Ground State D_2 Dissociation Energy from the Near-dissociation Behavior of Rotational Level Spacings[1]

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A method of determining the dissociation energy of a diatomic molecule from the rotational term value(s) of a single vibrational level lying near dissociation is derived and tested. It is based on expressions relating the characteristic near-dissociation behavior of the rotational constants B_v, D_v, H_v,... etc., to the asymptotically dominant inverse power contribution to the long range intermolecular potential. Application of this procedure to data for ground state D_2 yields a dissociation energy of $D_0 = 36\,748.88(\pm0.3)\,\text{cm}^{-1}$, in essentially exact agreement with the value Herzberg determined from the onset of continuum absorption in the vacuum u.v., $36\,748.9(\pm0.4)$ cm^{-1}. This agreement between results obtained from completely different observables appears to confirm the existence of a small discrepancy between experiment and the most recent theoretical nonadiabatic dissociation energy of Kolos and Wolniewicz, $36\,748.2\,\text{cm}^{-1}$.

Une méthode permettant de déterminer l'énergie de dissociation d'une molécule diatomique à partir de valeurs de termes rotationnels d'un seul niveau de vibration situé près de l'énergie de dissociation a été formulée et essayée. Cette méthode est basée sur des expressions reliant le comportement caractéristique des constantes rotationnelles B_v, D_v, H_v, ... etc. dans le voisinage de la dissociation au terme asymptotiquement dominant dans le développement en puissances inverses de la distance pour le potentiel intermoléculaire à longue portée. L'application de cette façon de procéder aux données relatives à l'état fondamental de D_2 donne pour l'énergie de dissociation $D_0 = 36\,748.88(\pm0.3)\,\text{cm}^{-1}$, en accord essentiellement exact avec la valeur déterminée par Herzberg à partir du seuil d'absorption continue de l'ultraviolet dans le vide, $36\,748.9(\pm0.4)\,\text{cm}^{-1}$. Cet accord entre résultats obtenus à partir d'observables complètement différents semble confirmer l'existence d'un faible écart entre l'énergie de dissociation expérimentale et l'énergie nonadiabatique calculée théoriquement par Kolos et Wolniewicz, $36\,748.2\,\text{cm}^{-1}$.

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I. Introduction

The properties of ground state molecular hydrogen play an important role in molecular physics and theoretical chemistry. Since it is one species for which *ab initio* calculations should now be able to meet or surpass the accuracy of experimental measurements, the hydrogen molecule is an important testing ground for both theory and experiment. For this reason, considerable effort has been expended in attempting to resolve discrepancies between the experimental and theoretical dissociation energies (Herzberg and Monfils 1960; Kolos and Wolniewicz 1964, 1965, 1968) and vibrational spacings (Herzberg and Howe 1959; Wolniewicz 1966; Le Roy and Bernstein 1968) of ground state H_2. As a result, many of these

differences now appear to be resolved (Herzberg 1970; Stwalley 1970a; Kolos and Wolniewicz 1974, 1975).

Herzberg (1970) obtained the presently accepted experimental dissociation energy of ground state D_2, $D_0^H(D_2) = 36\,748.9(\pm0.4)$ cm^{-1}, from a study of the onset of continuum absorption in the vacuum u.v. His result is in reasonable accord with the theoretical value of Kolos and Wolniewicz (1975), $D_0^{KW}(D_2) = 36\,748.2\,\text{cm}^{-1}$. However, it would be interesting to determine whether the residual $0.7\,\text{cm}^{-1}$ difference is truly significant. To this end, the present paper presents a new type of data analysis whose application yields an independent experimental estimate of this dissociation energy.

