Wei Hua’s Four-Parameter Potential

Comments

and Computation of Molecular Constants

\(\alpha_e\) and \(\omega_e x_e\)

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Abstract

The value of adjustable parameter \(C\) and the four-parameter potential
\[ U(r) = D_e \left[ \frac{1 - \exp[-b(x-e)]}{1 - c \exp[-b(x-e)]} \right]^2 \]
has been expressed in terms of molecular parameters and its significance has been brought out. The potential so constructed, with \(C\) derived from the molecular parameters, has been applied to ten electronic states in addition to the states studied by Wei Hua. Average mean deviation has been found to be 3.47 as compared to 6.93, 6.95 and 9.72 obtained from Levine2, Varshni and Morse potentials, respectively. Also Dunham’s method has been used to express rotation-vibration interaction constant \((\alpha_e)\) and anharmonicity constant \((\omega_e x_e)\) in terms of \(C\) and other molecular constants. These relations have been employed to determine these quantities for 37 electronic states. For \(\alpha_e\), the average mean deviation is 7.2% compared to 19.7% for Lippincott’s potential which is known to be the best to predict the values. Average mean deviation for \((\omega_e x_e)\) turns out to be 17.4%

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which is almost the same as found from Lippincott’s potential function.

I. INTRODUCTION

A knowledge of exact potential function which governs the interaction between atoms as a function of internuclear distance, is of fundamental importance in a wide variety of fields ranging from gas kinetics to stellar structure. Besides, potential energy (PE) curves provide a good deal of information about the molecular structure. Accordingly, a number of methods have been developed to obtain these curves and the most satisfactory technique for this purpose is RKR method [1–3], which is based on the experimental spectroscopic data. This approach is, however, limited to the region for which the spectroscopic data exist. To overcome this limitation, one resorts to either Dunham method or to analytical functions. In the former, term values are expressed as:

\[ T = \sum_{i,j} Y_{i,j}(v + \frac{1}{2})^i J^j (J + 1)^j, \]  \( \text{(1)} \)

where \( v \) and \( J \) are the vibrational and rotational quantum numbers, respectively, and the coefficients \( Y_{i,j} \) are related to spectroscopic constants. The formulation of analytical functions is based on the assumption that bonding potential curves can be fitted to a certain form of algebraic expression. A comparative study of the empirical potential functions by Steele et al [4] and by Varshni [5] revealed that of all the three-parameter potential functions those suggested by Morse [7], Varshni [5] and Levine [8] have small average absolute deviation from the RKR curve with their respective values as 3.68%, 2.31% and 1.98%. The corresponding Schrödinger equation can, however, be exactly solved only for Morse function.

Some time back Wei Hua [9], introduced a four-parameter (FP) potential function which apart from the usual three parameters viz. \( \omega_e, r_e, D_e \), contains a fourth parameter, \( b \), which in turn, depends on an adjustable constant \( C \). The value of \( C \) was chosen to minimize the absolute deviation of the calculated values from the corresponding RKR - values. Wei Hua studied 15 electronic states and found that FP curves fit the RKR curves more closely.
compared to Morse curves. Moreover, the corresponding Schrodinger equation can be solved exactly for zero and approximately for non-zero total angular momentum \[9\]. Almost all the researchers who have put forward an empirical potential function including the FP potential or have performed the comparative studies, have confined themselves to the study of simple molecules H\(_2\), O\(_2\), N\(_2\), CO, NO, hydrogen and alkali halides or to alkali oxides. With a view to test the applicability of FP potential to a wider range of molecules, Morsagh \[10\] carried out their comparative study for diatomic molecules containing sulphur. It was found that for outer wall of the potential curve (\(r > r_e\)) the average mean absolute deviations from RKR curve for Morse, Varshni, Levine and four-parameter potentials are 1.34\%, 2.09\%, 2.67\% and 0.7\%, respectively. Encouraged by the results in respect of FP potential, we have now dwelt upon the significance of adjustable constant \(C\) and have assessed how faithfully the potential function predicts the values of molecular parameters \(\alpha_e\) and \(\omega_e x_e\). This communication is an outcome of these efforts.

II. THE RKR-METHOD

This method \[1–3\] provides the classical turning points,

\[
\begin{align*}
    r_{\text{max}} &= \left[ \frac{f}{g} + f^2 \right]^{\frac{1}{2}} + f, \\
    r_{\text{min}} &= \left[ \frac{f}{g} + f^2 \right]^{\frac{1}{2}} - f
\end{align*}
\]

(2)

where \(f\) and \(g\) depend on the experimentally determined molecular constants \((\omega_e, \omega_e x_e, B_e, \alpha_e)\) and are defined as

\[
\begin{align*}
    f &= \frac{\partial S}{\partial U}, \\
    g &= -\frac{\partial S}{\partial k}
\end{align*}
\]

(3)

with

\[
S(U,k) = \frac{1}{\pi(2\mu)^{\frac{3}{2}}} \int_0^{\prime} \left\{ U - E(I,k) \right\}^{\frac{3}{2}} dI
\]

(4)
Here $U$ is the potential energy and $E(I,k)$ is the sum of vibrational and rotational energies of the molecule,

$$I = h(v + \frac{1}{2}),$$
$$k = \frac{J(J + 1)h^2}{8\pi^2\mu}$$  \hspace{1cm} (5)

$\mu$ is the reduced mass of the molecule. However, for the present work RKR potentials have been taken from the literature and the references are given in tables 1 and 3.

