthesis are One Standard Error

TABLE IV-4

Final Spectroscopic Constants for PbO[3]

Merged Constants	State	Te (cm^{-1})	We (cm^{-1})	WeXe (cm^{-1})
This Study (Glessner and Snyder, Refs (19) and (42)	D	30115.8(46.1)	542.2(54.9)	-1.99(13.1)
	B	22282.80(3.67)	489.50(2.63)	0.149(0.363)
	AO+	19856.22(3.31)	447.88(3.50)	1.013(0.6007)
	[2]b	16335.44(2.89)	428.43(1.21)	-0.99552(0.0983)
	a	16021.51(1.69)	484.239(0.808)	2.949(0.109)
	x		721.905(0.620)	3.5900(0.0683)
Linton and Broida, Ref (33)	AO+	19862.6(1.5)	444.3(0.8)	0.54(0.12)
	a1	16024.9(1.45)	481.5(0.7)	2.45(0.07)
	XO+		720.97(0.36)	3.536(0.025)
Bloomenthal, Ref (8)	D	30197.0	530.6	1.05
	B	22289.8	496.3	2.33
	X		722.3	3.73
Oldenborg, Dickensen and Zare, (Ref 36)	b	16379±430[1]		

[1] This value is based upon estimate by Oldenborg, Dickensen and Zare that the b state is 350±430 cm^{-1} above the a state.

[2] Based upon six data points marked with asterisk in Table IV-7.

[3] Errors reported in parenthesis are one standard deviation.

TABLE IV-5

Lead-Oxide Spectral Lines Assigned to the D-X, B-X, A-X and a-X Transitions

Energy(cm^{-1})			Assignments	
Observed	Calculated	Obs-Calc	v',v"	Transition
Investigator: Snyder (Ref (42))				
28589.0	28607.2	-18.2	0,2	D-X
28432.8	28453.7	-20.9	1,3	D-X
27648.9	27625.7	23.2	2,5	D
27534.6	27501.3	33.3	3,6	D
27076.0	27075.5	00.5	1,5	D
26788.7	26829.9	-41.2	3,7	D
26555.3	26529.3	26.0	0,5	D
26394.0	26387.0	-3.0	1,6	D
24122.4	24120.5	1.9	4,0	B
23630.9	23632.5	-1.6	3,0	B
23146.1	23144.0	2.1	2,0	B
22640.3	22655.1	-14.8	1,0	B
22175.3	22165.8	9.5	0,0	B
21450.0	21452.0	2.0	0,1	B
20749.4	20745.2	4.2	0,2	B
20055.5	20045.5	10.0	0,3	B
19646.0	19645.5	0.5	2,5	B
19346.0	19352.9	-6.9	0,4	B
18772.8	18784.0	-11.2	3,7	B
17802.4	17806.7	-4.3	1,7	B
17631.6	17631.2	0.4	2,8	B
21054.4	21051.1	3.3	3,0	A
20166.0	20167.0	1.0	1,0	A
19811.0	19809.6	1.4	5,3	A

TABLE IV-5--Continued

Energy(cm-1)			Assignments	
Observed	Calculated	Obs-Calc	v',v"	Transition
19719.7	19723.0	-3.3	0,0	A
19456.0	19453.2	2.8	1,1	A
18996.1	19009.1	-3.0	0,1	A
18741.8	18746.4	-4.6	1,2	A
18293.3	18302.4	-9.1	0,2	A
17593.4	17602.7	-9.3	0,3	A
17338.3	17354.1	-15.7	1,4	A
16905.6	16910.0	-4.4	0,4	A
16224.6	16224.5	0.1	0,5	A
15315.4	15318.5	-3.1	1,7	A
19127.0	19137.9	-10.9	7,0	a
18679.9	18690.4	-10.5	6,0	a
18244.2	18238.2	6.0	5,0	a
17972.0	17976.6	4.6	6,1	a
17778.6	17781.0	-2.4	4,0	a
17520.3	17524.3	4.0	5,1	a
17320.6	17319.0	0.4	3,0	a
17064.6	17067.2	-2.6	4,1	a
16855.4	16852.1	3.3	2,0	a
16601.3	16605.2	-3.9	3,1	a
16384.7	16380.4	4.3	1,0	a
16135.6	16138.3	-2.7	2,1	a
15896.7	15898.4	-1.7	3,2	a
15662.6	15666.5	-3.9	1,1	a
15657.9	11650.4	7.5	4,3	a
15431.5	15431.5	0.0	2,2	a
15187.9	15189.9	-2.0	0,1	a
14958.6	14959.8	-1.2	1,2	a

TABLE IV-5--Continued

Energy(cm^{-1})			Assignments	
Observed	Calculated	Obs-Calc	v',v"	Transition
14732.2	14731.8	0.4	2,3	a
14481.2	14483.1	-1.9	0,2	a
14260.0	14260.1	-0.1	1,3	a
13782.7	13783.4	-0.7	0,3	a
13561.7	13567.4	-5.7	1,4	a
13353.6	13353.6	0.0	2,5	a
13083.0	13090.8	-7.8	0,4	a
12932.2	12932.5	-0.3	4,7	a
12874.0	12881.9	-7.9	1,5	a
12473.5	12470.5	3.0	3,7	a
12399.9	12405.2	-5.3	0,5	a
12266.0	12268.2	-2.2	4,8	a
12199.5	12203.3	-4.3	1,6	a
12065.8	12068.0	-2.2	5,9	a
11801.3	11806.1	-4.8	3,8	a
Investigator: Glessner (Ref (19))				
23629.2	23632.5	-3.3	3,0	B
23162.7	23144.0	18.7	2,0	B
22661.3	22655.1	6.2	1,0	B
21444.6	21452.0	-7.4	0,1	B
20745.1	20745.2	0.1	0,2	B
20042.7	20045.5	-2.8	0,3	B
19840.6	19842.2	-1.6	1,4	B
19453.7	19455.5	-1.8	3,6	B
18928.1	18924.9	3.2	6,9	B
18759.8	18761.3	-1.5	7,10	B

TABLE IV-5--Continued

Energy(cm^{-1})			Assignments	
Observed	Calculated	Obs-Calc	v',v"	Transition
21921.0	21929.9	-8.9	5,0	A
20163.9	20167.0	-3.1	1,0	A
19004.8	19009.1	-4.3	0,1	A
18299.6	18302.4	-2.8	0,2	A
17609.8	17602.7	7.1	0,3	A
16906.1	16910.0	-3.9	0,4	A
16219.6	16244.5	-25.0	0,5	A
15980.3	15990.0	-9.7	1,6	A
15762.6	15761.2	1.4	2,7	A
19127.7	19137.9	-10.2	7,0	a
18682.3	18690.4	-8.1	6,0	a
18237.9	18238.2	-0.3	5,0	a
17783.0	17781.0	2.0	4,0	a
17513.3	17524.3	-11.0	5,1	a
17316.7	17319.0	-2.3	3,0	a
17064.3	17067.2	-2.9	4,1	a
16852.8	16852.1	0.7	2,0	a
16603.2	16605.2	-2.0	3,1	a
16382.0	16380.4	1.6	1,0	a
16135.8	16138.3	-2.5	2,1	a
15898.0	15903.7	-5.7	0,0*	a
15668.5	15666.5	2.0	1,1	a
15433.4	15431.5	1.9	2,2	a
15193.0	15189.9	3.1	0,1	a
14963.5	14959.8	3.7	1,2	a
14732.4	14731.8	0.6	2,3	a
14483.8	14483.1	0.7	0,2	a
14261.4	14260.1	1.3	1,3	a

TABLE IV-5--Continued

Energy(cm-1)			Assignments	
Observed	Calculated	Obs-Calc	v',v"	Transition
13781.7	13783.4	-1.7	0,3	a
13564.1	13567.4	-3.3	1,4	a
13085.4	13090.8	-5.4	0,4	a
Investigator: Linton & Broida (Ref (33))				
22364	22367.4	-3.4	6,0	A
21930	21929.9	0.1	5,0	A
21654	21653.6	0.4	6,1	A
21494	21491.2	2.8	4,0	A
21221	21216.1	4.9	5,1	A
20949	20946.8	2.2	6,2	A
20777	20777.3	-0.3	4,1	A
20245	20247.1	-2.1	6,3	A
20069	20070.6	1.6	4,2	A
20168	20167.0	1.0	1,0	A
19366	19370.9	-4.9	4,3	A
19117	19117.0	0.0	5,4	A
18679	18678.2	0.8	4,4	A
17994	17992.7	1.3	4,5	A
17083	17081.5	1.5	5,7	A
14483	14880.9	2.1	3,9	A
14440	14439.5	0.5	2,9	A
14229	14230.7	-1.7	3,10	A
14217	14210.1	6.9	0,8	A
13998	13996.8	1.2	1,9	A
13789	13789.3	-0.3	2,10	A
13585	13587.5	-2.5	3,11	A
13390	13391.4	-1.4	4,12	A

TABLE IV-5--<u>Continued</u>

Energy (cm^{-1})			Assignments	
Observed	Calculated	Obs-Calc	v',v"	Transition
13201	13201.1	-0.1	5,13	A
13347	13346.6	0.4	1,10	A
13146	13146.1	-0.1	2,11	A
12951	12951.3	-0.3	3,12	A
12761	12762.3	-1.3	4,13	A
12580	15279.1	0.9	5,14	A
12511	12509.9	1.1	2,12	A
12323	12322.3	0.7	3,13	A
12141	12140.3	0.7	4,14	A
11964	11964.2	-0.2	5,15	A
20448	20450.9	-2.9	10,0	a
20022	20018.1	3.9	9,0	a
19582	19580.4	1.6	8,0	a
19307	19304.2	2.8	9,1	a
19139	19137.9	1.1	7,0	a
18877	18866.6	10.4	8,1	a
18691	18690.4	0.6	6,0	a
18597	18597.5	0.5	9,2	a
18431	18424.0	7.0	7,1	a
18236	18238.2	-2.2	5,0	a
18160	18159.8	0.2	8,2	a
17977	17976.6	0.4	6,1	a
17782	17781.0	1.0	4,0	a
17526	17524.3	1.7	5,1	a
17317	17319.0	-2.0	3,0	a
17272	17269.8	2.2	6,2	a
17067	17067.2	-0.2	4,1	a
16854	16852.1	1.9	2,0	a

TABLE IV-5--Continued

Energy(cm^{-1})			Assignments	
Observed	Calculated	Obs-Calc	v',v"	Transition
16819	16817.6	1.4	5,2	a
16609	16605.2	3.8	3,1	a
16386	16380.4	5.6	1,0	a
16361	16360.4	0.6	4,2	a
16140	16138.3	1.7	2,1	a
16117	16117.9	0.9	5,3	a
15902	15898.4	3.6	3,2	a
15668	15666.5	1.5	1,1	a
15662	15660.7	1.3	4,3	a
15434	15431.5	2.5	2,2	a
15423	15425.2	-2.2	5,4	a
15191	15189.9	1.1	0,1	a
14961	14959.8	1.2	1,2	a
14734	14731.8	2.2	2,3	a
14510	14506.1	3.9	3,4	a
14485	14483.1	1.9	0,2	a
14286	14282.5	3.5	4,5	a
14261	14260.1	0.9	1,3	a
14071	14061.1	9.9	5,6	a
13828	13820.5	7.5	3,5	a
13784	13783.4	0.6	0,3	a
13569	13567.4	1.6	1,4	a
13355	13353.6	1.4	2,5	a
13146	13142	5.2	3.6	a
13092	13090.9	1.1	0,4	a
12884	12881.9	2.1	1,5	a
12667	12675.1	1.9	2,6	a
12407	12405.2	1.8	0,5	a

TABLE IV-5--Continued

Energy(cm^{-1})			Assignments	
Observed	Calculated	Obs-Calc	v',v"	Transition
12006	12003.6	2.4	2,7	a
11807	11806.1	0.9	3,8	a
11728	11726.7	1.3	0,6	a
11534	11531.9	2.1	1,7	a
11341	11339.3	1.7	2,8	a
11149	11148.8	0.2	3,9	a
11057	11055.3	1.7	0,7	a
10869	10867.5	1.5	1,8	a
10498	10498.6	-0.6	3,10	a
10391	10390.9	0.1	0,8	a
10212	10210.2	1.8	1,9	a

*Later reassigned as the "(3,2) a-X" transition.

Examination of Table IV-1 reveals values of w_e for the X-state ranging from 715.7 to 731.5 cm^{-1}. DUNCON permits the merging of the data listed in Table IV-1 in a weighted-correlated least-squares fashion.

The results of the merging are presented in Table IV-2. Error limits for w_e of the X-state are reduced from a maximum standard error of ± 11.3 cm^{-1} to ± 0.620 cm^{-1} when the data in columns I and II of Table IV-1 are merged. The results are presented in column I, Table IV-2.

Column II, Table IV-2 contains the smallest error estimate for the constants of the a-, A-, and X-electronic states. The variances for the merged fits of columns I and II are similar, 1.0248 and 1.008, respectively. But when the data in columns I and II are merged to yield column III, Table IV-2, the estimated variance of the fit and, in many cases, the standard errors of the individual constants increase. Examination of (columns I and II) the a- and X-states reveals term electronic energies, T_e , with error limits of comparable magnitude which do not overlap. Because of this, when merged, the error limits reflect the equal weighting of the "almost significant" differences and, hence, the increased error limit reflects a bias in one or both of the data sets.

Column III of Table IV-2 reflects the most conservative error estimate of the three columns in Table IV-2. It is also based upon the largest quantity of data.

In reporting constants, a researcher may be tempted to manipulate the constants of the ground state and report the constants obtained from the least-squares fits for the upper state. For example, if a routine for merging fits is not available, one might average the constants for the ground state or obtain a weighted average based upon the error estimates. The temptation then is to report the averaged ground state constants and the upper state constants obtained from the original least-squares fits. Reporting constants in this fashion is undesirable for two reasons. First, the constants reported in this manner will not faithfully reproduce the experimentally observed data. Second, a better estimate of the ground state has been obtained. This new estimate of the ground state constants should, in turn, be used to ascertain how well the upper state constants are known. This can be done by removing (adding) the energy contributions of the ground state from the experimental data and performing a least-squares fit to obtain the upper state constants. These new upper state constants and the average ground state constants should provide an accurate reproduction of the experimental data and an accurate set of constants for the generation of potential energy curves. The approach just described is not necessary if a routine such as DUNCON is available for merging data. Even though it is available, the use of DUNCON to form a merged fit may not be desirable if large quantities of data are involved and the ground state constant has already been well defined.

Often the data merged from different investigators may contain different experimental values for the same assignment (v',v"). If after using DUNCON to obtain the best estimate of the constants, one of the experimental values agrees with the fit and the other does not, then one might remove the poorer data point and perform the fit again. This approach should be used with caution.

Presented in Table IV-4 are the constants obtained by merging the experimental data of Glessner and Snyder. Presented for comparison are results published by other researchers.

The data used to produce the constants of Tables IV-1 and IV-2 is presented in Table IV-5. The calculated values of Table IV-5 were obtained using the constants of column III, Table IV-2 and Table IV-3 for the D state.

The D-state constants were obtained in a separate merged fit from that used to obtain the other constants because of their large error. The values reported by Bloomenthal (Ref 8) produced a better fit for his data; hence, his constants are the preferred constants.

The B-state constants reported by Bloomenthal provide a better fit to his data than the constants reported here fit the B data listed in Table IV-5. This statement must be modified slightly. Bloomenthal did not provide "observed-calculated" values for all the data he listed. Hence, these values may not have been included in his estimate of the constants.

The A-state constants reported in Table IV-4 provide a reasonable agreement with those reported by Linton and Broida (Ref 33). The reported constants are based upon the merging of data reported by Glessner and Snyder.

The small a-state constants reported in Table IV-4 rival those reported by Linton and Broida in accuracy. Table IV-2 shows that the merged data of Glessner and Snyder produces constants with error limits of magnitude comparable to that reported by Linton and Broida.

The ground state (x) constants reported in Table IV-4 agree well with those reported by Linton and Broida. The merging of Glessner's and Snyder's data resulted in constants for the X-state with significantly smaller errors than those obtained in separate fits of their data.

The discussion of the b-state data was reserved until last, because they were obtained by making reassignments of many transitions that were published in previous works.

The b-state constants listed in Table IV-1, column I are based upon the six assignments marked by asterisks in Table IV-7. The assignments were made by Glessner and Snyder (Refs 19; 42) based upon the works of Kurylo, et.al. (Ref 31). The variance of the constants in Table IV-2 is remarkably small considering that only six data points with five constants were used yielding a degree of freedom of one. A review of Kurylo's tentative assignments and tentative assignments made by Oldenborg, Dickson, and Zare (Ref 36) show a much greater difference between the observed and calculated values than would be expected from the constants of Table IV-1.

Using the b-state constants of Table IV-1, new assignments were made for the experimental data which had been marked as belonging to the b-X transition by Kurylo and Oldenborg. It was possible to make new assignments for 29 of 34 observed values which had been reported as belonging to the b-state. Twenty-six of those were used in a least-squares fit to generate new b-state constants. DUNCON was used to perform separate least-squares fits to the data of Snyder and Glessner, and to the data of Kurylo and Oldenborg. Then DUNCON was used to merge the results of these fits. A copy of the program with the results is presented in Appendix A.

The resulting b-state and X-state constants are presented in Table IV-6. The 26 assignments used to obtain the constants are listed in Table IV-7. The "observed-calculated" values are presented for comparison with those of the original investigators. For the 26 values used in the new fit, a standard error of +10.5 cm was obtained. For the 15 values which the investigators reported "observed-calculated" values, their standard error was +47.4 cm. It should be noted

TABLE IV-6

Spectroscopic Constants for b-X
Transition for Lead Oxide

State	Te	We	WeXe
b	16325.1(11.2)	430.99(2.47)	-0.757(0.165)
X		721.41(4.35)	3.700(0.441)

that this error was due to uncertainties in the assignments and not the quality of the data.

The second part of Table IV-7 contains those values which were published as b-X transitions for which no assignments had been made at the time the fit was performed. After the new constants were calculated, assignments were made for three more b-X transitions.

The new assignments presented in this paper were made without access to the raw spectral data and, hence, information concerning the relative intensities of each transition. It is also probable that some of the assignments of the transitions to the b-state are incorrect. For example, the last value of Table IV-7, an experimentally observed value of 15672 cm^{-1} was assigned as a b-X transition. This value corresponds closely with the value of 15662 cm^{-1} observed by Linton and Broida and assigned to the a-X transition series.

TABLE IV-7
Lead-Oxide Spectrum for the b-X Transition

This Work				Original Investigator	
Assignment	Observed (cm^{-1})	Calculated (cm^{-1})	Obs-Calc	Assignments	Obs-Calc
(14,1)	21643	21659.8	-16.8	$(12,0)^{O}$	
	21636			$(12,0)^{K}$	-24
(13,1)	21200	21207.6	- 7.7	$(11,0)^{O}$	
(10,1)*	19869.8	19860.2	9.6	$(10,1)^{G}$	4
(7,1)	18515	18526.3	-11.3	$(5,0)^{K}$	-15
(3,0)	17488.4	17483.1	5.3	$(3,0)^{S}$	- 5.5
(4,1)	17212	17206.1	5.9	$(2,0)^{K}$	13
(7,3)	17108	17120.5	-12.5	$(8,4)^{K}$	56
(2,0)	17033	17047.5	-14.5	$(5,2)^{K}$	-75
(5,2)	16915	16938.0	-23.0	$(1,0)^{K}$	-62
(3,1)	16773	16769.0	4.0	$(1,0)^{K}$	16
(1,0)	16614	16613.5	- 0.5	$(4,2)^{K}$	50
(4.2)	16488	16499.5	-11.5	$(2,1)^{K}$	3
(7,4)	16434	16428.7	5.3	$(10,5)^{K}$	67
(17,11)	16297	16292.4	4.6	$(0,0)^{K}$	-18
(14,9)	16215	16214.1	0.9	$(3,2)^{K}$	- 5
(3,2)*	16066.8	16062.4	4.4	$(3,2)^{S}$	- 5.7

TABLE IV-7--Continued

This Work				Original Investigator	
Assignment	Observed (cm^{-1})	Calculated (cm^{-1})	Obs-Calc	Assignments	Obs-Calc
(13,9)	15773	15762.0	11.0	$(2,2)^K$	- 5
(2,2)	15623	15627.0	- 4.0	$(0,1)^K$	22
(3,3)	15363	15363.2	- 0.2	$(1,2)^K$	28
(9,7)*	15281.9	15285.4	- 3.5	$(9,7)^S$	- 6.1
(3,4)	14687.8	14671.4	15.6	$(3,4)^S$	8.4
(8,8)	14180.1	14178.5	1.6	$(8,8)^S$	- 2.2
(0.4)	13367.30	13369.4	- 2.1	$(0,4)^S$	10.5
(1,5)*	13117.5	13117.4	0.1	$(1,5)^S$	5.9
(1,6)*	12440.1	12440.4	- 0.3	$(1,6)^S$	- 7.4
(3,8)*	11968.9	11978.2	- 9.3	$(3,8)^S$	- 8.9
	20786			$(10,0)^O$	
	20354			$(9,0)^O$	
	19923			$(8,0)^O$	
(19,5)	21169	21161.4	7.6	$(11,0)^K$	58
	20338			$(9,0)^K$	24
	19904			$(8,0)^K$	37

TABLE IV-7--Continued

This Work				Original Investigator	
Assignment	Observed(cm^{-1})	Calculated (cm^{-1})	Obs-Calc	Assignments	Obs-Calc
(18,12)	16108	16618	-10	$(6,4)^{K}$	-52
(17,12)	15672	15660	12	$(5,4)^{K}$	-43
	or				
	15662			$a(4,3)^{L\&B}$	

*These are the six transitions used to obtain the b-state constants of Table IV-1, column I.

O - Oldenborg (Ref 36)
S - Snyder (Ref 42)
G - Glessner (Ref 19)
K - Kurylo (Ref 31)
L&B - Linton and Broida (Ref 33)

This concludes the discussion of program DUNCON and the results of its application to lead-oxide. Only a small portion of the PbO data available was used in the present analysis. Rotational data, if used, should increase the quality of the constants. A more extensive evaluation of the literature data with the selective discarding of "erroneous" data points should yield better constants.

Lead-Oxide RKR-IPA Curves

To demonstrate the use of the RKR-IPA program, the X-, a-, and A-states were selected for evaluation. Curves were drawn for the X-, a-, and A-states using the results of the RKR routine alone or using the combined RKR and IPA routine (RKR-IPA curve). The resulting potential energy curves are presented in Fig. IV-1 for the X-, A-, and the a-states. For the A-state, the curve presented in Fig. IV-1 is an RKR curve, while for the X- and a-states, they are RKR-IPA curves. The RKR and IPA results are presented for the X- and a-states in Tables IV-8 and IV-9, respectively. The RKR data for the A-state is presented in Table IV-10. The constants used to generate these curves for each state is presented in Table IV-11.

The ultimate use of a potential should be to predict what transitions should occur. A sophisticated analysis would involve the calculation of Franck-Condon factors from the wave functions resulting from the solution of the Schroedinger wave

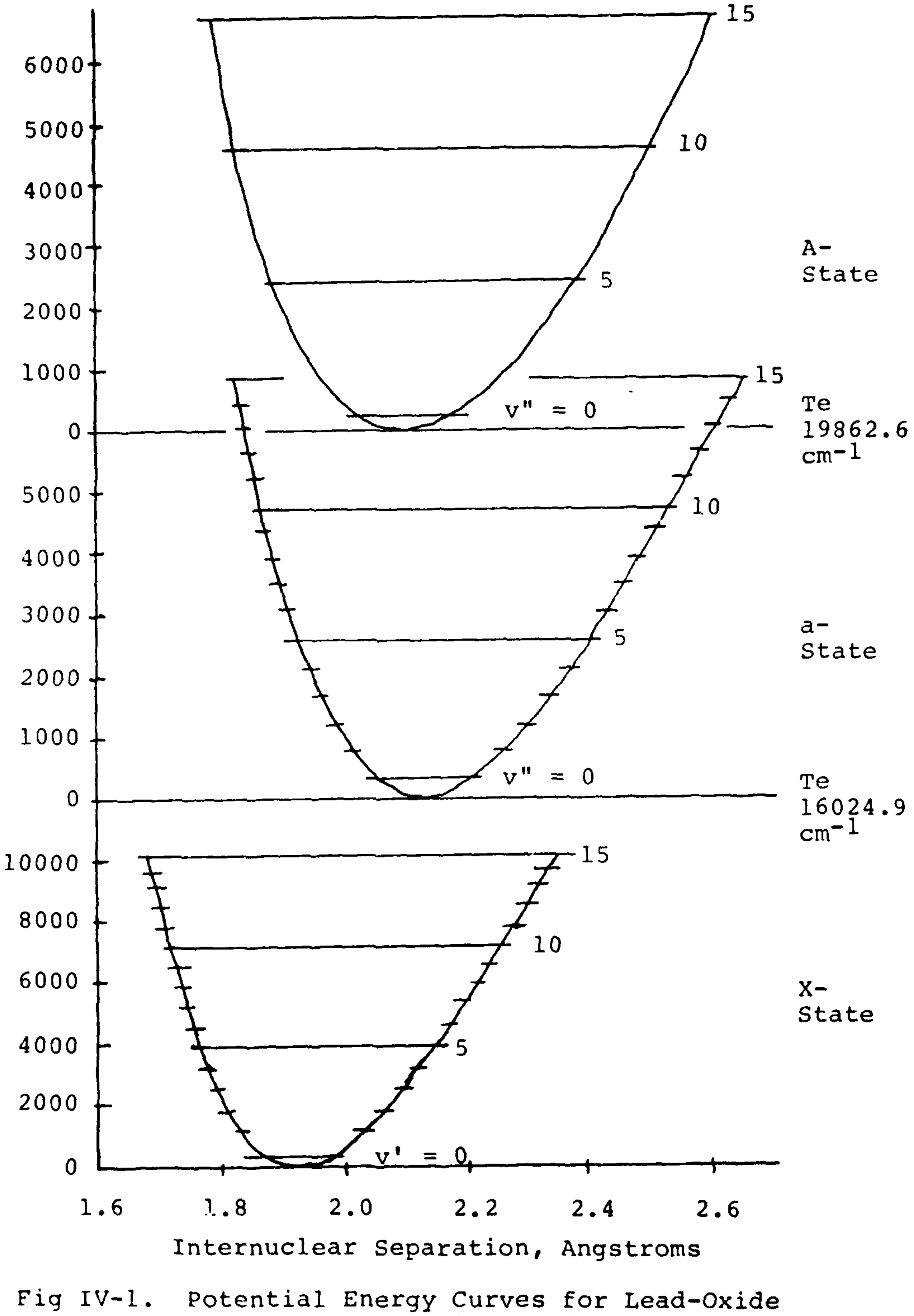

Fig IV-1. Potential Energy Curves for Lead-Oxide X, a, and A Electronic States

TABLE IV-8

RKR and IPA Potential for Ground State of Lead-Oxide

RKR				IPA			
V	Gv(cm^{-1})	R-(Å)	R+(Å)	Gv(cm^{-1})	R-(Å)	R+(Å)	Bv(cm^{-1})X100
-½		1.921					
0	359.62	1.868	1.980	359.918	1.867	1.979	30.687
1	1073.52	1.832	2.027	1073.901	1.831	2.027	30.469
2	1780.34	1.809	2.062	1780.716	1.808	2.062	30.256
3	2480.10	1.790	2.092	2480.445	1.791	2.092	30.048
4	3172.78	1.775	2.118	3173.120	1.776	2.119	29.844
5	3858.39	1.762	2.143	3858.743	1.763	2.144	29.645
6	4536.93	1.751	2.167	4537.299	1.752	2.168	29.452
7	5208.40	1.740	2.189	5208.773	1.741	2.190	29.264
8	5872.79	1.731	2.211	5873.161	1.732	2.212	29.082
9	6530.11	1.722	2.231	6530.471	1.723	2.236	28.905
10	7180.36	1.714	2.251	7180.713	1.715	2.253	28.731
11	7823.54	1.706	2.271	7823.891	1.707	2.273	28.557
12	8259.65	1.699	2.291	8459.997	1.700	2.292	28.378
13	9088.68	1.693	2.311	9089.028	1.693	2.311	28.192
14	9710.64	1.686	2.330	9711.015	1.686	2.330	27.998
15	10325.53	1.680	2.349	10326.059	1.680	2.349	27.796
$Y_{00} = 0.0233501$				$Y_{00} = 0.37952$			

TABLE IV-9

RKR and IPA Potential for the a-State of Lead-Oxide

	RKR			IPA			
V	Gv(cm^{-1})	R-(Å)	R+(Å)	Gv(cm^{-1})	R-(Å)	R+(Å)	Bv(cm^{-1})X100
-½		2.122					
0	240.13	2.075	2.172	240.23	2.054	2.192	25.163
1				716.87	2.011	2.250	24.988
2				1188.55	1.982	2.293	24.822
3				1655.34	1.960	2.329	24.658
4				2117.24	1.942	2.363	24.495
5	2574.13	1.928	2.394	2574.24	1.925	2.392	24.328
6				3026.34	1.911	2.421	24.157
7				3473.56	1.899	2.448	23.979
8				3915.90	1.887	2.457	23.795
9				4353.34	1.877	2.501	23.607
10	4785.63	1.868	2.528	4785.85	1.868	2.527	23.419
11				5213.45	1.859	2.552	23.236
12				5636.23	1.850	2.576	23.060
13				6054.34	1.842	2.600	22.893
14				6467.82	1.834	2.624	22.729
15	6874.63	1.827	2.647	6876.59	1.827	2.648	22.562
	$Y_{00} = 1.5566 \times 10^{-5}$			$Y_{00} = 0.16759$			

TABLE IV-10

RKR Potential for the A-State of Lead-Oxide

V	Gv(cm^{-1})	R-Å	R+Å
0.0	222.30	2.025	2.168
2.5	1328.32	1.937	2.288
5.0	2427.60	1.890	2.367
7.5	3520.12	1.856	2.432
10.0	4605.90	1.829	2.491
12.5	5684.92	1.807	2.546
15.0	6757.20	1.788	2.597

$Y_{00} = 0.28500$

TABLE IV-11

Input Constants and Data Used to Generate Potential Energy Curves

Constants	State		
	X	a	A
Te^*	0.0	16024.9(1.45)	19862.6(1.5)
$Y_{10}{}^*$	720.97(0.36)	481.5(0.70)	443.3(0.8)
$Y_{20}{}^*$	- 3.536(0.025)	- 2.45(0.07)	- 0.54(0.24)
Y_{01}	0.307519**	0.252(0.10)*	0.2588**
Y_{11}	$- 1.9167 X 10^{-3**}$	$- 1.6761 X 110^{-3\#}$	$1.4 X 10^{-3**}$
Y_{02}	$2.2 X 10^{-7**}$	$2.2 X 10^{-7\#\#}$	$3.3 X 10^{-7**}$

Mass : Oxygen - 1.5994 amu; Lead - 207.19 amu.

*Source: Linton and Broida (Ref 33).

**Source: Suchard (Ref 45).

#Source: Calculated from Linton and Broida's Y_{01} using Eq (104).

##Source: Used X-state value for a-state Y_{02} . The a-state Y_{02} should be calculated according to Eq (104´). The error due to this substitution should be small.

equation. But, it is possible to arrive at certain conclusions without calculation of the Franck-Condon factors. For example, examination of the a-state and X-state curves show that no overlap exists between the "v´=0" energy level for the a-state, and "v"=0" for the X-state. This indicates that such a transition is classically forbidden. In Table IV-5, a transition observed at 15898 cm had been assigned to the a-X (0,0) transition. Reevaluation showed that the 15898 band head should be the a-X (3,2) transition. Both assignments were acceptable within the error limits of fit. The relative positioning of the potentials indicate that only the (3,2) transition is possible. The calculated value for the a-X (3,2) transition is 15898.4 cm^{-1}.

The next step should be the generation of a new set of constants using the formulas for G_v and B_v and the newly obtained energy eigenvalues G_v and B_v values generated by the IPA routine. This technique was applied to the ground state IPA potential of Table IV-8. From this, the following constants were generated for the ground state:

$$Y_{10} = 720.991(0.058) \text{ cm}$$

$$Y_{20} = 3.5357(0.00479)$$

The calculation of new values for the rotational constants Y_{01} , Y_{11} , etc., from B_v was not performed.

The calculations using only Vidal's RKR-IPA method were halted at this point. Attempts to extend the curves to the dissociation limit "in one jump" produced a potential which diverged as the curve approached the dissociation limit (see Fig IV-2). Not having data for vibrational levels above about v=15, the iterative techniques of gradually extending the curve, as discussed by Vidal and Stawalley (Ref 43), were not attempted. They used the IPA method to improve the RKR curve at lower levels, and then on successive trials, extended the curve slowly to the dissociation limit.

The reader is referred to Vidal's works listed in the Bibliography and in Appendix C for further information concerning the generation of new constants and the extension of potential curves to the dissociation limit using the IPA routine.

This completes the discussion of the use of the RKR-IPA program by itself to generate potential curves. The next section presents use of the RKR-IPA technique in conjunction with Leroy's extension techniques to produce a potential energy curve which extends to the dissociation limit.

Extension of the X-State Lead-Oxide Potential Energy Curve to the Dissociation Limit, D_e

The potential energy curve for the ground state of lead-oxide was selected as the likely candidate for extension to the dissociation energy, D_e. This selection was based upon the fact that the constants for the ground state have the smallest standard errors.

The vibrational constants of Linton and Broida were selected as starting values because of their small error

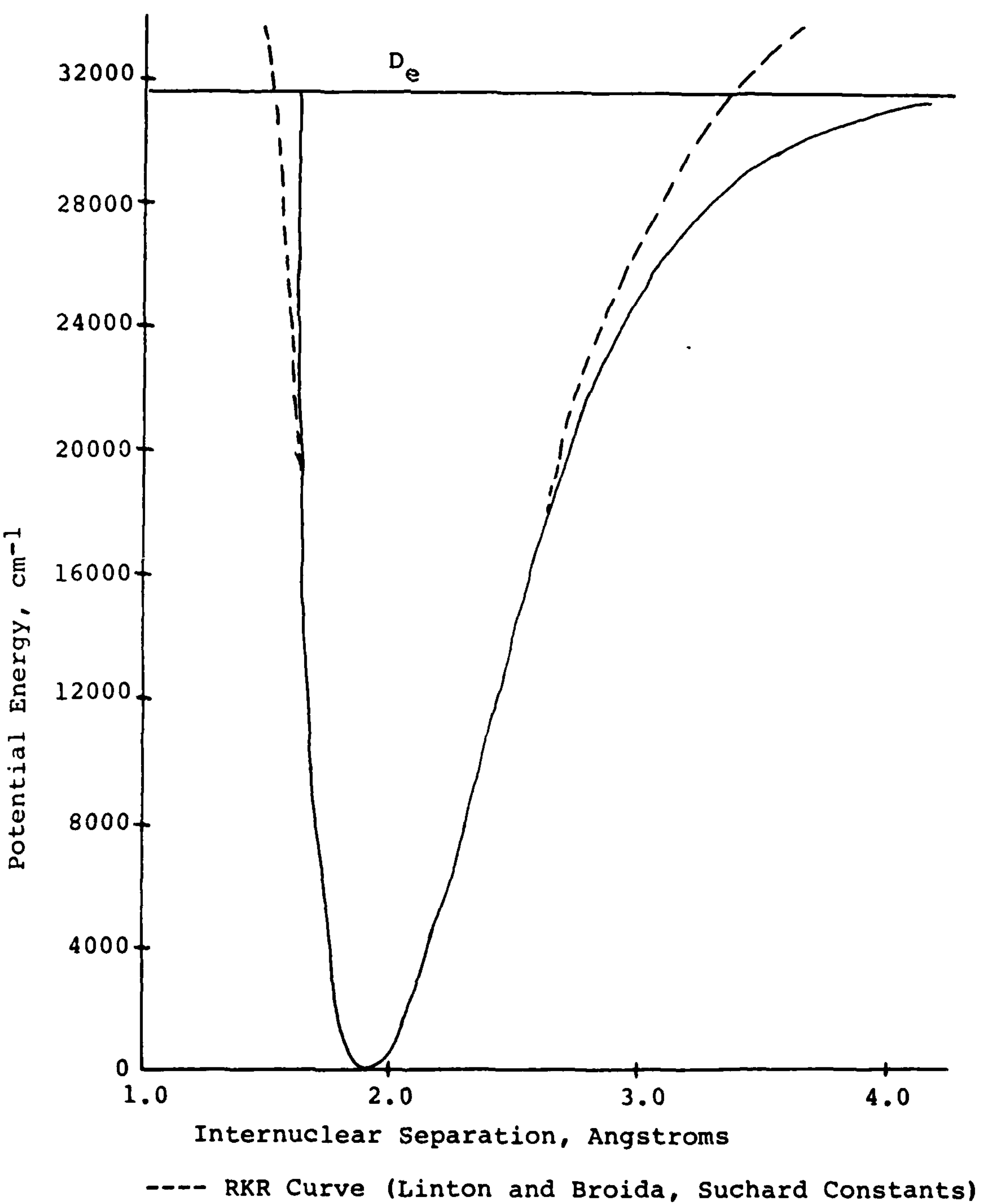

Fig IV-2. Lead-Oxide X-State Potential Energy Curves limits. The creation of potential energy curves also requires the knowledge of rotational constants. The rotational constants were selected from Suchard (Ref 45). Table IV-12 contains the original constants and the final set of constants used in extending the curve to the dissociation limit.

The method prescribed by Leroy was used. Linton and Broida's constants were used to generate a set of G(v)'s according to Eq (87) for v=0 to 15. A trial value was selected for Y_{40} and the other constants, Y_{30}, Y_{20}, and Y_{10} were solved for by performing a least-squares fit to the value obtained from Eq (98). Program DUNCON was modified to perform the fit. The process was repeated until the criterion of "$\Delta Gv+\frac{1}{2} = 0$" at D_e was satisfied.

Suchard's constants were used to generate a set of B_v's for v=0 to 15 according to Eq (93). A trial Y_{21} was selected and new Y_{01} and Y_{11} constants were obtained from a least squares fit to the values calculated by Eq (99).

The new vibrational constants and rotational constants were used as the inputs for the RKR-IPA program. The process of adjusting the rotational constants was repeated until the criteria expressed in Eqs (95), (96), and (97) were satisfied.

The last set of constants calculated are presented in Table IV-12 as the extended constants. The complete numerical results of the IPA-RKR routine are presented in Appendix B. The "Final Set of Turning Points," as output by the IPA routine was used to create the potential curve (solid line)

TABLE IV-12

Constants Used to Extend the Lead-Oxide X-State Potential Energy Curve to the Dissociation Limit, D_e

Constants	Original Values	Extended Values
Y_{10}	720.97(0.36)	721.062849
Y_{20}	- 3.536	- 3.57101904
Y_{30}		$3.85076374 \times 10^{-3}$
Y_{40}		$- 1.29 \times 10^{-4}$
Y_{01}	0.307519	0.30726775
Y_{11}	$- 1.9167 \times 10^{-3}$	$- 1.7667 \times 10^{-3}$
Y_{21}		$- 1.5 \times 10^{-5}$
Y_{02}	0.22×10^{-6}	0.22×10^{-6}

$D_e = 31570 \pm 410.\ \mathrm{cm}^{-1}$

in Fig IV-2 which satisfies the dissociation criteria. The dashed line in Fig IV-2 is the RKR curve, as defined by the original constants of Linton and Broida, and Suchard. It should be noted that the constants, as presented in Table IV-12, will only produce the curve in Fig IV-2 when input into an RKR-IPA routine. Examination of the "Final Set of Turning Points" yields a minimum inner turning radius of about 1.62 angstroms for vibrational quantum numbers from v=33 to v=69. Examination of the turning points for the initial "Potential Generated by RKR," listed at the beginning of the RKR-IPA program output in Appendix B, shows RMIN turning points as small as 1.54 angstroms for v=74. For v=69, the last vibrational quantum number investigated by the IPA routine, the RKR program returned an RMIN of 1.59 angstroms. This decreasing value in RMIN indicates that the left branch of the curve would diverge just as shown by the dashed line on the left-hand side in Fig IV-2. The turning points of the RKR potential were of sufficient quality that the IPA program was able to correct the potential to yield the solid curve of Fig IV-2. In this work, the procedure described above, was the final one used; however, continued refinements are possible by the use of the RKR-IPA program. The next step should be to take the G(v) [U(R)] and B(v) [BV*100] values as output by the IPA program and perform a least-squares fit to obtain a new set of Y_{n0} and Y_{n1} constants. These, in turn, would be used as input for the constants from the experimental data and calculating the higher $Y_{n+,n+}$ constants.

The convergence of the IPA routine became very sensitive as the "sought for value" of the last vibrational constant was approached. For the example, the IPA routine would not converge when values of $Y_{21} = -1.25 \times 10^{-5}$ or $Y = 1.75 \times 10^{-5}$ were used. The program would converge for values of Y_{21} larger and smaller than these, but the shape of the resulting curve diverged from the desired shape. An indication of the convergence of the IPA routine may be obtained by looking at the next to the last output of the IPA-RKR program, "The Summary of Errors of the Inverted Perturbation Approach."

Due to the fact that the "Final Set of Turning Points" fluctuates about 1.62 angstroms and the potential is increasing asymptotically along 1.62 angstroms, multiple potential energies are presented for the same RMIN turning point value. Thus, when searches are performed using a turning point radius value [XXX] as in DO-loop 55 of POTTAB, and PLYNN called from this loop, the routine stops at the first value satisfying the requirement [XXX]<X(J) (Subroutine PLYYN). The end result is that potential energies corresponding to turning points of magnitude of less than about 1.62 angstroms in the "Final Potential" should not be accepted as valid without close inspection. Improved constants and successive iterations of the RKR-IPA routine may remove this discrepancy.

V. Summary and Recommendations

The programs and techniques necessary to transform molecular spectra for diatomic molecules into potential energy curves have been presented and described in detail. The program DUNCON performs least-squares fits to separate data sets and then merges them in a weighted-correlated manner based upon the variances of the separate fits to yield spectroscopic constants. The RKR-IPA program presented first calculates "semi-classical" turning points based upon spectroscopic constants. It then adjusts the resulting RKR potential through an inverted perturbation technique to yield a potential energy curve whose energy eigenvalues are in best agreement with the model of a vibrating-rotating diatomic molecule as specified by the Schroedinger wave equation and with the experimentally observed data. The routing also calculates the wave functions for the potential energy curve.

Techniques were presented for extending potential energy curves to their dissociation limit when experimental data does not permit such an extension by straightforward application of the RKR technique.

Using DUNCON, constants for the a-X, A-X, B-X, and D-X transitions were calculated from experimental data. The results are presented in Tables IV-1, IV-2, and IV-3. The calculated values agree well with published values for these states.

A new set of assignments was made for b-X transitions. The new constants calculated for the b-state are presented in Table IV-6, and the new assignments are in Table IV-7. The new assignments and constants produced a fit with a standard error of 10.49 cm^{-1} versus 47.9 cm^{-1} for the previous published assignments.

Recommendations

1. The use of Leroy's technique for extending a curve to its dissociation limit in conjunction with the RKR-IPA routine should be tested upon a potential energy curve whose shape is known and for which experimental data is available all the way up to the dissociation energy. If the technique produces a curve and energy eigenvalues consistent with a curve based upon experimental data then, the validity of the method will be confirmed.

