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DIATOMIC MOLECULE PROPERTIES IN THE INTERMEDIATE ENERGY TO DISS--ETC(U)
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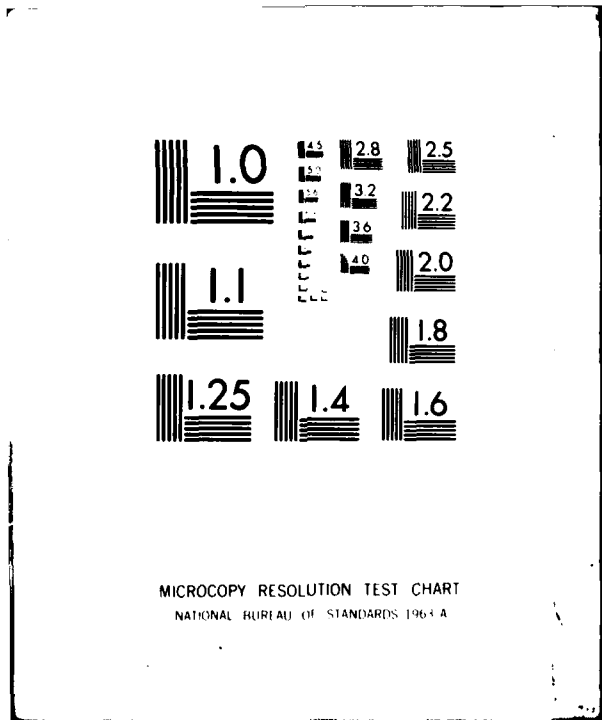
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REPORT DOCUMENTATION PAGE

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| 1. REPORT NUMBER AFOSR-TR- 82-0369 | | 2. GOVT ACCESSION NO. AD-A114867 | 3. RECIPIENT'S CATALOG NUMBER |
| 4. TITLE (and Subtitle) DIATOMIC MOLECULE PROPERTIES IN THE INTERMEDIATE ENERGY TO DISSOCIATION LIMIT RANGE | | 5. TYPE OF REPORT & PERIOD COVERED Final Technical Report Oct 1, 1976 to Sep 30, 1981 | |
| 7. AUTHOR(s) Charles L. Beckel | | 8. CONTRACT OR GRANT NUMBER(s) AFOSR 77-3132 | |
| 9. PERFORMING ORGANIZATION NAME AND ADDRESS Department of Physics and Astronomy The University of New Mexico Albuquerque, New Mexico 87131 | | 10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 61102 F 2301/A4 | |
| 11. CONTROLLING OFFICE NAME AND ADDRESS Directorate of Physical and Geophysical Sciences Air Force Office of Scientific Research Bolling Air Force Base, DC 20332 | | 12. REPORT DATE Sep 1981 | 13. NUMBER OF PAGES 15 |
| 14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office) | | 15. SECURITY CLASS. (of this report) Unclassified | |
| | | 15a. DECLASSIFICATION DOWNGRADING SCHEDULE | |

AD A114867

16. DISTRIBUTION STATEMENT (of this Report)

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17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)
Diatomic molecules; Vibrational potential curves; Vibrational energy levels; RKR method; Excited molecular states.

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)
To permit more reliable description of diatomic molecule properties in high-energy, high-temperature environments, new functional forms have been proposed for both vibrational energy levels and notations. These incorporate near-dissociation as well as near-equilibrium characteristics. The energy level expression was applied with considerable success to six electronic states; these include ground states of hydrogen species and excited states of molecular bromine and iodine. Use of the proposed eigenvalue representation reduced

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20. errors in RKR turning-point separations by two or three orders of magnitude, very near dissociation. Rational fraction representation of potentials was attempted for eight diatomic electronic states. The eight prototype potentials offer a diversity of forms. For all eight the rational fractions yielded very high levels of accuracy. Generally a single fraction was applicable over a wide range of nuclear separations, for example, from one-half to fifty angstroms. ↙

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Final Technical Report

"Diatomic Molecule Properties in the Intermediate
Energy to Dissociation Limit Range"