In recent years there have been great advances in our understanding of the properties of diatomic molecules in vibrational levels near dissociation. These developments arose from the realization that these properties are largely

determined by the intermolecular potential in the neighborhood of the levels' outer turning points. For rotationless ($J = 0$) levels sufficiently near dissociation, the potential in this region takes on its characteristic asymptotic long range form:

[1] $$V(R) = D - C_n/R^n$$

Substitution of this function into the semiclassical phase integral expressions for the vibrational level spacing (Le Roy and Bernstein 1970, 1971; Stwalley 1970a), for the rotational constant B_v (Le Roy 1972), and for the expectation value of the kinetic energy (Stwalley 1973) yielded simple analytic expressions which depend only on the parameters appearing in [1].[3]

The expression obtained for the characteristic near-dissociation behavior of vibrational level spacings has greatly facilitated the determination of accurate dissociation energies for a number of systems.[3] However, its use requires the observation of two or more vibrational levels lying sufficiently near dissociation that the intermolecular potential at their outer turning points is dominated by the asymptotic inverse power term of [1]. Such highly excited levels are often difficult to observe for Franck-Condon reasons. For molecules having a small reduced mass, this difficulty is compounded by the fact that the relatively low density of states will tend to minimize the number of levels lying in this region. The ground state of H_2 provides a good illustration of the latter difficulty, since its highest vibrational level is bound by ca. 143 cm^{-1}, and it has no levels lying in this limiting region.[4] The situation for ground state D_2 is not quite so bad, since it has one vibrational level ($v = 21$, bound by ca. 2 cm^{-1}) which definitely does lie in the 'near-dissociation' region.[4] However, the methods of analysis used previously[3] require the existence of more than one vibrational level in this region. The present paper therefore develops and applies a procedure which utilizes the characteristic near-dissociation behavior of the rotational spacings associated with a *single* vibrational level. It is based on a knowledge of

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[3]For a review of the development and applications of these techniques up to 1973, see Le Roy (1973).

[4]The delineation of this near-dissociation region is discussed by Stwalley (1970b) and Le Roy (1973).

the limiting behavior of the rotational constants B_v (Le Roy 1972), D_v, H_v, L_v, ... etc. (Barwell 1975).

In Sect. II, the new method of analysis is described and problems associated with it are pointed out. A quantitative examination of its utility is provided in Sect. III in the context of a 'model problem' analysis of rotation–vibration energy levels calculated by Li and Stwalley (1973) from their potential curve for ground state Mg_2. The experience gained there guides the analysis of the experimental data for ground state D_2, presented in Sect. IV.

II. Determining a Dissociation Limit from the Near-dissociation Behavior of Rotational Level Spacings

A. Description of the Method

The previously reported (Le Roy and Bernstein 1970; Le Roy 1972) expressions for the binding energies and B_v values of vibrational levels lying in the near-dissociation region may be written as

[2] $$D - G(v, J = 0) = X_n(0)(v_D - v)^{2n/(n-2)}$$

[3] $$B_v = X_n(1)(v_D - v)^{4/(n-2)}$$

where v_D is the effective (in general noninteger) vibrational quantum number at the dissociation limit and $X_n(k)$ is a constant depending on the reduced mass and the parameters n and C_n of [1]. More recently, Barwell (1975) obtained analogous expressions for the higher order rotational constants:

[4] $$D_v = -X_n(2)(v_D - v)^{-(2n-8)/(n-2)}$$

[5] $$H_v = X_n(3)(v_D - v)^{-(4n-12)/(n-2)}$$

[6] $$L_v = X_n(4)(v_D - v)^{-(6n-16)/(n-2)}$$

The constants $X_n(k)$ appearing in all of these equations may be written as

[7] $$X_n(k) = \bar{X}_n(k)/[\mu^n(C_n)^2]^{1/(n-2)}$$

where the constant $\bar{X}_n(k)$ is a known function of the integers n and k. For the $n = 6$ cases considered in the present work, the values of $\bar{X}_6(k)$ for $k = 0$-4 are: 7932.22, 546.658, -2.75404, -0.0191871, and -2.99430×10^{-4} respectively (assuming energies are expressed in cm^{-1} and lengths in Å). Note that $\bar{X}_n(k)$ (and hence $X_n(k)$) *is always negative* for $k \geq 2$.