Accuracy of a potential function can be judged in two ways: first by its comparison with the curve obtained from the experimental data and second, by using it to evaluate unused constants and comparing these with the respective experimental values. In the reported work the findings have been subjected to both the tests.

### III. POTENTIAL FUNCTIONS FOR COMPARATIVE STUDY

In the present work we have considered only those potential functions for comparative study, which fit more closely to the RKR potential curve [4]. The expressions for these potential functions and parameters $\alpha_e$ and $\omega_e x_e$ are as following:

(i) **Morse potential** [4,7]

$$U_M(r) = D_e \left[1 - e^{-a(r-r_e)}\right]^2,$$

$$\alpha_e = \left(\frac{6B_e^2}{\omega_e}\right) \left(\Delta\frac{1}{2} - 1\right),$$
$$\omega_e x_e = \left(\frac{\omega_e^2}{4D_e}\right);$$  \hspace{1cm} (7)

(ii) **Varshni potential** [5,6]

$$U_V(r) = D_e \left[1 - \frac{r_e}{r} e^{-b_e(r^2 - r_e^2)}\right]^2,$$

$$\alpha_e = \left(\frac{6B_e^2}{\omega_e \Delta\frac{1}{2}}\right) \left(\Delta - 2\Delta\frac{1}{2} + 2\right),$$
$$\omega_e x_e = \frac{B_e}{8} \left(8\Delta - 12 + 36 - \frac{56}{\Delta^2} + \frac{48}{\Delta}\right);$$  \hspace{1cm} (9)
(iii) Levine potential \[4,8\]

\[
U_L(r) = D_e \left[ 1 - \frac{r_e}{r} e^{-b_L(r^p - r_e^p)} \right]^2,
\]

\[
\alpha_e = \left( \frac{6B_e^2}{\omega_e} \right) \left( \frac{3}{4} \Delta \frac{1}{2} - \frac{1}{2} \right),
\]

\[
\omega_e x_e = \frac{B_e}{8} \left( 8\Delta - 12(p - 1)\Delta\frac{1}{2} + 8p^2 + 4 - \left( \frac{20p^2 - 12p}{\Delta\frac{1}{2}} \right) + \frac{12p^2}{\Delta} \right);
\]

(iv) Four-parameter potential \[9\]

\[
U(r) = D_e \left[ \frac{1 - \exp\{-b(r - r_e)\}}{1 - C \exp\{-b(r - r_e)\}} \right]^2
\]

The expressions for \(\alpha_e\) and \(\omega_e x_e\) for this potential have been obtained in Section IV.

Here, \(D_e\) is the dissociation energy, \(r_e\) is the equilibrium bond length and ‘a’ is related to force constant through

\[
k_e = 2D_e a^2 = U''(r_e) \quad \text{with}
\]

\[
k_e = \mu \omega^2;
\]

\[
\Delta \frac{1}{2} = ar_e;
\]

\[
b_v = \frac{1}{r_e^2} \left( \Delta \frac{1}{2} - 1 \right);
\]

\[
b_L = \frac{p^{-1}}{r_e^p} \left( \Delta \frac{1}{2} - 1 \right);
\]

\[
p = 2 + \frac{1}{3} (\Delta \frac{1}{2} - 4)(\Delta \frac{1}{2} - 2)
\]

\[
\frac{1}{(\Delta \frac{1}{2} - 1)}
\]

In order to obtain an analytical expression for \(C\), we have compared FP potential with five-parameter potential function of Hulburt and Hirschfelder \[11\] because a potential function with large number of parameters is more flexible. This gives \(C\) as

\[
C_{rel} = \left( -\frac{1}{12} + x \right) - \sqrt{\frac{120}{144} - \frac{37}{48} x^2 - \frac{2}{12} x + \frac{17}{144} \frac{G}{ar_e^2}}
\]

where
where \( x = \frac{1 + F}{ar_e} \),

\[
F = \frac{\alpha_e \omega_e}{6B_e^2},
\]

\[
G = \frac{8\omega_e x_e}{B_e}
\]

and

\[
a = \sqrt{\frac{k_e}{2D_e}}
\]

\( C \) has been denoted as \( C_{rel} \) to distinguish it from the \( C \), obtained by minimum deviation method adopted by Wei Hua.

The values of \( C_{rel} \) have been computed for the electronic states studied by Wei Hua using the data listed in Table 1 and are compared with \( C \) (columns 3 and 4 in Table 2). Value of \( C_{rel} \) depends on \( B_e, \alpha_e \) and \( \omega_e x_e \), apart from other parameters viz. \( \omega_e, r_e \) and \( D_e \), that are used in almost all the three-parameter potential functions. In other words, the value of \( C_{rel} \) also depends on the rotational constants. Furthermore, it is observed that a small change in \( \alpha_e \) changes \( C_{rel} \) significantly while a similar change in other parameters produces small variation. For example, in case of \( Li_2 \), if we change the value of either \( \alpha_e \) or \( \omega_e x_e \), then resulting variation in the value of \( C_{rel} \) due to the latter is nearly one-third that due to the former. Thus, \( C_{rel} \) is more sensitive to the rotation-vibration interaction constant compared to other parameters involved in the relation. Using the equation (18), values of \( C_{rel} \) for the electronic states studied by Wei Hua, have been calculated and this, in turn, has been used to calculate the FP potential curve.