Prepared by
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Submitted to
The U. S. Air Force Office of Scientific Research
in connection with
Grant No. AFOSR-77-3132

Period Covered: October 1, 1976 to September 30, 1981

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SUMMARY OF RESEARCH ACCOMPLISHMENTS

I. Introduction and Background

The vibrational potential V plays a central role in interpretation of diatomic molecule data. Experimental results are analyzed in terms of such potentials and the potentials in turn are used to predict unknown properties. In principle, V can be determined by solving a fixed-nucleus eigenproblem and correcting for nuclear-electronic interactions. In practice, however, except for 1- and 2-electron systems, such ab initio theoretical potentials are of quite limited reliability; in general, ab initio V 's cannot be used to determine accurate vibrational eigenenergies E_v or related spectral properties.

As a result of the intractability of the many-electron Schrödinger equation, a number of methods have been devised for characterizing and relating V and E_v . These include use of: power series expansions for V as a function of nuclear separation R , approximate integrals from which V is found at a finite set of R values through inversion of vibration-rotation data (the Rydberg-Klein-Rees or RKR method), long-range multipole forms of $V(R)$, and closed-form expressions for $V(R)$ containing adjustable parameters.

Unfortunately each of these methods has severe limitations. Near-equilibrium properties are well described through use of $V(R)$ power series. None of the methods are adequate for description of near-equilibrium and also intermediate energy and near-dissociation properties. Thus, it appeared at the outset of the project that additional research should focus on the intermediate to high energy range of diatomic molecule bound states. Better understanding and more useful techniques were both sought. Any improvements achieved would have a direct beneficial impact on Air Force laser and nuclear weapons effects technology areas.

II. A. Original Objectives and Proposed Work

The proposed research had two specific objectives:

(a) to develop expressions for the vibrational eigenenergies E_v as a function of vibrational quantum number v useful in the intermediate to high v regions for diatomic molecule bound states, and

(b) to evaluate various possible causes of RKR failure near dissociation and to devise such improvements as will make the RKR procedure useful at high v .

Consistent with these objectives, the proposed work had two parts. A set of model vibrational potentials V and a set of accurate potentials for actual molecular states were to be used, each with a variety of long-range V forms. For these potentials the eigenvalues E_v were to be found. To aid in determining E_v vs. v functional forms, reduced mass μ was to be varied. In the second part of the work the effects of numerical techniques, low density of data points, and the breakdown of semi-classical theory at high v were to be studied for their roles in the failure of RKR near dissociation.

B. Additional Objective

During the course of the project an additional objective was adopted:

(c) to assess the accuracy and utility of rational fraction representation of $V(R)$.

The assessment was to cover a variety of prototype diatomic molecule electronic states.

III. Progress and Accomplishments

A. Computer Codes

Work initially centered on testing available computer programs for eigenvalue extraction, function fitting, and RKR inversion.¹ As a result, we used a code designated SLEIGN² for precise eigenvalue determination, a Householder

reflection code for linear function fitting, a Davidson code³ (called VARMET) for non-linear fitting, and a modified RKR program. Both VARMET and the RKR routine are improved versions of programs that we originally obtained from Kirtland Air Force Base Computational Services.

SLEIGN was applied to the Born-Oppenheimer (BO) V for the ground state of H_2^+ to obtain precise E_v with both the true reduced mass μ_0 and the fictitious mass $9\mu_0$. This potential is an accurate prototype V for an actual molecular state with long-range $-C_4/R^4$ behavior. We also determined first-order WBK energy levels $E_v(\text{WBK}_1)$ with μ_0 and with $9\mu_0$ for the same V .

For the ground state of H_2 we employed SLEIGN to obtain accurate Born-Oppenheimer E_v with reduced masses μ_0 and $25\mu_0$. The latter high mass yields 77 bound states. $E_v(\text{WBK}_1)$ were also determined for this state with μ_0 and $25\mu_0$. Because $E_v(\text{WBK}_1)$ can be considered a continuous function of v , it was possible for us to determine WBK eigenenergies at a dense mesh of noninteger v in the immediate vicinity of the dissociation limit D .