2. This technique for extending curves might be further verified by applying it to two different states; for example, a- and b-states of lead-oxide, whose dissociation energies are the same. The coincidence of their potential energy curves at large separations should serve to verify both the extension technique and the quality of the constants used in construction of the curves.

3. A complete investigation of all published data using DUNCON should produce a better set of constants for lead-oxide. This is particularly true for cases where two

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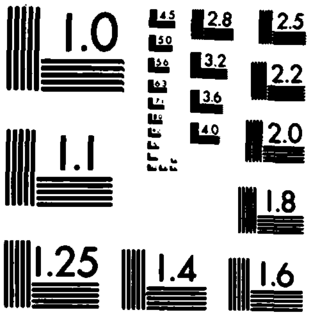

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investigators have given different energy levels for the same transition. The judgment as to which data is the more accurate should be based upon the constants produced by DUNCON.

4. Constants obtained from a least-squares fit should be reported as a group. If not, care should be taken to report how the constants were obtained.

5. The reassignments made for the b-X transitions should be evaluated by an investigator with access to data specifying the relative intensities of the experimental data. These were not available for the assignments made in this work.

Also, the b-state constants should be reevaluated using a more accurate set of X-state constants as opposed to those obtained from the least-squares fit of the b-X data. By fixing the value of the X-state constants, it may be possible to obtain a positive $w_e x_e$ for the b-state. Having a positive $w_e x_e$, then Eq (102) and Tellinghuisen's method for constructing a potential energy curve might be used. Alternatively, Eq (101) might be applied. From the potential energy curve, it might be possible to determine what transitions are more probable. Some information along these lines can be obtained by assuming a similarity between the a-state potential and estimating the position of the b-state curve relative to the a-state curve.

6. Vidal made use of the RKR-IPA routine to improve RKR curves for low energies and then used these improved

curves to extend the curves in small increments to higher energy levels. This technique has not been pursued and warrants further investigation. The RKR-IPA routine could even be used to improve constants for low energy levels, i.e., small "v", prior to using them in the previously described extension technique. Both techniques warrant further investigation.

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Appendix A

Program DUNCON

The following section contains the program DUNCON. The program has provisions for obtaining separate least-squares fits to separate data sets and then merging the resulting constants in a weighted-correlated fashion based upon the variances and covariances of the original separate fits.

Presented first is a written description of the program and instructions on how to use the program. Following that is a listing of the program with a sample output.

Merged Least-Squares Spectroscopic Constants Program

Program DUNCON is structured so the user can generate a least-squares fit to several different groups of data which have different standard errors and then merge the fits to obtain a weighted, correlated linear-least squares fit as described in the previous discussion on least-squares fits (Refs 2 and 3). DUNCON is written in Fortran V. A copy of DUNCON follows in this appendix.

The user must set up the model which will be used to fit his spectroscopic data, input the data, dimension the arrays used in his program, and call the subroutines WAVNUM, CONST, MATEQ, VECEQ, MATINV, and MERCN to obtain a merged least-squares fit. In turn, these routines call on a package of matrix manipulating routines (Ref 13) contained in the subroutine MATMULT.

Program DUNCON

The user has complete freedom in structuring this portion of the program. To perform a least-squares fit, the user must choose a model to represent his data. For data representing transitions between electronic states, the following is a typical model using Dunham coefficients (Ref 18):

$$\nu = T_e' + Y_{10}' + Y_{20}' - Y_{10}'' - Y_{20}'' \qquad (117)$$

where ν is the frequency of the transition expressed in units of cm^{-1}. As previously described, a series of transitions

(ν) may be represented in matrix notation as:

$$\nu_k = X_k B_k + \varepsilon_k \qquad k = 1,2,3 \tag{118}$$

where ν is a column matrix made of experimentally determined wavelengths or wavenumbers:

$$\nu = \begin{bmatrix} \nu_1 \\ \nu_2 \\ \vdots \\ \nu_n \end{bmatrix} \tag{119}$$

The X matrix is made up of the $v'+1/2$, $(v'+1/2)$, $v''+1/2$, and $(v''+1/2)$ terms:

$$X = \begin{bmatrix} 1 & v_1'+1/2 & (v_1'+1/2)^2 & v_1''+1/2 & (v_1''+1/2)^2 \\ 1 & v_2'+1/2 & (v_2'+1/2)^2 & v_2''+1/2 & (v_2''+1/2)^2 \\ \vdots & & & & \\ 1 & v_n'+1/2 & (v_n'+1/2)^2 & v_n''+1/2 & (v_n''+1/2)^2 \end{bmatrix} \tag{120}$$

This X matrix is calculated in lines 18-28 of the subroutine CONST. As the specific model chosen to represent spectroscopic data may vary, the user must define this section of CONST.

The β column matrix (vector) will contain the constants of the least-squares fits.

$$\beta = \begin{bmatrix} Te' \\ Y_{10}' \\ Y_{20}' \\ Y_{10}'' \\ Y_{20}'' \end{bmatrix} \qquad (121)$$

To operate the program, the user must input the following data:

1. $\underline{\nu}$--the experimentally determined energy of transition expressed in either angstroms (A) or wavenumbers (cm^{-1}). In the sample program in this appendix, ν is called ANUx, where the small "x" represents the additional characters necessary to identify a specific group of data. This convention is continued throughout the discussion in this section.

2. $\underline{v'}$--the vibrational quantum number associated with the upper state and referred to as QV1x in the program. It should be entered as a decimal.

3. $\underline{v''}$--the vibrational quantum number associated with the lower state and referred to as QV2x in the program. It should be entered as a decimal.

NOTE: the values of ANUx, QV1x, and QV2x for each observed transition must be associated with each other by subscripts. (The subscript is placed in parenthesis and the subscript must start with "0".) For example:

ANUx(0),QV1x(0),QV2x(0)
ANUx(1),QV1x(1),QV2x(1)
ANUx(2),QV1x(2),QV2x(2)
etc.

4. N--the number of constants minus one to be calculated in the initial least-squares fit. For the model in Eq (117), N should be defined as follows: N = 5 - 1 = 4.

5. Mx--corresponds to the number of experimental values to be included initially in a data set for least-squares fitting prior to the merging step.

6. MM--corresponds to the total number of constants minus one which are generated in the initial least-squares fits for each of the independent data sets. For example, if the calculation is for two different transitions, i.e., A-X, B-X, and, as in Eq (1), five constants are to be calculated then MM = 2*5 - 1 = 9.

7. NM--the number of constants to be obtained in the merged least-squares fit.

8. XM(0:MM,0:NM)--the coefficient matrix which relates the redundant variables obtained from independent least-squares fits to the desired final set of variables. It controls the merging of the constants obtained in the separate least-squares fits to yield the merged weighted, correlated least-squares constants by the following formula:

$$\beta^M = (X^T \theta I^{-1} X)^{-1} \quad X^T \theta I^{-1} Y \qquad (122)$$

For a problem involving five constants for each of two electronic transitions, the XM matrix would be of size 14x5 and contain the elements as follows:

State

$$\text{XM} = \begin{array}{c|cccccccc|}
 & \multicolumn{3}{c}{\underline{A}} & \multicolumn{3}{c}{\underline{B}} & \multicolumn{2}{c|}{\underline{X}} \\
 & Te & Y'_{10} & Y'_{20} & Te & Y'_{10} & Y'_{20} & Y''_{10} & Y''_{20} \\
\hline
Te & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
Y'_{10} & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
Y'_{20} & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
Y''_{10} & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
Y''_{20} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
Te & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
Y'_{10} & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
Y'_{20} & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
Y''_{10} & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
Y''_{20} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
\hline
\end{array}$$

← Merged Constant

Elements
Pertaining to
AX
Transitions

Elements
Pertaining to
B-X
Transitions

↓

Constants from Independent Least-Squares Fit

Fig A-1. Coefficient Matrix XM

9. THETAI(0:MM,0:MM)--this matrix is made by merging the variance-covariance matrices obtained from each of the independent least-squares fits. The details of its construction will be provided in the discussion of the subroutine MATEQ. The user must initially fill the matrix with zeros. The matrix has $(MM+1)^2$ elements. For example, if MM=9, then the statement, DATA THETAI (100*0D0) will initialize the matrix.

This concludes the data input required of the user. The only tasks remaining are the assembly of dimension statements and construction of statements in the main portion of the program to execute the least-squares and merging routines.

The sequence of statements required to perform a least-squares fit for each set of data are as follows:

```
CALL WAVNUM
CALL CONST
CALL MATEQ
CALL VECEQ
```

In the following section, the statement names and their arguments are listed along with a brief description of the routine.

WAVNUM(ANUx,Mx)

This subroutine converts data contained in the array ANUx(0:Mx) from angstroms to wavenumbers invacuo (cm^{-1}) by means of a correction for the index of refraction of air (Refs 7 and 21). ANUx is, as described above, an array of the Mx experimental values for one group of data. NOTE: If ANUx is entered as wavenumbers, this statement is omitted.

CONST(ANUx,QV1x,QV2x,BETx,THETx,Xx,Xtx,XTXx,XTXXTx,XBx,
   ANUXBx,CVRCx,Mx,N)

This routine does the work of obtaining minimum variance least-squares constants. It solves the matrix equation as outlined below:

$$\nu = X\beta + \varepsilon \tag{124}$$

$$\beta = (X^T X)^{-1} X^T \nu \tag{125}$$

$$\sigma^2 = (\nu - X\beta)^T (\nu - X\beta)/fm \tag{126}$$

$$\theta = \sigma^2 (X^T X)^{-1} \tag{127}$$

The correspondence between the arguments for CONST and these equations are as follows including the dimensions required for the arrays: ANUx(0:Mx) = ν

QV1x(0:Mx) and QV2x(0:Mx): These entries are the quantum mechanical vibration numbers which are for the upper (v´) and lower (v") states respectively, and are used to generate the Xx matrix as previously described.

Xx(0:Mx,0:N) = X: This matrix is generated by CONST in lines 18-28, as dictated by the user and by the model chosen to represent the data.

XTx(0:N,0:Mx) = X^T: This matrix is the transpose of matrix X and is generated by the subroutine TRNSPZ called from CONST.

XTXx = first(X^TX), then $(X^TX)^{-1}$: This matrix is the product of X^T and X formed by the subroutine MATMLT. The matrix is then replaced by its inverse by the routine MATINV.

XTXXTx(0;n,0:M) = $(X^TX)^{-1}X^T$: This matrix is the product of the inverse of the first matrix times the transpose of the second.

BETx(0:N) = $(X^TX)^{-1}X^T\nu$: This column matrix (vector) contains the least-squares estimate of the constants in Eq (1). It is formed by multiplying the matrix XTXXTx times the vector, ν , using the routine MATVEC.

XBx(0:Mx) = $X\beta$: This column matrix is the product obtained from the subroutine VECVEC. It is the calculated estimate of the original experimental values based upon the constants obtained from the least-squares fit of the experimental data.

ANUBx(0:Mx) = $(\nu - X\beta)$: This column matrix (vector) contains the differences between the measured and calculated values of wavelength for a given data set. The calculation is performed by the routine VECSUB.

VARINZ = $\sigma^2 = (\nu - X\beta)^T (\nu - X\beta)/f_m$: VARINZ is a scalar and is the estimated variance of the least-squares fit.

The variance is given in the output of the program. f_m is the degree of freedom, Mx - N. VARINZ is calculated in the routine CONST.

THETx(0:N,0:N) = $\theta = \sigma^2 (X^T X)^{-1}$: THETx is the variance-covariance matrix for the calculated constants. Estimates of the variance for the constants are contained on the diagonal with off diagonal elements being the covariances. The matrix is obtained from the product of the scalar, σ^2, and the matrix, $(X^T X)^{-1}$, using the routine SCAMAT.

CVRCx(0:N,0:N): This matrix is generated by CVRCOR which is called from CONST. It contains three types of data.

1. Above its diagonal it contains the same covariances of the constants as in THETx.

2. The diagonal contains the estimate of the standard error of each of the constants.

3. The elements below the diagonal are the correlation coefficients associated with the constants. The coefficients are calculated by the following formula:

$$C = \theta_{ij} / (\theta_{ii} \theta_{jj})^{\frac{1}{2}} \tag{129}$$

where θ_{ij} are the elements of the matrix θ. Since the matrix is symmetric, the procedure of reporting variances for the top half and covariances for the bottom half is sufficient. The results are printed in the program output.

This completes the description of the arrays required for the least-squares fit of one group of data. If it is necessary to perform a least-squares fit on several sets of data and merge them to obtain a correlated, weighted, least-squares estimate of the constants, then the MATEQ and VECEQ routines are used.

The merged least-squares calculation is based upon:

$$y = X\beta^M + \varepsilon \tag{130}$$

where the known values obtained from the previous least-squares fits of the experimental data are the y and X matrices and

$$y = \begin{bmatrix} Te \\ Y'_{10} \\ Y'_{20} \\ Y''_{10} \\ Y''_{20} \\ Te \\ Y'_{10} \\ Y'_{20} \\ Y''_{10} \\ Y''_{20} \end{bmatrix} \tag{131}$$

etc.

and X is the XM matrix as defined in the input data section. It relates the redundant values of y to the corresponding members of β^M (Ref 3). β^M is the best estimate of the constants obtained from the formula

$$\beta^M = (X^T \theta I^{-1} X)^{-1} X^T \theta^{-1} y \qquad (132)$$

where θI is of the form

$$\theta I = \begin{bmatrix} \theta_1 & 0 & 0 \\ 0 & \theta_2 & 0 \\ 0 & 0 & \theta_3 \end{bmatrix} \qquad (133)$$

MATEQ(THETx,THETAI,N,N,MM,MM,x,x)

This routine inserts the variance-covariance matrices, the THETx's from each least-squares fit, into the matrix THETAI.

THETx(0:N,0:N) : As previously defined.

THETAI(0:MM,0:MM) = I : As previously defined.

The last two arguments for MATEQ, "x,x", determine where the smaller matrices are inserted into THETAI. The user must input these values (as integers). For the first group of data, "x,x" should be "0,0". If the number of constants determined in each of the separate least-squares fits is "N+1", then "x,x" for the second THETx inserted into THETAI is "2*(N+1),2*(N+1)"; third, "3*(N+1),3*(N+1)", etc. The end result is the placement of the THETx matrices into THETAI as depicted by Eq (133).

CALL VECEQ(BETx,YM,N,MM,x)

VECEQ performs a similar insertion of the constants BETx obtained in the separate least-squares fits into the column matrix (vector) YM (y in Eqs (131) and (132)). The dimensions of these two parameters are BETx(0:N), and YM(0:MM).

The "x" value is again an integer and entered by the user. It corresponds to and is equal to the value used in the MATEQ statement. In this manner, the estimated constants and their variances are placed within the THETAI and YM matrices so their correspondence is retained in the merging calculations.

After the CALL WAVNUM through VECEQ statements have been executed for each of the separate groups of experimental data and the YM and THETAI matrices are loaded, the merging of the spectroscopic constants can be carried out. To accomplish this, the user must have constructed the XM matrix as previously described. Then the following statements will accomplish the merging:

```
        IPV = 0
        CALL MATINV
        CALL MERCN
```

CALL MATINV (THETAI,MM,MM,IPV)

This routine inverts the THETAI matrix. The routine was obtained from the computer program by C. R. Vidal contained in Appendix B.

```
CALL MERCN(XM,THETAI,YM,XTM,XTHM,XTHMX,XTXXTH,BETAM,XBM,YXBM,
        YXTH,THETAM,CVRCM,MM,NM)
```

This routine performs the calculations outlined in Eq (132) to yield a set of merged least-squared constants. MERCN estimates by the following formula, the variance to be obtained using the merged constants:

$$\sigma_m^2 = (y - X\beta^M)^T \theta I^{-1} (y - X\beta^M)/f_m \qquad (134)$$

It then calculates the variance-covariance matrix, θ^M , *for* the merged constants according to the following formula:

$$\theta^M = (X^T \theta I^{-1} X)^{-1} \qquad (135)$$

Listed next are the arguments of MERCN and their correspondence to the equations presented in other sections of the report.

XM(0:MM,0:MM) = X : In Eqs (130), (132), (134), and (135).

THETAI(0:MM,0:MM) = θI : Eqs (133), (134), and (135).

YM(0:MM) = y : Eqs (130), (131), (132), and (134).

XTM(0:NM,0:MM) = X^T : Eqs (132) and (135).

XTHM(0:NM,0:MM) = $X^T \theta I$: Eqs (132) and (135).

XTHMX(0:NM,0:NM) = first $(X^T \theta I^{-1} X)$ then $(X^T \theta I^{-1} X)^{-1}$: Eqs (132) and (135).

XTXXTH(0:NM,0:MM) = $(X^T \theta I^{-1} X)^{-1} X^T \theta I^{-1}$: Eq (132).

BETAM(0:NM) = β^M : Eqs (130), (132), and (134).

XBM(0:MM) = $X\beta M$: Eq (134).

YXBM(0:MM) = $y - X\beta^M$: Eq (134).

YXTH(0:MM) = $(y - X\beta^M)^T \theta I^{-1}$: Eq (134).

THETAM(0:NM,0:NM) = $\sigma^2 (X^T \theta I^{-1} X)^{-1}$: Eq (134).

This is the variance-covariance matrix for the merged constants.

CVRCM(0:NM,0:NM): CVRCM is the matrix containing the covariances, standard errors, and the correlation coefficients of the merged constants with the structure the same as described for the separate least-squares fits.

Calculations are performed in the subroutines CONST and MERCN using a group of matrix and vector manipulation routines (Ref 13).

The output of the program consists of the following for each separate set of data.

1. A listing of the experimental input values ν, ν' and ν'' with the calculated value $X\beta$.
2. The variance of the fit.
3. The complete variance-covariance matrix.
4. The matrix containing the covariances, standard errors and correlation coefficients.
5. The constants for the upper and lower levels.

For the merged data, the merged constants, the variance of the fit and variance, covariance, standard errors, and correlation coefficients of the merged constants are printed.

```
      PROGRAM DUNCON
C      DUN319, DUN317, DUN324, 10 DEC 82
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C         DIMENSIONING STATEMENTS FOR SNYDER-GLESSNER SMALL H-X
C         LEAD-OXIDE DATA
      DIMENSION ANUA(0:9),QVA1(0:9),QVA2(0:9)
      DIMENSION ABETA(0:4),THETA(0:4,0:4),XA(0:9,0:4),XTA(0:4,0:9)
      DIMENSION XTXXTA(0:4,0:9),XBA(0:9),XTXA(0:4,0:4),ANUXBA(0:9)
      DIMENSION CVRCA(0:4,0:4)
C         DIMENSION STATEMENTS FOR OLDENBORG, DICKSON, AND ZARE
      DIMENSION ANUB(0:5),QVB1(0:5),QVB2(0:5)
      DIMENSION ABETB(0:4),THETB(0:4,0:4),XB(0:5,0:4),XTB(0:4,0:5)
      DIMENSION XTXXTB(0:4,0:5),XBB(0:5),XTXB(0:4,0:4),ANUXBB(0:5)
      DIMENSION CVRCB(0:4,0:4)
C         DIMENSION STATMENTS FOR DATA OF KURYLO, ET.AL.
      DIMENSION ANUC(0:15),QVC1(0:15),QVC2(0:15)
      DIMENSION ABETC(0:4),THETC(0:4,0:4),XC(0:15,0:4),XTC(0:4,0:15)
      DIMENSION XTXXTC(0:4,0:15),XBC(0:15),XTXC(0:4,0:4),ANUXBC(0:15)
      DIMENSION CVRCC(0:4,0:4)
C         ARRAYS FOR MERGING 3 SEPARATE FITS
      DIMENSION XM(0:9,0:4),THETAI(0:9,0:9),YM(0:9)
      DIMENSION XTM(0:4,0:9),XTHM(0:4,0:9),XTHMX(0:4,0:4)
      DIMENSION YXTH(0:4),THETAM(0:4,0:4),CVRCM(0:4,0:4)
      DIMENSION XTXXTH(0:4,0:9),BETAM(0:4),XBM(0:9),YXBM(0:9)
C         DATA FOR SNYDER-GLESSNER
      DATA ANUA/5716.5D0,6606.5D0,7050.2D0,7476.9D0,6222.3D0,
     +6541.9D0,7621.3D0,8036.3D0,5352.7D0,5031.4D0/
      DATA QVA1/3D0,3D0,8D0,0D0,3D0,9D0,1D0,1D0,3D0,10D0/
      DATA QVA2/6D0,4D0,8D0,4D0,2D0,7D0,5D0,6D0,3D0,1D0/
C         DATA FOR OLDENBORG
C              AND
C     DATA FOR KURYLO
C        DATA IN INVERSE CENTIMTERS
      DATA ANUC/21643D0,21200D0,15515D0,
     +17212D0,17108D0,17033D0,16915D0,16773D0,
     +16614D0,16466D0,16434D0,16297D0,16215D0,15773D0,
     +15623D0,15363D0/
      DATA QVC1/14D0,13D0,7D0,4D0,7D0,2D0,5D0,3D0,
     +1D0,4D0,7D0,17D0,14D0,13D0,2D0,3D0/
      DATA QVC2/1D0,1D0,1D0,1D0,3D0,0D0,2D0,1D0,0D0,
     +2D0,4D0,11D0,9D0,9D0,2D0,3D0/
C         INTIALIZING MERGING MATRICES
      DATA XM/1D0,4*0D0,1D0,5*0D0,
     +1D0,4*0D0,1D0,5*0D0,
     +1D0,4*0D0,1D0,5*0D0,
     +1D0,4*0D0,1D0,5*0D0,
     +1D0,4*0D0,1D0 /
      DATA THETAI/100*0D0/
.     .
.

      N=4
      MA=9
      MB=5
      MC=15
      MM=5

      N=4
C         CALCULATION OF CONSTANTS FOR SNYDERS DATA
      CALL WAVNUM(ANUA,MA)
      CALL CONIT (ANUA,QVA1,QVA2,ABETA,THETA,XA,XTA,XTXA,XTXXTA,
     +XBA,ANUXBA,CVRCA,MA,N)
      CALL MATEQ(THETA,THETAI,N,N,MM,MM,0,0)
      CALL VECEQ(ABETA,YM,N,MM,0)
C         CALULATION OF CONSTANTS FOR KURYLOS DATA
      CALL CONIT(ANUC,QVC1,QVC2,ABETC,THETC,XC,XTC,XTXC,XTXXTC,
     +XBC,ANUXBC,CVRCC,MC,N)
      CALL MATEQ(THETC,THETAI,N,N,MM,MM,5,5)
      CALL VECEQ(ABETC,YM,N,MM,5)
      IPV=1
      CALL MATINV(THETAI,MM,MM,IPV)
      CALL MERGN(XM,THETAI,YM,XTM,XTHM,XTHMX,XTXXTH,
     +BETAM,XBM,YXBM,YXTH,THETAM,CVRCM,MM,NM)
      END
```

```
      SUBROUTINE MATINV(A,N,M,IPV)
C         REFERENCE:  OBTAINED FROM PROGRAM PREPARED BY C.R. VIDAL
C         MATRIX INVERSION
C         IPV.EQ.1:  NO SEARCH FOR PIVOT.  IPV.NE.1: SEARCH FOR PIVOT
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION IPIVOT(0:63),INDEXR(0:63),INDEXC(0:63)
      DIMENSION A(0:N,0:M)
C     ....................INITIALIZATION
.
      DO 20 J=0,N
 20   IPIVOT(J) = 0
      DO 500 I=0,N
      IF (IPV.NE.1) GO TO 40
       ICLM=I
      GO TO 260
C     ..................SEARCH FOR PIVOT ELEMENT
 40   AMAX=0.0
      DO 105 J=0,N
      IF (IPIVOT(J).EQ.1) GO TO 105
C     FOR UNSYMMETRIC MATRIX:  A(I,J).NE.A(J,I)
      DO 100 K=0,N
C     FOR SYMMETRIC MATRIX:  A(I,J).EQ.A(J,I)
C     DO K=J,N
      IF (IPIVOT(K).EQ.1) GO TO 100
      IF (ABS(AMAX).GE.ABS(A(J,K))) GO TO 100
      IROW=J
      ICLM=K
      AMAX=A(J,K)
 100   CONTINUE
 105   CONTINUE
      IPIVOT(ICLM)=IPIVOT(ICLM) + 1
      INDEXR(I)= IROW
      INDEXC(I)= ICLM
C     .......INTERCHANGE ROWS TO PUT PIVOLT ELEMENT ON DIAGONAL
      IF (IROW.EQ.ICLM) GO TO 260
.
      DO 200 L=0,N
      SWAP= A(IROW,L)
      A(IROW,L)=A(ICLM,L)
 200  A(ICLM,L) = SWAP
.
.
.
.
.
 260  PIVOT = A(ICLM,ICLM)
      IF (N.GT.10) GO TO 330
.
C     ................DIVIDE PIVOT ROW BY PIVOT ELEMENT
 330  A(ICLM,ICLM) = 1.0
 .    DO 350 L = 0,N
 350  A(ICLM,L)=A(ICLM,L)/PIVOT
.
.
.
```

```
      C        ................REDUCE NON-PIVOT ROWS
       380     DO 550 L1 = 0,N
               IF (L1.EQ.ICLM) GO TO 550
               T = A(L1,ICLM)
               A(L1,ICLM) = 0.0
               DO 450 L= 0,N
       450     A(L1,L) = A(L1,L) - A(ICLM,L)*T
      .
      .
      .
       550     CONTINUE
               IF (IPV.EQ.1) RETURN
      C        .....................INTERCHANGE COLUMNS
               DO 710 I= 0,N
               L= N-I
               IROW = INDEXR(L)
               ICLM = INDEXC(L)
               IF (IROW.EQ.ICLM) GO TO 710
               DO 705 K = 0,N
               SWAP=A(K,IROW)
      .
               A(K,IROW) = A(K,ICLM)
       705     A(K,ICLM) = SWAP
       710     CONTINUE
               RETURN
               END
```

```
C     THE FOLLOWING ROUTINES PERFORM STANDARD MATRIX OPERATIONS
C     AND VECTOR OPERATIONS
*
*
      SUBROUTINE MATMLT(A,U,T,M,N,P)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION A(0:M,0:N),U(0:N,0:P),T(0:M,0:P),B(0:M,0:N)
      DIMENSION D(0:P1,0:P2)
      DIMENSION X(0:N),Y(0:N),Z(0:M),V(0:N,0:M),Z1(0:N)
      INTEGER I,J,M,N,C,P
      INTEGER P1,P2
*
      DO 1 I=0,M
      DO 1 J=0,P
 1    T(I,J)=0D+0
      DO 2 I=0,M
      DO 2 J=0,P
      DO 2 K=0,N
*
 2    T(I,J)= A(I,K)*U(K,J) + T(I,J)
      RETURN
*
      ENTRY VECSUB(X,Y,Z1,N)
C     THIS ROUTINE SUBTRACTS TWO VECTORS
      DO 3 I=0,N
      Z1(I)=X(I)-Y(I)
 3    CONTINUE
      RETURN
*
      ENTRY MATVEC (A,X,Z,M,N)
*THIS ROUTINE MULTIPLIES A MATRIX TIMES A VECTOR YEILDING A VECTOR
      DO 5 I=0,M
 5    Z(I)=0D+0
      DO 6 I=0,M
      DO 6 J=0,N
 6    Z(I)=A(I,J)*X(J) + Z(I)
      RETURN
*
      ENTRY SCAVEC (S,X,Y,N)
*     THIS ROUTINE MULTIPLIES A SCALAR TIMES A VECTOR TO YEILD A VECTOR.
      DO 7 I=0,N
 7    Y(I)=S*X(I)
      RETURN
*
      ENTRY SCAMAT (S,A,B,M,N)
*     ROUTINE MULTIPIES A SCALAR TIMES A MATRIX
      DO 8 I=0,M
      DO 8 J=0,N
      B(I,J)=S*A(I,J)
      RETURN
*
      ENTRY VECVEC (X,Y,S,N)
*     THIS ROUTINE MULTIPLIES TWO VECTORS TOGETHER YEILDING A SCALAR
      S=0D+0
      DO 9 I=0,N
```

```
    9 S= S + X(I)*Y(I)
      RETURN
*
      ENTRY VECMAT (Z,A,X,M,N)
C     THIS ROUTINE MULTIPLIES A VECTOR TIMES A MATRIX TO YEILD A VECTOR
      DO 10 J=0,N
      X(J)= 0D+0
      DO 10 K=0,M
   10 X(J)=X(J) + Z(K)*A(K,J)
      RETURN
*
      ENTRY TRANSPZ (A,V,M,N)
C     THIS ROUTINE TRAPOSES A MATRIX
      DO 14 I=0,M
      DO 14 J=0,N
   14 V(J,I)=A(I,J)
      RETURN
*
*
*
      ENTRY CVRCOR(A,T,M,N,P)
C         THIS ROUTINE CREATES A MATRIX FOR PRINT OUT OF
C       STANDARD ERRORS, COVARIANCES, AND CORRELATION COEFFICIENTS OF
C     THE *DUNHAM COEFFICENTS*.
*
*
      DO 15 I=0,M
      DO 15 J=0,M
      IF (I.LT.J) THEN
      T(I,J)=A(I,J)
      ELSE IF (I.EQ.J) THEN
      T(I,J)=DSQRT(A(I,J))
      ELSE IF (I.GT.J) THEN
      T(I,J)=A(I,J)/(DSQRT(A(I,I))*DSQRT(A(J,J)))
      END IF
   15 CONTINUE
      RETURN
      ENTRY WAVNUM(X,N)
C        THIS ROUTINE CONVERTS WAVELENGTHS IN ANGSTROMS TO
C        WAVE NUMBERS(INVERSE CENTIMETERS).
C        WITH CORRECTION FOR INDEX OF REFRACTION OF AIR
C     REFERENCE:  R.T. BIRGE, PHYSICAL REVIEW, VOL. 60, 766-785(1941).
      DO 16 I=0,N
      WL = X(I)/1000.0D0
      XREF = 272.5[illegible]1D0 + 1.5453D0/WL**2D0 + 0.02168D0/WL**4D0
      XREF = 1D0 + XREF/1D6
   16 X(I) = 1D5/(WL*XREF)
      RETURN
      ENTRY MATEQ(A,D,M,N,P1,P2,K1,K2)
C        THIS ROUTINE TRANSFERS MATRIX A(M,N) INTO MATRIX D
C         STARTING AT POSITION X(K1,K2)
      M2=K1+M
      N2=K2+N
      DO 17 I=K1,M2
      DO 18 J=K2,N2
      I2=I-K1
      J2=J-K2
      D(I,J)=A(I2,J2)
   18 CONTINUE
   17 CONTINUE
      RETURN
*
*
      ENTRY VECEQ(X,Z,N,M,P1)
C        THIS ROUTINE TRANSFERS MATRIX X(N) INTO VECTOR Z(M)
C        STARTING AT POSITION Z(P1)
      N2=N+P1
      DO 19 I=P1,N2
      I2=I-P1
      Z(I)=X(I2)
   19 CONTINUE
      RETURN
      END
```

```
                SUBROUTINE CONST(ANU,QV1,QV2,BETA,THETA,X,XT
               +,XTX,XTXXT,XB,ANUXB,CVRC,M,N)
C                  THIS ROUTINES PERFORMS THE ACTUAL CALCULATION OF THE
C                  "DUNHAM MOLECULAR CONSTANTS."
                IMPLICIT DOUBLE PRECISION (A-H,O-Z)
                DIMENSION ANU(0:M),QV1(0:M),QV2(0:M)
                DIMENSION BETA(0:N),THETA(0:N,0:N)
                DIMENSION XT(0:N,0:M),X(0:M,0:N),XTX(0:N,0:N),XTXXT(0:N,0:M)
                DIMENSION XB(0:M),ANUXB(0:M),CVRC(0:N,0:N)
                DOUBLE PRECISION L1
                N2=N/2
                N3=N2+1
C                  THIS SECTION CALCULATES THE X MATRIX WIHCH IS MADE UP
C                  OF THE VIBRATIONAL AND/OR ROTATIONAL QUANTUM NUMBERS
C                     WITH "V+1/2" AND "J*(J+1)" RAISED TO POWERS MAKING UP
C                  THE X(I,J) TERMS.
*
                DO 2001 I = 0,M
                DO 2000 L = 0,N2
                L1 =L
                L2 = L + N2 + 1
                X(I,L)=(QV1(I)+0.5D0)**L1
          2000  CONTINUE
                DO 2002 L=N3,N
                L1=L-N2
                X(I,L)=-(QV2(I)+0.5D0)**L1
          2002  CONTINUE
          2001  CONTINUE
C                  CALCULATION OF CONSTANTS
                CALL TRNSFZ(X,XT,M,N)
                CALL MATMLT(XT,X,XTX,N,M,N)
                IPV=0
                CALL MATINV(XTX,N,N,IPV)
                CALL MATMLT(XTX,XT,XTXXT,N,N,M)
                CALL MATVEC(XTXXT,ANU,BETA,N,M)
C                  CALCULATION OF VARIANCE OF ENERGY LEVEL.  DF IS DEGREES
C                  OF FREEDOM.
                DF=1.0D+0/DBLE(M-N)
                CALL MATVEC(X,BETA,XB,M,N)
                CALL VECSUB(ANU,XB,ANUXB,M)
                PRINT*,' QV1  QV2     OBSERVED                        CALCULATED'
                DO 996 I=0,4
                PRINT 999 ,QV1(I),QV2(I),ANU(I),XB(I)
          999   FORMAT (2X,F3.0,2X,F3.0,2X,F19.7,2X,F19.7)
          996   CONTINUE
                CALL VECVEC(ANUXB,ANUXB,STEMP,M,M)
                VARINZ=STEMP*DF
                PRINT*,' ',' VARIANCE ',VARINZ
                PRINT*,' ','VARIANCE COVARIANCE MATRIX ELEMENTS'
                CALL SCAMAT(VARINZ,XTX,THETA,N,N)
                DO 123 I=0,N
                DO 123 J=0,N
                PRINT*,' ',I,J,THETA(I,J)
          123   CONTINUE
C
```

```
      C        THIS SECTION PLACES THE COVAIANCES ABOVE THE DIAGONAL
      C        OF THE MATRIX 'CVRC.'  IT PLACES THE STANDARD ERRORS
      C        FOR THE CONSTANTS ON THE DIAGONAL.  ITS CALCULATES THE
      C        CORRELATION COEFFICIENTS AND PLACES THEM BELOW THE DIAGONAL.
            CALL CVRCCR(THETA,CVRC,M,N,N)
            PRINT *,'STANDARD ERROR(I=J), CORRELCOEFF(I>J),COVARIANCE(I<J)'
            DO 615 I=0,N
            DO 614 J=0,N
        614 PRINT*,'  ',I,J,CVRC(I,J)
        615 CONTINUE
      C        PRINT OUT THE CONSTANTS FOR THE TWO ELECTRONIC STATES
            PRINT *,'1'
            PRINT*,'  ','VIBRATIONAL CONSTANTS FOR UPPER LEVEL'
            DO 2010 I=0,N2
       2010 PRINT*,'  ',I,BETA(I)
            PRINT *,'0'
            PRINT*,'   ','VIBRATIONAL CONSTANTS FOR LOWER STATE'
            DO 2020 I=N3,N
       2020 PRINT*,'   ',I,BETA(I)
            PRINT *,'1'
            END
```

```
      SUBROUTINE MERGCN(XM,THETAI,YM,XTM,XTHM,XTHMX,XTXXTH,
     +BETAM,XBM,YXBM,YXTH,THETAM,CVRCM,M,N)
C         THIS ROUTINE MERGES RESULTS TO OBTAIN A BEST ESTIMATE
C         OF THE SPECTROGRAPHIC CONSTANTS
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION XM(0:M,0:N),THETAI(0:M,0:M),YM(0:M)
      DIMENSION XTM(0:N,0:M),XTHM(0:N,0:M),XTHMX(0:N,0:N),XTXXTH(0:N,0:M
     +)
      DIMENSION BETAM(0:N),XBM(0:M),YXTH(0:M),THETAM(0:N,0:N)
      DIMENSION YXBM(0:M)
      DIMENSION CVRCM(0:N,0:N)
C         CALCULATE DEGREES OF FREEDOM AND DIVIDE INTO 1
      DF=1D0/(M-N)
C         CALCULATE MERGED CONSTANTS
      CALL TRNSFZ(XM,XTM,M,N)
      CALL MATMLT(XTM,THETAI,XTHM,N,M,M)
      CALL MATMLT(XTHM,XM,XTHMX,N,M,N)
      IPV=0
      CALL MATINV(XTHMX,N,N,IPV)
      CALL MATMLT(XTHMX,XTHM,XTXXTH,N,N,M)
      CALL MATVEC(XTXXTH,YM,BETAM,N,M)
      PRINT*,' ',' MERGED CONSTANTS'
      DO 2500 I=0,N
 2500 PRINT*,' ',I,BETAM(I)
C         CALCULATE ESTIMATED VARIANCE OF MERGED FIT
      CALL MATVEC(XM,BETAM,XBM,M,N)
      CALL VECSUB(YM,XBM,YXBM,M)
      CALL VECMAT(YXBM,THETAI,YXTH,M,M)
      CALL VECVEC(YXTH,YXBM,TEMP,M)
      VARM=DF*TEMP
      PRINT*,' ','ESTIMATED VARIANCE OF MERGED FIT'
      PRINT*,' ',' ',VARM
C         CALCULATE VARIANCE-COVARIANCE MATRIX
      CALL SCAMAT(VARM,XTHMX,THETAM,N,N)
      PRINT*,' ','VARIANCE-COVARIANCE MATRIX'
      DO 2510 I=0,N
      DO 2520 J=0,N
 2520 PRINT*,' ',I,J,THETAM(I,J)
 2510 CONTINUE
C         CALCULATE MATRIX CONTAINING STANDARD ERRORS,COVARIANCES,
C         AND CORRELATION COEFFICIENTS.
      PRINT*,' ','STANDARD ERROR(I=J),COVARIANCE(I<J),CORRELATION '
      PRINT*,' ','COEFFICIENTS(I>J)'
      CALL CVRCOR(THETAM,CVRCM,N,N,N)
      DO 2530 I=0,N
      DO 2540 J=0,N
 2540 PRINT*,' ',I,J,CVRCM(I,J)
 2530 CONTINUE
      END
```

```
 QV1   QV2      OBSERVED                       CALCULATED
 3.    0.         17486.4535292              17487.5335259
 3.    4.         14687.6345667              14682.0419301
 8.    8.         14180.1271055              14175.5752521
 0.    4.         13367.3042301              13367.6563264
 3.    2.         16066.6475222              16072.9523207
 9.    7.         15281.9128564              15287.3239519
 1.    5.         13117.5951259              13118.5212743
 1.    6.         12440.1462036              12437.5603405
 3.    8.         11968.913857               11971.2336055

   VARIANCE  27.1915530473326595545346-6
  VARIANCE COVARIANCE MATRIX ELEMENTS
  0 0 106.943773547659125535351
  0 1 -24.823005275304619886537406
  0 2 1.85548063271301953682941617
  0 3 29.7283146782022265361505984
  0 4 -3.03942206996610594956146727
  1 0 -24.823005275304619886537404
  1 1 9.6550118425412619750547072
  1 2 -.693722958795163151594637059
  1 3 -5.33970877953061435484753739
  1 4 .590342278864380529899535251
  2 0 1.85548063271301953682941615
  2 1 -.693722958795163151594637059
  2 2 .057672348852256607885234411
  2 3 .3823139216616248845298590695
  2 4 -.0423019804899164476142194149
  3 0 29.7283146782022265361505985
  3 1 -5.33970877953061435484753746
  3 2 .382319216616248845298590701
  3 3 10.8103680779663898684347119
  3 4 -1.12878957131627880276969448
  4 0 -3.03942206996610594956146727
  4 1 .590342278864380529899535256
  4 2 -.0423019804899164476142194155
  4 3 -1.12878957131627880276969448
  4 4 .12213769322157105367305532
STANDARD ERROR(I=J), CORRELCOEF(I>J),COVARIANCE(I<J)
  0 0 10.34136250524647603521 1765
  0 1 -24.8230052753046198865379406
  0 2 1.85548063271301953682941617
  0 3 29.7283146782022265361505984
  0 4 -3.03942206996610594556146726
  1 0 -.815910954530275794487410141
  1 1 2.94194014938123477429046276
  1 2 -.693722958795163151594637059
  1 3 -5.33970877953061435484753739
  1 4 .590342278864380529899535251
  2 0 .747127709611386315365481693
  2 1 -.981902610730813605940960774
  2 2 .240150679474901355252424936
  2 3 .382319216616249845298590695
  2 4 -.0423019804899164476142194149
  3 0 .874323771734915617085590976
  3 1 -.552031039636677918637007376
  3 2 .494196969797379890867983281
  3 3 3.29791241944651072678435463
  3 4 -1.12878957131627880276969448
  4 0 -.840985278867382339124252159
  4 1 .574176214296088263911799752
  4 2 -.594024737192207731212117987
  4 3 -.982353713159175053120706125
  4 4 .349482035620675435408365922
1
  VIBRATIONAL CONSTANTS FOR UPPER LEVEL
  0 16312.026857255936565862943
  1 436.758636992113042918613853
  2 .342474361766086486615621136
0
   VIBRATIONAL CONSTANTS FOR LOWER STATE
   3 716.167161677627612431597851
   4 -2.95885234656566905815542633
1
  QV1   QV2     OBSERVED                        CALCULATED
 14.    1.          21643.0000000            21645.5697255
```

```
  7.   1.        17515.0000000        17517.1503100
  4.   1.        17212.0000000        17199.6906566
  7.   3.        17107.0000000        17114.7119709
  2.   0.        17033.0000000        17041.7092610
  5.   2.        16915.0000000        16932.2802129
  3.   1.        16773.0000000        16763.6231663
  1.   0.        16614.0000000        16608.7402309
  4.   2.        16488.0000000        16494.6631921
  7.   4.        16434.0000000        16424.8376563
 17.  11.        16297.0000000        16300.2472034
 14.   9.        16215.0000000        16217.5145372
 13.   9.        15773.0000000        15765.9517442
  2.   2.        15623.0000000        15624.0777412
  3.   3.        15363.0000000        15361.1448271
   VARIANCE  84.8443137233809409472913037
  VARIANCE COVARIANCE MATRIX ELEMENTS
  0 0 69.9946554789276497208087301
  0 1 -18.3193667032877357317447143
  0 2 .96792810382089162866712156
  0 3 .656206970696071063059103397-
  0 4 .128530805840288421747521572
  1 0 -16.3193697032877357317447143
  1 1 12.7322975417575115351766951
  1 2 -.746534674235597031190447673
  1 3 13.0926491601496321953180176
  1 4 -1.27946175017026015676640097
  2 0 .967928103820851628667121557
  2 1 -.746534674235597031190447673
  2 2 .045283145415657263866536071
  2 3 -.7944483568043629649685615 5
  2 4 .0799805775413012916145822767
  3 0 .65620697069607106009103404
  3 1 13.0926491601486321853160177
  3 2 -.7944483568043629649685615 5
  3 3 24.710283012876976337858083
  3 4 -2.2876362343286097298660028 6
  4 0 .128530805840288421747521565
  4 1 -1.27946175017026015676640097
  4 2 .0799805775413012916145822766
  4 3 -2.2876362343286097298660028 6
  4 4 .220771981172538061928726964
STANDARD ERROR(I=J), CORRELCOEF(I>J),COVARIANCE(I<J)
  0 0 8.3603023557122412078896695
  0 1 -18.3193687032877357317447143
  0 2 .96792810382089182866712156
  0 3 .65620697069607106059103397
  0 4 .128530805840288421747521572
  1 0 -.514094389671820491416082998
  1 1 3.56823451327929279295364109
  1 2 -.746534674235597031190447673
  1 3 13.0926491601496321953180174
  1 4 -1.27946175017026015676640097
  2 0 .5440675494530600192346386 25
  2 1 -.983169283497392652108167776
  2 2 .212799367951659317666419827
  2 3 -.7944483568043629649685615 5
  2 4 .0799805775413012916145822767
  3 0 .0157899223919782759736377623
  3 1 .7341341202566763495111561203
  3 2 -.75103213439325961947526638-
  3 3 4.97094387545031291091131824
  3 4 -2.2876362343286097296680028 6
  4 0 .0327199980167859501284377335
  4 1 -.763135377706114958900364143
  4 2 .7799157423106246472063552343
```

```
 4 4 .40986379033061657265426117
1
 VIBRATIONAL CONSTANTS FOR UPPER LEVEL
 0 16321.3368038700816922543911
 1 429.369369587596502949386772
 2 .77476512225549496369511713
0
  VIBRATIONAL CONSTANTS FOR LOWER STATE
  3 720.18064535671168402472235
  4 -3.788295160865423351878651 45
1
   MERGED CONSTANTS
 0 16325.0860013430724641323019
 1 430.992738763138642018619323
 2 .757137465765772610872945945
 3 721.406462578690950569385459
 4 -3.69962785672620310479666648
 ESTIMATED VARIANCE OF MERGED FIT
   4.68365986021832319542077275
 VARIANCE-COVARIANCE MATRIX
 0 0 126.363261426977672167649463
 0 1 -14.8847784025539974174710745
 0 2 .636266650636370599569294269
 0 3 34.7536415518213556546556575
 0 4 -3.10748812164827308613720658
 1 0 -14.8847784025539974174710795
 1 1 6.08785529072724516123847419
 1 2 -.382724311901454576840520447
 1 3 .931640599155044541753524962
 1 4 -.134496379759094055850511191
 2 0 .636266650636370599569294266
 2 1 -.382724311901454576840520447
 2 2 .0271778217946922233681551316
 2 3 -.185417894407544335325907809
 2 4 .023127104722574241157378831
 3 0 34.7536415518213556546556575
 3 1 .931640599155044541753524952
 3 2 -.185417894407544335325907809
 3 3 18.8993081111965760822846654
 3 4 -1.86325815351165874859706127
 4 0 -3.10748812164827308613720658
 4 1 -.134496379759094055850511189
 4 2 .023127104722574241157378831
 4 3 -1.86325819351165874859706127
 4 4 .1346110604996165231458645 05
 STANDARD ERROR(I=J),COVARIANCE(I<J),CORRELATION
 COEFFICIENTS(I>J)
 0 0 11.2411414645923690629616723
 0 1 -14.8847784025539974174710795
 0 2 .636266650636370599569294266
 0 3 34.7536415518213556546556575
 0 4 -3.10748812164827308613720658
 1 0 -.536660706761101032779425021
 1 1 2.46735795755849647467935622
 1 2 -.382724311901454576840520447
 1 3 .931640599155044541753524962
 1 4 -.134496379759094055850511191
 2 0 .343337645134132077449334746
 2 1 -.340903671344469126015325347 9
 2 2 .164856973752074620472748857
 2 3 -.185417694407544335325937809
 2 4 .023127104722574241157378631
 3 0 .711159394668212126981648991
 3 1 .086854693700464577484 1321711
 3 2 -.258714856816529546415697774


 3 4 -1.86325819351165874859706127
 4 0 -.626635946663486074714521612
 4 1 -.12355477270461259777744252
 4 2 .314002243535114569975731 34
 4 3 -.971552620270823232296620879 7
 4 4 .441147436238252699523241266
```

Appendix B

RKR-IPA Program

The following section contains the RKR-IPA program as provided by C. R. Vidal.