Mean square deviations in

\[
\Delta Y_j = \frac{\sqrt{(U_j - U_{RKR})^2}}{D_e}
\]

where \( j \) denotes four-parameter (FP), Morse (M), Levine (L), Varshni (V) potential functions, have been calculated for all the cases. The results are projected in Table 2. It has been found that the mean square deviations with \( C_{rel} \) are not far off from the corresponding values derived with \( C \) which makes us to have faith in their correctness. In view of this,
$C_{rel}$ has been employed to calculate the potential curve for additional ten electronic states (Table 3) and deduce the values of $\alpha_e$ and $\omega_e x_e$ for a total of 37 electronic states of various molecules including the ones studied by Wei Hua.

**IV. DERIVATION OF $\alpha_E$ AND $\omega_EX_E$**

On the basis of wave mechanics Dunham [12] has shown that molecular parameters can be expressed in terms of the derivatives of potential functions if it can be expanded in the form of a power series. Applying this method, we get

$$\alpha_e = [ar_e(1 + C) - 1] \frac{6B_e^2}{\omega_e}$$

and

$$\omega_e x_e = \frac{h}{8\pi^2 c \mu} a^2 (1 + C + C^2)$$

$$= B_e \Delta (1 + C + C^2)$$

where $B_e = \frac{h}{8\pi^2 c \mu}$ as obtained from the solution of equation for a rotator. The relation for $\alpha_e$ is of the same form as obtained by Pekeris [12] using the Morse potential function, viz.

$$\alpha_e = \left[ \frac{\left( \omega_e x_e \right)^{\frac{1}{2}}}{B_e} \right] - 1 \right] \frac{6B_e^2}{\omega_e} = [ar_e - 1] \frac{6B_e^2}{\omega_e}$$

and that of Lippincott’s relation [4] i.e.

$$\alpha_e = \left( \frac{6B_e^2}{\omega_e} \right) ab \Delta^\frac{1}{2}$$

where

$$a = \frac{4}{5} \left( 1 - \frac{1}{b \Delta^\frac{1}{2}} \right) ;$$

and

$$b = 1.065$$

The expression for $\omega_e x_e$ is to be compared with
\[
\omega_{e}x_{e} = \frac{B_{e}}{8}\left(3 + 12ab\Delta^{\frac{1}{2}} + 6\Delta + 15a^{2}b^{2}\Delta - 12ab^{2}\Delta\right)
\]  
(26)

obtained from Lippincott’s potential function [1].

Values of these two parameters have been calculated for 37 electronic states and are given in Tables 4 and 5 for \(\alpha_{e}\) and \(\omega_{e}x_{e}\), respectively. These Tables also include the corresponding experimental values and the values found by employing Morse (eqn. 7), Varshni (eqn. 9) and Lippincott’s (eqns. 23, 26) potential functions. Values of molecular constants used in these calculations are listed in Table 1.

**V. RESULTS AND DISCUSSION**

The adjustable constant \(C\) is determined by finding the mean square deviation of the FP potential from the RKR potential curve, which itself is calculated using the molecular parameters \(\omega_{e}, \omega_{e}x_{e}, \alpha_{e}, r_{e}\) and \(B_{e}\) of the individual energy levels [1, 3]. Thus, any variation in the parameters from level to level is taken care of and hence most of the variations are absorbed indirectly. On the other hand, the least square fitted values of the parameters are used in the expression for \(C_{rel}\). These values of parameters, therefore, do not take care of level to level variations. Inspite of this \(C_{rel}\) is quite close to the value of \(C\) calculated by minimum deviation method. Among the electronic states which were studied by Wei Hua [3] the values of \(C_{rel}\) are within \(\pm 6\%\) of the values of the \(C\) except for \(\text{Li}_{2}X^{1}\Sigma_{g}^{+3}, \text{H}_{2}X^{1}\Sigma_{g}^{+}, \text{COX}^{1}\Sigma_{g}^{+}\) and \(\text{XeOd}^{1}\Sigma^{+}\) where the deviations are, respectively, 11%, 15.9%, 24% and 24%. These deviations can be understood from the fact that the molecular constants vary in going to higher energy levels. In \(\text{Li}_{2}, v = 0\) to 4 and \(v > 10\) levels have \(\alpha_{e}\) values 0.00704 and 0.0077, respectively (corresponding \(\gamma_{e}\) values are also different). In the case of those electronic states for which complete and accurate data are available, \(C_{rel}\) is very close to \(C\); the differences may be attributed to the fact that in \(C_{rel}\), finer interactions are not included.

The mean square deviations of the FP potential with \(C\) (i.e. \(\Delta Y_{FP,C}\)) and \(C_{rel}\) (i.e. \(\Delta Y_{FP,C_{rel}}\)) from RKR potential curve have been compared in Table 2. The mean
square deviations are within ±5% except for those states for which \( C_{\text{rel}} \) departs significantly from \( C \).