B. Representation of E_v as a Function of v (Objective a)

There is theoretical basis for a power-series expansion of E_v in $(v + \frac{1}{2})$ near equilibrium,⁴ i.e., at low v , and for a $(v_D - v)^m$ form near dissociation,⁵ i.e., at high v . Here v_D is the value of the vibrational quantum number at the dissociation limit D , and m is a parameter dependent on the long-range form of V . Hence, we sought a composite functional form of E_v which satisfies these two requirements and which interpolates well at intermediate v . In particular, we proposed use⁶ of the expression $E_v = D - (v_D - v)^m [L/N]$, where $[L/N]$ is a rational fraction in $(v_D - v)$. The degrees of numerator and denominator polynomials are L and N , respectively.

A thorough study was carried out⁶ on the use of the proposed composite E_v expression for the H_2^+ ground state BO eigenenergies. A variety of $[L/N]$ were

investigated. With $L + N = 4$, a polynomial ($N = 0$) yielded one of the poorest fits. As our proposed E_v form is nonlinear, the possibility exists of having several minima in each space of variable parameters; hence, it was necessary to carry out least-squares searches from a variety of starting points. Our best overall fit, with $L = 2$ and $N = 4$, had an RMS error of only 0.006 cm^{-1} in first differences $\Delta E(v + \frac{1}{2})$. Difficulties that might be encountered with use of the E_v expression were considered in some detail. The effect of neglecting terms of degree less than L or N in either numerator or denominator was investigated.

The proposed functional form for E_v was next applied to the H_2 ground electronic state.⁷ With the exception of [4/0] all $L + N = 4$ fits had an rms error in calculated BO $\Delta E(v + \frac{1}{2})$ of 0.02 cm^{-1} , attributable to the error in the theoretical V . The error in calculated $D - E_{14}$ ($v = 14$ is the highest bound state) could be made negligible. Mass 25 μ_0 levels were used to check applicability of the proposed expression to a large number of eigenenergies; several fits yielded all seventy-six ΔE with an rms error of only 0.04 cm^{-1} . The proposed composite form was also applied to the experimental vibrational energies. For these, best fits had an rms error of $\sim 0.07 \text{ cm}^{-1}$, larger than for theoretical energies presumably due to experimental errors.

The same form that had been applied to the ground electronic state of H_2 was used with isotopic substitution and mass-reduced quantum numbers to predict energy differences $\Delta E(v + \frac{1}{2})$ for D_2 and HD .⁸ Direct conversion from H_2 fittings yielded rms errors from experimental ΔE 's of 0.49 cm^{-1} and 0.43 cm^{-1} for D_2 and HD , respectively. Least-squares fitting to D_2 and HD ΔE 's lowered the rms errors to 0.034 and 0.045 cm^{-1} , significantly smaller than the best fittings to experimental H_2 data. The formula-predicted dissociation energies differed from recommended theoretical nonadiabatic values by 0.03 cm^{-1} for D_2 but by 1.5 cm^{-1} for HD .

The expression for E_v was applied⁹ to the B state of Br_2 , a prototype with $-C_5/R^5$ long-range behavior. We fitted the functional form with a variety of $[L/N]$ to the fifty-five experimental first differences ΔE for $^{79}\text{Br}_2$. Our best fits each had an overall rms error of 0.015 cm^{-1} in the ΔE . Apparently erroneous experimental results were exposed through consistently large errors in the same ΔE 's among different fits. Twelve of the 56 E_v were excluded as data to test the interpolation and extrapolation power of the proposed formula. The rms error in the interpolated ΔE 's was essentially the same whether these ΔE 's were included or excluded as fitting data; the rms error in the extrapolated ΔE at the three lowest v increased significantly, however. Our extrapolation for $D-E_{55}$ yields 1.00 cm^{-1} . Using the best $^{79}\text{Br}_2$ fits and mass reduced quantum numbers, we fitted to $^{81}\text{Br}_2$ and found an rms error of $<0.03 \text{ cm}^{-1}$ in the ΔE . Polynomial fits to the $^{79}\text{Br}_2 E_v$ and ΔE were attempted.¹⁰ The results indicated that our composite functional form was clearly superior to polynomials (a) near the dissociation limit, and (b) in extrapolation from above to near-equilibrium energies. Point (b), however, requires careful scrutiny.

