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THEORETICAL DETERMINATION OF METAL OXIDE - f - NUMBERS

H. Harvey Michels

United Aircraft Corporation

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United Aircraft Research Laboratories
East Hartford, Connecticut 06108

May 1975

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This technical report has been reviewed and is approved for publication.

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Calculations have been performed for band-to-band transition probabilities. The systems under study were LiO, AlO, FeO, UO^+, UO and TiO. Electronic wavefunctions have been constructed for selected states of these molecules and expectation values of the electronic energy and electric dipole transition moments have been calculated. The calculated electric dipole transition moments were combined with accurate numerical vibrational-rotational wavefunctions, based on RKR potential functions, to yield estimates of the system f-numbers, band

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strengths and integrated IR band absorption coefficients. Data are presented for the transitions $(X\,{}^2\Pi - X\,{}^2\Pi)$ and $(A\,{}^2\Sigma^+ - X\,{}^2\Pi)$ of LiO, $(B\,{}^2\Sigma^+ - X\,{}^2\Sigma^+)$ and $(X\,{}^2\Sigma^+ - X\,{}^2\Sigma^+)$ of AlO, $({}^5\Sigma^+$ II $- X\,{}^5\Sigma^+)$ and $(X\,{}^5\Sigma^+ - X\,{}^5\Sigma^+)$ of FeO, $(X\,{}^4\Pi - X\,{}^4\Pi)$ of UO^+, for an averaged vibrational-rotational band system of UO, and $(X\,{}^3\Delta - X\,{}^3\Delta)$, $(A\,{}^3\Phi - X\,{}^3\Delta)$ and $(B\,{}^3\Pi - X\,{}^3\Delta)$ of TiO. With the exception of the vibrational-rotational band system of the ground state of AlO, the calculated data are probably accurate to within a factor of two. An examination of the location of the excited state curves for AlO and TiO relative to AlO^+ and TiO^+ indicates that dissociative-recombination will occur in both of these systems for both thermal and higher energy electrons. A limited study of UO_2 and UO_2^+ using a multiple-scattering X_α approach indicates that the positive ion is stable in a linear $D_{\infty h}$ configuration. The lowest order symmetry of UO_2 is not well defined within this approximation.

SUMMARY

The release of certain chemical species into the upper atmosphere results in luminous clouds that display the resonance electronic-vibrational-rotation spectrum of the released species. Such spectra are seen in rocket releases of chemicals for upper atmospheric studies and upon reentry into the atmosphere of artificial satellites and missiles. Of particular interest in this connection is the observed spectra of certain metallic oxides. From band intensity distribution of the spectra, and knowledge of the f-values for electronic and vibrational transitions, the local conditions of the atmosphere can be determined.

Present theoretical efforts which are directed toward a more complete and realistic analysis of the transport equations governing atmospheric relaxation and the propagation of artificial distrubances require detailed information of thermal opacities and LWIR absorption in regions of temperature and pressure where molecular effects are important. Because of inherent difficulties in the experimental determination of such properties, a theoretical program for calculating band absorption and emission coefficients was initiated. This theoretical program is based on current quantum mechanical techniques and capabilities for determining electronic and vibrational transition probabilities.

Calculations have been performed for band-to-band transition probabilities. The systems under study were LiO, AlO, FeO, UO^+, UO and TiO. Electronic wavefunctions have been constructed for selected states of these molecules and expectation values of the electronic energy and electric dipole transition moments have been calculated. The calculated electric dipole transition moments were combined with accurate numerical vibrational-rotational wavefunctions, based on RKR potential functions, to yield estimates of the system f-numbers, band strengths and integrated IR band absorption coefficients. Data are presented for the transitions ($X\,^2\Pi$ - $X\,^2\Pi$) and ($A\,^2\Sigma^+$ - $X\,^2\Pi$) of LiO, ($B^2\Sigma^+$ - $X\,^2\Sigma^+$) and ($X\,^2\Sigma^+$ - $X\,^2\Sigma^+$) of AlO,

$({}^5\Sigma^+ \text{ II} - X\ {}^5\Sigma^+)$ and $(X\ {}^5\Sigma^+ - X\ {}^5\Sigma^+)$ of FeO, $(X^4\Pi - X\ {}^4\Pi)$ of UO^+, for an averaged vibrational-rotational band system of UO, and $(X\ {}^3\Delta - X^3\Delta)$, $(A\ {}^3\Phi - X\ {}^3\Delta)$ and $(B\ {}^3\Pi - X\ {}^3\Delta)$ of TiO. With the exception of the vibrational-rotational band system of the ground state of AlO, the calculated data are probably accurate to within a factor of two. An examination of the location of the excited state curves for AlO and TiO relative to AlO^+ and TiO^+ indicates that dissociative-recombination will occur in both of these systems for both thermal and higher energy electrons. A limited study of UO_2 and UO_2^+ using a multiple-scattering X_α approach indicates that the positive ion is stable in a linear $D_{\infty h}$ configuration. The lowest order symmetry of UO_2 is not well defined within this approximation. Further more detailed theoretical studies of AlO are indicated as a result of this investigation. Experimental spectroscopic studies of FeO are in progress and a final resolution of the properties of this system should be possible in the near future.

PREFACE

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SECTION I

INTRODUCTION

The release of certain chemical species into the upper atmosphere results in luminous clouds that display the resonance electronic-vibrational-rotation spectrum of the released species. Such spectra are seen in rocket releases of chemicals for upper atmospheric studies and upon reentry into the atmosphere of artificial satellites and missiles. Of particular interest in this connection is the observed spectra of certain metallic oxides. From band intensity distribution of the spectra, and knowledge of the f-values for electronic and vibrational transitions, the local conditions of the atmosphere can be determined (ref. 1).

Present theoretical efforts, which are directed toward a more complete and realistic analysis of the transport equations governing atmospheric relaxation and the propagation of artifical disturbances, require detailed information of thermal opacities and LWIR absorption in regions of temperature and pressure where both atomic and molecular effects are important (refs. 2 and 3). Although various experimental techniques have been employed for both atomic and molecular systems, theoretical studies have been largely confined to an analysis of the properties (bound-bound, bound-free and free-free) of atomic systems (refs. 4 and 5). This has been due in large part to the unavailability of reliable wavefunctions for diatomic molecular systems, and particularly for excited states or states of open-shell structures. Only recently (refs. 6-8) have reliable procedures been prescribed for such systems which have resulted in the development of practical computational programs.

Because of inherent difficulties in the experimental determination of transition probabilities for metal oxide systems and in light of the aforementioned recent progress in the <u>ab initio</u> calculation of electronic wavefunctions for diatomic systems, a research program was initiated and under-taken in order to assess the reliability of theoretically predicting diatomic transition probabilities. The systems studied under this program included the blue-green system and vibrational-rotational transition of aluminum oxide, the vibrational-rotational systems of lithium oxide, iron oxide, uranium oxide and UO^+. In the cases of FeO and LiO, transitions were also calculated between the ground state and an upper state defined from an analysis of the electronic wavefunctions, as the state giving rise to the strongest transition. All of these band systems arise from transitions between electronic molecular states characterized over a wide range of internuclear separations by smooth unperturbed potential curves. For such systems, the electronic transition moment is a slowly varying function of internuclear separation and can often be factored from the total transition moment integral. This slowly varying R-dependence can often be accounted for by use of the empirical R-centroid approximation. However, many molecular band systems arise from transitions between perturbed electronic states. The origin of these perturbations may be an avoided crossing or a mixing of nearly degenerate electronic states at some particular internuclear separation. For such molecular systems, the total transition moment cannot be cast into a factored form, and a direct calculation of the band strengths must be performed.

The general composition of this report is as follows. In section II, we present a review of the current status of quantum mechanical calculations for molecular systems. This is followed by section III which deals with a description of the mathematical methods which were employed in this research. Included in section III are sub-sections which deal with the construction of electronic wavefunctions, the calculations of expectation properties, and the evaluation of molecular transition probabilities. The calculated results and pertinent discussions are presented in section IV. Technical papers which have resulted from these research studies are presented in the appendixes.

SECTION II

CURRENT STATUS OF QUANTUM MECHANICAL METHODS FOR DIATOMIC SYSTEMS

The application of quantum mechanical methods to the prediction of electronic structure has yielded much detailed information about atomic and molecular properties (ref. 9). Particularly in the past few years, the availability of high-speed computers with large storage capacities has made it possible to examine both atomic and molecular systems using an ab initio approach, wherein no empirical parameters are employed (ref. 10). Ab initio calculations for diatomic molecules employ a Hamiltonian based on the non-relativistic electrostatic interaction of the nuclei and electrons, and a wavefunction formed by antisymmetrizing a suitable many-electron function of spatial and spin coordinates. For most applications it is also necessary that the wavefunction represent a particular spin eigenstate and that it have appropriate geometrical symmetry. Nearly all the calculations performed to date are based on the use of one-electron orbitals and are of two types: Hartree-Fock or configuration interaction (ref. 11).

Hartree-Fock calculations are based on a single assignment of electrons to spatial orbitals, following which the spatial orbitals are optimized, usually subject to certain restrictions. Almost all Hartree-Fock calculations have been subject to the assumption that the diatomic spatial orbitals are all doubly occupied as nearly as possible, and are all of definite geometrical symmetry. These restrictions define the conventional, or restricted, Hartree-Fock (RHF) method (refs. 12 and 13). Restricted Hartree-Fock calculations can be made with relatively large Slater-type orbital (STO) basis sets for diatomic molecules with first or second-row atoms, and the results are convergent in the sense that they are insensitive to basis enlargement. The RHF model is adequate to give a qualitatively correct description of the electron interaction in many systems and in favorable cases can yield equilibrium interatomic separations and force constants. However, the double-occupancy restriction makes the RHF method inappropriate in a number of circumstances of practical interest. In particular, it cannot provide potential curves for molecules dissociating into odd-electron atoms (e.g., AlO at large internuclear separation) or into atoms having less electron pairing than the original molecule, e.g., $AlO\,^2\Sigma^+ \rightarrow Al\,(^2P) + O\,(^3P)$; it cannot handle excited states having unpaired electrons; and, in general, it gives misleading results for molecules in which the extent of electron correlation changes with inter nuclear separation.

Configuration-interaction (CI) methods have the capability of avoiding the limitations of the RHF calculations. If configurations not restricted to doubly occupied orbitals are included, a CI can, in principle, converge to an exact wavefunction for the customary Hamiltonian. However, many CI calculations have in fact been based on a restriction to doubly occupied orbitals and therefore retain many of the disadvantages of the RHF method (ref. 11). The use of general CI formulations involves three considerations, all of which have been satisfactorily investigated: the choice of basis orbitals, the choice of configurations (sets of orbital assignments), and the specific calculations needed to make wavefunctions describing pure spin states (ref. 7). The last consideration has proved difficult to implement, but computer programs including it have been prepared, and the CI method has been found of demonstrable value in handling excited states and dissociation processes which cannot be treated with RHF techniques.

Either of the above described methods for ab initio calculations reduces in practice to a series of steps, the most important of which are the evaluation of molecular integrals, the construction of matrix elements of the Hamiltonian, and the optimization of molecular orbitals (RHF) or configuration coefficients (CI). For diatomic molecules, these steps are all comparable in their computing time, so that a point has been reached where there is no longer any one bottleneck determining computation speed. In short, the integral evaluation involves the use of ellipsoidal coordinates and the introduction of the Neumann expansion for the interelectronic repulsion potential (ref. 14); the matrix element construction depends upon an analysis of the algebra of spin eigenfunctions (ref. 15); and the orbital or configuration optimization can be carried out by eigenvalue techniques (ref. 16). All the steps have by now become relatively standard and can be performed efficiently on a computer having 32,000 to 65,000 words of core storage, a cycle time in the microsecond range, and several hundred thousand words of peripheral storage.

Both the RHF and CI methods yield electronic wavefunctions and energies as a function of the internuclear separation, the RHF method for one state, and the CI method for all states considered. The electronic energies can be regarded as potential curves from which may be deduced equilibrium internuclear separations, dissociation energies, and constants describing vibrational and rotational motion (including anharmonic and rotation-vibration effects). It is also possible to solve the Schrödinger equation for the motion of the nuclei subject to the potential curves to obtain vibrational wavefunctions for use in transition probability calculations. The electronic wavefunctions themselves can be used to estimate dipole moments of individual electronic states, transition moments between different electronic states, and other properties. While all of the calculations described in this paragraph have been carried out on some systems, the unavailability of good electronic wavefunctions and potential curves has limited actual studies of most of these properties to a very small number of molecules.

A few studies illustrating the scope of the current work in this field are cited. Exhaustive RHF calculations have been reported for first and second-row hydrides (ref. 17 and 18) for most first-row diatomic molecules (ref. 19), and for many other molecules containing second-row atoms (ref. 20). Configuration-interaction calculations restricted to double occupancy are illustrated by the work of Das and Wahl on Li_2 and F_2 (refs. 11 and 21). They determined an optimum choice of orbitals for a small number of configurations designed to permit proper description of the dissociation products, and obtained highly satisfactory potential curves. Davidson (refs. 22 and 23) has carried out doubly occupied CI studies with very large numbers of configurations to gain more insight into the description of correlation energy. The largest of the CI studies not restricted to doubly occupied orbitals have been carried out at UARL. The 62 states of O_2 dissociating into low-lying atomic oxygen states have been described in a qualitatively consistent manner (ref. 24). Many of these states involve several unpaired electrons, and the success of the treatment depended critically upon the inclusion of all types of pertinent configurations and upon proper handling of the spin. Similar work on the 102 low-lying N_2 states has now been completed (ref. 25). In striking contrast to the recent progress in obtaining electronic energies and wavefunctions, rather few calculations of electronic transition moments have been attempted. Among the few studies in this area is the work of Michels on $He\ H^+$ (ref. 8) and of Henneker and Popkie (ref. 26) on diatomic hydrides using Hartree-Fock wavefunctions. More recently a theoretical program for calculating band strengths for the system N_2 (1 PS), O_2 (SR), and NO (β) has been carried out. The results of this program indicate that reliable band strengths (10 to 25 percent) can be calculated, provided a CI approach is employed (ref. 27).

SECTION III

METHOD OF APPROACH

1. Electronic Structure

A spin-free, nonrelativistic, electrostatic Hamiltonian is employed in the Born-Oppenheimer approximation. In systems containing atoms as heavy as N or O, this approximation is quite good for low-lying molecular states. For a diatomic molecule containing n electrons, the approximation leads to an electronic Hamiltionian depending parametrically on the internuclear separation R:

$$\mathcal{H}(R) = -\frac{1}{2}\sum_{i=1}^{n} \nabla_i^2 - \sum_{i=1}^{n} \frac{Z_A}{r_{iA}} - \sum_{i=1}^{n} \frac{Z_B}{r_{iB}} + \frac{Z_A Z_B}{R} + \sum_{i>j\geq 1}^{n} \frac{1}{r_{ij}} \qquad (1)$$

where Z_A and Z_B are the charges of nuclei A and B, and r_{iA} is the separation of electron i and nucleus A. $\mathcal{H}$ is in atomic units (energy in Hartress, length in Bohrs).

Electronic wavefunctions $\Psi(R)$ are made to be optimum approximations to solutions, for a given R, of the Schrödinger equation

$$\mathcal{H}(R)\Psi(R) = E(R)\Psi(R) \qquad (2)$$

by invoking the variational principle

$$\delta W(R) = \delta \frac{\int \Psi^*(R)\mathcal{H}(R)\Psi(R)\,d\tau}{\int \Psi^*(R)\Psi(R)\,d\tau} \qquad (3)$$

The integrations in Eq. (3) are over all electronic coordinates and the stationary values of W(R) are approximations to the energies of states described by the corresponding $\Psi(R)$. States of a particular symmetry are studied by restricting the electronic wavefunction to be a projection of the appropriate angular momentum and spin operators. Excited electronic states corresponding to a particular symmetry are handled by construction of configuration interaction wavefunctions of appropriate size and form.

The specific form for $\Psi(R)$ may be written

$$\Psi(R) = \sum_{\mu} C_{\mu} \Psi_{\mu}(R) \tag{4}$$

where each $\Psi_{\mu}(R)$ is referred to as a configuration, and has the general structure

$$\Psi_{\mu}(R) = \mathcal{A}\mathcal{O}_{S} \prod_{i=1}^{n} \psi_{\mu i}(\underset{\sim}{r}_i, R)\,\theta_{M} \tag{5}$$

where ψ_{μ} is a spatial orbital, $\mathcal{A}$ is the antisymmetrizing operator, $\mathcal{O}_S$ is the spin-projection operator for spin quantum number S, and θ_M is a product of α and β one-electron spin functions of magnetic quantum number M. No requirement is imposed as to the double occupancy of the spatial orbitals, so Eqs. (4) and (5) can describe a completely general wavefunction.

In Hartree-Fock calculations, $\Psi(R)$ is restricted to a single Ψ_{μ} which is assumed to consist as nearly as possible of doubly occupied orbitals. The orbitals $\psi_{\mu i}$ are then selected to be the linear combinations of basis orbitals best satisfying Eq. (3). Writing

$$\psi_{\mu i} = \sum_{\nu} a_{\nu i} \chi_{\nu} \tag{6}$$

the $a_{\nu i}$ are determined by solving the matrix Hartree-Fock equations

$$\sum_{\nu} F_{\lambda\nu} a_{\nu i} = \epsilon_i \sum_{\nu} S_{\lambda\nu} a_{\nu i} \quad (\text{each } \lambda) \tag{7}$$

where ϵ_i is the orbital energy of $\psi_{\mu i}$.

The Fock operator $F_{\lambda\nu}$ has been thoroughly discussed in the literature (ref. 28) and depends upon one- and two- electron molecular integrals and upon the $a_{\nu i}$. This makes Eq. (7) nonlinear and it is therefore solved iteratively. Programs has been developed for solving Eq. (7) for both closed and open-shell systems, using basis sets consisting of Slater-type atomic orbitals. Examples of our use of these programs are in the literature (ref. 7).

In configuration interaction calculations, the summation in Eq. (4) has more than one term, and the C_μ are determined by imposing Eq. (3), to obtain the secular equation

$$\sum_{\nu}\left(H_{\mu\nu}-W\,S_{\mu\nu}\right)C_{\nu}=0 \quad \text{(each } \mu) \tag{8}$$

where

$$\begin{aligned} H_{\mu\nu} &= \int \Psi_{\mu}^{*}(R)\,\mathcal{H}(R)\,\Psi_{\nu}(R)\,d\tau \\ S_{\mu\nu} &= \int \Psi_{\mu}^{*}(R)\,\Psi_{\nu}(R)\,d\tau \end{aligned} \tag{9}$$

Equation (7) is solved by matrix diagonalization. The laboratory used a modified Givens method (ref. 16) or a method due to Nesbet (ref. 29). Both of these programs are available from the Quantum Chemistry Program Exchange (QPCE 62.1, 93).

The matrix elements $H_{\mu\nu}$ and $S_{\mu\nu}$ may be reduced by appropriate operator algebra to the forms

$$H_{\mu\nu} = \sum_{P} \epsilon_{P} \left\langle \theta_{M} \middle| \mathcal{O}_{S} P \middle| \theta_{M} \right\rangle \left\langle \prod_{i=1}^{n} \psi_{\mu i}\left(\mathbf{r}_{i}, R\right) \middle| \mathcal{H}(R) P \middle| \prod_{i=1}^{n} \psi_{\nu i}\left(\mathbf{r}_{i}, R\right) \right\rangle \tag{10}$$

$$S_{\mu\nu} = \sum_{P} \epsilon_{P} \left\langle \theta_{M} \middle| \mathcal{O}_{S} P \middle| \theta_{M} \right\rangle \left\langle \prod_{i=1}^{n} \psi_{\mu i}\left(\mathbf{r}_{i}, R\right) \middle| P \middle| \prod_{i=1}^{n} \psi_{\nu i}\left(\mathbf{r}_{i}, R\right) \right\rangle \tag{11}$$

where P is a permutation and ϵ_p its parity. The sum is over all permutations. $\left\langle \theta_{M} \middle| \mathcal{O}_{S} P \middle| \theta_{M} \right\rangle$ is a "Sanibel coefficient" and the remaining factors are spatial integrals which can be factored into one- and two-electron integrals. If the ψ_μ are orthonormal, Eqs. (10) and (11) become more tractable and the $H_{\mu\nu}$ and $S_{\mu\nu}$ may be evaluated by explicit methods given in the literature (ref. 30). Computer programs have been developed for carrying out this procedure, and they have been used for problems containing up to 40 total electrons, 10 unpaired electrons, and 530 configurations. Examples of the use of these programs are in the work on O_2 and N_2 (refs. 24 and 25).

The CI studies can be carried out for any orthonormal set of $\psi_{\mu i}$ for which the molecular integrals can be calculated. Programs developed at United Aircraft Research Laboratories (UARL) make specific provision for the choice of the $\psi_{\mu i}$ as Slater-type atomic orbitals, as symmetry molecular orbitals, as Hartree-Fock orbitals, or as more arbitrary combinations of atomic orbitals.

In summary, computer programs have been developed which are capable of carrying out all the steps needed to make diatomic Hartree-Fock or CI studies for closed- or open-shell systems, including excited states, based on Slater-type orbitals. These studies lead to electronic energies and wavefunctions as a function of the internuclear separation.

2. Vibrational and Rotational Properties

For an electronic state described by $\Psi(R)$ and $W(R)$, the relative motion of the nuclei is, in the Born-Oppenheimer approximation, subject to a potential having at internuclear separation R the value W(R). By considering the quantum mechanics of the nuclear motion, it is possible from W(R) to calculate the vibrational and rotational energy levels. It is convenient to report the vibration-rotation structure in terms of parameters r_e, D_e, $\omega_e \chi_e$, B_e, α_e, etc., which are also available by standard reduction of experimental data. Such an analysis can be routinely carried out for bound electronic states, using a Dunham analysis computer program which has been deposited in the Quantum Chemistry Program Exchange (QCPE 113).

From W(R) it is also possible to obtain vibrational wavefunctions by numerical integration of the radial Schrodinger equation for the nuclear motion. A computer program which carries out this calculation by the Numerov procedure has been developed. Any W(R) can be handled since the program fits it by a spline technique. This program has been used for several years on a variety of problems; a typical application has been to excitation transfer in collisions of normal and metastable He atoms (ref. 31). The input W(R) can be the calculated potential corresponding to the electronic wavefunctions (R) or it can be derived using an RKR procedure (refs. 32 and 33). The input can be either the basic B(v) and G(v) data or the derived experimental spectroscopic constants based on this data. Programs for implementing the RKR procedure have been described in the literature (ref. 34).

3. Transition Probabilities

The electronic and vibrational-rotational wavefunctions of a pair of states can be used to calculate transition probabilities. If two molecular states are separated in energy by an amount $E_{nm} = hc\nu$ (h = Planck's constant, c = velocity of light, ν = frequency in wave numbers), the semi classical theory of radiation (refs. 35 and 36) yields for the probability of a spontaneous transition from an upper state n to a lower state m

$$A_{nm} = \frac{4}{3}\,\frac{\Delta E_{nm}^{3}}{\hbar^{4}c^{3}}\,\frac{S_{nm}}{g_{n}} \tag{12}$$

Here A_{nm} is the Einstein coefficient for spontaneous transition from level n→m, g_n is the total degeneracy factor for the upper state

$$g_n = (2-\delta_{\sigma,\Lambda'})(2S'+1)(2J'+1) \tag{13}$$

and S_{nm} is the total strength of a component line in a specific state of polarization and propagated in a fixed direction. A related quantity is the mean radiative lifetime of state n defined by

$$\frac{1}{\tau_n} = \sum_{m<n} A_{nm} \tag{14}$$

the summation being over all lower levels which offer allowed connections. The intensity of the emitted radiation is

$$I_{nm} = \Delta E_{nm} N_n A_{nm} \tag{15}$$

where N_n is the number density in the upper state n. This analysis assumes that all degenerate states at the same level n are equally populated, which will be true for isotropic excitation. The total line strength S_{nm} can be written as the square of the transition moment summed over all degenerate components of the molecular states n and m:

$$S_{nm} = \sum_{i,j} |M_{ji}|^2 \tag{16}$$

where j and i refer to all quantum numbers associated collectively with upper and lower electronic states, respectively.

In the Born-Oppenheimer approximation, assuming the separability of electronic and nuclear motion, the wavefunction for a diatomic molecule can be written

$$\psi^{i}_{vJM\Lambda} = \psi^{i}_{el}(\underset{\sim}{r}, R)\psi_v(R)\psi_{JM\Lambda}(\theta, \chi, \phi) \tag{17}$$

where $\psi^{i}_{el}(\underset{\sim}{r}, R)$ is an electronic wavefunction for state i at fixed internuclear separation R, $\psi_v(R)$ is a vibrational wavefunction for level v and $\psi_{Jn\Lambda}(\theta, \chi, \phi)$ refers to the rotational state specified by electronic angular momentum Λ, total angular momentum J and magnetic quantum number M. The representation is in a coordinate system related to a space-fixed system by the Eulerian angles (θ, χ, ϕ). The transition moment M_{ji} can be written, using the wavefunction given by Eq. (17), as

$$M_{ji} = \int \psi^{j}_{v'J'\Lambda'M'} \left\{\underset{\sim}{M}^{e} + \underset{\sim}{M}^{n}\right\} \psi^{i}_{v''J''\Lambda''M''} \, d\tau_e d\tau_v d\tau_r \tag{18}$$

The subscripts e, v, and r refer to the electronic, vibrational, and rotational wavefunctions, and M^e and M^n are the electronic and nuclear electric dipole moments, respectively. Integration over the electronic wavefunction in the Born-Oppenheimer approximation causes the contribution of the nuclear moment M^n to vanish for $i \neq j$. The electronic dipole moment can be written (refs. 36 and 37) in the form

$$\underset{\sim}{M}^e = -\sum_k e\underset{\sim}{r}_k' = -\left\{\sum_k e\underset{\sim}{r}_k\right\}\cdot\underset{\sim}{\mathcal{D}}(\theta,\chi,\phi) \qquad (19)$$

where the primed coordinates refer to the space fixed system, the coordinates r_k refer to a molecule-fixed system and $\mathcal{D}(\theta,\chi,\phi)$ is a group rotation tensor whose elements are the direction cosines related to the Eulerian rotation angles (θ,χ,ϕ). Using bracket notation, Eqs. (18) and (19) can be combined to yield for the transition moment

$$M_{ji} = M^{jv'J'\Lambda'M'}_{iv''J''\Lambda''M''} = \left\langle jv'\right| -\sum_k e\underset{\sim}{r}_k \left|iv''\right\rangle \cdot \left\langle J'\Lambda'M'\right| \underset{\sim}{\mathcal{D}}(\theta,\chi,\phi) \left|J''\Lambda''M''\right\rangle \qquad (20)$$

The matrix elements $\left\langle J'\Lambda'M'\right|\underset{\sim}{\mathcal{D}}(\theta,\chi,\phi)\left|J''\Lambda''M''\right\rangle$ determine the group selection rules for an allowed transition and have been evaluated for many types of transitions (refs. 38, 39, and 40). Summing Eq. (20) over the degenerate magnetic quantum numbers M' and M'', we have Eq. (16)

$$S_{nm} = S^{nv'J'\Lambda'}_{mv''J''\Lambda''} = \mathcal{S}^{J'\Lambda'}_{J''\Lambda''}\,\rho^{nv'}_{mv''} \qquad (21)$$

where $\mathcal{S}^{J'\Lambda'}_{J''\Lambda''}$ is the Honl-London factor (refs. 41 and 42) and

$$\rho^{nv'}_{mv''} = \sum_{ij}\left|\left\langle jv'\right| -\sum_k e\underset{\sim}{r}_k \left|iv''\right\rangle\right|^2 \qquad (22)$$

is the band strength for the transition. Combining Eqs. (13, 15 and 21), we have for the intensity of a single emitting line from upper level n:

$$I_{nm} = I^{nv'J'}_{mv''J''} = \frac{4}{3} N_{J'} \frac{\left[\Delta E^{nv'J'}_{mv''J''}\right]^4 S^{nv'J'\Lambda'}_{mv''J''\Lambda''}}{\hbar^4 c^3 \omega_n} \tag{23}$$

where $N_{J'}$ is the number density in the upper rotational state J' and $\omega_n = (2 - \delta_{\sigma,\Lambda'})(2S' + 1)$ is the electronic degeneracy. Taking an average value of $E^{n\ v'\ J'}_{m\ v''\ J''}$ for the whole band, Eq. (23) can be summed to yield the total intensity in the (v', v") band:

$$I^{nv'}_{mv''} = \sum_{J',J''} I^{nv'J'}_{mv''J''} = \frac{4}{3} N_{v'} \frac{\left[\overline{\Delta E}^{nv'}_{mv''}\right]^4 p^{nv'}_{mv''}}{\hbar^4 c^3 \omega_n} \tag{24}$$

where $N_{v'} = \sum_{J} N_{J'}$ is the total number density in the upper vibrational level v' and where we make use of the group summation property

$$\sum_{J''} \mathcal{S}^{J'\Lambda'}_{J''\Lambda''} = (2J' + 1) \tag{25}$$

Comparing Eq. (15) and (24), we have for the Einstein spontaneous transition coefficient of the band (v', v ")

$$A^{nv'}_{mv''} = \frac{4}{3} \frac{\left[\overline{\Delta E}^{nv'}_{mv''}\right]^3 p^{nv'}_{mv''}}{\hbar^4 c^3 \omega_n} \tag{26}$$

Similarly, the lifetime of an upper vibrational level v' of state n can be written

$$\frac{1}{\tau_n} = \sum_{m<n} \sum_{v''} A^{nv'}_{mv''} \tag{27}$$

where the summation runs over all v " for each lower state m. Eq. (26) can be cast in the computational form

$$A^{nv'}_{mv''}(\text{sec}^{-1}) = \frac{(21.41759 \times 10^{9})}{\omega_n} \left[\Delta E^{nv'}_{mv''}(\text{a.u.})\right]^3 p^{nv'}_{mv''}(\text{a.u.}) \tag{28}$$

where $E^{n\,v'}_{m\,v''}$ and $\rho^{n\,v'}_{m\,v''}$ are in atomic units. It is also often convenient to relate the transition probability to the number of dispersion electrons needed to explain the emission strength classically. This number, the f-number or oscillator strength for emission, is given by

$$f_{nm,v'v''} = \frac{mc^3\hbar^2}{2e^2\left[\overline{\Delta E}^{nv'}_{mv''}\right]^2} A^{nv'}_{mv''} \tag{29}$$

The inverse process of absorption is related to the above development through the Einstein B coefficient. Corresponding to Eq. (15), we have for a single line in absorption

$$I_{mn} = I^{nv'J'}_{mv''J''} = \int_{line(v''v';J''J')} K(\nu)\,d\nu = \Delta E_{mn} N_m B_{mn} \tag{30}$$

where $K(\nu)$ is the absorption coefficient of a beam of photons of frequency ν and

$$B_{mn} = B^{nv'J'\Lambda'}_{mv''J''\Lambda''} = \frac{2\pi}{3\hbar^2 c}\,\frac{S^{nv'J'\Lambda'}_{mv''J''\Lambda''}}{\omega_m(2J''+1)} \tag{31}$$

is the Einstein absorption coefficient for a single line. Summing over all lines in the band (v'',v'), assuming an average band frequency, we obtain

$$I^{nv'}_{mv''} = \sum_{J',J''} I^{nJ'v'}_{mJ''v''} = N_{v''}\frac{2\pi}{3\hbar^2 c\,\omega_m}\rho^{nv'}_{mv''} \tag{32}$$

where $N''_v = \sum_{J''} N''_J$ is the total number density in the lower vibrational state v''. Corresponding to Eqs. (28) and (29) we can define an f-number or oscillator strength for absorption as

$$f_{mn,v''v'} = \frac{2m\,\overline{\Delta E}^{nv'}_{mv''}}{3\hbar^2 e^2\omega_n}\rho^{nv'}_{mv''} \tag{33}$$

In computational form, Eq. (33) becomes

$$f_{mn,v''v'} = \frac{2}{3}\cdot\frac{\overline{\Delta E}^{nv'}_{mv''}(a.u.)}{\omega_m}\,\rho^{nv'}_{mv''}(a.u.) \tag{34}$$

where $\overline{\Delta E}^{n\,v'}_{m\,v''}$ and $\rho^{n\,v'}_{m\,v''}$ are in atomic units. Combining Eqs. (26) and (29) and comparing with Eq. (33), we see that the absorption and emission f-numbers are related by

$$f_{mn,v''v'} = \left(\frac{\omega_n}{\omega_m}\right) f_{nm,v'v''} \tag{35}$$

Some caution must be observed in the use of f-numbers given either by Eq. (29) or (33) since both band f-numbers and system f-numbers are defined in the literature. The confusion arises from the several possible band averaging schemes that can be identified.

An integrated absorption coefficient (density corrected) can be defined from Eq. (32) as

$$S_{v'',v'} = \frac{1}{Pc} I^{nv'}_{mv''} = N_{v''}B_{v'',v'}\left(1-\exp\frac{-hc\nu_{v''v'}}{kT}\right)\frac{h\nu_{v''v'}}{Pc^2} \tag{36}$$

where the exponential factor corrects for stimulated emission. Eq. (36) can be written in terms of the absorption f-number as

$$S_{v'',v'} = \frac{\pi e^2}{mc^2}\,\frac{N_{v''}}{P}\left(1-\exp\frac{-hc\nu_{v''v'}}{kT}\right) f_{mn,v''v'} \tag{37}$$

Using h c/k = 1.43880 cm-K^0, we obtain a computational formula for the integrated absorption coefficient as

$$S_{v'',v'}(\text{cm}^{-2}\cdot\text{atm}^{-1}) =$$

$$2.3795\times10^{7}\left(\frac{273.16}{T(K^0)}\right)\left(\frac{N_{v''}}{N_T}\right)\left(1-\exp\frac{1.43880\,\nu_{v'',v'}(\text{cm}^{-1})}{T}\right)\cdot f_{mn,v''v'} \tag{38}$$

The total integrated absorption is found from

$$S_{TOTAL} = \sum_{v''} \sum_{v'} S_{v'',v'} \tag{39}$$

where, under normal temperature conditions, only the first few fundamentals and overtones contribute to the summations.

The developments given above are rigorous for band systems where an average band frequency can be meaningfully defined. Further approximations, however, are often made. For example, the electronic component of the dipole transition moment can be defined as

$$\mathcal{R}_{ji}(R) = \langle j | - \sum_{k} e\underline{r}_k | i \rangle \tag{40}$$

This quantity is often a slowly varying function of R and an average value can sometimes be chosen. Eq. (22) can then be written approximately in factored form as

$$p^{nv'}_{mv''} \simeq q_{v'v''} \sum_{ij} |\vec{\bar{\mathcal{R}}}_{ji}(\bar{R}|^2 \tag{41}$$

where $q_{v'v''}$, the square of the vibrational overlap integral, is called the Franck-Condon factor. $\mathcal{R}_{ji}$ is evaluated at some mean value of the internuclear separation R. In addition, it is sometimes possible to account for a weak R-dependence in $\underset{\sim}{\mathcal{R}}$ by a Taylor series expansion of this quantity about some reference value, $\mathcal{R}_{\alpha\beta}$, usually referred to the (0,0) band. We have

$$\mathcal{R}_{ji} \simeq \mathcal{R}^{\alpha\beta}_{ji}\left[1 + a(R - R_{\alpha\beta}) + b(R - R_{\alpha\beta})^2 + \cdots\right] \tag{42}$$

Substituting into Eq. (22) and integrating yields

$$p_{mv''}^{nv'} \simeq q_{v'v''} \sum_{i,j} \left| \mathcal{R}_{ji}^{\alpha\beta} \left[1 + a(\overline{R_{v'v''} - R_{\alpha\beta}}) + b(\overline{R_{v'v''} - R_{\alpha\beta}})^2 + \cdots \right] \right|^2 \tag{43}$$

where

$$(\overline{R_{v'v''} - R_{\alpha\beta}}) = \frac{\langle v' | (R - R_{\alpha\beta}) | v'' \rangle}{\langle v' | v'' \rangle} \tag{44}$$

is the R-centroid for the transition and

$$\overline{(R_{v'v''} - R_{\alpha\beta})^2} = \frac{\langle v' | (R - R_{\alpha\beta})^2 | v'' \rangle}{\langle v' | v'' \rangle} \tag{45}$$

is the R^2-centroid. Note that this last term differs (to second order) from the square of the R-centroid. An alternate procedure can be developed by evaluating Eq. (40) at each R-centroid, $\bar{R}_{v'v''}$. Then

$$p_{mv''}^{nv'} \approx q_{v'v''} \sum_{i,j} \left| \mathcal{R}_{ji}(\bar{R}_{v'v''}) \right|^2 \tag{46}$$

Eq. (46) assumes that the vibrational wavefunction product, $\psi_{v'} \psi_{v''}$, behaves like a delta function upon integration

$$\psi_{v'} \psi_{v''} = \delta(R - \bar{R}_{v'v''}) \langle v' | v'' \rangle \tag{47}$$

The range of validity of Eq. (46) is therefore questionable, particularly for band systems with bad overlap conditions such as oxygen Schumann-Runge. The range of validity of the R-centroid approximation has been examined by Frazer (ref. 43).

The final step in calculating transition probabilities is the determination of $\mathcal{R}_{ji}(R)$, the electronic dipole transition moment, for the entire range of internuclear separations, R, reached in the vibrational levels to be considered. This can be expressed in terms of the expansion of Eq. (4) as

$$\mathcal{R}_{ji}(R) = \sum_{\mu\nu} c_{\mu}^{j*} c_{\nu}^{i} \left\langle \psi_{\mu}(R) \middle| \underset{\sim}{M}^{e} \middle| \psi_{\nu}(R) \right\rangle \tag{48}$$

where c_{μ}^{j} and c_{ν}^{i} are coefficients for ψ_{el}^{j} and ψ_{el}^{i}, respectively.

An analysis similar to that yielding Eqs. (10) and (11) gives

$$\left\langle \psi_{\mu}(R) \middle| \underset{\sim}{M}^{e} \middle| \psi_{\nu}(R) \right\rangle =$$

$$\sum_{p} \epsilon_{p} \left\langle \theta_{M_S} \middle| \mathcal{O}_{S} P \middle| \theta_{M_S} \right\rangle \left\langle \prod_{k=1}^{n} \psi_{\mu k}(\underset{\sim}{r}_{k}, R) \middle| \underset{\sim}{M}^{e} P \middle| \prod_{k=1}^{n} \psi_{\nu k}(\underset{\sim}{r}_{k}, R) \right\rangle \tag{49}$$

The spatial integral in Eq. (49) reduces to one-electron integrals equivalent to overlap integrals, and the evaluation of Eq. (49) can be carried out by the same computer programs used for Eq. (11). Programs for evaluating $\mathcal{R}_{ji}(R)$ in Eq. (48) have been developed at UARL and examples of their applications have appeared in the literature (ref. 8).

For perturbed electronic systems, the transition dipole moment will have a strong R-dependence and R-centroid or other approximations will be invalid. A direct evaluation of Eq. (22) would therefore be required using the fully-coupled system of electronic and vibrational wavefunctions to properly account for the source of the band perturbations.

SECTION IV

DISCUSSION OF RESULTS

The theoretical research conducted under this program was concerned with the determination of f-numbers for selected band systems of certain metal oxides for use in the calculation of accurate absorption and emission coefficients. The band systems under study in this research program were the aluminum-oxide blue-green system ($B^2\Sigma^+$-$X^2\Sigma^+$), the aluminum-oxide vibrational-rotational transition ($X^2\Sigma^+$-$X^2\Sigma^+$), the lithium-oxide vibrational rotational transition ($X^2\Pi$-$X^2\Pi$), the lithium-oxide transitions ($A^2\Sigma^+$-$X^2\Pi$ and $A^2\Sigma^+$-$A^2\Sigma^+$), the iron-oxide orange system ($^5\Sigma^+$II-$X^5\Sigma^+$I), the iron-oxide vibrational rotational transition ($X^5\Sigma^+$I-$X^5\Sigma^+$I), the uranium-oxide vibrational rotational system, and the UO^+ vibrational rotational system ($X^4\Pi$-$X^4\Pi$).

1. Electronic Transition Probabilities

a. AlO

The first metal oxide systems studied were the AlO blue-green system and the vibrational-rotational system. Electronic wavefunctions were constructed using a single-zeta Slater-type orbital (STO) basis. Optimized SCF calculations were performed for the $X\ ^1\Sigma^+$ state of AlO^+ at three internuclear separations (R = 2.6, 3.0 and 3.4 bohrs). The optimized orbital basis obtained from these calculations is shown in table 1. The MOs obtained from these calculations were then used as input transformation vectors to convert the original atomic orbital basis to MO form. The lowest six MOs (1σ, 2σ, 3σ, $1\pi^+$, $1\pi^-$, 4σ) were taken as doubly occupied and a full CI was performed over the rest of the MOs for the $X\ ^2\Sigma^+$ and $A\ ^2\Pi$ states of AlO. This resulted in a wavefunction expansion as illustrated in Eq. 5, which consisted of 264 configurations for the $X\ ^2\Sigma^+$ state and 243 configurations for the $A\ ^2\Pi$ state of AlO. Table 2 lists the configuration sizes required for the VCI calculations performed and the number of states for other symmetries of AlO which were studied. By far, for all the molecules studied under this research program, the greatest amount of effort was devoted to construction of the electronic VCI wavefunctions. The symmetries of AlO which were studied are outlined in table 3. All states up to Al ^2P_u+O ^1D_g were included in these calculations. The energies of the aluminum and oxygen atomic states which represent the dissociation limits of the molecular states of AlO which were studied are given in table 4.

The results of the VCI calculations performed for AlO are illustrated in several ways. In table 5 we list the calculated electronic energies of all states of AlO which were studied. These data are also shown as calculated potential energy curves in figures 1-4. The derived spectroscopic constants for the calculated bound states of AlO are shown in table 6, where comparisons with experimental data are given wherever possible. A Rydberg-Klein-Rees (RKR) analysis of the experimental data yields the potential curve given in figure 5.

The calculated electronic transition probabilities and related properties for the AlO blue-green (BG) system and the vibrational-rotational (VR) system are given in tables 7 through 13. Tables 7 and 8 present the calculated oscillator strengths for the AlO (BG) and (VR) systems, respectively. The Franck-Condon factors, R-centroid factors and band strengths are given in tables 9 through 13 respectively.

The calculated f-numbers for the blue-green system are in good agreement with the lifetime studies of Johnson, Capelle, and Broida (ref. 44). The strength of this transition now seems to be established with a maximum error of about 50 percent. The calculated absorption for the $X^2\Sigma^+$ (VR) system of AlO is another matter. After considerable effort and many different trial wavefunctions, the behavior of the dipole moment of the $X^2\Sigma^+$ state is still not well understood. Table 8 shows the results based on the two most likely possibilities for the dipole moment. The first corresponds to a wavefunction expansion based on optimized orbitals from a Hartree-Fock calculation for the $^2\Pi$ state. The second corresponds to the $^2\Sigma^+$ HF orbitals from the outer (VB) HF solution. Two Hartree-Fock solutions exist for X $^2\Sigma^+$ near the equilibrium separation. The outer solution is neutral valence-bond in structure; the inner solution is nearly singly ionized Al^+O^-. These solutions are degenerate at a separation slightly greater than R_e and thus no single determined HF representation exists for this system. The optimized ${}^2\Sigma^+$ orbitals yield nearly a flat dipole moment curve in the region or R_e, a result similar to that found by the IBM group (ref. 45). Further studies are required to assess whether or not this anomalous result is real of an artifact of the orbital expansion for ${}^2\Sigma^+$ symmetry. Present experimental indications (ref. 46) are that AlO has strong LWIR absorption with a measured f-number of ~3×10^{-5}. This would be in agreement with our original valence-bond treatment of this system where no orbital transformation to MO form was carried out.

A survey of the higher electronic states of AlO was carried out to qualitatively study dissociative-recombination in this system. AlO^+ has two low-lying electronic states (ref. 47), a ${}^3\Pi$ state which correlates with $Al^+(^1S) + O(^3P)$ and a ${}^1\Sigma^+$ state which correlates with $Al^+(^1S) + O(^1D)$. Both states lie at about 9.5 eV and thus AlO^+ is a stable species with an indicated dissociation energy of ~1.5 eV. For either symmetry dissociative-recombination is highly likely since there are many repulsive molecular states both doublets and quartets, which connect with low-lying neutral states of Al + O and which pass through the minimum of the AlO^+ potential curve. Since these neutral AlO states can all couple with $e + AlO^+$ in first order, very rapid ($k > 10^{-7}$ cm^3/sec) dissociative-recombination should result.

b. LiO

The second metal-oxide system studied was lithium oxide. Electronic wavefunctions were constructed for this system using a single-zeta STO basis set. The screening parameters chosen for the lithium and oxygen atomic orbitals are given in table 14. The configuration sizes required for full VCI calculations and the number of states for the various symmetries of LiO which were studied is given in table 15. The symmetries of LiO which were studied are outlined in table 16. All states up to $Li\,^2P_u + O\,^1D_g$ were included in these calculations. The energies of the lithium and oxygen atomic states which represent the dissociation limits of the calculated molecular states of LiO are given in table 17.

The calculated electronic energies for LiO are given in table 18. These data are also shown as calculated potential energy curves in figures 6 through 10. The derived spectroscopic constants for the calculated bound states of LiO are given in table 19. Comparisons with experimental data are given wherever this is possible. A Rydberg-Klein-Rees (RKR) analysis of the experimental data yields the potential curve given in figure 11.

The calculated electronic transition probabilities and related properties for the LiO systems: $X^2\Pi - X^2\Pi$ (X-X), $A^2\Sigma^+ - A^2\Sigma^+$ (A-A), and $A^2\Sigma^+ - X^2\Pi$ (A-X) are given in tables 20 through 29. The calculated oscillator strengths are presented in tables 20 through 22 for the LiO (X-X), (A-A), and (A-X) systems, respectively. The Franck-Condon factors, R-centroid factors and band strengths are given in tables 23 through 29, respectively. These results are typical of those expected for an ionic molecule. The calculated integrated band absorption coefficient for $X^2\Pi$ of LiO is ≈550 cm^{-2} atm^{-1}. The electronic f_{00} number for A-A is 0.0041 which can be compared with the value of 0.012 (f_{00}) for the AlO (B-X) system.

The results reported herein are all similar (±25 percent) to those calculated by the IBM group (ref. 45). In addition, these results are in reasonable agreement with the experimental studies carried out in LiO (refs. 48 and 49) and no further theoretical studies are anticipated for this system.

c. FeO

The third group of metal-oxide systems studied were the iron oxide vibrational rotational system and the orange systems. Electronic wavefunctions were constructed for FeO in the single-zeta STO basis approximation. The optimized screening parameters for the atomic orbitals are given in table 30. The configuration sizes required for full VCI calculations for this system are given in table 31. All of the low-lying molecular states which were studied are shown in table 32. The energies of the separated atoms which represent the dissociation limits of the low-lying states of FeO are given in table 33.

All states up to the first ionic limit Fe$^{+6}S_g$+O$^{-2}P_u$ were included in the calculations. The calculated dissociation limits did not always correspond in order to those known experimentally (ref. 50). The Fe^5F_g+O^3P_g, Fe^3F_g+O^3P_g, and Fe^5P_g+O^3P_g have higher calculated than experimental energies (see table 33) but appear to yield repulsive potential curves.

The calculated electronic energies of FeO are given in the rather extensive compilation of table 34. The states dissociating to those calculated limits at a higher energy are also shown. Data of the more interesting states have been reduced to potential energy curves which are shown in figures 12 through 16. The derived spectroscopic constants for the calculated bound states of FeO are given in table 35 where comparisons with experimental data are also shown. A RKR analysis of the data yields the potential curve given in figure 17.

The calculated electronic transition probabilities results for the FeO vibrational-rotational (VR) system and the orange system ($^5\Sigma^+$II-X$^5\Sigma^+$I) are given in tables 36 through 42. The calculated oscillator strengths are presented in tables 36 through 37 for the FeO (VR) and the orange systems, respectively. The Franck-Condon factors, R-centroid factors and band strengths are given in tables 35 through 42, respectively.

We have been able to identify the principal band systems of FeO as a result of these theoretical studies of the excited electronic states. The ground state of FeO has $^5\Sigma^+$ symmetry and is well separated from the next lowest electronic state. We calculate an integrated band absorption coefficient of 155 cm^{-2} atm^{-1}, a value somewhat on the low side for a metal oxide. The orange system is identified as $^5\Sigma^+$II-X$^5\Sigma^+$I and we calculate for the electronic f-number (f_{00}) the value of 0.004, a result similar to that found for LiO. In addition, we identify the first excited electronic state as $^5\Pi$I with T_e = 1.29 eV. The IR bands of Callear and Norrish (ref. 51) can be identified with this transition ($^5\Pi$I-X$^5\Sigma^+$). The orange system corresponds to $^5\Pi$II-X$^5\Sigma^+$ with the upper state at T_e = 2.14 eV. A complete resolution of the spectroscopy of the low-lying excited electronic states of FeO now seems possible and further work on this system is warranted.

d. UO

The fourth metal-oxide system studied was the uranium oxide vibrational-rotational system. Electronic wavefunctions were constructed using the effective-z calculation method employing a single-zeta (SZO) basis approximation. The screening parameters for the atomic orbitals are given in table 43. The configuration sizes required for full WCI calculations for this system are given in table 44. The symmetries of UO up to $U\,{}^5K+O\,{}^3P$ are outlined in table 45. Only a selected group of symmetries was studied. The symmetries studied as possibly giving rise to the ground state were $^7\Sigma^{+-}$, $^{5,7}\Pi$, $^{5,7}\Delta$. The energies of the uranium and oxygen atomic states which represent the dissociation limits of the calculated molecular states of UO are given in table 46.

The compilation of calculated electronic energies for UO is given in table 47. These data are also shown as potential energy curves in figures 18 through 22. These curves represent electronic energy data adjusted to the ground state experimental curve. The derived spectroscopic constants for the adjusted calculated bound states of UO are given in table 48. A RKR analysis of available experimental data (refs. 52, 53, and 54) yields the potential curve in figure 23.

The calculated oscillator strengths for the UO vibrational-rotational system are given in table 49. The R-centroid factors and band strengths are given in tables 50 and 51, respectively. We find an integrated band absorption coefficient for UO of 288 cm^{-2} atm^{-1}, a value typical of other metal oxides. Only a limited analysis of the electronic structure of UO was attempted owing to the great number of low-lying states belonging to this system. We find a similar chemistry for all of the UO states which have the $5f^3$ electrons quartet coupled and a different chemistry for those states (which are much higher in energy) where the $5f^3$ electrons are doublet coupled. This effect seemed to dominate the interaction potential more than any effects of total spin or angular momentum. We did not investigate spin-orbit coupling effects in this first study of the UO system, but previous studies on U (ref. 55) have indicated that the 5f electrons are very nearly L-S coupled. A unique ground state symmetry cannot be assigned on the basis of these calculations. All of the symmetries studied yielded similar potential curves. A reasonable approximation for the electronic structure of UO is to assume a single state as indicated in figure 23, weighted in accordance with the multiplicities given in table 45. Further studies on this system are indicated.

e. UO^+, UO_2^+, UO_2^{++}, UO_2

The fifth metal-oxide system which was studied was the UO^+ vibrational-rotational system. Electronic wavefunctions were constructed using the effective-z calculation method employing a single-zeta (STO) basis approximation. The screening parameters for the atomic orbitals are given in table 52. The configuration sizes required for full VCI calculations for this system are given in table 53. The symmetries of UO^+ for the $U\,^4I_u + O\,^3P_g$ limit are outlined in table 54. Again, as in UO, only a selected group of symmetries was studied. The symmetries studied as likely to give rise to the ground state were $^{2,4,6}\Sigma^{+,-}$, $^{2,4,6}\Pi$, $^{2,4,6}\Delta$, and $^{2}\Phi$. The energies of the uranium ionic and oxygen atomic states which represent the dissociation limits of the low-lying calculated molecular states of UO^+ are given in table 55.

The calculated electronic energies for UO^+ are given in table 56. The data are also shown as potential energy curves in figures 24 through 33. These curves represent electronic energy data adjusted to the experimental ground state dissociation energy. The derived spectroscopic constants for the adjusted bound states of UO^+ are given in table 57. A RKR analysis of available experimental data (refs. 52, 53, and 54) yield the potential curve in figure 23.

The calculated oscillator strengths for the UO^+ vibrational-rotational system are given in table 58. The R-centroid factors and band strengths are given in tables 59 through 60, respectively. We find $^4\Pi$ to be the lowest L-S coupled state for this system, but again the chemistry is dominated by the 5f electrons. Two distinct sets of potential curves arise depending on whether the 5f electrons are predominately quartet or doublet coupled. Spin-orbit effects should be more important in this system than in UO, but they were not studied in this work. Further work is needed on this system.

The calculated integrated band absorption coefficient for UO$^+$ is 245 cm^{-2} atm^{-1}, a value slightly smaller than that found for UO. The absorption characteristics of this system can be estimated by assuming two different electronic states as indicated in figure 23 and weighing these states in accordance with the multiplicities given in table 54.

The systems UO$_2^{++}$, UO$_2^+$ and UO$_2$ were examined using the multiple-scattering (X$_\alpha$) method. We find UO$_2^{++}$ to be a linear molecule with a $^1\Sigma_g^+$ state as the indicated ground state of this system. The model chosen gives the inner uranium sphere an excess +2 charge initially so that the basic starting charge distribution is U^{+4}(O$^-$)$_2$. This initial charge distribution is allowed to relax in the pseudo-SCF X$_\alpha$ procedure. The calculated excitation spectra is in good agreement with the known absorption spectra for this ion. Low-lying excited states are of $^3\Pi_u$ and $^3\Delta_u$ symmetry. An energy-level diagram for UO$_2^{++}$ is given in figure 34.

The calculations indicate that UO$_2^+$ is also a stable linear molecule but we have not been able to precisely define the symmetry of the ground state. The 7s orbital of uranium is highly relativistic and (5f^{3}7s^2) is the lowest and correct ground state for U$^+$. However, (5f^{3}7s6d) is slightly lower in energy for U$^+$ in a non-relativistic calculation and we have not yet developed a relativistic X$_\alpha$ program for molecules. Molecular calculations which involve extensive hybridization of the 7s orbital, such as UO$_2^+$ and UO$_2$, probably will need a relativistic treatment for definitive calculations of the symmetries.

f. TiO

The sixth metal-oxide system studied was titanium oxide. Electronic wavefunctions were constructed for this system using a single-zeta STO basis set. The screening parameters chosen for the titanium and oxygen atomic orbitals are given in table 61. The configuration sizes required for full VCI calculations and the number of states for the various symmetries of TiO which were studied is given in table 62. The symmetries of TiO which were studied are outlined in table 63. All states up to Ti $^{3}F_g$ + O $^{1}D_g$ were included in these calculations. The energies of the titanium and oxygen atomic states which represent the dissociation limits of the calculated molecular states of TiO are given in table 64.

The calculated electronic energies for TiO are given in table 65. These data are also shown as calculated potential energy curves in figures 35 through 52. The derived spectroscopic constants for the calculated bound states of TiO are given in table 66. Comparisons with experimental data are given wherever this is possible. A Rydberg-Klein-Rees (RKR) analysis of the experimental data yields the potential curve in figure 53.

The calculated electronic transition probabilities and related properties for the TiO systems: vibrational-rotational $X\,^{3}\Delta - X\,^{3}\Delta$ (X-X), gamma $A\,^{3}\Phi - X\,^{3}\Delta$ (A-X), and gamma prime $B\,^{3}\Pi - X\,^{3}\Delta$ (B-X) are given in tables 67 through 77. The calculated oscillator strengths are presented in tables 67 through 69 for the TiO (X-X), (A-X) and (B-X) systems, respectively. The Franck-Condon factors, R-centroid factors and band strengths are given in tables 70 through 77, respectively. The calculated (A-X) or gamma system f-number is somewhat smaller (factor of ~4) than that reported by Price, et. al. (ref. 113). The LWIR absorption strength from the $X\,^{3}\Delta$ state is typical of most of the diatomic metal oxides studied herein. There are no experimental data with which to compare the gamma prime systems.

APPENDIX I

AB INITIO CALCULATION OF THE B $^2\Sigma^+$ - X $^2\Sigma^+$ OSCILLATOR STRENGTHS IN AlO

A theoretical calculation of the oscillator strengths for the B $^2\Sigma^+$ - X $^2\Sigma^+$ transitions in AlO (blue-green system) has been made. This system has often been labeled A $^2\Sigma^+$ - X $^2\Sigma^+$, a designation which has been corrected since the discovery of Innes (ref. 56), of a low-lying $^2\Pi$ state now labeled A$^2\Pi$. The pertinent potential curves are shown in figure I-1.

The calculation of oscillator strengths is dependent primarily on the knowledge of: (1) accurate vibration-rotation wavefunctions for the electronic states of interest, and (2) the dipole transition moment as a function of internuclear separation. Vibration-rotation wavefunctions can now be obtained from numerical solutions of the Schrödinger equation with accuracies such that many band spectra can be reproduced to within 1-2 wavenumbers. Electronic wavefunctions cannot be obtained to such a high degree of accuracy. Nevertheless, recent experience indicates that CI wavefunctions can be constructed with sufficient accuracy to yield reliable estimates of the electronic transition moment for diatomic molecular systems.

The electronic wavefunction is written in CI form as $\sum_i c_i \psi_i$ where each ψ_i differs by its orbital occupancy. In the Hartree-Fock model there is but one ψ_i and in the limit of a full CI there are all ψ_i which can be constructed to span the orbitals which are included in the calculation. In practice, Hartree-Fock calculations prove to be too restrictive and a full CI becomes impossible to construct when large basis sets are considered. For the studies performed here, the basis set was first transformed to Hartree-Fock form and the inner six Hartree-Fock orbitals were held frozen in all configurations. The wavefunction was reoptimized for each internuclear separation chosen for study. The final calculations included 190 configurations constructed for $^2\Sigma^+$ symmetry. A detailed report on the calculation procedure is in preparation (ref. 57).

These CI electronic wavefunctions were then used to evaluate the dipole transition moment, M (R). The calculated moment was fitted numerically using a spline fit and tabulated at 2000 mesh points in the internuclear separation. Integration of M (R) over the accurate vibrational wavefunctions yields directly our estimate of the band strengths.

The calculated f-numbers for the B-X transitions are shown in table I-1. For comparison, calculated Franck-Condon factors are also shown. These F-C factors are in good agreement with previous studies on this system (ref. 58); the differences are due to our use of slightly more accurate RKR potentials based on band origin data (ref. 59).

These data indicate an f-number of 0.012 for the strongest (0,0) transition, in agreement with previous theoretical studies on this system which were performed with less sophisticated wavefunctions (ref. 60). Previous calculations on N_2 IPS and NO-β band systems indicate an expected error of 25-30 percent for the analysis performed here.

The calculated result for f_{00} is in disagreement with the experimental results reported by Hooker and Main (ref. 61)(f_{00} =0.0035), by Vanpee (ref. 62)(f_{00} =0.0027) and by Daiber, et al (ref. 63)(f_{00} =0.13). Part of the discrepancy can be traced to their neglect of the low-lying A $^2\Pi$ state in the experimental analysis of number density. A 30 percent correction at 4000°K must be made for intensity measurements in absorption. This correction, however, is not large enough to fully account for the differences between the various experimental values and our calculated result. In contrast, a study of relative band intensities by Hebert and Tyte (ref. 64) yields a transition moment variation (1 - .46 R) in excellent agreement with our calculated variation over the range 1.5 - 1.85 Å.

Results of lifetime studies for the AlO blue-green transition have been reported by Johnson, Capelle, and Broida in this issue (ref. 65). Their studies yield a lifetime for B $^2\Sigma^+$ (v' = 0) of 129 nec, in reasonable agreement with our calculated lifetime of 234 nsec, considering the complexity of this metal oxide system. The calculated lifetime includes the contribution of the B-A transition which is characterized by f_{00} = 0.00014, q_{00} = 0.24, indicating that only 2 percent of the radiation is to this lower $A^2\Pi$ state.