Presented first is a written description of the program and instructions on the use of the program. Next, the original introductory comments by C. R. Vidal on the use of the program are presented.

Then a complete listing of the program and a sample output is presented.

Program Main (RKR-IPA Control)

Presented in the following section is a discussion of the RKR-IPA program provided by C. R. Vidal (Ref 41). The program MAIN contains a routine to perform RKR calculations and a routine to perform IPA calculations starting with the potential obtained from the RKR program. The program was originally written in Fortran IV to run on a CRAY-1 computer at the Max-Planck Institut fur Extraterrestrische Physik, Garching, Germany. It has been modified slightly to run on the CDC 6600 computer at the Air Force Institute of Technology, Wright-Patterson AFB, Ohio. The program, as presented in this appendix, is written in Fortran V. Comments provided by Vidal at the front of his program are included. PUNCH statements included by Vidal have been changed to comment cards. Many of the formatting statements have been changed from Hollerith editing to apostrophe editing formats.

Due to memory size constraints, 370 K octal, several arrays were reduced in size. Arrays now sized (2403) were originally sized (3601) in Vidal's program. Arrays sized (11,2403) were originally (24,3601) in size.

As sized, the program required a field length of 211,600 octal to run. A core memory size of 360 K was used. Maximum run times used for the RKR routine were less than 20 seconds. This involved the calculation of turning points (RMIN, RMAX) for 128 different energy levels.

Run time for the combined RKR-IPA routine ranged from 160 seconds for the calculation of parameters covering the following ranges:

v, vibrational quantum energy levels; v = 0 to 69

J, rotational quantum energy levels; J = 1

Iterations of IPA routine; n = 4

Array sizes; 1001 of 2403 maximum

to a maximum run time of 1150 seconds for:

v = 0 to 70

J = 2,6,10,14,17,20,21,23,28,30

n = 4

Array sizes; 1001 of 2403 maximum

One change has been made in the logic of Vidal's program. In the function subroutine FUNC, line 37, the third line after statement label 70, was changed from:

```
IF (XX.GT.RAA) RETURN
```

to

```
IF (KK.EQ.1) RETURN
```

The consequences of and reasons for suggesting this change are presented in the discussion of FUNC.

The discussion of Vidal's program is divided into two subsections: first, the discussion of the RKR portions of his program and, then, a discussion of the IPA portion. Within each section, the discussion is started with the inputs required of the user. Then the logic of the program is traced with explanations of the calculations and the subroutines used.

Numerical RKR Calculations

This section starts with the inputs required to perform the RKR calculations. The card number, the name of the input and the format of the input is given. The word CARD is used if only one card is required. CARDSET is used if more than one card (line of data) may be required.

CARD 1

NAME: ITEST

FORMAT: Integer.

ITEST should be placed in column 1. If ITEST = 0, the program stops. If ITEST = 1, the program is executed.

CARD 2 and 3

NAME: IHEAD

FORMAT: Lines 1-72 of these two cards.

These two cards contain the title to be printed at the top of the output. Relevant information that is suggested for the title includes the name of the molecule with the isotopes involved, the electronic state for which the calculations is performed, date, etc.

CARD 4

NAME: IIMS, ZMAS1, ZMAS2, ICODE

FORMAT: I4,2D16.9,32X,A4

IIMS must be 1 if the masses of the atoms are expressed in AMU's based upon the Carbon-12 scale and 2 if they are based upon the Oxygen-16 scale. ZMAS1 and ZMAS2 are the masses of the two atoms expressed in atomic mass units (AMU). The reduced mass of the two atoms may be entered in place of ZMAS1. If the reduced mass is used, ZMAS2 is left blank.

ICODE is the alphanumeric code used to describe the electronic state under investigation.

CARD 5

NAME: NDUN, JM(1), JM(2)...JM(NDUN)

FORMAT: 14I5

NDUN and JM specify the number of Dunham coefficients YDH and the order in which they will be read into the program.

CARDSET 6

NAME: YDH(1,1), YDH(2,1)...YDH(JM(2),1)
YDH(1,2), YDH(2,2)...YDH(JM(2),2)

.

.

.

YDH(1,NDUN), YDH(2,NDUN)...

YDN(JM(NDUN),NDUN)

FORMAT: 4D18.9

These cards contain the Dunham coefficients required as input for the RKR routine. The READ statement is structured so that JM(I) values of YDH(JM(I),I) are read in for each value of I with I ranging from 1 through NDUN. For each new value of I, the 1 through JM(I) values of YDH should be started on a new card. This means that the JM(1) coefficients Y(1,n) are read in, then the JM(2) YDH(2,n) coefficients, etc.

CARD 7

NAME: DE, TE

FORMAT: 2D15.8

DE is the dissociation energy and TE is the electronic term energy of the electronic state. Both are expressed in reciprocal centimeters. DE is the difference between the minimum in the potential of the electronic state and the dissociation energy. TE is the energy separation between the minimum of the potential curve and the minimum potential on the ground state of the molecule. If the ground state is being investigated, TE is omitted.

CARD 8

NAME: VFIN, VINC

FORMAT: 2F6.2

VFIN is the largest vibrational quantum number, v, for which the RKR routine calculates the classical turning points r minimum (RMIN) and r maximum (RMAX). The turning points are calculated starting with value of v = -0.25 and for each value of v from 0 to VFIN in increments of VINC. It is not necessary that either VINC or VFIN be whole numbers. That is, both may be decimal fractions. The quantity VFIN/VINC must not exceed 398.

CARD 9

NAME: IOPG

FORMAT: I1

IOPFG is the Klein action integral. "I" (see Eqs (32) and (81)), print switch.

All iterations are printed if IOPFG=1. If IOPFG=0, these values are not printed.

CARD 10

NAME: RLIM1, RLIM2, NEXT

FORMAT: 2F6.2,I2

FLIM1 and FLIM2 are the inner and outer limits of r, respectively to which the RKR curve will be extended. The curves will be extended by fitting formulas to points making the inner and outer portions of the curves plus any extra radius-potential energy pairs input as data to guide this fit. FLIM1 and RLIM2 also determine the range over which the final IPA curve will be expressed. RLIM1 and RLIM2 should be sized to contain any inner and outer radii generated by the RKR and IPA programs.

NEXT is the number of extra data points which will be used to guide the extension of the curve. NEXT must be less than 25 and may be 0 if no extra data points are to be added.

These data points must be obtained in one manner or another. The program does not specify how. But if these points are available, this card makes provision for entering them into the program.

CARDSET 11

NAME: R1(I),PE1(I), where I = 1 to NEXT

FORMAT: (4X,1PD16.9,7X,D16.9/)

If NEXT = 0, these cards are omitted. R1(I) and PE1(I) are the radius and potential energy pairs which will be used to guide the extension of the RKR curve which will be adjusted by the IPA program. R1(I) should be in angstroms. PE1(I) should be in reciprocal centimeters. These NEXT points, along with a given number of points from the inner and outer ends of the RKR curve, will be used to obtain a fit to formulas as described below to extend the original RKR curve to the RLIM1 and RLIM2 limits.

CARD 12

NAME: KFIT(1),KFIT(2),KOUT(1),KOUT(2),
KOUT(3),KOUT(4)

FORMAT: 6I5

KFIT(1) is the number of constants (An) used in fitting a formula to the inner portion of the RKR curves. The formula is of the form:

$$V(r) = 10^{A1+A2*X+A3*X^2...} \qquad (136)$$

where

$$x = \frac{r_e - r}{r_e}$$

KFIT(1)+2 is the number of data points taken from the inner portion of the RKR potential. These points, along with any extension data contained in CARDSET 11 for the inner portion of the curve, will be used to guide the extension of the curve to RLIM1. KFIT(2) is the number of constants (terms) used in the formula to extend the outer portion of the curve to RLIM2. The formula is of the form:

$$V(r) = A1\left(\frac{1}{r}\right)^{KOUT(1)} + A2\left(\frac{1}{r}\right)^{KOUT(2)} + A3\left(\frac{1}{r}\right)^{KOUT(3)} + \dots \qquad (137)$$

KOUT(I), as shown above, is the power to which each 1/r term is raised.
KFIT(2)+4 of the outermost turning points of the original RKR potential plus any

outer turning points included in CARDSET 11 are used in extending the curve to RLIIM2.

If CARD 12 is blank the default values for KFIT(1) through KOUT(4) are "2,4,0,6,8, and 10" respectively.

CARD 13

NAME: IPNRKR,IPNIPA

FORMAT: 2I2

These two values in Vidal's original program controlled the punching of an output deck for the RKR and IPA programs. As the PUNCH statements have been changed to comment cards, these two inputs should be 0 until the program in the appendix is modified. In the original program, if IPNRKR and IPNIPA equaled 1, the card decks were punched.

CARD 14

NAME: LTEST

FORMAT: I1

If LTEST = 0, the IPA routine is skipped and the program proceeds to read in the next set of data starting with the quantity ITEST. See CARD 1.

This completes the input required to run the RKR portion of the program. Input required for the IPA portion of the program will be presented with the discussion of the IPA calculations.

The following section discusses the functions of each of the major routines of the RKR program in the order which they are used. The headings used are the titles of the subroutines. Sections of the program which have a physical significance and are helpful in understanding the flow of the program are highlighted. Numerical techniques which perform the RKR calculations are discussed in more detail to aid the reader in understanding the technique. Calculations which are straightforward and not necessary to understanding the program are not described.

The line numbers in parenthesis refer to lines in the program in this appendix. In this development, program symbols corresponding to the mathematical symbols defined for the RKR calculation are given immediately following the mathematical symbols to which they correspond. The symbols are placed in brackets.

PROGRAM MAIN

PROGRAM MAIN acts as a controller directing the major objectives of the whole program, the calculation of an RKR curve and its adjustment by the IPA routine.

MAIN starts by insuring that mass units of the atoms are expressed in terms of the Carbon-12 system making conversions as directed by input data in IIMS (lines 12,23,24,28). The reduced mass, ZMU, is calculated in AMU's (line 27).

The Dunham constants, YDH, as specified by CARDSET 6, are read as a result of the statement CALL YDHP11 (line 30). The Dunham constant Y_{01} is assigned to "BE" the normal name of that spectroscopic constant as shown in Table I (line 31). Then using BE, the internuclear equilibrium distance, r_e , is calculated in angstroms according to the following formula:

$$r_e = \frac{FAC}{(BE)^{\frac{1}{2}}} = \left(\frac{h\ N_A}{4\pi c\mu Be}\right) \times 10^8 \qquad (138)$$

Then Y_{00} is calculated according to Eq (6) (lines 35 and 36).

SUBROUTINE RKR

This routine is called from line 70 of PROGRAM MAIN.

First a calculation is performed to determine the number of $G(v)$ energy levels which will be evaluated in the RKR routine. This number is assigned to the variable "M" (lines 34-39). Then values of the vibrational quantum number, v , for the $G(v)$ energy levels are calculated (lines 44 and 45). In the program, the term "TEMP" corresponds to "v" and the term "U" to $G(V)$. The function POLY performs the calculation of U [Gv] according to Eq (87) (line 46, statement label 110).

The program calculates, by an iterative technique, the value of "v_0" corresponding to Eq (90) (lines 51-62). It uses the Newton-Raphson method to find the value of "v_0" at which Gv+Y=0 (Eq 89)). The program uses "$v^* = Y_{00}/Y_{10}$" as its first estimate of "v_0" (line 55). From Eq (90), it can be determined that "v_0^*" is approximately "1/2" quantum units larger than the true value. Next, the value "$G(v_0^*)+Y_{00}$" is calculated (line 56). The Newton-Raphson method is used to converge to the value of "v_0" which satisfies "$G(v_0)+Y_{00}=0$" (lines 57-62, between statement labels 120 and 130).

For illustrative purposes, the Newton-Raphson method may be formulated as:

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} \tag{139}$$

By the definition of $f'(x)$:

$$f(x) = \frac{f(x_1)-f(x_2)}{x_1-x_2} \tag{140}$$

Hence:

$$x_2 = x_1 - f(x_1)\left[\frac{x_1 - x_2}{f(x_1) - f(x_2)}\right] \tag{141}$$

which corresponds directly to format of line 58. In Eq (141) $f(x)$ corresponds to "$G(v_0)+Y_{00}$". Loop 120 is repeated until a value of "v_0" is obtained such that "$G(v_0)+Y_{00}$" is close to 0 (line 57, statement label 120).

The remaining portion of the RKR routine, from statement label 130 to the end of the program, performs the integration required to solve Eqs (88) and (93) for "f" and "g". These, in turn, provide the classical turning points RMIN and RMAX of Eq (94). RMIN and RMAX values are obtained for each value of "v" [TEMP(I)] and corresponding "G(v)" [U(I)] as selected by inputs VFIN and VINC.

The solutions of the integrals for "f" and "g" contain a singularity. When "G(v´) = G(v)", the denominator [DENQ] of Eqs (88) and (93) go to 0 (lines 82,83,102, and 110). This singularity handled by assigning an "artificial" upper limit "v" [BS] to the integrals which is smaller than the true upper limit of the integral, TEMP(I), for the energy level "G(v)" [U(I)] involved. The artificial upper limit, BS, is allowed to approach the true value of "v" [TEMP(I)] in increasingly smaller steps until the solution of the integrals for two consecutive values of BS meet certain criteria. As BS is changed, the dv [d(BS)] contribution to the integrals is calculated and added to the sum for the integrals of "f" and "g". The rate at which BS approaches TEMP(I) is calculated in lines 72 and 130.

The criteria used for determining whether the solutions to the integrals are close enough to their true solution are given in lines 120-124 (statement labels 250-260). FEG is the value of the integral "f" for a given value of BS_n (line 120). FEG2 is the value by which the integral for "f" is in increased for the new value of BS_{n+} . Thus, if the ratio of the change in the value of the integral (FEG2) to the previous value for the integral (FEG) is less than 0.5×10^{-7} , the accuracy to which "f" has been determined is considered to be satisfactory. GEG2 and GEG in line 121 are tested in the same manner. In line 122, a ratio of changes (FEG2/FEG1) in the value of the integral "f" (FEG) for two consecutive calculations greater than 0.9 indicates that the accuracy of the integration is reaching a limit and should be halted. First, a ratio greater than 0.9 could indicate that the convergence to the true value is slower than desirable. Second, stopping the integration at this point is justified if the FEG1, FEG2 values are small. It is assumed that they are small. Similar arguments are given for GEG2 and GEG1.

The RKR program contains two integration routines. For the first three adjustments of BS, the upper limit of integration for "f" and "g", a Simpson rule integration is used. Lines 77-92 perform the integration of the functions for "f" and "g" over a range from VMIN (v) to BS on the first cycle. On the second cycle, VMIN is equated to BS, the lower limit of integration and a new upper limit BS is established as previously explained. In line 77-92, UV corresponds first to the v' and then to the $(G(v)-G(v'))$ of Eqs (88) and (93). And, expressed in the notation of the computer program, EV is the $G(v')$ and BI is the $B(v')$ of Eqs (88) and (93).

For the fourth through the twentieth adjustments of BS, a Gaussian integration routine is used to provide a higher degree of accuracy. The routine is contained in lines 93-113 (from statement label 180 through label 240). The abscissas [XGAUS] and weight factors [AGAUS] are listed at the start of the RKR routine for a Gaussian integration of moments where K=0 and N=4,6, or 8 depending upon the success of the iteration. The formula for the integration is (Ref 1:931):

$$\int x^k f(x)dx \approx \sum_{i=1}^{n} w_i f(x_i) \qquad (142)$$

Where

x_i = abscissas

w_i = weight factors

Finally, RMIN and RMAX for each v , *[TEMP] and* Gv , [U], are calculated in lines 139 and 140 per formula (95).

After all turning points have been calculated, control is transferred back to the program MAIN where CALL YDHP11(0) causes the input Dunham coefficients plus Y_{00} to be printed.

Routines EXTEND, GLSQ, FUNC, and EXTEND

The subroutine EXTEND, in conjunction with the above routines, performs a least-squares fit to the inner and outer portions of the RKR and extend them to RLIM1 and RLIM2 respectively. The fits are performed according to Eqs (117) and (118). Eq (117) expressed in the notation used in lines 16-31 of GLSQ and 31-39 of FUNC becomes:

$$\mathrm{Log}_{10}U(I) = Z(I) = B1[x(1)]^{0} + B2[X(I)]^{1} + B3[X(I)]^{2} + \ldots \qquad (143)$$

Z(1) is calculated in EXTEND and, as expressed, is the log to base ten of the energy. The inner turning radii, RMIN, are transferred into the X(I) array, and then the function FUNC (called from line 18 of GLSQ) transforms the variable X to the form given in Eq (117), i.e.,:

$$X = \frac{r_e - r_{min}}{r_e} \qquad (144)$$

Expressing Eq (124) in the notation of GLSQ yields a matrix equation of the form:

$$\begin{bmatrix} n & \Sigma x_i & \Sigma x_i^{2} & \Sigma x_i^{3} \\ \Sigma x_i & \Sigma x_i^{2} & \Sigma x_i^{3} & \Sigma x_i^{4} \\ \vdots & & & \vdots \\ \Sigma x_i^{3} & & & \Sigma x_i^{6} \end{bmatrix} \begin{matrix} B \\ B \\ \vdots \\ B \end{matrix} = \begin{matrix} Z \\ Z \\ \vdots \\ Z \end{matrix} \qquad (145)$$

or

A(J,K) * B(J) = BB(J)

where A(J,K) is formed in line 22 of GLSQ. BB(J) is formed in line 20. In line 23, the routine MATINV solves Eq (126) by inverting A(I,J), multiplying it times BB(J) and returns the B vector in place of the BB vector. The operation performed by MATINV may be expressed as follows:

$$B(J) = A(J,K)^{-1}BB(J) \qquad (146)$$

A similar pattern is followed for the outer portion of the curve except that formula (118) is used instead of (117).

After the fits have been performed, EXTEND calculates 20 additional points between the inner limit of the RKR curve and RLIM1, and 99 additional points between the outer end of the RKR curve and RLIM2. The points are calculated using fitting Eqs (117) and (118).

The change made in line 37 of FUNC affects the manner in which the curve fit is performed for values of r between the inner limit of the RKR curve and RLIM2. The difference occurs only if the extension data input in CARDSET 11 has an r , [R1(I)], between RLIM1 and the inner limit of the RKR curve. When FUNC is called from GLSQ which, in turn, has been called from EXTEND with an argument of "1" (CALL GLSQ(1)), the inner turning points are to be fit according to Eq (117). As written in Vidal's original program, line 37, "IF (XX.GT.AAA) RETURN", permitted the routine to continue on to the next statement when extra extension data was added with a radius less than the inner limit of the RKR curve [RAA]. This resulted in the returning of the energy [U(i)] of Eq (143) instead of the log of the energy, [Z(I)]. Then when the energy and the log of the energies are mixed in the fitting process, the fit is incorrect. By changing line 37 to "IF(KK.EQ.1) RETURN", the fit for the inner turning points is performed correctly. The variable "KK" is always "1" when the fit to the inner portion of the RKR curve is performed (line 31 of EXTEND). This change does not affect the operation of the program when FUNC is called from other routines. When FUNC is called from line 56 of FIPA, "KK" is equal to "0". Hence, the radius [XX] is the controlling factor in lines 7 and 8 of FUNC. Then when the potential energy for the extension points are being calculated, the routine proceeds through line 37 as it should.

This concludes the discussion of the RKR calculations.

Subroutine FIPA

Control of the program is transferred from MAIN to FIPA by line 83. This routine controls the IPA portion of the program. In the following section, the inputs required to run the FIPA routine are described.

FIPA Input

CARD 14

NAME: LTEST

FORMAT: I1

This input description is repeated from the RKR section. If LTEST is not equal to "0", the IPA calculation is continued and an IPA data deck is required as described below.

CARD 15

NAME: NI,NS,IPSIQ,MAXITT,EPSC

FORMAT: 4I4,D10.0

If NI=1, data from each SCHR iteration is printed.

If NI=0, the iterations are not printed.

If NS=1, the wavenumbers are printed at every IPSIQ points.

If NS=0, the wavenumbers are not printed.

EPSC is the convergence criterion for the solution of the Schroedinger wave equation for its energy eigenvalues, E_{vJ}. An EPSC of 0.001 wavenumbers is suggested as a good starting value.

MAXITT is the maximum number of times SCHR will attempt to satisfy the convergence criterion.

CARD 16

NAME: RMIN, RMAX, M NRPTT, NPL, MCH, LSW

FORMAT: 2F10.0,515

RMIN and RMAX are the minimum and maximum values over which the potential is evaluated by the IPA procedure. M is the number of points at which the potential will be evaluated. The maximum M should be 2401, for the program as written in the appendix.

Memory size limitations may dictate that fewer points be calculated.

NRPTT is the number of iterations performed in the IPA routine. On the last iteration, the rotationless potentials are calculated to obtain G_v and B_v .

NPL is the number of terms in the Legendre polynomial used to represent the correction, ΔV , to the energy potential.

MCH is the control used to punch a deck of the G_v and B_v values. As stated, all PUNCH cards have been changed to comment cards. If PUNCH statements are reactivated and MCH=1, the decks will be punched. Note that PUNCH is not a legitimate Fortran V statement.

If LSW=0, the first and last iterations of the IPA program are printed.

If LSW=1, all iterations are printed.

CARDSET 17

NAME: (MTRMIN(I),MTRIAL(I),BJTT(I),I=1,11)

FORMAT: (6(I2,I3,F7.0)/5(I2,I3,F7.0))

MTRMIN and MTRIAL defines the range of vibrational quantum numbers, v , which are investigated in the Schroedinger calculations.

These variables are input as "v+1" values.
Hence, an input of "1" corresponds to the
vibrational quantum number "0", etc.
BJTT determines the "J(J+1)" values for
which the corresponding MTRMIN-MTRIAL
range is calculated. The number of BJTT
values is limited to 11. The last BJTT
value must be "0" so that the rotationless
potentials may be calculated.

This completes the input required for the RKR-IPA program.

The IPA routine uses the Numerov-Cooley method to find numerical solutions to the Schroedinger equation (Refs 11:363; 14:1872). The routine presented here provides a method for finding solutions for bound states. Vidal also mentions methods for solving unbound states (Ref 43:7). They will not be presented here.

Terms initialized at the start of FIPA are described here. AZERO is the Bohr radius as measured in angstroms. Lines 47-49 repeat the calculation of "r_e", [RRE], the internuclear equilibrium separation according to Eq (119). Line 50 converts "r_e" [CRE] from angstroms to units of Bohr Radii.

Lines 51 and 52 insure that the limits of the extended RKR curve are beyond the RMIN-RMAX limits specified by the IPA input CARD 16. If not, the RMIN-RMAX limits are redefined to conform to the limits of the extended RKR curve.

Line 53 defines the step size of r [RH] for which the potential curve is calculated.

DO-loop 140 calculates the radius-potential energy pairs [P(J) and V(J)] which will be used in the IPA routine. The line of statement label 140 calls on the function FUNC to generate potential energies for each value of r . FUNC obtains the potential energies, V(r), for each value of r by performing a Lagrangian interpolation on the radius potential-energy pairs of the extended RKR curve. The Lagrangian technique may be expressed as follows (Ref 16):

$$V(r) = \sum_{i=0}^{n} \prod_{j=0}^{n} \frac{r-r_j}{r_i-r_j} \tag{147}$$

where r is the value for which V(r) is to be calculated. In FUNC, four points on both sides of r are used for the interpolation of each point. In this manner, the V(r) values are obtained for evenly spaced values of r from the unevenly spaced potentials of the RKR routine.

The section of FIPA following the comment "SEARCH FOR CENTRIFUGAL BARRIER," finds the maximum energy which a molecular system can have for a given rotational energy level, J , for a bound state. Expressed in the notation of the computer program, the effective potential energy, SX, is calculated by the formula:

$$SX = V(I)+ABE* \left[\frac{RE}{P(I)}\right]^2 *AJTT \qquad (148)$$

In lines 65-72, SX is calculated for rotationless potential energy and radius pairs, [V(I) and P(I)]. Hence, SX is the effective potential energy for a given radius and rotational quantum level, J . Fig B-1 shows the behavior of the potential for increasing J values.

The program first finds the minimum of the potential curve and assigns it to ASX. Once the minimum has been found, the potential increases with r . Each successive larger value of SX is assigned to TX. At the same time, ASX is equated to SX. This process is continued until the effective potential energy curves reaches a maximum as in Fig B-1. This maximum value of SX is retained in TX and is the sought for centrifugal barrier.

Having found the largest permissible value of SX (TX) for a given J value, the routine BETRL (line 73 of FIPA) finds the E_{vJ}[ETRIAL] which is just smaller than the centrifugal barrier, TX, and the corresponding rotational quantum number plus one (v+1). The "v+1" value is returned as NTRIAL to the FIPA routine. NTRIAL is then compared with input MTRIAL(KI) and the smaller value retained in the variable MTRIAL(KI) (lines 74-76). The ETRIAL corresponding to the retained MTRIAL(KI) is stored in the array variable ER(KI) (line 77).

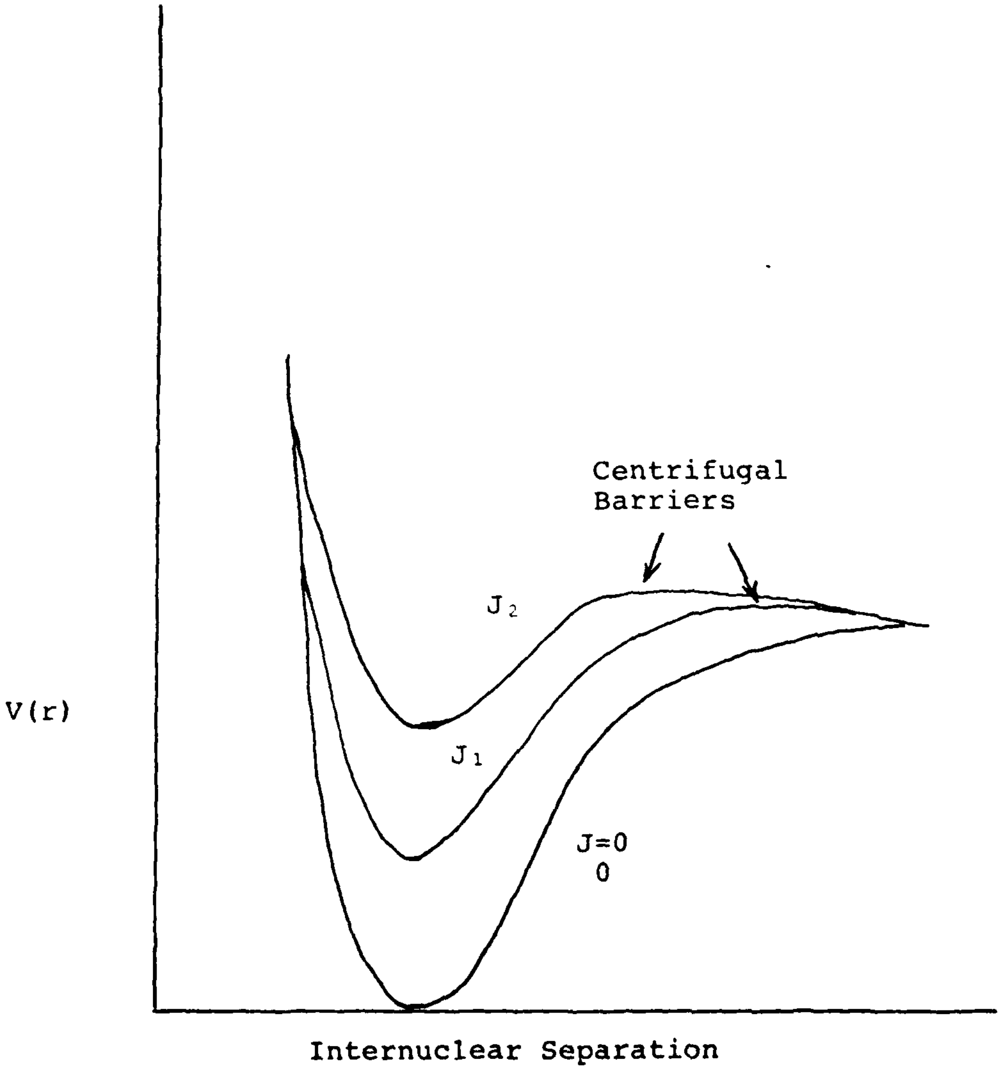

Fig B-1. Effective Potential Energy Curves for Three Rotational Energy Levels, J_1, J_2, and J_0

In addition to calculating the effective potential energy, the routine BETRL also calculates the values for B_v [BTRIAL], where J does not equal 0 . The variable B_v is determined according to the following relationship:

$$B_v\big|_J = \frac{\partial E_{vJ}}{\partial J(J+1)} = \frac{\partial \mathrm{ETRIAL}}{\partial J(J+1)} \qquad (149)$$

The next step is to determine the range of internuclear separations, r , which is to be considered in the IPA routine. This range is predetermined by the MTRIAL(J) and BJTT(J) values. This range is assigned to the variables RMII and RMAA.

DO-loop 200 performs the first step in identifying the RMII and RMAA values. The third line of the loop finds the first energy level, V(I), on the inner portion of the RKR curve which is smaller than or equal to the ER(KI) value being investigated. The value of the subscript for that V(I) is retained in N3AA. Line 88 finds the first energy level, V(I), on the outer portion of the RKR curve which is just larger or equal to the ER(KI) value being investigated. The subscript of that V(I) is retained in N3BB. The process is repeated for each ER(KI), and the smallest value of N3AA is retained as N3A (line 92, statement label 220). The largest value of N3BB is retained as N3B. The values N3A and N3B are the subscripts of the array P(I) which provide:

$$\mathrm{RMII} = P(\mathrm{N3A}) \qquad (150)$$

$$\mathrm{RMAA} = P(\mathrm{N3B}) \qquad (151)$$

In this manner, the limits of r over which the IPA routine and Schroedinger equation are to be investigated have been established so that they are consistent with the specified values BJTT(I) and MTRIAL(I) and the centrifugal barrier. The values MTRMIN(KI) along with the MTRIAL(KI) values which have been adjusted to be consistent with the centrifugal barrier, determine the range of vibrational quantum numbers, v, over which the RKR curve is evaluated for each value of BJTT(KI). This is true for all iterations of the IPA routine except the last iteration.

The range of vibrational quantum numbers, v, which are considered in the last iteration for each BJTT(KI) value may be different from that range specified by NTRMIN(KI) and MTRIAL(KI). The investigation of potential energy ranges specified by RMII and RMAA may uniquely define energy levels, E_{vJ}, for a specific BJTT(KI) value not included in the input NTRMIN(KI)-MTRIAL(KI) values. For the last IPA iteration, MTRIAL(KI) is replaced by LTRIAL(KI).

If the radius of the centrifugal barrier is greater than RMAA and, thus, outside the region investigated by previous iterations of the IPA routine, the maximum energy level to be investigated for a given value of BJTT is the smaller of the two following values:

$$TX = V(N3B) + ABE(RRE/RMAA) *AJTT \text{ (line 99)} \qquad (152)$$

$$SX = V(N3A) + ABE*(RRE/RMII) AJTT \text{ (line 101)} \qquad (153)$$

where V(N3A) is the potential energy corresponding to RMAA, and V(N3A) is the energy corresponding to RMII.

If the radius of the centrifugal barrier is smaller than RMAA, then the energy of the centrifugal barrier, YMAX(KI), for a given BJTT(KI) is compared with the value in Eq (152) and the smaller value retained for investigation and assigned to the variable. BETRL(TX) then identifies the first quantum vibrational-rotational energy level below TX for a given BJTT(KI). Then "v+1" is assigned to the LTRIAL(KI) variable.

Subroutine PLEGEN

Subroutine PLEGEN and lines 109-119 perform the calculations necessary to give a numerical value to the function f(r) which will be used to perform the calculations of Eqs (113), (114) and (115).

First, all the radii measurements are converted to units of Bohr radii.

Kosman and Hinze chose Legendre polynomials $P_i(x)$ to represent the $f_i(r)$ functions (Ref 23). Vidal found that attempting to extend calculations beyond RMII and RMAA, as specified by E_{vJ}, produced large oscillations. He finally settled upon a combination of Legendre polynomials and an exponential function to dampen the oscillations. This combination improved the convergence of the IPA method. The expression Vidal used is as follows (Ref 41:50):

$$\Delta V_0(r) = \sum_i c_i P_i(x)\exp(-x^{2n}) \tag{154}$$

where the typical range for "n" is 1<n<5. The Gaussian part of Eq (154) provides a smooth cutoff avoiding unphysical oscillations. The Legendre polynomials are calculated using the standard recursion relations (Ref 6:424):

$$(n+1)P_{n+1}(x) = (2n+1)XP_n(x)-nP_{n-1}(x) \tag{155}$$

where $P_1 = 1$ and $P_2 = X$.

Kosman and Hinze used a linear relationship between r and X such that X=1 for r=rmax and X=-1 for r=rmin . Vidal found this relationship to provide poor convergence when dealing with vibrational levels all the way to the dissociation limit and when dealing with anharmonic potentials. He stated that the reason for the poor convergence in the case of a highly anharmonic potential is that a linear interpolation tends to optimize only the outer turning points of the rotationless potential. To avoid this, Vidal chose a nonlinear interpolation given by:

$$X = \frac{(r-r_e)(r_{max}-r_{min})}{(r_{max}+r_{min})(r_e+r)-2r_{max}r_{min}-2r_e r} \tag{155'}$$

This relation assumes X=1, for $r=r_e$, and X=0 , for $r=r_{max}$ and X=1 , for $r=r_{min}$. The interpolation becomes linear for:

$$r_e = \frac{r_{max} + r_{min}}{2} \qquad (155)$$

This formulation treats the inner and outer turning points with comparable weight and reduces the number of Legendre polynomials in Eq (154).

Using these formulas, PLEGEN and DO-loop 270 calculate a Legendre polynomial F(J,I) with "NPL" terms (i.e., J=1 to NPL) for each of the turning points P(I) on the RKR potential where I=1 to M .

The section of FIPA from statement label 180 through the second line after statement label 780, contains the statements necessary to solve the Schroedinger wave equation (SWE) for its eigenvalues, E^0_{vJ} , and radial wave functions, ψ^0_{vJ} . It also calculates the correction to the potential, $\Delta v_0(r)$, necessary to make the eigenvalues obtained from the SWE consistent with those observed experimentally. The program returns to statement label 180 until all the "NRPTT" iterations have been completed. On the last iteration (NREP=NRPTT), lines 123-125 specify that NT3=NT1. The term "NTT" is equal to the number of BJTT values which are greater than "0".

As noted, the first use of the perturbation technique to adjust approximate potential energy curves is attributed to Hinze and Kosman (Ref 23). The technique used in this program to solve the Schroedinger equation is the Numerov-Cooley method (Refs 11; 14). The Numerov-Cooley method of solving the SWE was used by J. K. Cashion to test the validity of approximate eigenvalue equations developed by Pekeris for a rotating Morse oscillator (Ref 11).

The routine presented in this paper solves the SWE for bound states. Vidal discusses techniques for handling quasibound states. The techniques for evaluating quasibound states are not part of the present program but are here briefly discussed. One approach, Vidal used for quasibound states involved starting the integration of the SWE at small internuclear distances and looking for the maximum of the internal amplitude inside the centrifugal barrier as well as the phase shift of the partial wave outside the centrifugal barrier using a Breit-Wigner parametrization (Ref 12). Vidal also used a second approach in the same work (Ref 43). For quasibound states, he introduced an artificial barrier at large internuclear distances permitting the use of the Numerov-Cooley method. The eigenvalues he found in this manner were slightly higher than the energy eigenvalues derived from the maximum of the internal amplitude. Proper choice of the barrier kept the differences within the standard errors of the measurement. Using this technique, Vidal stated the same numerical method can be used for both quasibound and bound states.

Continuing with the program, as presented in this paper, it is necessary to transform the energy used in the SWE to units which are consistent with the units of length being used, Bohr radii. Thus far, energy has been expressed in terms of inverse centimeters, wavenumbers. To convert wavenumbers to energy units consistent with Bohr radii, it is necessary to divide by this factor (Ref 11:1873).

$$\frac{\hbar N_A}{4\pi c a_0 \mu_A} = \frac{60.19972628}{\mu_A} \text{ wavenumbers} \qquad (156)$$

where $a = 0.52197706$ and N_A = Avogadro's number. The inverse of this quantity is assigned to the variable ZEIN.

The effective potential energies (given according to Eq (148)) for the first BJTT value, for the whole range of the RKR curve, is calculated in DO-loop 340. The energy reference frame is shifted so that the dissociation energy [DE] is the zero energy level.

The lines between statement labels 340 and 360, establish the values of J(J+1) [BJTT(KI)] and the range of vibrational quantum numbers, NTRMIN through NTRIAL which will be considered for the experimental energy eigenvalue V(I) of statement label 340. Loop 660 also starts here.

If it is the last iteration of the IPA routine (NREP=NRPTT), the range of vibrational quantum numbers starts at "v+1=1" and extends through LTRIAL(KI) for each corresponding value of BJTT(KI). This range is specified by lines 140 and 141.

The value of J(J=1), to be investigated on a cycle of loop 660, is assigned to the variable AJTT in statement label 360.

CALL BETRL(TX) this time calculates all the term values, E_{vJ} [ETRIAL], for all values of "v+1" from 1 to NTRIAL with J specified by J(J+1) [AJTT]. B_v [BTRIAL] is also calculated over the same range. The rotational quantum number J corresponding to J(J+1) is assigned to the variable LJT in line 142.

The Schroedinger loop which calculates the radial wave functions [P(J)], B_{vJ} [BCALC], and E^0_{vJ} [ECALC] starts with line 152. The SWE loop (loop 600) starts by specifying the "v+1" values will be investigated, MTRMIN through MTRIAL. These variables were assigned their values in lines 137-141. Variables MA and MB are initiated to zero prior to entering the SWE routine.

Integer Function SCHR

The SCHR routine solves the Schroedinger equation by the Numerov-Cooley method. The routine is called by line 158 of FIPA. Using this method, each of the experimental term values is adjusted to be consistent with the whole RKR curve. Hence, all term values which were used to produce the RKR curve are indirectly used to adjust each eigenvalue, E_{vJ}, solution found by the SCHR routine.

Numerov-Cooley Method for Solving the SWE

The Numerov-Cooley method for solving the SWE is outlined here. Using Cooley's notation, the SWE may be expressed as follows:

$$P^{2}(r) = [U(R)-E]P(R) \tag{157}$$

$$P^{(n)} = \frac{d^{n}P}{d\,R^{n}}$$

where P(R) is the radial wavefunction and E are the eigenvalues of the SWE. Cooley defines the potential energy U(R):

$$U(R) = [J(J+1)-\Lambda^{2}]R^{-2}-Z_{a}Z_{b}R^{-1}+E_{el}(R) \tag{158}$$

In this paper, the contribution of the Λ quantum number, the z-component, due to the electronic angular momentum, is ignored. The electrostatic Coloumb repulsion energy of the nuclei, $Z_{a}Z_{b}R^{-1}$, and the electronic energy, $E_{el}(R)$, make up the vibrational (v+1/2) term of the E_{vJ}'s as expressed by Eq (2). The boundary conditions used are:

$$P(0) = 0, \text{ and } P(R) \text{ bounded} \tag{158'}$$

The following definitions are used to convert Eq (157) to a finite difference equation:

$$\begin{aligned} R_{i} &= h \qquad i = 0,1,2...n+1 \\ P_{i} &= P(R_{i}) \qquad (159) \\ U_{i} &= U(R_{i}) \end{aligned}$$

By dropping fourth order and higher terms in the series:

$$P_{i+1} + P_{i-1} = \sum_{k=0}^{\infty} \frac{2h^{2k}}{(2k)} P_{i}^{2k} \tag{160}$$

and by using the different equation to replace P_{i}^{2}, Cooley obtained the integration formula:

$$P_{i+1} + P_{i-1} - 2P_i = h^2(U_i - E)P_i \tag{161}$$

The error involved in Eq (161) is approximately $\frac{h^4}{12} P_i^{(4)}$. He then presented a higher order integration formula, developed by Numerov, which does not involve the calculation of additional P_i's. The formula is obtained by subtracting the product of $\frac{h^2}{12}$ times the following series:

$$P_{i+1}^{(2)} + P_{i-1}^{(2)} = \sum_{k=0}^{\infty} \frac{2h}{(2k)} P_1^{(2k+2)} \tag{162}$$

from Eq (160). Then dropping sixth and higher order terms in h , gives the differencing scheme used in Vidal's program:

$$Y_{i+1} + Y_{i-1} - 2Y_i = h^2(U_i - E)P_i \tag{163}$$

where:

$$Y_i = P_i - (h^2/12)\ P_i^{(2)} = [1-(h^2/12)\ (U_i-E)]\ P_i \tag{164}$$

The error for this formula is approximately $-\frac{h^6}{240} P_i^{(6)}$.