We also fitted our E_v vs. v representation to $^{127}\text{I}_2$ B state experimental values¹¹ of $\Delta E(v + \frac{1}{2})$ for $4 \leq v \leq 82$. Our formula proved to be useful for (a) accurate representation of known energy differences, (b) highlighting and correcting inaccurate levels, and (c) interpolation and extrapolation of missing I_2 vibrational energies. Following completion of our calculations, more recent and accurate experimental I_2 data were brought to our attention. We did not have opportunity to use these data; however, their high level of accuracy and completeness should make them very useful for testing our proposed E_v formula.

C. RKR Failure near Dissociation (Objective b)

We studied in detail the errors in RKR turning point differences δR at the highest vibrational levels, $v = 60$ for H_2^+ ($9 \mu_0$), and $v = 76$ for H_2 ($25 \mu_0$). With a cubic spline representation for E_v the errors for the SLEIGN levels E_{60}

and E_{76} were 41.1 a.u. (atomic units, i.e., Bohr radii) and 12.9 a.u., respectively. Even for the WBK levels, the errors were 31.9 a.u. for $E_{60}(\text{WBK}_1)$ and 7.4 for $E_{76}(\text{WBK}_1)$, respectively. The latter values are especially significant because RKR determination of δR is a first-order WBK inversion; the extremely large errors cannot be blamed on breakdown of the semi-classical theory. Further, our numerical techniques yield very precise E_v , the high masses lead to a high density of data points, and we found no evidence of integration difficulties or related errors. We attributed the error to the E_v form used in RKR integrals, and switched to our proposed form described in Section B. When we represented $E_v = [2/5](v_D - v)^4$ in the RKR integral for $\text{H}_2^+(9 \mu_0)$, the δR error for $E_{60}(\text{WBK}_1)$ was reduced from 31.9 to 0.0 a.u.¹² Similarly with $[2/5](v_D - v)^3$ for $\text{H}_2(25 \mu_0)$ the δR error for $E_{76}(\text{WBK}_1)$ changed from 7.4 to 0.0 a.u. The error reduction is not so dramatic for R associated with SLEIGN E_v ; nevertheless, the δR error was reduced by at least two orders of magnitude at the highest integer v when $(v_D - v)^m$ was used as a factor in the E_v representation.

Not all RKR error near D appears attributable to the E_v representation. However, incorporation of the long-range term $(v_D - v)^m$ in a hybrid representation for E_v removes the key source of error at high v both for $1/R^4$ and $1/R^6$ prototype states. It is not clear that significant additional effort is warranted in isolating causes of residual error.

D. Rational Fraction Representation of V (Objective c)

In work not originally proposed, we fitted rational fractions $[L/N]$ in R to $V(R)$ for the ground states of H_2^+ ; L and N were chosen to give the correct long-range form for V . A $[5/9]$ fitting yielded^{13,14} an approximate V with a maximum error of 0.04 cm^{-1} in the domain $1.0 \leq R \leq 100$ a.u. This V_{approx} had only a single pole for real $R \geq 0$ and this was at 0.002 a.u. (This pole should be exactly at $R = 0$.) Further, all E_v but E_{19} obtained by solving a Schrödinger

equation containing this approximate V are accurate to within 0.01 cm^{-1} and E_{19} is only in error by 0.016 cm^{-1} .

The success of the rational fraction potential representation led us to apply this expression to the Born-Oppenheimer potential for the ground electronic state of H_2 . We restricted N to $L + 6$ to yield the correct long-range form for this state. Our best [5/11] fit had an rms error from Kolos and Wolniewicz' V of 0.01 cm^{-1} on $0.7 \leq R \leq 12$ Bohr radii.¹⁵ The [5/11] fitting has a pole at 1.9×10^{-4} a.u. with a residue of 0.98 instead of the correct values of 0 and 1, respectively.