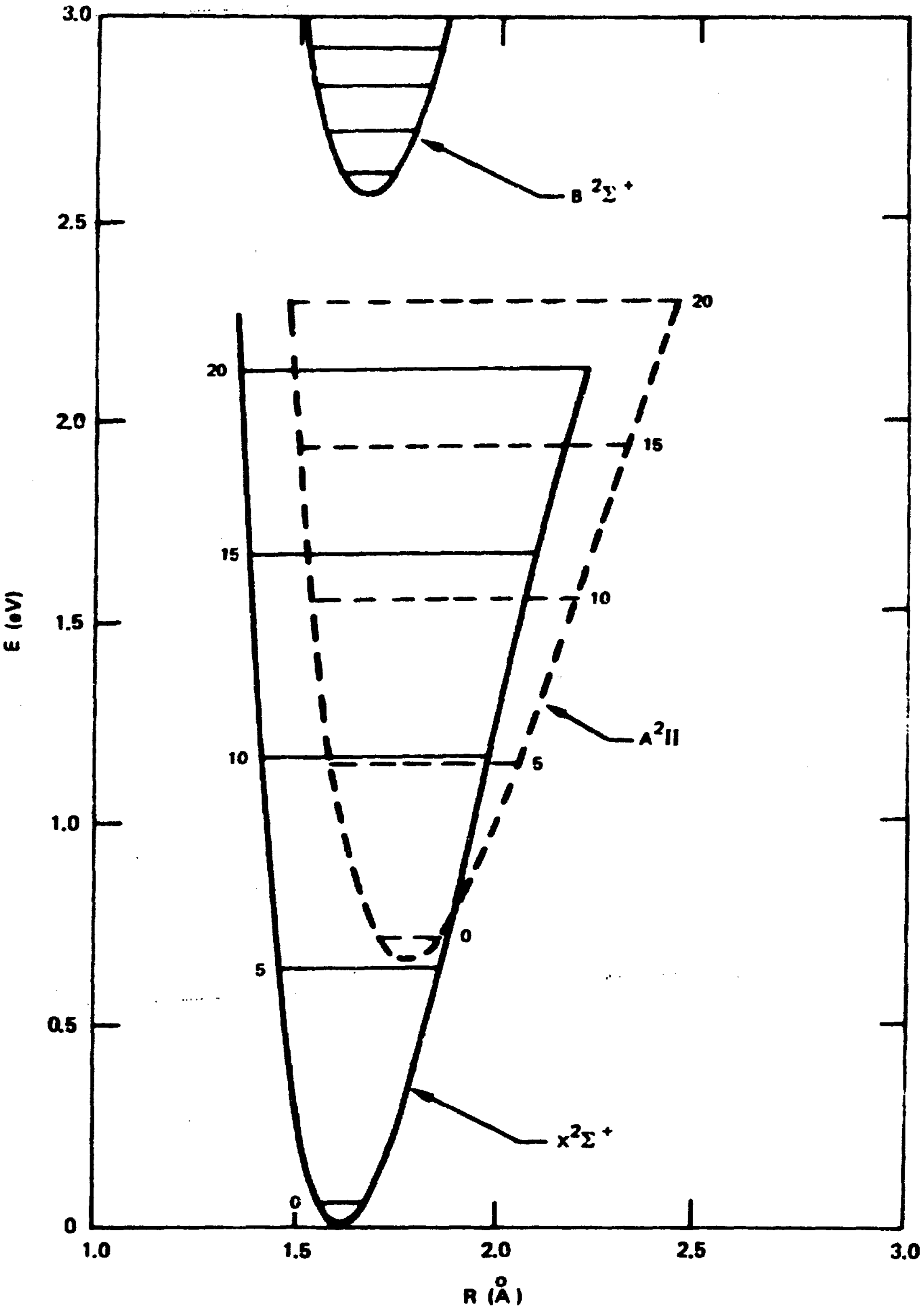

FIGURE I-1. POTENTIAL ENERGY CURVES FOR AlO

Table I-1

f-Numbers and Franck-Condon Factors for AlO $B\ {}^2\Sigma^+ - X\ {}^2\Sigma^+$

v" v'	0	1	2	3	4	5
0	1.171-2* 7.234-1**	4.417-3 2.267-1	9.954-4 4.280-2	1.718-4 6.101-3	2.519-5 7.061-4	3.326-6 6.794-5
1	3.146-3 2.426-1	5.380-3 3.388-1	5.787-3 3.014-1	2.171-3 9.466-2	5.262-4 1.903-2	9.866-5 2.879-3
2	3.299-4 3.193-2	4.435-3 3.518-1	2.120-3 1.375-1	5.612-3 2.964-1	3.136-3 1.389-1	9.978-4 3.692-2
3	1.367-5 1.837-3	7.688-4 7.653-2	4.720-3 3.846-1	6.127-4 3.983-2	4.757-3 2.549-1	3.754-3 1.691-1
4	1.455-7 3.450-5	4.246-5 5.854-3	1.201-3 1.233-1	4.504-3 3.764-1	6.864-5 4.565-3	3.712-3 2.016-1
5	5.045-12 5.595-9	4.095-7 1.208-4	8.252-5 1.169-2	1.578-3 1.673-1	4.069-3 3.488-1	1.834-5 1.199-3

*f-Numbers; **Franck-Condon factors.

APPENDIX II

ANALYSIS OF DIPOLE-ALLOWED ELECTRONIC TRANSITIONS IN DIATOMIC MOLECULES*

by

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APPENDIX II

ANALYSIS OF DIPOLE-ALLOWED ELECTRONIC TRANSITIONS IN DIATOMIC MOLECULES

If two molecular states are separated in energy by an amount $E_{nm} = hc\nu$ (h = Planck's constant, c = velocity of light, ν = frequency in wave numbers), the semi-classical theory of radiation (ref. 66, 67, 68) yields for the probability of a spontaneous transition from an upper state n to a lower state m

$$A_{nm} = \frac{4}{3} \frac{\Delta E_{nm}^3}{\hbar^4 c^3} \frac{S_{nm}}{g_n} \tag{50}$$

Here A_{nm} is the Einstein coefficient for spontaneous transition from level $n \rightarrow m$, g_n is the total degeneracy factor for the upper state

$$g_n = \left(2 - \delta_{\sigma,\Lambda'}\right) (2S'+1) (2J'+1) \tag{51}$$

and S_{nm} is the total strength of a component line in a specific state of polarization and propagated in a fixed direction. A related quantity is the mean radiative lifetime of state n defined by

$$\frac{1}{\tau_n} = \sum_{m<n} A_{nm} \tag{52}$$

the summation being over all levels which offer allowed connections. The intensity of the emitted radiation is

$$I_{nm} = \Delta E_{nm} N_n A_{nm} \tag{53}$$

where N_n is the number density in the upper state n. This analysis assumes that all degenerate states at the same level n are equally populated, which will be true for isotropic excitation. The total line strength S_{nm} can be written as the square of the transition moment summed over all degenerate components of the molecular states n and m:

$$S_{nm} = \sum_{ij} |M_{ij}|^2 \tag{54}$$

where j and i refer to all quantum numbers associated collectively with upper and lower electronic states, respectively.

In the Born-Oppenheimer approximation, assuming the separability of electronic and nuclear motion, the wavefunction for a diatomic molecule can be written as

$$\psi^{i}_{vJM\Lambda} = \psi^{i}_{el}(\underset{\sim}{r}, R)\, \psi_{v}(R)\, \psi_{JM\Lambda}(\theta, \chi, \phi) \tag{55}$$

where $\psi^{i}_{el}(\underset{\sim}{r}, R)$ is an electronic wavefunction for state i at fixed internuclear separation R, $\psi_{v}(R)$ is a vibrational wavefunction for level v and $\psi_{JM\Lambda}(\theta, \chi, \phi)$ refers to the rotational state specified by electronic angular momentum Λ, total angular momentum J and magnetic quantum number M. The representation is in a coordinate system related to a space-fixed system by the Eulerian angles (θ, χ, ϕ). The transition moment M_{ji} can be written, using the wavefunction given by Eq. (55), as

$$M_{ji} = \int \psi^{j*}_{v'J'\Lambda'M'} \left\{ \underset{\sim}{M}^{e} + \underset{\sim}{M}^{n} \right\} \psi^{i}_{v''J''\Lambda''M''}\, d\tau_{e}\, d\tau_{v}\, d\tau_{r} \tag{56}$$

The subscripts e, v and r refer to the electronic, vibrational and rotational wavefunctions and M^{e} and M^{n} are the electronic and nuclear electric dipole moments, respectively. Integration over the electronic wavefunction, in the Born-Oppenheimer approximation, causes the contribution of the nuclear moment M^{n} to vanish for i ≠ j. The electronic dipole moment can be written (refs. 67, 69) in the form

$$\underset{\sim}{M}^{e} = -\sum_{k} e\underset{\sim}{r}'_{k} = -\left\{ \sum_{k} e\underset{\sim}{r}_{k} \right\} \cdot \underset{\sim}{D}(\theta, \chi, \phi) \tag{57}$$

where the primed co-ordinates refer to the space fixed system, the co-ordinates r_k refer to a molecule-fixed system and $\mathcal{D}(\theta, \chi, \phi)$ is a group rotation tensor whose elements are the direction cosines related to the Eulerian rotation angles (θ, χ, ϕ). Using bracket notation, Eqs. (56) and (57) can be combined to yield for the transition moment

$$\mathcal{M}_{ji} = \mathcal{M}^{jv'J'A'\omega'}_{iv''J''A''\omega''} = \left\langle jv' \middle| -\sum_k e\underset{\sim}{r}_k \middle| iv'' \right\rangle \cdot \left\langle J'A'\omega' \middle| \underset{\sim}{\mathcal{D}}(\theta,\chi,\phi) \middle| J''A''\omega'' \right\rangle \tag{58}$$

An equivalent formulation (within the Born-Oppenheimer approximation) yields for the dipole velocity form of the transition moment

$$\mathcal{M}_{ji} = \frac{1}{\Delta E_{nm}} \left\langle jv' \middle| -\sum_k \underset{\sim}{\nabla}_k \middle| iv'' \right\rangle \cdot \left\langle J'A'\omega' \middle| \underset{\sim}{\mathcal{D}}(\theta,\chi,\phi) \middle| J''A''\omega'' \right\rangle \tag{59}$$

The matrix elements $\left\langle J'A'\omega' \middle| \underset{\sim}{\mathcal{D}}(\theta,\chi,\phi) \middle| J''A''\omega'' \right\rangle$ determine the group selection rules for an allowed transition and have been evaluated for many types of transitions (refs. 70, 71, 72). Summing Eq. (56) over the degenerate magnetic quantum numbers M' and M'', we have from Eq. (54)

$$S_{nm} = S^{nv'J'A'}_{mv''J''A''} = \mathcal{S}^{J'A'}_{J''A''} \rho^{nv'}_{mv''} \tag{60}$$

where $\mathcal{S}^{J'A'}_{J''A''}$ is the Hönl-London factor (refs. 73, 74) and

$$\rho^{nv'}_{mv''} = \sum_{i,j} \left| \left\langle jv' \middle| -\sum_k e\underset{\sim}{r}_k \middle| iv'' \right\rangle \right|^2 \tag{61}$$

is the band strength for the transition. Combining Eqs. (51), (53), and (60), we have for the intensity of a single emitting line from upper level n:

$$I_{nm} = I^{nv'J'}_{mv''J''} = \frac{4}{3} N_{J'} \frac{\left[\Delta E^{nv'J'}_{mv''J''}\right]^4 S^{nv'J'A'}_{mv''J''A''}}{\hbar^4 c^3 \omega_n} \tag{62}$$

where N_{J}'' is the number density in the upper rotational state J' and $\omega_n = (2-\delta_{\sigma},\Lambda'_J)$. (2S' + 1) is the electronic degeneracy. Taking an average value of $\Delta E^{n\,v'\,J'}_{m\,v''\,J''}$ for the whole band, Eq. (62) can be summed to yield the total intensity in the (v', v") band:

$$I^{nv'}_{mv''} = \sum_{J',J''} I^{nv'J'}_{mv''J''} = \frac{4}{3} N_{v'} \frac{\left[\overline{\Delta E}^{nv'}_{mv''}\right]^4 \rho^{nv'}_{mv''}}{\hbar^4 c^3 \omega_n} \tag{63}$$

where $N_{v}' = \sum_{J'} N_{J'}$ is the total number density in the upper vibrational level v' and where we make use of the group summation property

$$\sum_{J''} S^{J'\Lambda'}_{J''\Lambda''} = (2J' + 1) \tag{64}$$

Comparing Eqs. (53) and (63), we have for the Einstein spontaneous transition coefficient of the band (v', v")

$$A^{nv'}_{mv''} = \frac{4}{3} \frac{\left[\overline{\Delta E}^{nv'}_{mv''}\right]^3 \rho^{nv'}_{mv''}}{\hbar^4 c^3 \omega_n} \tag{65}$$

Similarly, the lifetime of an upper vibrational level v' of state n can be written

$$\frac{1}{\tau_n} = \sum_{m<n} \sum_{v''} A^{nv'}_{mv''} \tag{66}$$

where the summation runs over all v" for each lower state n. Eq. (65) can be cast in the computational form

$$A^{nv'}_{mv''}\,(\mathrm{sec}^{-1}) = \frac{(21.41759 \times 10^9)}{\omega_n} \left[\Delta E^{nv'}_{mv''}(\mathrm{a.u.})\right]^3 \rho^{nv'}_{mv''}\,(\mathrm{a.u.}) \tag{67}$$

where $\Delta E^{n\,v'}_{m\,v''}$ and $\rho^{n\,v'}_{m\,v''}$ are in atomic units. It is also often convenient to relate the transition probability to the number of dispersion electrons needed to explain the emission strength classically. This number, the f-number or oscillator strength for emission, is given by

$$f_{nm,v'v''} = \frac{m c^3 \hbar^2}{2e^2 \left[\overline{\Delta E}^{nv'}_{mv''}\right]^2} A^{nv'}_{mv''} \tag{68}$$

The inverse process of absorption is related to the above development through the Einstein B coefficient. Corresponding to Eq. (53), we have for a single line in absorption.

$$I_{mn} = I^{nv'J'}_{mv''J''} = \int_{\text{line}(v''v',\,J''J')} K(\nu)\,d\nu = \Delta E_{mn} N_m B_{mn} \tag{69}$$

where K(ν) is the absorption coefficient of a beam of photons of frequency and

$$B_{mn} = B^{nv'J'\Lambda'}_{mv''J''\Lambda''} = \frac{2\pi}{3\hbar^2 c} \frac{S^{nv'J'\Lambda'}_{mv''J''\Lambda''}}{\nu_{nm}(2J''+1)} \tag{70}$$

is the Einstein absorption coefficient for a single line. Summing over all lines in the band (v", v'), assuming an average band frequency, we obtain

$$I^{nv'}_{mv''} = \sum_{J',J''} I^{nJ'v'}_{mJ''v''} = N_{v''} \frac{2\pi}{3\hbar^2 c\,\omega_{m}} p^{nv'}_{mv''} \tag{71}$$

where $N_{v''} = \sum_{J''} N_{J''}$ is the total number density in the lower vibrational state v". Corresponding to Eqs. (67) and (68) we can define an f-number or oscillator strength for absorption as

$$f_{mn,v''v'} = \frac{2m\,\overline{\Delta E}^{nv'}_{mv''}}{3\hbar^2 e^2 \omega_{n}} p^{nv'}_{mv''} \tag{72}$$

In computation form, Eq. (72) becomes

$$f_{mn,v''v'} = \frac{2}{3} \cdot \frac{\overline{\Delta E}^{nv'}_{mv''}\,(\mathrm{a.u.})}{\omega_m} \; \rho^{nv'}_{mv''}\,(\mathrm{a.u.}) \tag{73}$$

where $\overline{\Delta E}^{n\,v'}_{m\,v''}$ and $\rho^{n\,v'}_{m\,v''}$ are in atomic units. Combining Eqs. (65) and (68) and comparing with Eq. (72), we see that the absorption and emission f-numbers are related by

$$f_{mn,v''v'} = \left(\frac{\omega_n}{\omega_m}\right) f_{nm,v'v''} \tag{74}$$

Some caution must be observed in the use of f-numbers given either by Eq. (68) or (72) since both band f-numbers and system f-numbers are defined in the literature. The confusion arises from the several possible band averaging schemes that can be identified.

An integrated absorption coefficient (density corrected) can be defined from Eq. (71) as

$$S_{v'',v'} = \frac{1}{Pc}\, I^{nv'}_{mv''} = N_{v''}\, B_{v'',v'} \left(1 - \exp \frac{-hc\nu_{v'',v'}}{kT}\right) \frac{h\nu_{v'',v'}}{Pc^2} \tag{75}$$

where the exponential factor corrects for stimulated emission. Eq. (75) can be written in terms of the absorption f-number as

$$S_{v''v'} = \frac{\pi e^2}{mc^2}\, \frac{N_{v''}}{P} \left(1 - \exp - \frac{hc\nu_{v'',v'}}{kT}\right) f_{mn,v''v'} \tag{76}$$

Using h c/k = 1.43880 cm-K^{o}, we obtain a computational formula for the integrated absorption coefficient as

$$S_{v'',v'}\,(\mathrm{cm}^{-2}\ \mathrm{atm}^{-1}) = \tag{77}$$

$$2.3786 \times 10^{7} \left(\frac{273.16}{T(K^{o})}\right)\left(\frac{N_{v''}}{N_T}\right)\left(1 - \exp \frac{-1.43880\,\nu_{v'',v'}(\mathrm{cm}^{-1})}{T\ (K^{o})}\right) f_{mn,v''v'}$$

The total integrated absorption is found from

$$S_{\mathrm{TOTAL}} = \sum_{v''} \sum_{v'} S_{v'',v'} \tag{78}$$

where, under normal temperature conditions, only the first few fundamentals and overtones contribute to the summations.

The developments given above are rigorous for band systems where an average band frequency can be meaningfully defined. Further approximations, however, are often made. For example, the electronic component of the dipole transition moment can be defined as

$$\mathcal{R}_{ji}(R) = \left\langle j \left| -\sum_k e\underset{\sim}{r}_k \right| i \right\rangle \tag{79}$$

This quantity is often a slowly varying function of R and an average value can sometimes be chosen. Eq. (61) can then be written approximately in factored form as

$$\rho^{nv'}_{mv''} \simeq q_{v'v''} \sum_{i,j} \left| \bar{\mathcal{R}}_{ji}(\bar{R}) \right|^2 \tag{80}$$

where $q_{v', v''}$, the square of the vibrational overlap integral, is called the Franck-Condon factor. $\mathcal{R}_{ji}$ is evaluated at some mean value of the internuclear separation R. In addition, it is sometimes possible to account for a weak R-dependence in $\underset{\sim}{M}^e$ by a Taylor series expansion of this quantity about some reference value, $\mathcal{R}_{\alpha\beta}$. Usually the reference is to the (0, 0) band. We have

$$\mathcal{R}_{ji} \simeq \mathcal{R}^{\alpha\beta}_{ji} \left[1 + a(R - R_{\alpha\beta}) + b(R - R_{\alpha\beta})^2 + \dots \right] \tag{81}$$

Substituting into Eq. (61) and integrating yields

$$\rho^{nv'}_{mv''} \simeq q_{v'v''} \sum_{i,j} \left| \mathcal{R}^{\alpha\beta}_{ji} \left[1 + a\,\overline{(R_{v'v''} - R_{\alpha\beta})} + b\,\overline{(R_{v'v''} - R_{\alpha\beta})^2} + \dots \right] \right|^2 \tag{82}$$

where

$$\overline{(R_{v'v''} - R_{\alpha\beta})} = \frac{\langle v'|(R - R_{\alpha\beta})|v''\rangle}{\langle v'|v''\rangle} \tag{83}$$

is the R-centroid for the transition and

$$\overline{(R_{v'v''} - R_{\alpha\beta})^2} = \frac{\langle v'|(R - R_{\alpha\beta})^2|v''\rangle}{\langle v'|v''\rangle} \tag{84}$$

is the R^2-centroid. Note that this last term differs (to second order) from the square of the R-centroid. An alternate procedure can be developed by evaluating Eq. (79) at each R-centroid, $\bar{\bar{R}}_{v', v''}$. Then

$$\rho^{nv'}_{mv''} \approx q_{v'v''} \sum_{ij} |R_{ij} (\bar{R}_{v'v''})|^2 \tag{85}$$

Eq. (85) assumes that the vibrational wavefunction product, $\psi_{v'} \psi_{v''}$, behaves like a delta function upon integration,

$$\psi_{v'} \psi_{v''} = \delta (R - \bar{R}_{v'v''}) \langle v'|v''\rangle \tag{86}$$

The range of validity of Eq. (85) is therefore questionable, particularly for band systems with bad overlap conditions such as oxygen Schumann-Runge. The range of validity of the R-centroid approximation has been examined by Frezer (ref.75). For perturbed electronic systems, the transition dipole moment will have a strong R-dependence and R-centroid or other approximations will be invalid. A direct evaluation on Eq. (61) would therefore be required using the fully-coupled system of electronic and vibrational wavefunctions to properly account for the source of the band perturbations.

The final step in calculating transition probabilities is the determination of $\mathcal{R}_{ji}(R)$, the electronic dipole transition moment, for the entire range of internuclear separations, R, reached in the vibrational levels to be considered. Expanding the wavefunction in configuration interaction form

$$\psi_{el}^{i}(R) = \sum_{\nu} C_{\nu}^{i}\, \psi_{\nu}(R) \tag{87}$$

we can write Eq. (79) as

$$\mathcal{R}_{ji}(R) = \sum_{\mu\nu} C_{\mu}^{j*}\, C_{\nu}^{i} \left\langle \psi_{\mu}(R) \middle| \underset{\sim}{M}^{e} \middle| \psi_{\nu}(R) \right\rangle \tag{88}$$

where C_{μ}^{j} and C_{ν}^{i} are expansion coefficients for ψ_{el}^{j} and ψ_{el}^{i}, respectively. The matrix elements appearing in Eq. (88) can finally be reduced, by appropriate operator algebra, to products of one-electron integrals over the spatial coordinates.

It is clear from Eq. (80) that the Franck-Condon factor plays a dominant role in the determination of intensities for a particular transition in a band system. The experimental evidence (refs. 68, 69, 76-82) is overwhelming that observed vibrational intensities can be correlated by a relative intensity scale determined from the Franck-Condon factors, modified in some cases by a slowly varying factor of the internuclear separation which is required to put the calculated intensities on an absolute scale. This implies that an accurate solution to the vibrational-rotational Schrödinger equation is required for the molecular states of interest, but that the electronic transition moments are, in general, smooth functions of the internuclear separation and can be conveniently parameterized.

The vibrational-rotational wavefunctions $\psi_{VJ}^{i}(R)$ satisfy

$$\frac{d^2\psi_{VJ}^{i}(R)}{dR^2} + \frac{2\mu}{\hbar^2}\left\{E_{VJ}^{i} - \left[U^{i}(R) + \frac{J(J+1)\hbar^2}{R^2}\right]\right\}\psi_{VJ}^{i}(R) \tag{89}$$

where μ is the reduced mass, $U^{i}(R)$ is total potential energy of interaction for the electronic state ψ^{i} and E^{i}_{VJ} are the vibrational energies belonging to this state. Studies of the sensitivity of the E^{i}_{VJ} to an assumed potential indicate that (with the possible exception of H_2 and HeH^{+}) theoretical estimates of $U^{i}(R)$, which result from electronic structure calculations for a molecule, are never as accurate as those obtained from spectroscopic data. The best procedure is to determine $U^{i}(R)$ as a numerical function using the RKR procedure (ref. 83) or modifications to this method proposed by Jarmain. (refs. 84 , 85) Vanderslice (ref. 86), Zelezaik (ref. 87) and others. The use of "experimental" RKR potential curves is especially critical where there is a bad Franck-Condon overlap such as is evidenced by the Schumann-Runge system of oxygen. Here a change in the potential of approximately 1% reflects in an order-of-magnitude change in predicted Franck-Condon factors. In addition, the use of potential functions derived from Hartree-Fock solutions to the electronic wavefunctions will yield increasingly poorer estimates of the Franck-Condon factors for higher vibrational levels owing to the improper connections of Hartree-Fock wavefunctions in both the united and separated atom limits. The accurate numerical solution of Eq. (89) using RKR potential functions has now become routine using the procedure of Cooley (ref. 88) based on the Numerov method of integration. Convenient programs for accomplishing this type of calculation have been written by Zare (ref. 89), Nicholls (ref. 90), and others for bound-bound transitions and by Allison and Dalgarno (ref. 91) and Nicholls (ref. 92) for bound-free transitions. Using accurate RKR potentials based on spectroscopic data, Eq. (89) can be routinely solved with errors of ±1 cm^{-1} or less in the derived $G(v)$ value.

The ab initio calculation of electronic transition moments has not achieved such high accuracy. Until recently, only a few calculations of absolute oscillator strengths have been attempted. Mulliken and Rieke (ref. 93) employed various approximate LCAO wavefunctions in an examination of the oscillator strength of the Lyman and Werner band systems in H_2. Bates (ref. 94) examined the N_2^+ first negative band system using LCAO wavefunctions. Stephenson (ref. 95) and Bates (ref. 96) studied the X $^2\Pi$ - A $^2\Delta$ transition of the CH radical using LCAO wavefunctions. In 1950 (refs. 97, 98) Shull carried out calculations for the N_2^+ first negative system, the C_2 Swan bands and the C_2 Deslandres - d'Azambuja band systems using LCAO wavefunctions within both dipole length and dipole velocity formulations. The H_2 first positive and second positive systems were first reported by Fraser (ref. 99). Shull in 1952 (ref. 100) repeated, within the dipole velocity approximation, the earlier calculations on H_2 of Mulliken and Rieke (ref. 93). A more thorough study was carried out for the Lyman band system by Ehrenson and Phillipson (ref. 101) using improved CI wavefunctions. Clementi (ref. 102) recalculated the Swan bands using the dipole length approximations within an SCF framework. A very accurate analysis of the Σ - Π transitions in H_2 has been reported by Rothenberg and Davidson (ref. 103).

In the last several years there has been a rapidly increasing number of ab initio calculations of transition moments. Among these is the work of Huo (ref. 104) on NH and CH, the studies of transitions in BeH and MgH by Chan and Davidson (refs. 105, 106), and the work of Henneker and Popkie on hydrides (ref. 107), on the 13 electron systems, C_2^-, CN, CO, N_2^+, BO, BF^+, and BeF (ref. 108) and on BeH and MgH (ref. 109). Very accurate theoretical results have been reported for band systems in H_2 by Wolniewicz (ref. 110) and for band systems in HeH^+ by Michels (ref. 111) and Wolniewicz (ref. 112). Although definitive theoretical results can be obtained for two-four electron molecules, calculations of electronic transition moments for heavier systems still can only be expected to have order-of-magnitude accuracy. A major role of such calculations, however, can be to gain insight into the validity of R-centroid or other approximate analyses of band intensities.

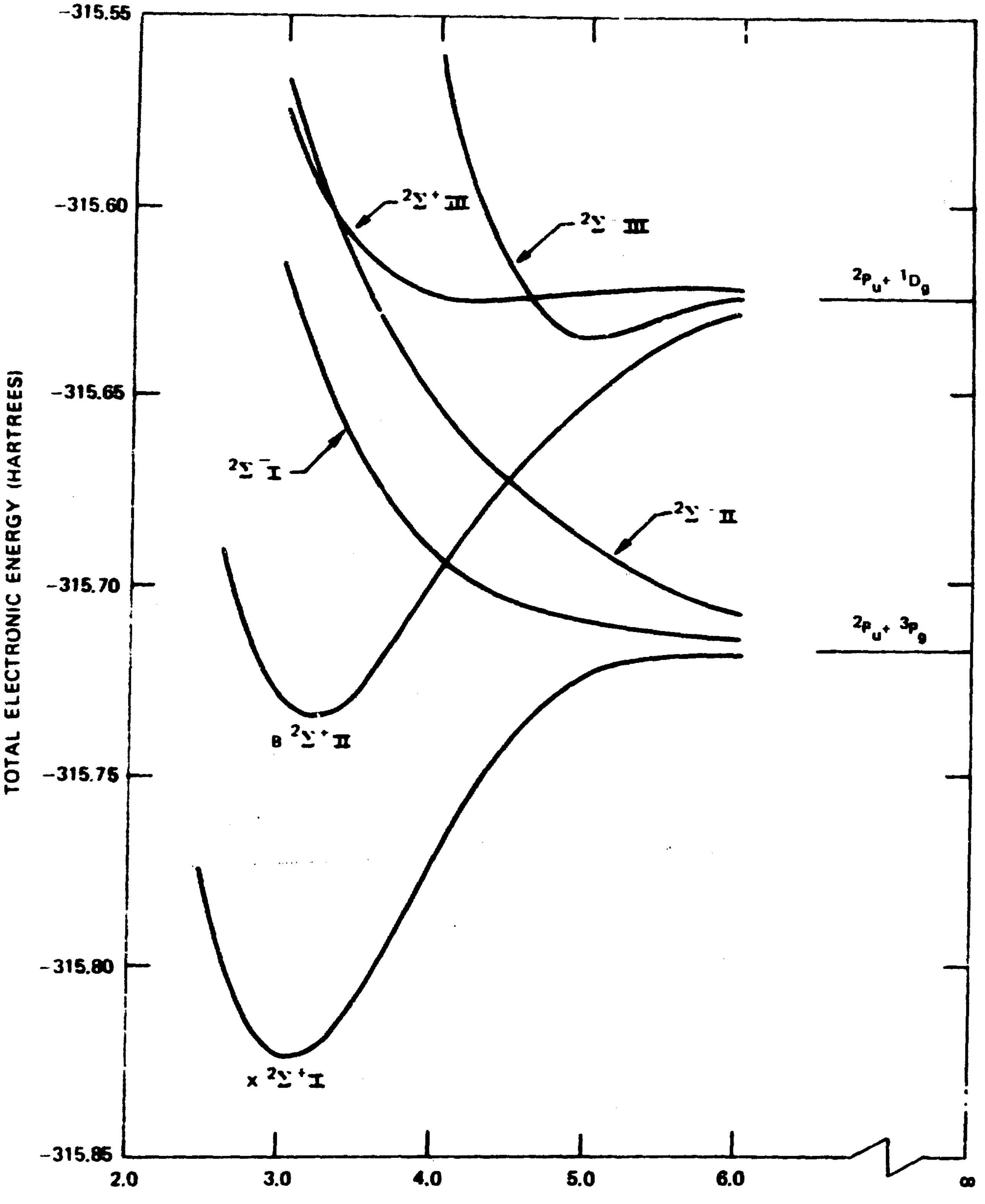


FIGURE 1. THE CALCULATED $^2\Sigma^{+,-}$ STATES OF AlO

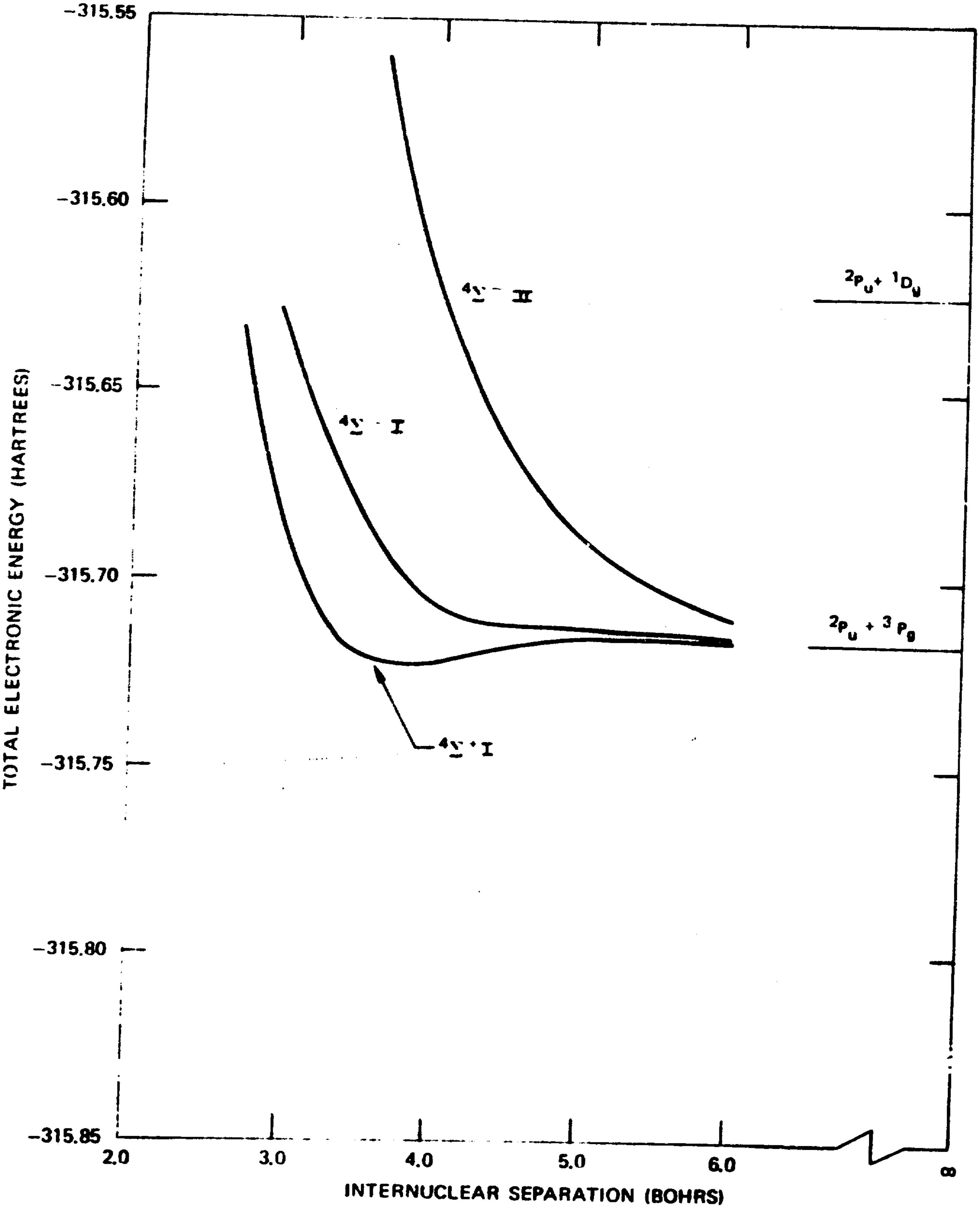


FIGURE 2. THE CALCULATED $^4\Sigma^{+,-}$ STATES OF AlO

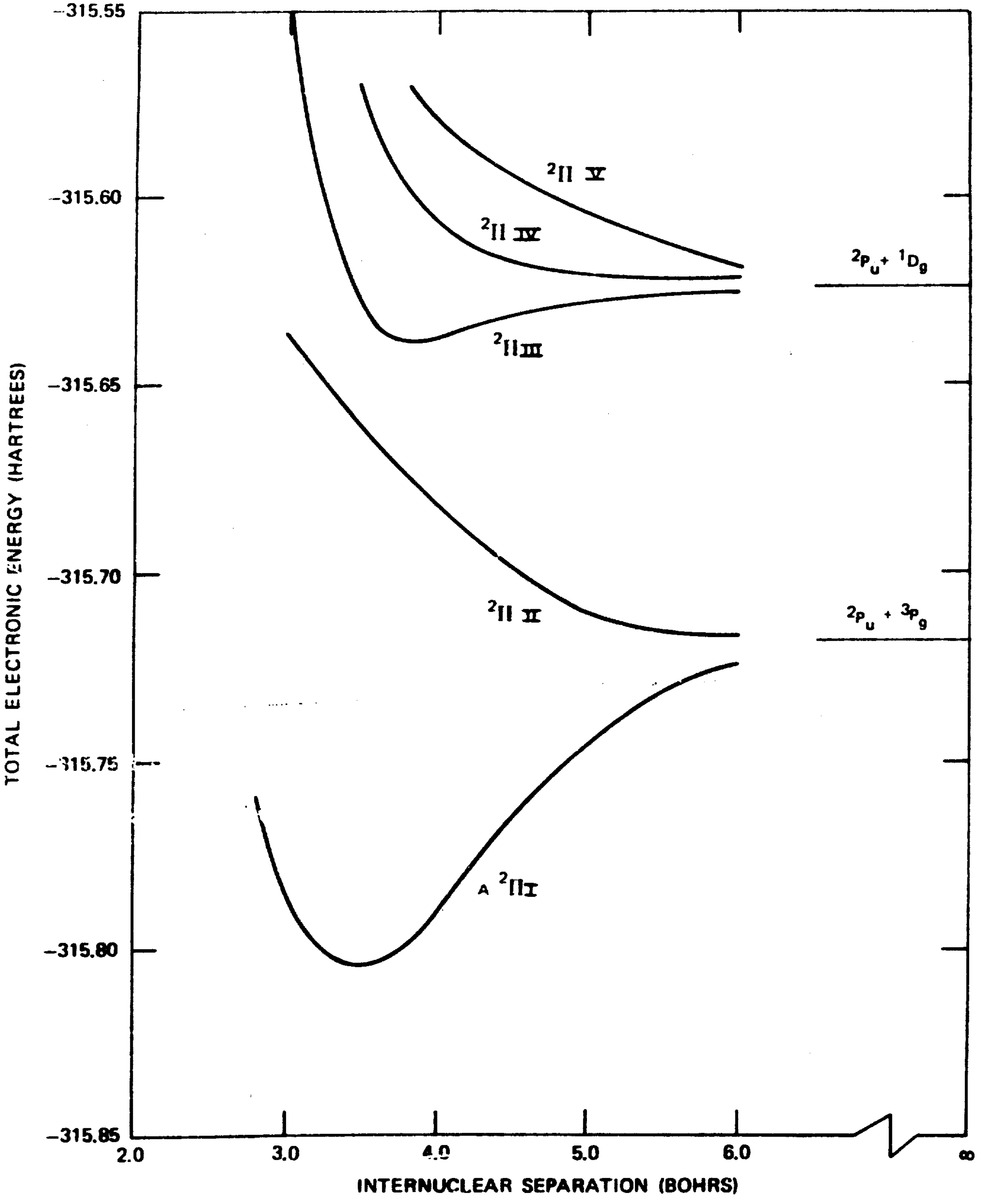


FIGURE 3. THE CALCULATED $^2\Pi$ STATES OF AlO.

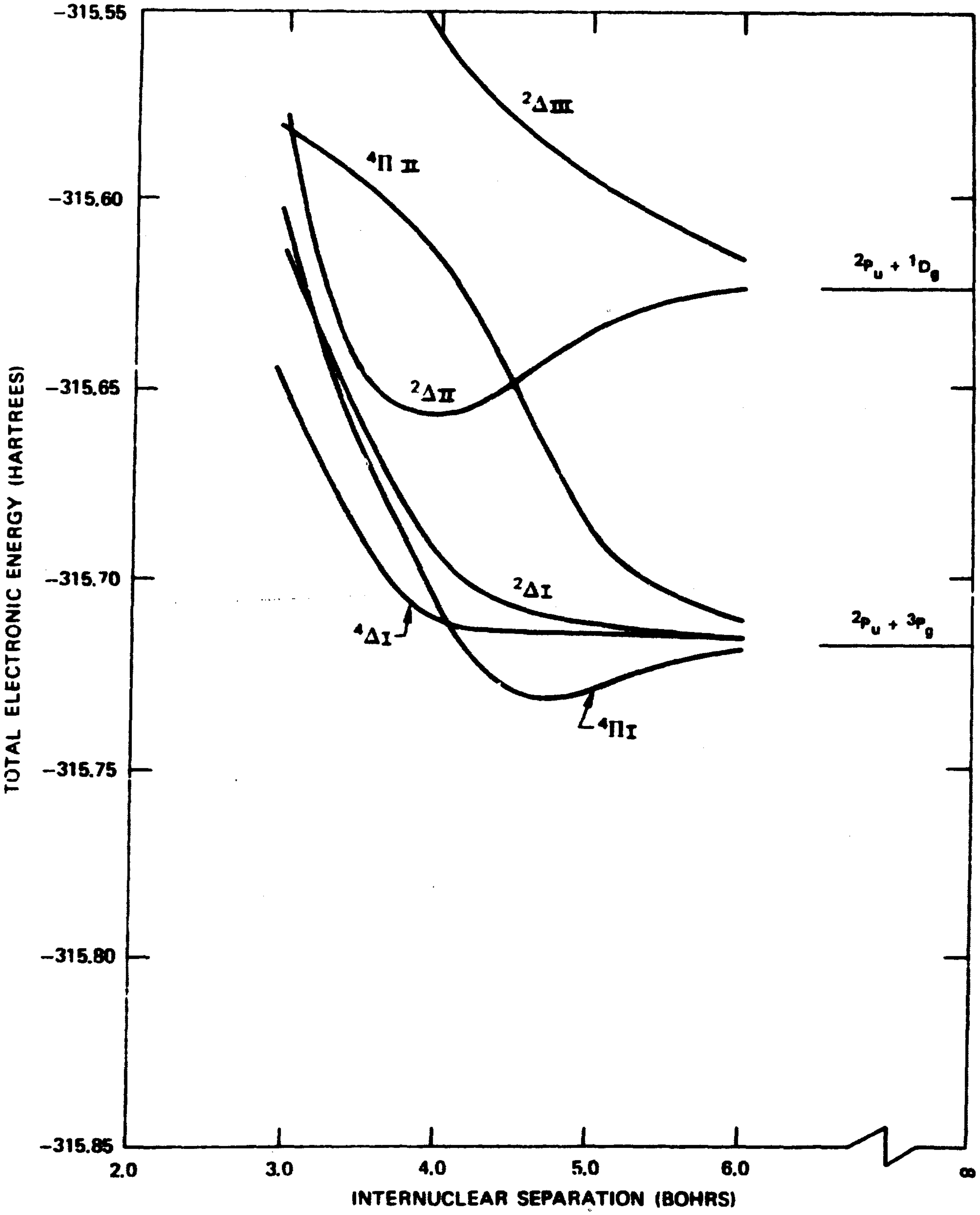


FIGURE 4. THE CALCULATED $^4\Pi$, $^2\Delta$, AND $^4\Delta$ STATES OF AlO.