For all unbound states, $E>U(\infty)$, solutions exist for all E and, according to Cooley, may be approximated by using Eqs (161) or (163) to integrate outward starting with boundary values:

$$P = 0\ ,\ P = \text{a small arbitrary number} \tag{165}$$

For bound states, $E<U(\infty)$, only discrete eigenvalues, E , exist. The boundary conditions for solution to Eq (163) are:

$$P(0) = 0 \tag{166}$$

and for P(R) bounded:

$$P_{n+1} = \text{a small arbitrary number} \tag{167}$$

$$P_n = P_{n+1}\exp\left(R_{n+1}\sqrt{U_{n+1} - E} - R_n\sqrt{U_n - E}\right) \tag{167′}$$

The second condition results from the assumption that at R_n , U(R) is slowly approaching a constant value.

The method of solution involves starting with some E (i.e., the experimentally obtained term values) and with the boundary conditions specified by Eq (166) integrate outward to some point R_M using Eq (163). Then the wavefunctions P_i to P_m are normalized to P_m:

$$P_i^{out} = P_i/P_m \qquad i = 1,2,3,...m \tag{168}$$

Then the same procedure is followed starting at P_{n+1} and integrating inward to P_m . Again, the P_i values are normalized, this time, using the P_m^{in} value obtained in the inward integration. Hence, $p_m^{out} = p_m^{in} = 1$. At this point, a correction for E is determined from the difference in slopes of the two portions of the curve ($R<R_m$ and $R>R_m$). The inward-outward, E correction cycle is repeated until the value for E on successive iterations differs by some established limit, ε [EPS]. When this occurs, a satisfactory eigenvalue E has been obtained.

The correction formula is expressed as follows:

$$D(E) = (P'_{out} - P'_{in}) / \int_0^{\infty} [P(R)]\, dR \qquad (169)$$

where the P' terms are derivatives of the wavefunctions at R_m resulting from the inward and outward integration. Expressed as a difference equation which is consistent with Eq (163) D(E) is:

$$D(E) = [(-Y_{m-1}+2Y_m-Y_{m+1})h^{-2}+(U_m-E)P_m] / \sum_{i=1}^{n} P_i^2 \qquad (170)$$

Convergence difficulties with this approach may be encountered. Cooley describes the convergence of the technique and how to recognize what types of difficulties can be encountered. These will not be covered here.

Problems with convergence will be encountered if a P(R) is selected so that the magnitude of radial wavefunction at R_m is "0". Recalling that the procedure calls for normalizing the radial wavefunction P(R) at the point P_m , it is clear that dividing by a number close to "0" into larger numbers can introduce significant errors.

Cooley's program used the Numerov method to solve the SWE. His program was structured so that D(E) must be decreasing in magnitude from one iteration to the next; then, the $D(E)<\varepsilon$ convergence criterion is applied.

The problem of stopping at a radius R_m when $P_m(R)$ is zero, is handled rather nicely from the knowledge that for the anharmonic motion of a diatomic molecule, the wavefunction P(R) reaches a maximum at a radius near the outer portion of the potential. Thus, Cooley started his inward integration and stopped at the value of R_m such that P_m had stopped increasing, i.e., it had reached its maximum. This method finds the largest P and, hence, keeps the correction technique from becoming accidentally unstable due to a poor choice of P_m. This value of R_m is retained and the outward integration is then performed. This concludes the discussion of Cooley's article. His article includes a derivation of D(E) and further discussion of the convergence of the method.

The discussion of the SCHR routine is now continued. As in previous sections, the notation in Vidal's program will be placed in brackets following the notation of Cooley when use of both is desirable.

The routine SCHR starts by initializing the values H [H], h^2[H2], and $h^2/12$ [HV] of difference Eqs (159), (163) and (164). The value "NN" corresponds to the "M" of input CARD 16. Line 13 sets E_{vJ} [E] equal to the value of ETRIAL(I) where "I" corresponds to a "V+1" vibrational quantum number. The "I" value is specified by FIPA, DO-loop 600.

The rotational quantum number J being considered corresponds to the J(J+1) [AJTT] specified by statement label 360 of FIPA. The E_{vJ} [ETRIAL(I)] was calculated by CALL BETRL(TX), line 144 of FIPA.

Next, DO-loop 10 finds the value on the potential curve which is just greater than E_{vJ}[E] and identifies it temporarily by the subscript of V(LCRIT). If the inner potential V(IPP) does not extend above E_{vJ}[E], then an error message is printed indicating the failure of the integration routine with KERR=1. The loop 16 decreases the starting subscript of the potential to either V(1) or until "WCRIT>20.0" is satisfied. It is assumed that this criterion is sized so that for the minimum value of R considered, the magnitude of the wavefunction P(R) will be sufficiently small to satisfy the assumed boundary conditions, Eqs (166) and (167).

This assumption may be checked in the printout. Values for the inner and outer wavefunctions $P(R_{min})$ [S(MA)] and $P(R_{max})$ [S(MB)] are printed. In the introductory comments to his program, Vidal states that S(MA) and S(MB) should typically be of a magnitude of 1×10^{-10}, if the RMIN and RMAX limits are wide enough. This implies that the "WCRIT>20.0" will produce S(MA) and S(MB) of similar magnitude.

The process is repeated to find the first value greater than E_{vJ}[E] at the outer end of the potential. The routine then extends the potential to sufficient magnitude of R so that the value of the outer wavefunction S(MB) will be sufficiently small. Again, an error message is printed with "KERR=2" if the outer portion of the potential does not extend above E_{vJ}[E].

The values of NL1 and NL2 are assigned such that V(NL1) is the second value on the inner portion of the curve less than E_{vJ}[E] and V(NL2) is the first value greater than E_{vJ}[E] (lines 23 and 130). These values will be used as the limits S(NL1) and S(NL2) between which the number of codes (i.e., the number of times P(R) [S(R)] becomes zero) associated with each E are counted. This count is the determination of the vibrational quantum number v[KV] associated with that eigenvalue E_{vJ} (lines 120-123, DO-loop 70). These values are printed out in the program listing.

Following Cooley's method, the inward integration is started first. The outer numerical value for the wavefunction P_{n+1} [S(MB)] is assigned an arbitrary value of $1x10^{-10}$ (Eq (117)). The next point P_n [S(MB-1)] is evaluated according to Eq (167´).

The lines between statement labels 36 and 40 perform the inward integration until P(R) [S(I)] stops increasing. The largest value of the wavefunction, P_m , is assigned to the variable PM. The correspondence beween Eq (163) and the program is as follows:

$$Y_{i+1} + Y_{i-1} - 2Y_i = h^2 (U_i - E)\ P_i \qquad (163)$$

YA + YC - 2YB = H2*(GI)*S(M+1)   Line 66

$$Y_i = [1 - h^2/12\ (U_i - E)]\ P_i \qquad (164)$$

YC = [1.D0 - HV*GI] (SM)   Line 68

The portion of the wavefunction obtained from the inward integration is normalized by PM_{in} .

If S(I) goes negative on the inward integration, an error message indicating the failure of the SCHR routing is printed with "KERR=3" indicating the source of the failure.

The process is repeated starting at the inner portion of the potential curve and integration continued out to the radius corresponding to the previously identified PM, the point at which the wavefunction first reached a maximum for the inward integration. This wavefunction from S(MA) to PM is normalized with PM_{out} . The variable DF corresponds to the denominator ΣP_i^2 of Eq (170) (statement label 53). The variable F corresponds to numerator and the correction to E_{vJ}[E] is DE. This DE should not be confused with the DE of the rest of the program which is the dissociation energy.

The convergence criterion, as outlined by Cooley, is satisfied by the lines between statement labels 56 and 60. Restating that criterion, DE [DE=ABS($E_{new}-E_{old}$)] must be less than some ε [EPS] with the stipulation that E is converging on consecutive iterations. A converging E requires that DE be getting smaller and smaller. Vidal's program handles these requirements in the following manner. TEST is assigned a value of "-1". If the SCHR routine converges on every iteration, i.e., DE gets smaller on every iteration, TEST is assigned a positive value. Then line 112 is never applied. On the other hand, if DE increases, the

ε [EPS] criterion is never applied because TEST will remain negative. Hence, DE must get smaller which results in TEST being assigned a positive value before the convergence criterion is checked. This prevents the routine from accidentally satisfying the convergence criterion without true convergence being obtained. This still does not prevent the program from jumping from a solution for one vibrational quantum number v to an eigenvalue associated with a different v. This error can be detected in the printout by observing that a proper ordering of v[KV] is not maintained.

DO-loop 70 counts the number of times the wavefunction P(R) [S(J)] becomes "0". This number, as noted, corresponds to the vibrational quantum number v for eigenvalue E_{vJ}[E].

The last computation is the normalization of the wavefunction P(R) [S(J)] so that

$$\int_{J=MA}^{MB} S(J)*S(J)dH = 1 \tag{171}$$

The remainder of the SCHR routine is concerned with the option of printing the solution of the routine. This option is controlled by the "NS" input of CARD 15.

FIPA (Continued)

At this point, control is returned to FIPA. If the SCHR routine has been successful, a wavefunction ranging from

S(MA) to S(MB) is returned along with a new eigenvalue E_{vJ} [ECALC]. In this case, "SCHR=0" and the programs proceed to statement label 420.

When "SCHR=1", this indicates that the SCHR routine was converging towards the limit ε [DE], but that the limit was not achieved in the number of iterations permitted, MAXITT, specified by input CARD 15. In this case, the program proceeds to statement label 400, and LLK is incremented. The variable "LLK" is used to report the number of times the convergence criterion ε is not satisfied. This value is printed by the command in statement label 620.

If "SCHR=2" is returned from the routine SCHR, the routine has failed to converge for a specific E_{vJ} . The reason for the failure is specified by the value "KERR" specified in SCHR (lines 21, 37, or 69) and printed out by the command in statement label 83 of SCHR.

If SCHR fails, the program proceeds to statement label 300 and KLK is incremented. If the SCHR routine fails "KLIM" times (where KLIM is specified as "2" in line 147), the program is halted by CALL EXIT (line 163).

If SCHR has been successful at finding the wavefunction S(J) for a given eigenvalue ECALC, then control proceeds to label 420 where the limits of the Schroedinger loop are, if necessary, adjusted to be consistent with MA and MB. The expectation values of "$\left(\frac{1}{r}\right)^2$" are calculated for a specific of v and J by lines 169 through 173. Simpson's rule is used to perform the required integration:

$$B_v = \frac{\hbar}{4\pi\mu c} \left\langle \psi_{vJ} \left| \frac{1}{r^2} \right| \psi_{vJ} \right\rangle \qquad (172)$$

where ψ_{vJ} is the numerical wavefunction S(MA) to S(MB) returned from SCHR.

The eigenvalue ECALC is converted to the proper units and the reference changed so the bottom of the potential well is zero by adding the dissociation energy DE to the potential (line 157).

The experimentally determined eigenvalue, ETRIAL(I), (calculated from the Dunham coefficients by the routine PETRL), is also returned to the reference frame where the bottom of the potential well is zero (line 175). The difference [DIFF] between the experimental eigenvalue (ETRIAL) and the eigenvalue (ECALC) is then calculated. The variable DIFF is the ΔE_{vJ} of Eq (109).

Line 177 directs the program to advance to statement label 540, if the program is in the last iteration of the IPA routine as specified by NRPTT. This skips several calculations necessary to obtain the ΔV of Eq (113). These are not necessary because the last values calculated by the program will be printed and the routines necessary to calculate Eq (113) will be skipped.

If the program is not on the last iteration of the IPA routine, it calculates (Eq (114)) the expectation values

[FPL(k)] of the f(r)'s [FX(K,J)] of Eq (113) where the f(r)'s are expressed in terms of Legendre polynomials as expressed in Eqs (154), (155), and (155′). The polynomials for f(r) were calculated in DO-loop 270 FIPA (lines 180-186).

The reason for the statistical weight EWG in line 189 has not been determined at this time. It might be used to reflect the different uncertainties in the determination of ΔE_{vJ} for different positions on the potential curve.

Next I shall discuss the solving of Eq (115) for the coefficients c_i [COEFF(K)] . The equation is manipulated and constants calculated in the normal least-squares fashion according to Eqs (12-16).

The least-squares fit is performed according to the general formula:

$$B = (X^T X)^{-1} X^T \tag{13}$$

where X^T corresponds to:

$$BL(K) = \sum_{k=1}^{NPL} DIFF*FPL(K) \tag{172}$$

as defined by DO-loop 520. And $(X^T X)$ in notation of the computer program is:

$$AL(K,J) = \sum_{k=1}^{NPL} \sum_{j=1}^{NPL} FPL(j)*FPL(k) \tag{173}$$

The errors associated with the calculations are tabulated in several ways. The sum of the errors, $\sum_v \Delta E_{vJ}$

[DIFF] are calculated for each value of AJTT. This sum of differences expressed in the notation of the computer program is:

$$\mathrm{GVDIF} = \sum_{v\,=\,\mathrm{MTRMIN(KI)}}^{\mathrm{MTRIAL}} \mathrm{DIFF} \tag{174}$$

The average difference is calculated in line (219) as the variable GVDA. The root mean square error, GVDF2, is calculated in lines 199 and 217 according to the formula:

$$\mathrm{GVDF2} = \left[\frac{\Sigma\ \mathrm{DIFF}}{\mathrm{APLTST}}\right]^{\frac{1}{2}} \tag{175}$$

where APLTST is as defined in line 216.

The difference DIFB between B_v as calculated by Eq (172), and B_v as calculated by Eq (91) is obtained in line 202. This quantity is multiplied by 1000 and 1000*DIFB is the value printed in the output of the program.

The variable "NL" of lines 197 and 133 is a count of the total number of "v,J" combinations for which calculations are performed for one iteration of the FIPA. DO-loops 640 and 650 adjust the potential V(I) to reflect a new J(J+1) value for the next solution of the Schroedinger wave equation.

The average variance and the standard error of the fit used to obtain the "NPL" coefficients of the Legendre polynomials (Eqs (113) and (115)) for the "NL" combinations of "v,J" are calculated in lines 228 and 229.

On the first iteration, line 230 transfers the program to statement label 700 where the coefficients of the Legendre polynomials of Eq (115) are calculated. The routine MATINV called by line 242 inverts the matrix AL(K,J) which then corresponds to the (X^TX) of Eq (13) and returns the inverted value in the same matrix. The MATINV routine, using the inverted AL(K,J) matrix and BL(K) calculates the coefficients of the Legendre polynomials of Eq (115), and returns the coefficients in the BL(K) array. DO-loop 720 then assigns the BL(K) coefficients to the array COEFF(K). DO-loops 740 and 760, then use the coefficients c_i[BL(k)] and the expectation value FX(K,I) to calculate the correction potential $\Delta V(r)$ of Eq (113). Then in the same line, a new corrected potential is obtained (Eq (110)).

The minimum of the potential curve is found (VMIN) and a new Y_{00} [YDH(1,1)] Dunham coefficient is calculated (line 253).

At this point, program control returns to statement label 253 for the "NREP"th iteration of the inverse perturbation routine.

On the second and following iterations, the program continues on from line 230. The standard error of E_{vJ} for all combinations of "v,J" is assigned to GVT. Using the coefficients COEFF(K) and the "error" ERROR(K) of the previous cycle (see DO-loop 720, DO-loop 680 prints the constants [DBAA] of the Legendre polynomials used to calculate ΔV , the standard error of that constant [$T^{\frac{1}{2}}$ (line 236), and the ratio of the error to the constant, i.e., T/DBAA.

After the last iteration, iteration number "NRPTT", line 241 transfers the program out of the loop which performs the IPA calculations. DO-loops 820 and 840 calculate the correlation coefficients for the Legendre polynomials (Eq (16)).

The routine POTTAB (called from line 264 of FIPA) then takes the potential energy curve generated by the IPA routine and produces the final set of turning points for the eigenvalues E_{vJ} of the routine and a second potential arranged in order of increasing "r" from P(I) minimum to P(I) maximum.

POTTAB starts by finding the minimum potential V(I) and assigns that value of "I" to IMIN. Next, starting with the inner portion of the adjusted IPA potential, from V(1) to V(IMIN), CALL PLLYNN finds the inner turning radii (AINN(I) for each of the eigenvalues E_{vJ} [EEE(I)] which were defined in line 203 of FIPA. PLLYNN obtains the turning points by doing a Lagrangian interpolation to the IPA potential. The process is repeated from V(IMIN) to V(M) for each EEE(I) to obtain the turning points on the outer portion of the IPA potential. The vibrational quantum numbers, v[IA], the energy eigenvalues [EEE(I)], the inner and outer turning points [AINN(I) and AOUT(I)], and the corresponding B_v [BBB(I)] values are printed.

POTTAB then using the new IPA potential, P(I) and V(I), where I=I,M, and the original RKR curve XI(I) and Yi(I) where I-1,N, determines an "IPA" potential energy for each RKR turning point, XI(I), by interpolation of the IPA curve. The difference in RKR and IPA energies for that radius is calculated.

Next POTTAB estimates the standard error of the potential for each value of "r" [XI(I)]. This standard error is based upon Eq (110):

$$V(r) = V(r) + \Delta V_0(r) \tag{110}$$

The validity of the calculation used, is based upon the assumption that the routine has converged within some acceptable error limits to some V(r). Any error in V(r) is then associated with calculation of $\Delta V(r)$. The correction ΔV to the energy potential has been obtained using the Legendre polynomials of Eq (154). From the errors of the coefficients "c_i" used to calculate the correction potential, the error of the correction can be estimated. DO-loop 99 calculates the estimated standard error of the potential and prints it, the potential, the turning point, the difference between the RKR and IPA potential and the standard error of the potential.

Control of the program is returned from POTTAB to FIPA. FIPA prints out a summary of the sum of the differences for each value of J(J+1) calculated on each IPA iteration. It also prints out the average errors for all values of J(J+1) for each iteration. The program last of all prints out the original Dunham coefficients with the new Y_{00} which has been calculated to set the minimum of the potential energy curve to zero.

This completes the description of the RKR-IPA program for one of set data. Control is then passed back to MAIN. If new data is provided, the RKR-IPA calculations are repeated for the new data.

To avoid any loss of information, Vida's original comments on input and output are included in this appendix with the revised program.

```
      1.         PROGRAM MAIN
            C AMOS:  GCR.JLTHIND
            C       MAIN PROGRAM: RIPA SYSTEM
            C
            C        THIS PROGRAM IS A UNIFICATION OF THE RKR AND IPA PROGRAMS WHERE
            C        THE RKR POTENTIAL IS USED AS AN INITIAL POTENTIAL IN THE IPA
            C        PROCEDURE.
            C
            C        RIPA CONSTRUCTS A POTENTIAL CURVE FOR AN ELECTRONIC STATE OF A
            C        ROTATIONLESS DIATOMIC MOLECULE -- I.E., PAIRS OF INNER AND OUTER
            C        CLASSICAL TURNING POINTS AND ASSOCIATED ENERGY LEVELS -- FROM
            C        DUNHAM EXPANSION COEFFICIENTS BY USING THE RYDBERG-KLEIN-REES
            C        METHOD. IT THEN PERFORMS AN EXTRAPOLATION OF THE INNER AND OUTER
            C        TURNING POINTS. FINALLY, RIPA PERFORMS AN INVERTED PERTURBATION
            C        APPROACH WHERE THE MEASURED TERM VALUES ARE FITTED TO THE QUANTUM
            C        MECHANICAL ENERGY EIGENVALUES OF A ROTATING VIBRATOR BY MEANS OF
            C        A LEAST SQUARES FIT USING A VARIATIONAL METHOD.
            C
            C        THE INPUT CARD DECK OF THE PROGRAM RIPA MUST BE AS FOLLOWS.
            C
            C        THE FIRST CARD HAS ITEST IN COLUMN 1.  IF ITEST = 0, THE
            C        PROGRAM WILL STOP.  IF ITEST = 1, THE PROGRAM WILL START A
            C        COMPLETE CALCULATION SEQUENCE, AND THE DATA DECK MUST BE AS
            C        FOLLOWS.
            C
            C        THE NEXT TWO CARDS HAVE THE OUTPUT PAGE TITLE IN COLUMNS 1
            C        THROUGH 72.
            C
            C        THE NEXT CARD HAS IIMS,THE VALUES OF THE MASSES OF THE TWO ATOMS
            C        AND THE IDENTIFICATION CODE OF THE ELECTRONIC STATE UNDER STUDY
            C        IN FORMAT I4,2D16.9,32X,A4. THE VALUES OF THE MASSES SHOULD BE
            C        EXPRESSED IN ATOMIC UNITS.  IIMS MUST BE 1 IF THE CARBON SCALE
            C        IS USED AND MUST BE 2 IF THE OXYGEN SCALE IS USED.  THERE IS AN
            C        OPTIONAL WAY OF USING THIS MASS CARD.  INSTEAD OF LISTING THE
            C        MASSES OF THE TWO ATOMS SEPARATELY, THE REDUCED MASS OF THE
            C        MOLECULE (IN ATOMIC UNITS) MAY BE ENTERED IN THE FIRST MASS FIELD
            C        THE SECOND MASS FIELD MUST THEN BE LEFT BLANK. THE CHOICE OF
            C        CARBON OR OXYGEN SCALE MUST, OF COURSE, STILL BE ENTERED.
            C
            C        THE NEXT CARD READS NDUN,(JM(I),I=1,NDUN) IN FORMAT 11I5. THE
            C        NDUN VALUES OF JM: N1, N2, N3, .... SPECIFY THE NUMBER OF DUNHAM
            C        COEFFICIENTS Y(I,1), Y(I,2), Y(I,3), ....
            C        THE NEXT CARDS CONTAIN THE DUNHAM COEFFICIENTS Y(I,K) WHICH ARE
            C        READ IN GOING FROM I=1 TO NDUN: (Y(I,1),I=1,N1), (Y(I,2),I=1,N2),
            C        (Y(I,3),I=1,N3),...... IN FORMAT (4D18,9).
            C
            C        THE NEXT CARD CONTAINS THE DISSOCIATION ENERGY DE AND THE ELEC-
            C        TRONIC TERM TE IN FORMAT 2D15.8 AND EXPRESSED IN RECIPROCAL
            C        CENTIMETERS.  DE IS THE ENERGY SEPARATION BETWEEN THE POTENTIAL
            C        MINIMUM OF THE ELECTRONIC STATE UNDER STUDY AND ITS DISSOCIATION
            C        LIMIT. TE IS THE ENERGY SEPARATION BETWEEN THE POTENTIAL MINIMA
            C        OF THE ELECTRONIC STATE UNDER STUDY AND OF THE GROUND ELECTRONIC
            C        STATE OF THE MOLECULE.IF THE ELECTRONIC STATE UNDER STUDY IS
            C        ITSELF THE GROUND STATE, THIS CARD MUST BE BLANK.
            C
            C        THE NEXT CARD CONTAINS VFIN, AND VINC IN FORMAT 2F6.2. RIPA CAL-
            C        CULATES INNER AND OUTER TURNING POINTS FOR V = -0.25 AND FOR
            C        EACH VALUE OF V FROM ZERO TO VFIN IN STEPS OF VINC. IT IS NOT
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C         NECESSARY THAT VFIN, AND/OR VINC BE INTEGRAL. THE QUANTITY
C         VFIN/VINC MUST NOT EXCEED 399.
C
C         THE NEXT CARD IS THE KLEIN ACTION INTEGRAL PRINT SWITCH AND
C         CONTAINS IOPFG IN FORMAT I1. IT IS USED IN GENERATING THE
C         INITIAL RKR POTENTIAL. IF IOPFG=1, THE VALUES OF THE KLEIN ACTION
C         INTEGRALS ARE PRINTED FOR ALL OF THE ITERATIONS ASSOCIATED WITH
C         EACH OF THE VALUES OF V FOR WHICH PAIRS OF TURNING POINTS ARE
C         CALCULATED.  IF IOPFG=0, THESE VALUES ARE NOT PRINTED.
C
C         THE NEXT CARD CONTAINS RLIM1, RLIM2, AND NEXT IN FORMAT 2F6.2,I2.
C         RLIM1 AND RLIM2 ARE THE INNER AND OUTER LIMITS, RESPECTIVELY,
C         TO WHICH EXTENSIONS OF THE RYDBERG-KLEIN-REES TURNING POINTS
C         WILL BE ESTIMATED, IN A FASHION TO BE DESCRIBED BELOW. THE
C         INPUT QUANTITY NEXT IS THE NUMBER OF EXTRA EXTENSION DATA
C         POINTS TO FOLLOW. NEXT MAY NOT EXCEED 25 AND MAY BE ZERO, IF
C         NO EXTRA DATA POINTS ARE TO BE ADDED.
C
C         THE NEXT NEXT CARDS EACH CONTAIN R1(I) AND PE1(I) IN FORMAT
C         2D15.9. THE R1(I) AND PE1(I) ARE R AND POTENTIAL ENERGY PAIRS
C         WHICH MAY BE USED TO GUIDE THE EXTENSION TO THE RYDBERG-
C         KLEIN-REES TURNING POINTS, AS DESCRIBED BELOW. THE UNITS OF
C         THE R1(I) AND PE1(I) SHOULD BE ANGSTROMS AND RECIPROCAL
C         CENTIMETERS, RESPECTIVELY. NOTE....IF NEXT IS ZERO, THESE
C         CARDS MUST BE OMITTED FROM THE INPUT DECK.
C
C         THE NEXT CARD CONTAINS THE FITTING PARAMETERS KFIT(I),I=1,2 AND
C         KOUT(I),I=1,4 IN FORMAT 6I5. IF THE CARD IS BLANK THE PROGRAM
C         TAKES THE DEFAULT VALUES 2, 4, 0, 6, 5,10. FOR EXTRAPOLATING THE
C         INNER TURNING POINTS KFIT(1) CONSTANTS INSIDE AN EXP-FUNCTION
C         OF THE FORM EXP(A(1)+A(2)*X+...) ARE USED WHICH ARE DETERMINED
C         BY A LEAST SQUARES FIT OF THE KFIT(1)+2 INNERMOST RKR TURNING
C         POINTS. FOR EXTRAPOLATING THE OUTER TURNING POINTS KFIT(2) CON-
C         STANTS ARE USED IN A FUNCTION OF THE FORM SUM(A(K)*R**(-KOUT(K)))
C         WHERE KOUT SPECIFIES THE INVERSE POWERS OF THE INTERNUCLEAR DIS-
C         TANCE R IN THE LONG RANGE INTERACTION FUNCTION. THE CONSTANTS ARE
C         DETERMINED BY A LEAST SQUARES FIT OF THE KFIT(2)+4 OUTERMOST RKR
C         TURNING POINTS.
C
C         THE NEXT DATA CARD IS THE PUNCH CONTROL CARD AND CONTAINS IPNRKR
C         AND IPNIPA IN FORMAT 2I2. IF IPNRKR=1, AN OUTPUT DATA DECK (RKR)
C         IS PUNCHED. IF IPNIPA=1, AN OUTPUT DATA DECK (IPA) IS PUNCHED.
C
C         THE NEXT CARD HAS LTEST IN COLUMN 1. IF LTEST=0, THE VARIATIONAL
C         PROCEDURE IS SKIPPED AND THE PROGRAM RETURNS TO THE BEGINNING TO
C         RESUME THE NEXT PROBLEM BY READING ITEST (SEE ABOVE).
C
C         IF LTEST=1, THE FOLLOWING ADDITIONAL CONTROL CARDS ARE NEEDED TO
C         RUN THE INVERTED PERTURBATION APPROACH.
C
C         THE NEXT CARD CONTAINS CONTROL VARIABLES FOR SCHR AS FOLLOWS--
C         NI,NS,IPSIQ,MAXIT, AND EPS IN FORMAT 4I4,D10.0.
C         IF NI = 1 DATA FROM EACH ITERATION IS PRINTED.
C         IF NI = 0 THE ITERATIONS ARE NOT PRINTED.
C         IF NS = 1 THE WAVE FUNCTIONS ARE PRINTED AT EVERY IPSIQ POINTS.
C         IF NS = 0 THE WAVE FUNCTIONS ARE NOT PRINTED.
C         EPS IS THE CONVERGENCE CRITERION.  0.001 WAVENUMBERS IS A GOOD
C         STARTING VALUE.
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C      MAXIT IS THE MAXIMUM NUMBER OF TIMES SCHR WILL ATTEMPT TO SATISFY
C      THE CONVERGENCE CRITERION.  TEN IS A GOOD STARTING VALUE.
C
C      THE NEXT CARDS CONTAIN RMIN,RMAX,M,NRPTT,NPL,MCH,LSW
C      AND (NTRMIN(I),NTRIAL(I),BJTT(I),I=1,11)
C      IN FORMAT 2F10.0,5I5/5(I2,I3,F5.0)/3(I2,I3,F5.0).
C      RMIN AND RMAX ARE THE LOWER AND UPPER LIMITS OVER WHICH THE
C      POTENTIAL CURVE IS TO BE CONSIDERED IN THE IPA PROCEDURE.
C      M IS THE NUMBER OF POINTS TO BE USED IN THE INTERPOLATED WELL
C      MAXIMUM M IS 2401
C      NRPTT DEFINES THE NUMBER OF ITERATIONS FOR THE INVERTED PERTURBA-
C      TION APPROACH, WHERE THE LAST ITERATION CALCULATES THE ROTATION-
C      LESS POTENTIAL FOR THE DEFINITION OF THE GV AND BV.
C      NPL IS THE ORDER OF THE CORRECTION FUNCTION OF THE POTENTIAL
C      WHICH IS DESCRIBED BY A SUM OF LEGENDRE POLYNOMIALS.
C      NTRMIN AND NTRIAL ARE THE MINIMUM AND MAXIMUM VALUE OF V+1 FOR
C      WHICH TRIAL VALUES ARE GENERATED (USING THE DUNHAM COEFFICIENTS)
C      FOR CALCULATING THE SCHROEDINGER EQUATION. THE PROGRAM STOPS
C      AUTOMATICALLY AT THE LAST BOUND STATE.
C      BJTT ARE THE VALUES OF J(J+1) FOR WHICH THE POTENTIAL  IS CALCU-
C      LATED.
C      FOR MCH=1 THE PROGRAM PUNCHES A DECK OF ALL THE GV AND BV VALUES
C      CALCULATED IN THE LAST ITERATION.
C      FOR LSW=0 THE PROGRAM PRINTS THE FIRST AND LAST ITERATION OF THE
C      INVERTED PERTURBATION APPROACH. FOR LSW=1 ALL ITERATIONS ARE
C      PRINTED.
C
C      THIS COMPLETES THE INPUT DATA DECK FOR ONE ELECTRONIC STATE.
C      THERE ARE NOW TWO OPTIONS.  IF NO OTHER POTENTIAL CURVES ARE TO
C      BE CALCULATED, A BLANK CARD MUST BE AT THE END OF THE DATA DECK,
C      I.E., ITEST=0.  IF A SECOND INPUT DATA DECK IS TO FOLLOW FOR
C      ANOTHER ELECTRONIC STATE, THE ABOVE INSTRUCTIONS SHOULD BE
C      REPEATED, I.E., ITEST=1.
C
C      THE FOLLOWING COMMENTS APPLY TO THE PRINTED OUTPUT OF RIPA.
C
C      THE FIRST LISTING STARTS WITH THE TITLE AND THE IDENTIFICATION
C      NUMBER OF THE ELECTRONIC STATE. THE VALUES OF THE ATOMIC MASSES
C      (OR THE VALUE OF THE REDUCED MASS OF THE MOLECULE) ARE ALSO
C      PRINTED AND THE CHOICE OF CARBON OR OXYGEN SCALE IS NOTED.  THE
C      LISTING ALSO CONTAINS THE RESULTS OF THE RKR CALCULATIONS. FOR
C      EACH VALUE OF V IN STEPS OF VINC UP TO VFIN, THE POTENTIAL AND
C      INERTIAL ENERGIES, THE INNER AND OUTER TURNING POINTS, AND THE
C      FINAL VALUES OF THE KLEIN ACTION INTEGRALS ARE LISTED.  THE
C      POTENTIAL ENERGY IS THE EXPANSION FOR GV + Y(0,0) EVALUATED AT
C      V. THE INERTIAL ENERGY IS THE EXPANSION FOR BV EVALUATED AT V.
C      BOTH ARE EXPRESSED IN RECIPROCAL CENTIMETERS.  THE TWO TURNING
C      POINTS ARE EXPRESSED IN ANGSTROMS.  THIS LISTING WILL ALSO
C      INCLUDE THE INTERMEDIATE VALUES OF THE KLEIN INTEGRALS IF
C      IOPEG=1.
C
C      THE SECOND LISTING CONTAINS THE PARAMETERS THAT PERTAIN TO THE
C      FIT OF THE INNER AND OUTER EXTENSIONS OF THE RKR POTENTIAL.
C      FOR THE FUNCTIONS INDICATED ABOVE THE LISTING GIVES THE CONSTANTS
C      AND THEIR STANDARD ERRORS AND THE TOTAL STANDARD ERROR. IT SHOWS
C      THE FIT FOR THE EXTENSION OF THE INNER AND OUTER TURNING POINTS.
C      FINALLY, IF EXTRA EXTENSION DATA POINTS ARE USED, THE DIFFERENCES
C      BETWEEN THESE AND THE FIT FUNCTION ARE GIVEN FOR EACH OF THE
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C         INPUT R1(1).
C         FURTHERMORE, THE DUNHAM COEFFICIENTS ARE LISTED WITH THE CALCU-
C         LATED VALUE Y(0,0).
C
C         THE FOLLOWING PRINTOUT EXCEPT FOR THE DUNHAM COEFFICIENTS DOES
C         NOT APPEAR IF LTEST=0.
C
C         THE FOLLOWING LIST PRESENTS THE PARAMETERS OF THE INVERTED PER-
C         TURBATION APPROACH.
C
C         THE PROGRAM THEN GENERATES A PRINTOUT OF THE FIRST AND LAST ITE-
C         RATION OF THE INVERTED PERTURBATION APPROACH AND A PRINTOUT OF
C         THE INTERMEDIATE ITERATIONS IF LSQ = 1. FOR EVERY VALUE OF BJIT
C         IT GENERATES A TABLE WHICH CONTAINS FOR ALL VALUES OF V SPE-
C         CIFIED BY MTRMIN AND MTRIAL, THE QUANTUM MECHANICAL ENERGY EIGEN-
C         VALUE, THE MEASURED TERM VALUE, THE DIFFERENCE, THE CALCULATED
C         BV VALUE, THE DIFFERENCE TO THE MEASURED VALUE AND THE VALUES
C         OF THE WAVE FUNCTIONS FOR THE INNERMOST AND OUTERMOST MEMBERS
C         OF THE ARRAY S. MA AND MB ARE DETERMINED BY THE SCHROEDINGER
C         ROUTINE SUCH THAT S(MA) AND S(MB) ARE TYPICALLY 1.D-10 IF THE
C         LIMITS RMIN AND RMAX ARE MADE WIDE ENOUGH.
C         FOR THE LAST ITERATION THE TABLE CONTAINS VIBRATIONAL LEVELS
C         ABOVE THE UPPER DASHED LINE AND BELOW THE LOWER DASHED LINE WHICH
C         WERE NOT SPECIFIED BY THE DATA FIELD ABOVE, BUT WHICH ARE UNIQUE-
C         LY SPECIFIED BY THE RANGE OF INTERNUCLEAR DISTANCES WHICH HAD TO
C         BE ADJUSTED IN THE INVERTED PERTURBATION APPROACH.
C         THE MEASURED VALUES ARE THOSE DEFINED BY THE DUNHAM COEFFICIENTS.
C         EVERY TABLE IS CLOSED WITH THE AVERAGE DEVIATION AND THE STANDARD
C         ERROR IN CM**(-1).
C
C         AFTER EVERY ITERATION THE PROGRAM PRINTS THE COEFFICIENTS OF THE
C         LINEAR COMBINATION OF LEGENDRE POLYNOMIALS OBTAINED IN THE IN-
C         VERTED PERTURBATION APPROACH. IT ALSO LISTS THE STANDARD ERROR
C         AND THE RELATIVE STANDARD ERROR. IF THE LATTER QUANTITY IS LARGER
C         OR COMPARABLE TO 1 AFTER THE FIRST ITERATION, NPL CAN BE LOWERED
C         IN THE NEXT RUN OF THE PROGRAM. THE LAST SET OF COEFFICIENTS IS
C         FOLLOWED BY THE CORRESPONDING CORRELATION MATRIX.
C
C         THE NEXT LISTING GIVES THE INTERPOLATED INNER AND OUTER TURNING
C         POINTS AND THE BV VALUES FOR THE CALCULATED QUANTUM MECHANICAL
C         ENERGY EIGENVALUES OF THE ROTATIONLESS MOLECULE AS OBTAINED AFTER
C         THE LAST ITERATION.
C
C         THE FINAL LISTING CONTAINS A TABULATION OF THE ENTIRE POTENTIAL
C         WELL. THESE DATA ARE (1) THE TURNING POINTS AND ENERGIES FORM THE
C         LAST IPA ITERATION, (2) THE DIFFERENCE TO THE INITIAL RKR POTEN-
C         TIAL AND (3) THE CORRESPONDING STANDARD ERROR OF THE POTENTIAL.
C         IN ADDITION, IT CONTAINS THE 20 INNER AND 99 OUTER EXTENSION
C         POINTS FROM THE EXTRAPOLATION METHOD DESCRIBED ABOVE. THE 20
C         INNER EXTENSION POINTS ARE EQUALLY SPACED IN R BETWEEN RLIM1 AND
C         THE INNERMOST RKR TURNING POINT, AND THE 99 OUTER EXTENSION
C         POINTS ARE EQUALLY SPACED IN R BETWEEN THE OUTERMOST RKR TURNING
C         POINT AND RLIM2. ALL UNITS ARE ANGSTROMS AND RECIPROCAL CENTI-
C         METERS.
C
C         THE PRINT OUT CLOSES WITH A RECOMMENDED SET OF INTEGRATION LIMITS
C         RMIN AND RMAX AS OBTAINED IN THE IPA PROCEDURE. THEY SHOULD BE
C         USED IN THE FOLLOWING RUNS. IT IS FOLLOWED BY A SUMMARY OF THE
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C     STANDARD ERRORS OF ALL ITERATIONS AND A TABLE OF THE DUNHAM COEF-
C     FICIENTS WITH A CORRECTED VALUE OF Y(0,0) SUCH THAT THE POTENTIAL
C     MINIMUM DEFINES ZERO ENERGY.
C
C     THIS COMPLETES THE PRINTED OUTPUT FOR ONE ELECTRONIC STATE.  IF
C     DATA FOR MORE THAN ONE STATE ARE INCLUDED IN THE INPUT DECK, THE
C     ABOVE OUTPUT IS REPEATED.
C
C     THE FOLLOWING COMMENTS APPLY TO THE PUNCHED OUTPUT OF RKR.
C
C     IF IPNRKR=1 AND/OR IPNIPA=1, A DECK IS PUNCHED WHICH IS TAILORED
C     TO SERVE AS INPUT TO OTHER PROGRAMS. ALL UNITS ARE ATOMIC MASS
C     UNITS (CARBON SCALE), ANGSTROMS, OR RECIPROCAL CENTIMETERS.
C     FOR IPNRKR=1 ONE OBTAINS THE RKR-POTENTIAL.
C     FOR IPNIPA=1 ONE OBTAINS THE IPA-POTENTIAL.
C
C     THE FIRST CARD CONTAINS THE REDUCED MASS OF THE MOLECULE
C     (AND EXPRESSED IN ATOMIC MASS UNITS, CARBON SCALE) AND ICODE IN
C     FORMAT 36X,D16.9,16X,A4.
C     THE NEXT CARD READS NDUN,(JM(I),I=1,10) IN FORMAT 11I5. THE NDUN
C     VALUES OF JM: N1, N2, N3, .... SPECIFY THE NUMBER OF DUNHAM
C     COEFFICIENTS Y(I,1), Y(I,2), Y(I,3), ....(AS EXPLAINED ABOVE)
C
C     THE NEXT CARD CONTAINS DE AND TOE IN FORMAT 2D15.8.  DE IS THE
C     ENERGY SEPARATION BETWEEN THE BOTTOM OF THE ROTATIONLESS
C     POTENTIAL WELL OF THE ELECTRONIC STATE UNDER STUDY AND ITS
C     DISSOCIATION LIMIT.  TOE IS THE ENERGY SEPARATION BETWEEN THE
C     BOTTOM OF THE ROTATIONLESS POTENTIAL WELL OF THE NEUTRAL OR IONIC
C     ELECTRONIC STATE UNDER STUDY AND THE V=0, J=0 LEVEL OF THE
C     GROUND ELECTRONIC STATE OF THE NEUTRAL MOLECULE.  NOTE.... IF
C     ELECTRONIC STATE UNDER STUDY IS ITSELF THE GROUND STATE OF THE
C     NEUTRAL MOLECULE, THEN TOE=-Y(0,0).
C
C     THE NEXT CARD CONTAINS N IN FORMAT I3, WHICH IS THE NUMBER OF R
C     AND POTENTIAL ENERGY PAIRS TO FOLLOW.
C
C     THE NEXT N CARDS CONTAIN THE R AND POTENTIAL ENERGY PAIRS WITH
C     TWO PAIRS PER CARD IN FORMAT 2D16.9,4X,2D16.9. THE DATA ON THESE
C     CARDS IS THAT TABULATED IN THE FIRST TWO COLUMNS OF THE THIRD
C     OUTPUT LISTING.
C
C     THIS COMPLETES THE PUNCHED OUTPUT FOR ONE ELECTRONIC STATE.  IF
C     DATA FOR MORE THAN ONE STATE ARE INCLUDED IN THE INPUT DECK, THE
C     ABOVE OUTPUT IS REPEATED.
      DIMENSION KIMS(2),ZIMS(2),NFT(2),LOUT(4),IHEAD(36)
      COMMON/RPW/R1(25),PE1(25),NEXT
      COMMON/YD/YDH(20,10),IN(10)
      COMMON/FC/F(11),G(11),RE,RAA,RBB,KFIT(2),KOUT(4)
      COMMON/EX/EV(921),UV(921),N
      DATA KIMS/4HC=12,4HO=16/
      DATA NFT/ 2, 4/
      DATA LOUT/ 0, 6, 8, 10/
      DATA ZIMS/ 1.0, 0.999682165/
C     RKR USES THE FOLLOWING FACTORS FOR CONVERTING BETWEEN MASS SCALES
C     AND DIFFERENT PHYSICAL UNITS.
C     ZIMS(2) IS 15.99491464/16, WHICH IS THE MASS OF OXYGEN ON THE
C    CARBON SCALE DIVIDED BY THE MASS OF OXYGEN ON THE OXYGEN SCALE.
C     FACMU=SQRT(H-BAR*AVOGADROS NUMBER/(4*PI*C))*10**8
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DO=-LONG/-OT,ARG=-COMMON/-FIXED,CS= USER/-FIXED,DB= TB/ SB/ SL/ ER/-ID/ PMD/-ST,AL
FTN5,DB.

              PROGRAM MAI
        C        RKR1N1.1 0, 10 DEC .9-2
              DIMENSION ZIMS(2),NFT(2),LCUT(4),IHEAD(36)
              COMMON/RPW/R1(25),PE1(25),NEXT
              COMMON/YD/YDH(20,10),IY(10)
              COMMON/FC/F(11),H(11),RE,RAA,RBB,KFIT(2),KCUT(4)
              COMMON/EX/EV(521),LV(521),M
              CHARACTER KIMS(2)*4
              DATA (KIMS(I),I=1,2)/'C=12','O=16'/
              DATA NFT/ 2, 4/
              DATA LCUT/ 0, 6, 6,10/
              DATA ZIMS/ 1.0, 0.999682165/
        C        RKR USES THE FOLLOWING FACTORS FOR CONVERTING BETWEEN
        C        MASS SCALES AND DIFFERENT PHYSICAL UNITS.  ZIMS(2) IS
        C        15.99491464/16, WHICH IS THE MASS OF OXYGEN ON THE CARBON SCALE
        C         DIVIDED BY THE MASS OF OXYGEN ON THE OXYGEN SCALE.
        C        FACNUM=SQRT(H-BAR*AVOGADROS NUMBER/(4*PI*C))*10**8
              FACNUM=4.105804548
        C     .........READ IN INPUT DATA
         10   READ 109,ITEST
              IF(ITEST.EQ.0) STOP
              READ 110,IHEAD
              READ 111,IIMS,ZMAS1,ZMAS2,ICODE
              IF((IIMS.NE.1).AND.(IIMS.NE.2)) IIMS=1
        C     .........PUT REDUCED MASS INTO ZMU
              ZMU=ZMAS1
              IF(ZMAS2.GT.0.) ZMU=ZMAS1*ZMAS2/(ZMAS1+ZMAS2)
              ZMU=ZMU*ZIMS(IIMS)
              FAC=FACNUM/SQRT(ZMU)
              CALL YDHF11(3)
              BE = YDH(1,2)
              RE=FAC/SQRT(BE)
              READ 112,DE, E
        C     ..........CALCULATE Y00
              A2=-YDH(2,2)*YDH(2,1)/(12.0D+0*BE)
              YDH(1,1)=(BE+YDH(3,1))/4.0D+0+A2+A2*A2/BE
              READ 113,VFIN,VINC
              READ 109,ICFFG
              READ 113,RLM1,RLM2,NEXT
        C     ..........READ EXTRA EXTENSION DATA IF NECESSARY
              IF (NEXT.LE.25) GO TO 20
              PRINT 103
              STOP
         20   IF (NEXT.LT.1) GO TO 40
              DO 30 I=1,NEXT
          30  READ 104,R1(I),PE1(I)
         40   READ 116,(KFIT(I),I=1,2),(KCUT(I),I=1,4)
              DO 50 I=1,2
              IF(KFIT(I).EQ.0) KFIT(I) =NFT(I)
              IF(KFIT(I).GT.11) KFIT(I)=11
         50   CONTINUE
              DO 60 I=1,4
              IF(KCUT(I).EQ.0) KCUT(I) = LCUT(I)
         60   CONTINUE
              READ 109,IPNRKR,IPNIFA
```

```
C     ............PRINT OUT THE INPUT DATA
      PRINT 114,IHEAD
      PRINT 115,ICODE
C     ............PRINT THE MASSES AND THEIR UNITS
      IF (ZMAS2.LE.0.0) GO TO 70
      PRINT 116,KIMS(IIMS),ZMAS1,ZMAS2
      GO TO 80
 70   PRINT 117,KIMS(IIMS),ZMAS1
 80   PRINT 105,DE,TE
      PRINT 106,RLM1,RLM2,VFIN,VINC,ICRFG,IPNRKR,IPNIPA
C     ............PRINT EXTRA EXTENSION DATA IF NECESSARY
      IF(NEXT.LT.1) GO TO 90
      PRINT 107
      PRINT 108,(R1(I),RE1(I),I=1,NEXT)
 90   CALL RKR(VFIN,VINC,ICRFG,FAC)
      CALL YDHP11(0)
      PRINT 114,IHEAD
C     ......EXTRAPOLATE FOR END POINTS OF POTENTIAL FUNCTION
      CALL EXTEND(RLM1,RLM2)
      M=2*M+120
      IF(IPNRKR.NE.1) GO TO 95
C     PUNCH 102,IIMS,ZMAS1,ZMAS2,ZMU,ICODE
C     CALL YDHP11(IPNRKR)
C     PUNCH,112,DE,TE
C     PUNCH 119,M
C     PUNCH 120,(EV(I),UV(I),I=1,M)
 95   PRINT 121
      CALL FIPA(ZMU,DE)
      CALL YDHP11(0)
      IF (IPNIPA.NE.1) GO TO 10
C     PUNCH 102,IIMS,ZMAS1,ZMAS2,ZMU,ICODE
      CALL YDHP11(IPNIPA)
C     PUNCH 112,DE,TE
C     PUNCH 119,M
C     PUNCH 120,(EV(I),UV(I),I=1,M)
      GO TO 10
 102  FORMAT (I4,3D16.9,16X,A4)
 103  FORMAT(37H0TOO MANY EXTRA EXTENSION DATA POINTS)
 104  FORMAT (2D16.9)
 105  FORMAT(//6H DE = ,D15.7,10X,6H TE = ,D15.7/)
 106  FORMAT(2X,'LIM1 = ',F9.4,' LIM2 = ',F9.4,' VFIN = ',F7.2,
     +'  VINC = ',F7.2//'  ICRFG = ',I1,'  IPNRKR = ',I1,
     +' IPNIPA = ',I1/)
 107  FORMAT('  THE FOLLOWING DATA WERE INCLUDED IN THE LEAST-SQUARES
     +FIT THAT DETERMINED THE COEFFICIENTS OF THE XTEN-'/'
     +  SION FUNCTION  TO THE RKR TURNING POINTS..'//
     +10X,'R',15X,'POTENTIAL ENERGY '/)
 108  FORMAT(4X,1PD16.9,7X,D16.9/)
 109  FORMAT(2I2)
 110  FORMAT(18A4)
 111  FORMAT(I4,2D16.9,32X,A4)
 112  FORMAT(2D15.9)
 113  FORMAT(2F6.2,I2)
 114  FORMAT(2X,18A4/2X,18A4)
 115  FORMAT(//'  THE CODE NUMBER FOR THIS STATE IS  ',A4)
 116  FORMAT(//'THE MASSES OF THE TWO ATOMS,'/'  BASED ON ',A4,' ARE ',
     +1PD16.9,'  AND  ',D16.9/)


 117  FORMAT(//'  THE REDUCED MASS OF THE TWO ATOMS,BASED ON  ',A4,'
     +  IS  ',1PD16.9)
 118  FORMAT(10I5)
 119  FORMAT(I3)
 120  FORMAT(2D16.9,4X,2D16.9,4X)
 121  FORMAT('   BEGINNING OF INVERTED PERTURBATION APPROACH '/)
      END
```

```
      SUBROUTINE RKR(VFIN,VINC,IOPFG,FAC)
C        RKR PROCEDURE
      DIMENSION HI(101),TEMP(400),DERQ(8),MZ(3),IZ(3),XG(4),YG(4)
      DOUBLE PRECISION AGAUS(3,8),XGAUS(3,8)
      COMMON/YD/YDH(20,10),IM(10)
      COMMON/EX/EV(521),UV(521),M
      COMMON/RX/RMIN(400),RMAX(400),U(400)
C     ........INTEGRATION CONSTANTS(ABRAMOWITZ,P.921)
C        THE XGAUS ARE THE ABSCISSAS AND AGAUS ARE THE WEIGHTING FACT
C        FOR A GAUSSIAN INTEGRATION OF MOMENTS WHERE N=8 ARE [illegible]
C        4,6, OR 8 DEPENDING ON THE DEGREE OF SUCCESS OF THE
C        ITERATION.
         DATA XGAUS/0.0198550717512320D0,0.0337652428984240D0,0.[illegible]
     +0297400,
     +0.1016667612931860D0,0.169395306766867D0,0.33[illegible]D0,
     +0.2372337950418360D0,0.3806904069584020D0,0.6699905217924280D0,
     +0.4082826787521750D0,0.6193095930415980D0,0.9305681557970 2.D0,
     +0.5917173212478250D0,0.8306046932331320D0,0.0D0,0.7627662049581640D0,0
     +0.9662347571015760D0,0.0D0,0.8983332387068140D0,0.0D0,0.0D0,0.980144
     +928248768D0,
     +0.0D0,0.0D0/
      DATA AGAUS/0.0506142681451880D0,0.0856622461895850D0,0.173 274.25[illegible]
     +27D0,
     +0.1111905172266870D0,0.1803807865240700D0,0.3260725774312[illegible]D0,
     +0.1568533229389440D0,0.2339569672863450D0,0.3260725774312[illegible]D0,
     +0.1813418916891810D0,0.2339569672863450D0,0.1739274225687270D0,
     +0.1813418916891810D0,0.1803807865240700D0,0.0D0,0.1568533[illegible]44D0,
     +0.0856622461895850D0,0.0D0,0.1111905172266870D0,0.0D0,0.0D0,0.0506[illegible]
     +2681451880D0,
     +0.0D0,0.0D0/
      DATA MZ/101,81,61/
      DATA IZ/8,6,4/
C     ..CALCULATE TEMP(THE V) AND U(THE GV) FOR EACH TURNING POINT
      M=VFIN/VINC+0.5D0
      M=M+2
      IF(M.LE.400) GO TO 100
      IVINC=100./(VFIN/3.5+1.)
      VINC=1./FLOAT(IVINC)
      M=VFIN/VINC + 2.5
      PRINT 291,VINC
  100 TEMP(1)=0.25D+0
      U(1)=POLYN(TEMP(1),1)
      DO 110 I=2,M
      TMP=FLOAT(I-2)*VINC+0.5D0
      TEMP(I)=TMP
  110 U(I)=POLYN(TMP,1)
      STEP=.9D0
      PRINT 294
C        COMMENCE FINDING TURNING POINTS BY INTEGRATION AND
C     ITERATE TO A BUILT IN LIMIT OF PRECISION
      SVTR=0.0
      VTR=0.0D0
      SETR=POLYN(VTR,1)
      IF (ABS(SETR).LT.1.0D-8) GO TO 130
      VTR=-YDH(1,1)/YDH(2,1)
```

```
            ETR=POLYN(VTR,1)
      120   IF (ABS(ETR).LT.1.0D-6) GO TO 130
            XTR=SVTR-(SETR*(SVTR-VTR))/(SETR-ETR)
            SVTR=VTR
            VTR=XTR
            SETR=ETR
            ETR=POLYN(XTR,1)
            GO TO 120
      130   VMINS=VTR-0.5
            DO 280 I=1,N
            VMIN=VMINS+0.5
            FEG=0.D0
            GEG=0.D00
            LT=1
            IGD=0
            IFD=0
      140   BS=VMIN+(TEMP(I)-VMIN)*STEP
            IF(LT.GT.3) GO TO 180
            MQ=MZ(LT)
            KM=MQ-2
            A=(BS-VMIN)/FLOAT(MQ-1)
            DO 160 J=1,MQ
            UV(J)=VMIN+FLOAT(J-1)*A
            EV(J)=POLYN(UV(J),1)
            IF (IGD.EQ.0) BI(J)=POLYN(UV(J),2)
            DENQ(1)=U(I)-EV(J)
            UV(J)=1.D0/SQRT(ABS(DENQ(1)))
      160   EV(J)=BI(J)*UV(J)
            FSUM=UV(1)+4.D0*UV(MQ-1) +UV(MQ)
            GSUM = EV(1) + 4D0*EV(MQ-1) + EV(MQ)
            DO 170 J=2,KM,2
            FSUM=FSUM + 4.D0*UV(J) + 2.D0*UV(J+1)
      170   GSUM = GSUM + 4.D0*EV(J) + 2.D0*EV(J+1)
            FEG2=A*FSUM/3.D0
            GEG2=A*GSUM/3.D0
            IF (LT.GT.1) GO TO 250
            GO TO 260
      180   IZDO=(LT-1)/3
            IF(IZDO.GT.3) IZDO=3
            NGAS=IZ(IZDO)
            DO 190 J=1,NGAS
            XG(J)=(BS-VMIN)*XGAUS(IZDO,J) +VMIN
      190   UV(J)=XG(J)
            EPSH = TEMP(I) -XG(NGAS)
            IF(EPSH.LE.0.) GO TO 270
            DO 200 K=1,NGAS
      200   DENQ(K)=POLYN(TEMP(I),1)-POLYN(XG(K),1)
            IF (IGD.NE.0) GO TO 220
            DO 210 J=1,NGAS
      210   BI(J)=POLYN(UV(J),2)
      220   FSUM=0.0D0
            GSUM=0.0D0
            DO 240 J=1,NGAS
            IF (DENQ(J).LE.0.) GO TO 270
            XG(J)=AGAUS(IZDO,J)/SQRT(DENQ(J))
            YG(J)=BI(J)*XG(J)
            FSUM=FSUM+XG(J)
```

```
  240 GSUM=GSUM+YG(J)
      HSN=HS-VMIN
      FEG2=BSV*FSUM
      GEG2=BSV*GSUM
C         CHECK IF ITERATION CRITERION IS ME
C         IT MAY HAVE TO BE ADJUSTED IN STATEMENTS 250
C         FOR PROPER CONVERGENCE WHEN RUN ON OTHER MACHINES
  250 IF ((FEG2/FEG).LE.5.D-7) IFD=1
      IF ((GEG2/GEG).LE.5.D-7) IGD=1
      IF (ABS(FEG2/FEG1).GT.0.9) IFD =1
      IF (ABS(GEG2/GEG1).GT.0.9) IGD=1
  260 LT=LT+1
      FEG1=FEG2
      GEG1=GEG2
      IF (IFD.EQ.0) FEG = FEG + FEG2
      IF (IGD.EQ.0) GEG = GEG + GEG2
      IF ((IFD.NE.0).AND.(IGD.NE.0)) GO TO 270
      VMIN=HS
C            IF INTERMEDIATE EVALUATIONS OF KLEIN ACTION INTEGRALS
C            ARE TO BE OUTPUT THEN WRITE OUT THE FEG AND GEG
      IF (IOPFG.NE.0) PRINT 295,FEG,GEG
      IF (LT.LE.20) GO TO 140
      PRINT 297
      RETURN
  270 F=FEG*FAC
      GF=GEG/FAC
      RMAX(I)=SQRT(F*F+F/GF)+F
      RMIN(I)=RMAX(I)-2.D0*F
C            WRITE OUT THE TURNING POINTS AND THE
C            CORRESPONDING KLEIN ACTION INTEGRALS
      TEMP(I)=TEMP(I)-0.5
      PRINT 296,TEMP(I),U(I),BI(NGAS),RMIN(I),RMAX(I),F,GF
  280 CONTINUE
C     .........END OF INTEGRATION AND ITERATION LOOP
      RETURN
  291 FORMAT(1X,'VFIN, AND VINC GIVE MORE THAN 400 TURNING POINT PAIR
     +--INCREMENT HAS BEEN ADJUSTED TO VINC= ',F5.2)
  294 FORMAT( / ' POTENTIAL GENERATED BY RKR IS AS FOLLOWS'//10X,
     +'POTENTIAL',10X,'INERTIAL',55X,'KLEIN ACTION INTEGRALS'/'     V','
     +,'ENERGY',13X,'ENERGY',15X,'RMIN',16X,'RMAX',18X,'F',19X,'G'/)
  295 FORMAT(6X,'FEG = ',D16.6,', GEG = ',D16.6)
  296 FORMAT(1X,F5.2,F15.4,D22.9,F16.9,F20.9,3X,2D20.9)
  297 FORMAT('  LT REACH MAXIMUM VALUE OF 20--RKR INTEGRATION ITERA
     +TION NOT LIKELY TO SUCCEED. ')
      END
```

```
      FUNCTION POLYN(X,N)
C          SUBROUTINE FOR RKR SYSTEM
C            SOLVES FOR ROOTS OF POLYNOMIAL FUNCTIONS OF TYPE
C           POLYN=SUM FOR I=1 TO IM(N) OF Y(I,N)*X**(I-1)
      COMMON/YD/Y(20,10),IM(10)
      POLYN=0.
      J=IM(N)
      IF (J.EQ.0) RETURN
      S=1.
      DO 10 I=1,J
      POLYN= POLYN +Y(I,N)*S
   10 S=S*X
      RETURN
      END
```