Next, we applied the $V(R)$ expression to the $2p\pi_u$ state of H_2^+ . This state is bound but has a repulsive long-range $1/R^3$ form. Thus, with a potential minimum at $R = 7.9$ a.u. and a small maximum at $R \sim 26$ a.u., this state places strong demands on a $V(R)$ representation. In spite of this, we found that a [6/9] fitting achieves an rms error at 74 R values in $5 \leq R \leq 90$ a.u. of only 0.0014 cm^{-1} .¹⁶ The [6/9] is reliable for interpolation. It extrapolates at low R to a pole at -1.5×10^{-6} a.u. with residue 0.92 in place of correct values 0 and 1, respectively. The reliability of the extrapolation near $R = 0$, even though no fitting points below 5 a.u. were used, is probably due to the dominance at intermediate R of the nuclear repulsion over the purely electronic energy.

Rational fraction representation applied to the Born-Oppenheimer potential V for $\text{H}_2^+ 2p\sigma_u$ is of interest because this is a prototype $-1/R^4$ van der Waals electronic state. A [6/10] fraction, least-squares fitted on $0.8 \leq R \leq 90$ Bohr radii, has an rms error of 0.003 cm^{-1} at fitted points.¹⁷ The [6/10] accurately reproduces the shallow, large- R minimum, and yields reasonably reliably the Coulomb pole at $R = 0$.

The vibrational potential of the $3d\sigma_g$ electronic state of H_2^+ was represented

by rational fractions in nuclear separation R over the range $R = 1$ to 90 a.u.¹⁸ This state with a deep well is characterized by a strong $1/R^2$ attraction with significant higher-order multipole contribution even at very large R . The long-range form of the potential was reproduced by using either one or three constraints on the denominator polynomial. The best overall fit achieved over the entire range (1-90) has an rms of 0.03 cm^{-1} . However, fits over restricted ranges, 1-28 a.u. and 5-90 a.u. each achieve an order of magnitude smaller error.

To complete consideration of prototype V, three purely repulsive states of H_2^+ were considered. These are: the $3d\pi_g$ with $1/R^3$ long-range repulsion and promotion from $n = 2$ at $R = \infty$ to $3d$ at $R = 0$, $2s\sigma_g$ with $1/R^2$ repulsion and no promotion, and $3p\sigma_u$ with $1/R^2$ repulsion and promotion from $n = 2$ to $3p$ in the united atom. In spite of this diversity, all three had best fits on $1 \leq R \leq 90$ a.u. with rms errors of about 0.015 cm^{-1} . Work on these three states has not yet been reported at a scientific meeting or submitted for publication in a journal.

Rational fraction representations have thus yielded a very high level of accuracy for eight diatomic states with diverse $V(R)$ forms. Generally, a single fraction was applicable over a very wide R range.

IV. References

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- ⁹"A New Functional Form for Representing Vibrational Eigenenergies of Diatomic Molecules: Application to the Br₂ B State," C. L. Beckel, R. B. Kwong and A. R. Hashemi-Attar, Paper TB2, 35th Symposium on Molecular Spectroscopy, Columbus, Ohio, 17 June 1980.
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PUBLICATIONS AND INTERACTIONS

I. Papers Presented

"A Functional Form for Representing Vibrational Energy Levels of Diatomic Molecules," Ali-Reza Hashemi-Attar, Charles Beckel, and William N. Keepin, Paper RB 10, 33rd Symposium on Molecular Spectroscopy, Columbus, Ohio, June 15, 1978.

"Representation of Diatomic Vibrational Potentials by Rational Fractions with Correct Long-Range Behavior," Charles L. Beckel and Paul R. Findley, Paper RB 11, 33rd Symposium on Molecular Spectroscopy, Columbus, Ohio, June 15, 1978.