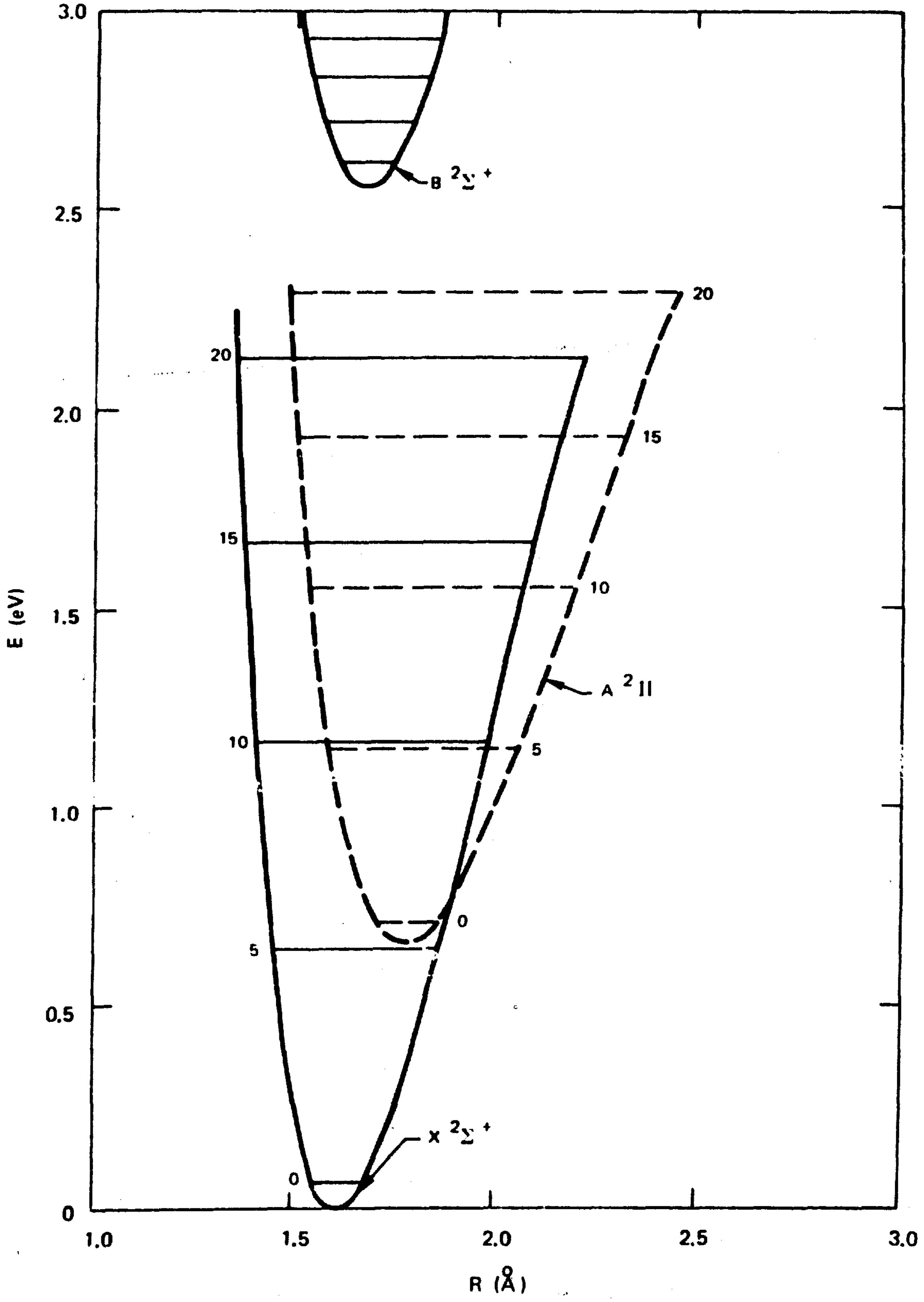


FIGURE 5. RKR POTENTIAL ENERGY CURVES FOR AlO

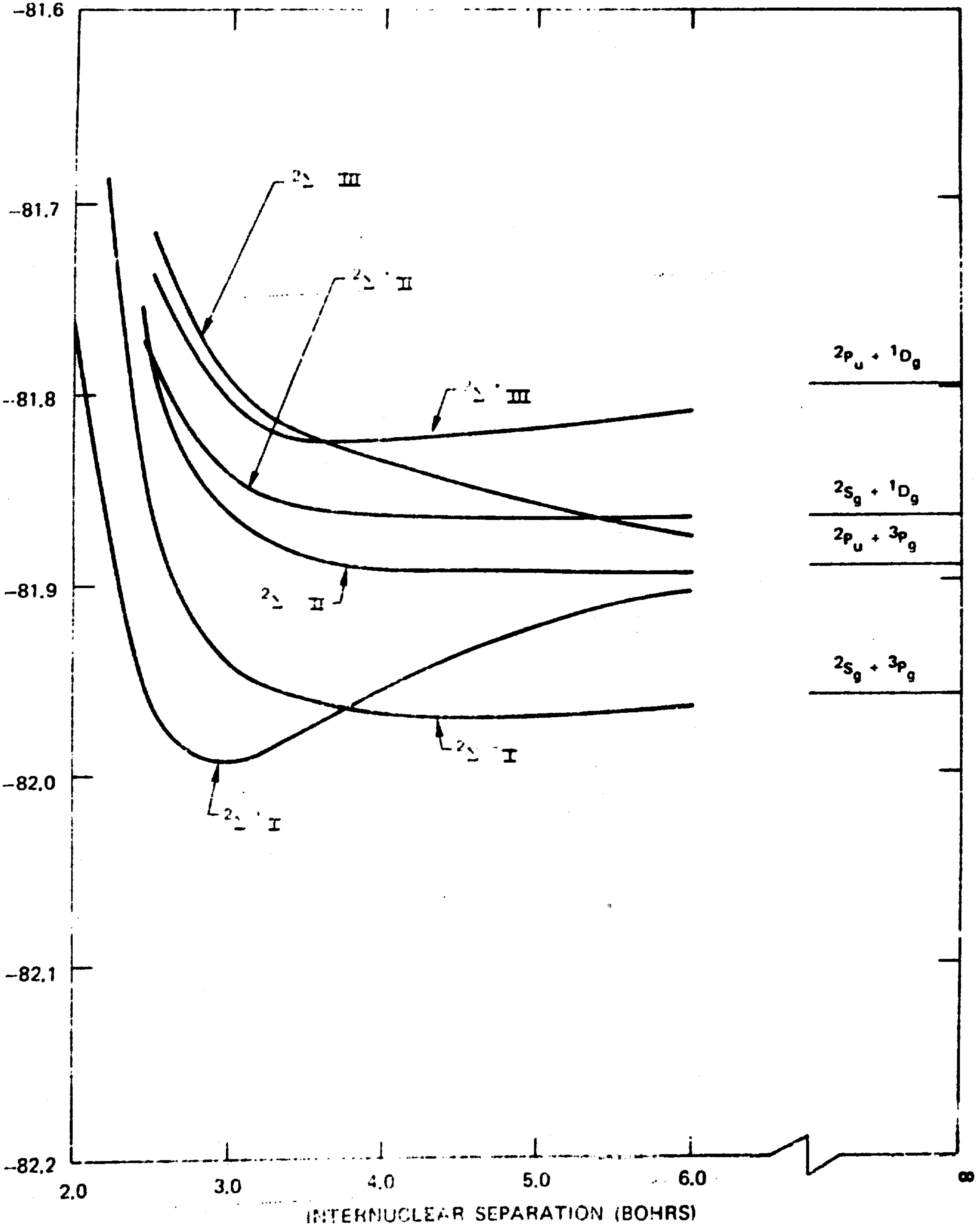


FIGURE 6. THE CALCULATED $^2\Sigma^{+,-}$ STATES OF LiO

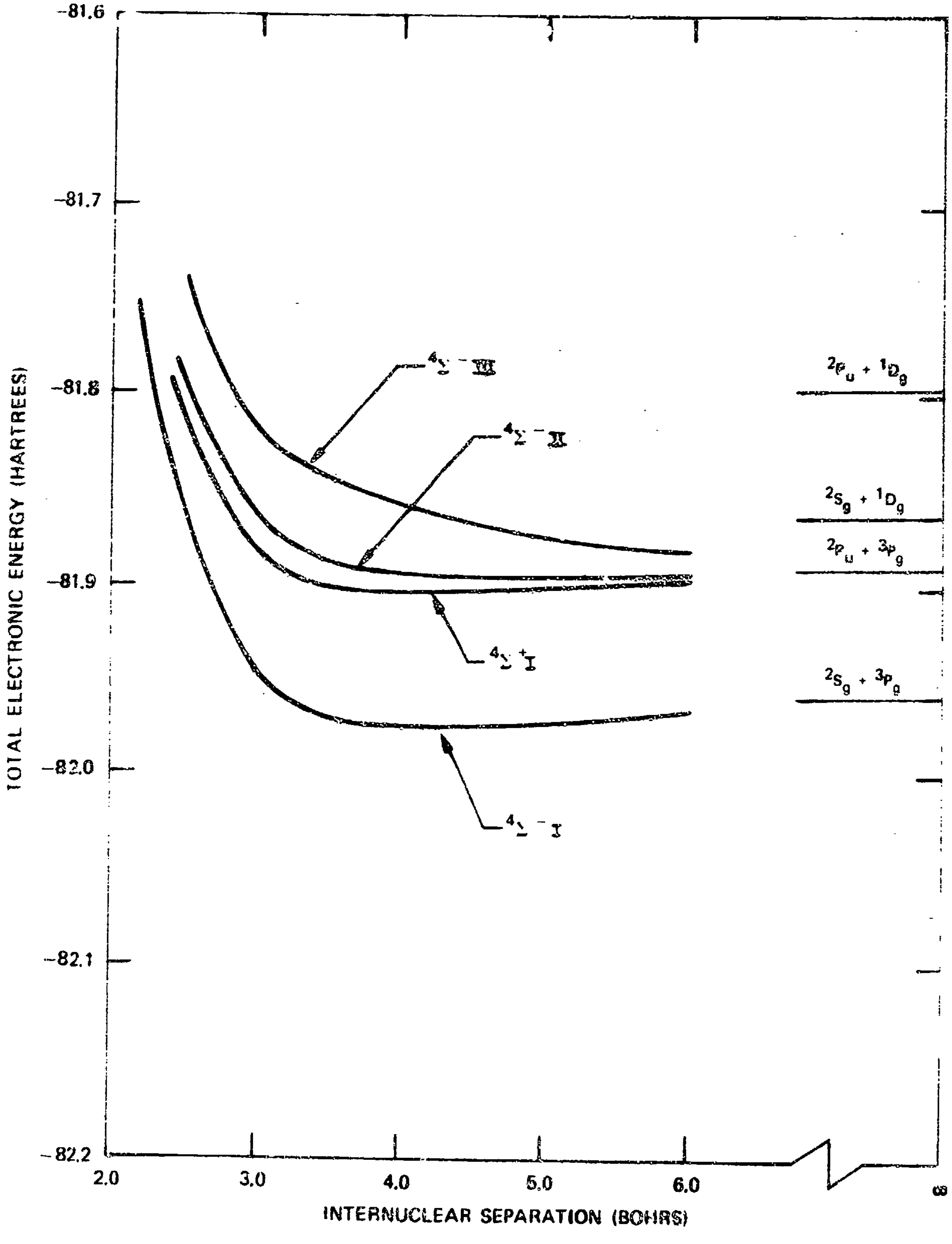


FIGURE 7. THE CALCULATED $^4\Sigma^{+,-}$ STATES OF LiO

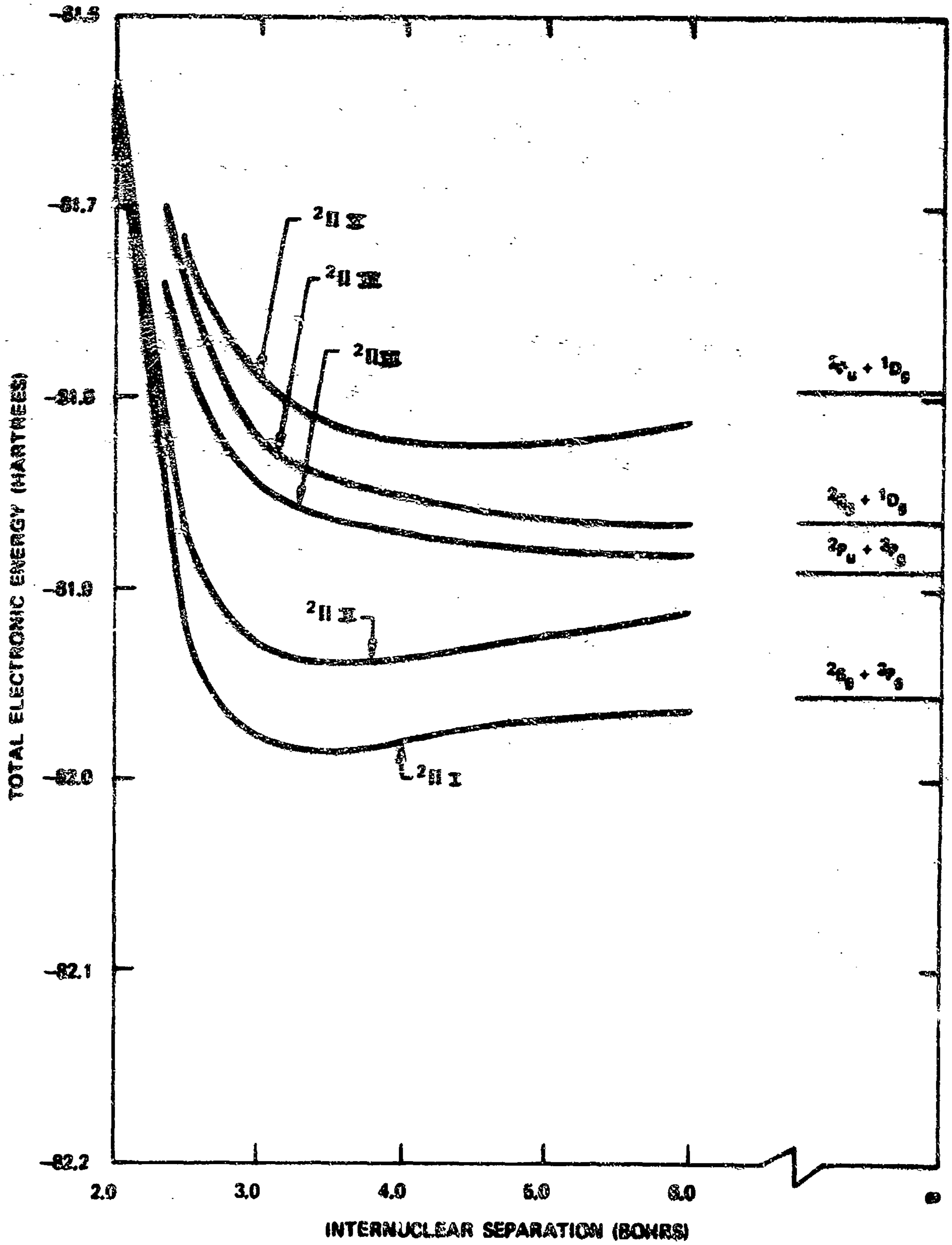


FIGURE 8. THE CALCULATED $^2\Pi$ STATES OF LiO

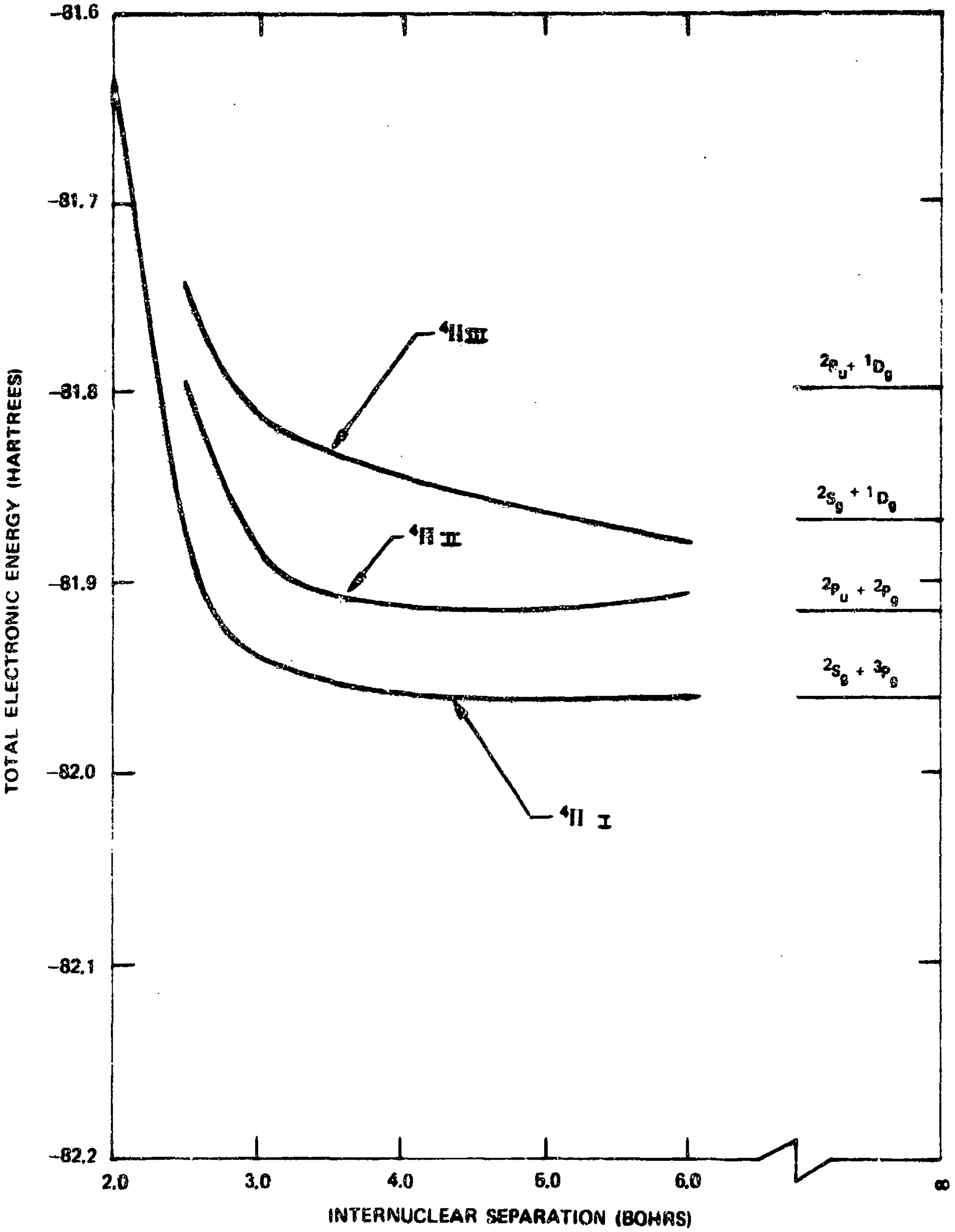


FIGURE 9. THE CALCULATED $^4\Pi$ STATES OF LiO

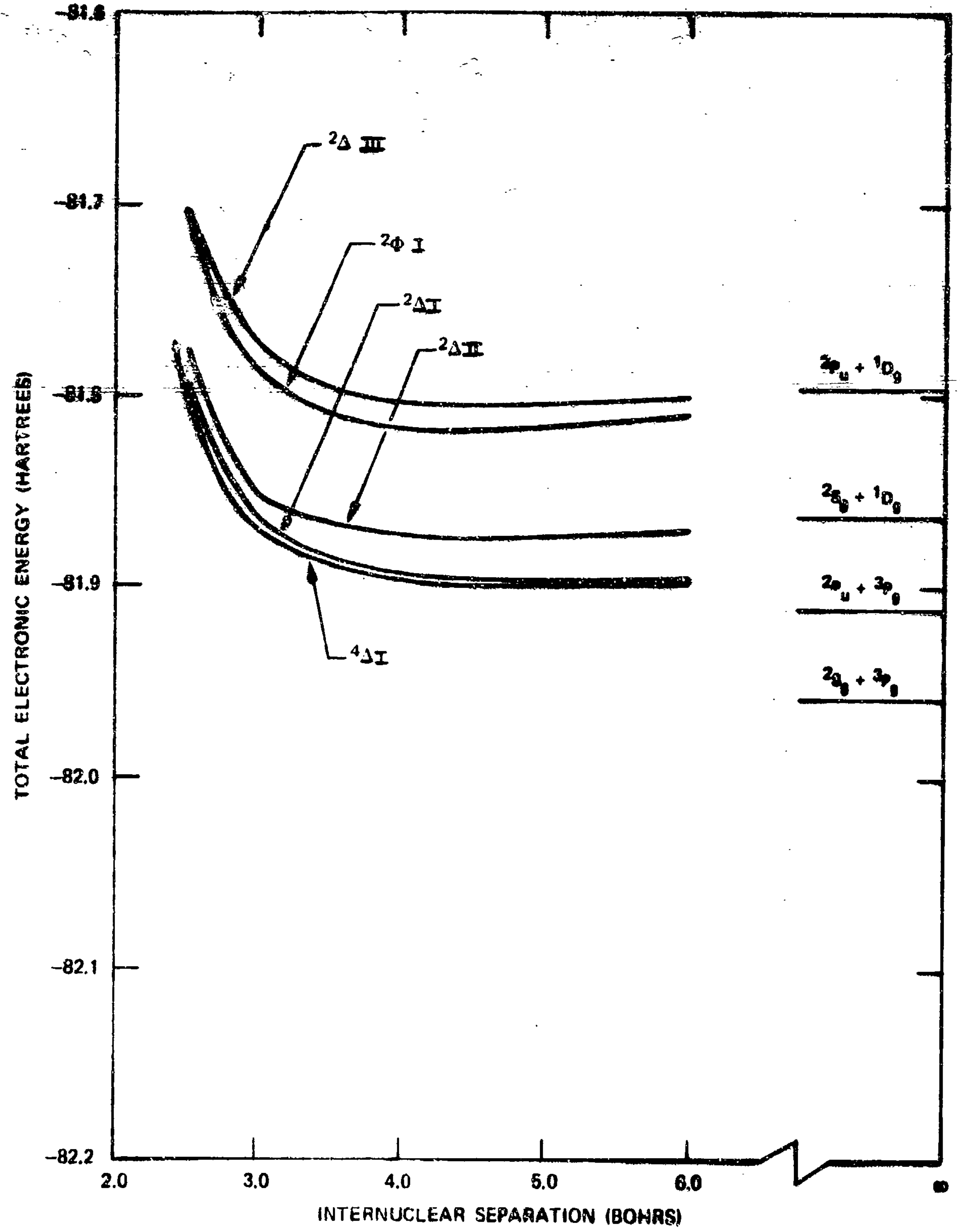


FIGURE 10. THE CALCULATED $^2\Delta$, $^4\Delta$ AND $^2\Phi$ STATES OF LiO

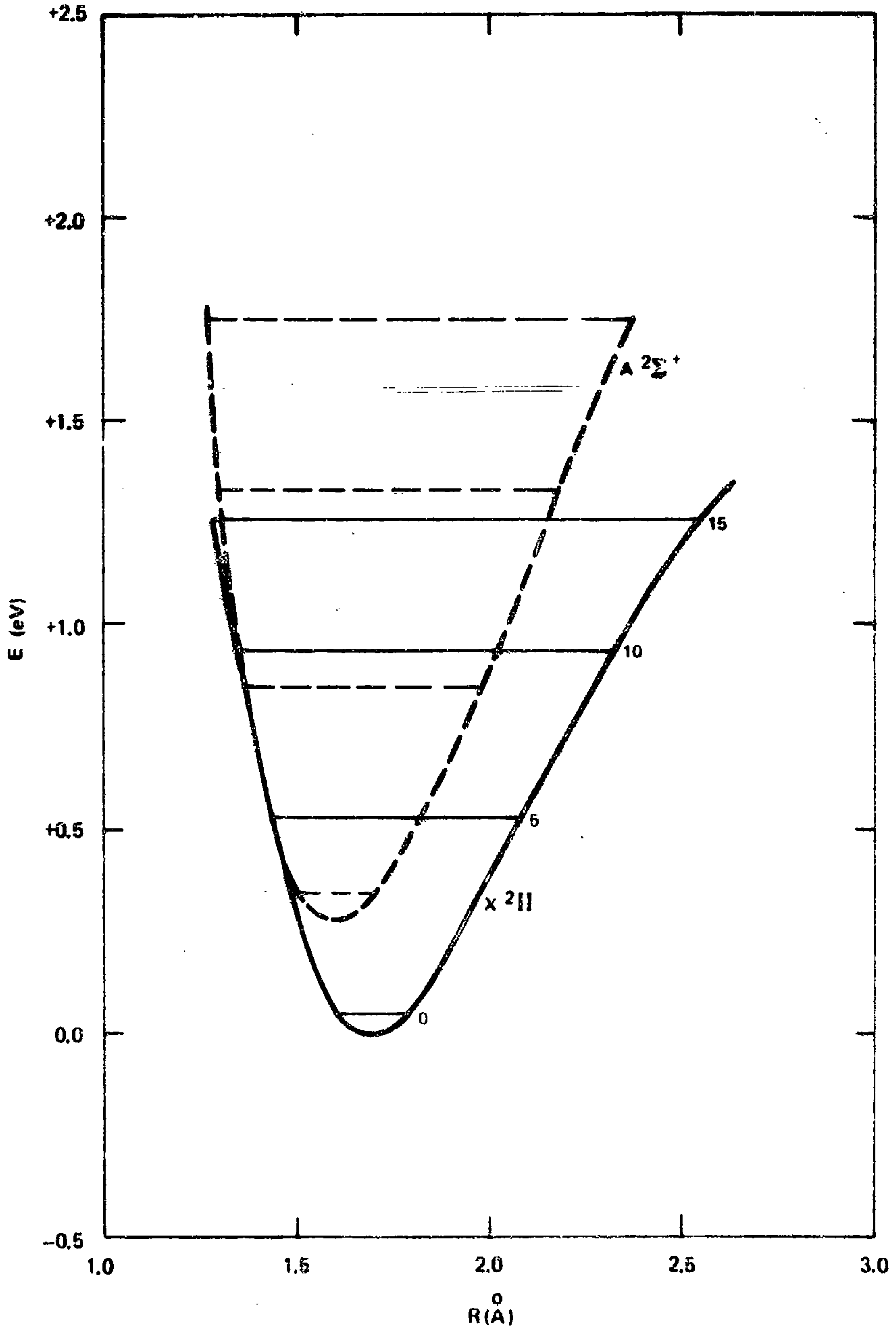


FIGURE 11. RKR POTENTIAL ENERGY CURVES FOR LiO

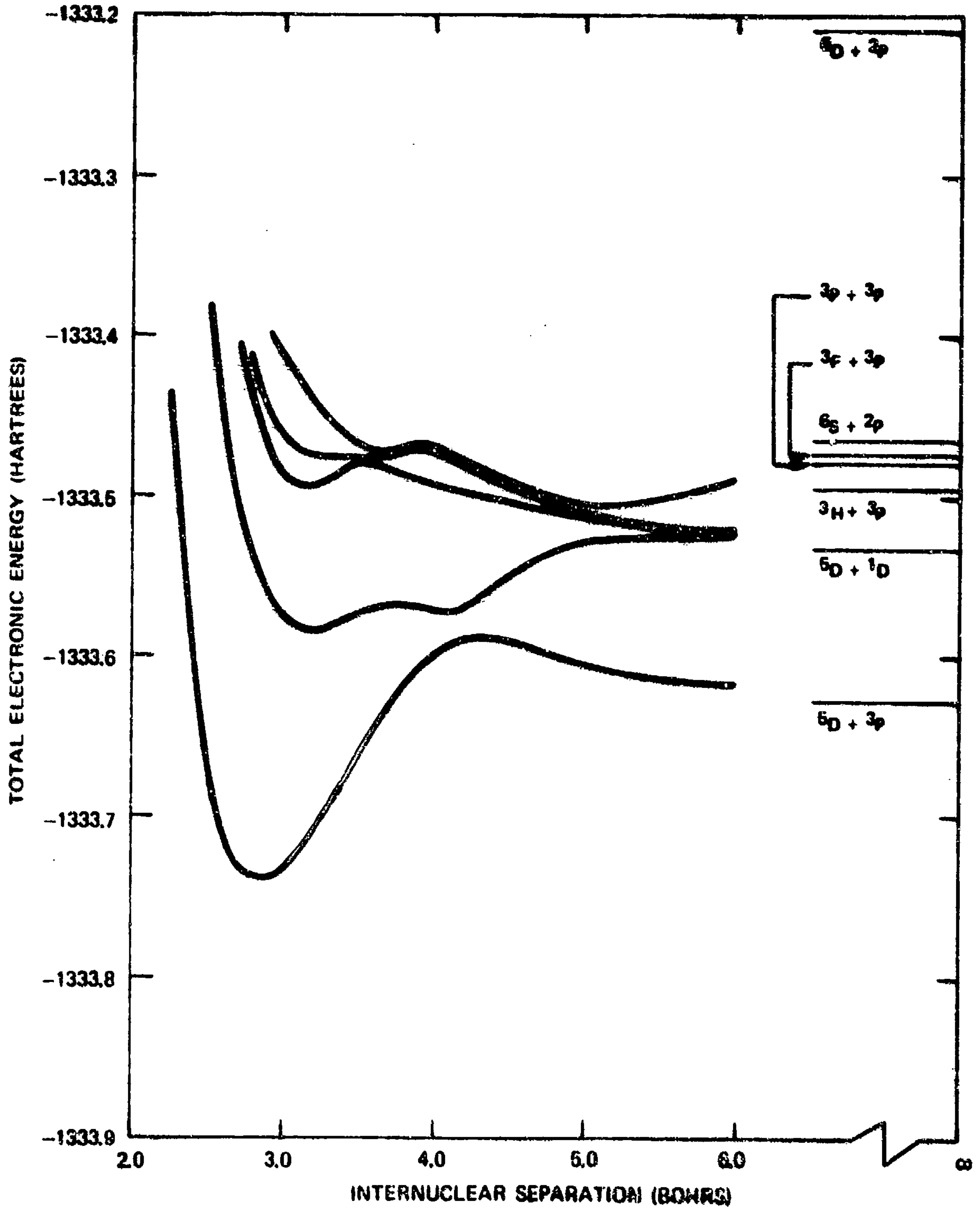


FIGURE 12. THE CALCULATED $^5\Sigma^+$ STATES OF FeO

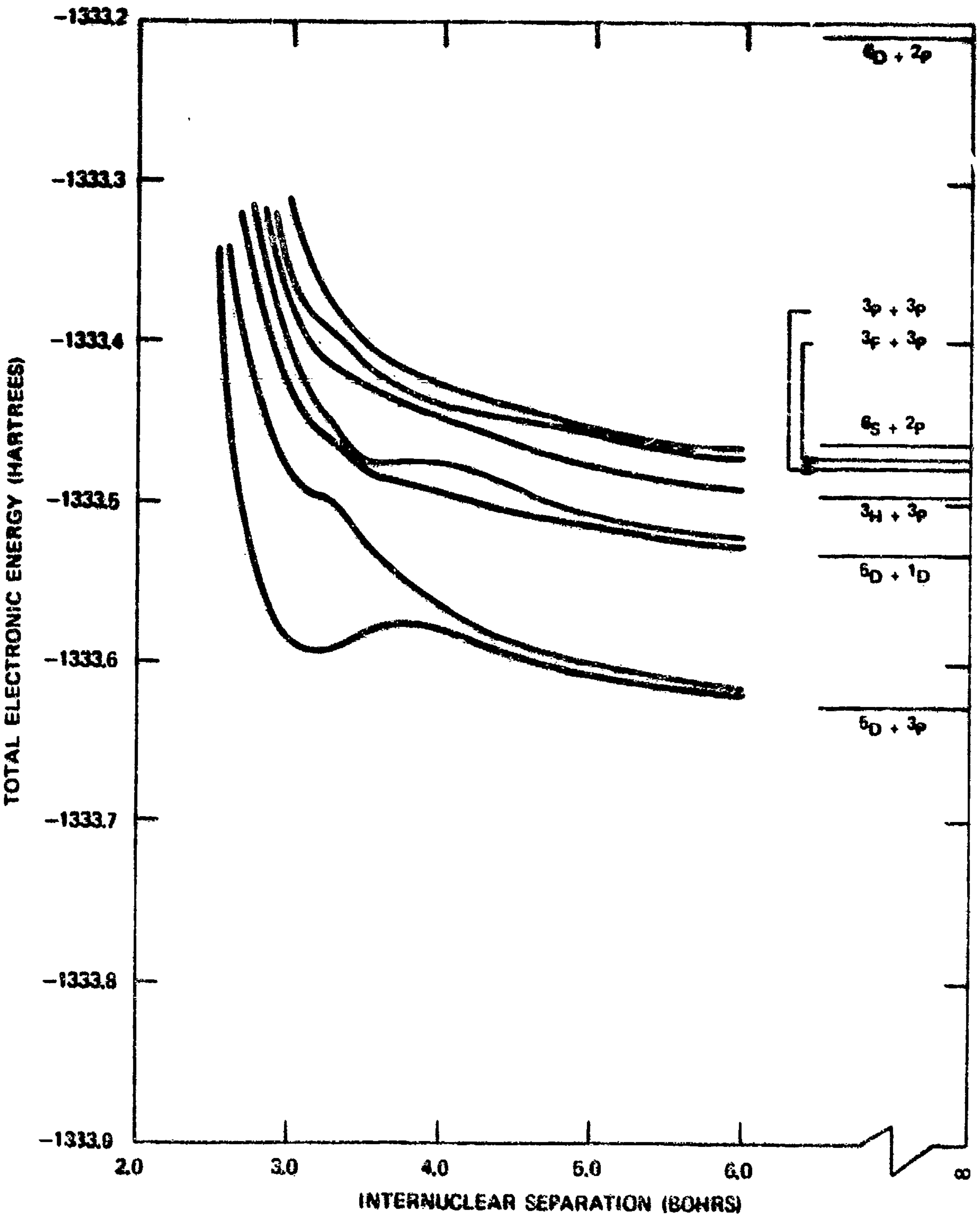


FIGURE 13. THE CALCULATED $^6\Sigma^-$ STATES OF FeO

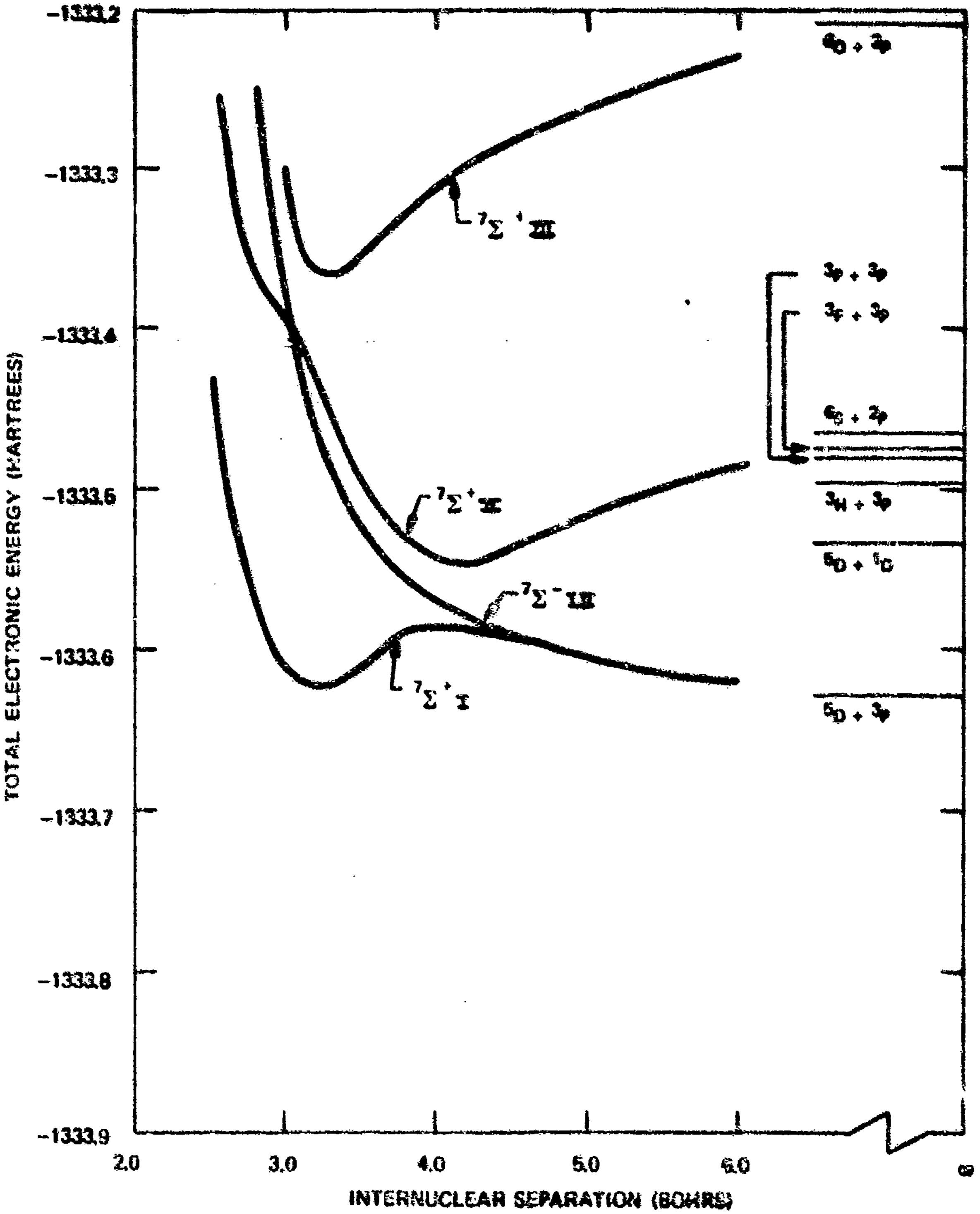


FIGURE 14. THE CALCULATED $^7\Sigma^{+,-}$ STATES OF FeO

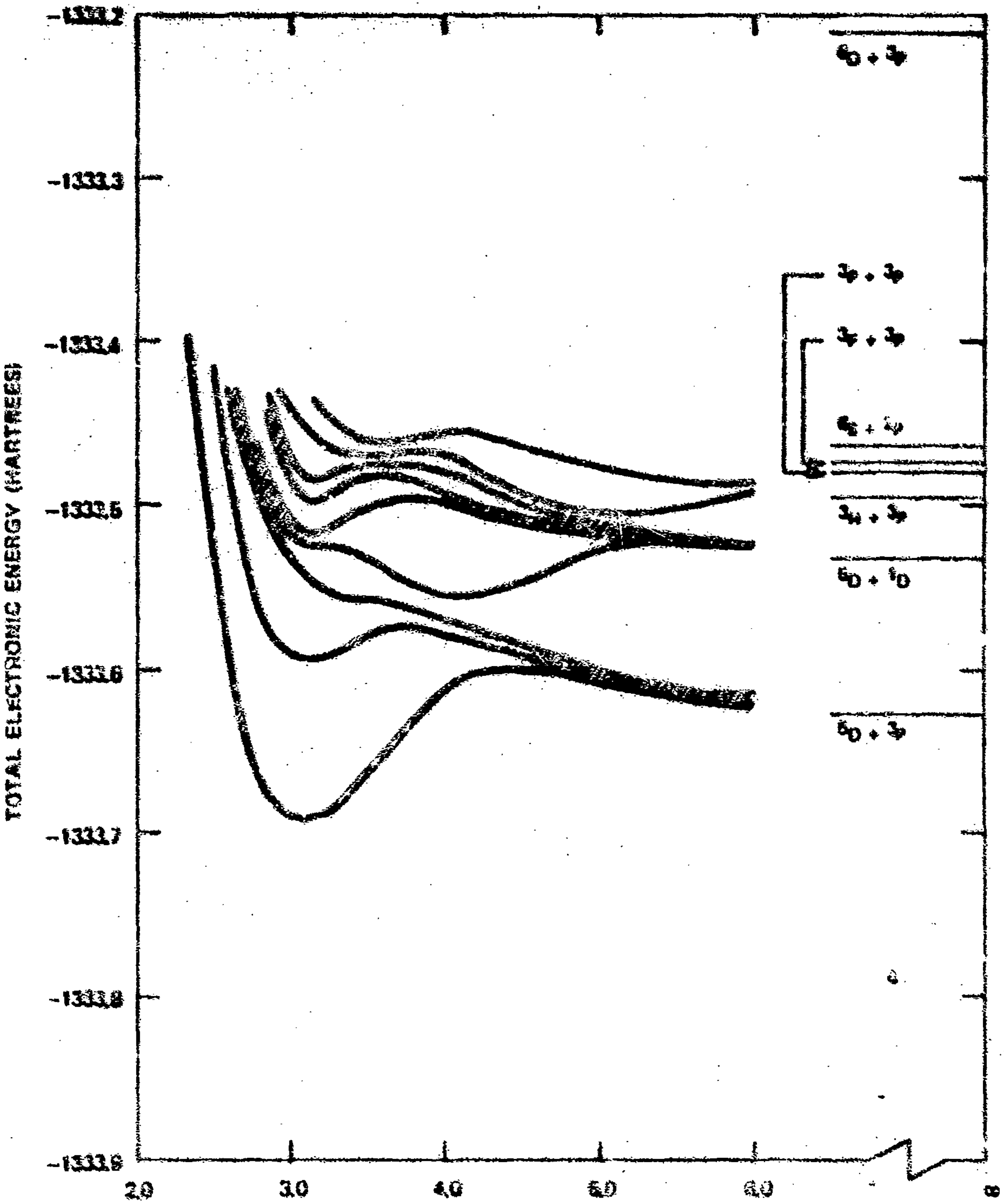


FIGURE 15. THE CALCULATED $^5\Pi$ STATES OF FeO

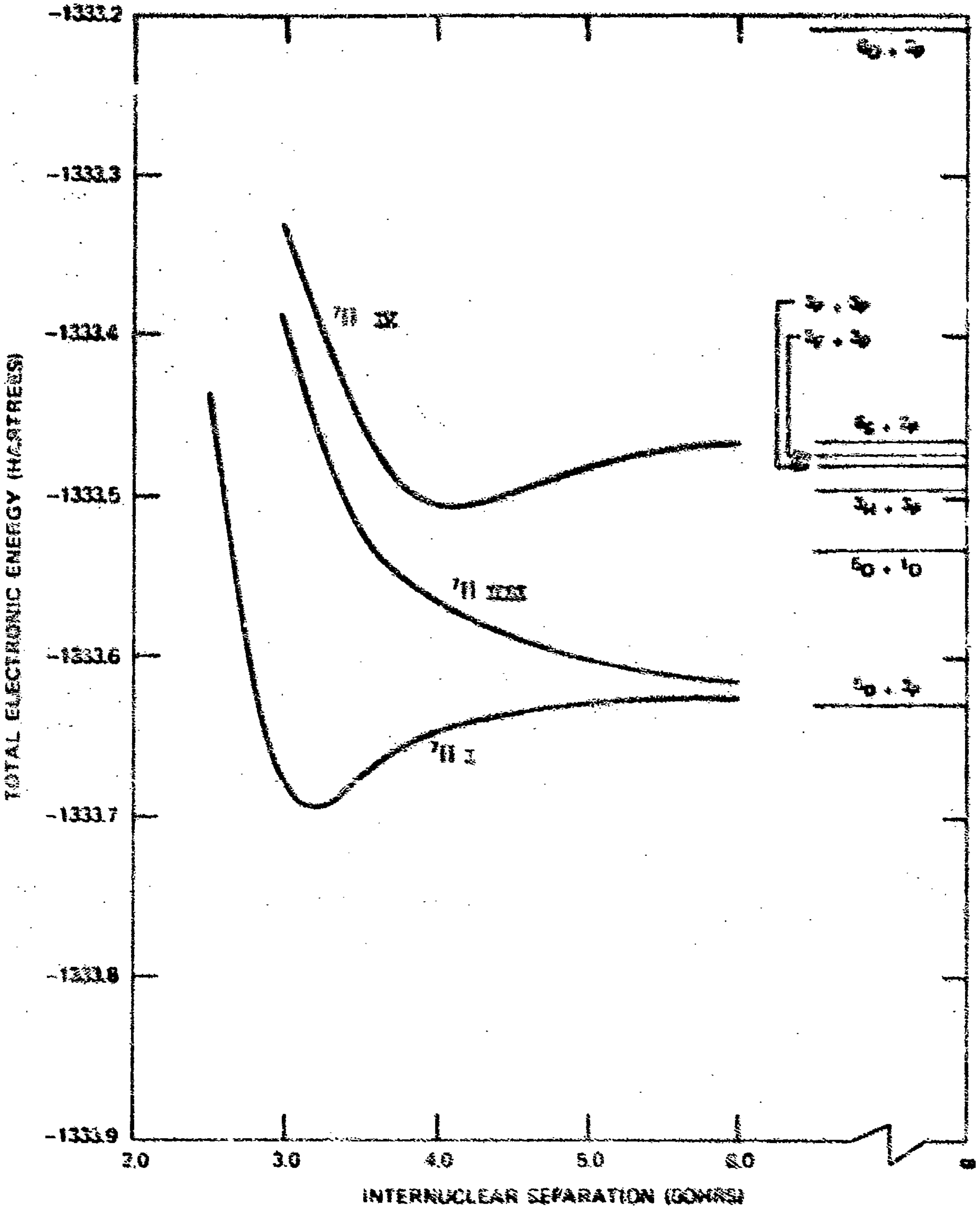


FIGURE 16. THE CALCULATED $^7\Pi$ STATES OF FeO

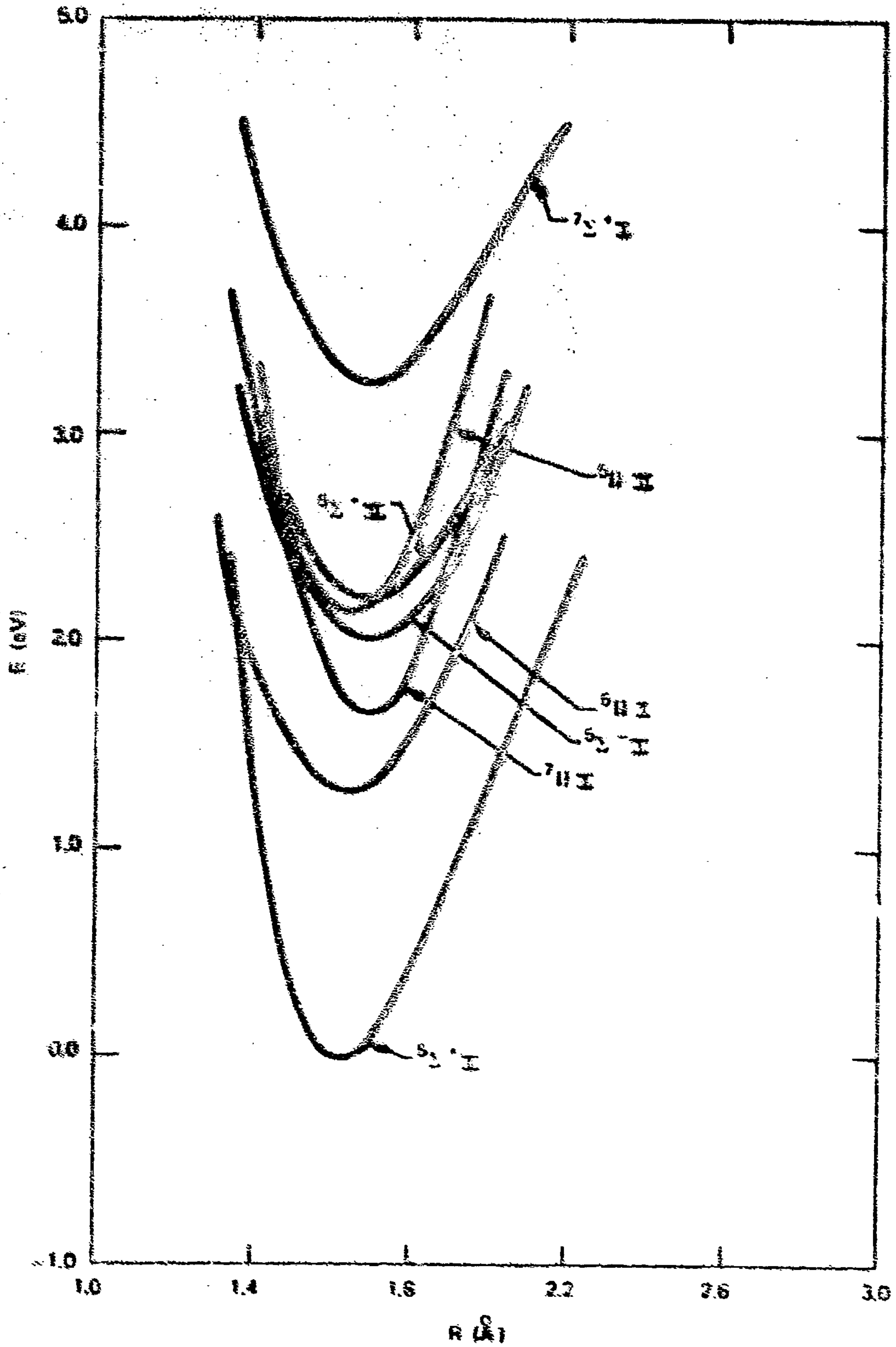