The problem encountered in the present

work is one in which the observable is a rotational term value for a single vibrational level of a molecule for which n and C_n, and hence the $X_n(k)$'s, are known. According to the familiar vibrating rotor model of a diatomic molecule, this term value may be expressed as[5]

[8] $G(v,J) - G(v,0) = B_v[J(J + 1)]$

$\quad - D_v[J(J + 1)]^2 + H_v[J(J + 1)]^3$

$\quad\quad + L_v[J(J + 1)]^4 + \cdots$

For $n = 6$, substituting [3]–[6] into [8] transforms it into an expression in which the only unknown is the parameter v_D,

[9] $G(v,J) - G(v,0)$

$$= \sum_{k=1}^{N} X_6(k)(v_D - v)^{3-2k}[J(J + 1)]^k$$

This equation is readily solved for the value of v_D, whose substitution into [2] determines the binding energy of the level in question. Addition of this binding energy to the vibrational term value for this level then yields the desired dissociation energy. This is the procedure used below.

B. Problems Associated with the Method

Two main questions are raised by the approach described above. The first of these concerns the effect of truncating the $J(J + 1)$ power series in [8] and [9] after a finite number of terms. For vibrational levels near dissociation, Dickinson and Bernstein (1970) showed that the highest unpredissociated rotational level for a given v corresponds to a value of $J(J + 1)$, here denoted $[J(J + 1)]_v^{\mp}$, which decreases as $(v_D - v)^2$ for v approaching v_D. More particularly, for the $n = 6$ case considered here, they showed that

[10] $[J(J + 1)]_v^{\mp} \simeq \dfrac{2\pi^2}{(6 - 3\sqrt{3})} (v_D - v)^2$

This limiting behavior ensures that the term value contributions associated with the centrifugal distortion constants D_v, H_v, ... etc. remain finite in this limit, in spite of the singularities in the values of the coefficients themselves (see

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[5]Note that in spite of the customary (Herzberg 1950) sign convention for the centrifugal distortion constants (see [8]), their contributions to the rotational term values of highly excited vibrational levels are all inherently negative (cf. [4]–[7]).

[4]–[6] for $n = 6$). However, combining [10] with the $\bar{X}_6(k)$ values given above shows that in this high J limit the term value contribution arising from each of these distortion constants is a significant fraction of that for the preceding term in [9]. Thus, any truncation of the power series in [8] and [9] should be accompanied by an estimate of the effect of the missing terms. A procedure for making such estimates is developed in the analysis of the model problem presented in Sect. III.

The second question which must be considered concerns the reliability of the near-dissociation expressions for the vibrational binding energy and rotational constants, [2]–[6]. Their derivation is based on the assumption that the intermolecular potential near the outer turning points of the levels under consideration is solely due to the asymptotically dominant inverse power contribution to the intermolecular potential (here, the R^{-6} term). In practice, this assumption is never completely true, and the effect of its breakdown is relatively more serious for the higher order rotational constants (Le Roy 1972, 1973; Barwell 1975). On the other hand, the net influence of these constants on the rotational term values decreases with increasing order.

In the model problem analysis presented below, the relative magnitudes of the errors in predictions based on [9] are correlated with the error in the single term ([1]) approximation for the long range potential. This then allows one to estimate the effect of this approximation on the final result for ground state D$_2$.

III. Testing the Method on a Model Problem

The long-range intermolecular potential for ground state Mg$_2$ has the same form as that for the ground state of molecular hydrogen,

[11] $V(R) = D - C_6/R^6 - C_8/R^8$

$\quad\quad - C_{10}/R^{10} - \cdots$

Vibration–rotation energy levels calculated from a precisely known Mg$_2$ potential energy curve are therefore used to generate simulated experimental data for use in testing and extending the method described above.

The highest observed levels of Mg$_2$ lie sufficiently close to dissociation that their outer turning points lie in the region described by

[11]. From an analysis of these turning points, Stwalley (1970*b*) determined the long range potential for Mg_2 to be

[12] $V(R) = 403.704 - (3.29 \times 10^6)/R^6$

$$- (0.48 \times 10^8)/R^8$$

where energies are in cm^{-1} and lengths in Å.[6] Li and Stwalley (1973) then calculated the eigenvalues of a number of levels of the potential curve obtained on combining [12] with the RKR turning points for the observed levels $v = 0$–12. In particular, they reported the energies of all (even J) rotational levels lying below its dissociation limit. In order to maximize similarities with the D_2 problem considered later, the present analysis of these 'data' only utilized the rotational term value for the highest J associated with each v.