"On Non-Uniqueness of the Inverse Eigenvalue Problem and the RKR Method," Charles L. Beckel and Eugene S. Hertel, Jr., Paper RB 12, 33rd Symposium on Molecular Spectroscopy, Columbus, Ohio, June 15, 1978.

"On the Cause of RKR f-Integral Error near a Diatomic Molecule Dissociation Limit," E. S. Hertel, Jr., and Charles L. Beckel, Paper JQ 7, American Physical Society Meeting, Chicago, Illinois, 22 March 1979.

"A New Functional Form for Representing Vibrational Eigenenergies of Diatomic Molecules. Application to H_2 Ground State," A. R. Hashemi-Attar and Charles L. Beckel, Paper MQ 11, American Physical Society Meeting, Chicago, Illinois, 23 March 1979.

"On Use of Rational Fractions in Representing Diatomic Molecule Vibrational Energy Levels and Potentials," Charles L. Beckel, Paper 2-II-6, Third International Congress of Quantum Chemistry, Kyoto, Japan, 2 November 1979.

"Use of Rational Fractions for Representing Diatomic Molecule Vibrational Energy Levels and Potentials," Charles L. Beckel, A. R. Hashemi-Attar, E. S. Hertel, Jr., R. B. Kwong, and P. R. Findley, Paper MM8, Eighth Symposium on Molecular Structure, Austin, Texas, 3 March 1980.

"Representation of the H_2 Ground State Vibrational Potential by Rational Fractions," C. L. Beckel, R. B. Kwong, and A. R. Hashemi-Attar, Paper 14, 35th Symposium on Molecular Spectroscopy, Columbus, Ohio, 17 June 1980.

"A New Functional Form for Representing Vibrational Eigenenergies of Diatomic Molecules: Application to the Br_2 B State," C. L. Beckel, R. B. Kwong, and A. R. Hashemi-Attar, Paper TB2, 35th Symposium on Molecular Spectroscopy, Columbus, Ohio, 17 June 1980.

"On the Cause of RKR f-Integral Error near a Diatomic Molecule Dissociation Limit," E. S. Hertel, Jr., and C. L. Beckel, Paper TB3, 35th Symposium on Molecular Spectroscopy, Columbus, Ohio, 17 June 1980.

II. Papers Published

"A new functional form for representing vibrational eigenenergies of diatomic molecules. Application to H_2^+ ground state," Ali-Reza Hashemi-Attar, Charles L. Beckel, William N. Keepin, and Stephanie A. Sonnleitner, Journal of Chemical Physics, Vol. 70, 3881 (1979).

"A new functional form for representing vibrational eigenenergies of diatomic molecules. II. Application to H_2 ground state," Ali-Reza Hashemi-Attar and Charles L. Beckel, Journal of Chemical Physics, Vol. 71, 4596 (1979).

"Rational fraction representation of diatomic vibrational potentials. Application to H_2^+ ground state," C. L. Beckel and P. R. Findley, J. Chem. Phys. 73, 3517 (1980).

"A new functional form for representing vibrational eigenenergies of diatomic molecules. III. Application to D_2 and HD ground states," C. L. Beckel and R. B. Kwong, J. Chem. Phys. 73, 4698 (1980).

"Rational fraction representation of diatomic vibrational potentials. II. Application to H_2 ground state," C. L. Beckel, R. B. Kwong, and A. R. Hashemi-Attar, J. Chem. Phys. 73, 5385 (1980).

"Rational fraction representation of diatomic vibrational potentials. III. Application to $\text{H}_2^+ 2p\pi_u$ electronic state," C. L. Beckel, E. R. Scaggs and R. B. Kwong, J. Chem. Phys. 73, 5398 (1980).

"Rational fraction representation of diatomic vibrational potentials. IV. The $2p\sigma_u$ vander Waals state of H_2^+ ," S. A. Sonnleitner and C. L. Beckel, J. Chem. Phys. 73, 5404 (1980).