A stringent condition for the acceptance of a potential function is the exact solution of the corresponding Schrodinger wave equation. As discussed by Wei Hua [9], FP potential provides eigenvalues:

\[
E_n = \frac{D_e}{4} \left[ 2 + (Q^2 + 1) - \frac{(\rho_c - \bar{n})^2}{t^2} - \frac{(Q^2 - 1)^2 t^2}{(\rho_c - \bar{n})^2} \right]
\]

(27)

where

\[
Q = \frac{1}{C}, \quad t = \frac{2D_e}{\omega_e(1 - C)}, \quad \bar{n} = n + \frac{1}{2}, \quad n = 0, 1, 2, 3;
\]

\[
\rho_c = \text{sign of}(C)\rho \quad \text{and} \quad \rho = \left[ \frac{1}{4} + (Q^2 - 1)^2 t^2 \right]^2
\]

(28)

The mean square deviation of the energy values \( (E_{\text{cal}}) \) with \( C(\Delta E_C) \) and \( C_{\text{rel}}(\Delta E_{C_{\text{rel}}}) \) from the observed levels \( (E_{\text{obs}} \text{ i.e. } U_{\text{RKR}} \text{ values}) \) have been calculated using the above equation and are given in the last two columns of Table 2. Corresponding \( \Delta E_C \) and \( \Delta E_{C_{\text{rel}}} \) are very close to each other supporting that \( C_{\text{rel}} \) equals \( C \) within the accuracy of molecular parameters and can be computed from these (eqn. 18). To reinforce the above conclusions, the mean square deviations viz. \( \Delta Y_j \) and \( \Delta E_{C_{\text{rel}}} \) from the RKR potential have been compared for additional ten states using \( C_{\text{rel}} \) in the FP potential function and the results are compiled in Table 3.

Taking \( C_{\text{rel}} \) as the correct value of \( C \) parameters, \( \alpha_e \) and \( \omega_e \) have been calculated using equation 21 and equation 22, for 37 electronic states including those studied by Wei Hua. The FP potential with \( C_{\text{rel}} \) yields \( \alpha_e \) values within ±15% of the corresponding experimental values. The observed variation is a consequence of uncertainty in the values of the molecular parameters which, in turn, determine the accuracy of \( C_{\text{rel}} \). It may, however, be pointed out that the results are closer to the experimental values as compared to the ones obtained from Lippincott’s potential function (eqn. 24) which is claimed to be the best potential for predicting the \( \alpha_e \) values [4]. The average mean deviations for FP, Morse, Varshni and
Lippincott’s potentials are 7.2%, 27.6%, 18.7% and 19.7%, respectively, establishing the supremacy of FP potential over other three-parameter potentials in predicting the $\alpha_e$ values.

As regards $\omega_e x_e$ the average mean deviations have been found to be 17.4%, 26.9%, 15.5% and 13.9%, respectively for FP, Morse, Varshni and Lippincott’s potential functions. Obviously, the accuracy is not as good as for $\alpha_e$. This is perhaps because $C_{rel}$ itself is not as much sensitive to $\omega_e x_e$. However, the results are better than the Morse potential for which, unlike the Varshni and Lippincott’s potential functions, Schrödinger equation is solvable. The calculated values are slightly larger than the experimental values for almost all the molecules. A graph between $C_{rel}$ for the individual level and $r_{max}$ (corresponding to $v$) (fig. 1) reveals that $C$ increases almost exponentially to large negative values at higher $v$. The nature of the curve at large $v$ and the fact that the factor $(1+C+C^2)$ may be approximated to $e^C(=1+C+C^2)$ because $|C|<1$, have prompted us to write $\omega_e x_e$ in the light of equation 22, as

$$\omega_e x_e = \frac{h}{8\pi^2 c \mu a^2} e^C$$

The use of this relation reduces the average mean deviation to 15.9% (column 12 in Table 5) which is comparable to the value obtained from Lippincott’s potential function.

VI. CONCLUSIONS

The constant $C$ has been expressed in terms of molecular constants implying that the FP potential manifests the contribution of vibration, rotation, rotation-vibration interaction constants. Furthermore, the potential may be preferred over all the known three-parameter potentials for the prediction of the rotation-vibration interaction constant, $\alpha_e$ and it yields the value of $\omega_e x_e$ as good as provided by Lippincott’s function which is known to be the best analytical function for its prediction.
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TABLE I. Experimental Molecular Constants Used in this work.