FIGURE 17. RKR POTENTIAL ENERGY CURVES FOR FeO

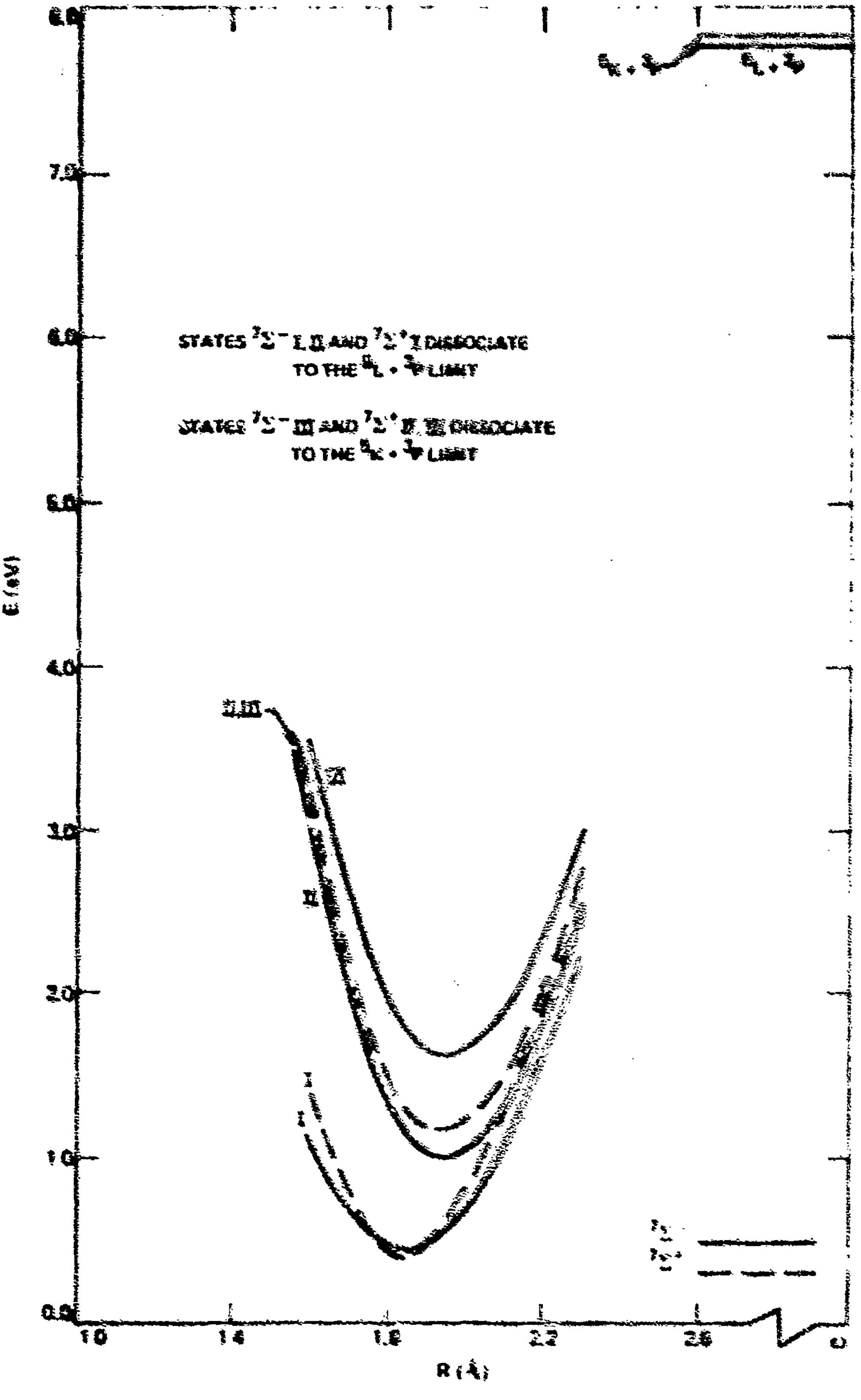


FIGURE 12. THE $^7\Sigma^{+,-}$ STATES OF UO

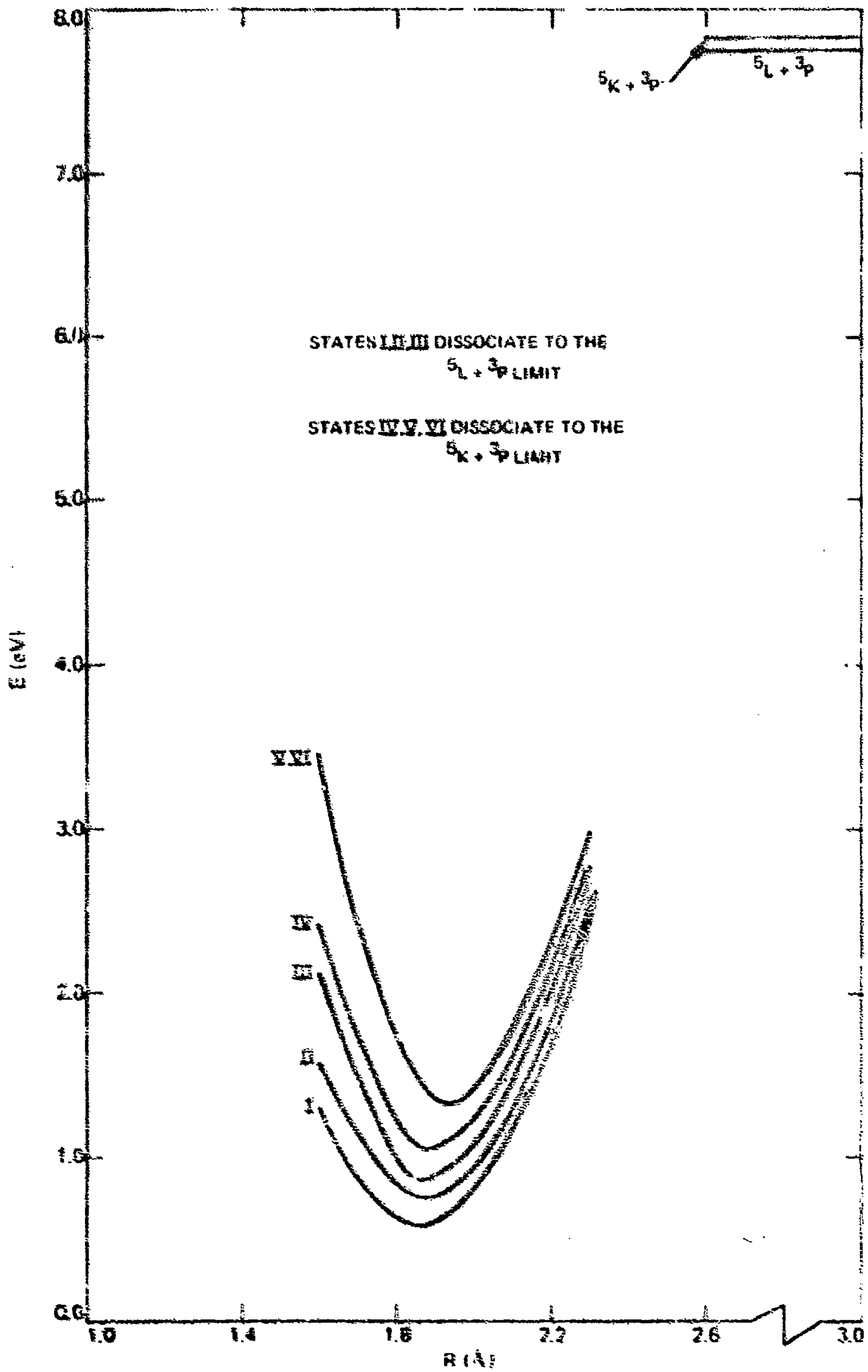


FIGURE 10. THE $^5\Pi$ STATES OF UO

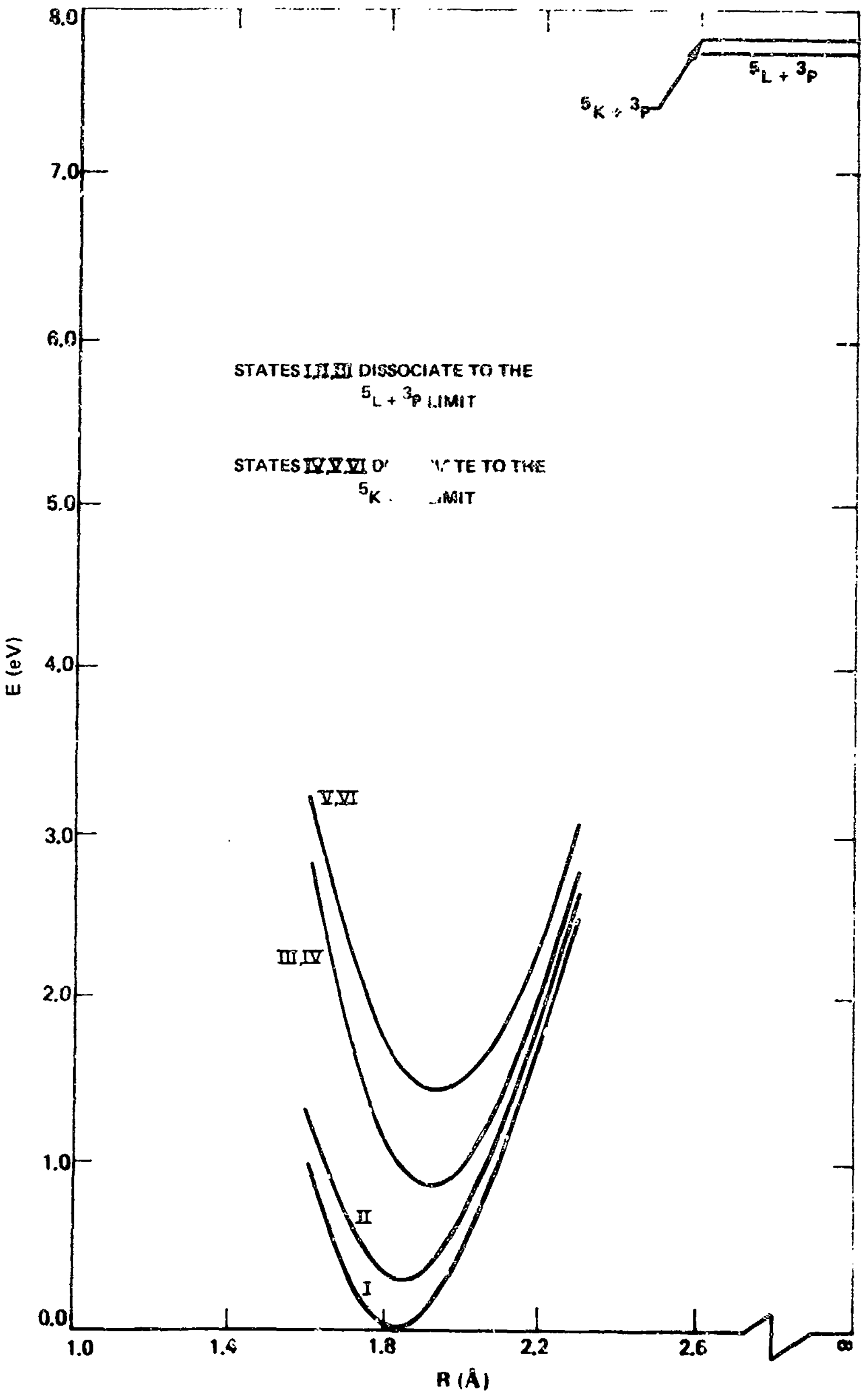


FIGURE 20. THE $^7\Pi$ STATES OF UO

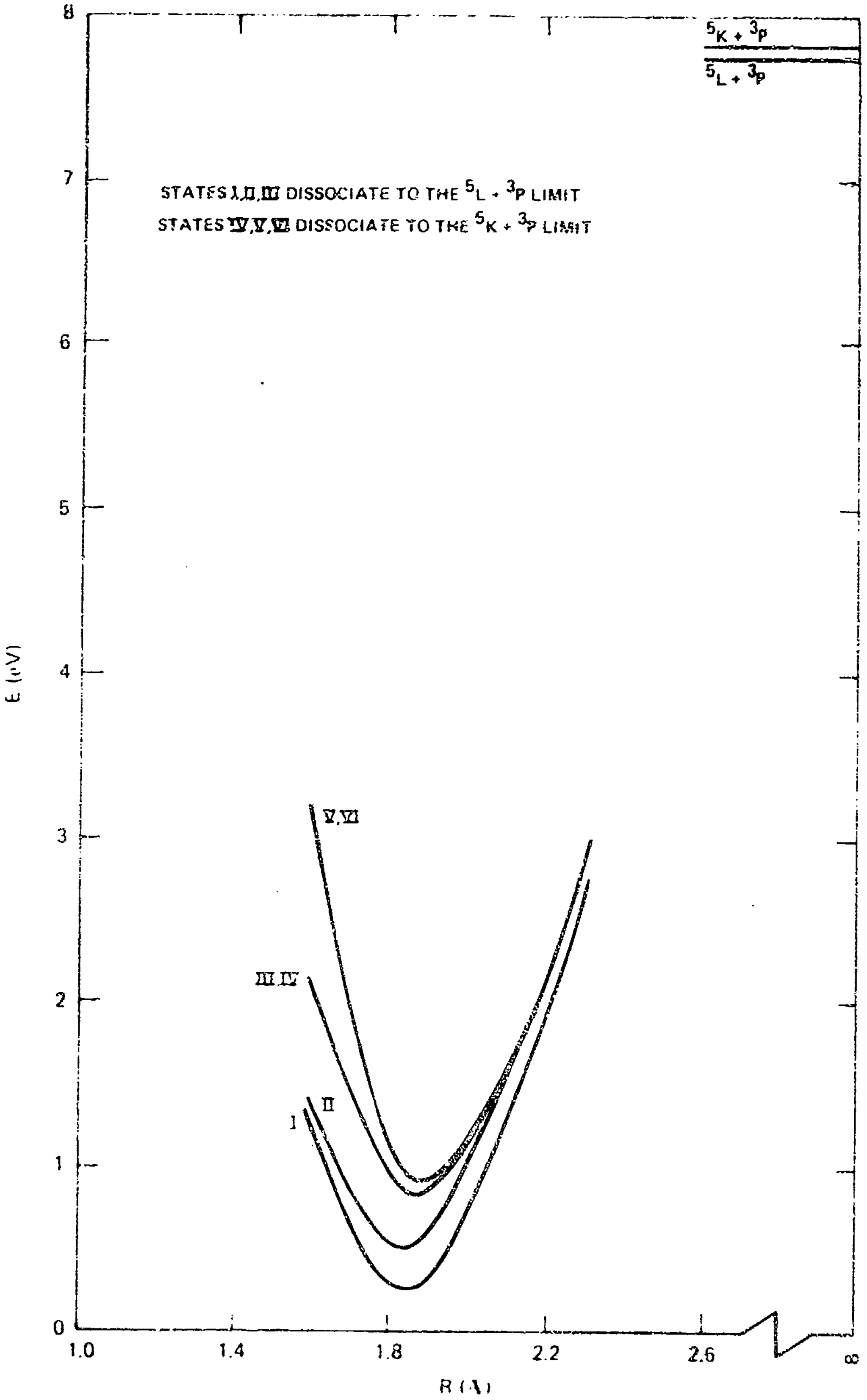


FIGURE 21. THE $^5\Delta$ STATES OF UO

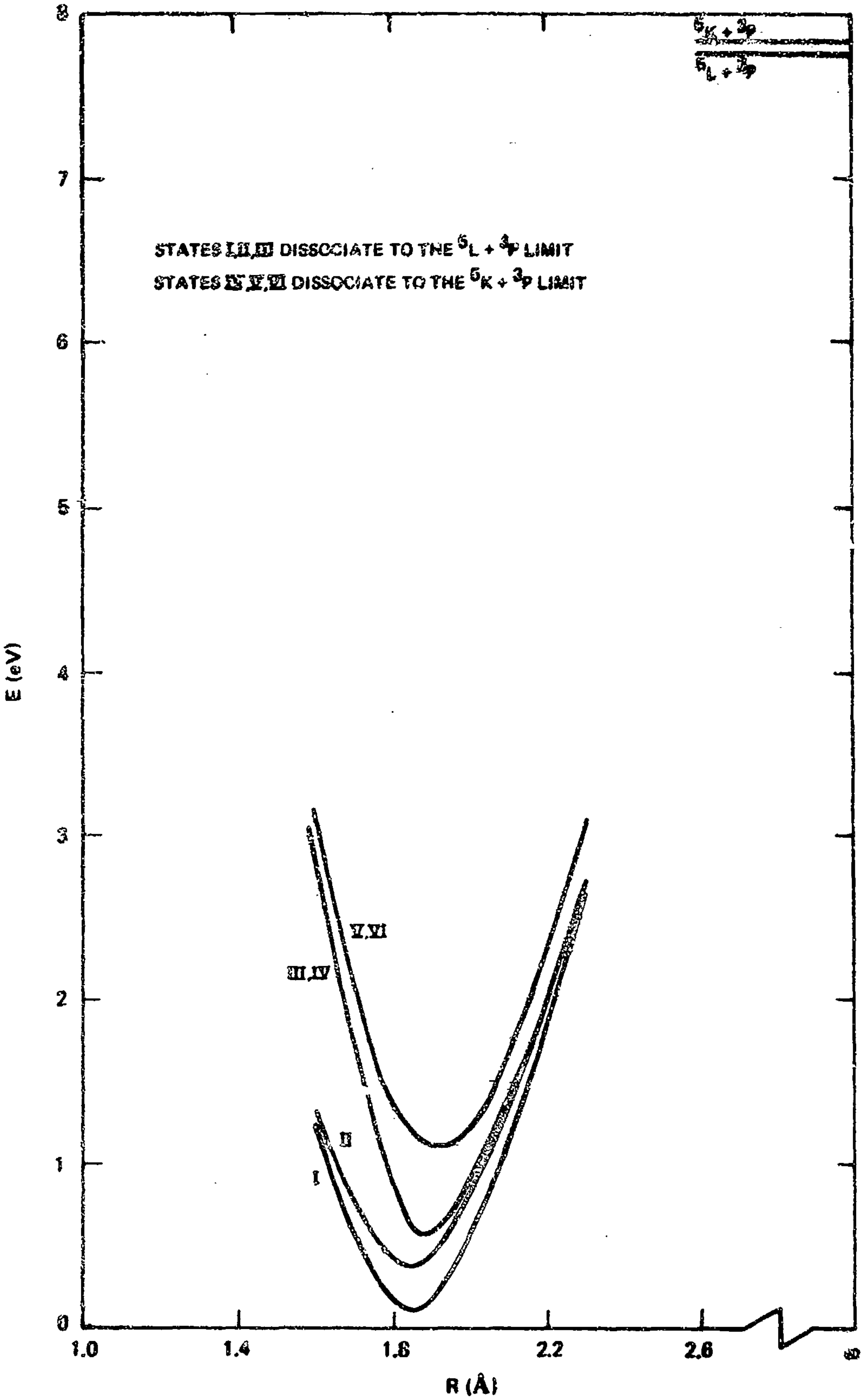


FIGURE 22. THE $^7\Delta$ STATES OF UO

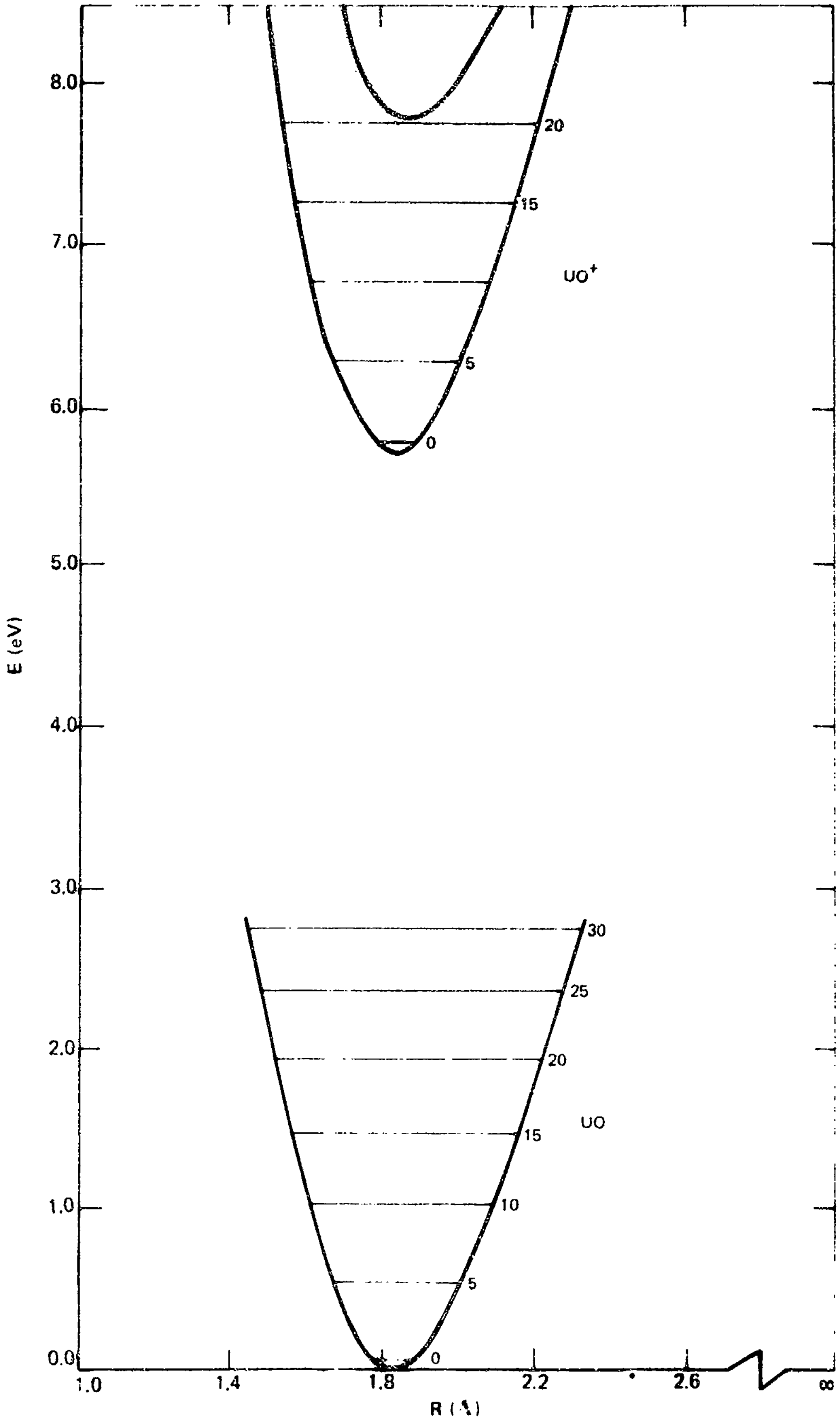


FIGURE 23. RKR POTENTIAL ENERGY CURVES FOR UO AND UO$^+$

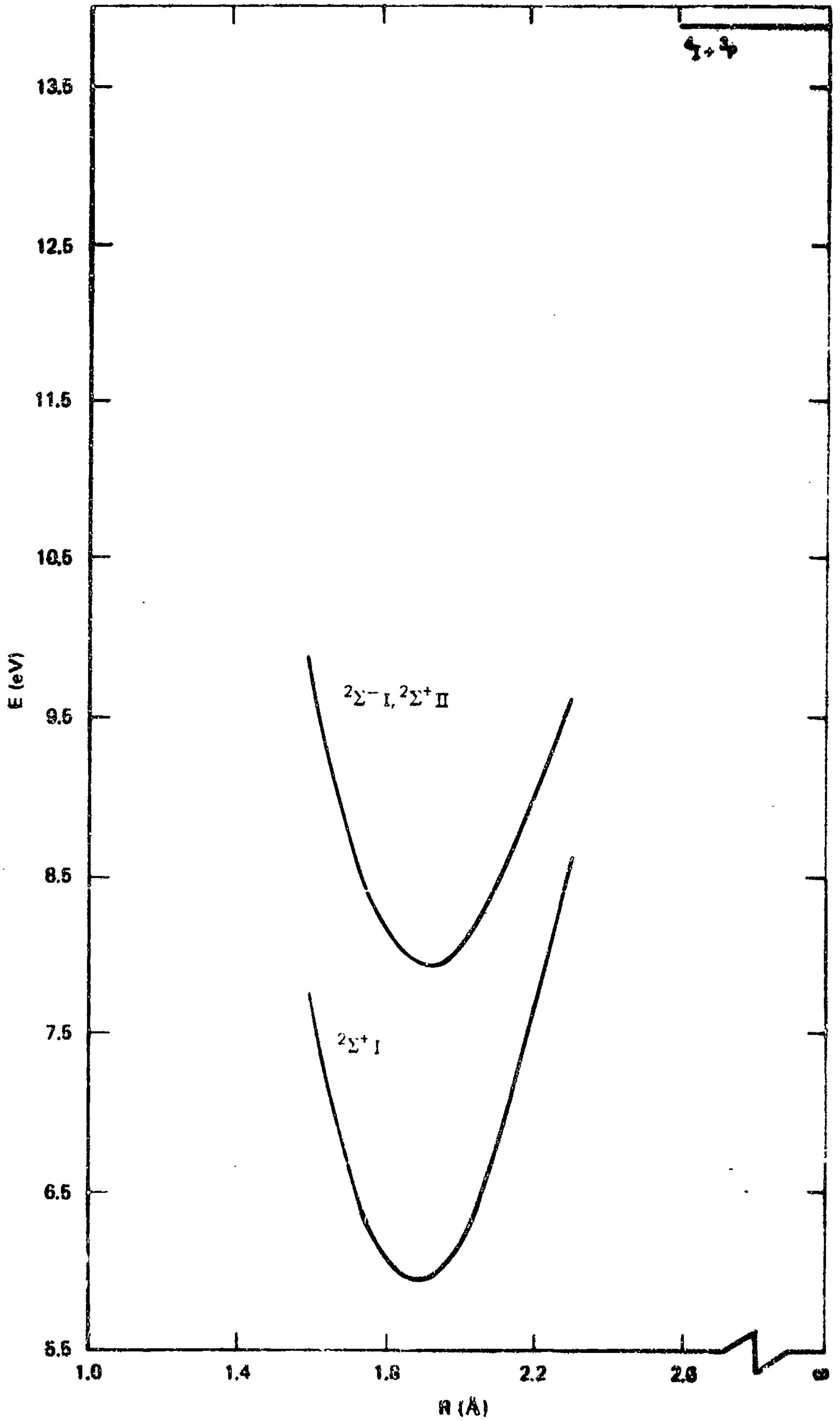


FIGURE 24. THE $^2\Sigma^{+,-}$ STATES OF UO^+

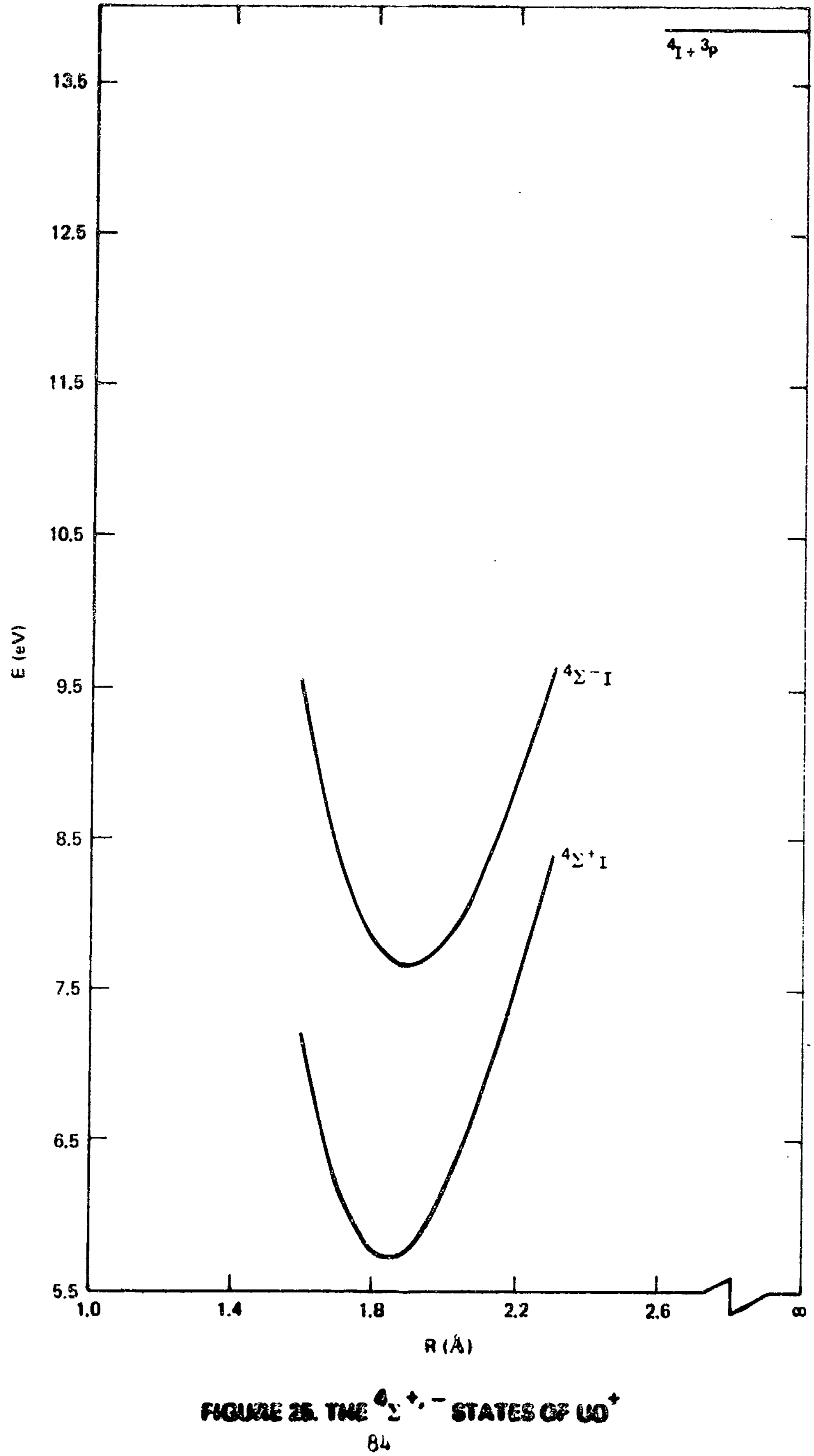


FIGURE 25. THE $^4\Sigma^{+,-}$ STATES OF UO$^+$

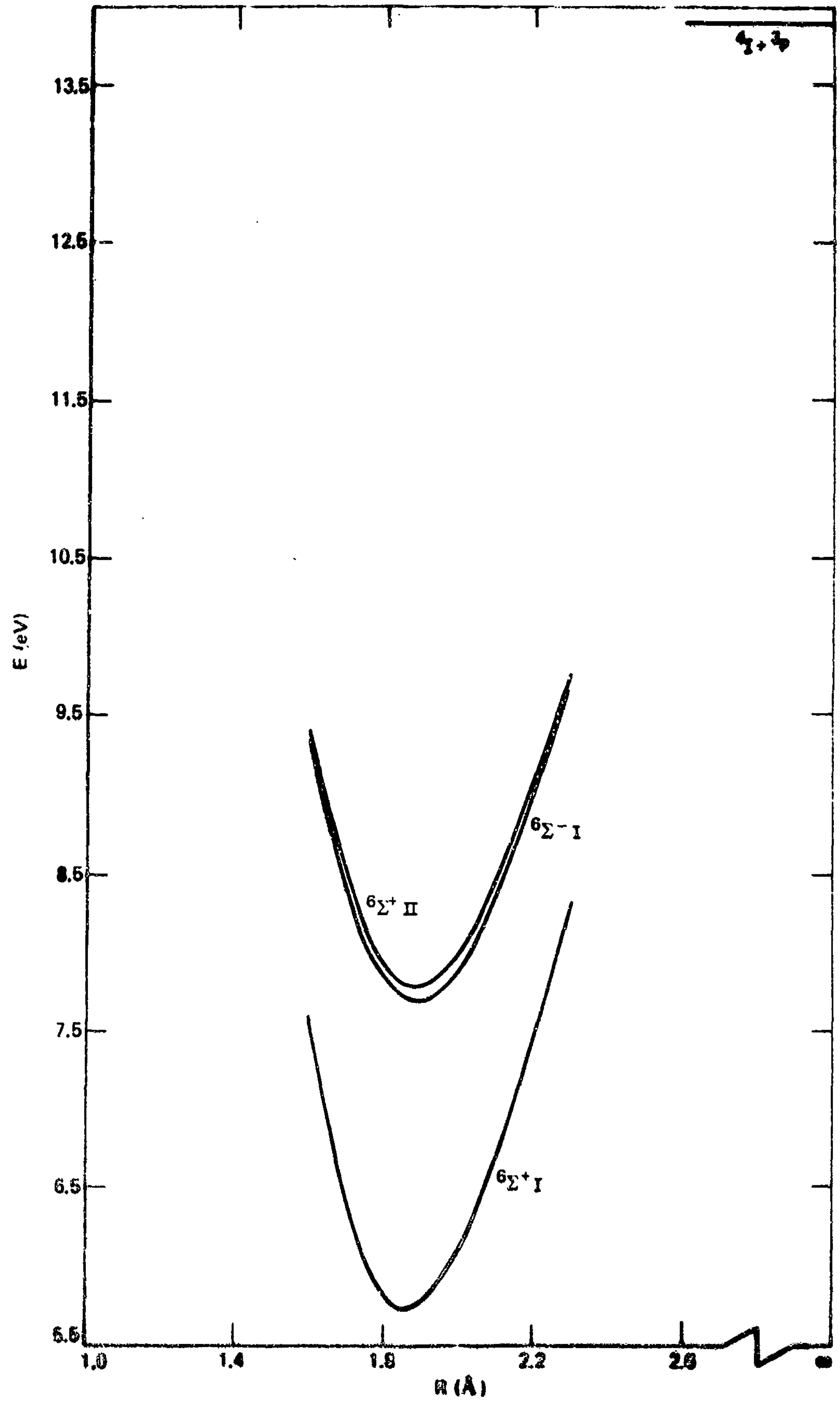


FIGURE 38. THE $^6\Sigma^{+,-}$ STATES OF UO^+

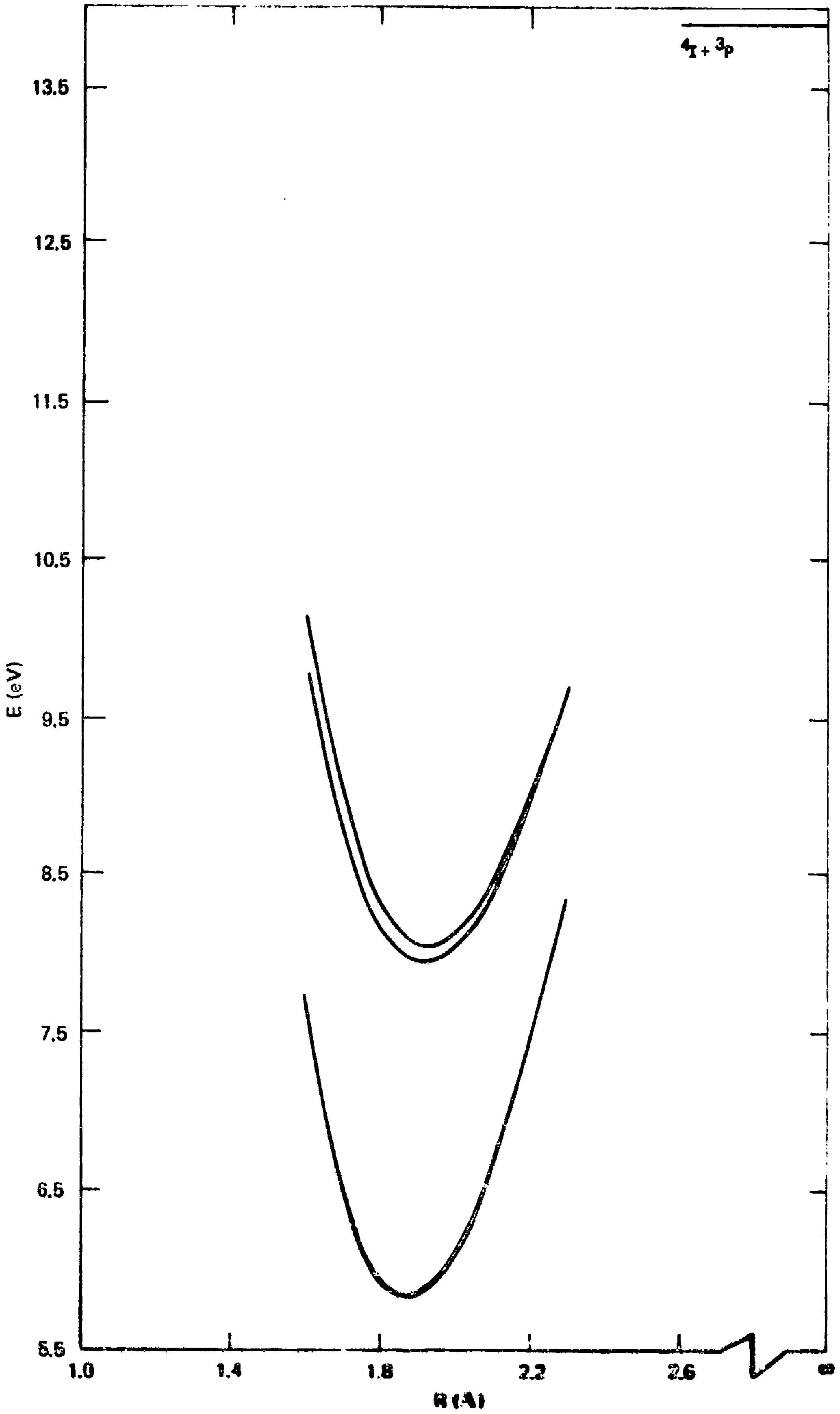


FIGURE 27. THE $^2\Pi$ STATES OF UO^+

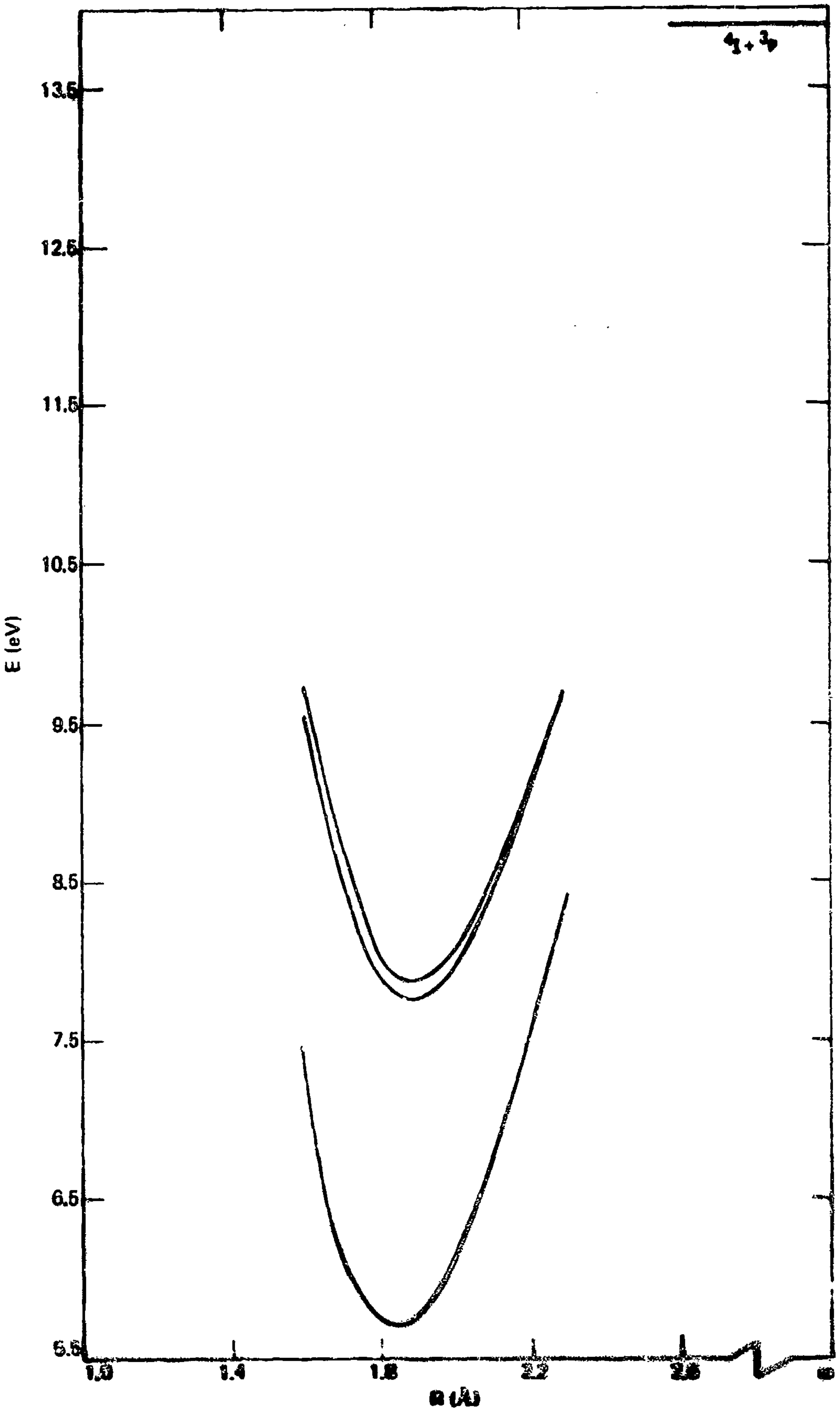


FIGURE 28. THE $^4\Pi$ STATES OF CO$^+$

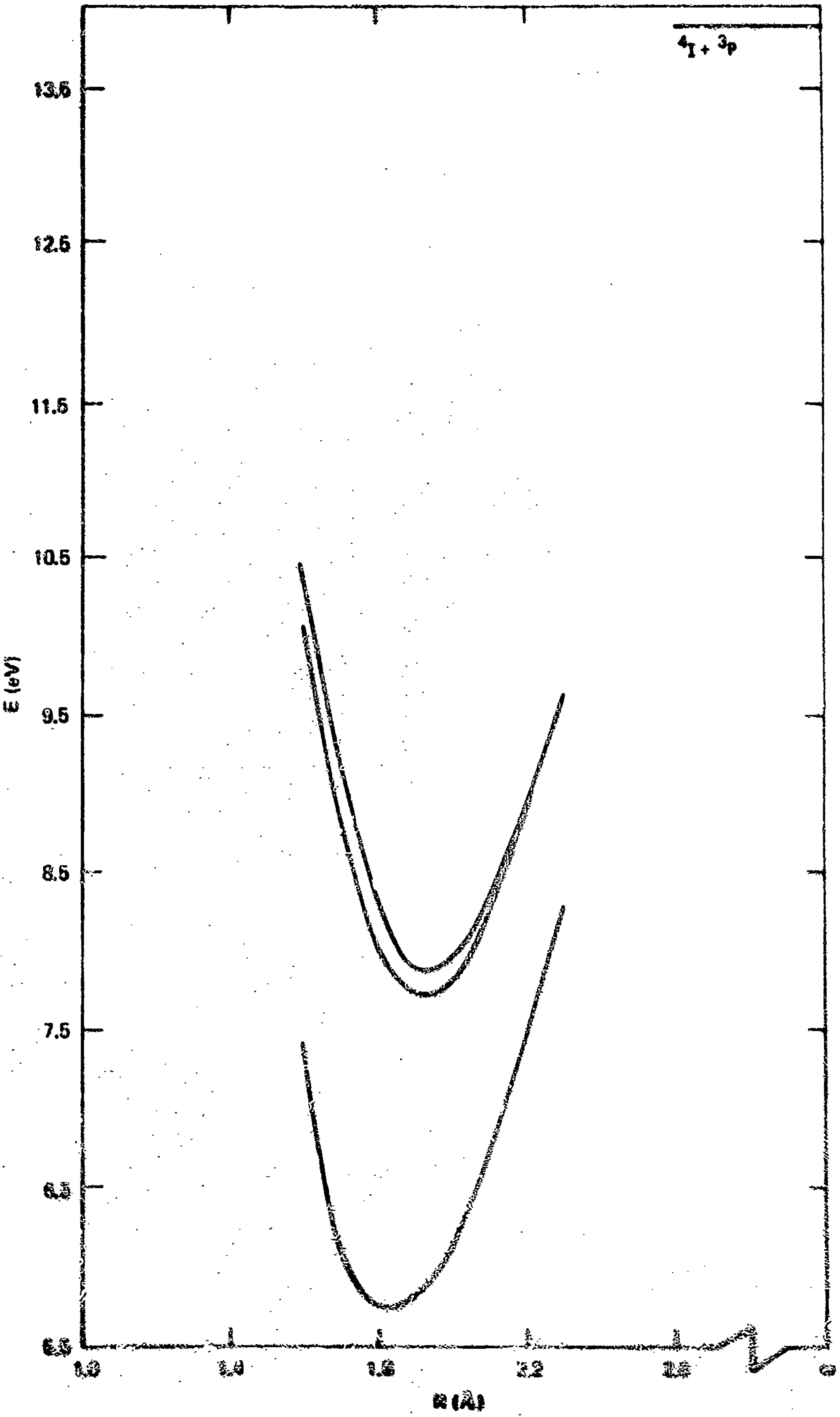
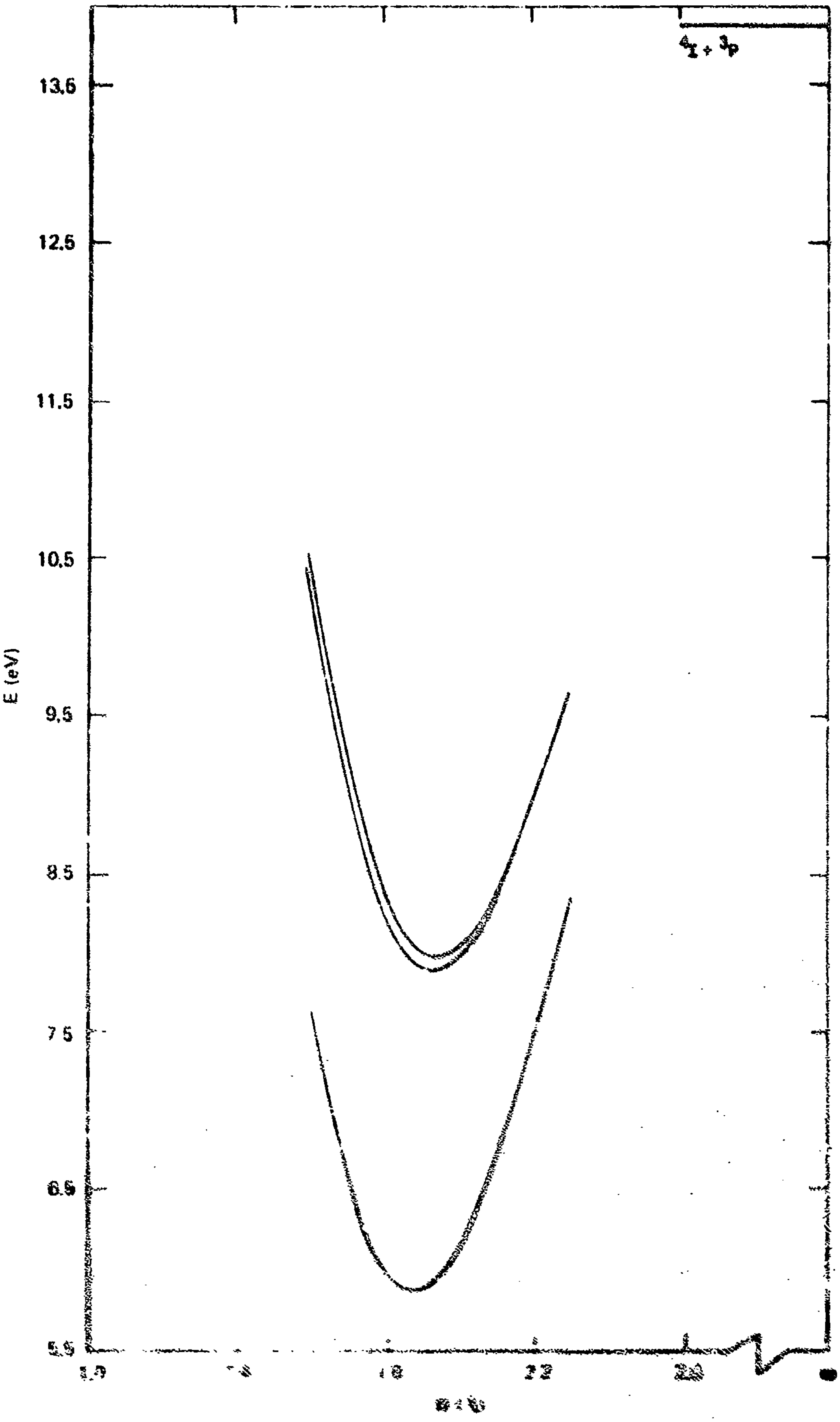


FIGURE 22. THE $^4\Pi$ STATES OF UO$^+$

$^4I + ^3P$
13.6
12.5
11.5
10.5
E (eV)
9.5
8.5
7.5
6.5
5.5
1.0
2.2

[illegible]