Applying the method of Sect. IIA to these model Mg_2 term values yielded the 'predicted' molecular dissociation energies which are plotted in Fig. 1 as functions of N, the number of terms retained in the sum in [9]. The $N = 0$ points are simply the vibrational term values of the indicated levels, while the dashed line labelled D_0 (true) denotes the actual dissociation energy of the given potential energy curve. The $N = \infty$ asymptote of each of the curves in Fig. 1 represents the best estimate of D_0 obtainable by the present method from the rotational term values for that vibrational level. However, since it is difficult to determine reliable values of the asymptotes from this type of plot, two alternate extrapolation procedures are shown in Fig. 2. There, the various predicted binding energies, each divided by the true binding energy of that level, are plotted against both $1/N^2$ (upper half) and $1/N^3$ (lower half of the figure). The near linearity of these plots for $N \geq 2$ implies that a short linear extrapolation beyond the last two points should yield a very reasonable estimate of the effect of truncating the sum in [9]. Moreover, the negative curvature of the $1/N^2$ plots implies that the intercepts obtained from them by linear extrapolation will be upper bounds to the true '$N = \infty$' limits for the various vibrational levels. Similarly, the positive curvature seen in the $1/N^3$ plots im-

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[6]While Li and Stwalley (1973) later determined slightly more reliable values of the constants D and C_8, the values in [12] were used in their calculation of the eigenvalues comprising the present model problem.
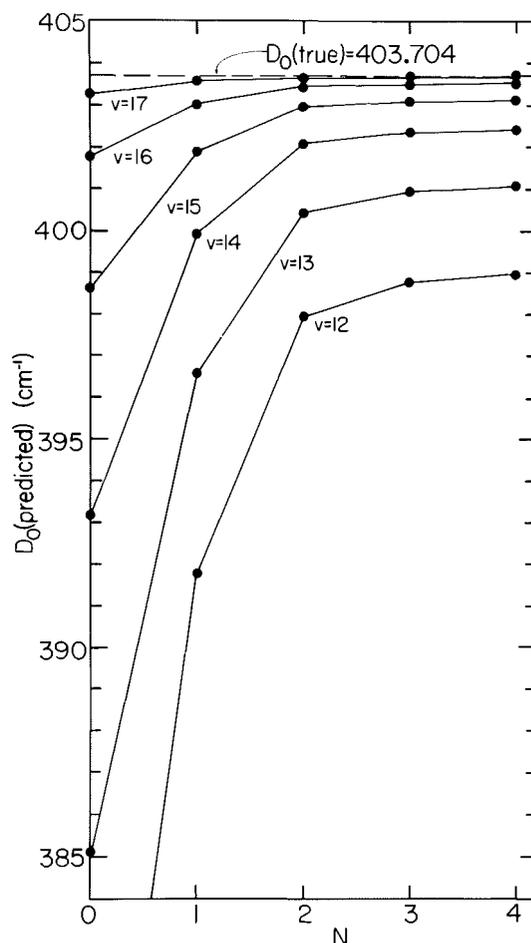

FIG. 1. Predicted dissociation energies for the model problem, obtained by applying [2] and [9] to the largest rotational term value for each of $v = 12$–17. N is the number of terms retained in the sum in [9]; $N = 0$ corresponds to the rotationless ($J = 0$) term value of the indicated level.

plies that their linear extrapolation will yield lower bounds to the limiting values. Therefore, the averages of these linearly extrapolated $N^{-2} = 0$ and $N^{-3} = 0$ intercepts are used to approximate the true values of these limits. This type of extrapolation solves the first problem raised in Sect. IIB.