| S.No. | Molecular State ($A^0$) | $r_e$ ($cm^{-1}$) | $D_e$ ($cm^{-1}$) | $\omega_e$ ($10^3 cm^{-1}$) | $\alpha_e$ ($cm^{-1}$) | $B_e$ ($cm^{-1}$) | $\omega_e x_e$ | $\mu_e$ | Ref. |
|-------|--------------------------|-------------------|-------------------|-----------------------------|-------------------------|-----------------|---------------|--------|------|
|       |                          |                   |                   |                             |                         |                 |               |        |      |
|   | Species | \( \omega \text{cm}^{-1} \) | \( \rho \) | \( \sigma \) | \( \varpi \text{cm}^{-1} \) | \( \Omega \text{cm}^{-1} \) | \( \sigma \text{cm}^{-1} \) |
|---|---------|-----------------|-----------|-----------|-----------------|-----------------|-----------|
| 1. | \( \text{Li}_2X^1\Sigma_g^+ \) | 2.6729 | 8516.780 | 351.430 | 7.040 | 0.6726 | 2.6100 | 3.5080 | 17.14 |
| 2. | \( \text{Na}_2X^1\Sigma_g^+ \) | 3.0788 | 6022.600 | 159.177 | 0.873 | 0.1547 | 0.7254 | 11.4949 | 18.14 |
| 3. | \( \text{K}_2X^1\Sigma_g^+ \) | 3.9244 | 4440.000 | 92.405 | 0.212 | 0.0562 | 0.3276 | 19.4800 | 19 |
| 4. | \( \text{Cl}_2X^1\Sigma_g^+ \) | 1.9872 | 20276.440 | 559.751 | 1.516 | 0.2442 | 2.6943 | 17.4844 | 20 |
| 5. | \( \text{Cl}_2B^3\Pi \) | 2.4311 | 3341.170 | 255.3800 | 2.511 | 0.1631 | 4.8000 | 17.48442 | 21 |
| 6. | \( \text{I}_2XO_g^+ \) | 2.6664 | 12547.335 | 214.520 | 0.113 | 0.037367 | 0.6079 | 63.4522 | 22.23 |
| 7. | \( \text{IClX}^1\Sigma_g^+ \) | 2.3209 | 17557.600 | 384.275 | 0.532 | 0.1142 | 1.4920 | 27.4147 | 24 |
| 8. | \( \text{IClA}^3\Pi_1 \) | 2.6850 | 3814.700 | 211.030 | 0.744 | 0.08529 | 2.1200 | 27.4147 | 24.25 |
| 9. | \( \text{IClA}^3\Pi_2 \) | 2.6651 | 4875.520 | 224.571 | 0.674 | 0.0865 | 1.8823 | 27.4147 | 25 |
|10. | \( \text{HFXX}^1\Sigma_g^+ \) | 0.9168 | 49384.000 | 4138.320 | 772.400 | 20.9557 | 89.8800 | 0.9571 | 26 |
|11. | \( \text{H}_2X^1\Sigma_g^+ \) | 0.7416 | 38297.000 | 4401.265 | 3051.300 | 60.8477 | 120.6020 | 0.5039 | 27 |
|12. | \( \text{COX}^1\Sigma_g^+ \) | 1.1283 | 90529.000 | 2169.813 | 17.504 | 1.93137 | 13.2883 | 6.8562 | 14 |
|13. | \( \text{xeOd}^1\Sigma_g^+ \) | 2.8523 | 693.000 | 156.832 | 5.400 | 0.1456 | 9.8678 | 14.2327 | 28 |
|14. | \( \text{Cs}_2X^1\Sigma_g^+ \) | 4.6480 | 3649.500 | 42.020 | 0.022 | 0.0117 | 0.0826 | 66.4527 | 30 |
|15. | \( \text{Rb}_2X^1\Sigma_g^+ \) | 4.2099 | 3950.000 | 57.7807 | 0.055 | 0.0224 | 0.1391 | 42.4559 | 31 |
|16. | \( \text{xeOb}^1\Sigma_g^+ \) | 2.5480 | 461.000 | 113.636 | 14.593 | 0.1820 | 11.8410 | 14.2651 | 28 |
|17. | \( \text{Ar}_2CO^+_u \) | 3.5960 | 465.800 | 66.820 | 2.500 | 0.0652 | 4.0000 | 19.9810 | 16 |
|18. | \( \text{Ar}_2XO^+_g \) | 3.7610 | 99.500 | 30.6800 | 3.641 | 0.05965 | 2.4200 | 19.9810 | 16 |
|19. | \( \text{O}_2X^3\Sigma_u^- \) | 1.2075 | 42047.000 | 1579.247 | 15.466 | 1.4456 | 11.5008 | 7.9975 | 15 |
|20. | \( \text{O}_{2b1}\Sigma_g^+ \) | 1.2268 | 28852.000 | 1432.775 | 18.198 | 1.4004 | 14.0065 | 7.9975 | 29 |
|21. | \( \text{O}_2A^3\Sigma_u^+ \) | 1.5215 | 6643.000 | 815.648 | 18.053 | 0.9105 | 19.8513 | 7.9975 | 15 |
|22. | \( \text{O}_2B^3\Sigma_u^- \) | 1.6042 | 8121.000 | 709.050 | 11.922 | 0.8189 | 10.6100 | 7.9975 | 15 |
|23. | \( \text{O}_2^+X^2\Pi_g \) | 1.1171 | 54681.000 | 1905.335 | 18.970 | 1.6905 | 16.3040 | 7.9973 | 25 |
|24. | \( \text{NOX}^2\Pi_{1/2} \) | 1.15077 | 53323.758 | 1904.204 | 17.100 | 1.67195 | 14.0750 | 7.4664 | 14 |
|25. | \( \text{NOB}^2\Pi \) | 1.4167 | 26544.888 | 1037.200 | 12.000 | 1.0920 | 7.7000 | 7.4664 | 14 |
|26. | \( \text{N}_2X^1\Sigma_g^+ \) | 1.0976 | 78742.304 | 2358.570 | 17.318 | 1.9982 | 14.3240 | 7.0015 | 14 |
|27. | \( \text{N}_2A^3\Sigma_u^+ \) | 1.2866 | 29772.23 | 1460.640 | 18.000 | 1.4546 | 13.8720 | 7.0015 | 14 |
|28. | \( \text{N}_2\alpha^1\Pi_g \) | 1.2203 | 48974.915 | 1694.248 | 17.930 | 1.6169 | 13.9490 | 7.0015 | 14 |
|29. | \( \text{N}_2B^3\Pi_g \) | 1.2126 | 39534.94 | 1733.390 | 17.910 | 1.6374 | 14.1220 | 7.0015 | 14 |
TABLE II. Mean square deviations (eqn. 20) from the RKR curves for the various potentials.