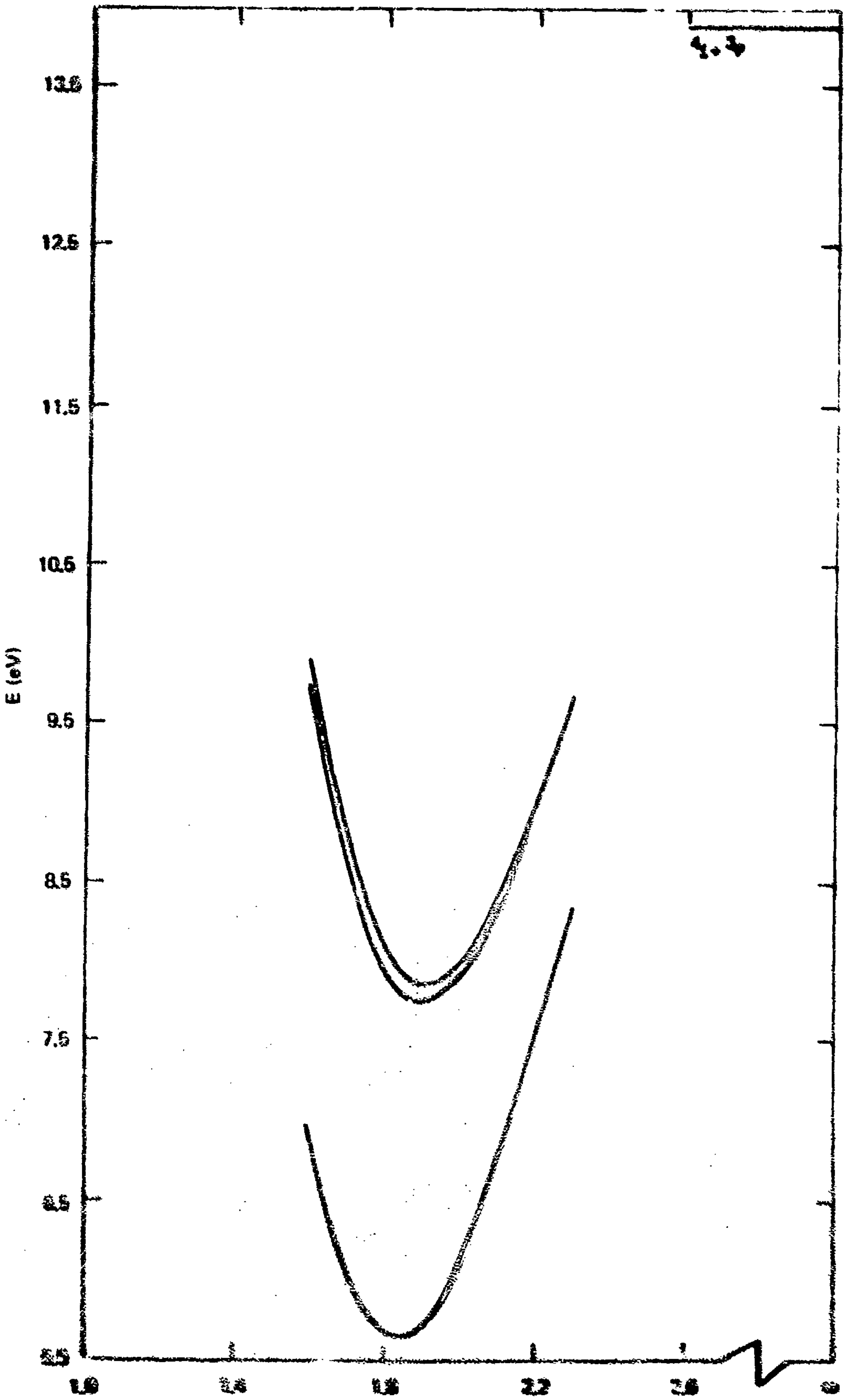


FIGURE 32. THE $^4\Sigma$ STATES OF UO$^+$

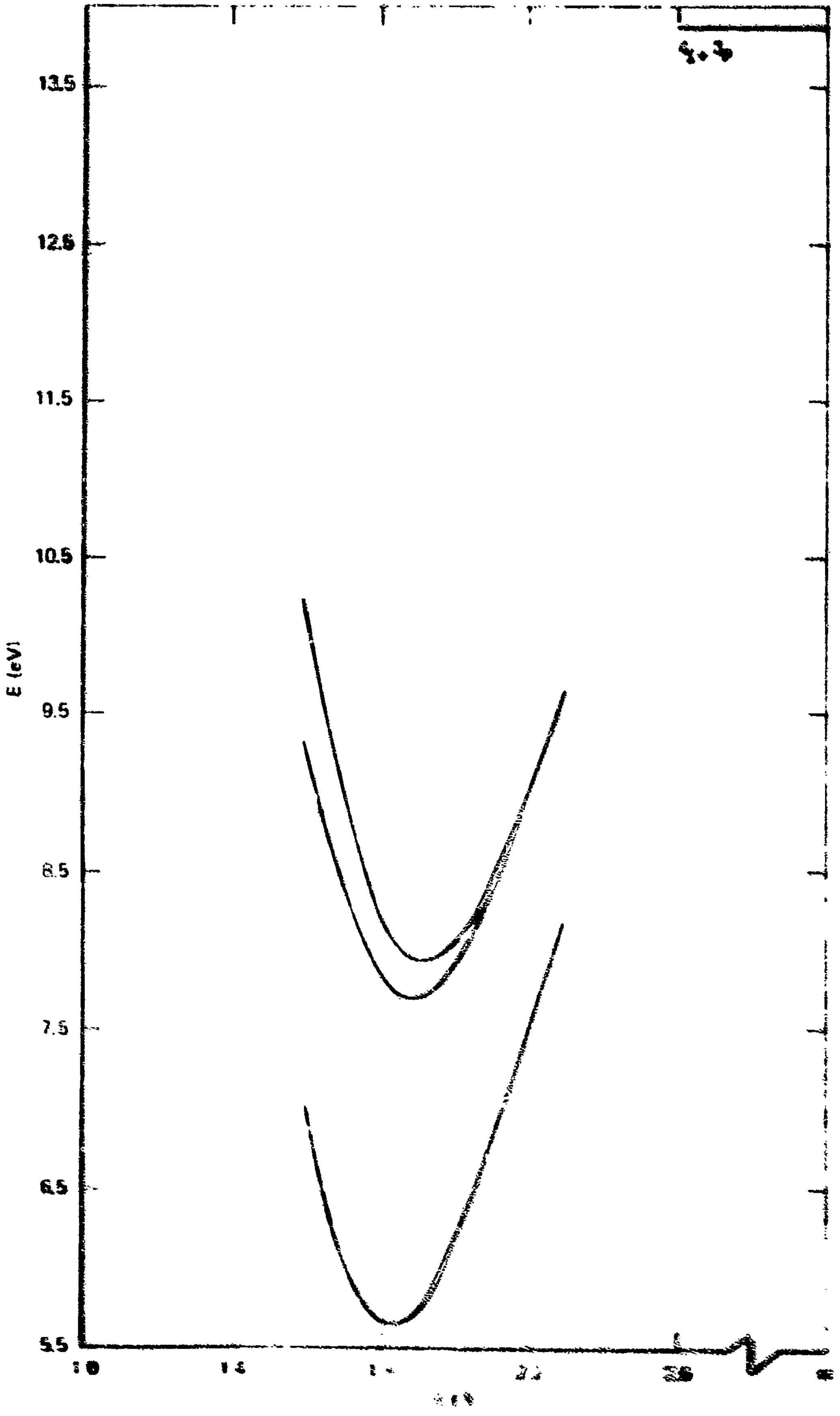


FIGURE 12 THE $^6\Sigma$ STATES OF CO$^+$

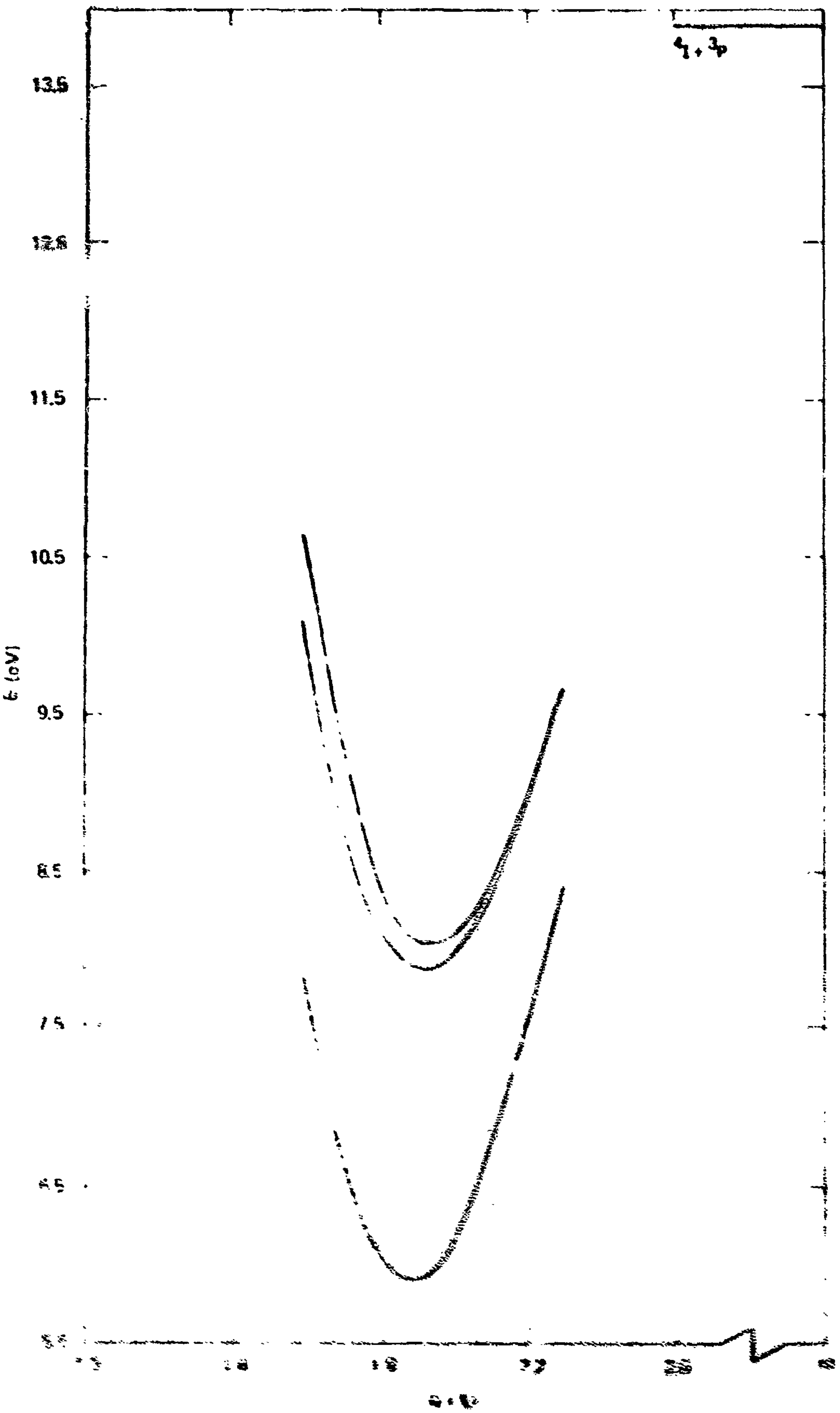


FIGURE 33 THE $^2\Phi$ STATES OF CO$^+$

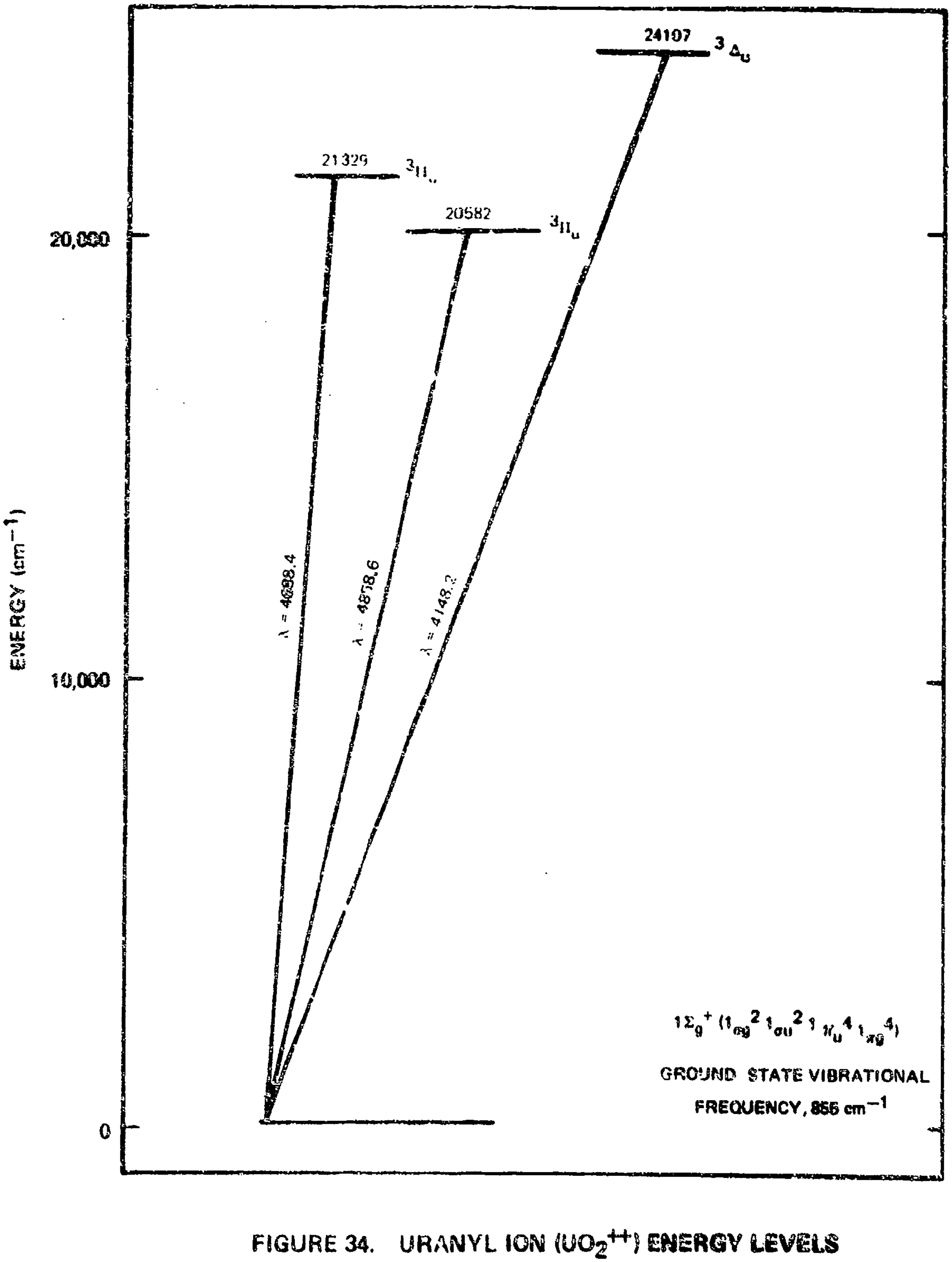


FIGURE 34. URANYL ION (UO_2^{++}) ENERGY LEVELS

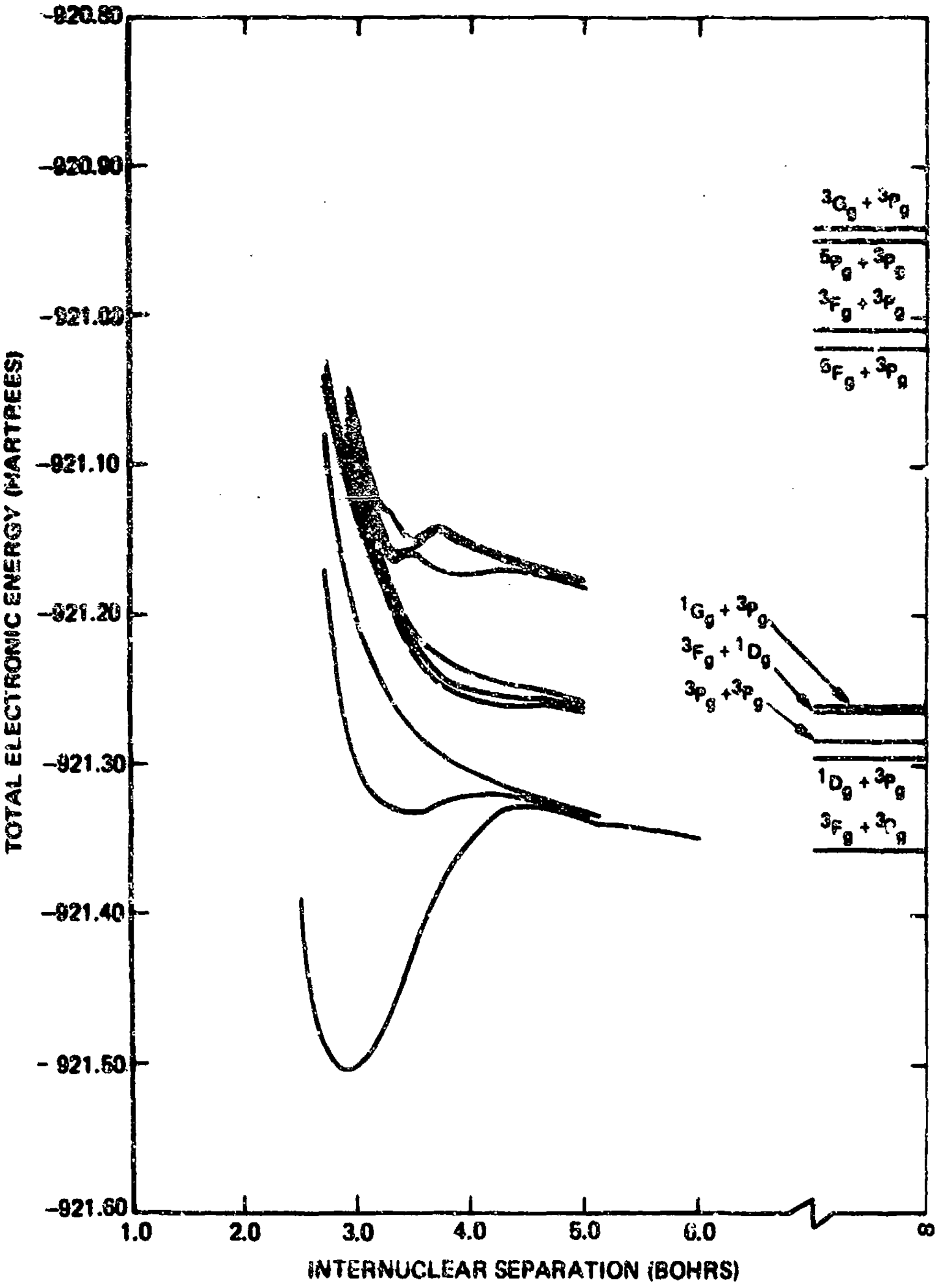


FIGURE 35. THE CALCULATED $^1\Sigma^+$, – STATES OF TiO

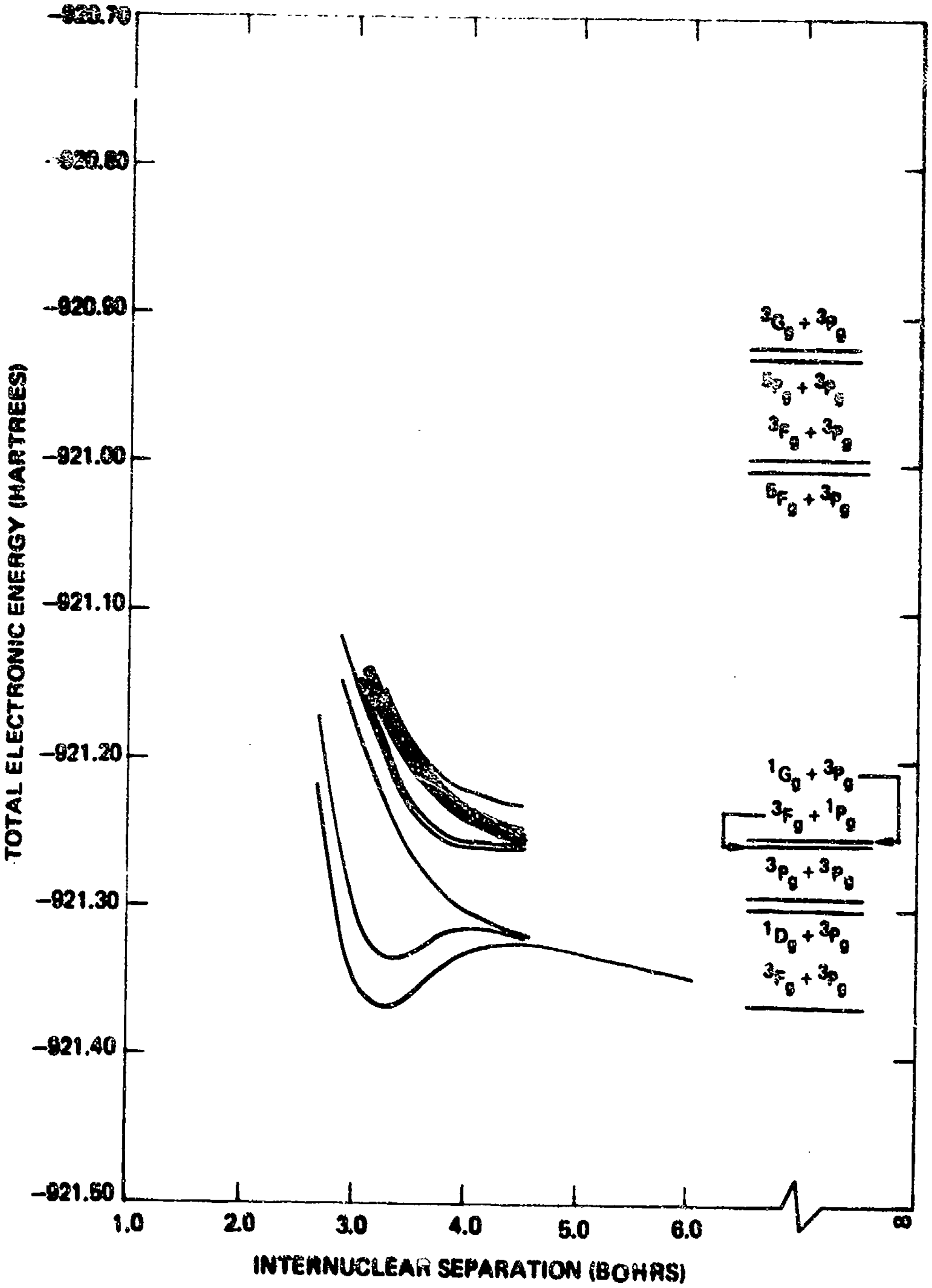


Figure 38. The calculated $^3\Sigma^{+,-}$ states of TiO

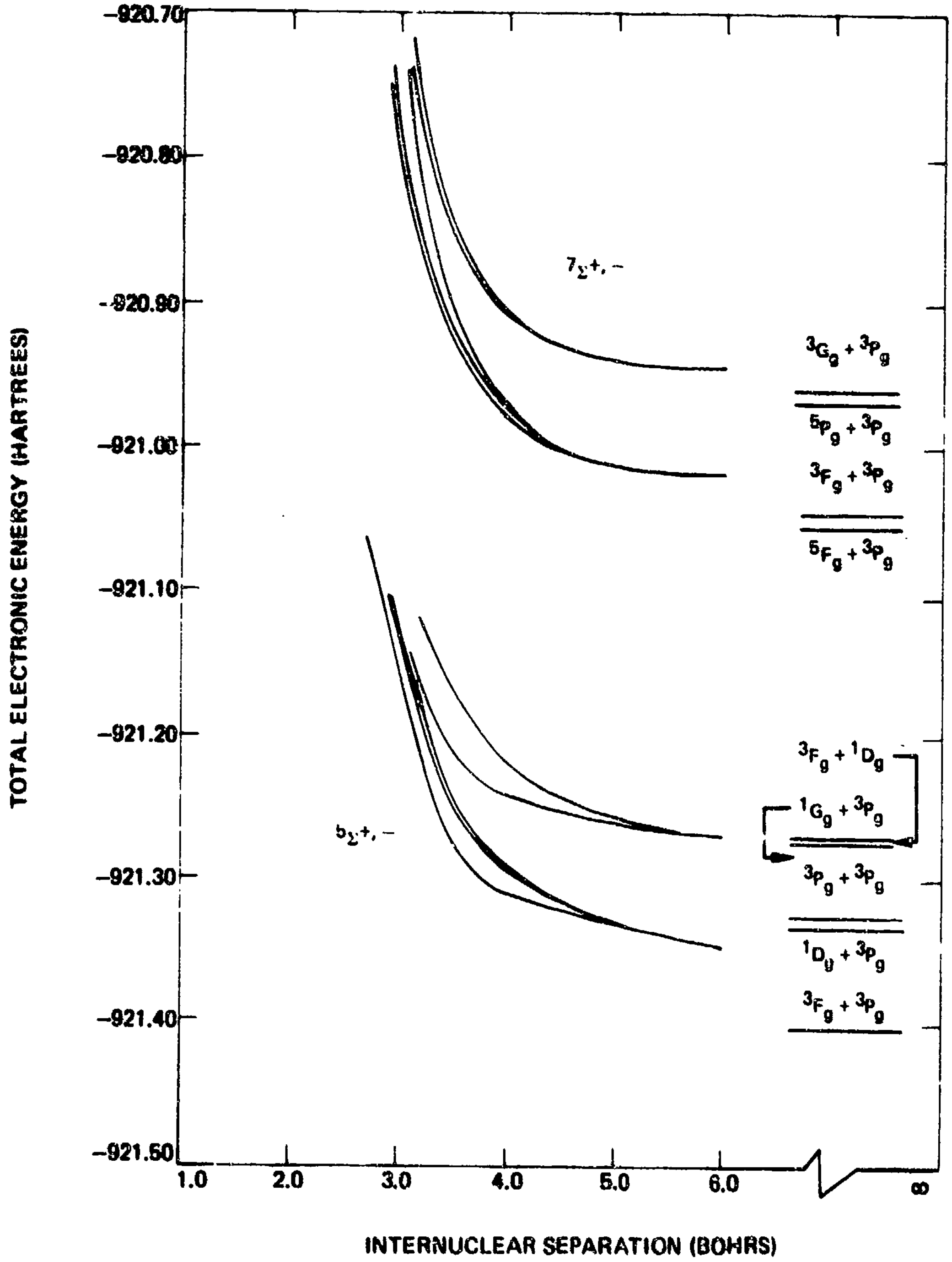


Figure 37. The calculated $^5\Sigma^{+,-}$ and $^7\Sigma^{+,-}$ states of TiO

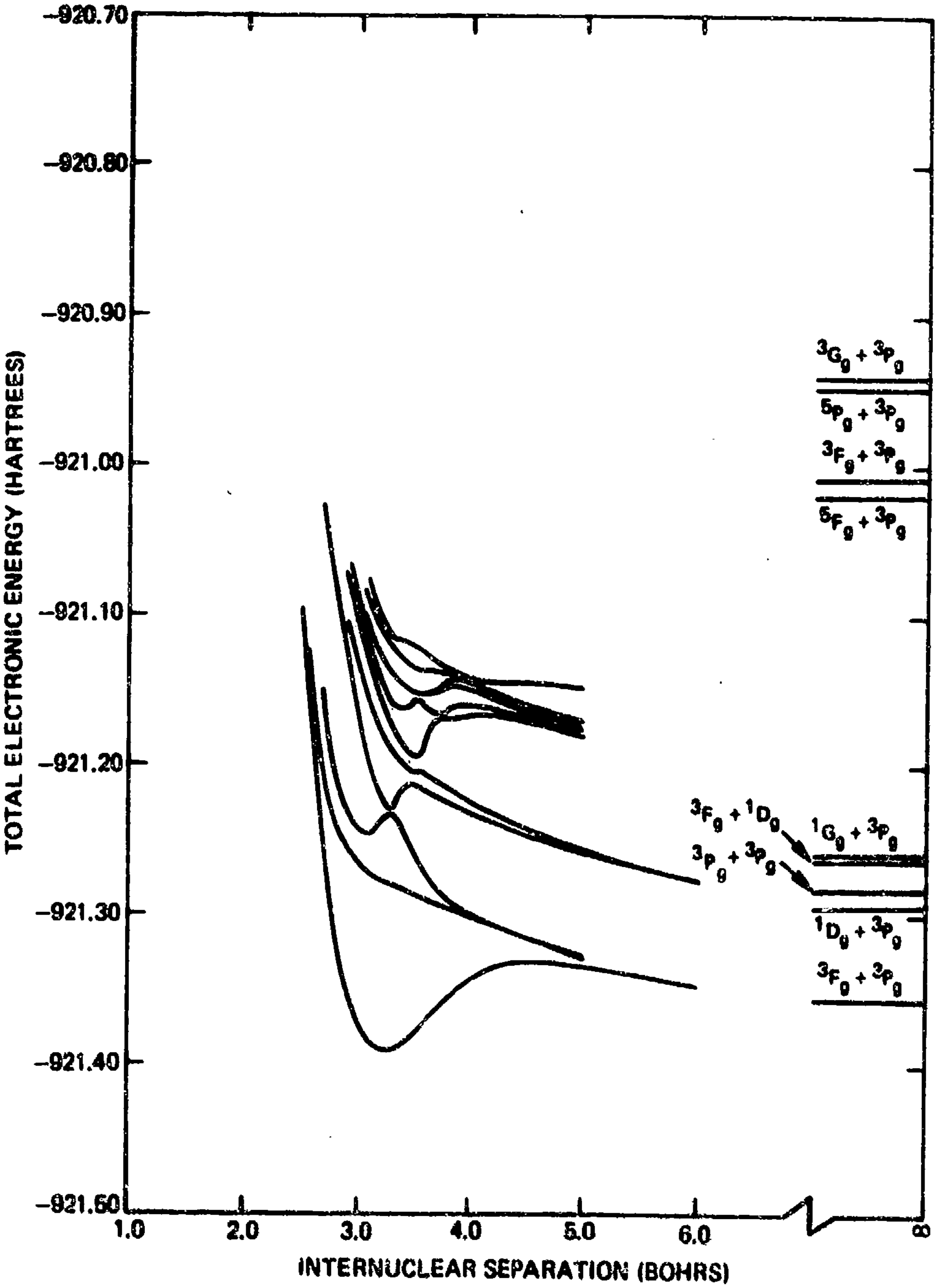


FIGURE 38. THE CALCULATED $^1\Pi$ STATES OF TiO

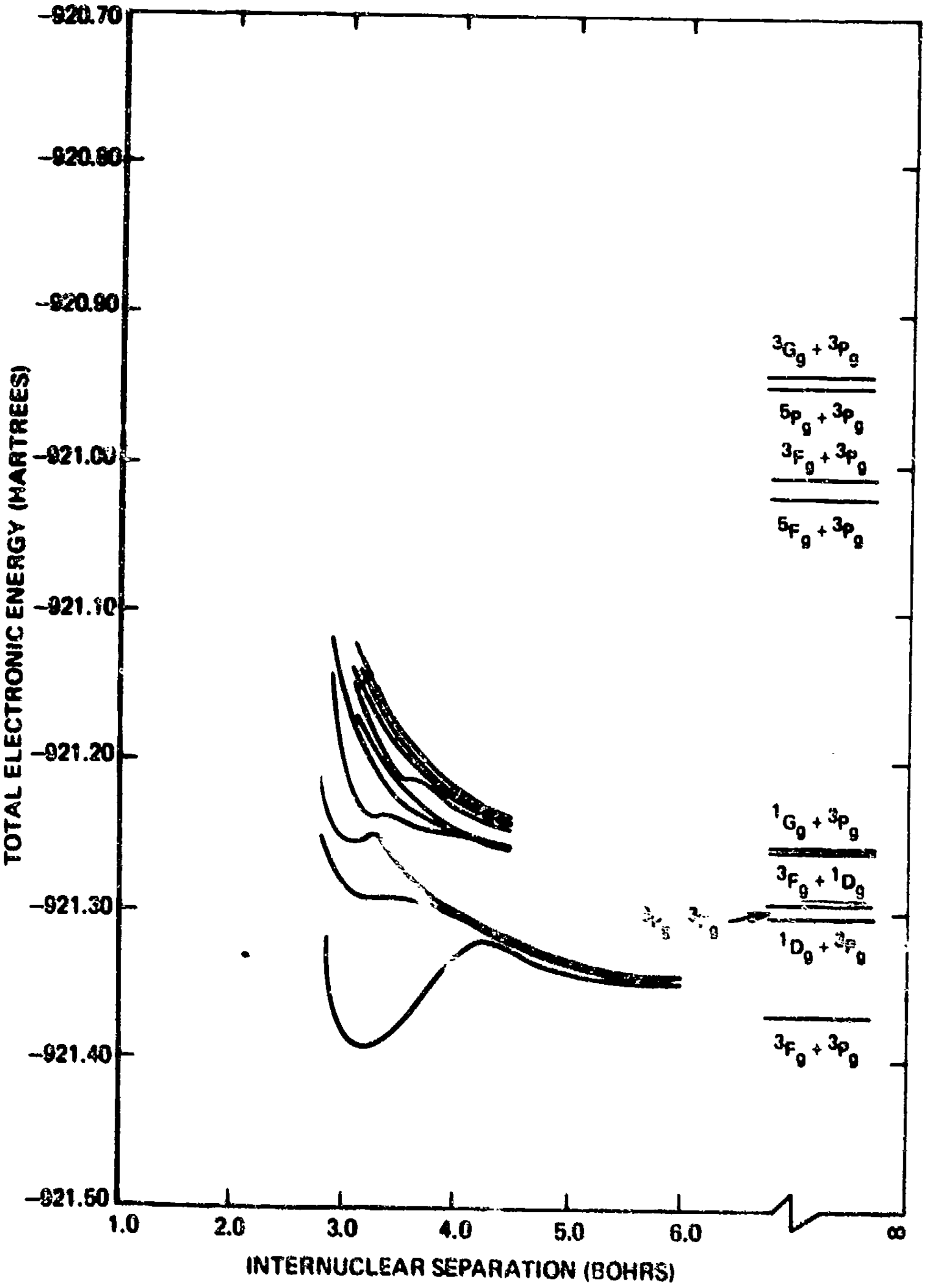


FIGURE 38. THE CALCULATED $^3\Pi$ STATES OF TiO

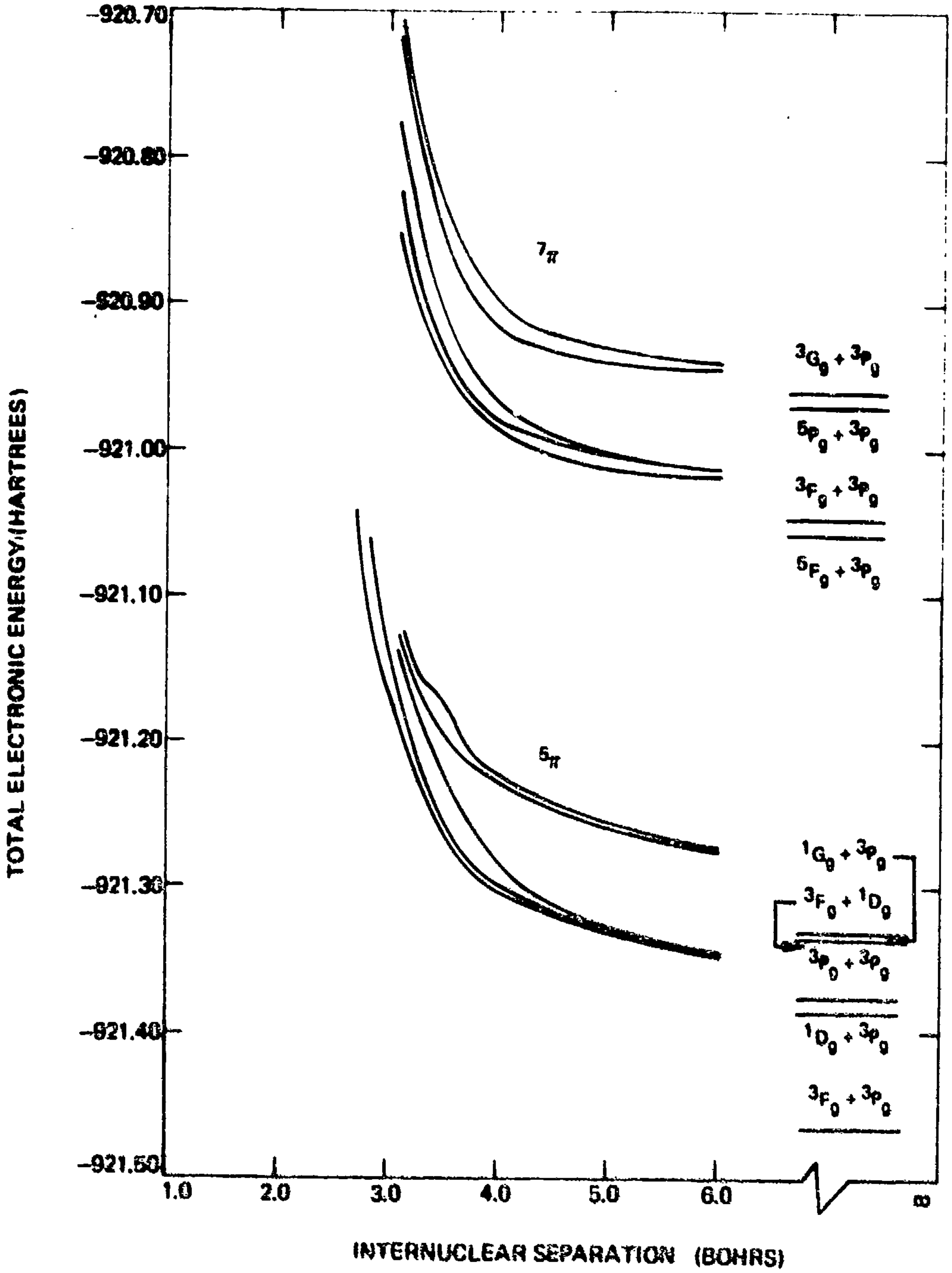


Figure 40. The calculated $^5\Pi$ and $^7\Pi$ states of TiO

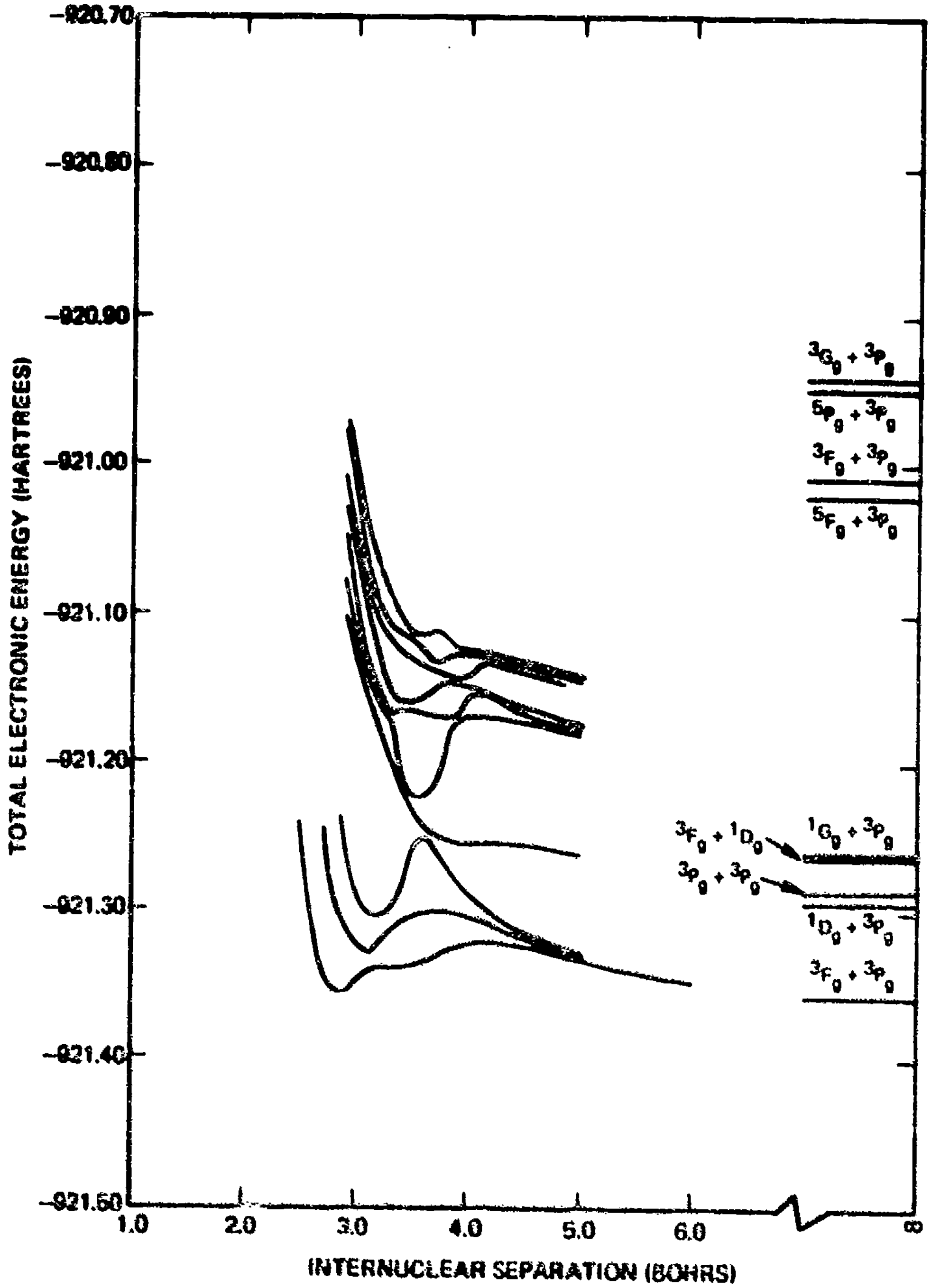


FIGURE 41. THE CALCULATED $^1\Delta$ STATES OF TiO

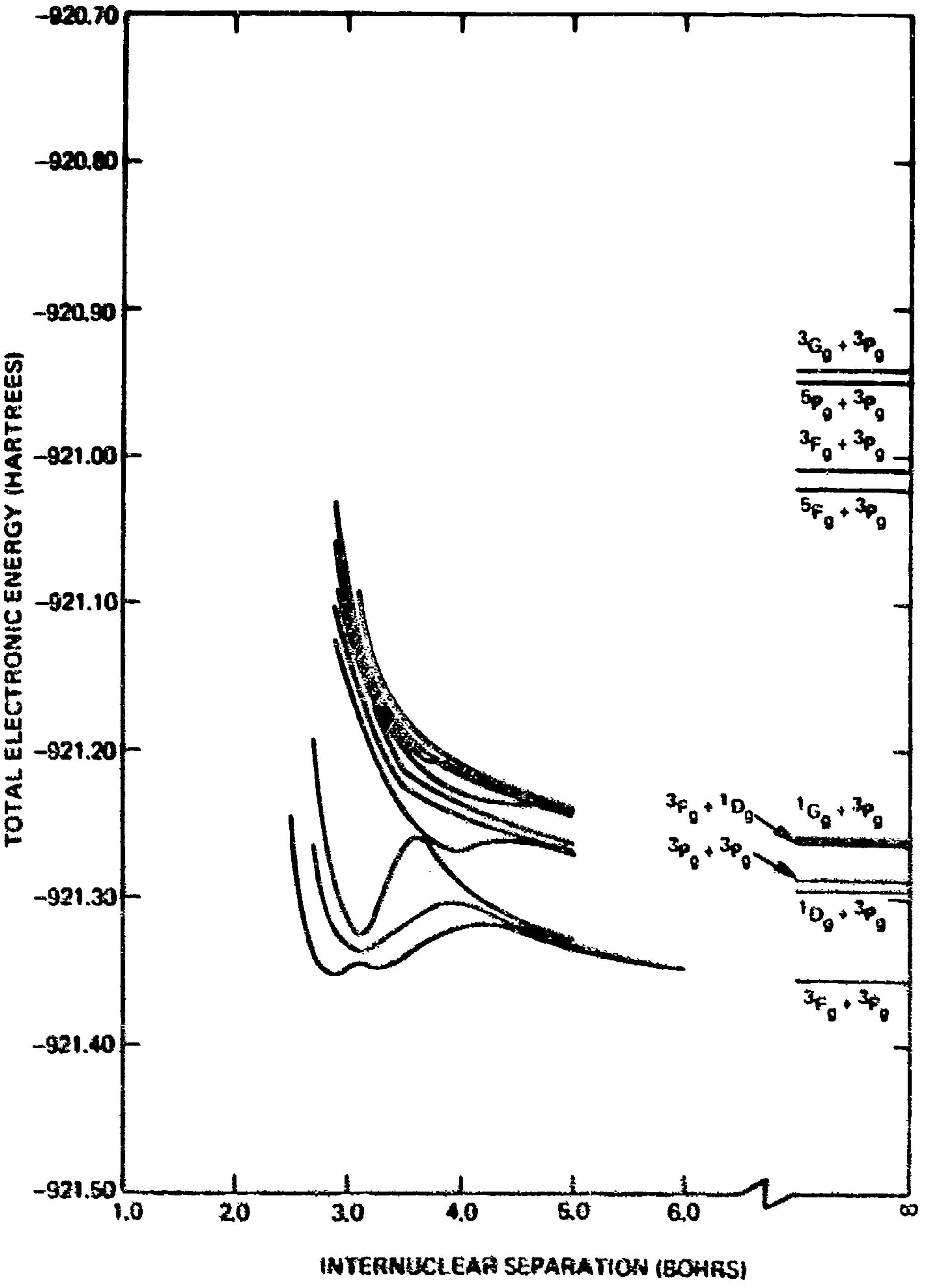


FIGURE 42. THE CALCULATED $^3\Delta$ STATES OF TiO

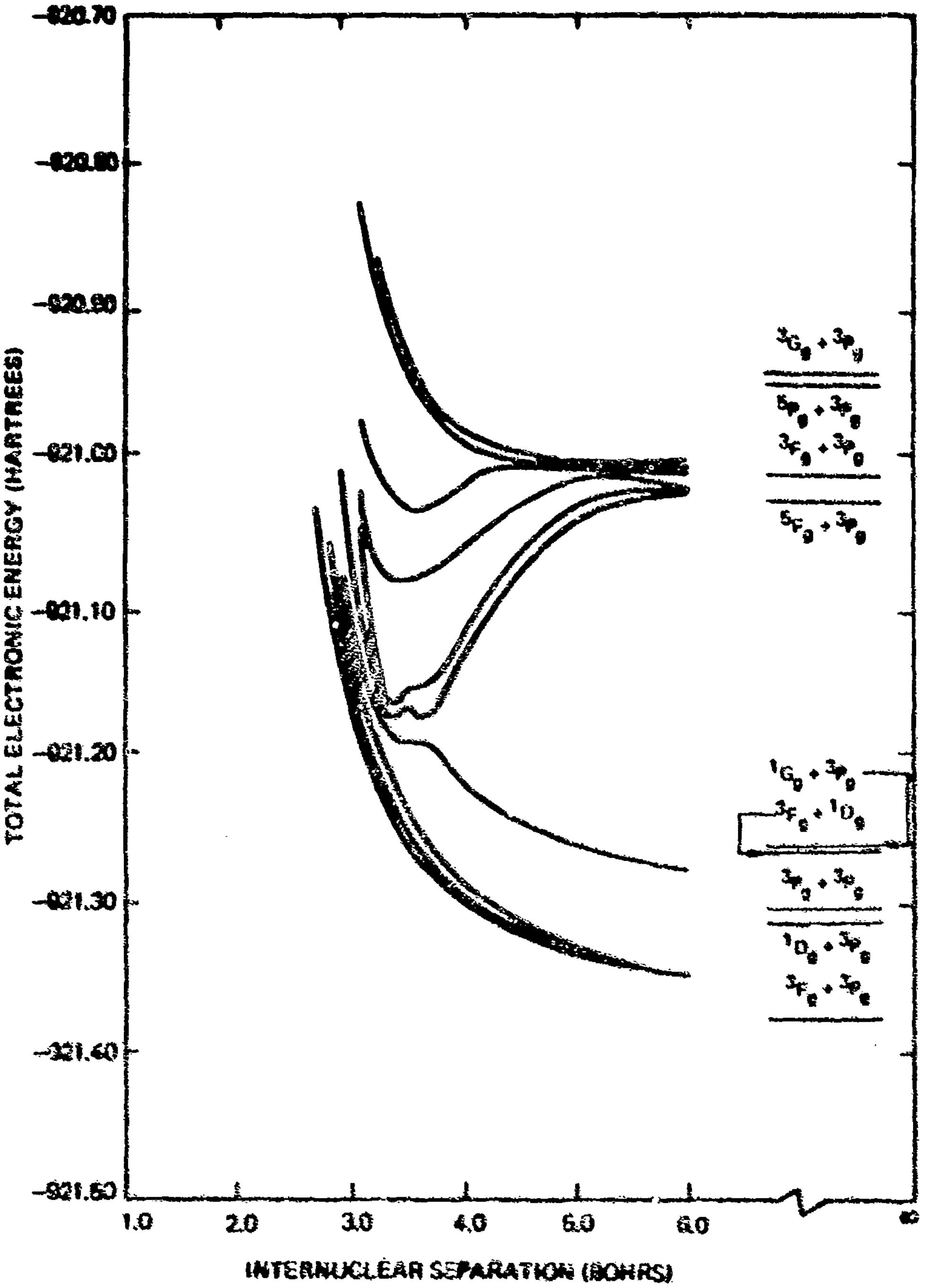


FIGURE 43. THE CALCULATED $^5\Delta$ STATES OF TiO

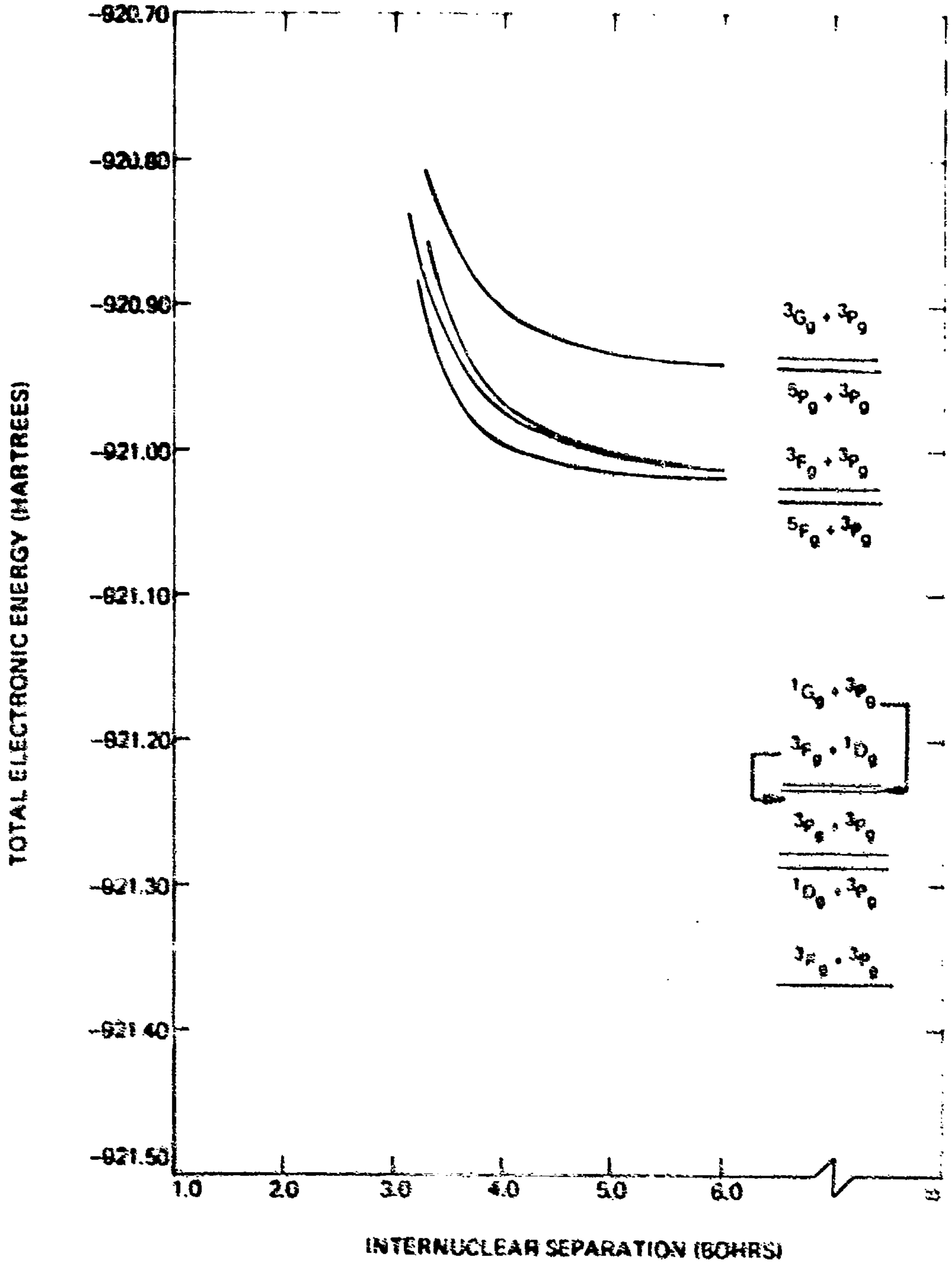


Figure 44. The calculated $^7\Delta$ states of TiO

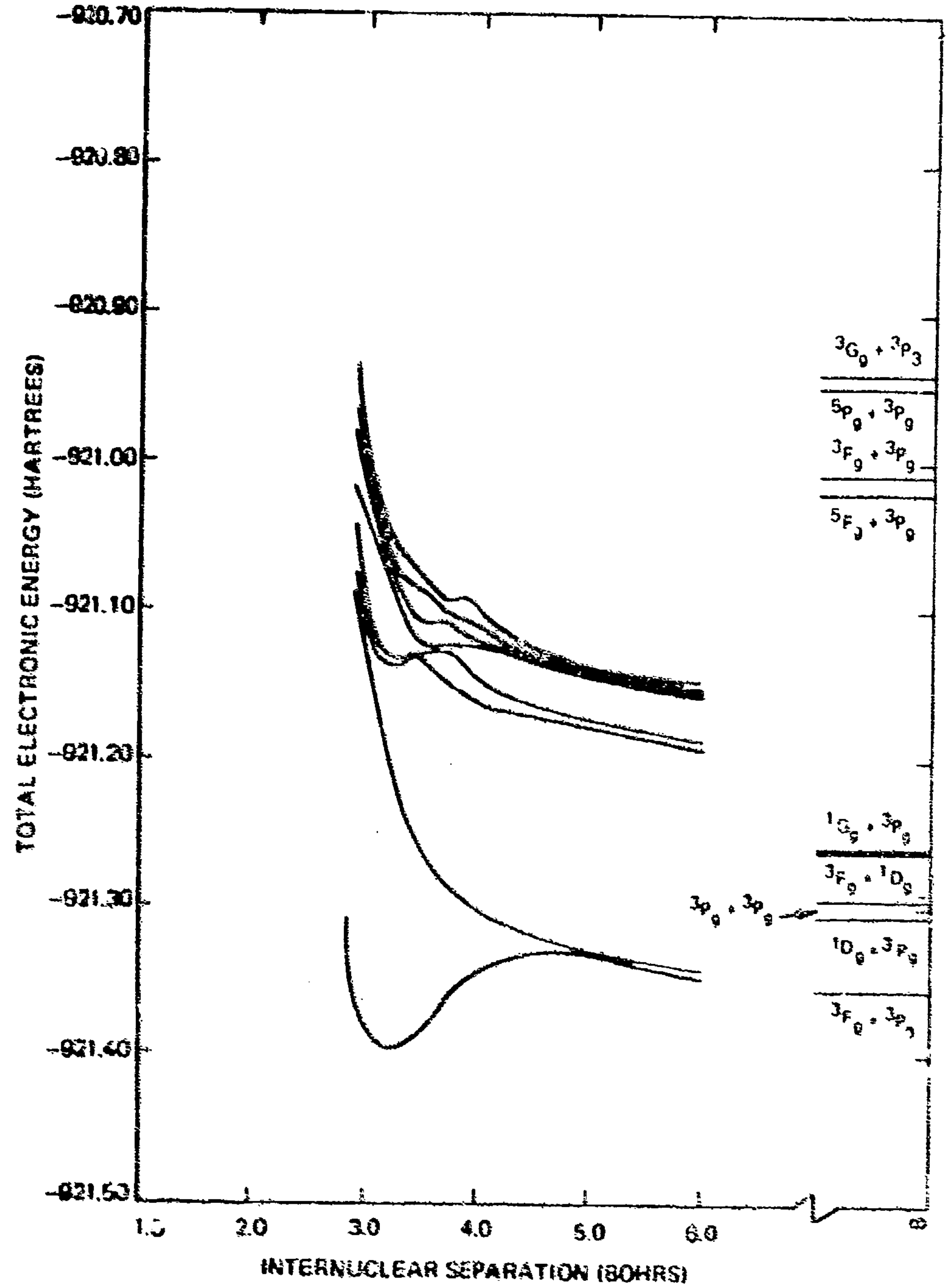


FIGURE 46. THE CALCULATED $^1\Phi$ STATES OF TiO

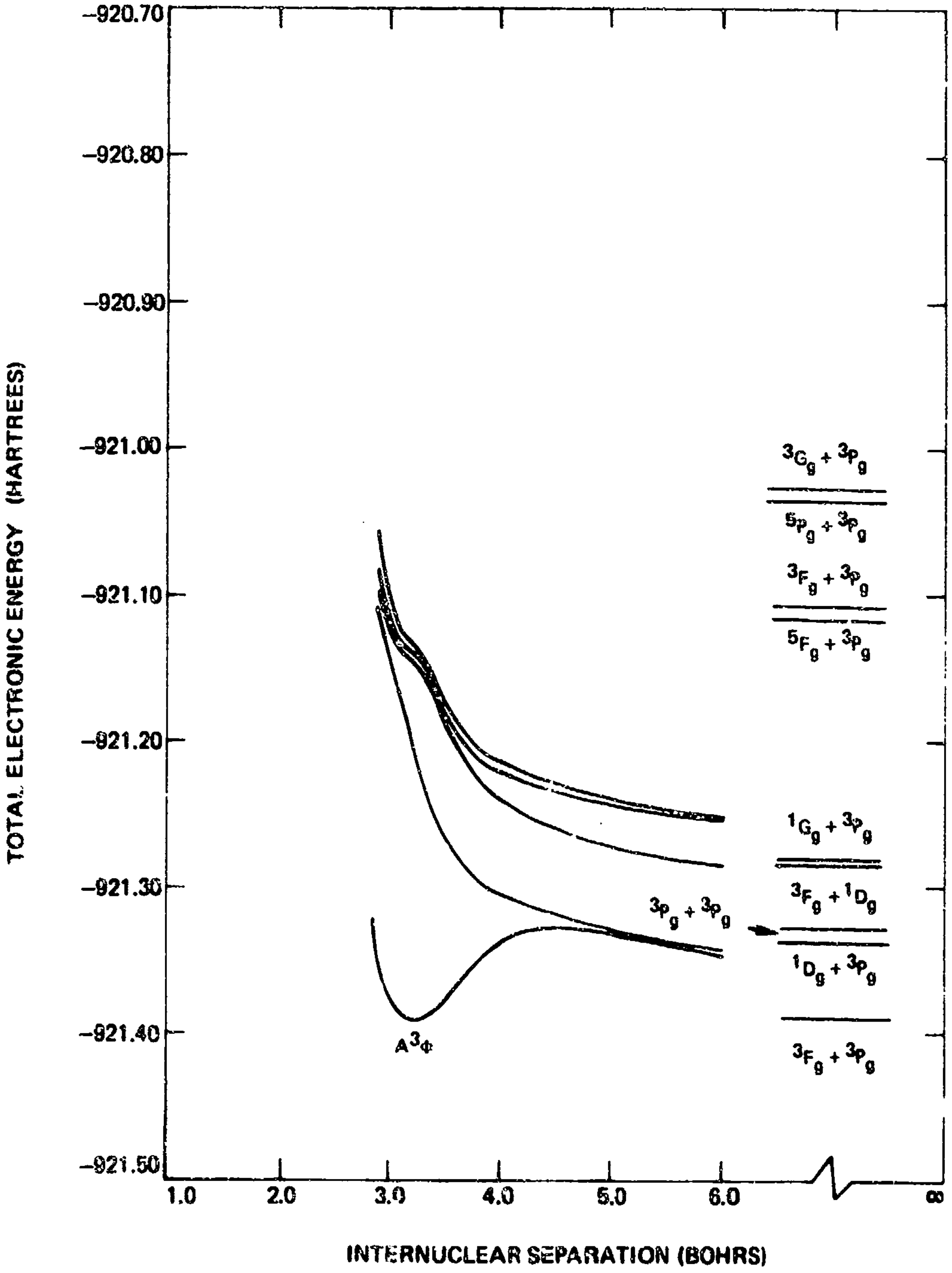


Figure 40. The calculated $^3\Phi$ states of TiO

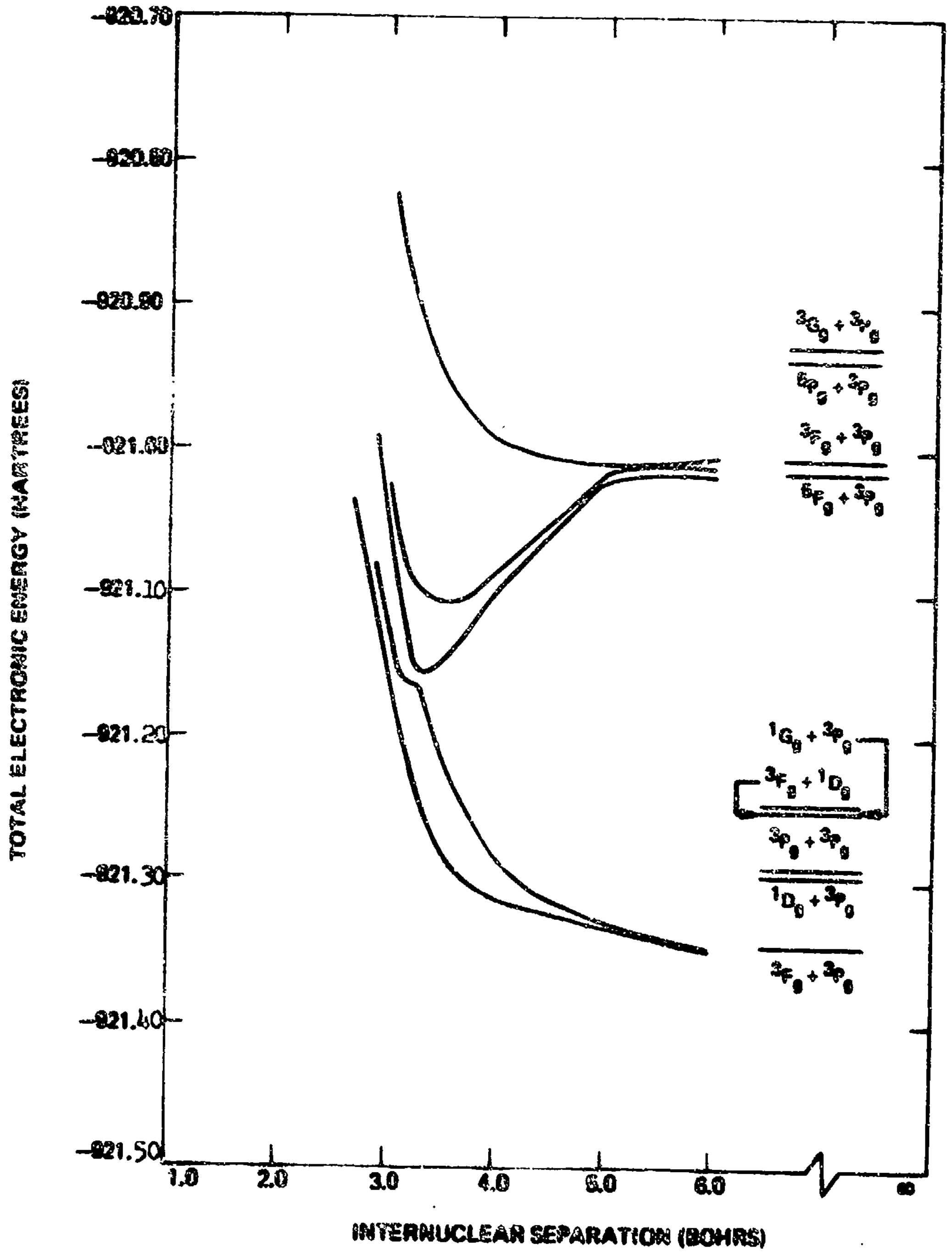


Figure 47. The calculated $^5\Phi$ states of TiO

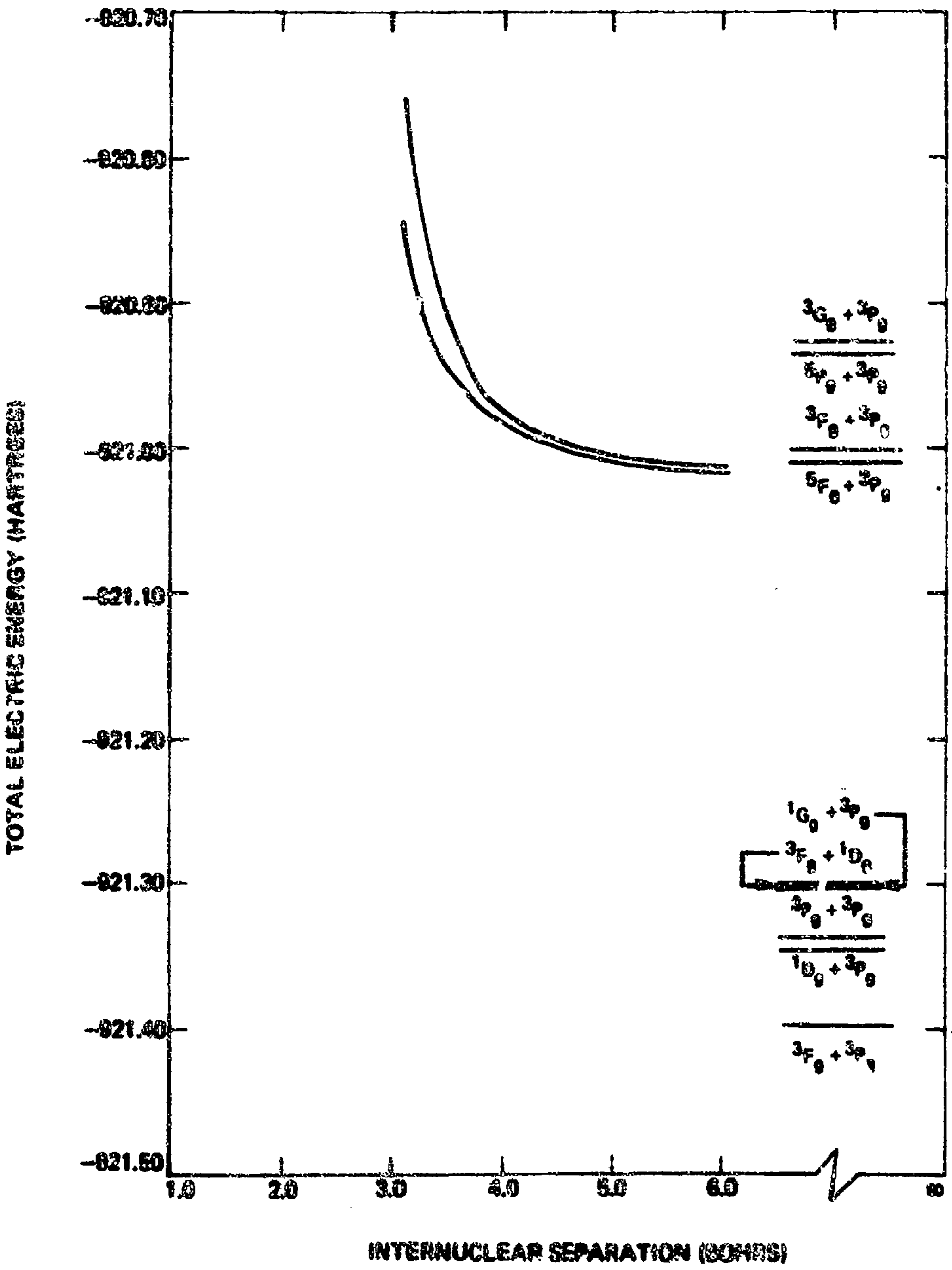


Figure 48. The calculated $^7\Phi$ states of TiO

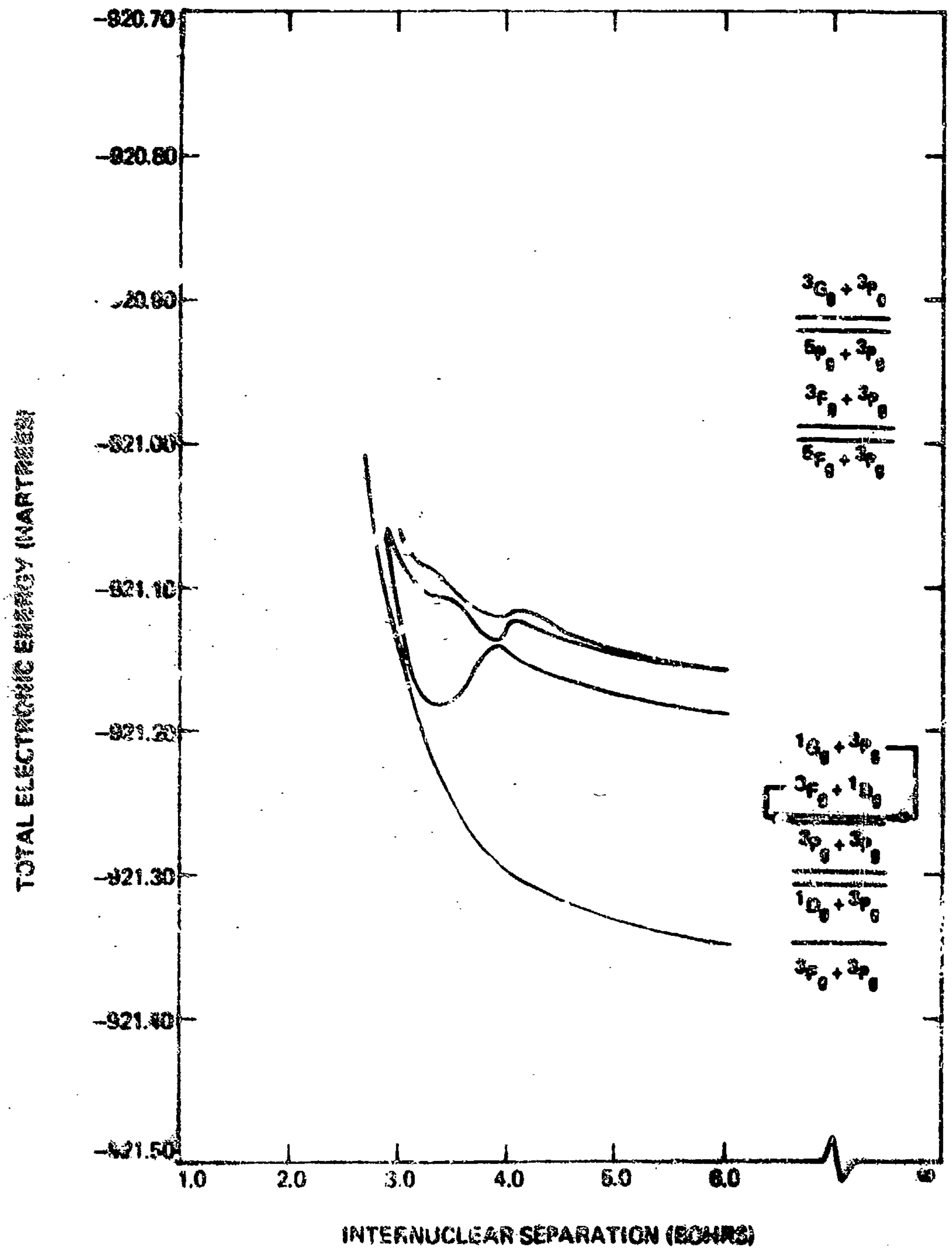


Figure 49. The calculated $^1\Gamma$ states of TiO

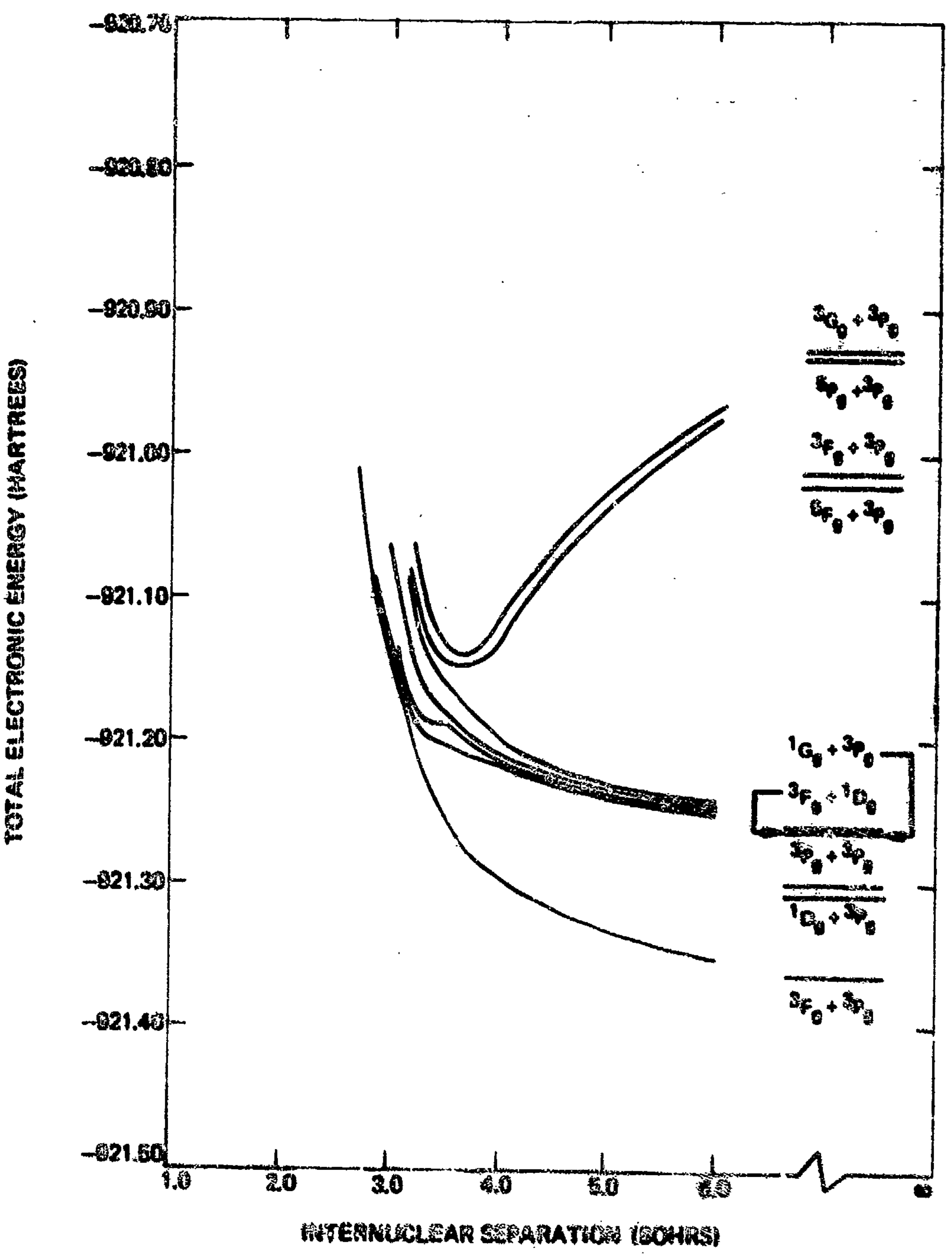


Figure 50. The calculated $^3\Gamma$ states of TiO

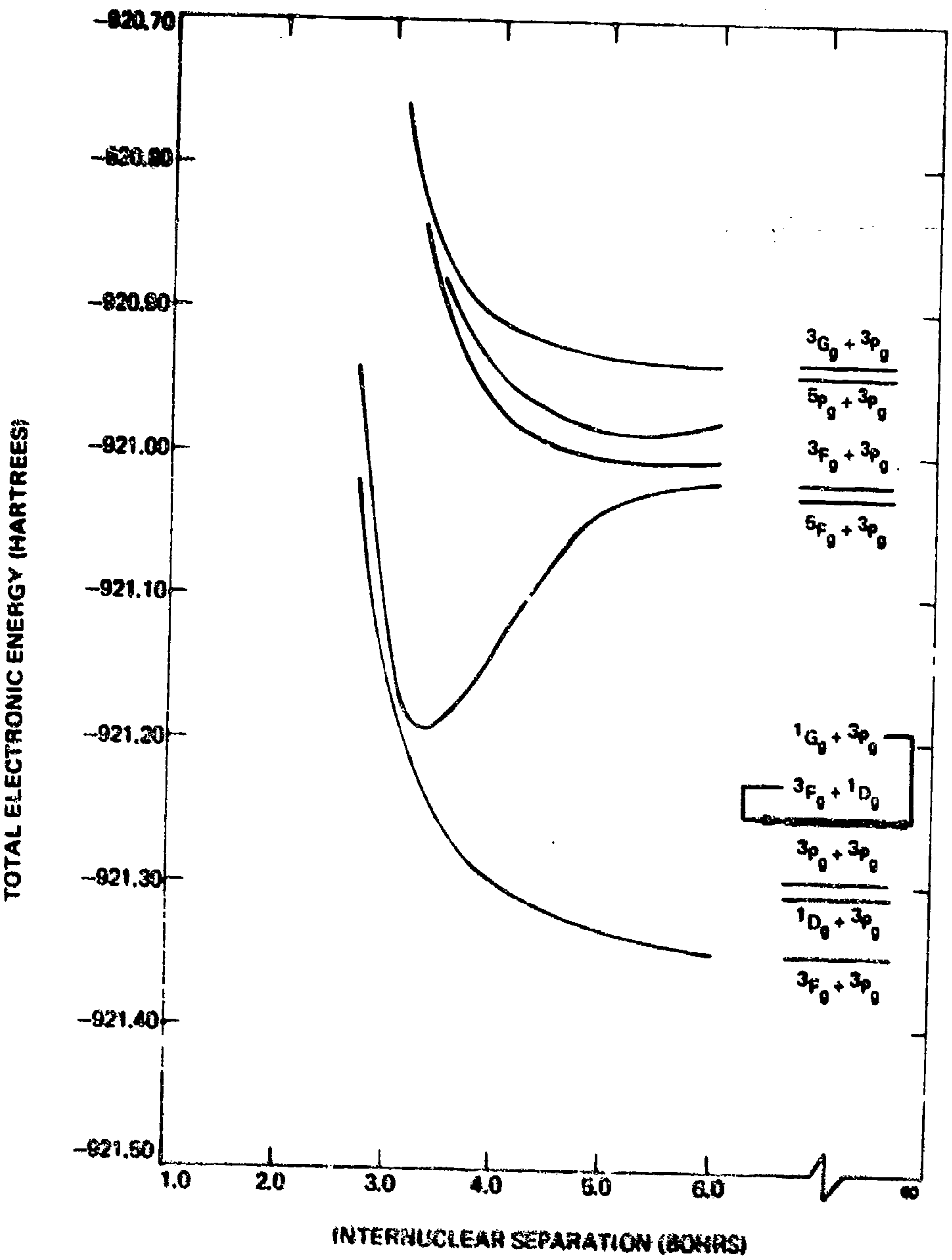


Figure 51. The calculated $^5\Gamma$ states of TiO

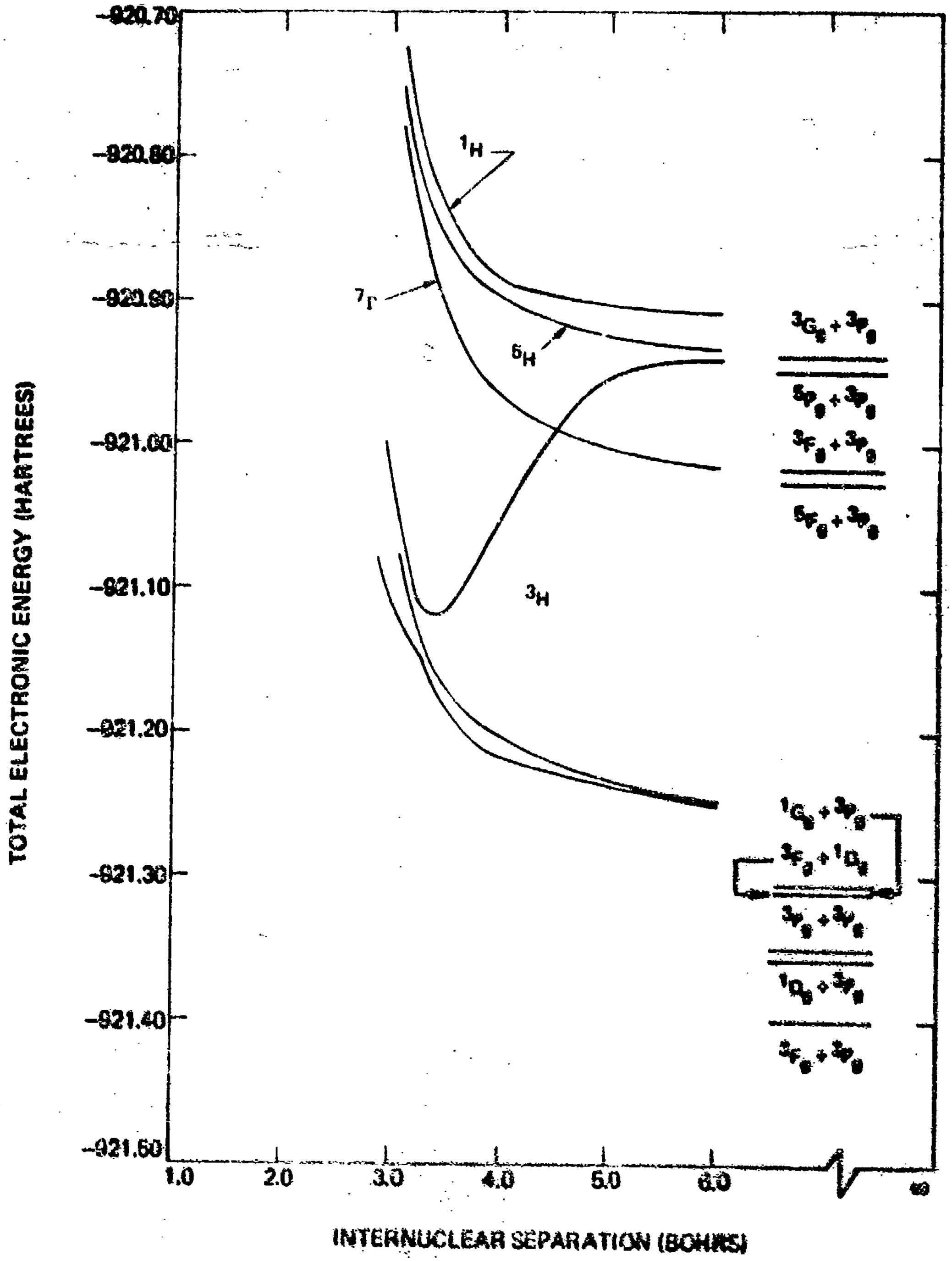


Figure 52. The calculated $^7\Gamma$, ^1H, ^3H and ^5H states of TiO

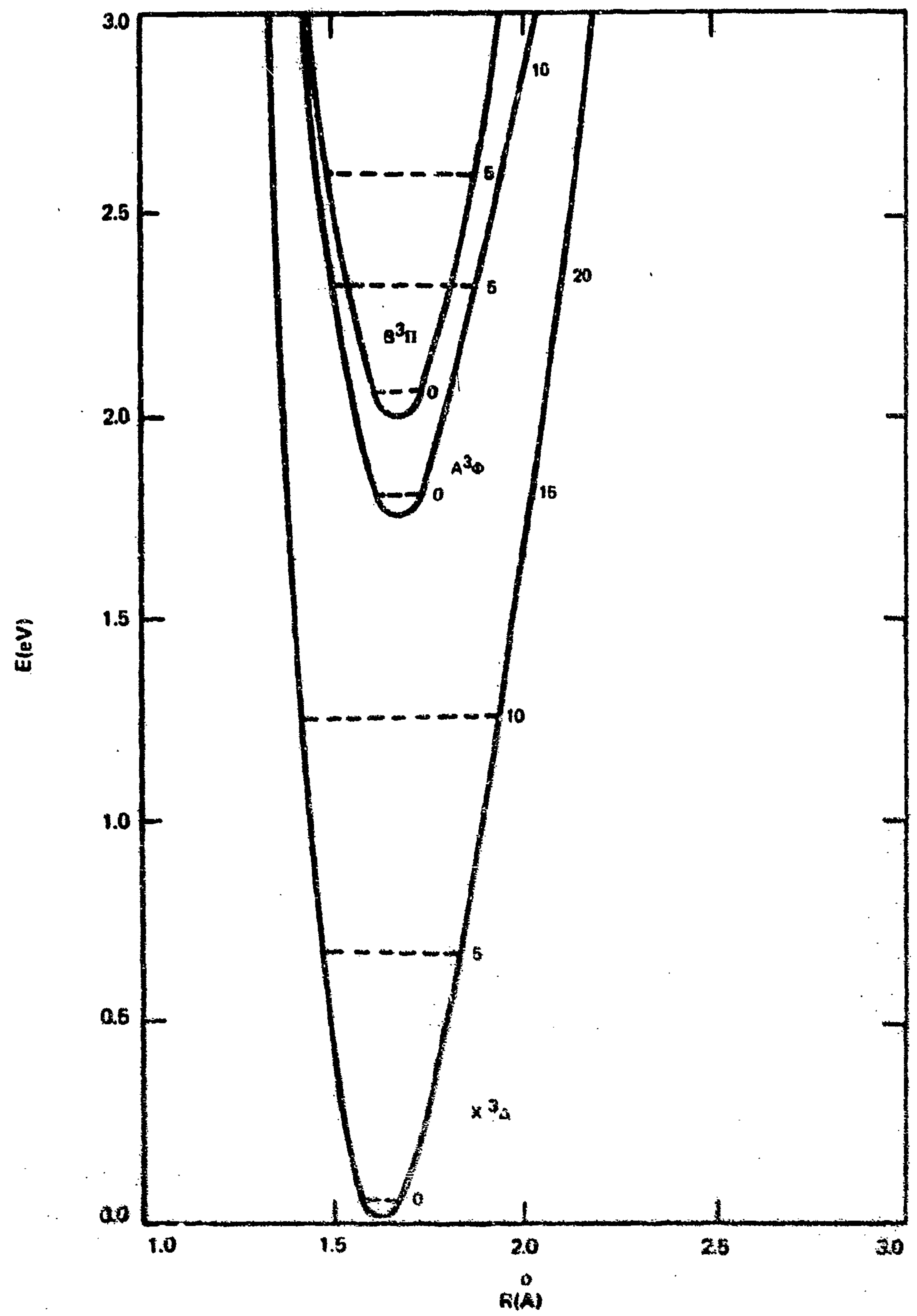


FIGURE 63. RKR POTENTIAL ENERGY CURVES FOR TiO

Table 1

Atomic and Molecular Orbital Basis for AlO and AlO$^+$

Molecular Orbital		Screening Parameters for Atomic Orbitals			
		AlO$^+$			AlO
		R = 2.6	R = 3.0	R = 3.4	All R's
1σ	1s (Al)	12.5902	12.5902	12.5902	12.5910
2σ	1s (O)	7.6568	7.6568	7.6568	7.6579
3σ	2s (Al)	4.1034	4.1034	4.1034	4.1068
$1\pi^{+,-}$	$2p\pi^{+,-}$ (Al)	4.4270	4.4270	4.4270	4.4817
4σ	$2p\sigma$ (Al)	4.4270	4.4270	4.4270	4.4817
5σ	2s (O)	2.2420	2.2508	2.2371	2.2458
6σ	$2p\sigma$ (O)	2.2141	2.1948	2.1400	2.2266
$2\pi^{+,-}$	$2p\pi^{+,-}$ (O)	2.1994	2.2156	2.1991	2.2266
7σ	3s (Al)	1.6472	1.5767	1.5591	1.3724
8σ	$3p\sigma$ (Al)	1.2383	1.4974	1.7198	1.3552
$3\pi^{+,-}$	$3p\pi^{+,-}$ (Al)	1.5754	1.5171	1.9690	1.3552

Table 2

Configuration Sizes and Number of States for VCI Calculations of Various Symmetries for AlO

Symmetry	No. Cfgs.	No. of States (to two lowest dissociation limits)
$^2\Sigma$	109	3(+), 3(-)
$^4\Sigma$	106	1(+), 2(-)
$^2\Pi$	159	5
$^4\Pi$	84	2
$^2\Delta$	92	3
$^4\Delta$	46	1
$^2\Phi$		1

Table 3

Low-Lying Molecular States of AlO and their Dissociation Limits

Dissociation Limit	Molecular States
Al + O	
${}^2P_u(3p) + {}^3P_g(2p^4)$	${}^2\Sigma^-(2)$, ${}^4\Sigma^-(2)$, ${}^2\Sigma^+(1)$, ${}^4\Sigma^+(1)$, ${}^2\Pi(2)$, ${}^4\Pi(2)$, ${}^2\Delta(1)$, ${}^4\Delta(1)$.
${}^2P_u(3p) + {}^1D_g(2p^4)$	${}^2\Sigma^-(1)$, ${}^2\Sigma^+(2)$, ${}^2\Pi(3)$, ${}^2\Delta(2)$, ${}^2\Phi(1)$.

( ) Indicates number of states for specified symmetry.

Table 4

Energies of Aluminum and Oxygen Atomic States Representing Dissociation Limits of Low Lying AlO States

Atomic States	Total Energy (hartrees)	Energy Relative to $^2P_u + ^3P_g$ (ev)	
		Calc.	Exp.
$^2P_u + ^3P_g$	-315.71895	0.00	0.00
$^2P_u + ^1D_g$	-315.62503	2.56	1.97

Table 5

Calculated Energies of Electronic States of AlO
(Energies are in hartrees; internuclear separations are in bohrs)

R	$^2\Sigma^+$ I	$^2\Sigma^-$ I	$^2\Sigma^-$ II	$^2\Sigma^+$ II	$^2\Sigma^-$ III	$^2\Sigma^+$ III
1.0	-305.53107	-305.43[illegible]		-305.46389		-305.06194
2.0	-315.08223	-314.69110	-314.62397	-314.98373		-314.74476
3.0	-315.82313	-315.61520	-315.56754	-315.72892	-315.45673	-315.57442
4.0	-315.7707[illegible]	-315.69[illegible]	-315.65351	-315.69895	-315.55911	-315.62358
5.0	-315.76247	-315.7105[illegible]	-315.67921	-315.64938	-315.63424	-315.62264
6.0	-315.71774	-315.71598	-315.70308	-315.62749	-315.62404	-315.62226
7.0	-315.71776	-315.71741	-315.71558	-315.62485	-315.62365	-315.62362
8.0	-315.71788	-315.71782	-315.71727	-315.62443	-315.62391	-315.62380
∞	-315.71895	-315.71895	-315.71895	-315.62503	-315.62503	-315.62503

R	$^4\Sigma^-$ I	$^4\Sigma^-$ II	$^4\Sigma^+$ I	$^2\Pi$ I	$^2\Pi$ II	$^2\Pi$ III
1.0	-304.82157	-305.63295	-304.79941	-305.71324	-305.31505	-305.25554
2.0	-314.76146	-314.71028	-314.60753	-314.90354	-314.88569	-314.75209
3.0	-315.68190	-315.63339	-315.50720	-315.78306	-315.63714	-315.53792
4.0	-315.72166	-315.70651	-315.62139	-315.79131	-315.68106	-315.63743
5.0	-315.71582	-315.71358	-315.69050	-315.74561	-315.71233	-315.62871
6.0	-315.71717	-315.71658	-315.71105	-315.72464	-315.71743	-315.62672
7.0	-315.71772	-315.71756	-315.71621	-315.71949	-315.71793	-315.62494
8.0	-315.71788	-315.71787	-315.71774	-315.71842	-315.71796	-315.62444
∞	-315.71895	-315.71895	-315.71895	-315.71895	-315.71895	-315.62503

Table 5 (Continued)

R	$^2\Pi$ IV	$^2\Pi$ V	$^4\Pi$ I	$^4\Pi$ II	$^2\Delta$ I	$^2\Delta$ II
1.0	-305.23165	-304.94929	-305.40196	-304.96776	-305.52115	-305.05736
2.0	-314.62782	-314.57458	-314.87165	-314.59255	-314.69329	-314.63663
3.0	-315.49823	-315.46148	-315.60633	-315.58155	-315.61318	-315.57797
4.0	-315.60822	-315.58075	-315.70584	-315.61595	-315.69441	-315.65659
5.0	-315.62149	-315.60408	-315.72091	-315.68750	-315.71111	-315.63516
6.0	-315.62274	-315.62054	-315.71963	-315.71126	-315.71620	-315.62449
7.0	-315.62364	-315.62335	-315.71851	-315.71687	-315.71746	-315.62390
8.0	-315.62397	-315.62373	-315.71822	-315.71786	-315.71778	-315.62400
∞	-315.62503	-315.62503	-315.71895	-315.71895	-315.71895	-315.62503

R	$^2\Delta$ III	$^4\Delta$ I
1.0	-304.78775	-304.81133
2.0	-314.56002	-314.73018
3.0	-315.45817	-315.65042
4.0	-315.55623	-315.71088
5.0	-315.59492	-315.71440
6.0	-315.61613	-315.71677
7.0	-315.62208	-315.71755
8.0	-315.62344	-315.71779
∞	-315.62503	-315.62503

Table 6

Calculated (Single-Zeta Results) and Experimental Spectroscopic Constants for Bound States of AlO

State			D_e(ev)	D_o^o(ev)	r_e(Å)	ω_e(cm^{-1})	$\omega_e X_e$(cm^{-1})	B_e(cm^{-1})	α_e(cm^{-1})
X	$^2\Sigma^+{}_{I}$	Calc	2.88	2.83	1.63	718.63	-0.93051	0.63	0.00008
		Exp.[a]	-	5.14	1.62	979.23	6.97	0.64	0.0058
B	$^2\Sigma^+{}_{II}$	Calc.	2.98	2.94	1.71	687.28	0.2978	0.57	-0.00014
		Exp.[a]	-	-	1.67	870.05	3.5	0.60	0.00447
A	$^2\Pi_{I}$	Calc.	2.34	2.31	1.84	588.54	2.9984	0.49	+0.00352
		Exp.[a]	-	4.38	1.78	728.5	4.15	-	0.0050
	$^2\Sigma^-{}_{III}$	Calc.	2.68	2.38	2.66	486.84	6.836	0.24	0.00183
	$^2\Pi_{III}$	Calc.	3.83	3.50	2.03	537.16	21.564	0.41	0.00975
	$^2\Delta_{II}$	Calc.	0.88	0.84	2.15	653.74	17.93	0.36	-0.00052

[a] B. Rosen (Director), Spectroscopic Data Relative to Diatomic Molecules, Pergamon Press, New York, 1970.