Stwalley (1970*b*) obtained his estimate of the Mg_2 dissociation energy, $D_0 = 403.7(\pm 0.7)$ cm^{-1}, from an analysis of the RKR turning points for levels $v \leq 12$. However, Fig. 1 shows that the present method could not yield a value of D_0 within these bounds unless rotational term values were accurately known for levels
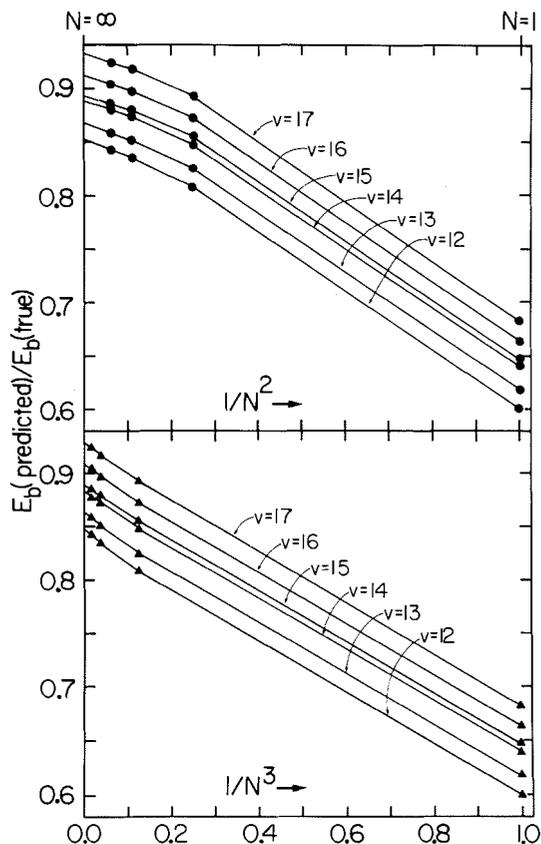
FIG. 2. Predicted binding energies $[E_b(v) = D - G(v)]$ for the model problem, each scaled by the true binding energy of that level, plotted vs. $1/N^2$ (upper half), and $1/N^3$ (lower half).
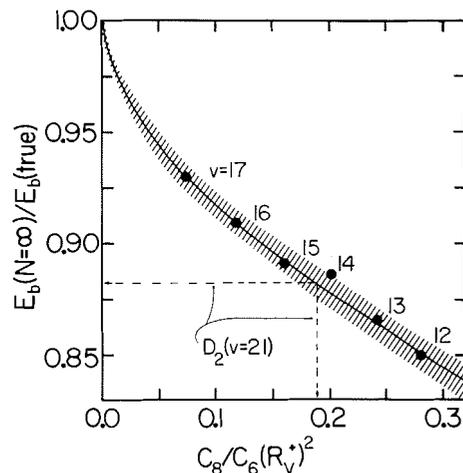

FIG. 3. Relative error in the $N = \infty$ binding energies for the model problem, plotted vs. the relative strength of the second inverse power contribution to [12], evaluated at the outer turning point $R_v{}^+$ of the level in question.

$v \geq 15$. This weakness of the present approach is due to the fact that it only considers the effect of the leading inverse power contribution to [11]. The magnitude of such errors depends on the relative strength of the other (non-R^{-6}) contributions to the long-range potential. One should therefore examine how the errors in the $N = \infty$ model-problem predictions depend on the ratio of the strengths of the two leading terms in [11]. The outer turning point of the level under consideration, $R_v{}^+$, is the distance at which these terms should be compared, since the potential in its neighborhood has a dominant influence on the values of the rotational constants for highly excited levels (Le Roy 1972; Barwell 1975).

Figure 3 plots the averaged $N = \infty$ intercepts from Fig. 2 vs. $C_8/C_6(R_v{}^+)^2$, the ratio of the first two inverse power terms in [12], evaluated

at the appropriate turning point. Since [2]–[6] are exact for a potential with a single inverse power term, a curve through these points must approach unity as $C_8/C_6(R_v{}^+)^2 \rightarrow 0$. The differences between the $N^{-2} = 0$ and $N^{-3} = 0$ intercepts in Fig. 2 lie within the diameters of the points in Fig. 3. The irregularity of the point for $v = 14$ is almost certainly due to the effect on the calculated eigenvalues of discontinuities in the model potential in the region where the RKR turning points for $v \leq 12$ are joined to the long range tail of [12]. The shaded region is an estimate of the uncertainties associated with this irregularity and with the extrapolation to $C_8/C_6(R_v{}^+)^2 = 0$.