"Rational fraction representation of diatomic vibrational potentials. V. The $3d\sigma_g$ state of H_2^+ ," S. A. Sonnleitner, C. L. Beckel, A. J. Colucci, and E. R. Scaggs, J. Chem. Phys. 75, 2018 (1981).

III. Papers Planned for Submission to Journals

"Rational fraction representation of diatomic vibrational potentials. VI. Purely repulsive $3p\sigma_u$, $2s\sigma_g$, and $3d\pi_g$ states of H_2^+ ," S. A. Sonnleitner and C. L. Beckel.

"A new functional form for representing vibrational eigenenergies of diatomic molecules. IV. The Br_2 B state," C. L. Beckel, R. B. Kwong, A. R. Hashemi-Attar, and R. J. LeRoy.

"On the cause of RKR f-integral error near a diatomic molecule dissociation limit," E. S. Hertel, Jr. and C. L. Beckel.

"Applicability of the WBK approximation at the dissociation limit for long-range potential forms," C. L. Beckel.

These papers will likely be submitted to the Journal of Chemical Physics or the Journal of Molecular Spectroscopy.

IV. Theses and Dissertations Completed

"Polynomial and Rational Fraction Representations of a Diatomic Molecular Potential," Master of Science Thesis, Paul R Findley, May, 1978.

"RKR f-integrals and their Breakdown near the Diatomic Molecular Dissociation Limit," Doctor of Philosophy Dissertation, Part I, Eugene S. Hertel, Jr. December 1980.

V. Seminar Talks

University of New Mexico, Department of Physics and Astronomy Colloquium, C. L. Beckel, "Diatomic Molecules and Small Segments of Biological Molecules," March 4, 1977.

University of New Mexico, Department of Physics and Astronomy Seminar, C. L. Beckel, "Some Research Problems in Molecular Physics and Biophysics," September 6, 1979.

Memorial University of Newfoundland, Canada, Physics Seminar, C. L. Beckel, "Vibrational Potentials and Energy Levels of H_2 and H_2^+ ," September 25, 1980.

University of Waterloo, Ont., Canada, Chemical Physics Research Seminar, C. L. Beckel, "Mathematical Representation of Diatomic Potentials and Vibrational Energy Levels," November 12, 1980.

Kirtland Air Force Base, Albuquerque, New Mexico, Seminar, C. L. Beckel, "Accurate Mathematical Representation of Diatomic Molecule Potentials and Vibrational Energy Levels," March 15, 1982.

VI. Other Interactions

C. L. Beckel served as Visiting Staff Member (Short Term-Intermittent Services) to Group M-3, Los Alamos Scientific Laboratory, October 1979 to February 15, 1980. Subject matter--structure of explosives' molecules. Individual involved--Ray Engelke.

During the period August 11, 1980-August 10, 1981, C. L. Beckel served as a Physical Science Officer at the U. S. Arms Control and Disarmament Agency, Washington, D.C., under an Intergovernmental Personnel Act Agreement.

PERSONNEL

Charles L. Beckel, Principal Investigator, October 1976 to August 1980; August 1981 to September 1981.

R. Marcus Price, Co-Principal Investigator, August 1980 to September 1981.

Ali-Reza Hashemi-Attar, Research Assistant, January to April 1977; Research Associate, May 1977 to July 1979.

Robin B. Kwong, Research Associate, August 1979 to August 1980.

Stephanie A. Sonnleitner, Research Assistant, May to August 1978; December 1978 to January 1979; May to July 1979; April to December 1980. Research Associate, December 1980 to September 1981.

Eugene S. Hertel, Jr., Research Assistant, January 1977 to November 1978.

Paul R. Findley, Research Assistant, January to August 1977.

William N. Keepin, Research Assistant, May to August 1977.

Edward Moy, Research Assisnat, August 1978.

Marilyn Glaubensklée, Research Assistant, January to May 1979.

E. Rodney Scaggs, Jr., Research Assistant, June 1979 to August 1979; December 1979 to July 1980.

Anthony J. Colucci, Technical Assistant, March to July 1980.

Stephen Elston, Technical Assistant, May to July 1980.

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