Table 7

Calculated Oscillator Strengths ($f_{v'v''}$) for the Blue-Green System of AlO ($B^2\Sigma^+ - X^2\Sigma^+$)

v'/v"	0	1	2	3	4	5
0	1.172-02	3.147-03	3.298-04	1.367-05	1.453-07	4.943-12
1	4.417-03	5.392-03	4.436-03	7.687-04	4.244-05	4.089-07
2	9.955-04	5.788-03	2.121-03	4.721-03	1.201-03	8.249-05
3	1.718-04	2.172-03	5.613-03	6.133-04	4.506-03	1.578-03
4	2.519-05	5.262-04	3.136-03	4.759-03	6.882-05	4.070-03
5	3.326-06	9.866-05	9.979-04	3.754-03	3.714-03	1.825-05
6	3.915-07	1.544-05	2.305-04	1.509-03	4.034-03	2.724-03
7	3.111-08	2.031-06	4.275-05	4.202-04	1.997-03	4.035-03
8	7.549-11	1.970-07	6.614-06	9.154-05	6.565-04	2.411-03
9	1.522-09	7.523-09	8.313-07	1.652-05	1.653-04	9.207-04
10	8.799-10	2.288-10	7.269-08	2.495-06	3.414-05	2.645-04

v'/v"	6	7	8	9	10
0	7.396-10	2.328-11	5.825-11	1.102-10	3.410-11
1	2.297-10	1.674-09	6.285-11	5.467-10	2.674-10
2	6.989-07	7.824-09	1.445-09	4.450-10	8.077-10
3	1.274-04	9.138-07	4.442-08	1.638-09	3.948-10
4	1.889-03	1.716-04	8.989-07	1.310-07	3.132-09
5	3.570-03	2.135-03	2.110-04	5.974-07	3.010-07
6	1.889-04	3.091-03	2.323-03	2.424-04	1.796-07
7	1.889-03	4.322-04	2.668-03	2.464-03	2.630-04
8	3.832-03	1.239-03	6.721-04	2.315-03	2.569-03
9	2.726-03	3.499-03	7.616-04	8.738-04	2.032-03
10	1.194-03	2.932-03	3.100-03	4.311-04	1.026-03

Table 8

Calculated Oscillator Strengths ($f_{v'v''}$) for the Vibrational-Rotational Transition of AlO ($X\,^2\Sigma^+ - X\,^2\Sigma^+$)

v'/v"	0	1	2	3	4	5
0						
1	1.203-06* 4.589-08**					
2	7.879-15 1.978-08	2.514-06 8.014-08				
3	3.356-11 1.746-09	2.857-11 5.822-08	3.938-06 1.075-07			
4	1.431-14 2.319-10	6.447-11 7.955-09	1.491-10 1.137-08	5.463-06 1.058-07		
5	5.472-12 9.629-11	7.659-13 1.311-09	1.097-11 1.919-08	1.402-10 1.830-07	7.074-06 1.339-07	
6	1.408-12 4.391-11	5.131-11 2.886-10	4.663-11 3.586-09	4.104-11 3.498-08	3.996-11 2.618-07	8.770-06 1.342-07
7	1.443-12 1.930-12	5.360-12 7.269-11	6.439-11 5.970-10	1.101-10 6.936-09	3.303-10 5.648-08	2.680-11 3.471-07
8	3.286-13 7.976-12	2.307-12 1.085-12	4.687-11 6.424-11	3.430-11 1.230-09	1.709-10 1.172-08	1.148-09 8.366-08
9	1.398-12 1.350-11	1.844-13 2.730-11	8.061-13 1.138-13	8.694-11 [illegible]	1.828-11 2.218-09	1.879-10 1.818-08
10	3.375-12 4.314-12	2.970-13 4.098-11	1.035-11 2.159-11	5.889-12 4.148-13	1.390-10 2.068-10	5.237-13 3.610-09

Table 8 (Continued)

v'/v"	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6					
7	1.054-05 1.278-07				
8	5.340-10 4.362-07	1.237-05 1.162-07			
9	2.396-09 1.163-07	1.974-09 5.287-07	1.429-05 9.971-08		
10	9.522-11 2.703-08	3.786-09 1.525-07	4.467-09 6.251-07	1.632-05 8.004-08	

* Using optimized π vectors
** Using optimized σ vectors

Table 9

Calculated Franck - Condon Factors ($q_{v'v''}$) for the Blue - Green System of AlO ($B\ ^2\Sigma^+ - X\ ^2\Sigma^+$)

v' \ v''	0	1	2	3	4	5
0	7.236-01	2.426-01	3.193-02	1.837-03	3.448-05	5.531-09
1	2.268-01	3.389-01	3.518-01	7.653-02	5.852-03	1.207-04
2	4.280-02	3.015-01	1.358-01	3.847-01	1.234-01	1.168-02
3	6.101-03	9.467-02	2.965-01	3.987-02	3.766-01	1.673-01
4	7.060-04	1.903-02	1.389-01	2.549-01	4.577-03	3.489-01
5	6.793-05	2.879-03	3.692-02	1.692-01	2.017-01	1.193-03
6	5.460-06	3.488-04	6.998-03	5.710-02	1.846-01	1.497-01
7	3.726-07	3.480-05	1.035-03	1.316-02	7.699-02	1.873-01
8	2.449-08	2.955-06	1.248-04	2.318-03	2.111-02	9.464-02
9	2.460-09	2.408-07	1.283-05	3.309-04	4.350-03	3.034-02
10	6.292-10	2.722-08	1.262-06	4.038-05	7.227-04	7.206-03

v' \ v''	6	7	8	9	10
0	1.407-08	5.988-11	7.573-12	1.104-13	3.734-14
1	1.523-08	9.379-08	1.037-10	7.495-11	3.446-13
2	2.469-04	5.009-07	3.379-07	5.444-12	3.719-10
3	1.869-02	3.795-04	3.224-06	8.624-07	2.006-09
4	2.062-01	2.620-02	4.757-04	1.201-05	1.719-06
5	3.142-[illegible]	2.398-01	3.358-02	4.985-04	3.304-05
6	1.268-02	2.793-01	2.648-01	4.029-02	4.302-04
7	1.049-01	2.933-02	2.479-01	2.929-01	4.587-02
8	1.803-01	6.938-02	4.593-02	2.215-01	3.143-01
9	1.088-01	1.668-01	4.289-02	5.997-02	2.007-01
10	4.021-02	1.188-01	1.494-01	2.431-02	7.047-02

Table 10

Calculated R-Centroid Factors $(\langle \bar{r} \rangle_{v'v''})$ for the Blue - Green System of AlO ($B\ ^2\Sigma^+ - X\ ^2\Sigma^+$)

v'/v"	0	1	2	3	4	5
0	1.647+00	1.726+00	1.812+00	1.924+00	2.130+00	5.816+00
1	1.575+00	1.658+00	1.738+00	1.824+00	1.940+00	2.170+00
2	1.509+00	1.583+00	1.672+00	1.749+00	1.836+00	1.956+00
3	1.442+00	1.517+00	1.591+00	1.694+00	1.760+00	1.848+00
4	1.368+00	1.450+00	1.524+00	1.598+00	1.765+00	1.773+00
5	1.281+00	1.379+00	1.459+00	1.531+00	1.605+00	1.478+00
6	1.171+00	1.296+00	1.389+00	1.467+00	1.538+00	1.612+00
7	1.027+00	1.195+00	1.310+00	1.400+00	1.474+00	1.544+00
8	8.763-01	1.069+00	1.216+00	1.323+00	1.408+00	1.481+00
9	8.848-01	9.401-01	1.104+00	1.235+00	1.335+00	1.416+00
10	1.127+00	9.289-01	9.914-01	1.133+00	1.252+00	1.346+00

v'/v"	6	7	8	9	10
0	1.859+00	3.025+00	1.805+00	2.513+00	1.644+00
1	-3.119+00	1.932+00	4.290+00	1.938+00	3.020+00
2	2.218+00	5.107-01	2.003+00	-1.918+01	2.061+00
3	1.974+00	2.277+00	1.164+00	2.076+00	6.724-02
4	1.861+00	1.991+00	2.355+00	1.448+00	2.156+00
5	1.786+00	1.873+00	2.010+00	2.463+00	1.615+00
6	1.617+00	1.799+00	1.886+00	2.030+00	2.631+00
7	1.619+00	1.641+00	1.814+00	1.899+00	2.051+00
8	1.550+00	1.626+00	1.651+00	1.830+00	1.913+00
9	1.487+00	1.555+00	1.633+00	1.656+00	1.847+00
10	1.423+00	1.493+00	1.560+00	1.640+00	1.658+00

Table 11

Calculated R-Centroid Factors ($\langle \bar{\bar{s}} \rangle_{v'v''}$)
For the Vibrational-Rotational Transition
of AlO ($X\,^2\Sigma^+ - X\,^2\Sigma^+$)

v'/v"	0	1	2	3	4	5
0	1.623+00					
1	4.154-02	1.634+00				
2	-2.492-03	5.897-02	1.644+00			
3	2.441-04	-4.339-03	7.249-02	1.655+00		
4	-3.019-05	4.910-04	-6.170-03	8.401-02	-1.666+00	
5	4.078-06	-6.787-05	7.809-04	-8.010-03	9.429-02	1.678+00
6	-4.769-07	1.001-05	-1.181-04	1.111-03	-9.865-03	1.037-01
7	-1.015-08	-1.243-06	1.877-05	-1.814-04	1.479-03	-1.174-02
8	4.944-08	-3.364-08	-2.495-06	3.078-05	-2.579-04	1.882-03
9	-3.286-08	1.380-07	-6.020-08	-4.326-06	4.632-05	-3.479-04
10	1.624-08	-9.132-08	3.019-07	-1.151-07	-6.844-06	6.577-05

v'/v"	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6	1.689+00				
7	1.124-01	1.701+00			
8	-1.364-02	1.207-01	1.712+00		
9	2.320-03	-1.555-02	1.285-01	1.724+00	
10	-4.518-04	2.790-03	-1.749-02	1.360-01	1.737+00

Table 12

Calculated Band Strengths ($p_{v'v''}$) for the Blue - Green System of AlO ($B\ ^2\Sigma^+ - X\ ^2\Sigma^+$)

v'/v"	0	1	2	3	4	5
0	1.874-01	5.281-02	5.818-03	2.538-04	2.847-06	1.024-10
1	6.781-02	8.652-02	7.478-02	1.361-02	7.908-04	8.032-06
2	1.470-02	8.931-02	3.426-02	7.991-02	2.134-02	1.542-03
3	2.444-03	3.222-02	8.703-02	9.948-03	7.657-02	2.814-02
4	3.456-04	7.524-03	4.677-02	7.412-02	1.121-03	6.941-02
5	4.410-05	1.361-03	1.434-02	5.625-02	5.809-02	2.983-04
6	5.024-06	2.059-04	3.197-03	2.179-02	6.071-02	4.276-02
7	3.869-07	2.621-05	5.731-04	5.856-03	2.896-02	6.097-02
8	9.107-10	2.464-06	8.582-05	1.233-03	9.192-03	3.512-02
9	1.783-08	9.129-08	1.045-05	2.155-04	2.238-03	1.295-02
10	1.003-08	2.697-09	8.870-07	3.154-05	4.475-04	3.597-03

v'/v"	6	7	8	9	10
0	1.623-08	5.429-10	1.447-09	2.926-09	9.714-10
1	4.767-09	3.678-08	1.466-09	1.357-08	7.088-09
2	1.376-05	1.626-07	3.178-08	1.038-08	2.003-08
3	2.388-03	1.803-05	9.244-07	3.604-08	9.201-09
4	3.379-02	3.222-03	1.776-05	2.730-06	6.889-08
5	6.108-02	3.828-02	3.971-03	1.182-05	6.270-06
6	3.098-03	5.302-02	4.174-02	4.568-03	3.556-05
7	2.977-02	7.110-03	4.589-02	4.455-02	4.962-03
8	5.812-02	1.958-02	1.109-02	3.989-02	4.631-02
9	3.986-02	5.325-02	1.208-02	1.445-02	3.508-02
10	1.686-02	4.304-02	4.732-02	6.854-03	1.[illegible]-02

Table 13

Calculated Band Strengths ($p_{v'v''}$) for the Vibrational-Rotational Transition of AlO ($X\,^2\Sigma^+ - X\,^2\Sigma^+$)

v'/v"	0	1	2	3	4	5
0	7.406-01* 5.976-01**					
1	4.103-04 1.565-05	7.287-01 5.956-01				
2	1.354-12 3.398-06	8.701-04 2.774-05	7.162-01 5.934-01			
3	3.871-09 2.015-07	4.980-09 1.015-05	1.383-03 3.774-05	7.032-01 5.910-01		
4	1.247-12 2.021-08	7.548-09 9.313-07	2.638-08 2.011-05	1.948-03 4.485-05	6.898-01 5.885-01	
5	3.844-10 6.764-09	6.775-11 1.160-07	1.304-09 2.281-06	2.518-08 3.287-05	2.561-03 4.848-05	6.763-01 5.861-01
6	8.303-11 2.590-09	3.659-09 2.058-08	4.188-09 3.221-07	4.952-09 4.222-06	7.288-09 4.775-05	3.224-03 4.934-05
7	7.348-11 9.831-11	3.210-10 4.352-09	4.662-09 4.322-08	1.004-08 6.326-07	4.049-08 6.922-06	4.965-09 6.431-05
8	1.475-11 3.582-10	1.193-10 5.612-11	2.850-09 3.906-09	2.522-09 9.046-08	1.583-08 1.086-06	1.489-07 1.041-05
9	5.624-11 5.450-10	8.406-12 1.245-09	4.234-11 5.977-12	5.369-09 6.554-09	1.365-09 1.657-07	1.768-08 1.711-06
10	1.231-10 1.574-10	1.213-11 1.674-09	4.796-10 1.000-09	3.142-10 2.213-11	8.721-09 1.257-08	3.975-11 2.740-07

Table 13 (Continued)

v'/v"	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6	6.625-01 5.835-01				
7	3.934-03 4.775-05	6.485-01 5.808-01			
8	1.005-07 8.210-05	4.696-03 4.410-05	6.342-01 5.780-01		
9	3.031-07 1.470-05	3.775-07 1.011-04	5.514-03 3.845-05	6.197-01 5.751-01	
10	9.106-09 2.535-06	4.867-07 [illegible]	8.685-07 1.215-04	6.396-03 3.138-05	6.048-01 5.720-01

* Using optimized r vectors
** Using optimized s vectors

Table 14

Screening Parameters for the Atomic Orbitals of LiO

Atomic Orbitals		Screening Parameters
1s	(O)	7.6579
1s	(Li)	2.6906
2s	(O)	2.2458
2pπ+	(O)	2.2266
2pπ−	(O)	2.2266
2s	(Li)	0.6396
2pσ	(O)	2.2266
2pπ+	(Li)	0.5243
2pπ+	(Li)	0.5243
2pσ	(Li)	0.5243

Table 15

Configuration Sizes and Number of States for VCI Calculations of Various Symmetries for LiO

Symmetry	No. of Cfgs.	No. of States
$^2\Sigma^{+,-}$	264	5 (+), 5 (-)
$^4\Sigma^{+,-}$	180	1 (+), 3 (-)
$^2\Pi$	243	8
$^4\Pi$	245	3
$^2\Delta$	230	4
$^4\Delta$	130	1
$^2\Phi$	88	1

Table 16

Low-Lying Molecular States of LiO and their Dissociation Limits

Dissociation Limit	Molecular States
Li + O	
^2S_g (2s) + ^3P_g ($2p^4$)	$^2\Sigma^-(1)$, $^4\Sigma^-(1)$, $^2\Pi(1)$, $^4\Pi(1)$.
^2P_u (2p) + ^3P_g ($2p^4$)	$^2\Sigma^-(2)$, $^4\Sigma^-(2)$, $^2\Sigma^+(1)$, $^4\Sigma^+(1)$, $^2\Pi(2)$, $^4\Pi(2)$, $^2\Delta(1)$, $^4\Delta(1)$.
^2S_g(2s) + ^1D_g ($2p^4$)	$^2\Sigma^+(1)$, $^2\Pi(1)$, $^2\Delta(1)$.
^2P_u(2p) + ^1D_g ($2p^4$)	$^2\Sigma^-(1)$, $^2\Sigma^+(2)$, $^2\Pi(3)$, $^2\Delta(2)$, $^2\Phi(1)$.
^2S_g (2s) + ^1S_g ($2p^4$)	$^2\Sigma^+(1)$.
^2P_u (2p) + ^1S_g ($2p^4$)	$^2\Sigma^-(1)$, $^2\Pi(1)$.

( ) Indicates number of states for specified symmetry.

Table 17

Energies of Lithium Atomic and Oxygen Atomic States Representing Dissociation Limits of Low-Lying LiO States

Atomic States	Total Energy (Hartrees)	Energy Relative to $^2S_g + {}^3P_g$ (ev)	
$^2S_g + {}^3P_g$	-81.95830	0.0000	0.0000
$^2P_u + {}^3P_g$	-81.89089	1.6980	1.8479
$^2S_g + {}^1D_g$	-81.86438	2.5552	1.9674
$^2P_u + {}^1D_g$	-81.79697	4.2532	3.8153
$^2S_g + {}^1S_g$	-81.78339	4.7593	4.1898
$^2P_g + {}^1S_g$	-81.71598	6.4573	6.0377

Table 18

Calculated Energies of Electronic States for LiO (Energies are in hartrees; internuclear separations are in bohrs)

R	$^2\Sigma^-_{\mathrm{I}}$	$^2\Sigma^+_{\mathrm{I}}$	$^2\Sigma^-_{\mathrm{II}}$	$^2\Sigma^-_{\mathrm{III}}$	$^2\Sigma^+_{\mathrm{II}}$	$^2\Sigma^+_{\mathrm{III}}$
1.0	-78.31310	-79.13734	-78.23786	-	-78.95344	-78.24726
1.5	-80.65297	-80.05037	-80.56132	-	-80.95780	-80.60696
2.0	-81.54805	-81.76570	-81.53373	-	-81.59824	-81.48777
2.5	-81.86385	-81.96519	-81.79053	-81.71566	-81.78255	-81.73528
3.0	-81.94227	-81.99300	-81.86281	-81.79417	-81.84206	-81.80273
4.0	-81.96676	-81.95773	-81.89169	-81.83347	-81.86314	-81.82326
5.0	-81.96755	-81.92372	-81.89486	-81.85786	-81.86540	-81.81799
6.0	-81.96498	-81.90553	-81.89421	-81.87379	-81.86574	-81.80978
7.0	-81.96247	-81.89748	-81.89317	-81.88252	-81.86559	-81.80381
8.0	-81.96081	-81.89417	-81.89248	-81.88705	-81.86535	-81.80062
∞	-81.95830	-81.89089	-81.89089	-81.89089	-81.86438	-81.79697

R	$^4\Sigma^-_{\mathrm{I}}$	$^4\Sigma^+_{\mathrm{I}}$	$^4\Sigma^-_{\mathrm{II}}$	$^4\Sigma^-_{\mathrm{III}}$	$^2\Pi_{\mathrm{I}}$	$^2\Pi_{\mathrm{II}}$
1.0	-78.31751	-78.33289	-78.14652	-77.95753	-79.00379	-78.39834
1.5	-80.65898	-80.68133	-80.41929	-80.37120	-80.92722	-80.77663
2.0	-80.55360	-81.56029	-81.53988	-81.42288	-81.65981	-81.65254
2.5	-81.86818	-81.81345	-81.79589	-81.73955	-81.92116	-81.87261
3.0	-81.94596	-81.88167	-81.86737	-81.81893	-81.97653	-81.92831
4.0	-81.97000	-81.90289	-81.89483	-81.85594	-81.97932	-81.93573
5.0	-81.97015	-81.90074	-81.89668	-81.87325	-81.96919	-81.92502
6.0	-81.96667	-81.89710	-81.89511	-81.88229	-81.96369	-81.91221
7.0	-81.96335	-81.89458	-81.89358	-81.88674	-81.96116	-81.90263
8.0	-81.96119	-81.89318	-81.89266	-81.88905	-81.95995	-81.89712
∞	-81.95830	-81.89089	-81.89089	-81.89089	-81.95830	-81.89089

Table 18 (Continued)

R	$^2\Pi$ III	$^2\Pi$ IV	$^2\Pi$ V	$^4\Pi$ I	$^4\Pi$ II	$^4\Pi$ III
1.0	-78.28919	-78.24525	-78.17445	-78.29774	-78.18420	-78.09669
1.5	-80.67706	-80.61916	-80.53684	-80.77296	-80.62795	-80.40114
2.0	-81.50559	-81.48287	-81.48237	-81.63500	-81.50811	-81.47150
2.5	-81.78069	-81.74460	-81.73020	-81.87675	-81.79767	-81.75127
3.0	-81.84495	-81.82258	-81.79155	-81.93880	-81.88341	-81.81264
4.0	-81.87019	-81.85071	-81.82107	-81.95776	-81.91329	-81.84318
5.0	-81.87711	-81.86257	-81.82113	-81.95886	-81.91202	-81.86244
6.0	-81.88387	-81.86582	-81.81324	-81.95899	-81.90544	-81.87582
7.0	-81.88807	-81.86599	-81.80639	-81.95909	-81.89954	-81.88354
8.0	-81.89018	-81.86565	-81.80221	-81.95909	-81.89580	-81.88795
∞	-81.89089	-81.86438	-81.79697	-81.95830	-81.89089	-81.89089

R	$^2\Delta$ I	$^2\Delta$ II	$^2\Delta$ III	$^4\Delta$ I	$^2\Phi$ I
1.0	-78.31641	-78.24599	-78.14462	-78.32315	-78.15414
1.5	-80.65652	-80.56889	-80.41544	-80.66720	-80.28244
2.0	-81.53721	-81.46194	-81.45076	-81.54753	-81.37613
2.5	-81.79318	-81.77641	-81.70442	-81.80234	-81.70239
3.0	-81.86508	-81.85316	-81.77529	-81.87259	-81.78807
4.0	-81.89327	-81.87498	-81.80317	-81.89765	-81.17413
5.0	-81.89585	-81.87443	-81.80507	-81.89805	-81.81618
6.0	-81.89480	-81.87132	-81.80286	-81.89577	-81.81015
7.0	-81.89351	-81.86859	-81.80064	-81.89391	-81.80482
8.0	-81.89267	-81.86686	-81.79926	-81.89283	-81.80146
∞	-81.78339	-81.86438	-81.79697	-81.89089	-81.79697

Table 19

Calculated (Single-Zeta Results) and Experimental Spectroscopic Constants for Bound States of LiO

State		D_e(ev)	D_o^o(ev)	r_e(Å)	ω_e(cm^{-1})	$\omega_e X_e$(cm^{-1})	B_e(cm^{-1})	α_e(cm^{-1})
X $^2\Pi$ I	Calc.	0.6988	0.6929	1.88	290.51	391.18	0.98	0.11289
	Exp.[a]	3.54	3.49					
A $^2\Sigma^+$ I	Calc.	2.78	2.71	1.58	1051.5	13.22	1.39	0.00699
$^2\Sigma^+$ III	Calc.	0.74	0.72	1.97	468.91	22.38	0.89	0.03283
$^4\Sigma^+$ I	Calc.	0.33	0.31	2.07	362.27	20.40	0.81	0.03324
$^2\Pi$ II	Calc.	1.28	1.25	1.85	508.62	35.13	1.01	0.03973
$^2\Pi$ V	Calc.	0.71	0.69	2.35	306.49	31.65	0.63	0.00703
$^2\Phi$ I	Calc.	0.55	0.53	2.43	266.38	2.69	0.58	0.00619

[a] D. L. Hildenbrand: "Thermochemical Studies of Some Gaseous Metal Oxides", to be published in the Journal of Chemical Physics.

Table 20

Calculated Oscillator Strengths ($f_{v'v''}$)
for the Vibrational - Rotational Transition
of LiO ($X\ ^2\Pi - X\ ^2\Pi$)

v'/v"	0	1	2	3	4	5
0						
1	2.364-05					
2	1.786-07	4.717-05				
3	2.063-09	5.329-07	7.042-05			
4	5.165-13	5.600-09	1.128-06	9.247-05		
5	9.547-11	3.431-10	4.233-09	2.152-06	1.125-04	
6	5.940-14	8.123-10	2.776-09	1.003-09	3.686-06	1.308-04
7	4.119-14	1.558-10	4.654-10	2.402-09	1.541-09	5.558-06
8	1.127-11	9.860-11	2.076-09	5.897-10	4.405-10	1.781-08
9	9.132-13	8.662-12	5.256-12	4.258-09	5.627-09	1.649-08
10	9.133-12	4.464-11	4.061-10	1.091-09	1.406-09	4.332-09

v'/v"	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6					
7	1.484-04				
8	7.499-06	1.659-04			
9	8.259-08	9.509-06	1.832-04		
10	4.142-08	2.120-07	1.159-05	2.001-04	

Table 21

Calculated Oscillator Strengths ($f_{v'v''}$) for the $A\,^2\Sigma^+ - A\,^2\Sigma^+$ System of LiO

v'/v"	0	1	2	3	4	5	6	7	8	9	10
0											
1	3.698-05										
2	3.005-07	7.329-05									
3	4.432-09	9.135-07	1.091-04								
4	1.244-10	2.216-08	1.821-06	1.444-04							
5	8.074-11	6.193-10	6.009-08	3.029-06	1.792-04						
6	3.487-11	1.191-10	2.477-09	1.221-07	4.572-06	2.129-04					
7	1.851-15	1.103-10	1.703-10	7.974-09	1.988-07	6.609-06	2.446-04				
8	7.227-12	1.551-11	2.258-10	1.313-10	2.442-08	2.634-07	9.348-06	2.736-04			
9	3.306-12	2.085-12	4.133-11	4.903-10	8.554-11	5.699-08	3.309-07	1.267-05	3.0127-04		
10	7.485-14	1.258-11	3.372-13	1.909-10	2.160-10	1.760-09	7.878-08	4.869-07	1.618-05	3.285-04	

Table 22

Calculated Oscillator Strengths
($f_{v'v''}$) for the $A^2\Sigma^+ - X^2\Pi$ System of LiO

v'/v"	0	1	2	3	4	5
0	4.138-03	8.632-04	9.960-05	-1.860-06	-4.652-06	-1.338-06
1	4.816-03	1.054-03	8.480-04	1.844-04	2.858-06	-1.152-05
2	1.515-03	6.164-03	9.391-05	5.866-04	2.261-04	1.620-05
3	1.260-04	3.572-03	5.915-03	4.356-05	3.262-04	2.296-04
4	9.288-07	4.438-04	5.689-03	4.993-03	3.360-04	1.398-04
5	2.223-12	5.850-06	9.807-04	7.619-03	3.858-03	7.198-04
6	1.137-08	1.968-09	2.038-05	1.740-03	9.242-03	2.739-03
7	2.438-09	4.307-08	3.915-08	5.320-05	2.716-03	1.050-02
8	1.273-11	7.984-09	1.204-07	3.083-07	1.168-04	3.904-03
9	5.215-10	7.431-11	1.473-08	2.845-07	1.628-06	2.310-04
10	1.324-10	1.382-09	4.015-10	1.052-08	6.934-07	6.203-06

v'/v"	6	7	8	9	10
0	-1.566-07	-1.056-09	-4.634-08	-6.030-08	-3.912-08
1	-4.110-06	-5.517-07	-3.720-09	-1.972-07	-2.852-07
2	-1.675-05	-7.566-06	-1.143-06	-8.813-09	-4.823-07
3	3.541-05	-1.774-05	-1.084-05	-1.868-06	-1.862-08
4	2.081-04	5.641-05	-1.346-05	-1.298-05	-2.589-06
5	3.522-05	1.737-04	7.576-05	-4.163-06	-1.336-05
6	1.091-03	1.964-07	1.352-04	9.180-05	9.180-06
7	1.751-03	1.409-03	2.216-05	9.757-05	1.044-04
8	1.136-02	9.531-04	1.656-03	9.250-05	6.320-05
9	5.297-03	1.184-02	3.796-04	1.828-03	2.072-04
10	4.258-04	6.888-03	1.189-02	5.818-05	1.920-03

Table 23

Calculated Franck-Condon Factors ($q_{v'v''}$) for the A $^2\Sigma^+$ - X $^2\Pi$ System of LiO

v'/v"	0	1	2	3	4	5
0	5.814-01	2.766-01	9.886-02	3.121-02	8.957-03	2.318-03
1	3.542-01	1.327-01	2.481-01	1.571-01	7.077-02	2.619-02
2	6.167-02	4.372-01	8.204-03	1.553-01	1.657-01	1.014-01
3	2.715-03	1.439-01	3.988-01	8.897-03	7.681-02	1.447-01
4	7.459-06	9.546-03	2.247-01	3.163-01	4.930-02	2.843-02
5	3.289-09	5.146-05	2.108-02	2.933-01	2.272-01	8.492-02
6	6.922-08	7.563-08	2.037-04	3.730-02	3.450-01	1.481-01
7	3.529-10	4.383-07	1.447-06	5.939-04	5.786-02	3.786-01
8	4.019-11	6.618-09	1.473-06	8.993-06	1.432-03	8.216-02
9	2.996-12	2.629-10	3.194-08	3.874-06	3.578-05	3.028-03
10	2.781-12	1.161-10	3.181-11	9.115-08	8.947-06	1.098-04

v'/v"	6	7	8	9	10
0	5.217-04	9.339-05	1.027-05	[illegible].065-07	5.402-07
1	8.237-03	2.164-03	4.373-04	5.187-05	3.627-07
2	4.666-02	1.735-02	5.206-03	1.166-03	1.469-04
3	1.176-01	6.577-02	2.836-02	9.555-03	2.335-03
4	1.130-01	1.210-01	8.090-02	3.984-02	1.486-02
5	5.691-03	8.134-02	1.158-01	9.134-02	5.067-02
6	1.128-01	1.843-06	5.494-02	1.058-01	9.749-02
7	8.541-02	1.279-01	3.997-03	3.496-02	9.395-02
8	3.946-01	4.048-02	1.319-01	1.265-02	2.082-02
9	1.094-01	3.942-01	1.267-02	1.269-01	2.294-02
10	5.809-03	1.385-01	3.757-01	7.060-04	1.151-01

Table 24

Calculated R-Centroid Factors ($\langle \bar{r} \rangle_{v'v''}$) for the Vibrational Rotational Transition of LiO ($X\,^2\pi - X\,^2\pi$)

v'/v"	0	1	2	3	4	5
0	1.705+00					
1	6.441-02	1.723+00				
2	-4.316-03	9.205-02	1.742+00			
3	3.221-04	-7.623-03	1.140-01	1.761+00		
4	7.951-06	6.484-04	-1.099-02	1.332-01	1.781+00	
5	-1.961-05	2.277-05	1.057-03	-1.449-02	1.506-01	1.802+00
6	9.879-06	-4.643-05	3.853-05	1.543-03	-1.813-02	1.671-01
7	-3.434-06	2.314-05	-8.799-05	5.560-05	2.111-03	-2.193-02
8	4.844-07	-8.969-06	4.589-05	-1.457-04	7.342-05	2.764-03
9	3.274-07	2.524-06	-1.852-05	8.053-05	-2.222-04	8.999-05
10	-2.114-07	-9.844-08	5.928-06	-3.407-05	1.297-04	-3.193-04

v'/v"	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6	1.824+00				
7	1.628-01	1.846+00			
8	-2.591-02	1.979-01	1.868+00		
9	3.510-03	-3.009-02	2.128-01	1.892+00	
10	1.036-04	4.356-03	-3.445-02	2.275-01	1.917+00

Table 25

Calculated R-Centroid Factors
($\bar{r}_{v'v''}$) for the A $^2\Sigma^+$ - A $^2\Sigma^+$
System of LiO

v'/v"	0	1	2	3	4	5
0	1.610+00					
1	6.330-02	1.630+00				
2	-4.571-03	8.977-02	1.650+00			
3	6.009-04	-7.944-03	1.102-01	1.670+00		
4	-1.135-04	1.214-03	-1.128-02	1.276-01	1.691+00	
5	2.908-05	-2.577-04	1.925-03	-1.461-02	1.430-01	1.712+00
6	-9.648-06	7.020-05	-4.476-04	2.732-03	-1.796-02	1.571-01
7	3.577-06	-2.365-05	1.311-04	-6.847-04	3.625-03	-2.133-02
8	-1.253-06	9.371-06	-4.628-05	2.133-04	-9.696-04	4.601-03
9	4.030-07	-4.009-06	1.900-05	-7.923-05	3.194-04	-1.302-03
10	-1.879-07	1.741-06	-8.704-06	3.397-05	-1.242-04	4.505-04

v'/v"	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6	1.754+00				
7	1.701-01	1.756+00			
8	-2.473-02	1.824-01	1.770+00		
9	5.654-03	-2.814-02	1.939-01	1.801+00	
10	-1.664-03	6.781-03	-3.155-02	2.046-01	1.824+00

Table 26

Calculated R-Centroid Factors ($\langle \bar{r} \rangle_{v'v''}$) for the A $^2\Sigma^+$ - X $^2\Pi$ System of LiO

v'/v"	0	1	2	3	4	5
0	1.658+00	1.572+00	1.510+00	1.459+00	1.412+00	1.363+00
1	1.748+00	1.693+00	1.583+00	1.516+00	1.463+00	1.415+00
2	1.874+00	1.764+00	1.853+00	1.598+00	1.523+00	1.468+00
3	2.120+00	1.887+00	1.785+00	1.482+00	1.619+00	1.531+00
4	3.328+00	2.126+00	1.901+00	1.810+00	1.607+00	1.657+00
5	1.397+00	3.054+00	2.133+00	1.917+00	1.841+00	1.649+00
6	1.751+00	2.671+00	2.863+00	2.143+00	1.934+00	1.880+00
7	-3.904-01	1.831+00	2.478+00	2.734+00	2.155+00	1.953+00
8	3.191+00	5.160-01	1.915+00	2.448+00	2.643+00	2.169+00
9	1.526+00	3.528+00	7.024-01	2.003+00	2.446+00	2.577+00
10	1.868+00	2.662+00	1.235+01	7.312-01	2.092+00	2.456+00

v'/v"	6	7	8	9	10
0	1.305+00	1.223+00	1.049+00	-5.518-01	1.811+00
1	1.366+00	1.308+00	1.225+00	1.046+00	-1.125+00
2	1.419+00	1.370+00	1.312+00	1.228+00	1.041+00
3	1.474+00	1.424+00	1.374+00	1.316+00	1.230+00
4	1.541+00	1.479+00	1.429+00	1.378+00	1.320+00
5	1.752+00	1.552+00	1.485+00	1.434+00	1.383+00
6	1.683+00	-6.400+00	1.565+00	1.492+00	1.439+00
7	1.932+00	1.716+00	1.475+00	1.550+00	1.490+00
8	1.973+00	2.012+00	1.752+00	1.578+00	1.596+00
9	2.165+00	1.994+00	2.176+00	1.793+00	1.636+00
10	2.530+00	2.203+00	2.016+00	3.229+000	1.840+00

Table 27

Calculated Band Strengths ($p_{v'v''}$) for the Vibrational Rotational Transition of LiO ($X\,^2\pi - X\,^2\pi$)

v'/v"	0	1	2	3	4	5
0	7.160+00					
1	9.422-03	7.312+00				
2	3.614-05	1.938-02	7.472+00			
3	2.826-07	1.112-04	2.986-02	7.637+00		
4	5.389-11	7.916-07	2.432-04	4.052-02	7.800+00	
5	8.098-09	3.696-08	6.183-07	4.795-04	5.098-02	7.962+00
6	4.267-12	7.118-08	3.092-07	1.515-07	8.498-04	6.136-02
7	2.579-12	1.157-08	4.219-08	2.769-07	2.411-07	1.328-03
8	6.276-10	6.384-09	1.596-07	5.536-08	5.263-08	2.859-06
9	4.599-11	4.993-10	3.524-10	3.391-07	5.476-07	2.044-06
10	4.212-10	2.328-09	2.426-08	7.584-08	1.162-07	4.379-07

v'/v"	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6	8.128+00				
7	7.223-02	8.302+00			
8	1.859-03	8.384-02	8.490+00		
9	1.391-05	2.450-03	9.627-02	8.658+00	
10	5.335-06	3.714-05	3.109-03	1.095-01	8.897+00

Table 28

Calculated Band Strengths ($p_{v'v''}$) for the $A\ ^2\Sigma^+ - A\ ^2\Sigma^+$ System of LiO

v'/v"	0	1	2	3	4	5
0	5.698+00					
1	1.426-02	5.883+00				
2	5.841-05	2.873-02	6.074+00			
3	5.789-07	1.805-04	4.345-02	6.272+00		
4	1.228-08	2.942-06	3.657-04	5.848-02	6.477+00	
5	6.432-09	6.217-08	8.109-06	6.182-04	7.376-02	6.689+00
6	2.333-09	9.646-09	2.528-07	1.675-05	9.489-04	8.914-02
7	1.070-13	7.502-09	1.402-08	8.275-07	2.774-05	1.395-03
8	3.688-10	9.121-10	1.562-08	1.099-08	2.577-06	3.739-05
9	1.512-10	1.082-10	2.472-09	3.450-08	7.286-09	6.121-06
10	3.107-12	5.851-10	1.779-11	1.162-08	1.547-08	1.526-07

v'/v"	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6	6.905+00				
7	1.041-02	7.123+00			
8	2.008-0[illegible]	1.156-01	[illegible]		
9	[illegible].750-05	2.771-0[illegible]	[illegible]	7.572+00	
10	8.612-06	7.161-0[illegible]	[illegible]	1.476-02	7.811+00

Table 29

Calculated Band Strength ($p_{v'v''}$)
for the A $^2\Sigma^+$ - X $^2\Pi$ System of LiO

v'/v"	0	1	2	3	4	5
0	1.163+00	3.749-01	9.179-02	1.980-02	3.767-03	5.720-04
1	9.923-01	2.929-01	3.560-01	1.533-01	4.652-02	1.105-02
2	2.473-01	1.265+00	2.568-02	2.367-01	1.691-01	6.927-02
3	1.706-02	5.828-01	1.204+00	1.16[illegible]-02	1.258-01	1.542-01
4	1.078-04	6.026-02	9.254-01	1.005+00	8.778-02	5.132-02
5	2.261-10	6.818-04	1.332-01	1.232+00	7.652-01	1.827-01
6	1.031-06	2.014-07	2.381-03	2.359-01	1.482+00	5.335-01
7	1.998-07	3.934-06	4.024-06	6.[illegible]-03	3.665-01	1.664+00
8	9.533-10	6.598-07	1.106-05	3.176-05	[illegible].364-02	5.232-01
9	3.599-08	5.614-09	1.226-06	2.625-05	1.679-04	2.688-02
10	8.484-09	9.633-08	3.058-06	[illegible]903-07	6.4[illegible]-05	6.390-04

v'/v"	6	7	8	9	10
0	4.601-05	2.385-07	8.551-06	[illegible]	5.[illegible]-08
1	1.950-03	1.740-04	9.[illegible]	3.8[illegible]-05	4.7[illegible]-05
2	2.015-02	4.071-03	4.0[illegible]	2.[illegible]	1.023-04
3	8.370-02	2.941-02	6.808-05	7.343-04	5.[illegible]-06
4	1.254-01	6.927-02	3.766-02	[illegible]	1.165-03
5	1.226-02	9.409-02	5.[illegible]37-02	4.[illegible]-02	1.3[illegible]-02
6	2.682-01	6.459-05	6.58[illegible]-02	2.[illegible]-02	4.[illegible]
7	3.340-01	3.343-01	6.87[illegible]-03	4.290-02	7.672-02
8	1.777+00	1.[illegible]-01	[illegible].772-01	2.6[illegible]-02	7.913-02
9	7.035-01	1.821+00	[illegible].875-02	4.2[illegible]-01	5.678-02
10	4.927-02	9.049-01	1.[illegible]	1.0[illegible]-02	4.[illegible]

Table 30

Screening Parameters for the Atomic Orbitals of FeO

Atomic Orbitals	Screening Parameters
1s (Fe)	25.3810
2s (Fe)	9.2995
$2p\sigma$ (Fe)	11.0444
$2p\pi^{+}$ (Fe)	11.0444
$2p\pi^{-}$ (Fe)	11.0444
1s (O)	7.6579
3s (Fe)	4.5587
$3p\sigma$ (Fe)	4.2593
$3p\pi^{+}$ (Fe)	4.2593
$3p\pi^{-}$ (Fe)	4.2593
2s (O)	2.2458
$2p\pi^{+}$ (O)	2.2266
$2p\pi^{-}$ (O)	2.2266
4s (Fe)	1.3585
$3d\sigma$ (Fe)	3.7266
$3d\delta^{+}$ (Fe)	3.7266
$3d\delta^{-}$ (Fe)	3.7266
$2p\sigma$ (O)	2.2266
$3d\pi^{+}$ (Fe)	3.7266
$3d\pi^{-}$ (Fe)	3.7266

Table 31

Configuration Sizes and Number of States for VCI Calculations of Various Symmetries for FeO

Symmetry	No. of Cfgs. (full CI)	No. of States (to and including first ionic level)
$^1\Sigma$	382	8(+), 4(-)
$^3\Sigma$	528*	13(+), 8(-)
$^5\Sigma$	182	17(+), 10(-)
$^7\Sigma$	18	6(+), 4(-)
$^1\Pi$	348	11
$^3\Pi$	498**	19
$^5\Pi$	166	24
$^7\Pi$	16	9
$^1\Delta$	292	10
$^3\Delta$	396	16
$^5\Delta$	130	19
$^7\Delta$	10	6
$^1\Phi$	204	7
$^3\Phi$	278	10
$^5\Phi$	80	12
$^7\Phi$	6	3
$^1\Gamma$	128	5

* Actual CI used was 329 which included all configurations of the type Fe+O, $Fe^+ + O^-$, and $Fe^{++} + O^{--}$.

**Actual CI used was 157 normal valence (Fe+O) configurations.

Table 31 (Continued)

Symmetry	No. of Cfgs. (full CI)	No. of States (to and including first ionic level)
$^3\Gamma$	158	6
$^5\Gamma$	41	6
$^7\Gamma$	1	1

Table 32

Low-Lying Molecular States of FeO and Their Dissociation Limits

Dissociation Limit	Molecular States
Fe + O	
^5D_g $(3d^6 4s^2)$ + ^3P_g $(2p^4)$	$^3\Sigma^+(1)$, $^5\Sigma^+(1)$, $^7\Sigma^+(1)$, $^3\Sigma^-(2)$, $^5\Sigma^-(2)$, $^7\Sigma^-(2)$, $^3\Pi(3)$, $^5\Pi(3)$, $^7\Pi(3)$, $^3\Delta(2)$, $^5\Delta(2)$, $^7\Delta(2)$, $^3\Phi(1)$, $^5\Phi(1)$, $^7\Phi(1)$.
^5F_g $(3d^7 4s)$ + ^2P_g $(2p^4)$	$^3\Sigma^+(2)$, $^5\Sigma^+(2)$, $^7\Sigma^+(2)$, $^3\Sigma^-(1)$, $^5\Sigma^-(1)$, $^7\Sigma^-(1)$, $^3\Pi(3)$, $^5\Pi(3)$, $^7\Pi(3)$, $^3\Delta(3)$, $^5\Delta(3)$, $^7\Delta(3)$, $^3\Phi(2)$, $^5\Phi(2)$, $^7\Phi(2)$, $^3\Gamma(1)$, $^5\Gamma(1)$, $^7\Gamma(1)$.
^3F_g $(3d^7 4s)$ + ^3P_g $(2p^4)$	$^1\Sigma^+(2)$, $^3\Sigma^+(2)$, $^5\Sigma^+(2)$, $^1\Sigma^-(1)$, $^3\Sigma^-(1)$, $^5\Sigma^-(1)$, $^1\Pi(3)$, $^3\Pi(3)$, $^5\Pi(3)$, $^1\Delta(3)$, $^3\Delta(3)$, $^5\Delta(3)$, $^1\Phi(2)$, $^3\Phi(2)$, $^5\Phi(2)$, $^1\Gamma(1)$, $^3\Gamma(1)$, $^5\Gamma(1)$.

( ) Indicates number of states for specified symmetry.

Table 32 (Continued)

Dissociation Limit	Molecular States
Fe + O	
$^5D_g\ (3d^6 4s^2) + {}^1D_g\ (2p^4)$	$^5\Sigma^+(3),\ ^5\Sigma^-(2),\ ^5\Pi(4),$ $^5\Delta(3),\ ^5\Phi(2),\ ^5\Gamma(1).$
$^5P_g\ (3d^7 4s) + {}^3P_g\ (2p^4)$	$^3\Sigma^+(2),\ ^5\Sigma^+(2),\ ^7\Sigma^+(2),$ $^3\Sigma^-(1),\ ^5\Sigma^-(1),\ ^7\Sigma^-(1),$ $^3\Pi(2),\ ^5\Pi(2),\ ^7\Pi(2),$ $^3\Delta(1),\ ^5\Delta(1),\ ^7\Delta(1).$
$^3P_g\ (3d^6 4s^2) + {}^3P_g\ (2p^4)$	$^1\Sigma^+(2),\ ^3\Sigma^+(2),\ ^5\Sigma^+(2),$ $^1\Sigma^-(1),\ ^3\Sigma^-(1),\ ^5\Sigma^-(1),$ $^1\Pi(2),\ ^3\Pi(2),\ ^5\Pi(2),$ $^1\Delta(1),\ ^3\Delta(1),\ ^5\Delta(1).$
$^3H_g\ (3d^6 4s^2) + {}^3P_g\ (2p^4)$	$^1\Sigma^+(2),\ ^3\Sigma^+(2),\ ^5\Sigma^+(2),$ $^1\Sigma^-(1),\ ^3\Sigma^-(1),\ ^5\Sigma^-(1),$ $^1\Pi(3),\ ^3\Pi(3),\ ^5\Pi(3),$ $^1\Delta(3),\ ^3\Delta(3),\ ^5\Delta(3),\ ^1\Phi(3),$ $^3\Phi(3),\ ^5\Phi(3),\ ^1\Gamma(3),\ ^3\Gamma(3),$ $^5\Gamma(3),\ ^1H(2),\ ^3H(2),\ ^5H(2),$ $^1I(1),\ ^3I(1),\ ^5I(1).$

( ) Indicates number of states for specified symmetry.

Table 32 (Continued)

Dissociation Limit	Molecular States
Fe + O	
^3F_g ($3d^64s^2$) + ^3P_g ($2p^4$)	$^1\Sigma^+$(2), $^3\Sigma^+$ (2), $^5\Sigma^+$ (2), $^1\Sigma^-$(1), $^3\Sigma^-$(1), $^5\Sigma^-$(1), $^1\Pi$ (3), $^3\Pi$ (3), $^5\Pi$ (3), $^1\Delta$(3), $^3\Delta$(3), $^5\Delta$(3), $^1\Phi$ (2), $^3\Phi$ (2), $^5\Phi$ (2), $^1\Gamma$ (1), $^3\Gamma$ (1), $^5\Gamma$ (1).
$Fe^+ + O^-$	
^6S_g ($3d^54s^2$) + ^2P_u($2p^5$)	$^5\Sigma^+$(1), $^5\Pi$ (1), $^7\Sigma^+$ (1), $^7\Pi$ (1)

( ) Indicates number of states for specified symmetry.

Table 33

Energies of Iron and Oxygen Atomic States Representing Dissociation Limits of Low-Lying FeO States

Atomic States	Total Energy (Hartrees) (Calc.)	Energy Relative to $^5D + {}^3P$ (ev)	
		Calc.	Exptl.[a]
$^5D + {}^3P$	-1333.62565	0.0000	0.0000
$^5F + {}^3P$	-1332.83456	21.5268	0.9464
$^3F + {}^3P$	-1332.82818	21.7005	1.5499
$^5D + {}^1D$	-1333.53173	2.5557	1.9673
$^5P + {}^3P$	-1332.73559	24.2200	2.1986
$^3P + {}^3P$	-1333.47896	3.9917	2.3956
$^3H + {}^3P$	-1333.49520	3.5498	2.4298
$^3F + {}^3P$	-1333.47411	4.1236	2.5849
$^6S + {}^2P$	-1333.46338	4.4156	13.297

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[a] C.E. Moore, "Atomic Energy Levels", Nat. Bur. Std. (U.S.) Circ. No. 467(1949)

Table 34

Calculated Energies of Electronic States of FeO.

(Energies are in hartrees; internuclear separations are in bohrs.)

R	$^1\Sigma^+$ I	$^1\Sigma^-$ I	$^1\Sigma^+$ II	$^1\Sigma^+$ III	$^1\Sigma^+$ IV	$^1\Sigma^-$ II
3.0	-1333.56038	-1333.47510	-1333.53884	-1333.43394	-1333.41494	-1333.47136
4.0	-1333.45477	-1333.45099	-1333.44268	-1333.43811	-1333.42567	-1333.44047
7.0	-1333.49308	-1333.49230	-1333.49230	-1333.47930	-1333.47503	-1333.47502
∞	-1333.49520	-1333.49520	-1333.49520	-1333.47896	-1333.47896	-1333.47896

R	$^1\Sigma^-$ III	$^1\Sigma^+$ V	$^1\Sigma^-$ VI	$^3\Sigma^-$ I	$^3\Sigma^+$ I	$^3\Sigma^-$ II
3.0	-1333.40917	-1333.40047	-1333.37769	-1333.46728	-1333.47111	-1333.45593
4.0	-1333.42522	-1333.42430	-1333.47670	-1333.56725	-1333.49283	-1333.49223
7.0	-1333.47118	-1333.47118	-1333.46932	-1333.62362	-1333.62338	-1333.62334
∞	-1333.47411	-1333.47411	-1333.47411	-1333.62565	-1333.62565	-1333.62565

R	$^3\Sigma^+$ II	$^3\Sigma^-$ III	$^3\Sigma^+$ III	$^3\Sigma^+$ IV	$^3\Sigma^+$ V	$^3\Sigma^-$ IV
3.0	-1333.45603	-1333.42146	-1333.41750	-1333.39784	-1333.39614	-1333.40644
4.0	-1333.43168	-1333.43161	-1333.40353	-1333.40099	-1333.39883	-1333.40008
7.0	-1333.49308	-1333.49307	-1333.49229	-1333.47929	-1333.47502	-1333.47502
∞	-1333.49520	-1333.49520	-1333.49520	-1333.47896	-1333.47896	-1333.47896

R	$^3\Sigma^-$ V	$^3\Sigma^+$ VI	$^3\Sigma^+$ VII
3.0	-1333.39523	-1333.37477	-1333.36003
4.0	-1333.39575	-1333.37633	-1333.38067
7.0	-1333.47119	-1333.47118	-1333.46931
∞	-1333.47411	-1333.47411	-1333 47411

Table 34 (Continued)

R	$^5\Sigma^-$ I	$^5\Sigma^+$ I	$^5\Sigma^-$ II	$^5\Sigma^+$ II	$^5\Sigma^+$ III
2.00	-1332.35710	-1332.98587	-1332.28619	-1332.40190	-1332.34040
2.25	-1333.04300	-1333.47247	-1332.91692	-1333.04980	-1332.98433
2.50	-1333.38792	-1333.67707	-1333.26520	-1333.37985	-1333.29140
2.75	-1333.53664	-1333.73600	-1333.42699	-1333.52650	-1333.42817
3.00	-1333.58591	-1333.72878	-1333.48548	-1333.57716	-1333.48612
3.25	-1333.58962	-1333.69630	-1333.49890	-1333.58189	-1333.49282
3.50	-1333.57966	-1333.65796	-1333.52792	-1333.57220	-1333.47961
4.00	-1333.57967	-1333.59676	-1333.56651	-1333.57122	-1333.49364
4.50	-1333.59405	-1333.59489	-1333.58720	-1333.54745	-1333.50502
5.00	-1333.60605	-1333.60629	-1333.60116	-1333.52691	-1333.51493
5.50	-1333.61412	-1333.61424	-1333.61096	-1333.52569	-1333.52170
6.00	-1333.61906	-1333.61913	-1333.61742	-1333.52849	-1333.52593
7.00	-1333.62362	-1333.62362	-1333.62337	-1333.53121	-1333.52965
∞	-1333.62565	-1333.62565	-1333.62565	-1333.53173	-1333.53173

R	$^5\Sigma^-$ III	$^5\Sigma^+$ IV	$^5\Sigma^-$ IV	$^5\Sigma^+$ V	$^5\Sigma^-$ V
2.00	-1332.22735	-1332.29406	-1332.20361	-1332.28913	-1332.15152
2.25	-1332.90742	-1332.93099	-1332.85699	-1332.91964	-1332.78347
2.50	-1333.22236	-1333.26647	-1333.16325	-1333.23499	-1333.12110
2.75	-1333.35608	-1333.42161	-1333.33155	-1333.36392	-1333.30421
3.00	-1333.43461	-1333.46671	-1333.41220	-1333.41833	-1333.38571
3.25	-1333.48358	-1333.47398	-1333.44898	-1333.45102	-1333.41491
3.50	-1333.47669	-1333.47853	-1333.47553	-1333.46737	-1333.42439
4.00	-1333.49244	-1333.47461	-1333.47448	-1333.47235	-1333.44648
4.50	-1333.50433	-1333.49505	-1333.49268	-1333.49266	-1333.46310
5.00	-1333.51457	-1333.50631	-1333.50630	-1333.50520	-1333.47562
5.50	-1333.52156	-1333.51607	-1333.51607	-1333.49676	-1333.48381
6.00	-1333.52585	-1333.52251	-1333.52251	-1333.48880	-1333.48877
7.00	-1333.52961	-1333.52865	-1333.52865	-1333.49310	-1333.49308
∞	-1333.53173	-1333.53173	-1333.53173	-1333.49520	-1333.49520

Table 3 (Continued)

R	$^5\Sigma^+$ VI	$^5\Sigma^+$ VII	$^5\Sigma^+$ VIII	$^5\Sigma^-$ VI	$^5\Sigma^-$ VII
2.00	-1332.20764	-1332.20115	-1332.15708	-1332.10525	-1332.05400
2.25	-1332.90593	-1332.83448	-1332.78924	-1332.74036	-1332.70040
2.50	-1333.21662	-1333.13595	-1333.11184	-1333.09600	-1333.09330
2.75	-1333.33773	-1333.33085	-1333.26555	-1333.29613	-1333.24162
3.00	-1333.39060	-1333.36765	-1333.33893	-1333.36751	-1333.32488
3.25	-1333.41594	-1333.39725	-1333.37933	-1333.41594	-1333.37410
3.50	-1333.42393	-1333.41925	-1333.40985	-1333.41744	-1333.40495
4.00	-1333.44881	-1333.43889	-1333.43843	-1333.43657	-1333.42857
4.50	-1333.46339	-1333.45676	-1333.44541	-1333.44538	-1333.44312
5.00	-1333.47571	-1333.47026	-1333.45770	-1333.45770	-1333.45410
5.50	-1333.48386	-1333.47973	-1333.46672	-1333.46534	-1333.46200
6.00	-1333.48616	-1333.48439	-1333.47315	-1333.47076	-1333.46690
7.00	-1333.49230	-1333.47930	-1333.47504	-1333.47504	-1333.47120
∞	-1333.49520	-1333.47896	-1333.47896	-1333.47896	-1333.47411

R	$^5\Sigma^+$ IX	$^5\Sigma^+$ X	$^5\Sigma^+$ XI	$^5\Sigma^-$ (71)	$^5\Sigma^+$ (72)
2.00	-1331.97019	-1331.91161	-1331.85726	-1331.09811	-1331.09271
2.25	-1332.69562	-1332.59244	-1332.69562	-1331.94151	-1331.94524
2.50	-1333.09323	-1333.02692	-1333.09322	-1332.38851	-1332.46139
2.75	-1333.24283	-1333.23382	-1333.17141	-1332.59015	-1332.66253
3.00	-1333.31468	-1333.28539	-1333.31468	-1332.65962	-1332.72307
3.25	-1333.37721	-1333.36247	-1333.35083	-1332.70148	-1332.70850
3.50	-1333.39739	-1333.38957	-1333.38603	-1332.76019	-1332.76019
4.00	-1333.42693	-1333.41739	-1333.41739	-1332.81387	-1332.81374
4.50	-1333.44265	-1333.43367	-1333.42941	-1332.83076	-1332.83069
5.00	-1333.44702	-1333.44702	-1333.44054	-1332.83495	-1332.83492
5.50	-1333.45672	-1333.45672	-1333.44846	-1332.83516	-1332.83514
6.00	-1333.46316	-1333.46316	-1333.45334	-1332.83458	-1332.83456
7.00	-1333.46338	-1333.46338	-1333.46338	-1332.83411	-1332.83410
∞	-1333.47411	-1333.47411	-1333.46338	-1332.83456	-1332.83456

Table 34 (Continued)

R	$^5\Sigma^+$ (73)	$^5\Sigma^-$ (74)	$^5\Sigma^+$ (75)	$^5\Sigma^+$ (76)	$^5\Sigma^+$ (82)
2.0	-1331.07463	-1331.01188	-1331.01447	-1331.00622	-1330.93686
2.25	-1331.93946	-1331.89026	-1331.91594	-1331.77915	-1331.70693
2.50	-1332.39482	-1332.31053	-1332.35819	-1332.23636	-1332.13893
2.75	-1332.59423	-1332.50907	-1332.55149	-1332.44801	-1332.40383
3.00	-1332.66142	-1332.60222	-1332.62327	-1332.60059	-1332.50999
3.25	-1332.70271	-1332.70148	-1332.69746	-1332.69014	-1332.60904
3.50	-1332.75982	-1332.73424	-1332.75613	-1332.74532	-1332.65919
4.00	-1332.80297	-1332.78503	-1332.79070	-1332.78513	-1332.70393
4.50	-1332.81771	-1332.80496	-1332.80677	-1332.80490	-1332.72233
5.00	-1332.82427	-1332.81509	-1332.81511	-1332.81504	-1332.73112
5.50	-1332.82812	-1332.82157	-1332.82105	-1332.82019	-1332.73537
6.00	-1332.83054	-1332.82448	-1332.82446	-1332.82323	-1332.73573
7.00	-1332.83285	-1332.82683	-1332.82682	-1332.82585	-1332.73524
∞	-1332.83456	-1332.82818	-1332.82818	-1332.82818	-1332.73559

R	$^5\Sigma^-$ (83)	$^5\Sigma^+$ (84)	$^7\Sigma^-$ I	$^7\Sigma^+$ 1	$^7\Sigma^-$ II
2.0	-1330.94625	-1330.09646	-1331.77539	-1332.48129	-1331.68339
2.25	-1331.69444	-1331.64713	-1332.55921	-1333.11906	-1332.50390
2.50	-1332.21438	-1332.09655	-1332.99027	-1333.42906	-1332.96036
2.75	-1332.40683	-1332.34763	-1333.23493	-1333.56335	-1333.19486
3.00	-1332.55818	-1332.50757	-1333.38315	-1333.61096	-1333.36957
3.25	-1332.60996	-1332.60295	-1333.47069	-1333.61764	-1333.46510
3.50	-1332.65938	-1332.65791	-1333.52101	-1333.60711	-1333.51740
4.00	-1332.70447	-1332.70143	-1333.56964	-1333.58445	-1333.56516
4.50	-1332.72239	-1332.71893	-1333.59246	-1333.59386	-1333.58702
5.00	-1332.73114	-1332.72545	-1333.60588	-1333.60619	-1333.60114
5.50	-1332.73537	-1332.72925	-1333.61416	-1333.61430	-1333.61095
6.00	-1332.73563	-1332.73162	-1333.61910	-1333.61918	-1333.61742
7.00	-1332.73520	-1332.73384	-1333.62362	-1333.62342	-1333.62338
∞	-1332.73559	-1332.73559	-1333.62565	-1333.62565	-1333.62565

Table 34 (Continued)

R	$^7\Sigma^+$ II	$^7\Sigma^+$ V	$^7\Sigma^-$ IV	$^7\Sigma^+$ VI	$^7\Sigma^+$ VII
2.00	-1332.32987	-1331.35172	-1331.04002	-1331.03909	-1330.79639
2.25	-1332.95515	-1332.16092	-1331.77694	-1331.77415	-1331.65874
2.50	-1332.24907	-1332.59467	-1332.20766	-1332.20519	-1332.15927
2.75	-1332.36378	-1332.80382	-1332.45650	-1332.45810	-1332.43940
3.00	-1332.39813	-1332.87956	-1332.60795	-1332.61707	-1332.59998
3.25	-1332.44812	-1332.87742	-1332.69741	-1332.71202	-1332.69333
3.50	-1332.49976	-1332.83417	-1332.74753	-1332.76419	-1332.74525
4.00	-1332.54356	-1332.80662	-1332.79206	-1332.79186	-1332.70916
4.50	-1332.53157	-1332.82017	-1332.80974	-1332.80966	-1332.72154
5.00	-1332.51291	-1332.82618	-1332.81940	-1332.81937	-1332.72741
5.50	-1332.49743	-1332.82952	-1332.82552	-1332.82550	-1332.73066
6.00	-1333.48447	-1332.83145	-1332.82937	-1332.82935	-1332.73254
7.00	-1333.46338	-1332.83313	-1332.83291	-1332.83290	-1332.73416
∞	-1333.46338	-1332.83456	-1332.83456	-1332.83456	-1332.73559

R	$^7\Sigma^+$ VIII	$^7\Sigma^-$ V
2.00	-1330.69472	-1330.71952
2.25	-1331.58142	-1331.56505
2.50	-1332.08668	-1332.05608
2.75	-1332.36494	-1332.33934
3.00	-1332.52527	-1332.50255
3.25	-1332.61789	-1332.59511
3.50	-1332.66804	-1332.64671
4.00	-1332.70823	-1332.69265
4.50	-1332.71105	-1332.71072
5.00	-1332.72068	-1332.72047
5.50	-1332.72674	-1332.72661
6.00	-1332.73054	-1332.73046
7.00	-1332.73401	-1332.73401
∞	-1332.73559	-1332.73559

Table 34 (Continued)

R	$^{1}\Pi$ I	$^{1}\Pi$ II	$^{1}\Pi$ III	$^{1}\Pi$ IV
2.5	-1333.52455	-1333.35602	-1333.33215	-1333.3[illegible]
3.0	-1333.50244	-1333.48505	-1333.46693	-1333.4574[illegible]
3.5	-1333.45377	-1333.46218	-1333.45028	-1333.44223
4.0	-1333.46403	-1333.45137	-1333.44020	-1333.43776
5.0	-1333.47569	-1333.47556	-1333.46998	-1333.46299
7.0	-1333.49511	-1333.49294	-1333.49226	-1333.48015
∞	-1333.49520	-1333.49520	-1333.49520	-1333.47896

R	$^{1}\Pi$ V	$^{1}\Pi$ VI	$^{1}\Pi$ VII	$^{1}\Pi$ VIII
2.5	-1333.28339	-1333.27435	-1333.26716	-1333.26014
3.0	-1333.44289	-1333.43223	-1333.40801	-1333.39866
3.5	-1333.43543	-1333.41376	-1333.40382	-1333.40169
4.0	-1333.43579	-1333.42369	-1333.42144	-1333.41963
5.0	-1333.45629	-1333.45271	-1333.45183	-1333.44793
7.0	-1333.47415	-1333.47342	-1333.47035	-1333.47016
∞	-1333.47896	-1333.47411	-1333.47411	-1333.47411

Table 34 (Continued)

R	$^3\Pi$ I	$^3\Pi$ II	$^3\Pi$ III	$^3\Pi$ IV
3.0	-1333.49289	-1333.46253	-1333.38360	-1333.37743
4.0	-1333.57943	-1333.49356	-1333.46514	-1333.42621
7.0	-1333.62436	-1333.6231	-1333.62248	-1333.49293
∞	-1333.62565	-1333.62565	-1333.62565	-1333.49520

R	$^3\Pi$ V	$^3\Pi$ VI	$^3\Pi$ VII	$^3\Pi$ VIII
3.0	-1333.36959	-1333.36052	-1333.34240	-1333.32750
4.0	-1333.42597	-1333.40747	-1333.40681	-1333.40251
7.0	-1333.49276	-1333.49225	-1333.47998	-1333.4741
∞	-1333.49520	-1333.49520	-1333.47896	-1333.47896

R	$^3\Pi$ IX	$^3\Pi$ X	$^3\Pi$ XI
3.0	-1333.32426	-1333.32009	-1333.31140
4.0	-1333.39033	-1333.38281	-1333.38232
7.0	-1333.47324	-1333.47034	-1333.46998
∞	-1333.47411	-1333.47411	-1333.47411

Table 34 (Continued)

R	$^5\Pi$ I	$^5\Pi$ II	$^5\Pi$ III	$^5\Pi$ IV	$^5\Pi$ V
2.00	-1332.69868	-1332.56269	-1332.44998	-1332.44553	-1332.42165
2.25	-1333.26839	-1333.12411	-1333.09529	-1333.01289	-1333.00570
2.50	-1333.53641	-1333.41520	-1333.38501	-1333.30413	-1333.27708
2.75	-1333.65000	-1333.54860	-1333.48620	-1333.46672	-1333.45096
3.00	-1333.68725	-1333.58923	-1333.52902	-1333.51680	-1333.51206
3.25	-1333.68491	-1333.58850	-1333.55004	-1333.52329	-1333.51066
3.50	-1333.66347	-1333.57720	-1333.55413	-1333.53167	-1333.50077
4.00	-1333.61365	-1333.57857	-1333.56883	-1333.55492	-1333.49776
4.50	-1333.59956	-1333.59357	-1333.58673	-1333.54572	-1333.50844
5.00	-1333.60794	-1333.60580	-1333.60018	-1333.52555	-1333.51773
5.50	-1333.61450	-1333.61399	-1333.60988	-1333.52372	-1333.52346
6.00	-1333.62031	-1333.61899	-1333.61632	-1333.52718	-1333.52714
7.00	-1333.62456	-1333.62336	-1333.62249	-1333.53080	-1333.53002
∞	-1333.62565	-1333.62565	-1333.62565	-1333.53173	-1333.53173