According to the WKB approximation, the rotational constants B_v, D_v, H_v, ... etc. may always be expressed in terms of various quadratures over the potential function in the region between the turning points of the given vibrational level (Le Roy 1972; Barwell 1975). For levels near dissociation these constants are largely determined by the intermolecular potential in the neighborhood of the levels' outer turning points. The fractional effect of a change in the potential on a property derived from the rotational constants will therefore depend only on the fractional change in the potential, and not on the vibrational quantum number or binding energy, or even on the identity of the species. For this reason we believe that Fig. 3

TABLE 1. Values of C_6, C_8, and $X_6(k)$ for the ground states of Mg_2 and D_2; energies are in cm^{-1} and lengths in Å

	$C_6 (\times 10^{-4})$	$C_8 (\times 10^{-6})$	$X_6(0)$	$X_6(1)$	$X_6(2)$	$X_6(3)$	$X_6(4)$
$Mg_2(X^1\Sigma_g^+)$	329^a	48^a	0.10530	7.2569×10^{-3}	-3.6560×10^{-5}	-2.5471×10^{-7}	-3.9750×10^{-9}
$D_2(X^1\Sigma_g^+)$	3.1364^b	0.16820^b	44.320	3.0544	-1.5388×10^{-2}	-1.0720×10^{-4}	-1.6730×10^{-6}

[a]From Stwalley (1970b), as used by Li and Stwalley (1973).
[b]From Hirschfelder and Meath (1967).

TABLE 2.   Results obtained on applying the present method to the D_2 ($v = 21$) term value of [13];
N is the number of terms retained in the power series expansion of [9]

N	B_v	D_v	H_v	L_v	v_D	$D - G(21,0)$
1	0.9438	—	—	—	21.309($\pm$0.016)	1.313($\pm$0.17)
2	1.0354	0.04539	—	—	21.339($\pm$0.015)	1.728($\pm$0.19)
3	1.0446	0.04499	−0.00268	—	21.342($\pm$0.015)	1.779($\pm$0.19)
4	1.0477	0.04486	−0.00266	−0.00035	21.343($\pm$0.015)	1.791($\pm$0.19)
.						.
.						.
.						.
∞	1.0507[a]	0.04473[a]	−0.00263[a]	−0.00035[a]	21.344($\pm$0.015)	1.803($\pm$0.20)

[a]Calculated from v_D (N = ∞) and [3]–[6].

is a 'universal' error function for cases in which the two leading contributions to the long range potential are C_6/R^6 and C_8/R^8. It will therefore be used to estimate the magnitude of the correction required by the $N = \infty$ binding energy for D_2, obtained by the present method.

IV. Results and Discussion: Application to D₂

Bredohl and Herzberg's (1973) high resolution measurements of the Lyman and Werner bands of D_2 provided the first experimental observation of the weakly bound $v = 21$, $J = 0$ and 1 levels of this species. More recently, Herzberg[7] noted a couple of minor errors in the original paper; their correction yields improved term values of $G(21,0) = 36\,746.84$ and $G(21,1) = 36\,748.73$ cm^{-1} for these levels. Since $v = 21$, $J = 0$ is bound by less than 2 cm^{-1} and has an outer turning point of $ca.$ 5.3 Å, it is an appropriate candidate for application of the present method.[4]

The long range potential constants for ground state D_2 are well known (Hirschfelder and Meath 1967); values of C_6, C_8, and the constants $X_6(k)$ appearing in [2]–[7] are given in Table 1. Substituting these coefficients and the experimental rotational term value

[13] $[G(21,1) - G(21,0)] = 1.89(\pm0.1)$ cm^{-1}

into [9] then yields the results shown in Table 2. The uncertainties seen there (in parentheses) arise from the ±0.1 cm^{-1} uncertainty in the experimental term value. The predicted binding energies for $N = 1$–4 are plotted in Fig. 4, and the average of the linearly extrapolated $N^{-2} = 0$ and $N^{-3} = 0$ intercepts shown there is the '$N = \infty$' binding energy given in Table 2.
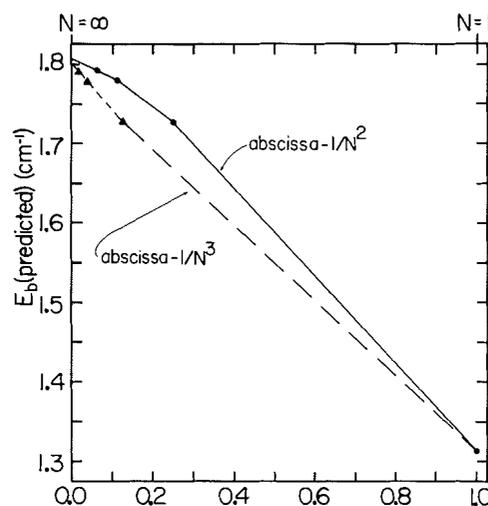
Examination of the (improved) long range

[7]Herzberg, G. 1974. Private communication.