| S.No. | State | $C^a$ | $C_{rel}$ | $\Delta Y_L$ (\%) | $\Delta Y_V$ (\%) | $\Delta Y_M$ (\%) | $\Delta Y_{FPC}$ (\%) | $\Delta Y_{FPC_{rel}}$ (\%) | $\Delta E_C$ (\%) | $\Delta E_{C_{rel}}$ (\%) |
|-------|-------|-------|-----------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|
| 1.    | $Li_2X^1\Sigma_g^+$ | -0.1460 | -0.1298 | 9.879            | 8.498            | 9.952            | 2.842            | 2.985            | 2.576            | 2.707            |
| 2.    | $Na_2X^1\Sigma_g^+$ | -0.2024 | -0.2031 | 18.721          | 16.058          | 21.372          | 2.028          | 2.027          | 2.878          | 2.872          |
| 3.    | $K_2X^1\Sigma_g^+$ | -0.2780 | -0.2694 | 10.448          | 9.155          | 13.622          | 2.034          | 2.062          | 1.374          | 1.409          |
| 4.    | $Cl_2X^1\Sigma_g^+$ | -0.1097 | -0.0910 | 2.063          | 2.047          | 7.628          | 3.502          | 3.665          | 3.105          | 3.265          |
| 5.    | $Cl_2B^3\Pi$ | -0.1036 | -0.1034 | 3.971          | 3.378          | 7.780          | 2.258          | 2.258          | 2.876          | 2.874          |
| 6.    | $I_2XO^+_g$ | -0.1460 | -0.1547 | 1.954          | 3.416          | 10.439          | 2.428          | 2.474          | 2.176          | 2.117          |
| 7.    | $IClX^1\Sigma^+$ | -0.1000 | -0.1020 | 1.822          | 1.828          | 6.842          | 3.298          | 3.300          | 3.306          | 2.989          |
| 8.    | $IClA^3\Pi_1$ | -0.1680 | -0.1780 | 3.036          | 5.452          | 12.181          | 1.104          | 1.244          | 0.910          | 0.925          |
| 9.    | $IClA^3\Pi_2$ | -0.1540 | -0.1610 | 2.171          | 3.940          | 10.375          | 1.260          | 1.320          | 0.905          | 0.882          |
| 10.   | $HFX^1\Sigma^+$ | 0.1120  | 0.1210  | 4.170          | 4.313          | 6.313          | 3.211          | 3.245          | 2.816          | 2.921          |
| 11.   | $H_2X^1\Sigma_g^+$ | 0.1510  | 0.1752  | 5.437          | 9.986          | 8.051          | 3.961          | 4.153          | 3.553          | 3.852          |
| 12.   | $COX^1\Sigma^+$ | 0.0370  | 0.0460  | 2.551          | 3.408          | 1.210          | 0.548          | 0.603          | 0.292          | 0.347          |
| 13.   | $XeOd^3\Sigma^+$ | -0.0940 | -0.0683 | 7.478          | 6.192          | 7.570          | 5.183          | 5.398          | 5.140          | 4.957          |
| 14.   | $Cs_2X^1\Sigma_g^+$ | -0.2949 | -0.3114 | 16.507         | 14.965         | 22.449         | 1.889         | 2.100         | 1.601         | 1.512          |
| 15.   | $Rb_2X^1\Sigma_g^+$ | -0.2890 | -0.2898 | 10.444         | 9.271         | 14.103         | 2.208         | 2.207         | 1.446         | 1.443          |
| Average |       | 6.710  | 6.794  | 10.659         | 2.517         | 2.802         | 2.348         | 2.338         |                |                |