--VARIABLE MAP--(IO-A)

```
      SUBROUTINE EXTEND(PLM1,PLM2)
C        SUBROUTIN FOR RKR SYSTEM
C        ROUTINE FOR FINDING INNERMOST 20 POINTS AND OUTERMOST 20 POI
C        OF POTENTIAL FUNCTION BY EXTRAPOLATION.  THIS ROUTINE AL
C      REORDERS THE POINTS DEFINING THE POTENTIAL FUNCTION IN ASCENDI
C     MAGNITIUDE OF R (THE INTERNUCLEAR DISTANCE).
      COMMON/GL/X(828),Z(828),L
      COMMON/RPW/R1(25),PE1(25),NEXT
      COMMON/FC/F(11),B(11),RE,RAA,RBB,NIN,NOUT,LOUT(4)
      COMMON/EX/XO(921),YO(921),N
      COMMON/RX/RMIN(400),RMAX(400),U(400)
      DO 10 I=1,11
   10 B(I) =0.
C     .........SPECIFIY LIMITS OF FIT FUNCTION
      RAA=RMIN(N) - 1.D-8
      RBB=RMAX(N) +1.D-8
C     .........FIR OF THE INNER TURNING POINTS
      L=NIN + 2
      DO 20 I = 1,L
      X(I) = RMIN(N-I+1)
   20 Z(I)= ALOG10(U(N-I+1))
      IF (NEXT.EQ.0) GO TO 30
      DO 25 I= 1,NEXT
      IF (R1(I).GE.RAA) GO TO 25
      L=L+1
      X(L)=R1(I)
      Z(L)= ALOG10(PE1(I))
   25 CONTINUE
   30 PRINT 92,RAA,NIN
      PRINT 93
      CALL GLSQ(1)
C     .........FIT OF THE OUTER TURNING POINTS
      L=NOUT +4
      DO 40 I= 1,L
      X(I) = RMAX(N-I+1)
   40 Z(I) = U(N-I+1)
      IF (NEXT.EQ.0) GO TO 60
      DO 50 I =1,NEXT
      IF (R1(I).LE.RBB) GO TO 50
      L=L+1
      X(L)=R1(I)
      Z(L) = PE1(I)
   50 CONTINUE
   60 PRINT 94,RBB,NOUT
      PRINT 95
      CALL GLSQ(2)
C     .........FINAL FIT OF THE POTENTIAL
      F6 = (RMIN(N) - PLM1)/20.
      DO 70 I=1,20
      XMO=PLM1+FLOAT(I-1) *F6
      XO(I) =XMO
   70 YO(I) = FUNC(0,XMO)
      DO 80 I=1,N
      J=N-I+1
      K = 20+I
```

```
      XO(K) = RMIN(J)
 80   YO(K) = U(J)
      DO 85 I=1,N
      K= N+I+21
      XO(K)= RMAX(I)
 85   YO(K)= U(I)
      K=N +21
      XO(K)=RE
      YO(K)= 0.000
      F6 = (RLM2 -RMAX(N))/99.
      DO 90 I=1,99
      K=2*N +I+21
      XMC = RMAX(N) +FLOAT(I)*F6
      XO(K) =XMO
 90   YO(K)=FUNC(0,XMO)
      RETURN
 92   FORMAT('  FIT OF INNERMOST TURINING POINTS FOR EXTRAPOLATING U(R)
     *WITH R LESS THAN ',1PD15.7,' USING '//'A FUNCTION OF THE FORM
     *EXP(B(1)+B(2)*X+B(3)*X*X.....+B(K)*X**(K-1)) WITH K=NIN= ',I2/)
 93   FORMAT(12X,'R',15X,'LOG(U(R))',13X,'FCALC',15X,'DIFF'/)
 94   FORMAT('  FIT OF OUTERMOST TURINING POINTS FOR EXTRAPOLATING U(R)
     *WITH R GREATER THAN ',1PD15.7,' USING '//'A FUNCTION OF THE FORM
     *B(1)+B(2)*R**(-6)+B(3)*R**(-8)+.....B(K)*..WITH K=KNOUT= ',I2/)
 95   FORMAT(12X,'R',18X,'U(R)',15X,'FCALC',15X,'DIFF'/)
      END
```

AD-A127 315 NUMERICAL METHODS FOR THE PREPARATION OF POTENTIAL
ENERGY CURVES OF DIATO..(U) AIR FORCE INST OF TECH
WRIGHT-PATTERSON AFB OH SCHOOL OF SYST.. L L RUTGER
UNCLASSIFIED MAR 83 AFIT/GNE/PH/83M-12 F/G 20/10 NL

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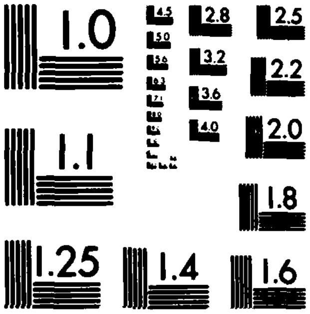

MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

```
      SUBROUTINE GLSQ(KK)
C        GENERAL LEAST SQUARES ROUTINE TO FIT A SET OF N DATA POINTS
C        KK=1: FIT RKR TURNING POINTS BY LEGENDRE POLYNOMIALS
C        KK=2: FIT INNER TURNING POINTS BY EXPONENTIAL FUNCTIONS
C        KK=3: FIT OF OUTER TURNING POINTS BY SUM OF C(N)*R**(-N)
      DIMENSION T(11)
      COMMON/GL/X(828),Z(828),N
      COMMON/FC/F(11),B(11),RE,RAA,RBB,NFIT(2),LCUT(4)
      COMMON/TM1/A(64,64),BB(64)
      M=NFIT(KK)
C     .............INITIALIZATION
 10   DO 20  J=1,M
      BB(J)=0.0D0
      DO 20 K=1,M
 20   A(J,K)=0.0D0
C     .............CALCULATION OF THE MATRIX
      DO 30 I=1,N
      DUMMY=FUNC(KK,X(I))
      DO 30 J=1,M
      BB(J)= BB(J)+Z(I)*F(J)
      DO 30 K=1,M
 30   A(J,K)=A(J,K)+F(J)*F(K)
      CALL MATINV(DETERM,M,1,0)
      DO 40 I=1,M
      NC=I
      IF (KK.GT.1) NC=NFIT(1) + I
 40   B(NC) = BB(I)
C        .........CALCULTION OF FIT AND STANDARD ERROR
      SIG =0.0
      DO 50 I=1,N
      XCRY =X(I)
      DUMMY=FUNC(KK,XCRY)
      DEL=Z(I) - DUMMY
      PRINT 104,XCRY,Z(I),DUMMY,DEL
 50   SIG=SIG+DEL*DEL
      SIGMA=SQRT(SIG/FLOAT(N-M))
C     .............ITERATION TEST
      IF (M.LE.2) GO TO 60
      DBDB =ABS(SQRT(ABS(A(M,M)))/BB(M))*SIGMA
      IF ((SIGMA.GT.1D-3).AND.(DBDB.LT.0.7)) GO TO 60
      M=M-1
      NFIT(KK) = M
      GO TO 10
C     .............PRINT OUT OF CONSTANTS AND ERRORS
 60   PRINT 101
      DO 70 I=1,M
      T(I)=SQRT(ABS(A(I,I)))*SIGMA
      DBDB= ABS(T(I)/BB(I))
 70   PRINT 102, I,BB(I),T(I),DBDB
      PRINT 103, N, SIGMA
 101  FORMAT('  CONSTANTS OF FIT'/)
 102  FORMAT('  B(',I2,' ) =',D18.8,5X,'RMS ERROR = ',D18.8,5X,'RELATIVE
     +RMS ERRO  =',D15.9)
 103  FORMAT(/'NUMBER OF ENTRIES : ',I3,' STANDARD ERROR = ',1PD14.5/)
 104  FORMAT (1PD20.9,3D20.9)

  SUBROUTINE GLSQ        74/74   OPT=0,-CUKO= A/ S/ M/-0,-DS      FTN 5.1+564

      RETURN
      END
```

```
      SUBROUTINE MATINV(DETERM,N,M,IPV)
C        MATRIX INVERSION WITH ACCOMPANYING SOLUTION OF LINEAR EQUATION
C        IPV.EQ.1: NO SEARCH FOR PIVOT,IPV.NE.1: SEARCH FOR PIVOT
C        IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION IPIVOT(64),INDEXR(64),INDEXC(64)
      COMMON/TM1/A(64,64),B(64,1)
C     .............INITIALIZATION
      DETERM=1.0
      DO 20 J=1,N
   20 IPIVOT(J) =0
      DO 550 I=1,N
      IF (IPV.NE.1) GO TO 40
      ICLM = I
      GO TO 260
C     ....................SEARCH FOR PIVOT ELEMENT
   40 AMAX = 0.0
      DO 105 J = 1,N
      IF (IPIVOT(J).EQ.1) GO TO 105
C        FOR UNSYMMETRIC MATRIX: A(I,J).NE.A(J,I)
C       DO 100 K=1,N
C       FOR SYMMETRIC MATRIX:  A(I,J).EQ.A(J,I)
      DO 100 K=J,N
      IF (IPIVOT(K).EQ.1) GO TO 100
      IF (ABS(AMAX).GE.ABS(A(J,K))) GO TO 100
      IROW =J
      ICLM=K
      AMAX=A(J,K)
  100 CONTINUE
  105 CONTINUE
      IPIVOT(ICLM) = IPIVOT(ICLM) + 1
      INDEXR(I) = IROW
      INDEXC(I) = ICLM
C     ......INTERCHANGE ROWS TO PUT PIVOT ELEMENT ON DIAGONAL
      IF (IROW.EQ.ICLM) GO TO 260
      DETERM = -DETERM
      DO 200 L = 1,N
      SWAP = A(IROW,L)
      A(IROW,L) = A(ICLM,L)
  200 A(ICLM,L) = SWAP
      IF (M.LE.0) GO TO 260
      DO 250 L=1,M
      SWAP = B(IROW,L)
      B(IROW,L)=B(ICLM,L)
  250 B(ICLM,L) = SWAP
  260 PIVOT = A(ICLM,ICLM)
      IF (N.GT.10) GO TO 330
      DETERM = DETERM*PIVOT
C     .........DIVIDE PIVOT ROW BY PIVOT ELEMENT
  330 A(ICLM,ICLM) = 1.0
      DO 350 L=1,N
  350 A(ICLM,L) =A(ICLM,L)/PIVOT
      IF (M.LE.0) GO TO 380
      DO 370 L =1,M
  370 B(ICLM,L)=B(ICLM,L)/PIVOT
C     .........REDUCE NON-PIVOT ROWS
```

```
      380  DO 550 L1=1,N
           IF (L1.EQ.ICLM) GO TO 550
           T=A(L1,ICLM)
           A(L1,ICLM) =0.0
           DO 450 L= 1,
      450  A(L1,L) = A(L1,L)-A(ICLM,L)*T
           IF (M.LE.0) GO TO 550
           DO 500 L=1,M
      500  B(L1,L) = B(L1,L) - B(ICLM,L)*T
      550  CONTINUE
           IF (IPV.EQ.1) RETURN
C          ............INTERCHANGE COLUMNS
           DO 710 I= 1,N
           L= N+1-I
           IROW = INDEXR(L)
           ICLM = INDEXC(L)
           IF (IROW.EQ.ICLM) GO TO 710
           DO 705 K =1,N
           SWAP=  A(K,IROW)
           A(K,IROW) = A(K,ICLM)
      705  A(K,ICLM) =SWAP
      710  CONTINUE
           RETURN
           END
```

```
      FUNCTION FUNC(KK,XX)
C        ROUTINE DEFINES THE LEGENDRE POLYNOMIALS FOR FITTING THE RK
C        POTENTIAL AND CONTAINS THE TWO EXTRAPOLATION FUNCTIONS BEYON
C        THE INNERMOST AND OUTERMOST TURNING POINTS, RESPECTIVELY.
      COMMON/FC/F(11),B(11),RE,RAA,RBB,NIN,NOUT,LCUT(4)
      COMMON/EX/XI(921),YI(921),N
      IF((XX.LT.RAA).OR.(KK.EQ.1)) GO TO 60
      IF ((XX.GT.RBB).OR.(KK.EQ.2)) GO TO 80
C     ..........FUNCTION FOR RKR TURNING POINTS
      NPOLY = 6
      FUNC= 0.0
      NM = (NPOLY +1)/2
      NM1 = NM +1
      NUP = N + NM1 -NPOLY
      DO 20 J = NM1,NUP
      IF (XX.LE.XI(J)) GO TO 30
   20 CONTINUE
      J=NUP
   30 L=J-NM
      LLL= L+ NPOLY -1
      DO 50 K = L,LLL
      TERM = 1.0
      DO 40 M = L,LLL
      IF (K.EQ.M) GO TO 40
      TERM = TERM* (XX-XI(M))/(XI(K)-XI(M))
   40 CONTINUE
      TERM = YI(K)*TERM
   50 FUNC= FUNC + TERM
      RETURN
C     ..........FUNCTION FOR INNER TURNING POINTS
   60 X = (RE-XX)/RE
      F(1) = 1.0
      FUNC = F(1) *B(1)
      DO 70 I = 2,NIN
      F(I) = F(I-1)*X
   70 FUNC = FUNC + F(I)*B(I)
      IF (KK.EQ.1) RETURN
      FUNC = 10.**FUNC
      RETURN
C     ........FUNCTION FOR OUTER TURNING POINTS
   80 X =1./XX
      FUNC = 0.0
      DO 90 I = 1,NOUT
      F(I) = X**LCUT(I)
   90 FUNC =   FUNC + F(I)*B(NIN+I)
      RETURN
      END
```

```
      SUBROUTINE YDHF11(NSW)
C        PRINT,PUNC AND READ SUBROUTINE OF DUNHAM COEFFICIENTS
C        (NSW.LE.0) PRINT, NSW=1:PRINT AND PUNCH, NSW=2: READ AND
C        PRINT, (NSW.GE.3):READ
      COMMON/YD/YDH(20,10),JM(10)
      IF (NSW.LT.2) GO TO 40
C     .................INITIALIZATION
      DO 10 IDH = 1,10
      JM(IDB) = 0
      DO 10 IDA = 1,20
 10   YDH(IDA,IDH)= 0.
C     .................READ INSTRUCTIONS
      READ 101,NDUN,(JM(I),I=1,NDUN)
      DO 20 IDN=1,NDUN
      NGBD = JM(IDN)
      IF (NGRD.EQ.0) GO TO 30
 20   READ 102,(YDH(I,IDN),I=1,NGBD)
 30   CONTINUE
      IF (NSW.GT.2) RETURN
C     .........PRINT INSTRUCTIONS
 40   PRINT 103
      DO 60 IDN = 1,20
      NMX =0
      DO 50 IY = 1,10
      IF (JM(IY).GE.IDN) NMX = IY
 50   CONTINUE
      IF (NMX.EQ.0) GO TO 70
 60   PRINT 104,(YDH(IDN,I),I=1,NMX)
 70   IF (NSW.NE.1) GO TO 90
C     .........PUNCH INSTRUCTIONS
C     PUNCH 101,NDUN,(JM(I),I=1,NDUN)
C     DO 80 IDN =1,NDUN
C     NGBD = JM(IDN)
C 80  PUNCH 102,(YDH(I,IDN),I= 1,NGBD)
 90   CONTINUE
      RETURN
 101  FORMAT (14I5)
 102  FORMAT (4D18.9)
 103  FORMAT (' THE DUNHAM COEFFICIENTS '/)
 104  FORMAT (1X,1P8D16.8)
      END
```

```
      SUBROUTINE FIPA(ZMU,DE)
C        ROUTINE RUNNING INVERTED PERTURBATION APP EACH
      DIMENSION GVSUM(10),FPL(64),MTRMIN(11),RCUT(11),YMAX(11),HJTT(11),
     + MTRIAL(11),GVST(11,10),LTRIAL(11),ER(11),COEFF(64),ERROR(64),
     + FX(11,2403),KA(11,98),KB(11,98)
      COMMON /EX/XI(921),YI(921),N
      COMMON /A2/V(2403)
      COMMON/A3/P(2403)
      COMMON /A4/ (2403)
      COMMON/AN2/MA,MB
      COMMON/AN4/ETRIAL(100),HTRIAL(100),AJTT,*TRIAL,KV(100)
      COMMON/YD/YDM(20,10),JM(10)
      COMMON/TM1/AL(64,64),BL(64)
      COMMON/PL/YPL(64),AA1,AA2,AA3,NPL
      COMMON/PO/AINN(100),AOUT(100),EEE(100),BBB(100)
      INTEGER SCHR
C        THE ATOMIC UNITS USED INTERNALLY IN THIS PROGRAM ARE DEFINED
C        BY THE FOLLOWING CONSTANTS.
C        FACMN = RYDBERG CONSTANT*MASS OF THE ELECTRON IN AMU.
C        AZERO = BOHR RADIUS
C        FACRT= SQRT(H-BAR*AVOGADRO-NUMBER/(4*PI*C)*10**5
      AZERO= 0.52917706
      ZIRA = 1.0/AZERO
      FACMN=60.19972628
      FACM=FACMN/ZMU
      ZIEN = 1.0/FACM
      FACRT=4.105204545
      READ 3002, LTEST
      IF (LTEST .EQ. 0) RETURN
C     ......READ CONTROL VARIABLES FOR SCHROEDINGER ROUTINE
      READ 3005, NI,NS,IPSIO,MAXIT,EPSC
      EPS = EPSC*ZIEN
      READ 3004,RMIN,RMAX,M,NRPTT,NPL,MCH,LSW
      READ 3021,(MTRMIN(I),MTRIAL(I),HJTT(I),I=1,11)
      IF ((M.EQ.0).OR.(M.GT.2403)) M=2403
      IF ((NPL.EQ.0).OR.(NPL.GT.31)) NPL=31
      IF ((NRPTT.EQ.0).OR.(NRPTT.GT.6)) NRPTT =6
      DO 80 J= 1,11
      DO 80 I=1,98
      KA(J,I) =0
 AC   KB(J,I)= 0
      NTT =0
      DO 100 IDA = 1,10
      IF (BJTT(IDA).LT.1.D-06) GO TO 120
  100 NTT = NTT + 1
  120 IF (NTT.EQ.0) NTT = 1
      ABE = YDM(1,2)
      CBE =ABE*ZIEN
      RRE = FACRT/SQRT(ZMU*ABE)
      CRE= RRE/AZERO
      IF (XI(1).GT.RMIN) RMIN = XI(1)
      IF ((XI(N).LT.RMAX).OR.(RMAX.LT.0.001)) RMAX =XI(N)
      RH = (RMAX-RMIN)/FLOAT(M-1)
      DO 140 J =1,M
      P(J) = FLOAT(J-1)*RH + RMIN
```

```
    140  V(J) = FUNC(C,P(J))
         NT1=NTT +1
         BJTT(NT1) =0.
         DO 180 KI = 1,NT1
         NTRIAL = 99
         AJTT = BJTT(KI)
C        ..........SEARCH FOR CENTRIFUGAL BARRIER
         TX = 0.
         ASX= 1.D+70
         DO 160 I=1,M
         SX = V(I) + ABE*(RRE/P(I))**2*AJTT
         IF (SX.LT.ASX) GO TO 180
         IF (SX.LE.TX) GO TO 160
         TX = SX
         ROUT(KI) = P(I)
         YMAX(KI)=SX
    160  ASX=SX
         CALL BETRL(TX)
         LTRIAL(KI)=NTRIAL
         IF (MTRIAL(KI).GT.NTRIAL) MTRIAL(KI) = NTRIAL
         NTRIAL = MTRIAL(KI)
    180  ER(KI) = ETRIAL(NTRIAL)
C        ......SEARCH FOR INNERMOST AND OUTERMOST TURNING POINTS
         N3A=M
         N3B=0
         DO 240 KI = 1,NTT
         N3AA = M
         N3BB = 0
         ASX = 1.D+70
         DO 200 I = 1,M
         SX = V(I) + ABE*(RRE/P(I))**2*BJTT(KI)
         IF ((SX.LE.ER(KI)).AND . (ASX.GE.ER(KI))) N3AA = I
         IF ((SX.GE.ER(KI)).AND.(ASX.LE.ER(KI))) N3BB = I
         IF (N3BB.GT.0)GO TO 220
    200  ASX = SX
    220  IF (N3AA.LE.N3A) N3A = N3AA
         IF (N3BB.GE.N3B) N3B = N3BB
    240  CONTINUE
         RMII = P(N3A)
         RMAA= P(N3B)
         DO 260 KI = 1,NT1
         AJTT = BJTT(KI)
         NTRIAL = LTRIAL(KI)
         TX =V(N3B) + AHE*(RRE/RMAA)**2*AJTT
         IF(RMAA.GT.RCUT(KI)) TX = YMAX(KI)
         SX = V(N3A) + AHE * (RRE/RMII)**2*AJTT
         IF (SX.LT.TX) TX =SX
         CALL BETRL(TX)
         LTRIAL(KI) = NTRIAL
         IF (NTRIAL.LT.MTRIAL(KI)) LTRIAL(KI) = MTRIAL(KI)
    260  CONTINUE
         NREP =1
         PRINT 3006,RMIN,RMAX,RH,EPSC,NRPTT,RMII,RMAA,RRE,NPL
         RMIN = RMIN *ZIRA
         RMAX = RMAX*ZIRA
         RH = RH*ZIRA
         AA1 = ZIRA*((RMAA+RMII)*RRE-2.*RMAA*RMII)/(RMAA-RMII)
```

```
           AA2= (RMAA+RMII-2.*RFE)/(RMAA-RMII)
           AA3 = ZIPA*RFE
           DO 270 I = 1,M
           P(I) = P(I)*ZIPA
           CALL PLEGEN(P(I))
           DO 270 J = 1,NPL
      270  FX(J,I) = YPL(J)
           N3A = M
           N3B=0
      260  ISW=LSW
           IF ((NREP.EQ.1).OR.(NREP.EQ.NRPTT)) ISW=1
           NT3 = NT1
           IF (NREP.EQ.NRPTT) GO TO 320
C          ...........INITIALIZATION
           DO 300 I = 1,NPL
           BL(I)= 0.0
           DO 300 J=1,NPL
      300  AL(I,J)= 0.0
           NT3 = NTT
      320  GVTT2 = 0.
           NL= 0
           DO 340 I = 1,M
      340  V(I) =(V(I)-DE)*ZIEN + CRE*(CRE/P(I))**2*BJTT(1)
           DO 660 KI = 1,NT3
           NTRIAL = MTRIAL(KI)
           NTRMIN = MTRMIN(KI)
           IF (NREP.LT.NRPTT) GO TO 360
           NTRIAL = LTRIAL(KI)
           NTRMIN = 1
      360  AJTT = BJTT(KI)
           TX = 1.0D+10
           CALL BETRL(TX)
           LJT = SQRT(AJTT)
           IF (ISW.EQ.1) PRINT 3007,AJTT,LJT
           KLIM = 2
           LLK = 0
           KLK = 0
           GVDIF = 0.
           GVDF2=  0.
C          ............DO SCHROEDINGER LOOP
           DO 600 I = NTRMIN,NTRIAL
           ETRIAL(I) = (ETRIAL(I) - DE)*ZIEN
           ECALC = ETRIAL(I)
           MA = KA(KI,I)
           MB = KB(KI,I)
           IF (SCHR(NI,NS,MAXIT,EPS,IPSIQ,M,RMIN,RMAX,KV(I),ECALC,FACM)-1)420
          + ,400,380
      380  KLK =  KLK +1
           IF (KLK.LT.KLIM) GO TO 420
           PRINT 3010
           CALL EXIT
      400  LLK =LLK +1
      420  IF (MA.LT.N3A) N3A = MA
           IF (MB.GT.N3B) N3B = MB
           KA(KI,I) = MA
           KB(KI,I) = MB
           HCALC = (S(1)/P(1))**2 + 4.*(S(2)/P(2))**2 + (S(M)/P(M))**2
```

```
      KSIMP = M-1
      DO 440 J=3,KSIMP,2
  440 BCALC=2.*(S(J)/P(J))**2 + 4.*(S(J+1)/P(J+1))**2 +BCALC
      BCALC = FACM*BCALC*RH/3.
      ECALC = DE + ECALC*FACM
      ETRIAL(I)=ETRIAL(I)*FACM + DE
      DIFF = ETRIAL(I) - ECALC
      IF(NREP.EQ.NRPTT) GO TO 540
      DO 460 K = 1,NPL
  460 FPL(K) = 0.0
      DO 490 J = MA,MB
      AJ = 4 + (J/2)*4 -2*J
      DO 480 K = 1,NPL
  480  FPL(K) = FPL(K) + AJ*S(J)**2*FX(K,J)
  490 CONTINUE
      DO 500 K = 1,NPL
  500  FPL(K) = FPL(K)*RH/3.
C     ************************************************************
C     STATISTICAL WEIGHT EWG
      EWG = 1.0
C     ************************************************************
      DO 520 K = 1,NPL
      BL(K) = BL(K) + DIFF*FPL(K)*EWG
      DO 520 J=1,NPL
  520 AL(K,J) = AL(K,J) + FPL(J)*FPL(K)*EWG
  540 IF ((I.LT.MTRMIN(KI)).OR.(I.GT.MTRIAL(KI)).OR.(KI.EQ.NT1))GO TO 56
     +
      NL= NL + 1
      GVDIF = GVDIF + DIFF
      GVDF2 = GVDF2 + DIFF*DIFF
      GVTT2 = GVTT2 + DIFF*DIFF*EWG
  560 IF (ISW.EQ.0) GO TO 600
      DIFB = (BTRIAL(I) -BCALC) *1000.0
      EEE(I) = ECALC
      BBB(I)= BCALC
      IF ((NREP.LT.NRPTT).OR.(KI.EQ.NT1)) GO TO 580
      IF (I.EQ.MTRMIN(KI)) PRINT 3020
C     ............PRINT SCHROEDINGER RESULTS
  580 PRINT 3008,KV(I),ECALC,ETRIAL(I),DIFF,BCALC,DIFB,S(MA),S(MB),MA,MB
      IF ((NREP.LT.NRPTT).OR.(KI.EQ.NT1)) GO TO 600
      IF (I.EQ.MTRIAL(KI)) PRINT 3020
  600 CONTINUE
      IF ((NREP.LT.NRPTT).OR.(MCH.NE.1)) GO TO 620
C     PUNCH 3018,NTRMIN,NTRIAL
C     PUNCH 3019,(KV(I),EEE(I),BBB(I),AJTT,I=NTRMIN,NTRIAL)
  620 IF(LLK.GE.1) PRINT 3009,LLK
      APLTST = MTRIAL(KI) - MTRMIN(KI) + 1
      GVDF2 = SQRT(GVDF2/APLTST)
      GVST(KI,NREP) = GVDF2
      GVDA = GVDIF/APLTST
      IF (ISW.EQ.1) PRINT 3011,GVDIF,GVDA,GVDF2
      DO 640 I = 1,M
  640 V(I)= V(I) - CBE*(CBE/P(I))**2*AJTT
      IF (KI.EQ.NT1) GO TO 660
      AJTT= BJTT(KI+1)
      DO 650 I = 1,M
  650 V(I) = V(I) + CBE*(CBE/P(I))**2*AJTT
```

```
      660 CONTINUE
          GVTT2= GVTT2/FLOAT(NL-NPL)
          GVSUM(NREP) = SQRT(GVTT2)
          IF (NREP.EQ.1) GO TO 700
          NRM1=NREP - 1
          PRINT 3012,NRM1
          GVT = GVSUM(NREP)
          DO 680 K= 1,NPL
          DBAA = COEFF(K)
          T = SQRT(ERROR(K))*GVT
          TEMP = ABS(T/DBAA)
      680 PRINT 3013,K,DBAA,T,TEMP
      700 DO 710 I = 1,M
      710 V(I) = V(I)*FACM + DE
          IF (NREP.EQ.NRPTT) GO TO 800
          CALL MATINV(DETERM,NPL,1,0)
          DO 720 K = 1,NPL
          COEFF(K) = BL(K)
      720 ERROR(K) = ABS(AL(K,K))
C         ............CORRETCTION OF POTENTIAL AND YOH(1,1)
          VMIN = 1.0D+10
          DO 760 I = 1,M
          DO 740 K =1,NPL
      740 V(I) = V(I) + BL(K)*FX(K,I)
          IF (V(I).LT.VMIN) VMIN = V(I)
      760 CONTINUE
          YOH(1,1) = YOH(1,1) - VMIN
          DO 780 I =1,M
      780 V(I) = V(I) - VMIN
          NREP = NREP + 1
          GO TO 260
      800 PRINT 3001
          DO 840 KE = 1,NPL
          COEFF(KE) = SQRT(ABS(AL(KE,KE)))
          DO 820 KEE = 1,KE
      820 FPL(KEE)= (ABS(AL(KE,KEE))/COEFF(KE))/COEFF(KEE)
      840 PRINT 3002,KE,(FPL(L),L=1,KE)
          CALL POTTAB(GVT,AZERO,DE,M,NTRIAL)
          PRINT 3014,N3A,P(N3A),N3B,P(N3B)
          PRINT 3015
          DO 860 I = 1,NTT
          PRINT 3016,BJTT(I),(GVST(I,L),L=1,NRPTT)
      860 CONTINUE
          PRINT 3020
          PRINT 3017,(GVSUM(I),I=1,NRPTT)
          RETURN
     3001 FORMAT('1','  CORRELATION MATRIX OF THE COEFFICIENTS'/)
     3002 FORMAT(/I5,10F10.6,4(/5X,10F10.6))
     3003 FORMAT(I1)
     3004 FORMAT (2F10.0,6I5)
     3005 FORMAT (4I4,D10.0)
     3006 FORMAT(' RMIN = ',F6.3,', RAMAX = ',F6.3,', SPACING = ',F10.7
         +/' CONVERGENCE CRITERION IS ERROR LESS THEN ',D9.2/
         +/' NUMBER OF ITERATIONS = ',I3//' PARAMETERS OF THE FITTING POLY
         +MIAL'//' RMIN = ',F7.3,'RMAX =',F7.3,' RE =',F7.3,','NPL=',I3//)
     3007 FORMAT ('  RESULTS OF SCHROEDINGER EQUATION FOR J(J+1) =',F5.0
         +,' AND J=',I3,//4X,'V     GV CAL      GV MEAS      GV M-C       BV CAL
```

```
     +    HV M-C    S(MA)     S(MH)     MA     MH '/)
3006 FORMAT (1X,I4,2F12.5,F11.5,F13.4,F10.5,2(1PD10.1),2I6)
3009 FORMAT ('0  PROGRAM SUCCESSFUL. (MAXIT REACHED ',I2,' TIMES)')
3010 FORMAT ('   SCHR NOT SUCCESSFUL')
3011 FORMAT(//'  SUM OF DIFF.=',1PD12.4,'   AVERAGE DIFF. =',D12.4,'
     +    RMS OF GV =',D12.4/)
3012 FORMAT ('0 COEFFICIENTS OF THE LEGENDRE POLYNOMIALS AFTER ITERAT
     +N NO. ',I2/)
3013 FORMAT(' H(',I2,') =',1PD15.9,4X,'RMS ERROR =',D16.6,4X,'RELATIVE
     + RMS ERROR =  ',D14.4)
3014 FORMAT(/ 'RECOMMENDED INTEGRATION LIMITS RMIN = R(',I4,') =', F6.
     +,'RMAX =R(',I4,')=',F7.3/)
3015 FORMAT (1H1,' SUMMARY OF ERRORS OF THE INVERTED PERTURBATION APP
     +ACH '//3X,'J(J+1)',4X,'1.',8X,'2.',8X,'3.',8X,'4.',8X,'5.',8X,
     +'6.',8X,'7.',8X,'8.',8X,'9.',7X,'10.ITERATION'/)
3016 FORMAT (1X,F8.1,10F10.5)
3017 FORMAT (/'  AVERAGE',10F10.5)
3018 FORMAT(2I10)
3019 FORMAT (I2,3D16.9)
3020 FORMAT (1X,57(2H--))
3021 FORMAT (6(I2,I3,F7.0)/5(I2,I3,F7.0))
     END
```

```
      INTEGER FUNCTION SCH (NI,NS,MX,EPS,IPSIQ,NN,RMIN,RMAX,KV,E0,FACM)
C        SCHROEDINGER EQUATION SOLVING ROUTINE FOR PSI**2+(E-V)*PSI=0
C        NI=1  PRINT ITERATIONS, OTHERWISE NO PRINTOUT
C      NS=1: PRINT SOLUTIONS WITH EACH ENERGY LEVEL, OTHERWISE NO PRINTOUT
      COMMON/A2/V(2403)
      COMMON/A4/S(2403)
      COMMON/AN2/MA,MB
      EPRIN = E0*FACM
      IF (NI.EQ.1) PRINT 201,KV,EPRIN
      H = (RMAX -RMIN)/FLOAT(NN-1)
      H2= H*H
      HV= H2/12.D0
      E=E0
      TEST = -1.D0
      DE = 0.D0
C     ...........DETERMINATION OF INNER INTEGRATION LIMIT
      DO 10 IPP = 1,NN
      LCRIT = IPP -1
      IF (V(IPP).LE.E) GO TO 13
 10   CONTINUE
 13   KERR =1
      IF (LCRIT.LT.1) GO TO 83
      NL1 = LCRIT + 2
      WCRIT = 0.
      DO 16 IPP = 1,LCRIT
      LCT =LCRIT + 1 - IPP
      WCRIT = WCRIT + SQRT(V(LCT) - E)*H
      IF (WCRIT.GE.20.0) GO TO 20
 16   CONTINUE
 20   MA = LCT
C     .............DETERMINATION OF OUTER INTEGRATION LIMIT
      DO 23 IPP= 1,NN
      LCT = NN + 1 - IPP
      IF (V(LCT).LE.E) GO TO 26
 23   CONTINUE
 26   LCRIT = LCT +1
      KERR = 2
      IF (LCRIT.GT.NN) GO TO 83
      WCRIT = 0.
      DO 30 IPP = LCRIT,NN
      LCT = IPP
      WCRIT=WCRIT +SQRT(V(IPP) - E)*H
      IF (WCRIT.GE.20.0) GO TO 33
 30   CONTINUE
 33   MB=LCT
      DO 35 IPP = NL1,NN
      IF (V(IPP).GT.E) GO TO 130
 35   CONTINUE
 130  NL2 = IPP
      DO 140 I = 1,MA
 140  S(I)=0.0
      DO 150 I = MB,NN
 150  S(I) = 0.0
      MAP1 = MA + 1
C     ............START ITERATION LOOP
```

```
      DO 60 IT = 1,MX
C     ............START INWARD INTEGRATION
      S(MB) = 1.D-10
      GN = V(MB) - E
      GI = V(MB-1) - E
      RMOX = RMIN + H*FLOAT(MB-1)
      S(MB-1) = S(MB)*EXP(RMOX*SQRT(GN)-(RMOX-H)*SQRT(GI))
      YA = (1.D0 - HV*GN)*S(MB)
      YB= (1.D0 - HV*GI)*S(MB-1)
      M =MB-2
   36 YC = YB + ((YB-YA) + H2*GI*S(M+1))
      GI = V(M) -E
      S(M) = YC/(1.D0-HV*GI)
      KER  =3
      IF (S(M).LT.0.0D0) GO TO 83
      IF (S(M).LE.S(M+1))GO TO 40
      YA = YB
      YB = YC
      M = M-1
      GO TO 36
   40 MSAVE = M
      PM = S(M)
      YIN = YB/PM
      DO 43 J = M,MB
   43 S(J)=S(J)/PM
C     ............START OUTWARD INTEGRATION
      S(MA) = 1.0D-10
      YA=0.0D0
      GI=V(MA) - E
      YB = (1.D0-HV*GI)*S(MA)
      DO 46 I = MA+1,M
      YC = YB + ((YB -YA) + H2*GI*S(I-1))
      GI = V(I) -E
      S(I) = YC/(1.D0-HV*GI)
      YA=YB
   46 YB=YC
      PM=S(M)
      YOUT= YA/PM
      YM=YC/PM
      DO 50 J=MA,M
   50 S(J)=S(J)/PM
C     ............CORRECTION
      DF = 0.0D0
      DO 53 J=MA,MB
   53 DF= DF - S(J)*S(J)
      F = (-YOUT -YIN + 2.0D0*YM)/H2+ (V(M) - E)
      DOLD = DE
      DE = -F/DF
      IF (NI.NE.1) GO TO 56
      EPRIN =E*FACM
      DEPRIN = DE*FACM
      PRINT 203,IT,EPRIN,F,DF,DEPRIN,MSAVE
   56 EOLD =E
      E=E +DE
      TEMP = ABS(DOLD) -ABS(DE)
      IF (TEMP.GT.TEST) TEST =TEMP
      IF (TEST.LT.0.0D+0) GO TO 60
```

```
            IF (ABS(E-EOLD).LE.ABS(EPS)) GO TO 63
   60       CONTINUE
            SCHR = 1
            GO TO 66
C.............COUNT NODES
   63       SCHR = 0
   66       KV = 0
            DO 70 J = NL1,NL2
             IF((S(J-1).LT.0.0).AND.(S(J).GE.0.0).AND.(S(J+1).GT.0.0)) KV=KV+1
            IF((S(J-1).GT.0.0).AND.(S(J).LE.0.0).AND.(S(J+1).LT.0.0)) KV=KV+1
   70       CONTINUE
C           .............NORMALIZE
            SN=SQRT(-H*DF)
            DO 73 J = MA,MB
   73       S(J) = S(J)/SN
C           ............PRINT SOLUTION
            IF (NS.NE.1) GO TO 80
            PRINT 204,KV,E
            PRINT 205,(I,S(I),I=1,MB,IPSIQ)
   80       E0=E
            RETURN
   83       PRINT 202,KERR
            SCHR = 2
            RETURN
  201       FORMAT('1',' SCHR- SOLUTION OF RADIAL SCHR. EQUATION FOR V= ',I3,5
           +X,'ETRIAL=',1PE15.7,'     (1/CM)'/
           +'  ITER,',5X,'E',14X,'F(E)',12X,'DF(E)',11X,'D(E)',4X)
  202       FORMAT(' KERR = ',I2,' DIFF EQATION SOLUTION TECHNIQUE FAILED')
  203       FORMAT(///I4,2X,1P4E16.7,5X,' THE CROSSING PT. OCCURS AT ',I4)
  204       FORMAT('1 SCHR-SOLUTION OF RADIAL SCHR. EQUATION FOR V= ',I3,' E=
           +',1PE15.7/'0    I',7X,'S(I)    ',5(20H    I          S(I)     ))
  205       FORMAT(6(I5,1PE15.7))
            END
```

```
            SUBROUTINE POLYN
            COMMON/TI/X(2403),Y(2403),NUMX,NPOLY,POLYN,XXX
C           THE ARRAY X HAS TO BE IN INCREASING ORDE
            NM = (NPOLY+1)/2
            NM1 = NM +1
            NUP = NUMX + NM1 - NPOLY
            DO 2 J = NM1,NUP
            IF (XXX.LE.X(J)) GO TO 4
    2       CONTINUE
            J=NUP
    4       L= J-NM
            LLL=L + NPOLY -1
            POLYN = 0.0
            DO 6 K=L,LLL
            TERM = 1.0
            DO 5 M =L,LLL
            IF (K.NE.M) TERM =TERM*(XXX-X(M))/(X(K)-X(M))
    5       CONTINUE
            TERM = Y(K)*TERM
    6       POLYN=POLYN +TERM
            RETURN
            END
```

```
      SUBROUTINE BETRL(TX)
C         THIS SUBROUTINE CALCULATES THE VALUES OF ETRIAL AND BTRIAL. IF
C     NTRIAL=0 THE VALUES ARE TAKEN WHICH HAVE BEEN READ IN FROM THE
C     RKP DECK.
      DIMENSION YIA(10)
      COMMON/YD/YDH(20,10),IM(10)
      COMMON/AN4/ETRIAL(100),BTRIAL(100),AJTT,NTRIAL,KV(100)
      IF (NTRIAL.EQ.0) RETURN
      NC=0
      NIN=NTRIAL
      EO=0.
      DO 40 I = 1,NIN
      KV(I) = NC
      NC = NC +1
      ANV =FLOAT(I) - 0.5
      NAB = 0
      DO 10 IA = 1,10
      NGBD = IM(IA)
      IF (NGBD.EQ.0) GO TO 20
      NAB = NAB +1
      FACV = 1.
      YIA(IA)= 0.
      DO 10 IB = 1,NGBD
      YIA(IA) = YIA(IA) + FACV*YDH(IB,IA)
   10 FACV = FACV*ANV
   20 YIA(NAB+1)=0.
      ETRIAL(I)=0.
      BTRIAL(I)=0.
      FACJ=1.
      DO 30 IA = 1,NAB
      ETRIAL(I)=ETRIAL(I) + YIA(IA)*FACJ
      AIA=IA
      BTRIAL(I)= BTRIAL(I) + YIA(IA+1)*FACJ*AIA
   30 FACJ=FACJ*AJTT
      IF (ETRIAL(I).LT.EO) GO TO 50
      IF (ETRIAL(I).GT.TX) GO TO 50
   40 EO = ETRIAL(I)
      GO TO 60
   50 NC=NC -1
   60 NTRIAL = NC
      RETURN
      END
```

```
      SUBROUTINE PLEGEN(Z)
C     THIS SUBROUTINE CALCULATES THE LEGENDRE POLYNOMIALS YPL BY MEANS
C     OF A RECURSION RELATION AND MULTIPLIES THEM BY AN EXPONENTIAL CUT
C     OFF FUNCTION AS REQUIRED FOR THE CORRECTION FUNCTION WHICH MODI-
C     FIES THE POTENTIAL AFTER EVERY ITERATION.
      COMMON/PL/YPL(64),AA1,AA2,AA3,NPL
      ZZ= (Z-AA3)/(AA1+AA2*Z)
      YPL(1) = 1.
      YPL(2)=ZZ
      DO 10 I = 3,NPL
      AI = I
   10 YPL(I)= (YPL(I-1)*ZZ*(2.*AI-1.)-YPL(I-2)*(AI-1.))/AI
      FAC= ZZ**10*3.
      IF (FAC.GT.50.) GO TO 20
      FAC = EXP(-FAC)
      GO TO 30
   20 FAC=0.0
   30 DO 40 I=1,NPL
   40 YPL(I) =YPL(I)*FAC
      RETURN
      END
```

```
SUBROUTINE POTTAB      74/74   OPT=0,ROUND= A/ S/ M/-D,-DS      FTN 5.1+
DO=-LONG/-OT,ARG=-COMMON/-FIXED,CS= USER/-FIXED,DB= TB/ SB/ SL/ ER/-ID/ PMD/-
FTN5,DB.

                  SUBROUTINE POTTAB(GVT,AZERO,DE,M,NTRIAL)
          C       ROUTINE FOR INTERPOLATION OF INNER AND OUTER TURNING POINTS
                  DIMENSION ZI(521)
                  COMMON/PO/AINN(100),AOUT(100),EEE(100),BBB(100)
                  COMMON/T1/XR(2403),YR(2403),NUMX,NPOLY,POLYN,XXX
                  COMMON/A2/V(2403)
                  COMMON/A3/P(2403)
                  COMMON/EX/XI(521),YI(521),N
                  COMMON/TM1/AL(64,64),BL(64)
                  COMMON/PL/YPL(64),AA1,AA2,AA3,NPL
          C       ............SEARCH FOR MINIMUM
                  DO 10 I = 1,M
           10     P(I) = P(I)*AZERO
                  TX = V(1)
                  DO 15 I = 2,M
                  IF (V(I).GE.TX) GO TO 15
                  TX=V(I)
                  IMIN = I
           15     CONTINUE
          C       .............INTERPOLATION OF THE POTENTIAL
                  NPOLY = 4
                  DO 30 NR = 1,2
                  NA =1
                  NB = IMIN
                  IF (NR.EQ.1) GO TO 20
                  NA=IMIN
                  NB=M
           20     DO 25 I = NA,NB
                  NUMX= I + 1 -NA
                  K=I
                  IF (NR.EQ.1) K = IMIN + 1 - I
                  XR(NUMX)= V(K)
           25     YR(NUMX)=P(K)
                  DO 30 I = 1,NTRIAL
                  XXX=EEE(I)
                  CALL POLYNN
                  IF (NR.EQ.1) AINN(I) = POLYN
                  IF (NR.EQ.2) AOUT(I) = POLYN
           30     CONTINUE
          C       .............PRINTOUT OF THE TURINING POINTS
                  PRINT 101
          C       PUNCH 101
                  DO 35 I = 1,NTRIAL
                  IA=I-1
                  BBB(I)=BBB(I)*100.0
                  IF (IA.EQ.40) PRINT 101
          C       PUNCH 102,IA,EEE(I),AINN(I),ANOUT(I),BBB(I)
           35     PRINT 102,IA,EEE(I),AINN(I),AOUT(I),BBB(I)
                  DO 40 I = 1,M
                  XR(I) = P(I)
           40     YR(I)=V(I)
                  NUMX =M
                  IA = 0
                  IB = N +1
                  DO 55 I=1,N
```

```
                  XXX = XI(I)
                  IF (XXX.GE.P(1)) GO TO 45
                  IA = I
                  GO TO 55
           45     IF (XXX.LE.P(M)) GO TO 50
                  IB = I
                  GO TO 60
           50     CALL POLYNM
                  ZI(I)= YI(I) - POLYN
                  YI(I) = POLYN
           55     CONTINUE
           60     IF(IA.EQ.0) GO TO 70
                  DO 65 I = 1, A
                  ZI(I) = ZI(IA+1)
           65     YI(I)=YI(I)-ZI(I)
           70     IF (IB.EQ.(N+1)) GO TO 80
                  DO 75 I = IB,N
                  ZI(I) =ZI(IB-1)
           75     YI(I)=YI(I) -ZI(I)
          C       .....PRINTOUT OF THE FINAL POTENTIAL AND OF THE STANDARD ERROR
           80     PRIN  103
                  DO 99 I = 1,N
                  ST = XI(I)/AZERO
                  CALL PLEGEN(ST)
                  ST=0.0
          C       DO 85 K = 1,NPL
          C 85    ST =ST + BL(K,1)*YPL(K)
          C       IF (ABS(ST).GT.1.0D-6) GO TO 90
          C       ST=0.0
          C       GO TO 99
          C 90    ST=0.0
                  DO 95 J=1,NPL
                  DO 95 K =1,NPL
           95     ST = ST + YPL(K)*AL(K,J)*YPL(J)
                  ST = SQRT(ABS(ST))*CVT
           99     PRINT 104,XI(I),YI(I),ZI(I),ST
          101     FORMAT(1H1,'   FINAL SET OF TURNING POINTS'//5X,1HV,3X,'L(M)',1
                 +,'RMIN',11X,'RMAX',10X,'RV*100'/)
          102     FORMAT(1X,I5,F15.3,F14.6,F15.6,F15.7)
          103     FORMAT(1H1,'  FINAL POTENTIAL'//12X,'R',16X,'L(R)',15X,'RK--IPA',1
                 +2X,'ERROR'/)
          104     FORMAT (1X,1PD20.9,3D20.9)
                  RETURN
                  END
```

```
        POTENTIAL OF THE PBO     MOLECULE   (TOTAL FIT)
              GROUND STATE FOR LEAD OXIDE


    THE CODE NUMBER FOR THIS STATE IS


   HE MASSES OF THE TWO ATOMS,
    BASED ON C=12 ARE  1.5999400000D+01  AND   2.0719000000D+02


   DE =    .3157000D+05            TE =    0.
```

```
LIM1 =    1.4000 LIM2 =    7.5000 VFIN =    74.0   VINC =      .25

IOPFG = 0  IPNRKR = 1  IPNIPA = 0

PCTENTIAL GENERATED BY RKR IS AS FOLLOWS

          POTENTIAL        INERTIAL                                                 KLEIN ACTION INTEGRAL
    V      ENERGY           ENERGY            RMIN             RMAX                  F                  G

  -.25     179.9606      .30682513D+00     1.86356 991     1.962982 24      .377 6518 0D- 1     .1 773  235D- 1
  0.00     359.5572      .30630065D+00     1.86031 6556    1.95 632 21      .58217  295D- 1     .151 [illegible]D- 1
   .25     538.7080      .30553428D+00     1.85703 2 6     1.99948 5267     . 32665 40D- 1      .1 7   424D- 1
   .50     717.4136      .30547605D+00     1.84763 6774    2.0069844 2      .7 7 7 7 20D- 1     .214 5   ( - 1
   .75     895.6741      .30503593D+00     1.83 4 5747     2.017838 06      . 17 1 2 41D- 1     .29 277  4 - 1
  1.00    1073.4898      .30456395D+00     1.832245644     2.0270142 2      . 77 4 9 0D- 1      .2631 4377D- 1
  1.25    1250. 612      .30413005 D+00    1.82566 144     2.03712 144      .1  7 3 30D+ 0      .2 42     D- 1
  1.50    1427.7884      .30367435D+00     1.81 624122     2.04592243       .11514 1 0D+ 0      .3 3 34 75 D- 1
  1.75    1604.2717      .30321673D+00     1.81401515      2.0542 2643      .12 1 7 7240D+      .3223  7  D- 1
  2.00    1780.3114      .30275725D+00     1.80877023      2.062310 2       .12 77  15 D+ 0     . 3  4446  D- 1
  2.25    1955.5077      .30229565 D+00    1.803835615     2.07903 0 85     .13   73  0D+ 0     .35644 4 4 D- 1
  2.50    2131.0609      .30183265D+00     1.79516 654     2.07749 41       .13 1C23  0D+ 0     .3723144 4 D- 1
  2.75    2305.7712      .30136753D+00     1.79473 403     2.0847 4 72      .144  73 40D+ 0     .3 7 32  D- 1
  3.00    2480.6388      .30090055D+00     1.79651 7 54    2.09177  67      .1566 30 570D+ 0    .4 21771 5 D- 1
  3.25    2653.8638      .30043168 D+00    1.7864 324      2.0 6647 7       .156  1 3 0D+ 0     .416307 3 D- 1
  3.50    2827.2465      .29996095D+00     1.7826169 6     2.1053 6 5       .16  71 4 0D+ 0     .42  74 4 D- 1
  3.75    3000.1 71      .29948833D+00     1.77  03513     2.11 93270       .166514 1 0D+ 0     .44322   D- 1
  4.00    3172.6657      .29901385D+00     1.77532 553     2.1163726        .1715243   D+ 0     .4 6   2 40D- 1
  4.25    3344.7425      .29853746D+00     1.77188365      2.1247082 5      .17641231 9D+ 0     .46 5 14 6 D- 1
  4.50    3516.3575      .29805925D+00     1.768555 74     2.130932774      .181  7450D+ 0      .4  77 1  D- 1
  4.75    3687.5310      .29757913 D+00    1.765337435     2.137060 01      .185 615  0D+ 0     .4 265727 D- 1
  5.00    3858.2630      .29709715D+00     1.762220 06     2.14309 212      .1 0 43   30D+ 0     .52425 112 D- 1
  5.25    4028.5536      .29661328 D+00    1.75919902      2.149055 76      .194 2 37 0D+ 0     .5 55  3 2 D- 1
  5.50    4198.4030      .29612755D+00     1.75626 076     2.15493630       .19 3351 6 D+ 0     .52 694 7 D- 1
  5.75    4367.8112      .29563993D+00     1.75 341 512    2.160746 24      .20366 1 60D+ 0     .5375 C471D- 1
  6.00    4536.7782      .29515045D+00     1.750645435     2.16649077       .2 7 2 5720D+ 0     .5 4 20  15 D- 1
  6.25    4705.3042      .29465908D+00     1.74754 421     2.1721741 5      .2121124 70D+ 0     .55 65    D- 1
  6.50    4873.3891      .29416585D+00     1.745321453     2.177 0C534      .21 2 35 3 D+ 0     .56   77  D- 1
  6.75    5041.0330      .29367073D+00     1.742760 73     2.18 373 31      .22 7 63 7 D+ 0     .57  76  5 D- 1
  7.00    5208.2359      .29317375D+00     1.740263341     2.188856 52      .2243167 5 D+ 0     .5   727 5 D- 1
  7.25    5374.9979      .29267488 D+00    1.737825796     2.19427371       .22 2737 D+ 0       .5 6 C 4 4 D- 1
  7.50    5541.3186      .29217415 D+00    1.735445420     2.1998C 1        .2321 02 5 D+ 0     .6  1 6   D- 1
  7.75    5707.1987      .29167153-D+00    1.733113622     2.20515726       .236 3-  20D+ 0     .6176  2 7 D- 1
  8.00    5872.6376      .29116705D+00     1.73084603      2.210545 03      .23 851 470D+ 0     .626  011 D- 1
  8.25    6037.6353      .29066066 D+00    1.72 622356     2.215 C6  1      .2436214 0D+ 0      .636  2  1 D- 1
  8.50    6202.1920      .29015245D+00     1.72 446607     2.221147 54      .2473506 9 D+ 0     .645 3  6 D- 1
  8.75    6366.3074      .28964233 D+00    1.724316 44     2.22 3 72        .251 40227D+ 0      . 5  1 4 7 D- 1
  9.00    6529.9815      .28913035D+00     1.7222312 1     2.231 16 27      . 546 247 D+ 0      .66  1   7 D- 1
```

```
  9.25   6693.2142   .28861648 D+00   1.72016 253   2.236806405   .25[illegible]30[illegible]1760+10   .67132[illegible]D-01
  9.50   6856.0054   .288190756D+00   1.718186198   2.241[illegible]6[illegible]43[illegible]   .261[illegible]16170+10   .6[illegible]D-01
  9.75   7018.3550   .28758313 D+00   1.716223659   2.247106 55   .2659915 0D+10   .6[illegible]71D-01
 10.00   7180.2628   .28706365 D+00   1.714299255   2.252220107   .26[illegible]4250D+10   .6[illegible]1[illegible]94D-01
 10.25   7341.7288   .28654228 D+00   1.712411702   2.257310564   .27244[illegible]310+10   .7[illegible]4 332 3D-01
 10.50   7502.7527   .286019050D+00   1.710559746   2.262237507   .27[illegible]0+10   .712[illegible]D-01
 10.75   7663.3345   .28549393 D+00   1.708742167   2.267428147   .27[illegible]3424 0D+10   .72[illegible]9711D-01
 11.00   7823.4738   .28496695 D+00   1.70695 361   2.272457764   .2[illegible]274 [illegible]0+10   .72[illegible]D-01
 11.25   7983.1706   .28443808 D+00   1.705206747   2.27746 101   .2[illegible]1171170+10   .7[illegible]7167 [illegible]D-01
 11.50   8142.4246   .28390735 D+00   1.703486557   2.282246[illegible]5   .2[illegible]1D+10   .7445[illegible]D-01
 11.75   8301.2357   .28337473 D+00   1.70179687[illegible]   2.287442007   .2[illegible]22[illegible]5D+10   .7[illegible]2 [illegible]D-01
 12.00   8459.6035   .28284025 D+00   1.700136 42   2.292405[illegible]4   .2[illegible]6134[illegible]0+10   .7[illegible]2464D-01
 12.25   8617.5279   .28230388 D+00   1.698505 31   2.297354617   .2[illegible]424[illegible]0+   .767747 74D-01
 12.50   8775.0086   .28176565 D+00   1.696902452   2.302256[illegible]4   .2[illegible]4[illegible]0+10   .7747 [illegible]11D-01
 12.75   8932.0453   .28122553 D+00   1.695326565   2.307214[illegible]1[illegible]   .2[illegible]9[illegible]0+10   .7[illegible]1[illegible]4[illegible]D-01
 13.00   9088.6378   .28068355 D+00   1.693777257   2.312125 1[illegible]   .2[illegible]174[illegible]0+10   .7[illegible]6[illegible]D-01
 13.25   9244.7[illegible]5[illegible]   .28013965 D+00   1.692253[illegible]54   2.317026604   .2[illegible]0+10   .7[illegible]7[illegible]14[illegible]D-01
```

```
13.75     9555.7471     .27904633 D+00     1.688[illegible]    [illegible]         [illegible]          [illegible]
14.00     9710.5597     .27849685 D+00     1.687832771         2.331671 1          [illegible]          [illegible]
14.25     9864.9265     .2779454  D+00     1.686406622         2.336[illegible]    .32 1  4 D+0         [illegible]
14.50    10018.6472     .2773 225 D+00     1.685003[illegible] 2.3413[illegible]   [illegible]          .  717 71 D-01
14.75    10172.3214     .27683713 D+00     1.683623261         2.346241751         [illegible]          [illegible]
15.00    10325.3487     .27628015 D+00     1.682264643         2.351[illegible]    [illegible]          [illegible]
15.25    10477.9286     .2757 12  D+00     1.680927 46         2.355522 7          [illegible]          [illegible]
15.50    10630.0613     .27516055 D+00     1.67 611343         2.360755463         [illegible]          [illegible]
15.75    10781.7458     .27459793 D+00     1.678315773         2.3655  3274        [illegible]          [illegible]
16.00    10932.5817     .27403345 D+00     1.677[illegible]    2.370 40  1         [illegible]          [illegible]
16.25    11083.7686     .27346706 D+00     1.675784695         2.375 22  7         [illegible]          .  147 4  D-01
16.50    11234.1065     .27289845 D+00     1.674548342         2.380043 82         .3527476  D+0        .  77     D-01
16.75    11383.9545     .2723287  D+00     1.673331059         2.3846 7777         .3557 63  D+0        .  18  2  D-01
17.00    11533.4322     .27175675 D+00     1.672132358         2.3896 9 22         .35 76  17D+0        .  7 544 1D-01
17.25    11682.4192     .27118288 D+00     1.670951939         2.394479684         .361763 72D+0        [illegible]
17.50    11830.9549     .2706071500D+00    1.669767453         2.39928839          .364747 73D+0        [illegible]
17.75    11979.0389     .27002553 D+00     1.668644592         2.404096195         .3677  3 7D+0        [illegible]
18.00    12126.6706     .2694560050D+00    1.667517014         2.408903 48         .37 6 32 7D+0        [illegible]
18.25    12273.8496     .26886268 D+00     1.666406450         2.413710683         .37365211 9D+0       [illegible]
18.50    12420.5753     .26822545 D+00     1.665312594         2.418518169         .3766 27  7D+0       .  5771 4 D-01
18.75    12566.8470     .26776033 D+00     1.664235160         2.42332640          .379 545  3D+0       .  411 3  2D-01
19.00    12712.6644     .2671133500D+00    1.663173485         2.428135 69         .3824   7  D+0       .3471 7   D-01
19.25    12858.0267     .26652448 D+00     1.662120492         2.43294647          .3 540     D+0       .353  764 D-01
19.50    13002.9335     .2659337500D+00    1.661098742         2.437759066         .3  37013  D+0       .95  51 7 6D-01
19.75    13147.3840     .26534113 D+00     1.660084369         2.442573 66         .3 124479  D+0       .364 7411 4D-01
20.00    13291.3776     .2647466500D+00    1.659085142         2.44739122          .394153 4  D+0       .37 7173  2D-01
20.25    13434.9141     .26415028 D+00     1.658100 22         2.452211 15         .3975553   D+00      .376522 4  D-01
20.50    13577.9523     .2635520550D+00    1.657131196         2.45703594          .3   51  5 D+0       .3822   2  D-01
20.75    13720.6118     .26295193 D+00     1.656176031         2.461 62197         .40 431    D+0       .   1   56 D-01
21.00    13862.7720     .2623499500D+00    1.655235117         2.466653274         .405722 1  D+0       .5937 1 7  D-01
21.25    14004.4721     .26174608 D+00     1.65430 253         2.4715 28 2         .40  101 7 D+0       .359 371 41D-01
21.50    14145.7114     .2611403500D+00    1.6533 5232         2.476368590         .4114 6 7  D+0       .1034  4   D+00
21.75    14286.4893     .26053273 D+00     1.652495862         2.481213477         .41435     D+0       .101 50 17 D+0
22.00    14426.8051     .2599232500D+00    1.651609951         2.486063615         .417226 32 D+00      .1016137 5 D+0
22.25    14566.6579     .25931188 D+00     1.650737315         2.49091  24         .42  911 4 D+0       .102165    D+0
22.50    14706.0472     .2586986500D+00    1.649877773         2.495780 17         .422 51 72 D+0       .102714 51 +0
                                                                                    .4     76  D+0       .10  6  21 D+0
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[illegible]  [illegible]   
22.75   14844.5722   .25808353-D+00   1.6490?1160   2.50UE4??9?    .4?      [illegible]   --
23.00   14983.4320   .25746655OD+00   1.6481572A-   2.505522?A5    .42?6621 ?0+0?    .103? ?2?27D+?(
23.25   15121.4260   .25684768rC+00   1.647376006   2.510404CA1    .4315141?-0+00    .104241??7D+?(
23.50   15258.?533   .25622695CD+00   1.646567144   2.515292955    .4343625?50+?)    .104?7???2D+?(
23.75   15396.0131   .25560433 0+00   1.645770547   2.520187 31    .437?056 .20+?0   .10?4111??D+ (
24.00   15532.6047   .25497585CD+00   1.644986064   2.525091377    .4401526 ?0+??    .105?412??D+?(
24.25   15668.7273   .2543534??D+00   1.644213540   2.530002?4     .442??943?40+?C   .10646 ?? 2D+?(
24.50   15804.3799   .25372525OD+00   1.643452-31   2.534722?34    .4457347?10+?)    .106?92 1(?+?(
24.75   15939.561A   .25309513?0+0?   1.642703791   2.539850437    .4485734?30+?0    .107514??D+?(
25.00   16074.2721   .25246315CD+00   1.641966294   2.544767? 25   .45141076?0+?)    .10??92 1?D+?(
25.25   16208.5099   .2518292??D+00   1.641240183   2.549734?36    .454?47??5D+?C    .10?54? ? 2D+?(
25.50   16342.2743   .25119355OD+00   1.640525337   2.554690134    .457??2???D+?0    .109?F1??7D+?(
25.75   16475.5646   .25055593?D+00   1.639821632   2.559655 01    .45??171?5D+?0    .10??5724??D+ (
26.00   16608.3797   .24991645CD+0?   1.639128521   2.564631?6?    .4627513?40+?0    .11 ??? ?2D+ (
26.25   16740.71A7   .24927508?C+00   1.638447097   2.569617695    .4655852??D+?0    .110?595?5D+?(
26.50   16872.5?08   .24863185?D+00   1.637776030   2.574614486    .46?41922?D+?0    .1110??217D+?(
26.75   17003.9649   .24798673?D+00   1.637115696   2.579622?20    .4712533?7D+?0    .1115?????D+?(
27.00   17134.8702   .24733975OD+00   1.636465704   2.584641?01    .474??77??D+?0    .112??4??C+?(
27.25   17265.2956   .2466908??D+00   1.635826179   2.589671741    .476?22771D+?0    .1125?12? 0D+?(
27.50   17395.2402   .24604C15CD+00   1.6351?7002   2.594714??)    .4797583?9D+?0    .1130?4???D+?(
27.75   17524.7030   .2453475??D+00   1.634577??    2.599776??43   .4825?5??1D+?)    .113?64?37D+?(
28.00   17653.6?31   .24471305CC+00   1.633969052   2.604835422    .4854331?50+?3    .114??2?41D+?(
28.25   17782.1793   .2440766??D+0C   1.633370096   2.609914 86    .488?27244?D+?)   .1145?3?43?D+.(
28.50   17910.1?07   .2434144?C+00    1.6327???9?   2.61500757?    .4911132 CD+?)    .115? ?1 ? D+.(
28.75   18027.7162   .2427563??C+00   1.632201?73   2.620117459    .4??????10+.?     .1155?????D+?(
29.00   18164.7548   .24209635?D+0C   1.631632013   2.625232?07    .4??0?4170+?3     .115??2???D+?(
29.25   18291.3054   .2414324?? C+00  1.631071 17   2.630366?7?    .49??4717?D+?     .1164??? CD+?(
29.50   18417.3670   .2407667?CC+00   1.630521?0?   2.635513 C5    .5?24??2??D+?     .116?34??7D+?(
29.75   18542.9?A4   .24005913?D+00   1.6295??05?   2.640?67? 31   .5??747? ?C+?0    .1174???1D+?(
                                                    [illegible]    [illegible]?D+?(   .117 77???D+?(

30.25   18752.6065   .22?7??2??C+00   1.62?-2?33?   2.6??1644 .    [illegible]       [illegible]
30.50   18?16.7009   .22?0?5?5?C+0C   1.628411?5?   2.656?251-?7   .?11 ?? ? ?D+ ?   .11  ??? ?D+ (
30.75   19040.?00?   .227405?? C+0C   1.6279076?7   2.661474? 17   .?1?7?? ?(+ ?     .11? ?7 ?+ (
31.00   19162.4045   .2267?255?C+0?   1.62741127?   2.66??712??54  .?1??51?7D+?      .11? 72? ???D+ (
31.25   19226.0121   .2260540?? C+00  1.6265243?4   2.67156 ?36    .???2?4?6D+ (     .1???????? ?+ (
31.50   194C8.1212   .225?723??C+0G   1.6264?-243   2.677241?6?    .?????? D+?       .1???(??  ?1+ (
31.75   19529.7211   .2246?C7? C+0C   1.625576?6?   2.682520?5     .?2??7?? ??+?     .1211?? ? ?+ (
32.00   19650.?406   .22405?2??C+00   1.6255156?3   2.6?7?3?6?2?   .?311C??????+?(   .121?714???+ (
32.25   19771.44?4   .2233315???D+00  1.6250635?1   2.69??1?C4??   .??4?4 4 ?D+??    .12???? ???+ (
32.50   19851.5534   .22263?1???C+0C  1.62461????   2.69??5?22C.   .??6?412 ?D+ C    .122?4?4 ??+ (
32.75   20011.1543   .2215?41?2?C+CC  1.6241833?6   2.70?3??2?5)   .???2? ?14D+?(    .122? ?6? ??+ (
33.00   20130.2498   .22124555CD+CC   1.6237565?6   2.70??241C1?   .?4??4??? D+?     .122?7?? ??+ (
33.25   20248.0?8?   .2205??6??C+00   1.6233374C?   2.714??2? ?C?  .?4??5?? ?D+?0    .1221?? ?1?+ (
33.50   20366.9200   .2298595?CC+C0   1.622926350   2.72?C5?4??    .?4? ?6???2D+?(   .124??(??1?+ (
33.75   20484.4?20   .2251623??C+00   1.622523331   2.725?451? C?  .??14??? ?D+?C    .124?(?  ?+ (
34.00   20??1.?536   .2284?2??CC+00   1.62212 265   2.73?C54F?C?   .?5?41(? ?D+?(    .12?1???4???+ (
34.25   20716.1034   .22776?4?-C+C0   1.6217410?4   2.736?42?C1?   .??7391??D+?(     .125?5?(4?3?+ (
34.50   20834.1403   .22705?825CD+00  1.621361716   2.741??22?6?   .?6?2???2?D+?(    .12????? ??+.(
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B-84

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34.75   20949.6628   .22635312 D+00   1.620590 07   2.74744072    [illegible]   [illegible]
35.00   21064.6696   .225646155D+00   1.620626103   2.752596474   [illegible]   [illegible]
35.25   21179.1593   .224937276D+00   1.62026 722   2.758584156   [illegible]   [illegible]
35.50   21293.1307   .224226550D+00   1.61992  60   2.764125962   [illegible]   [illegible]
35.75   21406.5822   .223513526D+00   1.61957 445   2.769321641   [illegible]   [illegible]
36.00   21519.5126   .222795545D+00   1.619245403   2.775260601   [illegible]   [illegible]
36.25   21631.9205   .222083086D+00   1.618851866   2.78101260    [illegible]   [illegible]
36.50   21743.6043   .221364855D+00   1.61855 174   2.786666655   [illegible]   [illegible]
36.75   21855.1628   .220644473D+00   1.618286 42   2.792286552   [illegible]   [illegible]
37.00   21965.5944   .219922755D+00   1.617981617   2.798112067   [illegible]   [illegible]
37.25   22076.2578   .219158886D+00   1.617683406   2.803662606   [illegible]   [illegible]
37.50   22186.0714   .218473155D+00   1.617392166   2.809636512   [illegible]   [illegible]
37.75   22295.3137   .217745536D+00   1.617107614   2.815426645   [illegible]   [illegible]
38.00   22404.0234   .217016056D+00   1.616830287   2.821262663   [illegible]   [illegible]
38.25   22512.1589   .216284666D+00   1.61655 510   2.827115671   [illegible]   [illegible]
38.50   22619.8287   .215551456D+00   1.616295423   2.832595431   [illegible]   [illegible]
38.75   22726.9413   .21481633 D+00   1.616037359   2.838502626   [illegible]   [illegible]
39.00   22833.5052   .214079356D+00   1.615787032   2.844623706   [illegible]   [illegible]
39.25   22939.5267   .213340486D+00   1.615542594   2.850601125   [illegible]   [illegible]
39.50   23045.0104   .212599756D+00   1.615304572   2.856702345   [illegible]   [illegible]
39.75   23149.9487   .21185712 D+00   1.615072897   2.862614552   [illegible]   [illegible]
40.00   23254.3420   .211112656D+00   1.614847492   2.868686159   [illegible]   [illegible]
40.25   23358.1886   .210366286D+00   1.614628295   2.874547712   [illegible]   [illegible]
40.50   23461.4871   .209618056D+00   1.614415235   2.881066036   [illegible]   [illegible]
40.75   23564.2358   .208867536D+00   1.614209252   2.887203643   [illegible]   [illegible]
41.00   23666.4331   .208115556D+00   1.614007262   2.893377066   [illegible]   [illegible]
41.25   23768.0773   .207362086D+00   1.613812206   2.899586705   [illegible]   [illegible]
41.50   23869.1667   .206606356D+00   1.613623010   2.905862727   [illegible]   [illegible]
41.75   23969.6597   .205848736D+00   1.613439602   2.912101356   [illegible]   [illegible]
42.00   24069.6747   .205089256D+00   1.613261915   2.918409276   [illegible]   [illegible]
42.25   24169.0895   .204327866D+00   1.613089874   2.924751604   [illegible]   [illegible]
42.50   24267.9437   .203564656D+00   1.612923403   2.931121556   [illegible]   [illegible]
42.75   24366.2342   .202799536D+00   1.612762439   2.937542535   [illegible]   [illegible]
43.00   24463.5599   .202032556D+00   1.612606906   2.943992617   [illegible]   [illegible]
43.25   24561.1189   .201262666D+00   1.612456720   2.950475254   [illegible]   [illegible]
43.50   24657.7056   .200492556D+00   1.612311915   2.957002459   [illegible]   [illegible]
43.75   24753.7301   .199720336D+00   1.612172116   2.96355 50    [illegible]   [illegible]
44.00   24849.1787   .198945856D+00   1.612037540   2.970167122   [illegible]   [illegible]
44.25   24944.0535   .19816594 D+00   1.611908017   2.976607102   [illegible]   [illegible]
44.50   25038.3529   .197391256D+00   1.611783466   2.98346860    [illegible]   [illegible]
44.75   25132.0749   .196611136D+00   1.611663758   2.990210 43   [illegible]   [illegible]
45.00   25225.2176   .195829156D+00   1.6115 4  47   .996574277    [illegible]   [illegible]
45.25   25317.7798   .19504528 D+00   1.611439827   3.003760287   [illegible]   [illegible]
45.50   25409.7565   .194259556D+00   1.611333342   3.010626266   [illegible]   [illegible]
45.75   25501.1532   .193471536D+00   1.611232432   3.017522062   [illegible]   [illegible]
46.00   25591.9612   .192682456D+00   1.611135990   3.024466655   [illegible]   [illegible]
46.25   25682.1867   .191895106D+00   1.611043940   3.031442440   [illegible]   [illegible]
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46.75   25860.8468   .1904 2727D+00   1.610[illegible]   3.0[illegible]    [illegible]          [illegible]
47.00   25945.2895   .189559750D+00   1.610793229   3.052671927   .72[illegible]        .14[illegible]
47.25   26037.1362   .188706880D+00   1.610717 25   3.059844 41   .724[illegible]       .14[illegible]
47.50   26124.3845   .187906150D+00   1.610646368   3.067067487   .72[illegible]        .14[illegible]
47.75   26211.0336   .187103526D+00   1.610577138   3.074240700   .731[illegible]       .147[illegible]
48.00   26297.0403   .186259050D+00   1.610514 40   3.081665485   .735575122D+00   .14[illegible]
48.25   26382.5232   .185452688D+00   1.610454590   3.088042747   .7352[illegible]      .14[illegible]
48.50   26467.3001   .1846 44500D+00   1.610397 43   3.096473521   .743[illegible]       .148[illegible]
48.75   26551.5651   .183874330D+00   1.610344534   3.103558188   .746[illegible]       .148[illegible]
49.00   26635.2081   .183062250D+00   1.610294540   3.111455550   .75[illegible]        .148[illegible]
49.25   26718.2152   .182248488D+00   1.610247753   3.119058957   .754424620D+00   .150[illegible]
49.50   26800.6062   .181432750D+00   1.610204063   3.126752065   .75 2742 1D+00   .150[illegible]
49.75   26882.3854   .180619128D+00   1.610163342   3.134465570   .7621512[illegible]   .1510106 6D+00
50.00   26963.5443   .179795650D+00   1.610125493   3.142225804   .766657156D+00   .1514126[illegible]
50.25   27044.0031   .178974288D+00   1.610090376   3.150074785   .76[illegible]        .1515[illegible]
50.50   27123.9595   .178151050D+00   1.610057 70   3.157972124   .773957127D+00   .1522[illegible]
50.75   27203.2916   .177325538D+00   1.610027848   3.165533067   .777552[illegible]    .152622311D+00
51.00   27281.9572   .176498950D+00   1.610000179   3.173595853   .781575[illegible]    .1530[illegible]
51.25   27359.9542   .175670098D+00   1.609974733   3.182050895   .78[illegible]        .153422[illegible]
51.50   27437.4004   .174835350D+00   1.609951363   3.190210466   .789129551D+00   .15[illegible]
51.75   27514.1737   .174006738D+00   1.609929333   3.198428576   .794254531D+00   .1540[illegible]
52.00   27590.3120   .173172250D+00   1.609910303   3.206737 23   .798412765D+00   .154054814D+00
52.25   27665.8130   .172335889D+00   1.609892300   3.215108802   .80260[illegible]     .155064090D+00
52.50   27740.6746   .171497650D+00   1.609875792   3.223552714   .806932841D+00   .155474[illegible]
52.75   27814.6546   .170657538D+00   1.609860609   3.232031771   .81110[illegible]     .1558[illegible]
53.00   27888.4708   .169815550D+00   1.609846595   3.240667357   .815410[illegible]    .1562[illegible]
53.25   27961.4009   .168971688D+00   1.609833559   3.249241228   .819753832D+00   .156712770D+00
53.50   28033.6828   .168125550D+00   1.609821349   3.258059594   .824136422D+00   .1571[illegible]
53.75   28105.3141   .167278338D+00   1.609809776   3.266520472   .828560248D+00   .157546[illegible]
54.00   28176.2527   .166428850D+00   1.609798652   3.275845468   .833025418D+00   .1579[illegible]
54.25   28246.6162   .165577488D+00   1.609787773   3.284852981   .837533184D+00   .158[illegible]
54.50   28316.2823   .164724250D+00   1.609776967   3.293549779   .842084[illegible]    .1588[illegible]
54.75   28385.2289   .163869138D+00   1.609766012   3.303126868   .846680477D+00   .1592242[illegible]
55.00   28453.6335   .163012150D+00   1.609754687   3.312295858   .851322[illegible]    .159658284D+00
55.25   28521.3138   .162153288D+00   1.609742791   3.321765510   .85601[illegible]     .1600[illegible]
55.50   28588.3276   .161292550D+00   1.609730083   3.331226030   .86074[illegible]     .16051[illegible]
55.75   28654.6725   .160429538D+00   1.609716324   3.340788208   .865[illegible]       .1605[illegible]
56.00   28720.3460   .159565450D+00   1.609701273   3.350449113   .870377[illegible]    .1613[illegible]
56.25   28785.3460   .158699088D+00   1.609684675   3.360212501   .875264111D+00   .16181 74D+00
56.50   28849.6695   .157830850D+00   1.609666269   3.370062268   .8802079 9D+00   .16225[illegible]
56.75   28913.3150   .15696677 D+00   1.609645781   3.380055808   .885207013D+00   .162[illegible]
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57.00  28976.2101  .156088750D+00  1.609622315  2.395014836  .450262126D+00  .162145500D+00
57.25  29028.5616  .155214887D+00  1.609597398  2.400250657  .555376630D+00  .162553027D+00
57.50  29100.1574  .154325150D+00  1.609556889  2.410665779  .500554380D+00  .164042412D+00
57.75  29161.0652  .15346153[illegible]D+00  1.609537117  2.421106868  .505785735D+00  .164456168D+00
58.00  29221.2524  .152582050D+00  1.609501695  2.431670727  .511084516D+00  .164852831D+00
58.25  29280.8066  .151706688D+00  1.609462326  2.442355007  .516449340D+00  .165412522D+00
58.50  29339.6352  .150817450D+00  1.609418597  2.453117704  .521875326D+00  .165877166D+00
58.75  29397.7660  .149932228D+00  1.609370171  2.464126847  .527275334D+00  .166244111D+00
59.00  29455.1963  .149045250D+00  1.609316626  2.475217655  .532505035D+00  .166[illegible]150[illegible]D+00
59.25  29511.9236  .148156488D+00  1.609257586  2.486447516  .535559565D+00  .167285624D+00
59.50  29567.9454  .147265750D+00  1.609192601  2.497822459  .544314545D+00  .167767613D+00
59.75  29623.2591  .146372138D+00  1.609121220  2.509346854  .550312837D+00  .168251557D+00
60.00  29677.8623  .145476650D+00  1.609042966  2.521025184  .555591150D+00  .168725826D+00
60.25  29731.7524  .144588228D+00  1.608957373  2.532861164  .561552246D+00  .169221524D+00
60.50  29784.5267  .1436[illegible]4050D+00  1.608863406  2.544866191  .567595500D+00  .169725061D+00
60.75  29837.3827  .142783528D+00  1.608762036  2.557030264  .574124114D+00  .170231207D+00
61.00  29889.1176  .141881550D+00  1.608651197  2.569372255  .580760540D+00  .170728748D+00
61.25  29940.1294  .140978098D+00  1.608530780  2.581895823  .586681425D+00  .171251700D+00
61.50  29990.4145  .140072350D+00  1.608400192  2.594555504  .592157856D+00  .171770267D+00
61.75  30039.9717  .139164728D+00  1.608259748  2.607459359  .595617325D+00  .172255000D+00
62.00  30088.7570  .138255250D+00  1.608105766  2.620552459  .100674330D+01  .172[illegible]25[illegible]75D+00
62.25  30136.8883  .13734286[illegible]D+00  1.607945534  2.633851420  .101297534D+01  .173226328D+00
62.50  30184.2925  .136430650D+00  1.607762273  2.647402557  .101882014D+01  .173711726D+00
62.75  30230.6581  .13551553[illegible]D+00  1.607570163  2.661132243  .102670154D+01  .174045143D+00

63.50  30366.2401  .132756550D+00  1.606902106  2.702311414  [illegible]  [illegible]
63.75  30409.8706  .131826330D+00  1.606645647  2.711402626  [illegible]  [illegible]
64.00  30452.7481  .130511850D+00  1.606370554  2.722252[illegible]61  [illegible]  [illegible]
64.25  30494.8695  .129965488D+00  1.606075740  2.745577[illegible]06  [illegible]  [illegible]
64.50  30536.2331  .129065725D+00  1.605759[illegible]24  2.764088814  [illegible]  [illegible]
64.75  30576.8351  .128127129D+00  1.605421[illegible]06  2.775855052  [illegible]  [illegible]
65.00  30616.6720  .127195150D+00  1.605060257  2.786000218  [illegible]  [illegible]
65.25  30655.7440  .126261288D+00  1.60467356[illegible]  2.811743822  [illegible]  [illegible]
65.50  30694.0453  .125325550D+00  1.604260246  2.825920452  [illegible]  [illegible]
65.75  30731.5742  .124387528D+00  1.603810664  2.849322728  [illegible]  [illegible]
66.00  30768.2276  .123448450D+00  1.603347003  2.863800455  [illegible]  [illegible]
66.25  30804.3029  .122507088D+00  1.60284341  2.881676570  [illegible]  [illegible]
66.50  30839.4971  .121563850D+00  1.602305[illegible]00  2.895554074  [illegible]  [illegible]
66.75  30873.9073  .120618720D+00  1.601731[illegible]72  2.911864257  [illegible]  [illegible]
67.00  30907.5208  .119671750D+00  1.601115558  2.927777213  [illegible]  [illegible]
67.25  30940.3645  .118722888D+00  1.600466039  2.957270528  [illegible]  [illegible]
67.50  30972.4056  .117772150D+00  1.599768595  2.977477257  [illegible]  [illegible]
67.75  31003.6511  .116815528D+00  1.599024265  3.998[illegible]  [illegible]  [illegible]
68.00  31034.0981  .115865050D+00  1.598229758  4.019234[illegible]60  [illegible]  [illegible]
68.25  31063.7437  .114908668D+00  1.597381577  4.040567000  [illegible]  [illegible]
68.50  31092.5649  .113950450D+00  1.596475[illegible]01  4.068311069  [illegible]  [illegible]
68.75  31120.6187  .112990338D+00  1.595508245  4.086303483  [illegible]  [illegible]
69.00  31147.[illegible]422  .112028350D+00  1.594474326  4.109588667  [illegible]  [illegible]
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69.25   31174.2523   .1110644840D+00   1.59336[illegible]60   4.1294[illegible]   [illegible]   [illegible]
69.50   31193.6461   .1100087500D+00   1.592186294   4.159607170   .1283710440D+01   .1532[illegible]45[illegible]
69.75   31212.6205   .1091311138D+00   1.590920372   4.188648678   .1297269310D+01   .1548276 2[illegible]
70.00   31231.5725   .1081616550D+00   1.589564304   4.212585[illegible]   .1311[illegible]12[illegible]50+[illegible]   .1958[illegible]57[illegible]
70.25   31250.6551   .1071502840D+00   1.588110302   4.240049750   .1326193[illegible]D+01   .1965[illegible]
70.50   31269.5572   .1062170550D+00   1.586545678   4.26544 350   .1341449240D+01   .1968[illegible]
70.75   31288.4637   .1052419320D+00   1.584873364   4.29[illegible]525653   .1357226140D+01   .19918[illegible]72 [illegible]
71.00   31306.0955   .1042645550D+00   1.583069706   4.330875063   .1373977[illegible]D+01   .2003505[illegible]
71.25   31325.8896   .1032860850D+00   1.581127164   4.363454551   .1391163[illegible]D+01   .20164[illegible]
71.50   31344.8425   .1023065350D+00   1.579031142   4.397523666   .1409252770+01   .20294[illegible]
71.75   31362.9522   .1013227380D+00   1.576765654   4.433213023   .1423[illegible]D+01   .20421[illegible]
72.00   31410.2144   .1003382500D+00   1.574312371   4.470643570   .1448165[illegible]D+01   .20575[illegible]
72.25   31426.6264   .9935188750D-01   1.571649533   4.510031662   .1465125[illegible]D+01   .207272 [illegible]
72.50   31442.1950   .9836265000D-01   1.568751947   4.551560244   .1481409200+01   .208 7226[illegible]
72.75   31456.8871   .9737253750D-01   1.565585960   4.595552522   .1514967680+01   .21058[illegible]
73.00   31470.7294   .9638155000D-01   1.562127994   4.642225844   .154[illegible] 20+01   .21226[illegible]
73.25   31483.7688   .9538766750D-01   1.558323193   4.692036161   .1566856490+01   .2142941[illegible]
73.50   31495.8222   .9439195000D-01   1.554123363   4.745412761   .1595645210+01   .2162[illegible]
73.75   31507.0662   .9339423750D-01   1.549463953   4.802924[illegible]   .1626732070+01   .218[illegible]
74.00   31517.4376   .9235948501D-01   1.544263655   4.865280400   .1660598390+01   .22100[illegible]
THE DUNHAM COEFFICIENTS

-8.19752144D-02  3.07267750D-01  2.20000000D-07
 7.21062849D+02 -1.76670000D-03
-2.57101904D+00 -1.50000000D-05
 2.85076374D-03
-1.29000000D-04
   POTENTIAL OF THE PBO     MOLECULE    (TOTAL FIT)
         GROUND STATE FOR LEAD OXIDE
FIT OF INNERMOST TURNING POINTS FOR EXTRAPOLATING U(R) WITH R LESS THAN   1.544263E+00 USING

FUNCTION OF THE FORM     EXP(B(1)+B(2)*X+B(3)*X*X....+B(K)*X**(K-1)) WITH K=MIN=  2

         R                  LOG(U(R))              UCALC              DIFF

   1.544263655D+00    4.458550902D+00    4.458564378D+00   -1.345316557D-05
   1.549463953D+00    4.458407565D+00    4.458392777D+00    1.458804775D-05
   1.554123363D+00    4.458252950D+00    4.458235386D+00    1.256435266D-05
   1.559323153D+00    4.458085867D+00    4.498100943D+00   -1.505603492D-05
CONSTANTS OF FIT

[illegible]          RMS ERROR=      [illegible]          RELATIVE RMS ERROR =     [illegible]
```