FIG. 4.   Predicted binding energy for the $v = 21$ level of D_2, plotted vs. both $1/N^2$ and $1/N^3$, where N is the number of terms retained in the sum in [9].

hydrogen potential of Kolos and Wolniewicz (1974) shows that a level bound by 1.7–2.1 cm^{-1} has an outer turning point of 5.33($\pm$0.09) Å. Combined with the known C_6 and C_8 constants for this species (see Table 1), this yields a value of $C_8/C_6(R_v^+)^2 = 0.189(\pm0.007)$ for the parameter characterizing the breakdown of the single-term (R^{-6}) approximation to the long range potential. This quantity defines the position of the vertical dashed line in Fig. 3, which in turn implies that the $N = \infty$ binding energy given in Table 2 is too small by a factor of 0.882($\pm$0.010). Application of this correction factor then yields the present method's best estimate of the $v = 21$, $J = 0$ binding energy for ground state D_2,

[14] $D - G(21,0) = 2.04(\pm0.22)$ cm^{-1}

The weakest step in the determination of the binding energy in [14] is the application of the

correction factor obtained from the model problem results in Fig. 3. The scaling of the predicted binding energies plotted in Fig. 2 was originally done in order to allow the results for the different vibrational levels to be shown in a single figure. The parallel behavior of the resulting curves for levels with binding energies differing by a factor of 65 also provided gratifying evidence of the essential soundness of the extrapolation procedure. However, if the D_2 results in Table 2 are scaled by the binding energy of [14] and then included in Fig. 2, they would be virtually superimposed on the model problem results for $v = 14$. This similarity of results for levels of different species, whose binding energies differ substantially, provides qualitative confirmation of the validity of the correction procedure based on Fig. 3.

V. Conclusions

Adding the binding energy of [14] to Herzberg's corrected $v = 21$, $J = 0$ term value yields the present estimate of the dissociation energy of ground state D_2,

$$D_0{}^{LB}(D_2) = 36\ 748.88(\pm0.3)\ cm^{-1}$$

This result is essentially identical to the value Herzberg (1970) obtained by locating the onset of the absorption continuum in the vacuum ultraviolet

$$D_0{}^{H}(D_2) = 36\ 748.9(\pm0.4)\ cm^{-1}$$

Since these two results were obtained from quite different experimental observables, their agreement is quite gratifying. Moreover, it appears to confirm the existence of a small disagreement with the most recent theoretical dissociation energy of Kolos and Wolniewicz (1975)

$$D_0{}^{KW}(D_2) = 36\ 748.2\ cm^{-1}$$

This $0.7\ cm^{-1}$ discrepancy is almost the same size as the difference between the analogous theoretical dissociation energy for ground state H_2,

$$D_0{}^{KW}(H_2) = 36\ 118.0\ cm^{-1}$$

and the experimental value which Stwalley (1970a) determined from a near-dissociation analysis of vibrational spacings of the $B(^1\Sigma_u{}^+)$ state,

$$D_0{}^{S}(H_2) = 36\ 118.6(\pm0.5)\ cm^{-1}$$

In view of the importance of molecular hydrogen in testing our understanding of molecular quantum mechanics, this $0.7\ cm^{-1}$ discrepancy may be quite significant.

The method of analysis utilized in the present work is a useful application of the characteristic near-dissociation behavior of diatomic molecule rotational constants. The rotational constant expressions [3]–[6] are relatively more sensitive than that for the binding energy ([2]) to the effect of deviations from the single-term approximation to the long range potential (Le Roy 1972; Barwell 1975). Thus, a near-dissociation analysis of the vibrational spacings is to be preferred over the present approach whenever suitable data are available. On the other hand, the empirical correction procedure based on Fig. 3 greatly improves the accuracy of predictions obtained by the present method, making this approach a reliable complement to the usual[3] vibrational analysis techniques.

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