$^a$The values are slightly different from those obtained by Wei Hua [9], possibly because of reduced mass which we have taken from ref. 14 for all the molecules.
| S.No. | State     | $C_F$ | $\Delta Y_L$ | $\Delta Y_V$ | $\Delta Y_M$ | $\Delta Y_{FPC_{rel}}$ | $\Delta E_{C_{rel}}$ | $E_{max}$ | Ref. for | $D_e$ | RKR Potential |
|-------|-----------|-------|---------------|---------------|---------------|--------------------------|-----------------------|-----------|----------|-------|----------------|
| 1.    | $XeOb^1\Sigma^+$ | 0.5410 | 20.478 | 18.962 | 15.985 | 5.168 | 2.984 | 0.6582 | 28 |
| 2.    | $Ar_2CO^+_u$  | 0.1105 | 17.744 | 16.530 | 14.136 | 13.406 | 10.313 | 0.7022 | 16 |
| 3.    | $Ar_2XO^+_g$  | -0.0223 | 7.302 | 5.967 | 6.881 | 6.038 | 2.015 | 0.9484 | 16 |
| 4.    | $O_2X^3\Sigma^-_g$ | -0.0242 | 1.867 | 1.998 | 3.244 | 2.914 | 1.745 | 0.7064 | 15 |
| 5.    | $O_2^1\Sigma^+_g$ | -0.0530 | 0.419 | 0.484 | 1.347 | 0.851 | 0.381 | 0.3870 | (b) |
| 6.    | $O_2A^3\Sigma^+_u$ | -0.2372 | 8.994 | 11.166 | 18.781 | 3.758 | 2.805 | 0.9849 | 15 |
| 7.    | $O_2B^3\Sigma^-_u$ | -0.2500 | 4.612 | 5.097 | 11.171 | 2.612 | 0.927 | 0.9031 | 15 |
| 8.    | $O_2^+X^2\Pi_g$ | 0.0036 | 0.968 | 1.220 | 0.110 | 0.094 | 0.102 | 0.3330 | 15 |
| 9.    | $COa^3\Sigma^+$ | 0.0169 | 7.654 | 8.274 | 5.998 | 5.951 | 3.820 | 0.7664 | (b) |
| 10.   | $N_2X^1\Sigma^+_g$ | -0.0561 | 2.459 | 2.095 | 5.573 | 4.049 | 2.787 | 0.9937 | (b) |
|       | Average    | 7.25  | 7.18  | 8.32  | 4.48  | 2.79  |          |         |         |

(\textsuperscript{(b)}) RKR potential is calculated using LeRoy's computer program \textsuperscript{[32]}. 

\textsuperscript{18}
TABLE IV. Comparison of experimental values of $\alpha_e$ with calculated values and the mean deviations $[\Delta X = (\alpha_e(exptl) - \alpha_e(i))/(\alpha_e(exptl))]$; where $\alpha_e(i)$ stands for, $\alpha_e(FPC_{rel})$, FP; $\alpha_e(M)$, Morse; $\alpha_e(V)$, Varshni; $\alpha_e(L)$, Lippincott for different electronic states.