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 B( 2 ) =     .6235435770-01        RMS ERROR=     .3705775470-02        RELATIVE RMS ERROR =     .[illegible]

NUMBER OF ENTRIES :   4 STANDARD ERROR =    2.021710-05

 FIT OF OUTERMOST TRAINING POINTS FOR EXTRAPOLATING U(R) WITH R GREATER THAN   4.652 C4E+00 USING

 FUNCTION OF THE FORM  B(1)+B(2)*R**(-6)+B(3)*R**(-8)+....B(K)*..WITH K=NPOLT=  4

           R                  U(R)                FCALC               DIFF

    4.865280409D+00    3.151743762D+04    3.151743645D+04     1.131283062D-03
    4.802524059D+00    3.150706617D+04    3.150706640D+04    -2.226824535D-03
    4.745413781D+00    3.149582217D+04    3.149582253D+04    -3.601415136D-04
    4.652036161D+00    3.148370814D+04    3.148370724D+04     1.602582240D-03
    4.642225644D+00    3.147072541D+04    3.147072759D+04     1.415750857D-03
    4.595525328D+00    3.145687070D+04    3.145687772D+04    -6.415685008D-04
    4.551560344D+00    3.144218500D+04    3.144218713D+04    -2.126727602D-03
    4.510019662D+00    3.142662640D+04    3.142662515D+04     1.205357055D-03
 CONSTANTS OF FIT

 B( 1 ) =     .3154834610+05        RMS ERROR=     .8472617850+00        RELATIVE RMS ERROR =     .26[illegible]D-04
 B( 2 ) =     .2516502940+07        RMS ERROR=     .8909682320+05        RELATIVE RMS ERROR =     .[illegible]D-01
 B( 3 ) =    -.7008951320+08        RMS ERROR=     .2920592550+07        RELATIVE RMS ERROR =     .4[illegible]D-[illegible]
 B( 4 ) =    -.2047831840+09        RMS ERROR=     .2549814040+08        RELATIVE RMS ERROR =     .124[illegible]D+00

NUMBER OF ENTRIES :   8 STANDARD ERROR =    2.08320D-03

  BEGINNING OF INVERTED PERTURBATION APPROACH

RMIN =  1.400, RMAX =  7.500, SPACING =   .0061000
CONVERGENCE CRITERION IS ERROR LESS THAN   .10D-02

NUMBER OF ITERATIONS =   4

PARAMETERS OF THE FITTING POLYNOMIAL

RMIN =   1.595RMAX =  4.115 RE =  1.522,NPL= 10
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RESULTS OF SCHROEDINGER EQUATION FOR J(J+1) =    2. AND J=  1

  V    GV CAL      GV MEAS       GV M-C        BV CAL      BV M-C     S(MA)       S(MF)       MA     MP

  0    360.18200    360.16593    -.01607     .30637699     .00454     6.3D-10     7.4D-11     33    155
  1   1074.14182   1074.09502    -.04680     .30457966     .00517    -5.2D-10     7.1D-11     31    160
  2   1780.99104   1780.91692    -.07412     .30275232     .00581     6.5D-10     6.6D-11     30    164
  3   2480.73620   2480.64056    -.09564     .30089457     .00646    -4.7D-10     6.6D-11     28    168
  4   3173.39293   3173.28374    -.10915     .29900762     .00711     5.8D-10     6.3D-11     27    172
  5   3858.97005   3858.85119    -.11886     .29709029     .00774    -6.6D-10     7.2D-11     26    176
  6   4537.47352   4537.36853    -.10499     .29514299     .00834     7.1D-10     1.0D-10     25    17[illegible]
  7   5206.90649   5206.82230    -.08419     .29316571     .00892    -7.2D-10     8.3D-11     24    1[illegible]3
  8   5873.26522   5873.21991    -.04531     .29115848     .00945     6.5D-10     1.1D-10     23    1[illegible]6
  9   6530.55919   6530.55972     .00053     .28912126     .00997    -6.5D-10     8.5D-11     22    1[illegible]
 10   7190.77098   7190.83695     .06598     .28705406     .01047     5.5D-10     1.1D-10     21    1[illegible]
 11   7823.85652   7824.04377     .18725     .28495647     .01096    -5.2D-10     8.3D-11     20    1[illegible]7
 12   8455.92436   8456.16920     .24484     .28282565     .01149     4.5D-10     1.1D-10     19    20[illegible]
 13   9088.84108   9089.19521     .35414     .28067239     .01204    -5.2D-10     1.4D-10     19    20[illegible]
 14   9710.62995   9711.11666     .48671     .27848500     .01273     7.7D-10     1.6D-10     18    2[illegible]7
 15  10325.27164  10325.90129     .62965     .27626741     .01362    -6.4D-10     1.2D-10     17    210
 16  10932.74420  10933.52975     .78555     .27401551     .01482     5.2D-10     1.0D-10     16    214
 17  11533.02202  11533.57571     .55369     .27174116     .01647    -5.7D-10     1.2D-10     16    217
 18  12126.08101  12127.20653    1.12552     .26943216     .01877     7.[illegible]D-10     1.0D-10     15    221
 19  12711.88861  12713.19863    1.31002     .26709229     .02114    -6.3D-10     1.4D-10     14    224
 20  13290.41387  13291.90728    1.49341     .26472125     .0262[illegible]     5.1D-10     1.1D-10     13    22[illegible]
 21  13861.62241  13863.29668    1.67427     .2623[illegible]76     .03[illegible]7    -[illegible]D-10     1.5D-10     12    231

 23  14941.49533  14[illegible]
 24  15530.96737  15533.11471    2.14734     .254[illegible]74     .[illegible]63[illegible]4     4.7D-10     1.[illegible]D-10     10    [illegible]
 25  16072.50891  16074.77655    2.26764     .2523[illegible]519     .[illegible]74[illegible]4    -7.[illegible]D-10     1.4D-10     10    24[illegible]
 26  16606.52072  16608.87950    2.35878     .2498[illegible]65     .[illegible]     6.9D-10     1.3D-10      9    [illegible]
 27  17132.94551  17135.36484    2.41933     .24723270     .107[illegible]3    -5.[illegible]D-10     1.2D-10      8    254
 28  17651.72713  17654.17252    2.44539     .2446[illegible]14     .127[illegible]    -.61-10     1.5D-10      8    257
 29  18162.78756  18165.23897    2.45141     .241[illegible]419     .1439[illegible]    -7.2D-10     2.[illegible]D-10      7    261
 30  18666.06660  18668.49750    2.43090     .23927212     .15[illegible]41     6.1D-10     2.[illegible]D-10      6    26[illegible]
 31  19161.48165  19163.87833    2.39668     .2365[illegible]379     .170[illegible]4    -[illegible].2D-10     1.4D-10      5    27[illegible]
 32  19648.94794  19651.30860    2.36066     .2234[illegible]     .1761[illegible]     4.5D-10     1.[illegible]D-10      4    [illegible]74
 33  20128.37497  20130.71234    2.33737     .23107563     .174[illegible]    -7.4D-10     1.[illegible]D-10      4    [illegible]7
 34  20595.66495  20598.01040    2.34545     .228[illegible]67     .1694[illegible]     [illegible]D-10     2.[illegible]D-10      3    [illegible]
 35  21062.71855  21065.12087    2.40232     .2255[illegible]     .14217    -[illegible]D-10     1.[illegible]D-10      2    [illegible]7
 36  21517.43027  21519.95825    2.52798     .22269269     .13744     5.4D-10     2.3D-10      1    [illegible]1
 37  21963.65234  21966.39426    2.74192     .21[illegible]6559     .[illegible]5[illegible]    -[illegible]D-10     2.[illegible]D-10      1    [illegible]
 38  22401.39483  22404.45747    3.06264     .2170[illegible]    -.00543     1.5D-09     1.5D-10      1    [illegible]1
 39  22830.42660  22833.93332    3.50672     .214165[illegible]2    -.04534    -3.4D-09     1.5D-10      1    [illegible]
 40  23250.67601  23254.76418    4.08817     .2112[illegible]     .18146     5.5D-09     1.5D-10      1    [illegible]1[illegible]
 41  23662.03154  23666.64931    4.61777     .20841661    -.29374    -6.9D-09     2.1D-10      1    31[illegible]
 4[illegible] [illegible]  [illegible]  5.[illegible]  [illegible]  -.4[illegible]  1.0D-08  2.4D-1[illegible]  1  [illegible]21
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42 24069.3[illegible]
43 24457.61829 24464.36298   6.74569   .20259853   -.56511   -1.7D-08   2.9D-10   1   326
44 24841.63092 24849.57656   7.94563   .19966503   -.72235    2.3D-08   2.6D-10   1   332
45 25216.31286 25225.60551   9.29265   .19672217   -.88214   -4.2D-08   2.5D-10   1   338
46 25581.55609 25592.34661  10.79052   .19375620  -1.07237    6.8D-08   2.6D-10   1   344
47 25937.26153 25949.66856  12.40703   .19076915  -1.26252   -1.1D-07   2.8D-10   1   350
48 26283.32083 26297.45294  14.13211   .18775471  -1.45678    1.7D-07   3.4D-10   1   356
49 26619.63207 26635.57426  15.94219   .18472227  -1.65904   -2.7D-07   3.1D-10   1   363
50 26946.09257 26963.90392  17.81135   .18165693  -1.86040    4.3D-07   3.1D-10   1   370
51 27262.60346 27282.31021  19.70675   .17855942  -2.05955   -6.8D-07   3.9D-10   1   377
52 27569.05574 27590.65434  21.59860   .17542618  -2.25305    1.1D-06   3.2D-10   1   385
53 27865.35574 27888.81044  23.45470   .17225325  -2.43642   -1.7D-06   3.2D-10   1   393
54 28151.39576 28176.62551  25.22975   .16903628  -2.60655    2.6D-06   3.6D-10   1   401
55 28427.01450 28453.95548  26.94098   .16577043  -2.75740   -4.1D-06   3.9D-10   1   410
56 28692.27646 28720.66518  28.38872   .16245034  -2.88401    6.4D-06   3.0D-10   1   420
57 28946.89527 28976.59232  29.69705   .15907006  -2.98043   -9.9D-06   3.9D-10   1   42
58 29190.81711 29221.58754  30.77043   .15562291  -3.03398    1.5D-05   3.4D-10   1   440
59 29423.92362 29455.49438  31.57057   .15210138  -3.05515   -2.4D-05   3.7D-10   1   451
60 29646.05224 29678.15328  32.06105   .14849695  -3.01746    3.7D-05   3.8D-10   1   463
61 29857.19308 29889.40159  32.20851   .14480002  -2.91719   -5.6D-05   3.9D-10   1   476
62 30057.09001 30089.07355  31.98354   .14099931  -2.74319    8.6D-05   3.3D-10   1   4 1
63 30245.63838 30277.00031  31.36194   .13708186  -2.48243   -1.3D-04   3.7D-10   1   506
64 30422.68381 30453.00994  30.32613   .13303237  -2.11464    2.0D-04   3.9D-10   1   523
65 30588.06073 30616.92739  28.86666   .12883249  -1.63646   -3.0D-04   4.0D-10   1   542
66 30741.59034 30768.57452  26.98418   .12445587  -1.01054    4.4D-04   3.7D-10   1   564
67 30883.07852 30907.77011  24.69159   .11988633   -.21370   -6.5D-04   3.6D-10   1   585
68 31012.31322 31034.32583  22.01261   .11507526    .79067    9.5D-04   4.0D-10   1   617
69 31129.06132 31148.06626  19.00494   .10997644   2.05273   -1.4D-03   4.0D-10   1   651

SUM OF DIFF.=  6.7912D+02   AVERAGE DIFF. =  9.7018D+00       RMS OF EV =  1.5049D+01

COEFFICIENTS OF THE LEGENDRE POLYNOMIALS AFTER ITERATION NO.  1

B( 1) =   5.8902515740D+02   RMS ERROR =   5.558021D+03   RELATIVE  RMS ERROR =   1.[illegible]
B( 2) =  -1.2859567090D+03   RMS ERROR =   2.276525D+04   RELATIVE  RMS ERROR =   1.[illegible]
B( 3) =   1.2149805070D+03   RMS ERROR =   1.641827D+04   RELATIVE  RMS ERROR =   1.[illegible]
B( 4) =  -6.5545320940D+02   RMS ERROR =   4.030265D+03   RELATIVE  RMS ERROR =   [illegible]
B( 5) =   7.2513377650D+02   RMS ERROR =   6.242624D+03   RELATIVE  RMS ERROR =   [illegible]
B( 6) =  -7.7468869510D+02   RMS ERROR =   1.227544D+04   RELATIVE  RMS ERROR =   1.[illegible]
B( 7) =   4.5354120390D+02   RMS ERROR =   6.798574D+03   RELATIVE  RMS ERROR =   1.[illegible]
B( 8) =  -2.0779258150D+02   RMS ERROR =   1.649701D+03   RELATIVE  RMS ERROR =   [illegible]
B( 9) =   9.7716269060D+01   RMS ERROR =   1.868205D+03   RELATIVE  RMS ERROR =   1.[illegible]
B(10) =  -5.6203792470D+01   RMS ERROR =   1.164599D+03   RELATIVE  RMS ERROR =   1.[illegible]

COEFFICIENTS OF THE LEGENDRE POLYNOMIALS AFTER ITERATION NO.  2
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```
B( 1) =  -1.032818846D+02    RMS ERROR =   1.329299D+03    RELATIVE  RMS ERROR =     [illegible]
B( 2) =   2.326286235D+02    RMS ERROR =   3.054679D+03    RELATIVE  RMS ERROR =     [illegible]
B( 3) =  -1.330419284D+02    RMS ERROR =   2.351419D+03    RELATIVE  RMS ERROR =     [illegible]
B( 4) =  -3.179065807D+01    RMS ERROR =   5.517142D+02    RELATIVE  RMS ERROR =     [illegible]
B( 5) =  -4.325265580D+01    RMS ERROR =   1.152552D+03    RELATIVE  RMS ERROR =     [illegible]
B( 6) =   1.875305485D+02    RMS ERROR =   1.542767D+03    RELATIVE  RMS ERROR =     [illegible]
B( 7) =  -1.103204262D+02    RMS ERROR =   8.124137D+02    RELATIVE  RMS ERROR =     [illegible]
B( 8) =   1.757473555D+01    RMS ERROR =   3.289116D+02    RELATIVE  RMS ERROR =     [illegible]
B( 9) =  -2.846576069D+01    RMS ERROR =   2.833562D+02    RELATIVE  RMS ERROR =     [illegible]
B(10) =   2.804516122D+01    RMS ERROR =   1.262784D+02    RELATIVE  RMS ERROR =     [illegible]
 RESULTS OF SCHROEDINGER EQUATION FOR J(J+1) =    2. AND J=  1
```

```
  V    GV CAL     GV MEAS      GV M-C     BV CAL      BV M-C    S(BA)      S(BE)    MA   MI
-----------------------------------------------------------------------------------------------
  0    359.71158   359.75318   .04160   .30427567   2.10516   [illegible].3E-10  7.1E-11  34  159
  1   1073.70618  1073.68227  -.02391   .30263144   1.94435   -7.1E-10   1.1E-10  32  162
  2   1780.53582  1780.50017  -.03565   .30095108   1.80705    4.5E-10   7.8E-11  30  166
  3   2480.24558  2480.22381  -.02178   .29922063   1.68040   -6.5E-10   8.0E-11  29  169
  4   3172.86762  3172.86679  -.00083   .29744630   1.56843    8.2E-10   7.3E-11  28  173
  5   3854.42349  3854.44044   .01695   .29562938   1.46465   -9.4E-10   1.1E-10  27  176
  6   4536.92570  4536.95178   .02608   .29377114   1.38019    1.0E-09   8.5E-11  26  180
  7   5208.37949  5208.40554   .02605   .29187281   1.30132   -1.0E-09   1.2E-10  25  183
  8   5872.78440  5872.80316   .01876   .28993549   1.23244    1.0E-09   9.4E-11  24  187
  9   6530.13553  6530.14297   .00744   .28796016   1.17107   -5.5E-10   1.2E-10  23  190
 10   7180.42461  7180.42020  -.00446   .28594763   1.11690    8.7E-10   9.2E-11  22  194
 11   7823.64100  7823.62702  -.01398   .28389861   1.06922   -7.7E-10   1.2E-10  21  197
 12   8459.77162  8459.75245  -.01917   .28181367   1.02746    6.7E-10   8.8E-11  20  201
 13   9088.80174  9088.78246  -.01928   .27969332    .99111   -5.8E-10   1.1E-10  19  204
 14   9710.71463  9710.69991  -.01472   .27753801    .95972    4.9E-10   1.4E-10  18  207
 15  10325.49139 10325.48454  -.00684   .27534825    .93278   -5.5E-10   1.1E-10  18  211
 16  10933.11061 10933.11304   .00243   .27312455    .90978    7.4E-10   1.4E-10  17  214
 17  11533.54792 11533.55896   .01104   .27086753    .89010   -6.4E-10   1.6E-10  16  218
 18  12126.77559 12126.79278   .01720   .26857790    .87303    5.2E-10   1.4E-10  15  221
 19  12712.76220 12712.78188   .01968   .26625647    .85776   -5.4E-10   1.1E-10  15  225
 20  13291.47248 13291.49053   .01806   .26390411    .84342    7.6E-10   1.4E-10  14  228
 21  13862.86719 13862.87993   .01274   .26152173    .82910   -6.2E-10   1.2E-10  13  232
 22  14426.90329 14426.90815   .00486   .25911026    .81387    5.0E-10   1.6E-10  12  235
 23  14983.53418 14983.53019  -.00399   .25667058    .79685   -8.6E-10   1.4E-10  12  239
 24  15532.70997 15532.69795  -.01202   .25420350    .77723    7.0E-10   1.2E-10  11  243
 25  16074.37788 16074.36024  -.01764   .25170975    .75428   -5.7E-10   1.8E-10  10  246
 26  16608.48246 16608.46275  -.01971   .24918997    .72736    4.7E-10   1.6E-10   9  250
 27  17134.96580 17134.94809  -.01771   .24664474    .69585   -7.9E-10   1.5E-10   9  254
 28  17653.76768 17653.75577  -.01191   .24407458    .65935    6.6E-10   1.5E-10   8  258
 29  18164.82543 18164.82222  -.00321   .24148002    .61721   -5.5E-10   1.5E-10   7  262
 30  18668.07382 18668.08075   .00693   .23886164    .56889    4.7E-10   1.5E-10   6  266
 31  19163.44479 19163.46158   .01679   .23622006    .51377   -7.6E-10   1.6E-10   6  270
 32  19650.86715 19650.89185   .02470   .23355597    .45116    6.8E-10   1.8E-10   5  274
 33  20130.26631 20130.29559   .02928   .23087016    .38027   -6.0E-10   2.0E-10   4  278
 34  20601.56412 20601.59373   .02961   .22816346    .30027    5.3E-10   1.6E-10   3  283
 35  21064.67870 21064.70412   .02541   .22543672    .21031   -4.5E-10   1.5E-10   2  287
 36  21519.52438 21519.54150   .01711   .22269077    .10956    8.1E-10   2.4E-10   2  291
 37  21966.01181 21966.01751   .00570   .21992632   -.00263   -7.5E-10   2.1E-10   1  296
 38  22404.04803 22404.04072  -.00732   .21714396   -.12703    1.3E-09   1.5E-10   1  301
 39  22833.53679 22833.51657  -.02022   .21434410   -.26387   -2.1E-09   1.5E-10   1  306
 40  23254.37870 23254.34743  -.03127   .21152686   -.41333    3.4E-09   2.0E-10   1  310
 41  23666.47144 23666.43256  -.03888   .20869210   -.57527   -5.6E-09   2.0E-10   1  316
 42  24069.70996 24069.66814  -.04182   .20583935   -.74922    9.1E-09   2.3E-10   1  321
 43  24463.98668 24463.94722  -.03946   .20296781   -.93436   -1.5E-08   2.7E-10   1  326
 44  24849.19157 24849.15981  -.03176   .20007631  -1.12958    2.4E-08   2.4E-10   1  332
 45  25225.21216 25225.19276  -.01940   .19716231  -1.33328   -3.8E-08   3.2E-10   1  337
 46  25591.93342 25591.92985  -.00357   .19422067  -1.54354    6.2E-08   3.2E-10   1  342
 47  25945.23781 25945.25181   .01400   .19126471  -1.75908   -9.9E-08   3.9E-10   1  346
 48  26297.00501 26297.03619   .03118   .18827412  -1.97419    1.6E-07   3.0E-10   1  351
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50 26563.43137 26563.48116     .05[illegible]      .1[illegible]        [illegible]       [illegible]      [illegible]
51 27281.83409 27281.89346     .05937      .17505569   -2.59886   -6.4D-07   4.2D-11     1    376
52 27590.18622 27590.24159     .05537      .17595521   -2.74600    1.0D-06   3.7D-11     1    384
53 27888.35018 27888.39369     .04351      .17277155   -2.95512   -1.6D-06   3.6D-11     1    392
54 28176.18433 28176.20876     .02443      .16953042   -3.10066    2.5D-06   4.3D-11     1    401
55 28453.54293 28453.54273   -.00020       .16622597   -3.21614   -4.0D-06   4.2D-11     1    40[illegible]
56 28720.27602 28720.24 42   -.02759       .16286386   -3.29793    6.2D-06   4.7D-11     1    41[illegible]
57 28976.22959 28976.17556   -.05403       .15942513   -3.33550   -9.7D-06   4.3D-11     1    4[illegible]
58 29221.24593 29221.17079   -.07515       .15590617   -3.32324    1.5D-05   4.4D-11     1    4[illegible]
59 29455.16396 29455.07763   -.08633       .15229471   -3.25294   -2.4D-05   4.5D-1      1    45[illegible]
60 29677.82007 29677.73653   -.08354       .14859372   -3.11413    3.7D-05   5.3D-11     1    46[illegible]
61 29889.04878 29888.98484   -.06394       .1447 122   -2.89832   -5.6D-05   5.7D-11     1    475
62 30088.68398 30088.65680   -.02718       .14085031   -2.59416    8.6D-05   6.2D-11     1    4[illegible]
63 30276.56002 30276.58356    .02354       .13678677   -2.18534   -1.3D-04   6.1D-11     1    5[illegible]
64 30452.51303 30452.59319    .08016       .13258282   -1.67039    2.0D-04   6.7D-11     1    5[illegible]
65 30616.38207 30616.51064    .12857       .12821652   -1.02849   -3.0D-04   6.2D-11     1    54[illegible]
66 30768.00985 30768.15777    .14792       .12367310    -.22147    4.5D-04   7.3D-11     1    563
67 30907.24262 30907.35336    .11074       .11892178     .75085   -6.8D-04   7.5D-10     1    5[illegible]
68 31033.92875 31033.91308   -.01567       .11393723    1.92810    9.9D-04   7.8D-10     1    617
69 31147.91491 31147.64951   -.26540       .10867409    3.35514   -1.3D-03   8.6D-10     1    651
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SUM OF DIFF.=  1.9422D-02   AVERAGE DIFF. =  2.7747D-04        RMS OF GV =  5.2590D-02

RESULTS OF SCHROEDINGER EQUATION FOR J(J+1) =    0. AND J=  0

  V    GV CAL      GV MEAS       GV M-C       BV CAL     BV M-C     S(MA)      S(ME)      MA    ME

  0    359.10303   359.14042     .03739     .20427655   2.10412    9.2D-10    7.1D-11    34   156
  1   1073.10090  1073.07210    -.02881     .20262733   1.94662   -7.1D-10    1.1D-10    32   160
  2   1779.93396  1779.89466    -.03931     .20095197   1.80524    4.5D-10    7.8D-11    30   165
  3   2479.64714  2479.62200    -.02514     .19922153   1.67902   -6.5D-10    8.0D-11    29   16[illegible]
  4   3172.27273  3172.26896    -.00377     .19744721   1.56684    4.2D-10    7.3D-11    28   173
  5   3857.83223  3857.84624     .01401     .19563029   1.46646   -[illegible].4D-10  1.1D-10    27   176
  6   4536.33816  4536.36148     .02332     .19377206   1.37839    1.0D-09    6.9D-11    26   1[illegible]
  7   5207.79575  5207.81920     .02345     .19187373   1.30002   -1.0D-09    1.2D-10    25   1[illegible]
  8   5872.20453  5872.22083     .01630     .18993641   1.23064    1.0D-09    5.4D-11    24   1[illegible]7
  9   6529.55961  6529.56471     .00510     .18796104   1.16927   -5.5D-10    1.2D-10    23   1[illegible]
 10   7179.85277  7179.84608    -.00670     .18594856   1.11509    4.1D-10    9.2D-11    22   1[illegible]4
 11   7823.07320  7823.05708    -.01612     .18389954   1.06741   -7.7D-10    1.2D-10    21   1[illegible]7
 12   8459.20799  8459.18677    -.02122     .18181455   1.02566    6.7D-10    8.[illegible]D-11  20   201
 13   9088.24235  9088.22109    -.02126     .17969423    .98932   -5.8D-10    1.1D-10    19   204
 14   9710.15955  9710.14291    -.01664     .17753893    .95792    4.5D-10    1.4D-10    18   207
 15  10324.94069 10324.93198    -.00871     .17534916    .93099   -[illegible].5D-10  1.1D-10    18   211
 16  10932.56436 10932.56497     .00061     .17312546    .90749    7.8D-10    1.4D-10    17   214
 17  11533.00618 11533.01545     .00926     .17086843    .88832   -6.9D-10    1.0D-10    16   21
 18  12126.23843 12126.25388     .01545     .16857680    .87125    5.2D-10    1.4D-10    15   221
 19  12712.22569 12712.24165     .01597     .16625737    .85598   -5.4D-10    1.1D-10    15   22[illegible]
 20  13290.94467 13290.96104     .01637     .16390500    .84165    7.6D-10    1.4D-10    14   22
 21  13862.34414 13862.35523     .01108     .16152262    .82733   -6.2D-10    1.2D-10    13   232
 22  14426.38507 14426.38830     .00323     .15911114    .81211    5.0D-10    1.6D-10    12   23[illegible]
 23  14983.02084 14983.01526    -.00556     .15667146    .79569   -6.6D-10    1.4D-10    12   2[illegible]
 24  15532.20157 15532.18800    -.01357     .15420437    .77544    7.0D-10    1.2D-10    11   24[illegible]
 25  16073.87446 16073.85532    -.01914     .15171062    .75253   -5.7D-10    1.8D-10    10   24[illegible]
 26  16607.98407 16607.96292    -.02116     .14919083    .72562    4.7D-10    1.6D-10     9   25[illegible]
 27  17134.47251 17134.45341    -.01910     .14664559    .69416   -7.5D-10    1.5D-10     9   [illegible]4
 28  17653.27953 17653.26631    -.01323     .14407543    .65762    6.6D-10    1.5D-1      8   25
 29  18169.34247 18169.33803    -.00444     .14148087    .61540   -5.5D-10    1.5D-10     7   262
 30  18667.59610 18667.60189     .00579     .13886249    .56716    4.7D-10    1.5D-10     6   26[illegible]
 31  19162.97235 19162.98811     .01576     .13622090    .51205   -7.[illegible]D-10  1.6D-10     6   [illegible]7[illegible]
 32  19650.40004 19650.42384     .02380     .13355881    .44944    6.[illegible]D-10  1.[illegible]D-10     5   274
 33  20129.80457 20129.83309     .02851     .13087100    .37955   -6.0D-10    2.0D-10     4   27
 34  20631.10780 20631.13680     .02901     .12816430    .29655    5.3D-10    1.[illegible]D-10     3   [illegible]
 35  21064.22782 21064.25283     .02499     .12543757    .20654   -4.5D-10    1.5D-10     2   [illegible]7
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37 21965.57196 21965.57766     .00571     .21[illegible]   [illegible]
38 22403.61375 22403.60666    -.00707     .21714434    -.12875   1.3D-09   1.5D-10      1   [illegible]
39 22633.10411 22633.08841    -.01570     .21434498    -.26563  -2.1D-09   1.6D-10      1   [illegible]
40 23253.95565 23253.92520    -.03045     .21152776    -.41511   3.4D-09   2.0D-10      1   [illegible]
41 23666.05406 23666.01633    -.03773     .20866103    -.57706  -5.6D-09   2.0D-10      1   [illegible]
42 24069.29829 24069.25796    -.04033     .20584030    -.75105   9.1D-09   2.3D-10      1   [illegible]
43 24463.58076 24463.54316    -.03760     .20296679    -.93624  -1.5D-08   2.7D-10      1   [illegible]
44 24848.79142 24848.76191    -.02951     .20007732   -1.13147   2.4D-08   2.4D-10      1   [illegible]
45 25224.81784 25224.80110    -.01674     .19716435   -1.33520  -3.8D-08   3.2D-10      1   [illegible]
46 25591.54498 25591.54449    -.00049     .19422795   -1.54550   6.2D-08   3.2D-10      1   [illegible]
47 25948.85530 25948.87280     .01750     .19126584   -1.76069  -9.9D-08   3.6D-10      1   [illegible]
48 26296.62848 26296.66355     .03512     .18827530   -1.97625   1.6D-07   3.0D-10      1   [illegible]
49 26634.74120 26634.79139     .05018     .18525923   -2.19068  -2.5D-07   3.8D-10      1   367
50 26963.06700 26963.12757     .06057     .18219613   -2.40048   4.0D-07   3.6D-10      1   [illegible]
51 27281.47591 27281.54046     .06455     .17910006   -2.60111  -6.4D-07   4.1D-10      1   376
52 27589.83432 27589.89525     .06092     .17596066   -2.78841   1.0D-06   3.7D-10      1   [illegible]
53 27888.00466 27888.05406     .04940     .17277308   -2.95753  -1.6D-06   3.6D-10      1   [illegible]
54 28175.84529 28175.87590     .03061     .16953205   -3.10320   2.5D-06   4.3D-10      1   [illegible]
55 28453.21049 28453.21671     .00622     .16623171   -3.21956  -4.0D-06   4.2D-10      1   [illegible]
56 28719.95031 28719.92929    -.02102     .16286573   -3.30028   6.2D-06   4.7D-10      1   41[illegible]
57 28975.91076 28975.86339    -.04737     .15942713   -3.33834  -9.7D-06   4.8D-10      1   [illegible]
58 29220.93414 29220.86562    -.06852     .15590133   -3.32623   1.5D-05   4.4D-10      1   [illegible]
59 29454.85939 29454.77554    -.07985     .15230106   -3.25571  -2.4D-05   4.9D-10      1   [illegible]
60 29677.52290 29677.44557    -.07733     .14859628   -3.11763   3.7D-05   5.3D-10      1   [illegible]
61 29888.75924 29888.70107    -.05816     .14478404   -2.90209  -5.6D-05   5.6D-10      1   475
62 30089.40230 30088.38029    -.02201     .14085342   -2.59817   8.6D-05   6.2D-10      1   [illegible]
63 30276.28646 30276.31436     .02790     .13679224   -2.19367  -1.3D-04   6.1D-10      1   [illegible]
64 30452.24788 30452.33136     .08349     .13258673   -1.67488   2.0D-04   6.7D-10      1   [illegible]
65 30616.12565 30616.25624     .13059     .12822097   -1.02552  -3.0D-04   6.2D-10      1   [illegible]
66 30767.76252 30767.91087     .14836     .12367594    -.22749   4.5D-04   7.3D-10      1   [illegible]
67 30907.00479 30907.11402     .10923     .11892780     .74355  -6.6D-04   7.5D-10      1   [illegible]
68 31033.70088 31033.68135    -.01953     .11394503    1.92022   9.5D-04   7.6D-10      1   617
69 31147.69757 31147.42545    -.27212     .10868287    3.34544  -1.4D-03   8.6D-10      1   651

 SUM OF DIFF.=  0.            AVERAGE DIFF. =  0.                RMS OF DV =  0.