R	$^5\Pi$ VI	$^5\Pi$ VII	$^5\Pi$ VIII	$^5\Pi$ IX	$^5\Pi$ X
2.00	-1332.30373	-1332.17532	-1332.14217	-1332.11108	-1332.09399
2.25	-1332.92338	-1332.89865	-1332.88339	-1332.85060	-1332.83493
2.50	-1333.27485	-1333.26881	-1333.23012	-1333.21822	-1333.18248
2.75	-1333.40617	-1333.39725	-1333.39457	-1333.36932	-1333.32345
3.00	-1333.47363	-1333.46541	-1333.44081	-1333.40061	-1333.38661
3.25	-1333.48840	-1333.47839	-1333.46244	-1333.44572	-1333.41059
3.50	-1333.48278	-1333.47710	-1333.46805	-1333.46037	-1333.43549
4.00	-1333.49218	-1333.47850	-1333.46658	-1333.45594	-1333.44641
4.50	-1333.50407	-1333.49765	-1333.49122	-1333.46423	-1333.46287
5.00	-1333.51442	-1333.50892	-1333.50535	-1333.47573	-1333.47562
5.50	-1333.52146	-1333.51599	-1333.50039	-1333.48386	-1333.48373
6.00	-1333.52580	-1333.52239	-1333.48881	-1333.48866	-1333.48736
7.00	-1333.52960	-1333.52856	-1333.49313	-1333.49295	-1333.49226
∞	-1333.53173	-1333.53173	-1333.49520	-1333.49520	-1333.49520

Table 34 (Continued)

R	$^5\Pi$ XI	$^5\Pi$ XII	$^5\Pi$ XII	$^5\Pi$ XIV	$^5\Pi$ XV
2.00	-1332.08745	-1332.03778	-1332.02304	-1332.01143	-1331.91789
2.25	-1332.77590	-1332.75717	-1332.74503	-1332.64931	-1332.60988
2.50	-1333.14270	-1333.12999	-1333.09759	-1332.99851	-1332.97305
2.75	-1333.30204	-1333.29646	-1333.25679	-1333.23304	-1333.18097
3.00	-1333.37776	-1333.34506	-1333.33272	-1333.32286	-1333.30145
3.25	-1333.40426	-1333.37757	-1333.37149	-1333.36745	-1333.35828
3.50	-1333.42361	-1333.40788	-1333.40662	-1333.39691	-1333.38663
4.00	-1333.44401	-1333.43850	-1333.43290	-1333.42910	-1333.42061
4.50	-1333.45661	-1333.45224	-1333.44478	-1333.44003	-1333.43846
5.00	-1333.47000	-1333.46313	-1333.45625	-1333.45270	-1333.45186
5.50	-1333.47968	-1333.47103	-1333.46425	-1333.46155	-1333.46090
6.00	-1333.48612	-1333.47590	-1333.46915	-1333.46799	-1333.46586
7.00	-1333.48017	-1333.47451	-1333.47343	-1333.47235	-1333.47017
∞	-1333.47896	-1333.47896	-1333.47411	-1333.47411	-1333.47411

R	$^5\Pi$ XVI	$^5\Pi$ LXV	$^5\Pi$ LXVI	$^5\Pi$ LXVII	$^5\Pi$ LXVIII
2.00	-1331.90024	---	---	---	---
2.25	-1332.59456	-1331.01637	-1331.96947	-1331.91630	-1331.85794
2.50	-1332.96914	-1331.48958	-1331.48762	-1331.42855	-1331.33816
2.75	-1333.16982	---	-1331.66340	-1331.62436	-1331.56618
3.00	-1333.29246	-1331.77164	-1331.70401	-1331.68923	-1331.64661
3.25	-1333.35245	-1331.73953	-1331.70963	-1331.70240	-1331.69594
3.50	-1333.38068	-1331.76400	-1331.75680	-1331.75417	-1331.74516
4.00	-1333.41821	-1331.81469	-1331.81238	-1331.80304	-1331.79875
4.50	-1333.43407	-1331.83094	-1331.83057	-1331.81605	-1331.80709
5.00	-1333.44792	-1331.83554	-1331.83452	-1331.82470	-1331.81565
5.50	-1333.45772	-1331.83583	-1331.83469	-1331.82858	-1331.82171
6.00	-1333.46218	-1331.83525	-1331.83410	-1331.83101	-1331.82514
7.00	-1333.46560	-1331.83478	-1331.83364	-1331.83331	-1331.82751
∞	-1333.46338	-1331.83456	-1331.83456	-1331.83456	-1331.82818

Table 34 (Continued)

R	$^5\Pi$ LXIX	$^5\Pi$ LXX	$^5\Pi$ LXXVI	$^5\Pi$ LXXVII	$^7\Pi$ I
2.00	---	---	---	---	---
2.25	-1331.83119	-1331.76212	-1331.65695	-1331.65170	-1333.04389
2.50	-1331.28585	-1331.19302	-1332.21149	-1331.11118	-1333.42981
2.75	-1331.49794	-1331.44686	-1332.36218	---	-1333.60924
3.00	-1331.63587	-1331.60873	-1332.51559	-1331.51292	-1333.67671
3.25	-1331.69194	-1331.68900	-1332.61013	-1331.60894	-1333.68673
3.50	-1331.73551	-1331.73272	-1332.65825	-1331.65753	-1333.67055
4.00	-1331.78525	-1331.78458	-1332.70402	-1331.70289	---
4.50	-1331.80522	-1331.80464	-1332.72213	-1331.71901	-1333.62408
5.00	-1331.81551	-1331.81465	-1332.73023	-1331.72573	-1333.60397
5.50	-1331.82064	-1331.82061	-1332.73434	-1331.72962	-1333.60870
6.00	-1331.82401	-1331.82369	-1332.73492	-1331.73207	-1333.62039
7.00	-1331.82637	-1331.82631	-1332.73450	-1331.73438	-1333.62458
∞	-1332.82818	-1332.82818	-1332.73559	-1332.73559	-1333.62565

R	$^7\Pi$ II	$^7\Pi$ III	$^7\Pi$ IV	$^7\Pi$ VIII	$^7\Pi$ IX
2.25	-1332.61728	-1332.61204	-1332.56493	-1331.78421	-1331.70241
2.50	-1333.02198	-1333.00176	-1332.98885	-1332.21376	-1332.16809
2.75	-1333.24631	-1333.22966	-1333.22032	-1332.46252	-1332.44939
3.00	-1333.38983	-1333.38689	-1333.30885	-1332.61544	-1332.61299
3.25	-1333.47686	-1333.47222	-1333.38973	-1332.71121	-1332.70207
3.50	-1333.52455	-1333.52096	-1333.45431	-1332.76355	-1332.75121
4.00	-1333.56975	-1333.56674	-1333.51891	-1332.80655	-1332.79331
4.50	-1333.59202	-1333.58672	-1333.53112	-1332.82048	-1332.80974
5.00	-1333.60563	-1333.60020	-1333.51687	-1332.82661	-1332.81987
6.00	-1333.61904	-1333.61632	-1333.48741	-1332.83191	-1332.83002
7.00	-1333.62337	-1333.62244	-1333.46561	-1332.83360	-1332.83358
∞	-1333.62565	-1333.62565	-1333.46338	-1332.83456	-1332.83456

Table 34 (Continued)

R	$^7\Pi$ X	$^7\Pi$ XI	$^7\Pi$ XII
2.25	-1331.68408	-1331.60688	-1331.45497
2.50	-1332.13546	-1332.12331	-1332.01789
2.75	-1332.41844	-1332.37648	-1332.33504
3.00	-1332.58888	-1332.52081	-1332.51186
3.25	-1332.68525	-1332.61101	-1332.60484
3.50	-1332.73966	-1332.66380	-1332.65212
4.00	-1332.78970	-1332.70733	-1332.69319
4.50	-1332.80956	-1332.72145	-1332.70984
5.00	-1332.81903	-1332.72764	-1332.71945
6.00	-1332.82890	-1332.73298	-1332.72964
7.00	-1332.83245	-1332.73468	-1332.73328
∞	-1332.83456	-1332.73559	-1332.73559

R	$^1\Delta$ I	$^1\Delta$ II	$^1\Delta$ III	$^1\Delta$ IV
3.0	-1333.53656	-1333.52466	-1333.49851	-1333.47347
4.0	-1333.45499	-1333.45135	-1333.44148	-1333.43874
7.0	-1333.49308	-1333.49257	-1333.49211	-1333.47503
∞	-1333.49520	-1333.49520	-1333.49520	-1333.47896

R	$^1\Delta$ V	$^1\Delta$ VI	$^1\Delta$ VII
3.0	-1333.41905	-1333.40247	-1333.39725
4.0	-1333.43352	-1333.42556	-1333.41712
7.0	-1333.47420	-1333.47258	-1333.47118
∞	-1333.47411	-1333.47411	-1333.47411

Table 34 (Continued)

R	$^3\Delta$ I	$^3\Delta$ II	$^3\Delta$ III	$^3\Delta$ IV	$^3\Delta$ IV
2.50	-1333.56943	-1333.48018	-1333.39581	-1333.32261	-1333.30220
2.75	-1333.63501	-1333.55454	-1333.47627	-1333.46056	-1333.42959
3.00	-1333.63725	-1333.56290	-1333.50676	-1333.48238	-1333.47665
3.25	-1333.61815	-1333.55008	-1333.49757	-1333.48392	-1333.47431
3.50	-1333.59779	-1333.54558	-1333.47849	-1333.47109	-1333.45658
4.00	-1333.58562	-1333.55799	-1333.45771	-1333.45012	-1333.43863
4.50	-1333.59529	-1333.58659	-1333.46444	-1333.46358	-1333.45622
5.00	-1333.60626	-1333.60023	-1333.47566	-1333.47542	-1333.46978
6.00	-1333.61906	-1333.61645	-1333.48875	-1333.48827	-1333.48596
7.00	-1333.62338	-1333.62259	-1333.49308	-1333.49257	-1333.49211
∞	-1333.62565	-1333.62565	-1333.49520	-1333.49520	-1333.49520

R	$^3\Delta$XI	$^3\Delta$ VII	$^3\Delta$ VIII	$^3\Delta$ IX
2.50	-1333.29881	-1333.28855	-1333.28209	-1333.27371
2.75	-1333.42596	-1333.41128	-1333.40134	-1333.39168
3.0	-1333.47008	-1333.46896	-1333.44906	-1333.43926
3.25	-1333.47104	-1333.46576	-1333.45358	-1333.44611
3.50	-1333.45445	-1333.45152	-1333.44534	-1333.42407
4.0	-1333.43707	-1333.43326	-1333.43056	-1333.42292
4.5	-1333.44670	-1333.44499	-1333.44217	-1333.43650
5.0	-1333.45790	-1333.45682	-1333.45385	-1333.45022
6.0	-1333.47073	-1333.46987	-1333.46686	-1333.46642
7.0	-1333.47503	-1333.47420	-1333.47258	-1333.47118
∞	-1333.47896	-1333.47411	-1333.47411	-1333.47411

Table 34 (Continued)

R	$^5\Delta$ I	$^5\Delta$ II	$^5\Delta$ III	$^5\Delta$ IV	$^5\Delta$ V	$^5\Delta$ VI
2.0	-1332.67106	-1332.55790	-1332.42881	-1332.36278	-1332.30169	-1332.24598
2.5	-1333.41[illegible]12	-1333.39234	-1333.33943	-1333.32158	-1333.29323	-1333.24392
3.0	-1333.53767	-1333.52604	-1333.51615	-1333.49748	-1333.43529	-1333.42519
3.5	-1333.58052	-1333.54020	-1333.49870	-1333.49166	-1333.47991	-1333.46060
7.0	-1333.62339	-1333.62259	-1333.52995	-1333.52969	-1333.52961	-1333.49309
∞	-1333.625[illegible]	-1333.[illegible]	-1333.53173	-1333.53173	-1333.53173	-1333.49520

R	$^5\Delta$ VII	$^5\Delta$ VIII	$^5\Delta$ IX	$^5\Delta$ X	$^5\Delta$ XI	$^5\Delta$ XII
2.0	-1332.17169	-1332.169[illegible]	-1332.01148	-1331.92254	-1331.90275	-1331.87562
2.5	-1333.22490	-1333.11959	-1333.10183	-1333.06090	-1333.01154	-1332.99740
3.0	-1333.40783	-1333.38772	-1333.37056	-1333.33165	-1333.32274	-1333.29085
3.5	-1333.43854	-1333.42488	-1333.40766	-1333.39608	-1333.39472	-1333.38737
7.0	-1333.49253	-1333.49211	-1333.47504	-1333.47421	-1333.47258	-1333.47119
∞	-1333.49520	-1333.49520	-1333.47896	-1333.47411	-1333.47411	-1333.47411

R	$^7\Delta$ I	$^7\Delta$ II	$^7\Delta$ V	$^7\Delta$ VI	$^7\Delta$ VII	$^7\Delta$ VIII
2.0	-1332.68411	-1332.56388	-1331.79160	-1331.73647	-1331.58469	-1331.56875
2.5	-1333.03512	-1332.99357	-1332.22130	-1332.18666	-1332.12737	-1332.05788
3.0	-1333.39978	-1333.38425	-1332.61603	-1332.61231	-1332.60317	-1332.50271
3.5	-1333.52723	-1333.52131	-1332.76265	-1332.75063	-1332.74655	-1332.64701
7.0	-1333.62340	-1333.62259	-1332.83429	-1332.83291	-1332.83243	-1332.73403
∞	-1333.62565	-1333.62565	-1332.83456	-1332.83456	-1332.83456	-1332.73559

Table 34 (Continued)

R	$^1\Phi$ I	$^1\Phi$ II	$^1\Phi$ III	$^1\Phi$ IV
3.0	-1333.55960	-1333.49924	-1333.48163	-1333.46182
4.0	-1333.45643	-1333.45281	-1333.43898	-1333.43528
7.0	-1333.49294	-1333.49172	-1333.49158	-1333.47342
∞	-1333.49520	-1333.49520	-1333.49520	-1333.47411

R	$^1\Phi$ V	$^3\Phi$ I	$^3\Phi$ II	$^3\Phi$ III
3.0	-1333.41303	-1333.64158	-1333.53989	-1333.51768
4.0	-1333.42721	-1333.58372	-1333.45809	-1333.45304
7.0	-1333.47338	-1333.62335	-1333.49244	-1333.49172
∞	-1333.47411	-1333.62565	-1333.49520	-1333.49520

R	$^3\Phi$ IV	$^3\Phi$ V	$^3\Phi$ VI
3.0	-1333.49301	-1333.46369	-1333.45744
4.0	-1333.43739	-1333.43585	-1333.43052
7.0	-1333.49158	-1333.47348	-1333.47338
∞	-1333.49520	-1333.47411	-1333.47411

Table 34 (Continued)

R	$^5\Phi$ I	$^5\Phi$ II	$^5\Phi$ III	$^5\Phi$ V
2.25	-1333.10034	-1333.01455	-1332.90666	-1332.86673
2.50	-1333.41829	-1333.29157	-1333.24964	-1333.22962
3.00	-1333.58973	-1333.49465	-1333.47906	-1333.44866
3.50	-1333.57720	-1333.49180	-1333.48812	-1333.47281
7.00	-1333.62336	-1333.52968	-1333.52856	-1333.49295
∞	-1333.62565	-1333.53173	-1333.53173	-1333.49520

R	$^5\Phi$ V	$^5\Phi$ VI	$^5\Phi$ VII	$^5\Phi$ VIII
2.25	-1332.84353	-1332.75848	-1332.67468	-1332.58895
2.50	-1333.18686	-1333.09622	-1332.99999	-1332.98833
3.00	-1333.35240	-1333.32338	-1333.30434	-1333.28952
3.50	-1333.42227	-1333.40979	-1333.40516	-1333.39237
7.00	-1333.49172	-1333.49160	-1333.47344	-1333.47338
∞	-1333.49520	-1333.49520	-1333.47411	-1333.47411

R	$^7\Phi$ I	$^7\Phi$ III	$^7\Phi$ IV
2.25	-1332.62011	-1331.69625	-1331.62318
2.50	-1333.02342	-1332.18268	-1332.13021
3.00	-1333.38875	-1332.62123	-1332.58903
3.50	-1333.52120	-1332.76578	-1332.73972
7.00	-1333.62337	-1332.83359	-1332.83319
∞	-1333.62565	-1332.83456	-1332.83456

Table 34 (Continued)

R	$^{1}\Gamma$ I	$^{1}\Gamma$ II	$^{1}\Gamma$ III	$^{1}\Gamma$ IV	$^{3}\Gamma$ I
3.0	-1333.53849	-1333.48855	-1333.43075	-1333.40524	-1333.58607
4.0	-1333.45872	-1333.45379	-1333.43516	-1333.43262	-1333.45712
7.0	-1333.49257	-1333.49071	-1333.48950	-1333.47420	-1333.49257
∞	-1333.49520	-1333.49520	-1333.49520	-1333.47411	-1333.49520

R	$^{3}\Gamma$ II	$^{3}\Gamma$ III	$^{3}\Gamma$ IV	$^{7}\Gamma$ I
3.0	-1333.49191	-1333.48280	-1333.45248	-1332.61899
4.0	-1333.45515	-1333.43638	-1333.43368	-1332.79297
7.0	-1333.49071	-1333.48950	-1333.47420	-1332.83243
∞	-1333.49520	-1333.49520	-1333.47411	-1332.83243

R	$^{5}\Gamma$ I	$^{5}\Gamma$ II	$^{5}\Gamma$ III	$^{5}\Gamma$ IV	$^{5}\Gamma$ V
2.25	-1332.94254	-1332.92368	-1332 79591	-1332.68459	-1332.59880
2.50	-1333.28313	-1333.24789	-1333.09812	-1333.08799	-1332.96820
3.0	-1333.50702	-1333.42451	-1333.36916	-1333.28618	-1333.25942
3.5	-1333.49926	-1333.43086	-1333.42626	-1333.39508	-1333.38771
7.0	-1333.52866	-1333.49258	-1333.49071	-1333.48951	-1333.47421
∞	-1333.53173	-1333.49520	-1333.49520	-1333.49520	-1333.47411

Table 35

Calculated and Experimental Spectroscopic Constants for Bound States of FeO

State		$T_e(\mathrm{cm}^{-1})$	$D_e(\mathrm{ev})$	$D_o^o(\mathrm{ev})$	$r_e(\mathrm{\AA})$	$\omega_e(\mathrm{cm}^{-1})$	$\omega_eX_e(\mathrm{cm}^{-1})$	$B_e(\mathrm{cm}^{-1})$	$\alpha_e(\mathrm{cm}^{-1})$
$X^5\Sigma^+$ I	Exp.[a]	0.	3.97	3.92	1.63	880.53	4.63	0.51	0.0038
$^5\Pi$ I	Calc.	10971.	6.16	6.10	1.64	1015.4	5.86	0.50	0.0028
	Exp.[c]	10406.							
$^7\Pi$ I	Calc.	13230.	6.10	6.04	1.69	1042.4	8.82	0.48	0.0036
	Exp.[a]					955.			
$^5\Sigma^-$ I	Calc.	16215.	1.62	1.56	1.67	890.3	20.77	0.49	0.0072
$^5\Pi$ II	Calc.	16134.	1.63	1.58	1.64	919.8	20.21	0.50	0.0072
	Exp.[a]	17263.				827.	2.00		
$^5\Sigma^+$ II	Calc.[b]	18231.	1.40	1.35	1.67	888.94	20.74	0.48	0.0069
	Exp.[a]	17909. 17989.	-	-	1.69	667.	-	0.47	-

Table 35 (Continued)

State		$T_e(cm^{-1})$	$D_e(ev)$	$D_o^o(ev)$	$r_e(\AA)$	$\omega_e(cm^{-1})$	$\omega_ex_e(cm^{-1})$	$B_e(cm^{-1})$	$\alpha_e(cm^{-1})$
$^7\Sigma^+$ I	Calc.	26299.	4.21	4.16	1.68	826.7	6.82	0.48	0.0051
	Exp.[a]	-	-	-	-	670.0	-	-	-

a. B. Rosen (Director), *Spectroscopic Data Relative to Diatomic Molecules*, Pergamon Press, New York, 1970.

b. Dissociation limit of curve taken to be $^5D + {}^1D$.

c. T. Wentick, unpublished results.

Table 36

Calculated Oscillator Strengths ($f_{v'v''}$) for the Vibrational-Rotational Transition of FeO ($X\ ^5\Sigma^+\ I - X\ ^5\Sigma^+\ I$)

v'/v"	0	1	2	3	4	5
0						
1	6.523-06					
2	8.693-08	1.296-05				
3	4.012-09	2.578-07	1.921-05			
4	3.584-10	1.198-08	4.901-07	2.523-05		
5	2.752-12	5.181-10	2.369-08	7.801-07	3.110-05	
6	1.298-10	6.707-11	8.410-10	4.380-08	1.114-06	3.695-05
7	9.339-11	2.861-10	2.712-11	1.311-09	7.944-08	1.432-06
8	2.206-12	6.916-11	3.361-10	3.287-11	8.589-10	1.454-07
9	3.801-11	7.638-12	3.703-11	6.320-10	4.395-10	2.028-10
10	5.928-11	9.773-11	6.648-12	1.169-10	6.099-10	4.098-10

v'/v"	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6					
7	4.301-05				
8	1.687-06	4.936-05			
9	2.445-07	1.949-06	5.546-05		
10	1.394-09	3.130-07	2.396-06	6.069-05	

Table 37

Calculated Oscillator Strengths
($f_{v'v''}$) for the Orange System of FeO
($^5\Sigma^+$II - X $^5\Sigma^+$I)

v'/v"	0	1	2	3	4	5
0	4.043-03	3.076-03	1.326-03	3.534-04	6.404-05	7.697-06
1	2.083-03	8.002-04	2.998-03	2.452-03	9.332-04	2.155-04
2	4.106-04	2.306-03	3.808-05	2.196-03	3.151-03	1.594-03
3	2.501-05	8.372-04	1.995-03	5.652-05	1.428-03	3.529-03
4	2.683-07	7.159-05	1.173-03	1.608-03	2.490-04	8.672-04
5	1.433-06	1.148-06	1.260-04	1.411-03	1.282-03	4.200-04
6	3.444-07	6.579-06	3.565-06	1.744-04	1.571-03	1.044-03
7	1.140-08	1.767-06	1.802-05	9.315-06	2.081-04	1.669-03
8	2.211-09	5.004-08	4.947-06	3.777.05	2.155-05	2.221-04
9	1.903-09	2.847-08	7.926-08	1.004-05	6.733-05	4.492-05
10	4.027-10	2.574-08	1.737-07	5.335-08	1.646-05	1.082-04

v'/v"	6	7	8	9	10
0	6.178-07	3.464-08	1.896-09	1.285-10	3.961-11
1	3.073-05	2.867-06	1.836-07	1.577-08	4.804-10
2	4.488-04	7.357-05	8.026-06	5.867-07	4.344-08
3	2.256-03	7.530-04	1.380-04	1.697-05	1.155-06
4	3.746-03	2.896-03	1.117-03	2.204-04	2.843-05
5	5.039-04	3.918-03	3.506-03	1.513-03	3.091-04
6	5.270-04	2.816-04	4.096-03	4.069-03	1.922-03
7	8.892-04	5.855-04	1.485-04	4.307-03	4.586-03
8	1.710-03	8.032-04	6.150-04	7.318-05	4.592-03
9	2.138-04	1.704-03	7.614-04	6.348-04	3.502-05
10	8.298-05	1.517-04	1.669-03	7.410-04	6.493-04

Table 38

Calculated Franck-Condon Factors ($q_{v'v''}$) for the Orange System of FeO ($^5\Sigma^+$II - X$^5\Sigma^+$I)

v'/v"	0	1	2	3	4	5
0	5.430-01	3.188-01	1.108-01	2.311-02	3.231-03	2.789-04
1	3.544-01	1.006-01	2.852-01	1.914-01	5.656-02	1.012-02
2	9.234-02	3.739-01	4.594-03	1.883-01	2.294-01	8.896-02
3	9.151-03	1.794-01	3.103-01	5.645-03	1.067-01	2.397-01
4	1.563-05	2.478-02	2.412-01	2.430-01	2.295-02	5.272-02
5	7.661-04	2.762-05	4.217-02	2.799-01	1.913-01	3.469-02
6	1.160-04	1.195-03	7.088-06	3.020-01	3.020-01	1.364-01
7	8.982-06	5.544-04	3.253-03	6.778-02	6.778-02	3.123-01
8	4.185-07	3.944-05	1.527-03	4.415-04	4.415-04	7.182-02
9	1.280-06	4.553-06	9.148-05	1.276-02	1.276-02	1.926-03
10	3.033-07	9.466-06	2.570-05	5.368-03	5.368-03	2.095-02

v'/v"	6	7	8	9	10
0	1.568-05	4.125-07	6.496-09	1.059-10	1.060-10
1	1.004-03	6.350-05	1.515-06	3.922-08	8.237-10
2	1.948-02	2.118-03	1.501-04	2.997-06	1.456-07
3	1.148-01	2.993-02	3.413-03	2.731-04	3.829-06
4	2.366-01	1.325-01	4.046-02	4.622-03	4.288-04
5	2.161-02	2.299-01	1.427-01	5.055-02	5.496-03
6	3.808-02	6.116-03	2.248-01	1.463-01	6.009-02
7	1.347-01	3.556-02	4.549-04	2.240-01	1.446-01
8	3.139-01	1.219-01	3.038-02	6.462-04	2.286-01
9	6.917-02	3.077-03	1.147-01	3.396-02	4.003-03
10	5.471-03	6.059-02	2.941-01	1.100-01	1.664-02

Table 39

Calculated R-Centroid Factors
$(\langle \overleftrightarrow{a} \rangle_{v'v''})$ for the Vibrational-Rotational
Transition of FeO $(X\,^5\Sigma^+ I - X\,^5\Sigma^+ I)$

v'/v"	0	1	2	3	4	5
0	1.630+00					
1	3.931-02	1.639+00				
2	-2.102-03	5.573-02	1.648+00			
3	1.887-04	-3.652-03	6.843-02	1.657+00		
4	-2.210-05	3.777-04	-5.179-03	7.921-02	1.666+00	
5	2.916-06	-4.939-05	6.043-04	-6.712-03	8.878-02	1.676+00
6	-3.675-07	8.319-06	-8.828-05	8.595-04	-8.255-03	9.751-02
7	2.199-07	-2.002-06	1.540-05	-1.366-04	1.141-03	-9.804-03
8	-2.721-07	5.044-07	-3.522-06	2.480-05	-1.933-04	1.448-03
9	1.289-07	-9.623-08	8.355-07	-5.065-06	3.692-05	-2.599-04
10	6.144-08	-4.265-09	5.859-08	1.097-06	-7.642-06	5.226-05

v'/v"	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6	1.685+00				
7	1.056-01	1.695+00			
8	-1.136-02	1.132-01	1.704+00		
9	1.780-03	-1.294-02	1.204-01	1.714+00	
10	-3.366-04	2.138-03	-1.452-02	1.272-01	1.724+00

Table 40

Calculated R-Centroid Factors ($\langle \bar{r} \rangle_{v'v''}$) for the Orange System of FeO ($^5\Sigma^+$II - X$^5\Sigma^+$I)

v'/v"	0	1	2	3	4	5
0	1.660+00	1.723+00	1.769+00	1.824+00	1.878+00	1.951+00
1	1.611+00	1.655+00	1.738+00	1.780+00	1.838+00	1.890+00
2	1.551+00	1.616+00	1.54[illegible]+00	1.757+00	1.783+00	1.854+00
3	1.444+00	1.558+00	[illegible]	1.882+00	1.791+00	1.800+00
4	-2.191-01	1.454+00	1.564+00	1.615+00	1.831+00	1.826+00
5	1.676+00	-8.143-01	1.460+00	1.568+00	1.608+00	1.850+00
6	1.510+00	1.664+00	-4.932+00	1.465+00	1.572+00	1.598+00
7	1.254+00	1.504+00	1.649+00	5.298+00	1.468+00	1.574+00
8	2.163+00	1.250+00	1.496+00	1.633+00	2.71[illegible]+00	1.470+00
9	1.585+00	1.953+00	1.199+00	1.487+00	1.618+00	2.158+00
10	1.399+00	1.566+00	1.866+00	1.113+00	1.462+00	1.604+00

v'/v"	6	7	8	9	10
0	2.022+00	2.151+00	2.228+00	1.028+00	1.545+00
1	1.970+00	2.036+00	2.254+00	2.110+00	9.823-01
2	1.902+00	1.992+00	2.046+00	2.360+00	1.968+00
3	1.871+00	1.914+00	2.019+00	2.049+00	2.558+00
4	1.[illegible]+00	1.[illegible]90+00	1.923+00	2.052+00	2.042+00
5	1.908+00	1.614+00	1.913+00	1.931+00	2.095+00
6	1.590+00	2.119+00	1.[illegible]17+00	1.939+00	1.936+00
7	1.584+00	1.94[illegible]+00	3.382+00	1.817+00	1.971+00
8	1.577+00	1.571+00	2.025+00	1.286+00	1.816+00
9	1.469+00	1.580+00	1.560+00	2.125+00	9.909-01
10	1.929+00	1.467+00	1.[illegible]85+00	1.553+00	2.245+00

Table 41

Calculated Band Strengths ($p_{v'v''}$) for the Vibrational-Rotational Transition of FeO ($X\,^5\Sigma^+$ I - $X\,^5\Sigma^+$ I)

v'/v"	0	1	2	3	4	5
0	2.374+00					
1	2.465-03	2.402+00				
2	1.651-05	4.952-03	2.432+00			
3	5.109-07	4.951-05	7.419-03	2.462+00		
4	3.441-08	1.542-06	9.514-05	9.849-03	2.493+00	
5	2.125-10	5.029-08	3.082-06	1.531-04	1.228-02	2.525+00
6	3.398-09	5.236-09	8.254-08	5.763-06	2.210-04	1.475-02
7	5.208-09	1.872-08	2.141-09	1.301-07	1.057-05	2.874-04
8	1.082-10	3.899-09	2.224-08	2.624-09	8.619-06	1.956-03
9	1.667-09	3.790-10	2.112-09	4.228-08	3.549-08	2.058-03
10	2.353-09	4.334-09	3.336-10	6.744-09	4.127-08	3.347-06

v'/v"	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6	2.559+00				
7	1.736-02	2.596+00			
8	3.425-04	2.015-02	2.634+00		
9	3.328-05	4.001-04	2.291-02	2.671+00	
10	1.432-07	4.310-05	4.978-04	2.536-02	2.706+00

Table 42

Calculated Band Strengths ($p_{v'v''}$)
for the Orange System of FeO
($^5\Sigma^+ II - X^5\Sigma^+ I$)

v'/v"	0	1	2	3	4	5
0	7.452-02	5.959-02	2.706-02	7.616-03	1.461-03	1.863-04
1	3.701-02	1.492-02	5.877-02	5.065-02	2.035-02	4.975-03
2	7.046-03	4.146-02	7.184-04	4.355-02	6.583-02	3.517-02
3	4.152-04	1.454-02	3.629-02	1.079-03	2.865-02	7.462-02
4	4.314-06	1.202-03	2.061-02	2.959-02	4.810-03	1.761-02
5	2.235-05	1.868-05	2.141-03	2.509-02	2.387-02	8.209-03
6	5.217-06	1.038-04	5.868-05	2.999-03	2.827-02	1.967-02
7	1.680-07	2.709-05	2.877-04	1.552-04	3.620-03	3.039-02
8	3.170-08	7.459-07	7.674-05	6.104-04	3.632-04	3.911-03
9	2.660-08	4.131-07	1.196-06	1.576-04	1.101-03	7.665-04
10	5.490-09	[illegible]	2.552-06	6.148-07	2.615-04	1.791-03

v'/v"	6	7	8	9	10
0	1.592-05	9.536-07	5.598-09	4.087-09	1.363-09
1	7.528-04	7.476-05	5.255-06	4.711-07	1.545-08
2	1.048-02	1.824-03	2.118-04	1.654-05	1.313-06
3	5.037-02	1.779-02	3.462-03	4.533-04	3.296-05
4	8.016-02	6.543-02	2.672-02	5.595-03	7.686-04
5	1.036-02	8.484-02	8.017-02	3.674-02	7.942-03
6	1.042-02	5.657-03	8.976-02	9.416-02	1.042-02
7	1.696-02	1.172-02	3.126-03	9.553-02	1.696-02
8	3.150-02	1.551-02	1.252-02	1.559-03	3.150-02
9	3.811-03	3.177-02	[illegible]	1.302-02	3.811-03
10	1.433-03	3.278-03	3.150-02	1.466-02	1.433-03

Table 43

Screening Parameters for the Atomic Orbitals of UO

Atomic Orbitals	Screening Parameter
1s (O)	7.6563
2s (O)	2.2472
7s (U)	3.0630
$5f\phi^+$ (U)	5.7200
$5f\phi^-$ (U)	5.7200
$5f\delta^+$ (U)	5.7200
$5f\delta^-$ (U)	5.7200
$5f\pi^+$ (U)	5.7200
$5f\pi^-$ (U)	5.7200
$5f\sigma$ (U)	5.7200
$6d\delta^+$ (U)	2.4240
$6d\delta^-$ (U)	2.4240
$6d\pi^+$ (U)	2.4240
$6d\pi^-$ (U)	2.4240
$6d\sigma$ (U)	2.4240
$2p\pi^+$ (O)	2.2262
$2p\pi^-$ (O)	2.2262
$2p\sigma$ (O)	2.2262

Table [illegible]

Configuration Sizes and Number of States for VCI Calculations of Various Symmetries for UO

Symmetry	No. of [illegible] (Full CI)	(Actual CI run)	No. of States (to the first two dissociation limits)
$^{1}\Sigma^{+,-}$	1791		-
$^{3}\Sigma^{+,-}$	[illegible]		3 (+), 3 (-)
$^{5}\Sigma^{+,-}$	[illegible]		3 (+), 3 (-)
$^{7}\Sigma^{+,-}$	[illegible]	[illegible]	3 (+), 3 (-)
$^{1}\Pi$	[illegible]		-
$^{3}\Pi$	[illegible]		6
$^{5}\Pi$	[illegible]	[illegible]	6
$^{7}\Pi$	[illegible]	[illegible]	6
$^{1}\Delta$	[illegible]		-
$^{3}\Delta$	[illegible]		6
$^{5}\Delta$	[illegible]	[illegible]	6
$^{7}\Delta$	[illegible]	[illegible]	6
$^{1}\Phi$	[illegible]		-
$^{3}\Phi$	[illegible]		6
$^{5}\Phi$	[illegible]		6
$^{7}\Phi$	[illegible]		6
$^{1}\Gamma$	[illegible]		-
$^{3}\Gamma$	[illegible]		[illegible]

Table 44 (Continued)

Symmetry	No. of Cfgs. (full CI) (Actual CI run)	No. of States (to the first two dissociation limits)
$^5\Gamma$	667	6
$^7\Gamma$	88	6
^1H	748	-
^3H	1148	6
^5H	459	6
^7H	59	6
^1I	508	-
^3I	748	6
^5I	289	6
^7I	33	6
^1K	306	-
^3K	448	5
^5K	159	5
^7K	17	5
$^1\Lambda$	173	-
$^3\Lambda$	234	3
$^5\Lambda$	78	3
$^7\Lambda$	6	3
^1M	81	-
^3M	109	1
^5M	30	1
^7M	2	1

Table 45

Low-Lying Molecular States of UO and their Dissociation Limits

Dissociation Limit	Molecular States
U + O	
$^5L_u\ (5f^37s^26d) + {}^3P_g\ (2p^4)$	$^3\Sigma^-(1)$, $^3\Sigma^+(2)$, $^5\Sigma^-(1)$, $^5\Sigma^+(2)$, $^7\Sigma^-(1)$ $^7\Sigma^+(2)$, $^3\Pi(3)$, $^5\Pi(3)$, $^7\Pi(3)$, $^3\Delta(3)$, $^5\Delta(3)$, $^7\Delta(3)$, $^3\Phi(3)$, $^5\Phi(3)$, $^7\Phi(3)$, $^3\Gamma(3)$, $^5\Gamma(3)$, $^7\Gamma(3)$, $^3H(3)$, $^5H(3)$, $^7H(3)$, $^3I(3)$, $^5I(3)$, $^7I(3)$, $^3K(3)$, $^5K(3)$, $^7K(3)$, $^3\Lambda(2)$, $^5\Lambda(2)$, $^7\Lambda(2)$, $^3M(1)$, $^5M(1)$, $^7M(1)$.
$^5K_u\ (5f^37s^26d) + {}^3P_g\ (2p^4)$	$^3\Sigma^-(2)$, $^3\Sigma^+(1)$, $^5\Sigma^-(2)$, $^5\Sigma^+(1)$, $^7\Sigma^-(2)$, $^7\Sigma^+(1)$, $^3\Pi(3)$, $^5\Pi(3)$, $^7\Pi(3)$, $^3\Delta(3)$, $^5\Delta(3)$, $^7\Delta(3)$, $^3\Phi(3)$, $^5\Phi(3)$, $^7\Phi(3)$, $^3\Gamma(3)$, $^5\Gamma(3)$, $^7\Gamma(3)$, $^3H(3)$, $^5H(3)$, $^7H(3)$, $^3I(3)$, $^5I(3)$, $^7I(3)$, $^3K(2)$, $^5K(2)$, $^7K(2)$, $^3\Lambda(1)$, $^5\Lambda(1)$, $^7\Lambda(1)$.

( ) Indicate [illegible]

Table 46

Energies of Uranium Atomic and Oxygen Atomic States Representing Dissociation Limits of Low-Lying UO States

Atomic States	**Total Energy (hartrees)**
$^5L + {}^3P$	-62.19842
$^5K + {}^3P$	-62.20129

Table 47

Calculated Energies of Electronic States of UO (Z effective = 6.0; energies are in hartrees; internuclear separations are in bohrs)

R	$^7\Sigma^-$ I	$^7\Sigma^+$ I	$^7\Sigma^-$ II	$^7\Sigma^+$ II	$^7\Sigma^-$ III
3.0	-61.67594	-61.67154	-61.60038	-61.59509	-61.59795
4.0	-61.99399	-61.98998	-61.98834	-61.98395	-61.96781
5.0	-62.15287	-62.15218	-62.14967	-62.14840	-62.14345
6.0	-62.19183	-62.19179	-62.18821	-62.18757	-62.18622
8.0	-62.19585	-62.19585	-62.19462	-62.19058	-62.18852
∞	-62.20129	-62.20129	-62.20129	-62.19842	-62.19842

R	$^7\Sigma^+$ III	$^5\Pi$ I	$^5\Pi$ II	$^5\Pi$ III	$^5\Pi$ IV
3.0	-61.59286	-61.67107	-61.66584	-61.63986	-61.63469
4.0	-61.96784	-61.98979	-61.98706	-61.98488	-61.98133
5.0	-62.14358	-62.15198	-62.15128	-62.14873	-62.14720
6.0	-62.18466	-62.19187	-62.19137	-62.18825	-62.18751
8.0	-62.18844	-62.19679	-62.19590	-62.19440	-62.19066
∞	-62.19842	-62.20129	-62.20129	-62.20129	-62.19842

R	$^5\Pi$ V	$^5\Pi$ VI	$^7\Pi$ I	$^7\Pi$ II	$^7\Pi$ III
3.0	-61.59799	-61.59365	-61.67648	-61.67174	-61.60259
4.0	-61.97666	-61.97450	-61.99384	-61.98968	-61.98822
5.0	-62.14359	-62.14265	-62.15282	-62.15204	-62.14969
6.0	-62.18633	-62.18443	-62.19217	-62.19145	-62.18860
8.0	-62.19031	-62.18845	-62.19680	-62.19590	-62.19440
∞	-62.19842	-62.19842	-62.20129	-62.20129	-62.20129

Table 47 (Continued)

R	${}^7\Pi$ IV	${}^7\Pi$ V	${}^7\Pi$ VI	${}^5\Delta$ I	${}^5\Delta$ II
3.0	-61.59385	-61.59826	-61.59512	-61.67170	-61.66686
4.0	-61.98390	-61.96927	-61.96644	-61.98973	-61.98656
5.0	-62.14847	-62.14407	-62.14332	-62.15182	-62.15051
6.0	-62.18782	-62.18637	-62.18474	-62.19178	-62.19142
8.0	-62.19066	-62.19031	-62.18845	-62.19665	-62.19628
∞	-62.19842	-62.19842	-62.19842	-62.20129	-62.20129

R	${}^5\Delta$ III	${}^5\Delta$ IV	${}^5\Delta$ V	${}^5\Delta$ VI	${}^7\Delta$ I
3.0	-61.64037	-61.63565	-61.59578	-61.59284	-61.67652
4.0	-61.98459	-61.98141	-61.97769	-61.97483	-61.99373
5.0	-62.14808	-62.13798	-62.13766	-62.13640	-62.15272
6.0	-62.18936	-62.18753	-62.18624	-62.18435	-62.19193
8.0	-62.19583	-62.19326	-62.19649	-62.18848	-62.19665
∞	-62.20129	-62.19842	-62.19842	-62.19842	-62.20129

R	${}^7\Delta$ II	${}^7\Delta$ III	${}^7\Delta$ IV	${}^7\Delta$ V	${}^7\Delta$ VI
3.0	-61.67274	-61.60007	-61.59983	-61.59516	-61.59295
4.0	-61.98920	-61.98789	-61.98408	-61.97085	-61.96770
5.0	-62.15154	-62.14978	-62.14863	-62.14482	-62.14349
6.0	-62.19184	-62.18961	-62.18768	-62.17890	-62.17558
8.0	-62.19629	-62.19583	-62.19326	-62.19050	-62.18848
∞	-62.20129	-62.20129	-62.19842	-62.19842	-62.19842

TABLE 48

Spectroscopic Constants* for Bound States of UO

D_e = 62588. cm^{-1}, 7.76 ev

ω_e = 820. cm^{-1}

$\omega_e x_e$ = 2.686 cm^{-1}

α_e = 0.00149 cm^{-1}

B_e = 0.3321 cm^{-1}

r_e = 1.84 Å

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*G. DeMaria, R. P. Burns, J. Drowart and M. G. Inghram: "Mass Spectrometric Study of Gaseous Molybdenum, Tungsten, and Uranium Oxides," Journal of Chemical Physics, Vol. 32, 1960, p. 1373.

S. D. Gabelnick, G. T. Reedy and M. G. Chasanov: "The Infrared Spectra of Matrix-Isolated Uranium Oxide Species. I. The Stretching Region", to be submitted to the Journal of Chemical Physics.

Table 49

Calculated Oscillator Strengths ($f_{v'v''}$) for the Vibrational - Rotational Transition of UO

v'/v"	0	1	2	3	4	5
0						
1	1.209-05					
2	2.294-07	2.398-05				
3	8.633-09	7.200-07	3.558-05			
4	1.455-09	3.417-08	1.458-06	4.705-05		
5	1.772-10	4.427-09	9.236-08	2.470-06	5.851-05	
6	1.526-11	1.218-09	1.308-08	[illegible].057-07	3.760-06	6.991-05
7	3.498-12	1.904-10	5.085-09	3.470-08	3.673-07	5.345-06
8	6.884-11	6.121-11	1.367-09	1.242-08	7.346-08	6.267-07
9	9.820-11	1.124-10	1.999-10	3.9[illegible]9-09	2.081-08	1.216-07
10	1.7[illegible]0-12	5.532-11	7.362-11	1.988-10	4.617-09	[illegible].544-08

v'/v"	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6					
7	5.106-05				
8	7.143-06	9.176-05			
9	8.9[illegible]-07	[illegible]	[illegible]		
10	1.[illegible]4-07	[illegible]	[illegible]	[illegible]	

Table 50

Calculated R-Centroid Factors ($\langle \bar{r} \rangle_{v'v''}$) for the Vibrational-Rotational Transition of UO

v'v"	0	1	2	3	4	5
0	1.843+00					
1	3.709-02	1.850+00				
2	-1.504-03	5.253-02	1.856+00			
3	1.001-04	-2.613-03	6.444-02	1.863+00		
4	8.831-06	2.028-04	-3.711-03	7.455-02	1.869+00	
5	1.149-06	-2.012-05	3.147-04	-4.799-03	8.349-02	1.876+00
6	-2.293-07	1.061-06	-3.190-05	4.476-04	-5.885-03	9.160-02
7	-2.567-07	6.972-07	3.304-06	-4.823-05	5.986-04	-6.990-03
8	3.544-07	-5.217-08	2.987-07	6.443-06	-7.159-05	7.597-04
9	-3.247-08	-1.629-07	4.307-08	-1.292-06	9.317-06	-9.707-05
10	-2.266-07	1.027-07	-6.019-07	1.121-07	-1.682-06	1.286-05

v'v"	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6	1.882+00				
7	9.911-02	1.889+00			
8	-8.098-03	1.061-01	1.896+00		
9	9.323-04	-9.200-03	1.128-01	[illegible]	
10	-1.238-04	1.117-03	-1.031-02	1.238-04	1.909+00

Table 51

Calculated Band Strengths ($p_{v'v''}$) for the Vibrational-Rotational Transition of UO

v'v"	0	1	2	3	4	5
0	7.267-01					
1	4.888-03	7.159-01				
2	4.650-05	9.754-03	7.059-01			
3	1.171-06	1.469-04	1.457-02	6.959-01		
4	1.485-07	4.665-06	2.995-04	1.940-02	6.866-01	
5	1.451-08	4.548-07	1.269-05	5.110-04	2.429-02	6.776-01
6	1.045-09	1.005-07	1.436-06	2.846-05	7.832-04	2.922-02
7	2.060-10	1.313-08	4.222-07	3.620-06	5.396-05	1.121-03
8	3.560-09	3.630-09	9.491-08	1.039-06	7.702-06	8.792-05
9	4.530-09	5.852-09	1.194-08	2.775-07	1.752-06	1.284-05
10	7.162-11	2.569-09	3.872-09	1.195-08	3.390-07	2.156-06

v'v"	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6	6.687-01				
7	3.411-02	6.598-01			
8	1.508-03	3.888-02	6.506-01		
9	1.266-04	1.926-03	4.350-02	1.266-04	
10	1.769-05	1.686-04	2.376-03	1.769-05	6.317-01

Table 52

Screening Parameters for the Atomic Orbitals of UO^+

Atomic Orbitals	Screening Parameters
1s (O)	7.6568
2s (O)	2.2472
7s (U)	3.0630
$5f\phi^+$ (U)	5.7200
$5f\phi^-$ (U)	5.7200
$5f\delta^+$ (U)	5.7200
$5f\delta^-$ (U)	5.7200
$5f\pi^{-,+}$ (U)	5.7200
$5f\sigma$ (U)	5.7200
$2p\pi^+$ (O)	2.2262
$2p\pi^-$ (O)	2.2262
$2p\sigma$ (O)	2.2262

Table 53

Configuration Sizes and Number of States for VCI Calculations of Various Symmetries for UO$^+$

Symmetry	**No. of Cfgs.** (Full C.I.)	(U^++O)	**No. of States** (to ^4I_u + ^4D_g level)
$^2\Sigma^{+,-}$	483	119*	2 (+), 1(-)
$^4\Sigma^{+,-}$	335	75*	2 (+), 1(-)
$^6\Sigma^{+,-}$	74*	13	2 (+), 1(-)
$^2\Pi$	469	116*	3
$^4\Pi$	332	72*	3
$^6\Pi$	72*	13	3
$^2\Delta$	427	105*	3
$^4\Delta$	293	65*	3
$^6\Delta$	63*	11	3
$^2\Phi$	368	89*	3
$^4\Phi$	245	53	3
$^6\Phi$	51*	9	3
$^2\Gamma$	295	69	3
$^4\Gamma$	194	40	3
$^6\Gamma$	38	6	3
^2H	222	50	3
^4H	139	27	3
^6H	26	4	3

Table 53 (Continued)

Symmetry	No. of Cfgs. (Full C.I.)	(U^{+}+O)	No. of States (to $^{4}I_u$ + $^{1}D_g$ level)
^{2}I	154	33	2
^{4}I	93	17	2
^{6}I	15	2	2
^{2}K	98	20	1
^{4}K	55	9	1
^{6}K	8	1	1

*Indicates actual configuration list used.

Table 54

Low-Lying Molecular States of UO$^+$ and their Dissociation Limits

Dissociation Limit	Molecular States
$U^+ + O$	
$^4I_u\,(5f^3 7s^2) + {}^3P_g(2p^4)$	$^2\Sigma^-(1)$, $^2\Sigma^+(2)$, $^4\Sigma^-(1)$, $^4\Sigma^+(2)$, $^6\Sigma^-(1)$, $^6\Sigma^+(2)$, $^2\Pi(3)$, $^4\Pi(3)$, $^6\Pi(3)$, $^2\Delta(3)$, $^4\Delta(3)$, $^6\Delta(3)$, $^2\Phi(3)$, $^4\Phi(3)$, $^6\Phi(3)$, $^2\Gamma(3)$, $^4\Gamma(3)$, $^6\Gamma(3)$, $^2H(3)$, $^4H(3)$, $^6H(3)$, $^2I(2)$, $^4I(2)$, $^6I(2)$, $^2K(1)$, $^4K(1)$, $^6K(1)$.

Table 55

Energies of Uranium Ionic and Oxygen Atomic States Representing Dissociation Limits of Low-Lying UO^+ States

Atomic States	Total Energy (hartrees)
$^4I_u + {}^3P_g$	-79.66736

Table 56

Calculated Energies of Electronic States of UO$^+$ (effective z = 10.)
(Energies are in hartrees; internuclear separation in bohrs)

R	$^{2}\Sigma^{+}$ I	$^{2}\Sigma^{-}$ I	$^{2}\Sigma^{+}$ II	$^{4}\Sigma^{+}$ I	$^{4}\Sigma^{-}$ II	$^{4}\Sigma^{+}$ II
3.0	-79.55572	-79.47943	-79.48008	-79.58866	-79.52379	-
3.5	-79.61696	-79.54079	-79.54094	-79.62454	-79.55180	-
4.0	-79.65748	-79.60141	-79.60129	-79.65896	-79.60208	-
5.0	-79.68222	-79.64916	-79.64912	-79.68222	-79.64917	-79.64913
6.0	-79.67707	-79.65724	-79.65722	-79.67707	-79.65724	-79.65782
8.0	-79.65889	-79.65334	-79.65334	-79.65889	-79.65334	-
∞	-79.66736	-79.66736	-79.66736	-79.66736	-79.66736	-79.66736

R	$^{6}\Sigma^{+}$ I	$^{6}\Sigma^{-}$ I	$^{6}\Sigma^{+}$ II	$^{2}\Pi$ I	$^{2}\Pi$ II	$^{2}\Pi$ III
3.0	-79.58966	-79.52508	-79.51818	-79.55642	-79.47817	-79.47404
3.5	-79.62475	-79.55205	-79.55010	-79.61717	-79.54041	-79.53473
4.0	-79.65900	-79.60239	-79.60226	-79.65730	-79.60141	-79.60127
5.0	-79.68227	-79.64[illegible]	-79.64917	-79.68223	-79.64916	-79.64912
6.0	-79.67707	-79.65[illegible]	-79.65722	-79.67784	-79.65874	-79.65647
8.0	-79.65889	-79.6[illegible]34	-79.65336	-79.66237	-79.65971	-79.64979
∞	-79.66736	-79.6[illegible]36	-79.66736	-79.66736	-79.66736	-79.66736

R	$^{4}\Pi$ I	$^{4}\Pi$ II	$^{4}\Pi$ III	$^{6}\Pi$ I	$^{6}\Pi$ II	$^{6}\Pi$ III
3.0	-79.59137	-79.51508	-79.51269	-79.59260	-79.51597	-79.47298
3.5	-79.62536	-79.54924	-79.54393	-79.62561	-79.54944	-79.54015
4.0	-79.65915	-79.60242	-79.60183	-79.65920	-79.60254	-79.60216
5.0	-79.68223	-79.64917	-79.64913	-79.68228	-79.64921	-79.64917
6.0	-79.67784	-79.65874	-79.65647	-79.67784	-79.65874	-79.65647
8.0	-79.66237	-79.65970	-79.64979	-79.66236	-79.65971	-79.64979
∞	-79.66736	-79.66736	-79.66736	-79.66736	-79.66736	-79.66736

Table 56 (Continued)

R	$^{2}\Delta$ I	$^{2}\Delta$ II	$^{2}\Delta$ III	$^{4}\Delta$ I	$^{4}\Delta$ II	$^{4}\Delta$ III
3.0	-79.55775	-79.48044	-79.47407	-79.59587	-79.51406	-79.51303
3.5	-79.61748	-79.54091	-79.53476	-79.62692	-79.54917	-79.54407
4.0	-79.65760	-79.60138	-79.60127	-79.65953	-79.60248	-79.60203
5.0	-79.68226	-79.64915	-79.64911	-79.68226	-79.64917	-79.64912
6.0	-79.67935	-79.65934	-79.65723	-79.67935	-79.65934	-79.65723
8.0	-79.66863	-79. 221	-79.65334	-79.66863	-79.66221	-79.65334
∞	-79.66736	-79.66736	-79.66736	-79.66736	-79.66736	-79.66736

R	$^{6}\Delta$ I	$^{6}\Delta$ II	$^{6}\Delta$ III	$^{2}\Phi$ I	$^{2}\Phi$ II	$^{2}\Phi$ III
3.0	-79.59754	-79.51545	-79.48166	-79.55806	-79.48237	-79.47454
3.5	-79.62724	-79.54947	-79.54049	-79.61752	-79.54166	-79.53433
4.0	-79.65958	-79.60267	-79.60232	-79.65761	-79.60139	-79.60102
5.0	-79.68232	-79.64921	-79.64917	-79.68229	-79.64915	-79.64907
6.0	-79.67936	-79.65935	-79.65723	-79.67998	-79.65874	-79.65783
8.0	-79.66863	-79.66221	-79.65334	-79.67109	-79.65971	-79.65587
∞	-79.66736	-79.66736	-79.66736	-79.66736	-79.66736	-79.66736

TABLE 57

Spectroscopic Constants for Selected Bound States of UO^+

State		$T_e(cm^{-1})$	$D_e(ev)$	$r_e(Å)$	$\omega_e(cm^{-1})$	$\omega_eX_e(cm^{-1})$	$B_e(cm^{-1})$	$\alpha_e(cm^{-1})$
$X^4\Pi$	Exp[a]	0.0	8.15	1.843	850.	2.748	0.3310	0.00145
$^4\Pi$ II		16449.	6.11	1.888	763.8	-1.456	0.3155	0.00104
$^4\Pi$ III	Calc.	17299.	6.01	1.896	859.8	5.765	0.3130	0.00074
$^2\Pi$ I	Calc.	1050.	8.02	1.867	807.7	0.405	0.3226	0.00174
$^2\Pi$ II	Calc.	17944.	5.92	1.922	718.8	-3.632	0.3044	-0.000007
$^2\Pi$ III	Calc.	18825.	5.81	1.927	740.9	-1.014	0.3030	0.00050

[a] G. DeMaria, R. P. Burns, J. Drowart and M. G. Inghram: "Mass Spectrometric Study of Gaseous Molybdenum, Tungsten, and Uranium Oxides", The Journal of Chemical Physics, Vol. 32, 1960, p. 1373.