 COEFFICIENTS OF THE LEGENDRE POLYNOMIALS AFTER ITERATION NO.  3

B( 1) =   1.4369155010D+01    RMS ERROR =    5.0754640D+01    RELATIVE  RMS ERROR =     6.315[illegible]D+01
B( 2) =  -3.3873805970D+01    RMS ERROR =    2.0788090D+02    RELATIVE  RMS ERROR =     6.1369D+00
B( 3) =   3.3711769023D+01    RMS ERROR =    1.5583130D+02    RELATIVE  RMS ERROR =     4.6[illegible]D+00
B( 4) =  -2.8684832020D+01    RMS ERROR =    5.2436950D+01    RELATIVE  RMS ERROR =     1.8[illegible]D+00
B( 5) =   2.6585983580D+01    RMS ERROR =    6.5283950D+01    RELATIVE  RMS ERROR =     2.4556D+00
B( 6) =  -1.8743753780D+01    RMS ERROR =    1.0186560D+02    RELATIVE  RMS ERROR =     5.4314D+00
B( 7) =   8.7384763930D+00    RMS ERROR =    5.3980790D+01    RELATIVE  RMS ERROR =     6.1774D+00
B( 8) =  -6.7548728960D+00    RMS ERROR =    1.6594350D+01    RELATIVE  RMS ERROR =     2.7954D+00
B( 9) =   5.1577965520D+00    RMS ERROR =    1.7593800D+01    RELATIVE  RMS ERROR =     3.4111D+00
B(10) =  -1.4933555090D+00    RMS ERROR =    8.6643350D+00    RELATIVE  RMS ERROR =     5.8152D+00
```

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CORRELATION MATRIX OF THE COEFFICIENTS

 1  1.000000

 2   .999991  1.000000

 3   .999053   .999222  1.000000

 4   .966866   .967502   .977042  1.000000

 5   .992274   .952756   .9[illegible]6420   .98[illegible]741  1.000000

 6   .998493   .998437   .956833   .961515   .9[illegible]1033  1.000000

 7   .997258   .997245   .956017   .963434   .951305   .99[illegible]70  1.000000

 8   .988955   .989452   .992116   .967154   .9[illegible]8617   .99[illegible]87   .951[illegible]62  1.000000

 9   .956893   .996810   .994951   .955526   .959489   .999513   .955717   .9[illegible]  1.000000

10   .976161   .975594   .968629   .907182   .957251   .985251   .985752   .960[illegible]32   .9[illegible]751  1.000000
```

```
FINAL SET OF TURNING POINTS

 V          U(R)          RMIN            RMAX            RV.120

 0        359.103       1.875111        1.967533        30.4276560
 1       1073.101       1.836694        2.034213        30.2637326
 2       1779.534       1.814851        2.066433        30.0551 72
 3       2475.647       1.796367        2.097640        29. 221537
 4       3172.273       1.780940        2.124004        29.7447207
 5       3857.832       1.767616        2.148505        29.5630200
 6       4536.338       1.755847        2.171701        29.377205
 7       5207.796       1.745249        2.193925        29.1873730
 8       5872.205       1.735712        2.215411        28.9936413
 9       6529.560       1.726953        2.236325        28.7561079
10       7179.853       1.718891        2.256789        28.5944556
11       7823.073       1.711432        2.276899        28.3897536
12       8459.208       1.704505        2.296730        28.1614591
13       9088.242       1.698050        2.316345        27.9694234
14       9710.160       1.692021        2.335793        27.7536930
15      10324.941       1.686379        2.355120        27.5349157
16      10932.564       1.681050        2.374361        27.3125457
17      11533.006       1.676126        2.393550        27.0864434
18      12126.238       1.671464        2.412716        26.8576 02
19      12712.230       1.667062        2.431886        26.6257366
20      13290.945       1.662960        2.451093        26.3904995
21      13862.344       1.659081        2.470329        26.1522617
22      14426.385       1.655425        2.489646        25.9111142
23      14983.021       1.651969        2.509052        25.6671456
24      15532.202       1.648745        2.528567        25.4204373
25      16073.874       1.645694        2.548208        25.1710620
26      16607.984       1.642814        2.567992        24.9190 33
27      17134.473       1.640098        2.587939        24.6645596
28      17653.280       1.637537        2.608063        24.4075431
29      18164.342       1.635121        2.628384        24.1480 73
30      18667.596       1.632845        2.648917        23.8662447
31      19162.972       1.630701        2.669682        23.6220 01
32      19650.400       1.628682        2.690656        23.3558 10
33      20129.805       1.626788        2.711978        23.0870596
34      20601.108       1.625012        2.733548        22. 164303
35      21064.228       1.623349        2.755425        22.543756
36      21519.079       1.621801        2.777631        22.2681622
37      21965.572       1.620365        2.800189        21.9527177
38      22403.614       1.619046        2.823121        21.7144 35
39      22833.108       1.617843        2.846454        21.4344 83
```

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FINAL SET OF TURNING POINTS

 V          U(R)            RMIN            RMAX            BV*100

40       23253.956        1.616741        2.872214        21.1527765
41       23666.054        1.615732        2.894431        20.8683027
42       24069.298        1.614812        2.918135        20.5840299
43       24463.581        1.613973        2.944361        20.2961770
44       24848.791        1.613735        2.970146        20.0077514
45       25224.818        1.614496        2.996532        19.7164351
46       25591.545        1.615416        3.023561        19.4227 53
47       25948.855        1.616414        3.051265        19.1265 42
48       26296.628        1.617435        3.079759        18.8275256
49       26634.741        1.618407        3.109041        18.525322
50       26963.067        1.619287        3.139202        18.2196127
51       27281.476        1.620034        3.170317        17.9100057
52       27589.834        1.620616        3.202471        17.5960655
53       27888.005        1.621010        3.235762        17.2773040
54       28175.845        1.621198        3.270295        16.9532047
55       28453.210        1.621171        3.306207        16.6231714
56       28719.950        1.620924        3.343628        16.2865724
57       28975.911        1.620460        3.382727        15.9427130
58       29220.934        1.619786        3.423693        15.590 332
59       29454.859        1.618914        3.466746        15.2301060
60       29677.523        1.617862        3.512145        14.8596280
61       29888.759        1.616649        3.560192        14.47 4040
62       30088.402        1.615299        3.611250        14.0 53424
63       30276.286        1.613837        3.665752        13.679223
64       30452.248        1.612293        3.724226        13.2586732
65       30616.126        1.610695        3.787324        12.8220 70
66       30767.763        1.609074        3.855863        12.367593
67       30907.005        1.607461        3.930893        11.8927 05
68       31033.701        1.617871        4.013796        11.3945030
69       31147.698        1.619633        4.106466        10.8662 72
```

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FINAL POTENTIAL

          R                      U(R)                  RKR-IPA                 ERROR

   1.4000000000D+00       3.1865019200D+04       4.1675115830D-01       0.
   1.4072131830D+00       3.1847577660D+04       4.1675115900D-01       0.
   1.4144263660D+00       3.1830146070D+04       4.1675115760D-01        .
   1.4216395480D+00       3.1812723620D+04       4.16751156 0D-01        .
   1.4288527310D+00       3.1795311100D+04       4.1675115510D-01        .
   1.4360659140D+00       3.1777907920D+04       4.1675115670D-01        .
   1.4432790970D+00       3.1760514260D+04       4.1675115970D-01        .
   1.4504922790D+00       3.1743130130D+04       4.1675115550D-01        .
   1.4577054620D+00       3.1725755500D+04       4.1675115710D-01       0.
   1.4649186450D+00       3.1708390390D+04       4.1675115740D-01       0.
   1.4721318280D+00       3.1691034780D+04       4.1675115890D-01       0.
   1.4793450100D+00       3.1673688680D+04       4.1675115770D-01       0.
   1.4865581930D+00       3.1656352060D+04       4.1675115800D-01        .
   1.4937713760D+00       3.1639024940D+04       4.1675115740D-01       0.
   1.5009845590D+00       3.1621707300D+04       4.1675115760D-01       0.
   1.5081977410D+00       3.1604399140D+04       4.1675115940D-01       0.
   1.5154105240D+00       3.1587100450D+04       4.1675115950D-01       0.
   1.5226241070D+00       3.1569811230D+04       4.1675115850D-01       0.
   1.5298372900D+00       3.1552531470D+04       4.1675115760D-01       0.
   1.5370504720D+00       3.1535267230D+04       4.1069432880D-01       0.
   1.5442636550D+00       3.1517848180D+04      -4.1055359680D-01       1.2024807460D-15
   1.5494639530D+00       3.1506311 00D+04       7.5437033940D-01       2.6534455560D-11
   1.5541233630D+00       3.1495448870D+04       3.7729459240D-01       2.5954757620D-0
   1.5583231930D+00       3.1483296710D+04       4.1213559950D-01       3.5565556800D-06
   1.5621275940D+00       3.1470314040D+04       4.1536626520D-01       1.4162425 10D-04
   1.5655859600D+00       3.1456428010D+04       4.5560499680D-01       2.0322686450D-03
   1.5687519480D+00       3.1441748060D+04       4.3694515880D-01       1.5354674860D-02
   1.5716495230D+00       3.1426553470D+04       7.2929597510D-02       7.31 4125550D-02
   1.5743122710D+00       3.1411180060D+04      -5.6564974010D-01       2.4  4425470D-01
   1.5767656540D+00       3.1397243610D+04      -4.2514193470D+00       6.5765634450D-01
   1.5790311420D+00       3.1384770240D+04      -9.9273506910D+00       1.4362906070D+00
   1.5811271640D+00       3.1375034910D+04      -1.9145283610D+01       2.70 5262020D+00
   1.5830699060D+00       3.1368503680D+04      -3.2405162310D+01       4.556564 650D+00
   1.5848733680D+00       3.1366465930D+04      -5.1002260590D+01       7.0065526330D+00
   1.5865498780D+00       3.1366834960D+04      -7.2837763640D+01       1.0070455450D+01
   1.5881103020D+00       3.1369033660D+04      -9.7334552370D+01       1.3558164060D+01
   1.5895693040D+00       3.1373655670D+04      -1.2508312430D+02       1.745271  D+01
   1.5909203720D+00       3.1380963230D+04      -1.5634270120D+02       2.1730205920D+01
   1.5921862940D+00       3.1387736320D+04      -1.8789219780D+02       2.6162491510D+01
   1.5933688600D+00       3.1393309580D+04      -2.1905723970D+02       3.0653758240D+01
   1.5944743280D+00       3.1397270660D+04      -2.4942845990D+02       3.5241053740D+01
   1.5955082850D+00       3.1401612040D+04      -2.8099331690D+02       3.9736072060D+01
   1.5964759010D+00       3.1408356250D+04      -3.1590535620D+02       4.4125262540D+01
   1.5973815770D+00       3.1411636850D+04      -3.4769316020D+02       4.8366526760D+01
   1.5982257580D+00       3.1410916050D+04      -3.7681794290D+02       5.2436373060D+01
   1.5990242650D+00       3.1406063620D+04      -4.0243274780D+02       5.6315225750D+01
   1.5997685990D+00       3.1397203500D+04      -4.2479794680D+02       5.9506513950D+01
   1.6004660290D+00       3.1384481200D+04      -4.4911672150D+02       6.3453678800D+01
   1.6011195580D+00       3.1368216640D+04      -4.6068786750D+02       6.6710615420D+01
   1.6017319720D+00       3.1407444070D+04      -5.3353673060D+02       6.9762071940D+01
   1.6023058000D+00       3.1460102540D+04      -6.2060546200D+02       7.2616811180D+01
   1.6028434180D+00       3.1459113510D+04      -6.9481062320D+02       7.5275529560D+01
   1.6033470030D+00       3.1523270220D+04      -7.5494259710D+02       7.7756870420D+01
   1.6038146640D+00       3.1532298500D+04      -8.0072433490D+02       8.0067532400D+01
   1.6042602460D+00       3.1526587060D+04      -8.3254170960D+02       8.2211895940D+01
   1.6046735680D+00       3.1506990140D+04      -8.5124612700D+02       8.4202425380D+01
   1.6050602670D+00       3.1474670210D+04      -8.5799720970D+02       8.6045760770D+01
   1.6054215060D+00       3.1430976430D+04      -8.5414132640D+02       8.7761592060D+01
   1.6057595340D+00       3.1377356260D+04      -8.4112322690D+02       8.9348301650D+01
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```
1.6063705560D+00   3.1246216420D+04   -7.9346831640D+02   9.2176[illegible]
1.6066456470D+00   3.1171547360D+04   -7.6167675300D+02   9.34341576[illegible]
1.6069021060D+00   3.1092602420D+04   -7.2626232710D+02   9.455[illegible]
1.6071410150D+00   3.1010599070D+04   -6.8673965450D+02   9.567[illegible]
1.6073633870D+00   3.0926645210D+04   -6.4551819430D+02   9.66[illegible]
1.6075701630D+00   3.0772830560D+04   -5.4197251240D+02   9.7575356230[illegible]
1.6077622730D+00   3.0610464410D+04   -4.2622152130D+02   9.84[illegible]
1.6079405340D+00   3.0455165170D+04   -3.1625653900D+02   9.92[illegible]1067[illegible]
1.6081057660D+00   3.0307496850D+04   -2.1865981300D+02   9.991177237[illegible]
1.6082587480D+00   3.0167701360D+04   -1.2773026650D+02   1.005771[illegible]
1.6084001920D+00   3.0035971470D+04   -4.5556523850D+01   1.01163[illegible]
1.6085307800D+00   2.9912341260D+04    2.7768191540D+01   1.017[illegible]917[illegible]
1.6086511970D+00   2.9796711140D+04    9.2406663620D+01   1.0223[illegible]652[illegible]
1.6087620360D+00   2.9688963120D+04    1.4841557940D+02   1.02719[illegible]
1.6088635000D+00   2.9588674300D+04    1.9604636290D+02   1.031464[illegible]42[illegible]
1.6089573720D+00   2.9496162090D+04    2.3557026490D+02   1.035[illegible]7634[illegible]
1.6090429660D+00   2.9410611410D+04    2.6725091300D+02   1.03[illegible]5444[illegible]
1.6091212200D+00   2.9331824730D+04    2.9143442200D+02   1.04219[illegible]2440[illegible]
1.6091926010D+00   2.9259514720D+04    3.0643066900D+02   1.0451[illegible]870[illegible]
1.6092575860D+00   2.9193329040D+04    3.1659454670D+02   1.0478[illegible]3723[illegible]
1.6093166260D+00   2.9132916310D+04    3.2227996490D+02   1.050264[illegible]
1.6093701710D+00   2.9077900450D+04    3.1986552800D+02   1.0524635020[illegible]
1.6094185970D+00   2.9027964940D+04    3.1167033710D+02   1.054447[illegible]25[illegible]
1.6094623260D+00   2.8982730880D+04    2.9607568240D+02   1.05623[illegible]
1.6095016950D+00   2.8941894720D+04    2.7938765880D+02   1.0578427[illegible]76[illegible]
1.6095371170D+00   2.8905063400D+04    2.5600177920D+02   1.0592862440[illegible]
1.6095688950D+00   2.8871947240D+04    2.2821020590D+02   1.060579315[illegible]
1.6095973980D+00   2.8842196860D+04    1.9636476120D+02   1.061737220[illegible]
1.6096229150D+00   2.8815516170D+04    1.6076396400D+02   1.062772[illegible]
1.6096457820D+00   2.8791570800D+04    1.2174454710D+02   1.06369[illegible]675[illegible]
1.6096662690D+00   2.8770091590D+04    7.9577926600D+01   1.064529294[illegible]
1.6096846790D+00   2.8750763350D+04    3.4576637450D+01   1.065274134[illegible]
1.6097012730D+00   2.8733334660D+04   -1.2958620510D+01   1.06594[illegible]
1.6097163240D+00   2.8717506520D+04   -6.2824466720D+01   1.06655[illegible]
1.6097300830D+00   2.8703027110D+04   -1.1469951450D+02   1.06710[illegible]
1.6097427910D+00   2.8689643430D+04   -1.6832960680D+02   1.067621224[illegible]
1.6097546870D+00   2.8677106660D+04   -2.2347320350D+02   1.068100[illegible]25[illegible]
1.6097660120D+00   2.8665164310D+04   -2.7967545370D+02   1.068[illegible]57345[illegible]
1.6097769670D+00   2.8653605310D+04   -3.3732299300D+02   1.06[illegible]626[illegible]
1.6097877730D+00   2.8642196810D+04   -3.9558066340D+02   1.069433653[illegible]
1.6097986520D+00   2.8630705070D+04   -4.5441241530D+02   1.06[illegible]871465[illegible]
1.6098097760D+00   2.8618947560D+04   -5.1363345010D+02   1.0703[illegible]
1.6098213490D+00   2.8606707770D+04   -5.7362498450D+02   1.070[illegible]764142[illegible]
1.6098335590D+00   2.8593787370D+04   -6.3238643610D+02   1.071274702[illegible]
1.6098465950D+00   2.8579984440D+04   -6.9151363310D+02   1.07179[illegible]131[illegible]
1.6098606090D+00   2.8565134750D+04   -7.5024010910D+02   1.07226[illegible]25[illegible]
1.6098757920D+00   2.8549036220D+04   -8.0836157530D+02   1.072[illegible]365[illegible]
1.6098923000D+00   2.8531516160D+04   -8.6570515140D+02   1.073630[illegible]54[illegible]
1.6099103030D+00   2.8512396780D+04   -9.2208677950D+02   1.074251720[illegible]
1.6099299330D+00   2.8491532410D+04   -9.7735667640D+02   1.075137024[illegible]
1.6099513630D+00   2.8468731570D+04   -1.0313311590D+03   1.07559[illegible]
1.6099747230D+00   2.8443841870D+04   -1.0836476850D+03   1.076[illegible]26505[illegible]
1.6100001790D+00   2.8416711800D+04   -1.1347545960D+03   1.077[illegible]41222[illegible]
1.6100278480D+00   2.8387176640D+04   -1.1838550290D+03   1.07[illegible]043265[illegible]
1.6100578700D+00   2.8355091450D+04   -1.2310915210D+03   1.0[illegible]237373[illegible]
1.6100903760D+00   2.8320307450D+04   -1.2762243660D+03   1.0[illegible]152[illegible]353[illegible]
1.6101254930D+00   2.8282677370D+04   -1.3191350430D+03   1.0[illegible]29207[illegible]
1.6101633420D+00   2.8242066320D+04   -1.359680 35D+      1.0[illegible]441[illegible]
1.6102040630D+00   2.8198305890D+04   -1.3977015540D+03   1.0[illegible]027[illegible]
1.6102477530D+00   2.8151294070D+04   -1.4330786200D+03   1.0[illegible]7750414[illegible]
1.6102945400D+00   2.8100868950D+04   -1.4656660120D+03   1.0[illegible]115[illegible]
1.6103445340D+00   2.8046905820D+04   -1.4953167430D+03   1.0[illegible]1553472[illegible]
1.6103978430D+00   2.7989277150D+04   -1.5219171060D+03   1.0[illegible]640[illegible]
1.6104545800D+00   2.7927651650D+04   -1.5453204750D+03   1.0[illegible]91[illegible]
1.6105148400D+00   2.7862516100D+04   -1.5654357540D+03   1.0[illegible]202[illegible]57[illegible]
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1.610646365D+00     2.771961154D+04     -1.600225635D+03     1.104225321D+02
1.610717839D+00     2.764111362D+04     -1.606467757D+03     1.106055024D+02
1.610793229D+00     2.755966024D+04     -1.610371298D+03     1.108551181D+02
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1.613261915D+00     2.493253605D+04     -8.638613417D+02     1.197612505D+02
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1.9629820240D+00   1.2623574670D+02    5.3724461260D+01    1.8520665810D+01
1.9808326210D+00   2.8462466110D+02    7.4732506610D+01    2.5730140110D+01
1.9948862670D+00   4.4942345210D+02    8.9245949550D+01    3.2495955530D+01
2.0069842260D+00   6.1697971190D+02    1.0643306450D+02    3.6596234550D+01
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2.0278145250D+00     5.5673308760D+02     1.1175676570D+02     4.3006021830D+01
2.0371231440D+00     1.1275267060D+03     1.2283446640D+02     4.5167649070D+01
2.0459224390D+00     1.2956233150D+03     1.2816507340D+02     4.8360564450D+01
2.0542926430D+00     1.4716471910D+03     1.3262451600D+02     5.0252011390D+01
2.0623109280D+00     1.6438693630D+03     1.3644234380D+02     5.1887324540D+01
2.0700305850D+00     1.8161901860D+03     1.3971754770D+02     5.3305940400D+01
2.0774544910D+00     1.9885321570D+03     1.4252602430D+02     5.4543064250D+01
2.0847345720D+00     2.1608348680D+03     1.4493632440D+02     5.5611900850D+01
2.0917740670D+00     2.3330452260D+03     1.4699353050D+02     5.6525840500D+01
2.0986470870D+00     2.5051216920D+03     1.4874211860D+02     5.7330795760D+01
2.1053600950D+00     2.6770285930D+03     1.5021754800D+02     5.8010243410D+01
2.1119327090D+00     2.8487357020D+03     1.5145141900D+02     5.8585652050D+01
2.1183782690D+00     3.0202169280D+03     1.5246678360D+02     5.9067074400D+01
2.1247082880D+00     3.1914497760D+03     1.5329268780D+02     5.9462031150D+01
2.1309327740D+00     3.3624145550D+03     1.5394295910D+02     5.9781125230D+01
2.1370605010D+00     3.5330539600D+03     1.5443700660D+02     6.0026059590D+01
2.1430992120D+00     3.7034726390D+03     1.5479015660D+02     6.0205823730D+01
2.1490557680D+00     3.8735375160D+03     1.5501612500D+02     6.0331672090D+01
2.1549363080D+00     4.0432760230D+03     1.5512695030D+02     6.0395365180D+01
2.1607463240D+00     4.2126774460D+03     1.5513374260D+02     6.0414272520D+01
2.1664907790D+00     4.3817321590D+03     1.5504607250D+02     6.0383232610D+01
2.1721741560D+00     4.5504313250D+03     1.5487286650D+02     6.0308607300D+01
2.1778005340D+00     4.7187670520D+03     1.5462206470D+02     6.0194228520D+01
2.1833736310D+00     4.8867321350D+03     1.5430085410D+02     6.0042454880D+01
2.1888968520D+00     5.0543200670D+03     1.5391586040D+02     5.9856195100D+01
2.1943733170D+00     5.2215247160D+03     1.5347305950D+02     5.9637958500D+01
2.1998055100D+00     5.3883410230D+03     1.5297778190D+02     5.9390037240D+01
2.2051972860D+00     5.5547636510D+03     1.5243506480D+02     5.9114563390D+01
2.2105495030D+00     5.7207880510D+03     1.5184948650D+02     5.8812509680D+01
2.2158660510D+00     5.8864102240D+03     1.5122512030D+02     5.8486707040D+01
2.2211478540D+00     6.0516261580D+03     1.5056580260D+02     5.8141457110D+01
2.2263972980D+00     6.2164323770D+03     1.4987488160D+02     5.7774545200D+01
2.2316162370D+00     6.3808255970D+03     1.4915585920D+02     5.7386249950D+01
2.2368064050D+00     6.5448027780D+03     1.4841136490D+02     5.6984352530D+01
2.2419694320D+00     6.7083611380D+03     1.4764422560D+02     5.6564146050D+01
2.2471068550D+00     6.8714980430D+03     1.4685692810D+02     5.6128683320D+01
2.2522201070D+00     7.0342110680D+03     1.4605175850D+02     5.5679560000D+01
2.2573105640D+00     7.1964981220D+03     1.4523067700D+02     5.5217396240D+01
2.2623795070D+00     7.3583570730D+03     1.4439566370D+02     5.4743329360D+01
2.2674281470D+00     7.5197859580D+03     1.4354851490D+02     5.4258297370D+01
2.2724576460D+00     7.6807830670D+03     1.4269076430D+02     5.3762196010D+01
2.2774691010D+00     7.8413466360D+03     1.4182398700D+02     5.3258662150D+01
2.2824635590D+00     8.0014752010D+03     1.4094944470D+02     5.2746076670D+01
2.2874420070D+00     8.1611672660D+03     1.4006842050D+02     5.2225548650D+01
2.2924053940D+00     8.3204215850D+03     1.3918193500D+02     5.1696068420D+01
2.2973546170D+00     8.4792367480D+03     1.3829116020D+02     5.1164250660D+01
2.3022905490D+00     8.6376116760D+03     1.3739692600D+02     5.0624659050D+01
2.3072140160D+00     8.7955452070D+03     1.3650013170D+02     5.0080026650D+01
2.3121258100D+00     8.9530362780D+03     1.3560156650D+02     4.9530762320D+01
2.3170266940D+00     9.1100841560D+03     1.3470167850D+02     4.8977513900D+01
2.3219173830D+00     9.2666875210D+03     1.3380148870D+02     4.8420717030D+01
2.3267986010D+00     9.4228458630D+03     1.3290119660D+02     4.7860866590D+01
2.3316710100D+00     9.5785582220D+03     1.3200144000D+02     4.7298422440D+01
2.3365352580D+00     9.7338236790D+03     1.3110240520D+02     4.6733606070D+01
2.3413919890D+00     9.8886415890D+03     1.3020516800D+02     4.6167424610D+01
2.3462417910D+00     1.0043011920D+04     1.2930946800D+02     4.5599660300D+01
2.3510852590D+00     1.0196533120D+04     1.2841561480D+02     4.5030855070D+01
2.3559229730D+00     1.0350404560D+04     1.2752385570D+02     4.4461457770D+01
2.3607554630D+00     1.0503426650D+04     1.2663466510D+02     4.3891686200D+01
2.3655832740D+00     1.0655597590D+04     1.2574775700D+02     4.3321392440D+01
2.3704069100D+00     1.0808113110D+04     1.2486360980D+02     4.2752374640D+01
2.3752268780D+00     1.0959786600D+04     1.2398219740D+02     4.2183915650D+01
2.3800436820D+00     1.1111003110D+04     1.2310343600D+02     4.1615291140D+01
2.3848577770D+00     1.1261766820D+04     1.2222767680D+02     4.1048224950D+01
2.3896696320D+00     1.1412077740D+04     1.2135445750D+02     4.0482459860D+01
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2.39528-399D+00     1.1711335836D+04    1.1961652770D+02    3.93[illegible]
2.4040561950D+00    1.1860257360D+04    1.1875152550D+02    3.8715491000D+01
2.4049534880D+00    1.2032781660D+04    1.1788956860D+02    3.8237231260D+01
2.4137136930D+00    1.2156620720D+04    1.1703088770D+02    3.7641357610D+01
2.4185181890D+00    1.2304404260D+04    1.1617100390D+02    3.7136001720D+01
2.4233264060D+00    1.2451531500D+04    1.1531514740D+02    3.6577355620D+01
2.4281356990D+00    1.2598202860D+04    1.1446154540D+02    3.60[illegible]
2.4329464700D+00    1.2744417640D+04    1.1360110610D+02    3.54[illegible]
2.4377590600D+00    1.2890174810D+04    1.1275866560D+02    3.494224[illegible]
2.4425738660D+00    1.3035474720D+04    1.1190532920D+02    3.4414547670D+01
2.4473912290D+00    1.3180316580D+04    1.1106120630D+02    3.3870[illegible]2610D+01
2.4522115150D+00    1.3324700470D+04    1.1021362700D+02    3.333[illegible]
2.4570350460D+00    1.3468625330D+04    1.0936695830D+02    3.2811117130D+01
2.4618621870D+00    1.3612091400D+04    1.0852044290D+02    3.2267241670D+01
2.4666932740D+00    1.3755097970D+04    1.0767400260D+02    3.1767243[illegible]
2.4715286280D+00    1.3897644620D+04    1.0682743310D+02    3.1251221[illegible]
2.4763685590D+00    1.4039731190D+04    1.0598020250D+02    3.0735266020D+01
2.4812134770D+00    1.4181357000D+04    1.0513225220D+02    3.0231465060D+01
2.4860636150D+00    1.4322521820D+04    1.0428323590D+02    2.97278[illegible]770D+01
2.4909193240D+00    1.4463225110D+04    1.03432 3310D+02    2.9228646770D+01
2.4957809170D+00    1.4603466670D+04    1.0258056140D+02    2.8733778460D+01
2.5006486900D+00    1.4743245480D+04    1.0172668970D+02    2.8243364290D+01
2.5055229850D+00    1.4882562020D+04    1.0086995560D+02    2.7757464390D+01
2.5104040810D+00    1.5021414950D+04    1.0001098220D+02    2.7276141200D+01
2.5152922950D+00    1.5159804320D+04    9.9148963300D+01    2.6795449710D+01
2.5201875310D+00    1.5297729570D+04    9.8263578570D+01    2.6327438600D+01
2.5250912770D+00    1.5435189950D+04    9.7414796060D+01    2.5866160130D+01
2.5300026490D+00    1.5572185360D+04    9.6541917-10D+01    2.5397656420D+01
2.5349223340D+00    1.5708715300D+04    9.5664510450D+01    2.4935969350D+01
2.5398506370D+00    1.5844776490D+04    9.47[illegible]1640D+01  2.4467136320D+01
2.5447878250D+00    1.5980375030D+04    9.3857032760D+01    2.4035194750D+01
2.5497342340D+00    1.6115504550D+04    9.30053273[illegible]D+01  2.3596172730D+01
2.5546901340D+00    1.6250166160D+04    9.2106187350D+01    2.3156101290D+01
2.5596558010D+00    1.6384359150D+04    9.1205426210D+01    2.2725008130D+01
2.5646315690D+00    1.6518083270D+04    9.0296395700D+01    2.2296[illegible]1315D+01
2.5696176950D+00    1.6651337630D+04    8.9351071430D+01    2.187[illegible]
2.5746144860D+00    1.6784121850D+04    8.8458905570D+01    2.1455806900D+01
2.5796222200D+00    1.6916435040D+04    8.7529856660D+01    2.1042825940D+01
2.5846412010D+00    1.7048276610D+04    8.6593547760D+01    2.0634022200D+01
2.5896717410D+00    1.7179646070D+04    8.5645515360D+01    2.0232093620D+01
2.5947140800D+00    1.7310542480D+04    8.4697730930D+01    1.9834357760D+01
2.5997685420D+00    1.7440965180D+04    8.3737653170D+01    1.944171[illegible]
2.6048354220D+00    1.7570913710D+04    8.2769345900D+01    1.905418[illegible]
2.6099149860D+00    1.7700386680D+04    8.1792598400D+01    1.8671755420D+01
2.6150075700D+00    1.7829384090D+04    8.0806570540D+01    1.8294432720D+01
2.6201134500D+00    1.7957904620D+04    7.9811551260D+01    1.7922215410D+01
2.6252329070D+00    1.8085947610D+04    7.8807171060D+01    1.7555111[illegible]
2.6303662700D+00    1.8213512360D+04    7.7793021320D+01    1.7193103590D+01
2.6355138050D+00    1.8340597760D+04    7.6769212960D+01    1.6836152590D+01
2.6406758310D+00    1.8467203070D+04    7.5735351770D+01    1.6484370110D+01
2.6458526610D+00    1.8593327640D+04    7.4690998250D+01    1.6137626710D+01
2.6510445600D+00    1.8718969560D+04    7.3626537180D+01    1.5795554640D+01
2.6562518970D+00    1.8844129690D+04    7.2571247570D+01    1.5459338140D+01
2.6614749170D+00    1.8968805530D+04    7.1455240540D+01    1.5127760070D+01
2.6667135540D+00    1.9092996520D+04    7.0406342330D+01    1.48[illegible]
2.6719693360D+00    1.9216701880D+04    6.9310185070D+01    1.447[illegible]
2.6772413610D+00    1.9339920170D+04    6.8201043540D+01    1.4163172820D+01
2.6825303590D+00    1.9462650820D+04    6.7080297120D+01    1.3851621670D+01
2.6878366200D+00    1.9584892290D+04    6.5946303160D+01    1.3545030410D+01
2.6931604910D+00    1.9706643760D+04    6.4804662180D+01    1.3242376830D+01
2.6985023080D+00    1.9827904030D+04    6.3649359060D+01    1.29466[illegible]
2.7039623570D+00    1.9948671780D+04    6.2482501720D+01    1.2659752400D+01
2.7092410150D+00    2.0068946120D+04    6.1303721170D+01    1.2367613550D+01
2.7146386050D+00    2.0188725590D+04    6.0113233060D+01    1.20[illegible]
2.7200554560D+00    2.0308009160D+04    5.8910851620D+01    1.18[illegible]
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2.7309483090D+00    2.0545062830D+04    5.6470724630D+01    1.1240312210D+0
2.7364250150D+00    2.0662876500D+04    5.5232930750D+01    1.1015007450D+0
2.7419223620D+00    2.0770156500D+04    5.3963386770D+01    1.0746683200D+0
2.7474407380D+00    2.0896940690D+04    5.2722093920D+01    1.0472885260D+01
2.7529809474D+00    2.1013222310D+04    5.1449264360D+01    1.0243742010D+01
2.7585415690D+00    2.1128994600D+04    5.0164735520D+01    9.9555005550D+0
2.7641255620D+00    2.1244261800D+04    4.8868876620D+01    9.7556257340D+0
2.7697316410D+00    2.1359020530D+04    4.7561720710D+01    9.5242834900D+0
2.7753606010D+00    2.1473269350D+04    4.6243292380D+01    9.2934341260D+0
2.7810128090D+00    2.1587006560D+04    4.4913916280D+01    9.0670444300D+0
2.7866846550D+00    2.1700230550D+04    4.3573786140D+01    8.8450752220D+0
2.7923885520D+00    2.1812539560D+04    4.2222829630D+01    8.6274856640D+0
2.7981128670D+00    2.1925132650D+04    4.0861762320D+01    8.4142458620D+0
2.8038620680D+00    2.2036807510D+04    3.9490249110D+01    8.2053042420D+0
2.8096365120D+00    2.2147962330D+04    3.8109020090D+01    8.0036252600D+0
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2.9504792540D+00    2.4556591840D+04    4.5271063400D+00    4.3654596200D+0
2.9570034540D+00    2.4654666970D+04    3.0426260640D+00    4.2491954520D+0
2.9635658500D+00    2.4752168260D+04    1.5618913760D+00    4.1355464270D+0
2.9701671220D+00    2.4849093080D+04    8.5578979110D-02    4.0256857970D+0
2.9768079020D+00    2.4945438730D+04   -1.3852007560D+00    3.9183637060D+0
2.9834889080D+00    2.5041202670D+04   -2.8497620660D+00    3.8135245120D+0
2.9902108430D+00    2.5136382180D+04   -4.3072440410D+00    3.7123144590D+0
2.9969743770D+00    2.5230974440D+04   -5.7565932100D+00    3.6134760350D+0
3.0037802570D+00    2.5324976700D+04   -7.1969192220D+00    3.5173600580D+0
3.010627266D+00     2.5418386260D+04   -8.6273611040D+00    3.4235047650D+0
3.0175220820D+00    2.5511200160D+04   -1.0046809280D+01    3.3330579140D+0
3.0244595580D+00    2.5603415740D+04   -1.1454493560D+01    3.2447630710D+0
3.0314424480D+00    2.5695029820D+04   -1.2849105590D+01    3.1585653670D+0
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3.0526719270D+00    2.5966235270D+04   -1.6945718510D+01    2.9155559340D+0
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3.1422398040D+00    2.6995049050D+04   -3.1504730020D+01    2.1342626590D+0
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3.2067378330D+00    2.7629224360D+04          -3.8912356830D+01           1.7496755710D+0
3.2151036020D+00    2.7705486040D+04          -3.9675013370D+01           1.707711[illegible]350D+0
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7.1806400500D+00   3.1558728210D+04   4.1733463260D-01   2.1253557030D-05
7.2072533790D+00   3.1558570800D+04   4.1728517270D-01   1.9492955680D-05
7.2338667080D+00   3.1558415040D+04   4.1723995070D-01   1.7656248710D-05
7.2604800370D+00   3.1558260960D+04   4.1719871330D-01   1.6355983750D-05
7.2870933660D+00   3.1558108590D+04   4.1716099610D-01   1.4551856880D-05
7.3137066960D+00   3.1557957940D+04   4.1712652750D-01   1.3740816560D-05
7.3403200250D+00   3.1557809050D+04   4.1709502220D-01   1.2596546560D-05
7.3669333540D+00   3.1557661930D+04   4.1706622100D-01   1.1545600020D-05
7.3935466830D+00   3.1557516580D+04   4.1703966800D-01   1.0552105130D-05
7.4201600120D+00   3.1557373040D+04   4.1701560790D-01   9.7157383200D-06
7.4467733420D+00   3.1557231250D+04   4.1699378400D-01   8.5136557520D-06
7.4733866710D+00   3.1557091350D+04   4.1697363750D-01   8.1754331260D-06
7.5000000000D+00   3.1556953200D+04   4.1697363750D-01   7.5072106730D-06

ECOMMENCED INTEGRATION LIMITS RMIN =R(    1) = 1.400RMAX =R( 651)=  5.265
```

```
SUMMARY OF ERRORS OF THE INVERTED PERTURBATION APPROACH

 J(J+1)    1.         2.         3.         4.         5.         6.         7.         8.         9.        10.ITERATION

    2.0  15.03964   3.85281    .79104     .05260
------------------------------------------------------------------------------------------------------------------------

AVERAGE  16.24466   4.16151    .65529     .05661
THE DUNHAM COEFFICIENTS

-4.987263730D-01  3.072677500D-01  2.200000000D-07
 7.210628490D+02 -1.766700000D-03
-3.571019040D+00 -1.500000000D-05
 3.850763740D-03
-1.290000000D-04
```

Appendix C

Supplementary References

The following are references which contain information about the reduction of spectroscopic data and the construction of potential energy curves. They were not cited elsewhere in this report.

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Vita

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Inverted Perturbation Approach (IPA)
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20. ABSTRACT *(Continue on reverse side if necessary and identify by block number)*

This thesis presents the tools necessary to transform spectral data from diatomic molecules into potential energy curves which are most consistent with the experimental data and the quantum mechanical model (i.e., the Schroedinger wave equation (SWE)) for a diatomic molecule. The first of these tools, a computer program called DUNCON, generates spectroscopic constants by performing least-squares fits to spectroscopic data. The program performs fits to

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separate groups of data and then merges the results in a manner based upon the relative errors and correlations of the separate data sets. The second tool is a computer program provided by C. R. Vidal which contains two major routines. The first routine generates potential energy curves using the Rydberg-Klein-Rees (RKR) method. The second routine through an inverted perturbation analysis (IPA) adjusts the RKR curve so it is consistent with the SWE model. Finally, techniques are presented for extending potential energy curves to the dissociation energy, De , when the spectroscopic data alone is inadequate for the purpose.

Use of the programs is demonstrated for the diatomic molecule lead-oxide. Constants are produced for the A, B, D, a, b, and X states from previously published experimental data. A new set of assignments is made for the b state experimental data producing constants with significantly improved accuracy over those reported in literature. The b state constants are:

$$T_e = 16325.1 \pm 11.2 \text{ cm}^{-1}$$

$$W_e = 430.99 \pm 2.47 \text{ cm}^{-1}$$

$$W_e X_e = -0.757 \pm 0.441 \text{ cm}^{-1}$$

These are one standard error limits. Potential energy curves are generated for the a, A, and X states of lead-oxide. The X state potential energy curve is extended to its dissociation energy.