Table 58

Calculated Oscillator Strengths ($f_{v'v''}$) for the Vibrational-Rotational Transition of UO$^+$($X^4\Pi$ - $X^4\Pi$)

v'v"	0	1	2	3	4	5
0						
1	1.031-05					
2	7.093-08	2.041-05				
3	7.074-10	2.003-07	3.036-05			
4	2.598-11	2.992-09	3.877-07	4.017-05		
5	6.028-12	6.191-12	7.806-09	6.249-07	4.987-05	
6	1.015-11	6.438-12	1.016-12	1.614.08	9.121-07	5.945-05
7	1.119-11	4.399-12	9.378-12	1.867-11	2.848-08	1.251-06
8	3.812-13	1.059-11	1.488-11	1.698-11	1.950-10	4.385-08
9	7.778-12	1.766-12	1.639-11	3.911-11	5.753-11	7.026-10
10	6.214-12	2.462-12	4.805-12	1.798-11	4.092-11	8.425-11

v'v"	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6					
7	6.883-05				
8	1.643-06	7.816-05			
9	6.303-08	2.081-06	8.728-05		
10	1.501-09	8.585-08	2.567-06	9.623-05	

Table [illegible]

Calculated R-Centroid Factors ($\langle\bar{R}\rangle_{v'v''}$) for the Vibrational-Rotational Transition of UO$^+$ (X^4[illegible] - ^{4}[illegible])

v'v"	0	1	2	3	4	5
0	1.846+00					
1	3.642-02	1.853+00				
2	-1.464-03	5.160-02	1.859+00			
3	9.487-05	-2.543-03	6.330-02	1.865+00		
4	-7.672-06	1.924-04	-3.605-03	7.321-02	1.872+00	
5	9.607-07	-1.774-05	3.064-04	-4.666-03	8.199-02	1.878+00
6	-2.237-07	1.908-06	4.305-04	4.330-04	-5.730-03	8.997-02
7	-2.594-08	-2.988-07	-4.755-05	-4.755-05	5.743-04	-6.798-03
8	7.294-08	-7.095-09	5.434-06	5.434-06	-6.738-05	7.283-04
9	-2.086-08	8.464-08	-5.596-07	-5.596-07	8.108-06	-9.063-05
10	-1.797-08	-4.072-08	-1.165-08	-1.165-08	-8.296-07	1.1[illegible]2-05

v'v"	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6	1.884+00				
7	9.734-02	1.891+00			
8	-7.872-03	1.042-01	1.897+00		
9	8.948-04	-8.948-03	1.108-01	1.904+00	
10	-1.171-04	1.074-03	-1.003-02	1.169-01	1.911+00

Table [illegible]

Calculated Band Strengths ($p_{v'v''}$)
for the Vibrational-Rotational
Transition of UO$^+$ ($X^4\pi$ - $X^4\pi$)

v'/v"	0	1	2		4	5
0	1.931+00					
1	4.018-03	1.956+00				
2	1.387-05	8.010-03	1.983+00			
3	9.253-08	3.943-05	1.199-02	[illegible]		
4	2.558-09	3.939-07	7.683-05	1.5[illegible]-02	[illegible]37+00	
5	4.763-10	6.134-10	1.035-06	1.[illegible]	1.996-02	2.065+00
6	6.704-10	5.120-10	1.013-10	2.1[illegible]	1.[illegible]32-04	2.396-02
7	6.358-10	2.926-10	7.508-10	1.8[illegible]	[illegible].525-06	2.529-04
8	1.901-11	6.055-10	9.961-10	1.36[illegible]	1.972-08	5.931-06
9	3.459-10	8.867-11	9.434-10	2.6[illegible]	[illegible].668-09	7.150-08
10	2.496-11	1.102-10	2.429-10	1.0[illegible]	[illegible].777-09	6.883-09

v'/v"	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6	2.093+00				
7	2.795-02	2.121+00			
8	3.344-04	3.193-02	2.151+00		
9	8.582-06	4.265-04	3.590-02	2.180+00	
10	1.538-07	1.177-05	5.296-04	3.985-02	[illegible]09+00

TABLE 41

Screening Parameters for the Atomic Orbitals of TiO

Atomic Orbitals		Screening Parameters
$1s$	(Ti)	21.4409
$1s$	(O)	7.6579
$2s$	(Ti)	7.6883
$2s$	(O)	2.2458
$2p\sigma$	(Ti)	9.0324
$2p\pi^{+}$	(Ti)	9.0324
$2p\pi^{-}$	(Ti)	9.0324
$3s$	(Ti)	3.6777
$3p\sigma$	(Ti)	3.3679
$3p\pi^{+}$	(Ti)	3.3679
$3p\pi^{-}$	(Ti)	3.3679
$2p\sigma$	(O)	2.2266
$2p\pi^{+}$	(O)	2.2266
$2p\pi^{-}$	(O)	2.2266
$4s$	(Ti)	1.2042
$3d\sigma$	(Ti)	2.7138
$3d\pi^{+}$	(Ti)	2.7138
$3d\pi^{-}$	(Ti)	2.7138
$3d\delta^{+}$	(Ti)	2.7138
$3d\delta^{-}$	(Ti)	2.7138

TABLE 62

Configuration Sizes and Number of States for VCI Calculations of Various Symmetries for TiO

Symmetry	No. of Cfgs.	No. of States (to ^3F_g + ^1D_g level)
$^1\Sigma^{+,-}$	754	7(+), 5(-)
$^3\Sigma^{+,-}$	1,110	15(+), 14(-)
$^5\Sigma^{+,-}$	440	11(+), 7(-)
$^7\Sigma^{+,-}$	61	4(+), 2(-)
$^1\Pi$	700	11
$^3\Pi$	1,050	27
$^5\Pi$	404	16
$^7\Pi$	56	5
$^1\Delta$	597	10
$^3\Delta$	861	23
$^5\Delta$	324	14
$^7\Delta$	39	4
$^1\Phi$	434	7
$^3\Phi$	626	16
$^5\Phi$	214	9
$^7\Phi$	22	2
$^1\Gamma$	287	4
$^3\Gamma$	382	9
$^5\Gamma$	120	5
$^7\Gamma$	8	1
^1H	152	1
^3H	200	3
^5H	50	1

TABLE 63

Low-Lying Molecular States of TiO and their Dissociation Limits

Dissociation Limit	Molecular States
Ti + O	
$^3F_g(3d^2 4S^2) + {}^3P_g(2p^4)$	$^1\Sigma^+(2)$, $^5\Sigma^+(2)$, $^1\Sigma^-(1)$, $^3\Sigma^-(1)$, $^5\Sigma^-(1)$, $^1\Pi(3)$, $^3\Pi(3)$, $^5\Pi(3)$, $^1\Delta(3)$, $^3\Delta(3)$, $^5\Delta(3)$, $^1\Phi(2)$, $^3\Phi(2)$, $^5\Phi(2)$, $^1\Gamma(1)$, $^3\Gamma(1)$, $^5\Gamma(1)$, $^3\Sigma^+(2)$
$^5F_g(3d^3 4s) + {}^3P_g(2p^4)$	$^3\Sigma^+(2)$, $^5\Sigma^+(2)$, $^7\Sigma^+(2)$, $^3\Sigma^-(1)$, $^5\Sigma^-(1)$, $^7\Sigma^-(1)$, $^3\Pi(3)$, $^5\Pi(3)$, $^7\Pi(3)$, $^3\Delta(3)$, $^5\Delta(3)$, $^7\Delta(3)$, $^3\Phi(2)$, $^5\Phi(2)$, $^7\Phi(2)$, $^3\Gamma(1)$, $^5\Gamma(1)$, $^7\Gamma(1)$
$^1D_g(3d^2 4s^2) + {}^3P_g(2p^4)$	$^3\Sigma^+(1)$, $^3\Sigma^-(2)$, $^3\Pi(3)$, $^3\Delta(2)$, $^3\Phi(1)$
$^3P_g(3d^2 4s^2) + {}^3P_g(2p^4)$	$^1\Sigma^+(2)$, $^3\Sigma^+(2)$, $^5\Sigma^+(2)$, $^1\Sigma^-(1)$, $^3\Sigma^-(1)$, $^5\Sigma^-(1)$, $^1\Pi(2)$, $^3\Pi(2)$, $^5\Pi(2)$, $^1\Delta(1)$, $^3\Delta(1)$, $^5\Delta(1)$
$^3F_g(3d^3 4s) + {}^3P_g(2p^4)$	$^1\Sigma^+(2)$, $^3\Sigma^+(2)$, $^5\Sigma^+(2)$, $^1\Sigma^-(1)$, $^3\Sigma^-(1)$, $^5\Sigma^-(1)$, $^1\Pi(3)$, $^3\Pi(3)$, $^5\Pi(3)$, $^1\Delta(3)$, $^1\Phi(2)$, $^3\Phi(2)$, $^5\Phi(2)$, $^1\Gamma(1)$, $^3\Gamma(1)$, $^5\Gamma(1)$, $^3\Delta(3)$, $^5\Delta(3)$
$^1G_g(3d^2 4s^2) + {}^3P_g(2p^4)$	$^3\Sigma^+(1)$, $^3\Sigma^-(2)$, $^3\Pi(3)$, $^3\Delta(3)$, $^3\Phi(3)$, $^3\Gamma(2)$, $^3H(1)$

TABLE 63 (Continued)

Dissociation Limit	Molecular States
$^5P_g(3d^34s) + {}^3P_g(2p^4)$	$^3\Sigma^+(2)$, $^5\Sigma^+(2)$, $^7\Sigma^+(2)$, $^3\Sigma^-(1)$, $^5\Sigma^-(1)$, $^7\Sigma^-(1)$, $^3\Pi(2)$, $^5\Pi(2)$, $^7\Pi(2)$, $^3\Delta(1)$, $^7\Delta(1)$, $^5\Delta(1)$
$^3G_g(3d^34s) + {}^3P_g(2p^4)$	$^1\Sigma^+(1)$, $^3\Sigma^+(1)$, $^5\Sigma^+(1)$, $^1\Sigma^-(2)$ $^3\Sigma^-(2)$, $^5\Sigma^-(2)$, $^1\Pi(3)$, $^3\Pi(3)$, $^5\Pi(3)$, $^1\Delta(3)$, $^3\Delta(3)$, $^5\Delta(3)$, $^1\Phi(3)$, $^3\Phi(3)$, $^5\Phi(3)$, $^1\Gamma(2)$ $^3\Gamma(2)$, $^5\Gamma(2)$, $^1H(1)$, $^3H(1)$, $^5H(1)$
$^3F_g(3d^24s^2) + {}^1D_g(2p^4)$	$^3\Sigma^+(2)$, $^3\Sigma^-(3)$, $^3\Pi(5)$, $^3\Delta(4)$, $^3\Phi(3)$, $^3\Gamma(2)$, $^3H(1)$

TABLE 64

Energies of Titanium Atomic and Oxygen Atomic States Representing Dissociation Limits of Low-lying TiO States

Atomic States	Total Energy (Hartrees)	Energy Relative to $^3F_g + {}^3P_g$ (eV) Calc.
$^3F_g + {}^3P_g$	-921.35604	0.0000
$^5F_g + {}^3P_g$	-921.02076	9.1235
$^1D_g + {}^3P_g$	-921.29370	1.6964
$^3P_g + {}^3P_g$	921.28385	1.9644
$^3F_g + {}^3P_g$	-921.00951	9.4296
$^1G_g + {}^3P_g$	-921.26001	2.6131
$^5P_g + {}^3P_g$	-920.94850	11.0876
$^3G_g + {}^3P_g$	-920.94126	11.2863
$^3F_g + {}^1D_g$	-921.26211	2.5559

Table 65

Calculated Energies of Electronic States of TiO
(Energies are in hartrees; internuclear distance in Bohrs.)

R	$^1\Sigma^+$	$^1\Sigma^+$	$^1\Sigma^-$	$^1\Sigma^+$	$^1\Sigma^+$
2.5	-921.39764	-920.98489	-920.90889	-920.90389	-920.88437
2.7	-921.48334	-921.17125	-921.07944	-921.04026	-921.02944
2.9	-921.50485	-921.27173	-921.17688	-921.10898	-921.10778
3.1	-921.49034	-921.31864	-921.22909	-921.15102	-921.14585
3.3	-921.45813	-921.33398	-921.25805	-921.19365	-921.18774
3.5	-921.42026	-921.33300	-921.27720	-921.22655	-921.22029
3.7	-921.38481	-921.32638	-921.29108	-921.24559	-921.23900
3.9	-921.35713	-921.32096	-921.30116	-921.25480	-921.24780
4.1	-921.33968	-921.31934	-921.30876	-921.25777	-921.25116
4.5	-921.32890	-921.32385	-921.32013	-921.25825	-921.25481
5.0	-921.33370	-921.33322	-921.33041	-921.26305	-921.26203
6.0	-921.34724	-	-	-	-
∞	-921.35604	-921.35604	-921.35604	-921.28385	-921.28385

R	$^1\Sigma^-$	$^1\Sigma^+$	$^1\Sigma^+$	$^1\Sigma^-$	$^1\Sigma^+$
2.5	-920.84473	-920.77111	-920.76765	-920.73990	-
2.7	-920.98986	-920.97094	-920.96123	-920.93819	-920.93682
2.9	-921.08053	-921.07193	-921.05529	-921.05034	-921.04417
3.1	-921.13451	-921.13095	-921.12876	-921.12315	-921.10748
3.3	-921.18655	-921.16409	-921.16069	-921.13181	-921.12909
3.5	-921.21383	-921.15990	-921.15917	-921.15705	-921.13665
3.7	-921.22682	-921.17003	-921.14450	-921.14413	-921.14264
3.9	-921.23490	-921.17131	-921.15233	-921.15207	-921.14742
4.1	-921.24056	-921.17060	-921.15918	-921.15898	-921.15406
4.5	-921.24897	-921.17291	-921.16886	-	-
5.0	-921.25814	-921.18106	-921.17892	-	-
6.0	-	-	-	-	-
∞	-921.28385	-921.00951	-921.00951	-921.00951	-920.94128

Table 65 (Continued)

R	$^3\Sigma^+$	$^3\Sigma^+$	$^3\Sigma^-$	$^3\Sigma^+$	$^3\Sigma^-$
2.7	-921.22161	-921.17247	-921.07226	-921.05931	-921.04860
2.9	-921.31668	-921.27258	-921.15088	-921.11879	-921.11593
3.1	-921.35808	-921.31881	-921.19534	-921.15930	-921.15391
3.3	-921.35778	-921.33307	-921.23008	-921.20568	-921.19646
3.5	-921.36087	-921.33053	-921.26208	-921.23277	-921.23051
3.7	-921.34786	-921.32215	-921.28390	-921.24971	-921.24788
3.9	-921.33582	-921.31587	-921.29783	-921.25783	-921.25502
4.1	-921.32831	-921.31498	-921.30721	-921.25882	-921.25715
4.5	-921.32579	-921.32202	-921.31991	-921.25957	-921.25925
5.0	-921.33307	-	-	-	-
6.0	-921.34725	-	-	-	-
∞	-921.35604	-921.35604	-921.35604	-921.29370	-921.29370

R	$^3\Sigma^-$	$^3\Sigma^+$	$^3\Sigma^+$	$^3\Sigma^-$	$^3\Sigma^+$
2.7	-921.02371	-920.99174	-920.98575	-920.98422	-920.97481
2.9	-921.11328	-921.09410	-	-	-
3.1	-921.15205	-921.15016	-921.14660	-921.13791	-921.13634
3.3	-921.18235	-921.17738	-921.17470	-921.16910	-921.16574
3.5	-921.20443	-	-	-	-
3.7	-921.22473	-921.22172	-921.21621	-921.21386	-921.20794
3.9	-921.23677	-921.23370	-921.22925	-921.22852	-921.21634
4.1	-921.24471	-921.24176	-921.23894	-921.23846	-921.22257
4.5	-921.25629	-921.25396	-921.25182	-921.24873	-921.23231
5.0	-	-	-	-	-
6.0	-	-	-	-	-
∞	-921.29370	-921.28385	-921.28385	-921.28385	-921.26211

Table 65 (Continued)

R	$^5\Sigma^+$	$^5\Sigma^+$	$^5\Sigma^-$	$^5\Sigma^+$	$^5\Sigma^+$
2.5	-920.93633	-920.80260	-920.80025	-920.77044	-920.69252
2.7	-921.06688	-920.99760	-	-	-
2.9	-921.13041	-921.10547	-	-	-
3.1	-921.17966	-921.16378	-921.16141	-921.15064	-921.14900
3.3	-921.24144	-921.21152	-	-	-
3.5	-921.27671	-921.24745	-921.24716	-921.21030	-921.16973
3.7	-921.29622	-921.27154	-921.27124	-921.22783	-921.19129
3.9	-921.30701	-921.28838	-921.28813	-921.23724	-921.21200
4.1	-921.31340	-921.30076	-921.30057	-921.24270	-921.22656
4.5	-921.32157	-921.31794	-	-	-
5.0	-921.33192	-921.33190	-921.33029	-921.26016	-921.25954
6.0	-921.34726	-	-	-	-
∞	-921.35604	-921.35604	-921.35604	-921.28385	-921.28385

R	$^7\Sigma^+$	$^7\Sigma^+$	$^7\Sigma^-$	$^7\Sigma^+$	$^7\Sigma^+$
2.5	-920.38730	-920.36547	-920.19994	-920.19850	-920.12743
2.7	-920.60857	-920.59389	-920.46127	-920.46066	-920.43253
2.9	-920.74845	-920.73884	-920.63946	-920.43124	-920.62636
3.1	-920.83662	-920.83068	-920.77051	-920.74098	-920.73838
3.3	-920.89256	-920.88911	-920.85702	-920.81084	-920.80878
3.5	-920.92865	-920.92680	-920.91296	-920.85452	-920.85295
3.7	-920.95244	-920.95164	-920.94867	-920.88151	-920.88068
3.9	-920.97184	-920.96845	-920.96782	-920.89921	-920.89832
4.1	-920.98637	-920.97949	-920.97918	-920.91305	-920.90913
4.5	-921.00202	-920.99321	-920.99313	-920.92904	-920.92189
5.0	-921.01057	-921.00306	-921.00306	-920.93788	-920.93112
6.0	-921.01728	-921.01381	-921.01379	-920.94482	-920.94163
∞	-921.02076	-921.02076	-921.02076	-920.94858	-920.94858

Table 65 (Continued)

R	$^1\Pi$ I	$^1\Pi$ II	$^1\Pi$ III	$^1\Pi$ IV	$^1\Pi$ V
2.5	-921.10065	-921.09583	-921.00741	-920.84785	-920.83398
2.7	-921.26628	-921.21151	-921.15421	-921.02620	-921.00194
2.9	-921.35057	-921.25797	-921.2266	-921.12509	-921.12097
3.1	-921.38455	-921.27328	-921.24684	-921.19279	-921.16251
3.3	-921.38935	-921.28133	-921.23268	-921.23159	-921.18857
3.5	-921.37928	-921.28643	-921.26207	-921.21234	-921.20640
3.7	-921.36400	-921.29288	-921.28320	-921.22186	-921.21233
3.9	-921.34959	-921.30037	-921.29715	-921.22903	-921.22273
4.1	-921.33916	-921.30762	-921.30655	-921.23583	-921.23159
4.5	-921.33128	-921.32011	-921.31885	-921.24702	-921.24554
5.0	-921.33494	-921.33228	-921.32961	-921.25915	-921.25716
6.0	-921.34731	-	"	-	-
∞	-921.35604	-921.35604	-921.35604	-921.28385	-921.28385

R	$^1\Pi$ VI	$^1\Pi$ VII	$^1\Pi$ VIII	$^1\Pi$ IX	$^1\Pi$ X
2.5	-920.82573	-920.79024	-920.77997	-920.68237	-920.66877
2.7	-920.95018	-920.97049	-920.96560	-920.89931	-920.88423
2.9	-921.07249	-921.05694	-921.04331	-921.03559	-921.02150
3.1	-921.13077	-921.13904	-921.11505	-921.10712	-921.07686
3.3	-921.17605	-921.16094	-921.13621	-921.12173	-921.11638
3.5	-921.19427	-921.15708	-921.15267	-921.13529	-921.12089
3.7	-921.17177	-921.16801	-921.15200	-921.13886	-921.13379
3.9	-921.16841	-921.16141	-921.14925	-921.14524	-921.14144
4.1	-921.16749	-921.16875	-921.15575	-921.15355	-921.14447
4.5	-921.17159	-921.17045	-921.16759	-921.16458	-921.14517
5.0	-921.18032	-921.17937	-921.17914	-921.17381	-921.14929
6.0	-	-	-	-	-
∞	-921.00951	-921.00951	-921.00951	-920.94128	-920.94128

Table 65 (Continued)

R	B $^3\Pi$ I	$^3\Pi$ II	$^3\Pi$ III	$^3\Pi$ IV	$^3\Pi$ V
2.7	-921.27263	-921.22046	-921.17090	-921.03174	-921.02985
2.9	-921.35443	-921.26893	-921.23832	-921.14966	-921.12729
3.1	-921.38615	-921.28668	-921.25262	-921.21436	-921.17254
3.3	-921.38871	-921.29109	-921.24739	-921.23673	-921.20803
3.5	-921.37641	-921.29045	-921.26797	-921.23686	-921.22472
3.7	-921.35906	-921.29310	-921.28517	-921.24516	-921.23639
3.9	-921.34323	-921.29981	-921.29772	-921.24752	-921.24522
4.1	-	-	-	-	-
4.5	-921.32721	-921.32004	-921.31884	-921.26049	-921.25805
5.0	-	-	-	-	-
6.0	-921.34728	-	-	-	-
∞	-921.35604	-921.35604	-921.35604	-921.29370	-921.29370

R	$^3\Pi$ VI	$^3\Pi$ VII	$^3\Pi$ VIII	$^3\Pi$ IX	$^3\Pi$ X
2.7	-921.02862	-921.01295	-920.99735	-920.97522	-920.96979
2.9	-	-	-	-	-
3.1	-921.16963	-921.14742	-921.13842	-921.12100	-921.11989
3.3	-921.19655	-921.18701	-921.17609	-921.17528	-921.15329
3.5	-921.21269	-921.21225	-921.19133	-921.18844	-921.18615
3.7	-921.23289	-921.21331	-921.20917	-921.20537	-921.20519
3.9	-921.23969	-921.22630	-921.22105	-921.22030	-921.21601
4.1	-	-	-	-	-
4.5	-921.25729	-921.24694	-921.24564	-921.23376	-921.23313
5.0	-	-	-	-	-
6.0	-	-	-	-	-
∞	-921.29370	-921.28385	-921.28385	-921.26211	-921.26211

Table 65 (Continued)

R	$^5\Pi$ I	$^5\Pi$ II	$^5\Pi$ III	$^5\Pi$ IV	$^5\Pi$ V
2.5	-920.87298	-920.86065	-920.72372	-920.70760	-920.64224
2.7	-921.04256	-921.02085	-920.93978	-920.92194	-920.89358
2.9	-921.13861	-921.09900	-921.07630	-921.06284	-921.04613
3.1	-921.18458	-921.16669	-921.16326	-921.13174	-921.10983
3.3	-921.22905	-921.22423	-921.19257	-921.16734	-921.15465
3.5	-921.26568	-921.25833	-921.21713	-921.19715	-921.17394
3.7	-921.28711	-921.28032	-921.25131	-921.21169	-921.20103
3.9	-921.30001	-921.29494	-921.27525	-921.22412	-921.21974
4.1	-921.30836	-921.30532	-921.29244	-921.23362	-921.23135
4.5	-921.31984	-921.31931	-921.31480	-921.24716	-921.24556
5.0	-921.33242	-921.33107	-921.32762	-921.25959	-921.25710
6.0	-921.34729	-921.34720	-921.34466	-921.27487	-921.27246
∞	-921.35604	-921.35604	-921.35604	-921.28385	-921.28385

R	$^7\Pi$ I	$^7\Pi$ II	$^7\Pi$ III	$^7\Pi$ IV	$^7\Pi$ V
2.5	-920.37959	-920.26619	-920.25423	-920.13398	-920.06214
2.7	-920.61397	-920.53630	-920.51132	-920.41184	-920.37775
2.9	-920.76333	-920.71261	-920.67746	-920.59471	-920.58273
3.1	-920.85547	-920.82396	-920.78722	-920.72211	-920.70719
3.3	-920.91147	-920.89357	-920.85975	-920.80658	-920.78475
3.5	-920.94516	-920.93697	-920.90762	-920.85931	-920.83501
3.7	-920.96548	-920.96412	-920.93924	-920.89129	-920.86779
3.9	-920.98136	-920.97788	-920.96027	-920.91035	-920.88931
4.1	-920.99231	-920.98595	-920.97448	-920.92173	-920.90366
4.5	-921.00426	-920.99586	-920.99139	-920.93315	-920.92042
5.0	-921.01120	-921.00382	-921.00261	-920.93946	-920.93124
6.0	-921.01733	-921.01386	-921.01378	-920.94526	-920.94189
∞	-921.02076	-920.02076	-921.02076	-920.94858	-920.94858

Table 65 (Continued)

R	$^1\Delta$ I	$^1\Delta$ II	$^1\Delta$ III	$^1\Delta$ IV	$^1\Delta$ V
2.5	-921.24234	-921.12289	-920.97241	-920.78649	-920.77550
2.7	-921.33218	-921.24979	-921.15885	-920.98613	-920.97023
2.9	-921.35530	-921.30910	-921.25879	-921.09769	-921.07736
3.1	-921.34206	-921.32983	-921.30224	-921.15246	-921.14069
3.3	-921.34014	-921.31208	-921.30117	-921.19886	-921.17190
3.5	-921.33719	-921.30576	-921.25841	-921.23250	-921.22419
3.7	-921.33042	-921.30105	-921.25935	-921.24875	-921.21342
3.9	-921.32464	-921.30253	-921.28153	-921.25416	-921.17295
4.1	-921.32208	-921.30777	-921.29640	-921.25458	-921.17110
4.5	-921.32483	-921.31956	-921.31402	-921.25583	-921.17348
5.0	-921.33342	-921.33183	-921.32829	-921.26236	-921.18133
6.0	-921.34725	-	-	-	-
∞	-921.35604	-921.35604	-921.35604	-921.28385	-921.00951

R	$^1\Delta$ VI	$^1\Delta$ VII	$^1\Delta$ VIII	$^1\Delta$ IX	$^1\Delta$ X
2.5	-920.72284	-920.71639	-920.69851	-920.66173	-920.65907
2.7	-920.91424	-920.89906	-920.89679	-920.88342	-920.83524
2.9	-921.04725	-921.02855	-921.00719	-920.97746	-920.97076
3.1	-921.12904	-921.08703	-921.08498	-921.07183	-921.05090
3.3	-921.14812	-921.14885	-921.11603	-921.10814	-921.08274
3.5	-921.15563	-921.15964	-921.13091	-921.11714	-921.11573
3.7	-921.16938	-921.14943	-921.13662	-921.13433	-921.11702
3.9	-921.16943	-921.14710	-921.14432	-921.12720	-921.12537
4.1	-921.16431	-921.15312	-921.13464	-921.13187	-921.12587
4.5	-921.16757	-921.16274	-921.14002	-921.13664	-921.13403
5.0	-921.17882	-921.17309	-921.14783	-921.14630	-921.14495
6.0	-	-	-	-	-
∞	-921.00951	-921.00951	-920.94858	-920.94858	-920.94858

Table 65 (Continued)

R	X $^3\Delta$ I	$^3\Delta$ II	$^3\Delta$ III	$^3\Delta$ IV	$^3\Delta$ V
2.5	-921.24565	-921.14373	-921.00892	-920.82504	-920.79073
2.7	-921.33507	-921.26625	-921.19202	-921.01869	-920.99012
2.9	-921.35773	-921.32170	-921.28858	-921.12545	-921.10249
3.1	-921.34308	-921.33950	-921.32860	-921.17731	-921.16017
3.3	-921.34641	-921.32969	-921.30606	-921.20910	-921.19743
3.5	-921.34034	-921.3178[illegible]	-921.26288	-921.24321	-921.22706
3.7	-921.32925	-921.30673	-921.26337	-921.25993	-921.23167
3.9	-921.32068	-921.30345	-921.28284	-921.26833	-921.23923
4.1	-921.31792	-921.30752	-921.29723	-921.26552	-921.24509
4.5	-921.32286	-921.31948	-921.31494	-921.26112	-921.25662
5.0	-921.33295	-921.33188	-921.32838	-921.26997	-921.26723
6.0	-921.34726	-	-	-	-
∞	-921.35604	-921.35604	-921.35604	-921.29370	-921.29370

R	$^3\Delta$ VI	$^3\Delta$ VII	$^3\Delta$ VIII	$^3\Delta$ IX	$^3\Delta$ X
2.5	-920.78358	-920.77699	-920.72764	-920.72142	-920.71396
2.7	-920.97832	-920.97609	-920.92481	-920.91067	-920.90517
2.9	-921.09052	-921.08243	-921.05761	-921.03587	-921.03473
3.1	-921.14851	-921.14588	-921.13304	-921.12310	-921.09209
3.3	-921.17863	-921.17566	-921.17425	-921.16742	-921.15531
3.5	-921.21509	-921.19836	-921.19315	-921.18694	-921.17689
3.7	-921.22203	-921.21592	-921.20830	-921.20083	-921.19645
3.9	-921.22977	-921.22495	-921.21243	-921.20934	-921.20498
4.1	-921.23893	-921.23117	-921.21997	-921.21742	-921.21553
4.5	-921.25184	-921.23613	-921.23138	-921.22978	-921.22765
5.0	-921.26157	-921.24382	-921.24148	-921.24090	-921.23727
6.0	-	-	-	-	-
∞	-921.28385	-921.26211	-921.26211	-921.26211	-921.26211

Table 65 (Continued)

R	$^5\Delta$ I	$^5\Delta$ II	$^5\Delta$ III	$^5\Delta$ IV	$^5\Delta$ V
2.5	-920.83895	-920.79174	-920.73050	-920.72213	-920.68570
2.7	-921.03124	-920.99066	-920.94582	-920.91552	-920.90663
2.9	-921.1369[illegible]	-921.10165	-921.08489	-921.06034	-921.0050[illegible]
3.1	-921.189[illegible]	-921.16825	-921.15942	-921.14722	-921.09941
3.3	-921.22918	-921.21098	-921.19532	-921.18044	-921.17094
3.5	-921.26088	-921.24714	-921.23176	-921.18968	-921.16917
3.7	-921.28148	-921.27137	-921.26418	-921.18980	-921.17123
3.9	-921.29[illegible]30	-921.28828	-921.28491	-921.21097	-921.14773
4.1	-921.305[illegible]	-921.30068	-921.298[illegible]6	-921.22589	-921.12287
4.5	-921.31945	-921.3178[illegible]	-921.31557	-921.24516	-921.07801
5.0	-921.33212	-921.33183	-921.32856	-921.25976	-921.03936
6.0	-921.34727	-921.34713	-921.34459	-921.27520	-921.02036
∞	-921.35604	-921.35604	-921.35604	-921.28385	-921.02076

R	$^5\Delta$ VI	$^5\Delta$ VII	$^5\Delta$ VIII	$^5\Delta$ IX	$^5\Delta$ X
2.5	-920.[illegible]1747	-920.47711	-920.4[illegible]8[illegible]	-920.38155	-920.36622
2.7	-920.77845	-920.7597[illegible]	-920.7[illegible]704	-920.58547	-920.58149
2.9	-920.97[illegible]97	-920.92132	-920.88782	-920.72829	-920.72586
3.1	-921.05507	-921.03265	-920.97339	-920.82778	-920.82468
3.3	-921.10[illegible]98	-921.07[illegible]92	-921.01[illegible]	-920.89693	-920.89378
3.5	-921.1[illegible]409	-921.08003	-921.03086	-920.93903	-920.93788
3.7	-921.1[illegible]00[illegible]	-921.07491	-921.03091	-920.96649	-920.96188
3.9	-921.12880	-921.06[illegible]29	-921.0[illegible]262	-920.98311	-920.97[illegible]70
4.1	-921.10[illegible]81	-921.05399	-921.011[illegible]1	-920.99334	-920.98386
4.5	-921.0[illegible]	-921.03183	-921.00465	-921.00[illegible]22	-920.99655
5.0	-921.02999	-921.01230	-921.0076[illegible]	-921.00658	-921.00470
6.0	-921.01987	-921.01040	-921.00589	-921.00555	-921.00480
∞	-921.02076	-921.0207[illegible]	-921.00951	-921.00951	-921.00951

Table 64 (Continued)

R	$^{7}\Delta$ I	$^{7}\Delta$ II	$^{7}\Delta$ III	$^{7}\Delta$ IV
2.5	-920.37612	-920.25931	-920.23380	-920.19432
2.7	-920.60097	-920.54581	-920.49838	-920.45778
2.9	-920.74370	-920.72869	-920.67086	-920.62888
3.1	-920.84316	-920.83324	-920.78414	-920.73918
3.3	-920.91221	-920.89070	-920.85857	-920.80935
3.5	-920.95332	-920.92745	-920.90745	-920.85326
3.7	-920.97728	-920.95193	-920.93959	-920.88048
3.9	-920.99109	-920.96820	-920.96085	-920.89749
4.1	-920.99914	-920.97938	-920.97513	-920.90849
4.5	-921.00720	-920.99321	-920.99196	-920.92150
5.0	-921.01207	-921.00316	-921.00292	-920.93089
6.0	-921.01739	-921.01394	-921.01379	-920.94154
∞	-921.02076	-921.02076	-921.02076	-920.94858

R	^{1}H I	^{3}H I	^{3}H II	^{3}H III	^{5}H I
2.5	-920.30641	-920.81[illegible]10	[illegible]	-920.54704	-920.27746
2.7	-920.98488	-920.99212	-920.86639	-920.81818	-920.51885
2.9	-920.61042	-921.08632	-920.99739	-920.98752	-920.67074
3.1	-920.72430	-921.12863	-921.09056	-921.07680	-920.76459
3.3	-920.79522	-921.1[illegible]113	-921.14614	-921.11169	-920.82280
3.5	-920.83843	-921.18517	-921.16754	-921.11444	-920.85807
3.7	-920.85441	-921.20383	-921.18552	-921.09392	-920.87969
3.9	-920.87983	-921.21401	-921.19834	-921.06778	-920.89340
4.1	-920.88912	-921.22000	-921.20791	-921.04071	-920.90268
4.5	-920.89892	-921.22777	-921.22214	-920.99251	-920.914[illegible]
5.0	-920.90[illegible]	-921.23641	-921.23519	-920.95195	-920.92370
6.0	-920.91182	-921.25087	-921.25083	-920.94182	-920.93418
∞	-920.94128	-921.2[illegible]11	-921.[illegible]001	-920.94128	-920.94128

Table 65 (Continued)

R	$^1\Phi$ I	$^1\Phi$ II	$^1\Phi$ III	$^1\Phi$ IV	$^1\Phi$ V
2.5	-921.10956	-920.85590	-920.80992	-920.79548	-920.63373
2.7	-921.27426	-921.01204	-920.98319	-920.94451	-920.86888
2.9	-921.35772	-921.09307	-921.07887	-921.04407	-921.01848
3.1	-921.39102	-921.15409	-921.12779	-921.12231	-921.05504
3.3	-921.39522	-921.22148	-921.13531	-921.13320	-921.09671
3.5	-921.38457	-921.26186	-921.13267	-921.13118	-921.12524
3.7	-921.36865	-921.28569	-921.14990	-921.12889	-921.12641
3.9	-921.35349	-921.29990	-921.15941	-921.14294	-921.12503
4.1	-921.34218	-921.30887	-921.16428	-921.15273	-921.12725
4.5	-921.33260	-921.32017	-921.17062	-921.16450	-921.13607
5.0	-921.33518	-921.33021	-921.17938	-921.17391	-921.14616
6.0	-921.34731	-921.34480	-921.19202	-921.18850	-921.15933
∞	-921.35604	-921.35604	-921.00951	-921.00951	-920.94128

R	$^1\Phi$ VI	$^1\Phi$ VII	$^7\Phi$ I	$^7\Phi$ II
2.5	-920.61513	-920.60656	-920.37536	-920.09706
2.7	-920.85255	-920.83098	-920.61376	-920.41544
2.9	-920.97930	-920.96598	-920.76317	-920.62542
3.1	-921.04524	-921.03893	-920.85535	-920.76298
3.3	-921.08588	-921.07646	-920.91140	-920.85240
3.5	-921.10953	-921.08861	-920.94514	-920.91002
3.7	-921.10918	-921.10103	-920.96548	-920.94686
3.9	-921.11544	-921.10798	-920.97805	-920.97027
4.1	-921.12471	-921.11831	-920.98669	-920.98469
4.5	-921.13494	-921.13326	-921.00160	-920.99579
5.0	-921.14569	-921.14451	-921.01030	-921.00380
6.0	-921.15833	-921.15792	-921.01714	-921.01385
∞	-920.94128	-920.94128	-921.02076	-921.02076

Table 65 (Continued)

R	A ^{3}●I	^{3}●II	^{3}●III	^{3}●IV	^{3}●V
2.5	-921.10954	-920.89138	-920.86480	-920.81423	-920.79233
2.7	-921.27293	-921.03532	-921.01933	-920.99028	-920.94530
2.9	-921.35514	-921.10884	-921.09928	-921.08456	-921.05800
3.1	-921.38720	-921.16496	-921.14021	-921.13401	-921.12695
3.3	-921.39014	-921.22877	-921.15299	-921.15078	-921.14521
3.5	-921.37826	-921.26623	-921.18951	-921.18266	-921.17596
3.7	-921.36134	-921.28792	-921.21554	-921.20446	-921.19720
3.9	-921.34581	-921.30072	-921.23283	-921.21719	-921.20937
4.1	-921.33512	-921.30893	-921.24415	-921.22490	-921.21672
4.5	-921.32856	-921.32000	-921.25815	-921.23339	-921.22922
5.0	-921.33392	-921.33023	-921.27026	-921.24203	-921.24166
6.0	-921.24728	-921.34480	-921.28499	-921.25531	-921.25428
∞	-921.35604	-921.35604	-921.29370	-921.26211	-921.26212

R	^{5}●I	^{5}●II	^{5}●III	^{5}●IV	^{5}●V
2.5	-920.89188	-920.64583	-920.63913	-920.56140	-920.36277
2.7	-921.04262	-920.91442	-920.86259	-920.81590	-920.59838
2.9	-921.11971	-921.08289	-920.99352	-920.98257	-920.74736
3.1	-921.18535	-921.15141	-921.09327	-921.06421	-920.84182
3.3	-921.24549	-921.16719	-921.15597	-921.09727	-920.90282
3.5	-921.27945	-921.21693	-921.14587	-921.10669	-920.94267
3.7	-921.29800	-921.25117	-921.12818	-921.10215	-920.96858
3.9	-921.30812	-921.27516	-921.10767	-921.09014	-920.98547
4.1	-921.31406	-921.29237	-921.08709	-921.07489	-920.99657
4.5	-921.32187	-921.31474	-921.09407	-921.04920	-921.04149
5.0	-921.33117	-921.33025	-921.02036	-921.01594	-921.01316
6.0	-921.34721	-921.34480	-921.01959	-921.01613	-921.00545
∞	-921.35604	-921.35604	-921.02076	-921.02076	-921.00951

Table 65 (Continued)

R	$^{1}\Gamma_{I}$	$^{1}\Gamma_{II}$	$^{1}\Gamma_{III}$	$^{1}\Gamma_{IV}$	$^{1}\Gamma_{I}$
2.5	-920.89115	-920.79920	-920.74012	-920.73457	-920.88130
2.7	-921.01251	-921.00803	-921.00112	-920.92330	-921.01251
2.9	-921.10994	-921.07010	-921.06336	-921.02223	-921.11719
3.1	-921.16487	-921.15625	-921.09207	-921.07496	-921.17249
3.3	-921.21625	-921.18110	-921.10421	-921.08621	-921.21999
3.5	-921.25277	-921.17701	-921.10970	-921.10480	-921.25520
3.7	-921.27616	-921.16051	-921.12752	-921.11374	-921.27777
3.9	-921.29180	-921.14122	-921.13813	-921.11949	-921.29285
4.0	-921.30294	-921.15025	-921.12540	-921.11787	-921.30363
4.5	-921.31839	-921.16227	-921.13514	-921.13234	-921.31870
5.0	-921.33162	-921.17317	-921.14552	-921.14483	-921.33175
6.0	-921.34701	-921.18840	-921.15898	-921.15815	-921.25211
∞	-921.35604	-921.00951	-920.94128	-920.94128	-921.35604

R	$^{3}\Gamma_{II}$	$^{3}\Gamma_{III}$	$^{3}\Gamma_{IV}$	$^{3}\Gamma_{V}$	$^{3}\Gamma_{VI}$
2.5	-920.81130	-920.80101	-920.72432	-920.69085	-920.62087
2.7	-921.00803	-921.00112	-920.92330	-920.92053	-920.84763
2.9	-921.11443	-921.07432	-921.06973	-921.02874	-921.00457
3.1	-921.17018	-921.15964	-921.10087	-921.09689	-921.09021
3.3	-921.19495	-921.18452	-921.15697	-921.12857	-921.12123
3.5	-921.20307	-921.18830	-921.11799	-921.16183	-921.14318
3.7	-921.20866	-921.05050	-921.15343	-921.16923	-921.16336
3.9	-921.21493	-921.21397	-921.19786	-921.19019	-921.14149
4.1	-921.22080	-921.21914	-921.20822	-921.20416	-921.11941
4.5	-921.23081	-921.22620	-921.22280	-921.22135	-921.07718
5.0	-921.24102	-921.23603	-921.23454	-921.23426	-921.04244
6.0	-921.25065	-921.24891	-921.02270	-921.00470	-920.97661
∞	-921.26211	-921.26211	-921.26001	-921.26001	-921.02076

Table 65 (Continued)

R	$^{3}\Gamma_{VII}$	$^{3}\Gamma_{VIII}$	$^{3}\Gamma_{IX}$	$^{5}\Gamma_{I}$	$^{5}\Gamma_{II}$
2.5	-920.61143	-920.58648	-920.38032	-920.82380	-920.71437
2.7	-920.84659	-920.83419	-920.68055	-921.01977	-920.94038
2.9	-920.98718	-920.98005	-920.87642	-921.12811	-921.08180
3.1	-921.07257	-921.06703	-921.00314	-921.18291	-921.16617
3.3	-921.09745	-921.08484	-921.08431	-921.22728	-921.19152
3.5	-921.13519	-921.09049	-921.06979	-921.25995	-921.18647
3.7	-921.14070	-921.07232	-921.04741	-921.28091	-921.16895
3.9	-921.12576	-921.04877	-921.02323	-921.29492	-921.14584
4.1	-921.10531	-921.02386	-920.99988	-921.30498	-921.12131
4.5	-921.05418	-921.09793	-920.97847	-921.32931	-921.07687
5.0	-921.02632	-920.98829	-920.97280	-921.33202	-921.03858
6.0	-920.96995	-920.94112	-920.96995	-921.34713	-921.02032
∞	-921.00951	-920.94128	-920.94128	-921.35604	-921.02076

R	$^{5}\Gamma_{III}$	$^{5}\Gamma_{IV}$	$^{5}\Gamma_{V}$	$^{7}\Gamma_{I}$
2.1	-920.30833	-920.27966	-920.21167	-920.23299
2.7	-920.53099	-920.50883	-920.47467	-920.49701
2.9	-920.67084	-920.65560	-920.64900	-920.67018
3.1	-920.76612	-920.76202	-920.75781	-920.78389
3.3	-920.84517	-920.83587	-920.82081	-920.85852
3.5	-920.89912	-920.89912	-920.86308	-920.90749
3.7	-920.93601	-920.93601	-920.88876	-920.93966
3.9	-920.96119	-920.96119	-920.90458	-920.96093
4.1	-920.97828	-920.97828	-920.91454	-920.97519
4.5	-920.99740	-920.99740	-920.92539	-920.99202
5.0	-921.00585	-921.00585	-920.93187	-921.00303
6.0	-921.00586	-921.00586	-920.93788	-921.01393
∞	-921.00951	-920.94128	-920.94128	-921.02076

Table 66

Spectroscopic Constants for Bound States of TiO

State	T_e (cm^{-1})	ω_e (cm^{-1})	$\omega_e X_e$ (cm^{-1})	B_o (cm^{-1})	r_e (Å)	α_e (cm^{-1})
X $^3\Delta$	0.0	1008.2	4.13	0.5338	1.620	.003
a $^1\Delta$	580.0	1016.3	3.93	0.5362	1.619	-
d $^1\Sigma^+$	2802.3	1023.8	4.60	0.5490	1.600	.00337
b $^1\Pi$	11899.6	918.7	3.75	0.5133	1.654	.0028
A $^3\Phi$	14192.3	867.71	3.94	0.5057	1.664	.0031
B $^3\Pi$	16248.0	865.	-	0.50613	1.6637	-
c $^1\Phi$	18470.09	917.55	4.42	0.52115	1.642	-
C $^3\Delta$	19437.4	837.86	4.54	0.4884	1.695	.0029

a. S. Suchard, Spectroscopic Constants for Selected Heteronuclear Diatomic Molecules, Vol. III., Aerospace Corpora-ion, 1974.

Table 67

Calculated Oscillator Strengths ($f_{v'v''}$) for the Vibrational-Rotational Transitions of TiO ($X\,^3\Delta - X\,^3\Delta$)

v'\v"	0	1	2	3	4	5
0						
1	2.494-05					
2	5.029-09	4.865-05				
3	1.755-08	3.002-08	7.140-05			
4	6.492-10	5.094-08	1.126-07	9.333-05		
5	1.943-10	7.489-10	9.087-08	2.613-07	1.145-04	
6	1.377-09	1.745-09	3.620-09	1.337-07	4.819-07	1.349-04
7	2.644-10	5.593-10	3.244-09	1.152-08	1.805-07	8.106-07
8	2.237-11	1.882-11	1.016-09	3.158-09	2.110-08	2.276-07
9	3.581-10	6.794-11	6.120-11	2.999-09	2.854-09	3.609-08
10	9.602-10	3.553-10	1.217-10	8.537-14	4.707-09	1.640-09

v'\v"	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6					
7	1.545-04				
8	1.249-06	1.733-04			
9	2.787-07	1.827-06	1.911-04		
10	5.458-08	3.318-07	2.559-06	2.081-04	

TABLE 68

Calculated Oscillator Strengths ($f_{v'v''}$) for the Gamma System of TiO ($A^3\Phi - X^3\Delta$)

v'/v"	0	1	2	3	4	5
0	3.102-02	8.105-03	1.095-03	8.689-05	4.240-06	1.413-07
1	1.271-02	1.319-02	1.084-02	2.547-03	2.922-04	1.908-05
2	2.713-03	1.720-02	4.057-03	1.039-02	3.886-03	6.147-04
3	3.976-04	6.397-03	1.666-02	4.933-04	8.384-03	4.365-03
4	4.419-05	1.360-03	9.862-03	1.347-02	1.050-04	5.881-03
5	3.793-06	2.018-04	2.858-03	1.234-02	9.416-03	1.190-03
6	2.367-07	2.171-05	5.365-04	4.750-03	1.351-02	5.634-03
7	5.616-09	1.426-06	7.124-05	1.105-03	6.798-03	1.338-02
8	2.372-09	1.771-08	6.026-0[illegible]	1.762-04	1.943-03	8.740-03
9	7.299-09	1.028-08	1.360-07	1.870-05	3.685-04	3.038-03
10	4.449-09	1.358-08	2.754-08	8.198-07	4.664-05	6.796-04

v'/v"	6	7	8	9	10
0	4.953-09	1.769-09	6.174-11	5.259-10	1.775-12
1	9.597-07	4.908-08	1.949-09	2.924-14	3.788-10
2	5.211-05	3.173-06	1.778-07	3.419-09	1.667-10
3	1.024-03	1.038-04	7.779-06	5.181-07	1.514-08
4	5.373-03	1.475-03	1.952-04	1.643-05	1.191-06
5	3.547-03	5.419-03	1.927-03	3.108-04	3.063-05
6	2.635-03	1.743-03	5.065-03	2.333-03	4.546-04
7	2.723-03	3.805-03	5.910-04	4.418-03	2.655-03
8	1.214-02	8.950-04	4.419-03	6.441-05	3.592-03
9	1.033-02	1.015-02	8.752-05	4.440-03	4.397-05
10	4.343-03	1.138-02	7.791-03	7.685-05	3.967-03

Table 69

Calculated Oscillator Strengths ($f_{v'v''}$) for the Gamma Prime System of TiO ($B^3\Pi - X^3\Delta$)

v'/v"	0	1	2	3	4	5
0	3.784-02	8.430-03	1.065-03	5.285-05	6.231-07	2.238-08
1	1.392-02	2.029-02	1.093-02	2.151-03	1.227-04	1.077-06
2	2.143-03	1.966-02	1.150-02	1.101-02	2.971-03	1.768-04
3	1.324-04	4.667-03	2.171-02	7.104-03	1.026-02	3.518-03
4	2.987-07	3.627-04	6.893-03	2.213-02	4.961-03	9.312-03
5	1.291-06	3.228-07	6.036-04	8.597-02	2.198-02	4.023-03
6	4.447-07	6.931-06	1.968-08	7.926-04	9.743-03	2.174-02
7	5.666-08	2.590-06	2.008-05	2.648-06	8.884-04	1.037-02
8	5.683-09	2.435-07	7.254-06	4.428-05	1.496-05	8.683-04
9	2.745-11	5.617-10	6.023-07	1.452-05	8.332-05	4.768-05
10	3.718-09	6.245-09	6.568-09	1.077-06	2.459-05	1.377-04

v'/v"	6	7	8	9	10
0	2.618-09	9.270-10	8.844-11	7.852-10	7.438-12
1	1.038-07	3.670-09	2.620-11	3.022-12	6.797-10
2	9.115-07	4.043-07	5.919-09	7.060-10	2.871-10
3	1.950-0[illegible]	2.561-07	1.156-06	2.052-09	3.043-10
4	3.838-03	1.732-04	5.015-08	2.343-06	1.392-09
5	8.391-03	3.987-03	1.225-04	1.312-06	3.99[illegible]-06
6	3.815-03	7.578-03	3.998-03	6.017-05	4.387-06
7	2.154-02	4.140-03	6.855-03	3.897-03	1.00[illegible]-05
8	1.052-02	2.139-02	4.954-03	6.181-03	3.609-03
9	7.425-04	1.023-02	2.124-02	6.284-03	5.498-03
10	1.132-04	5.398-04	9.544-03	[illegible].0[illegible]5-02	8.179-03

Table 70

Calculated Franck-Condon Factors ($q_{v'v''}$) for the Gamma System of TiO ($A\ ^3\Phi - X\ ^3\Delta$)

v'\v''	0	1	2	3	4	5
0	7.138-01	2.401-01	4.109-02	4.441-03	3.341-04	1.876-05
1	2.392-01	3.096-01	3.337-01	9.987-02	1.567-02	1.559-03
2	4.155-02	3.307-01	9.635-02	3.332-01	1.592-01	3.413-02
3	4.759-03	1.005-01	3.271-01	1.112-02	2.795-01	2.077-01
4	3.739-04	1.694-02	1.588-01	2.706-01	3.602-03	2.038-01
5	1.809-05	1.831-03	3.703-02	2.040-01	1.933-01	3.538-02
6	3.055-07	1.209-04	5.242-03	6.372-02	2.295-01	1.175-01
7	7.113-09	3.117-06	4.526-04	1.149-02	9.429-02	2.334-01
8	1.126-08	3.167-08	1.734-05	1.257-03	2.123-02	1.252-01
9	4.571-09	9.498-08	1.197-08	6.716-05	2.882-03	3.477-02
10	1.566-09	3.196-08	3.800-07	1.069-07	2.042-04	5.758-03

v'\v''	6	7	8	9	10
0	7.872-07	1.522-08	2.509-10	2.744-10	2.457-12
1	1.069-04	5.2[illegible]5-06	1.608-07	3.705-09	6.237-10
2	4.314-03	3.[illegible]78-04	2.0[illegible]8-05	7.863-07	2.151-08
3	5.890-02	9.222-03	9.102-04	6.061-05	2.707-06
4	2.387-01	8.80[illegible]-02	1.679-02	1.946-03	1.485-04
5	1.579-01	2.499-01	1.189-01	2.732-02	3.683-03
6	7.916-02	[illegible].944-02	2.423-01	1.489-01	4.087-02
7	5.694-02	1.174-01	2.318-02	2.188-01	1.751-01
8	2.175-01	1.79[illegible]-02	1.408-01	2.696-03	1.842-01
9	1.[illegible]27-01	1.8[illegible]6-01	1.141-03	1.463-01	1.711-03
10	5.187-02	1.73[illegible]-01	1.46[illegible]-01	3.319-03	1.354-01

Table 71

Calculated Franck-Condon Factors ($q_{v'v''}$) for the Gamma Prime System of TiO ($B\ ^3\Pi - X\ ^3\Delta$)

v'\v"	0	1	2	3	4	5
0	7.480-01	2.155-01	3.371-02	2.490-03	7.446-05	1.660-06
1	2.236-01	4.053-01	2.929-01	7.137-02	6.406-03	1.880-04
2	2.711-02	3.167-01	2.309-01	3.112-01	1.034-01	1.018-02
3	1.044-03	5.917-02	3.497-01	1.423-01	3.066-01	1.279-01
4	7.513-06	2.838-03	8.735-02	3.566-01	9.854-02	2.955-01
5	2.628-05	4.172-05	4.684-03	1.086-01	3.536-01	7.913-02
6	4.412-06	1.206-04	1.463-04	5.977-03	1.226-01	3.479-01
7	1.225-07	2.171-05	3.264-04	3.938-04	6.344-03	1.295-01
8	9.454-08	5.355-07	5.834-05	6.776-04	8.859-04	5.694-03
9	8.339-09	1.068-07	1.123-06	1.176-04	1.189-03	1.744-03
10	1.549-09	7.551-08	5.345-07	1.351-06	1.908-04	1.849-03

v'\v"	6	7	8	9	10
0	1.342-07	1.297-08	2.701-11	2.903-10	5.591-12
1	5.309-07	7.242-07	3.876-08	1.448-09	5.694-10
2	2.571-04	6.[illegible]-05	2.171-06	6.000-08	1.215-08
3	1.270-02	2.319-04	3.042-05	4.144-06	4.617-08
4	1.4[illegible]-01	1.339-02	1.278-04	8.575-05	5.307-06
5	2.846-01	1.587-01	1.214-02	2.130-05	1.822-04
6	7.463-02	2.764-01	1.324-01	9.293-03	1.747-05
7	3.420-01	8.137-02	2.709-01	1.627-01	5.562-03
8	1.299-01	3.359-01	9.889-02	2.670-01	1.574-01
9	4.211-03	1.246-01	3.284-01	1.265-01	2.628-01
10	3.082-03	2.328-03	1.142-01	3.171-01	1.724-01

Table 72

Calculated R-Centroid Factors ($\langle A \rangle_{v'v''}$)
for the Vibrational-Rotational Transition of TiO ($X\ ^3\Delta - X\ ^3\Delta$)

v'\v"	0	1	2	3	4	5
0	1.626+00					
1	3.740-02	1.633+00				
2	-1.701-03	5.301-02	1.640+00			
3	1.228-04	-2.955-03	6.506-02	1.648+00		
4	-1.085-05	2.531-04	-4.193-03	7.528-02	1.655+00	
5	1.910-06	-2.636-05	4.023-04	-5.431-03	8.434-02	1.663+00
6	-7.031-07	3.339-06	-4.628-05	5.715-04	-6.674-03	9.259-02
7	-1.642-08	-7.204-07	5.923-06	-7.122-05	7.594-04	-7.923-03
8	2.462-07	7.111-08	-9.471-07	9.633-06	-1.015-04	9.646-04
9	-1.079-07	1.959-07	1.341-07	-1.432-06	1.443-05	-1.368-04

v'\v"	6	7	8	9	10
0					
1					
2					
3					
4					
5					
6	1.670+00				
7	1.002-01	1.678+00			
8	-9.150-03	1.074-01	1.686+00		
9	1.165-03	-1.044-02	1.141-01	1.695+00	
10	-1.774-04	1.474-03	-1.172-02	1.206-01	1.701+00

Table 73

Calculated R-Centroid Factors ($\langle r \rangle_{v'v''}$) for the Gamma System of TiO ($A\,^3\Phi - X\,^3\Delta$)

v'\v"	0	1	2	3	4	5
0	1.647+00	1.719+00	1.783+00	1.846+00	1.909+00	1.970+00
1	1.586+00	1.654+00	1.726+00	1.791+00	1.853+00	1.916+00
2	1.518+00	1.594+00	1.657+00	1.736+00	1.799+00	1.861+00
3	1.440+00	1.529+00	1.603+00	1.641+00	1.745+00	1.807+00
4	1.336+00	1.454+00	1.539+00	1.610+00	1.753+00	1.754+00
5	1.159+00	1.358+00	1.467+00	1.549+00	1.617+00	1.717+00
6	5.929-01	1.203+00	1.376+00	1.460+00	1.559+00	1.622+00
7	3.047+00	7.653-01	1.238+00	1.394+00	1.492+00	1.568+00
8	1.696+00	3.709+00	9.009-01	1.269+00	1.410+00	1.504+00
9	1.486+00	1.750+00	9.295+00	1.001+00	1.296+00	1.426+00
10	1.441+00	1.486+00	1.828+00	-3.279+00	1.075+00	1.321+00

v'\v"	6	7	8	9	10
0	2.032+00	2.214+00	2.318+00	1.758+00	1.056+00
1	1.980+00	2.045+00	2.149+00	2.240+00	1.884+00
2	1.923+00	1.988+00	2.054+00	2.139+00	2.225+00
3	1.869+00	1.931+00	1.995+00	2.062+00	2.141+00
4	1.815+00	1.877+00	1.938+00	2.003+00	2.070+00
5	1.762+00	1.823+00	1.884+00	1.946+00	2.010+00
6	1.719+00	1.772+00	1.831+00	1.892+00	1.953+00
7	1.622+00	1.725+00	1.783+00	1.839+00	1.900+00
8	1.577+00	1.608+00	1.732+00	1.803+00	1.849+00
9	1.515+00	1.584+00	1.464+00	1.740+00	1.771+00
10	1.441+00	1.526+00	1.591+00	1.799+00	1.749+00

Table 74

Calculated R-Centroid Factors ($\langle r \rangle_{v'v''}$)
for the Gamma Prime System of TiO ($B^3\Pi - X^3\Delta$)

v'\v"	0	1	2	3	4	5
0	1.646+00	1.724+00	1.784+00	1.375+00	2.016+00	5.464+00
1	1.578+00	1.649+00	1.736+00	[illegible]	1.895+00	2.059+00
2	[illegible]	1.580+00	1.651+00	1.749+00	1.805+00	1.919+00
3	1.312+00	[illegible]	1.581+00	1.649+00	1.704+00	1.816+00
4	2.504+00	1.507+00	1.476+00	1.580+00	1.646+00	1.781+00
5	1.611+00	2.340+00	1.295+00	[illegible]	[illegible]	1.643+00
6	1.428+00	[illegible]	[illegible]	1.275+00	1.443+00	1.576+00
7	1.037+00	[illegible]	1.584+00	[illegible]	1.243+00	1.489+00
8	[illegible]	[illegible]	1.405+00	1.568+00	1.899+00	1.132+00
9	[illegible]	[illegible]	8.444-01	[illegible]	[illegible]	1.817+00
10	1.548+00	1.517+00	1.831+00	[illegible]	1.366+00	[illegible]

v'\v"	6	7	8	9	10
0	1.774+00	[illegible]	[illegible]	[illegible]	[illegible]
1	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
2	1.132+00	[illegible]	[illegible]	[illegible]	[illegible]
3	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
4	1.826+00	[illegible]	[illegible]	[illegible]	[illegible]
5	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
6	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
7	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
8	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
9	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
10	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

Table 75

Calculated Band Strengths ($p_{v'v''}$) for the Vibrational-Rotational Transition of TiO ($X\,^3\Delta - X\,^3\Delta$)

v'\v''	0	1	2	3	4	5
0	2.442+00	1.642-02	1.662-06	3.884-06	1.082-07	2.601-08
1	1.642-02	2.345+00	3.231-02	1.001-05	1.137-05	1.259-07
2	1.662-06	3.231-02	2.254+00	4.781-02	3.787-05	2.045-05
3	3.884-06	1.001-05	4.781-02	2.169+00	6.302-02	8.858-05
4	1.082-07	1.137-05	3.787-05	6.302-02	2.087+00	7.798-02
5	2.601-08	1.259-07	2.045-05	8.857-05	7.798-02	2.009+00
6	5.880-08	2.357-07	6.137-07	3.034-05	1.648-04	9.267-02
7	2.550-08	6.321-08	4.418-07	1.970-06	4.134-05	2.796-04
8	1.897-09	1.831-09	1.158-07	4.338-07	3.639-06	5.255-05
9	2.709-08	5.808-09	6.005-09	3.448-07	3.954-07	6.278-06
10	9.478-09	2.711-08	1.050-08	8.450-12	5.459-07	2.292-07

v'\v''	6	7	8	9	10
0	5.880-08	2.550-08	1.897-09	2.709-08	9.478-09
1	2.357-07	6.320-08	1.831-09	5.809-09	2.711-08
2	6.137-07	4.417-07	1.158-07	6.005-09	1.050-08
3	3.034-05	1.970-06	4.338-07	3.448-07	8.449-12
4	1.648-04	4.134-05	3.639-06	3.954-07	5.459-07
5	9.267-02	2.796-04	5.255-05	6.278-06	2.292-07
6	1.933-00	1.071-01	4.347-04	6.494-05	9.579-06
7	1.071-01	1.860+00	1.211-01	6.414-04	7.799-05
8	4.347-04	1.211-01	1.790+00	1.347-01	9.065-04
9	6.494-05	6.414-04	1.348-01	1.723+00	1.480-01
10	9.579-06	7.799-05	9.065-04	1.480-01	1.658+00

Table 76

Calculated Band Strengths ($p_{v'v''}$) for the Gamma System of TiO ($A^3\Phi - X^3\Delta$).

v'/v"	0	1	2	3	4	5
0	1.457-00	4.099-01	5.995-02	5.180-03	2.773-04	1.022-05
1	5.624-01	6.255-01	5.538-01	1.409-01	1.760-02	1.261-03
2	1.135-01	7.688-01	1.944-01	5.363-01	2.172-01	3.743-02
3	1.579-02	2.704-01	7.522-01	2.388-02	4.372-01	2.748-01
4	1.671-03	5.458-02	4.211-01	6.142-01	5.136-03	3.099-01
5	1.369-04	7.709-03	1.158-01	5.325-01	4.339-01	5.882-02
6	8.176-06	7.914-04	2.070-02	1.944-01	5.889-01	2.623-01
7	1.861-07	4.975-05	2.623-03	4.307-02	2.811-01	5.890-01
8	7.553-08	5.927-07	2.123-04	6.554-03	7.650-02	3.651-01
9	2.238-07	3.306-07	4.596-06	6.656-04	1.384-02	1.208-01
10	1.316-07	4.205-07	8.945-07	2.799-05	1.677-03	2.580-02

v'/v"	6	7	8	9	10
0	4.005-07	1.619-07	6.503-09	6.512-08	2.662-10
1	7.018-05	4.012-06	1.805-07	3.117-12	4.749-08
2	3.481-03	2.346-04	1.470-05	3.202-07	1.800-08
3	6.301-02	7.373-03	5.816-04	4.333-05	1.435-06
4	3.067-01	9.177-02	1.333-02	1.242-03	1.008-04
5	1.889-01	3.126-01	1.211-01	2.146-02	2.342-03
6	1.316-01	9.381-02	2.953-01	1.483-01	3.173-02
7	1.281-01	1.920-01	3.220-02	2.604-01	1.706-01
8	5.401-01	4.255-02	2.254-01	3.542-03	2.140-01
9	4.360-01	4.562-01	4.204-03	2.289-01	2.444-03
10	1.745-01	4.852-01	3.539-01	3.732-03	2.067-01

TABLE 77

Calculated Band Strengths ($p_{v'v''}$) for

The Gamma Prime System of TiO ($B^3\Pi - X^3\Delta$)

v'/v"	0	1	2	3	4	5
0	1.532-00	3.637-01	4.914-02	2.619-03	3.332-05	1.299-06
1	5.351-01	8.279-01	4.751-01	1.000-01	6.127-03	5.803-05
2	7.836-02	7.612-01	4.728-01	4.821-01	1.391-01	8.889-03
3	4.618-03	1.718-01	8.462-01	2.940-01	4.525-01	1.659-01
4	9.955-06	1.273-02	2.555-01	8.681-01	2.066-01	4.132-01
5	4.121-05	1.083-05	2.132-02	3.206-01	8.678-01	1.686-01
6	1.362-05	2.226-04	6.640-07	2.817-02	3.655-01	8.629-01
7	1.667-06	7.979-05	6.486-04	8.985-05	3.174-02	3.911-01
8	1.609-07	7.206-06	2.247-04	1.438-03	5.104-04	3.118-02
9	7.492-10	1.599-08	1.792-05	4.521-04	2.719-03	1.635-03
10	9.792-08	1.714-07	1.880-07	3.221-05	7.695-04	4.514-03

v'/v"	6	7	8	9	10
0	1.659-07	6.469-08	6.856-09	6.839-08	7.382-10
1	6.068-06	2.344-07	1.842-09	2.360-10	5.961-08
2	4.946-05	2.380-05	3.806-07	4.995-08	2.256-08
3	9.870-03	1.399-05	6.845-05	1.327-07	2.592-08
4	1.821-01	8.818-03	2.754-06	1.396-04	9.048-08
5	3.745-01	1.902-01	6.273-03	7.244-05	2.391-04
6	1.607-01	3.399-01	1.917-01	3.095-03	2.432-04
7	8.593-01	1.753-01	3.089-01	1.876-01	5.674-04
8	3.986-01	8.576-01	2.107-01	2.797-01	1.783-01
9	2.679-02	3.894-01	8.549-01	2.683-01	2.497-01
10	3.898-03	1.956-02	3.647-01	8.465-01	3.504-01

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