| S.No. | State | $C_{rel}$ | $\alpha_e(exptl)$ | $\alpha_e(FPC_{rel})$ | $\alpha_e(M)$ | $\alpha_e(V)$ | $\alpha_e(L)$ | $\Delta X_{FPC_{rel}}$ | $\Delta X_M$ | $\Delta X_V$ | $\Delta X_L$ |
|-------|-------|-----------|-------------------|----------------------|----------------|----------------|----------------|--------------------------|--------------|--------------|--------------|
|       |       | (10^3 cm⁻¹) | (10^3 cm⁻¹) | (10^3 cm⁻¹) | (10^3 cm⁻¹) | (%) | (%) | (%) | (%) | (%) | (%) |
|   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|
| 1. | $Li_2X^1\Sigma^+_g$ | -0.1298 | 7.040 | 7.875 | 10.206 | 9.137 | 9.097 | 11.9 | 45.0 | 29.8 | 29.2 |
| 2. | $Na_2X^1\Sigma^+_g$ | -0.2031 | 0.873 | 0.972 | 1.449 | 1.239 | 1.282 | 11.4 | 66.1 | 42.0 | 46.9 |
| 3. | $K_2X^1\Sigma^+_g$ | -0.2694 | 0.212 | 0.233 | 0.394 | 0.329 | 0.346 | 9.9 | 86.0 | 55.4 | 63.5 |
| 4. | $Cl_2X^1\Sigma_g$ | -0.0910 | 1.516 | 1.672 | 1.903 | 1.585 | 1.655 | 10.3 | 25.5 | 4.6 | 9.1 |
| 5. | $Cl_2B^3\Pi$ | -0.1034 | 2.511 | 2.439 | 2.793 | 2.396 | 2.412 | 2.8 | 11.2 | 4.6 | 3.9 |
| 6. | $I_2XO^+_g$ | -0.1547 | 0.113 | 0.125 | 0.154 | 0.131 | 0.134 | 10.1 | 36.5 | 15.9 | 18.1 |
| 7. | $IClX^1\Sigma^+$ | -0.1020 | 0.532 | 0.581 | 0.670 | 0.561 | 0.582 | 9.2 | 26.0 | 5.5 | 9.3 |
| 8. | $IClA^3\Pi_1$ | -0.1780 | 0.744 | 0.788 | 1.000 | 0.867 | 0.865 | 5.8 | 34.8 | 16.5 | 16.3 |
| 9. | $IClA^3\Pi_2$ | -0.1610 | 0.674 | 0.717 | 0.893 | 0.767 | 0.772 | 6.4 | 32.5 | 13.7 | 14.4 |
| 10. | $HFX^1\Sigma^+$ | 0.1210 | 772.400 | 801.900 | 658.200 | 647.600 | 593.900 | 3.8 | 14.8 | 16.1 | 23.1 |
| 11. | $H_2X^1\Sigma^+_g$ | 0.1752 | 3051.300 | 3502.874 | 2229.439 | 4183.994 | 2161.944 | 14.8 | 26.9 | 37.1 | 29.1 |
| 12. | $COX^1\Sigma^+$ | 0.0460 | 17.504 | 17.600 | 16.440 | 14.080 | 14.547 | 0.5 | 6.0 | 19.5 | 16.9 |
| 13. | $XeOd^1\Sigma^+$ | -0.0683 | 5.400 | 5.088 | 5.520 | 4.932 | 4.745 | 5.8 | 2.2 | 8.9 | 12.1 |
| 14. | $Cs_2X^1\Sigma^+_g$ | -0.3114 | 0.022 | 0.0238 | 0.0435 | 0.0361 | 0.0381 | 8.8 | 98.6 | 64.7 | 73.9 |
| 15. | $Rb_2X^1\Sigma^+_g$ | -0.2898 | 0.055 | 0.062 | 0.108 | 0.0897 | 0.0947 | 11.3 | 95.3 | 62.4 | 71.3 |
| 16. | $XeOb^1\Sigma^+$ | 0.5410 | 14.593 | 14.900 | 9.090 | 7.910 | 7.842 | 2.0 | 37.6 | 45.7 | 46.2 |
| 17. | $Ar_2CO^+_u$ | 0.1105 | 2.500 | 2.189 | 1.930 | 1.670 | 1.667 | 12.4 | 22.6 | 32.8 | 33.3 |
| 18. | $Ar_2XO^+_g$ | -0.0223 | 3.641 | 3.580 | 3.685 | 3.210 | 3.176 | 1.6 | 1.2 | 11.8 | 12.7 |
| 19. | $O_2X^3\Sigma^-_g$ | -0.0242 | 15.466 | 16.870 | 17.480 | 14.500 | 15.311 | 8.6 | 13.0 | 6.2 | 0.9 |
| 20. | $O_2b^1\Sigma^+_g$ | -0.0530 | 18.198 | 19.500 | 21.052 | 17.449 | 18.364 | 7.1 | 15.6 | 4.1 | 0.9 |
| 21. | $O_2A^3\Sigma^+_u$ | -0.2372 | 18.053 | 18.290 | 25.870 | 22.100 | 22.360 | 1.3 | 43.3 | 22.4 | 23.9 |
| 22. | $O_2B^3\Sigma^-_u$ | -0.2500 | 11.922 | 12.810 | 18.990 | 15.920 | 16.478 | 7.4 | 59.3 | 33.6 | 38.2 |
| 23. | $O_2^+X^2\Pi_g$ | -0.0036 | 18.970 | 19.130 | 18.880 | 15.690 | 16.680 | 1.7 | 0.5 | 17.4 | 12.2 |
| 24. | $NOX^2\Pi_1$ | -0.0352 | 17.100 | 18.180 | 19.000 | 15.770 | 16.600 | 5.8 | 11.1 | 7.7 | 2.6 |
| 25. | $NOB^2\Pi$ | -0.0371 | 12.000 | 13.030 | 13.802 | 11.500 | 12.120 | 8.3 | 15.0 | 4.1 | 1.0 |
| 26. | $N_2X^1\Sigma^+_g$ | -0.0561 | 17.318 | 18.478 | 20.030 | 16.710 | 17.598 | 6.6 | 15.6 | 3.5 | 1.6 |
| 27. | $N_2A^3\Sigma^+_u$ | -0.0836 | 18.000 | 19.250 | 21.808 | 18.070 | 19.030 | 6.7 | 21.1 | 0.4 | 5.7 |
| 28. | $N_2a^1\Pi_g$ | -0.0157 | 17.930 | 18.170 | 18.610 | 15.500 | 16.330 | 1.0 | 3.7 | 13.5 | 8.9 |
| 29. | $N_2B^3\Pi_g$ | -0.0915 | 17.910 | 19.400 | 22.300 | 18.490 | 19.500 | 8.0 | 24.6 | 3.2 | 8.9 |
TABLE V. Comparison of experimental values of $\omega_e x_e$ with calculated values and the mean deviations $[\Delta X=(\omega_e x_e(\text{exptl})-\omega_e x_e(i))/(\omega_e x_e(\text{exptl})]$, where $\omega_e x_e(i)$ stands for $\omega_e x_e(FC_{rel})$, FP; $\omega_e x_e(M)$, Morse; $\omega_e x_e(V)$, Varshni; $\omega_e x_e(L)$, Lippincott; $\omega_e x_e(\text{exp.})$ using equation 29 for the corresponding electronic states given in table 3.

| S.No. | $\omega_e x_e(\text{exptl.})$ cm\(^{-1}\) | $\omega_e x_e FC_{rel}$ cm\(^{-1}\) | $\omega_e x_e(M)$ cm\(^{-1}\) | $\omega_e x_e(V)$ cm\(^{-1}\) | $\omega_e x_e(L)$ cm\(^{-1}\) | $\omega_e x_e(\text{exp.})$ cm\(^{-1}\) | $\Delta X_{FC_{rel}}$ (%) | $\Delta X_M$ (%) | $\Delta X_V$ (%) | $\Delta X_L$ (%) | $\Delta X_{\text{exp.}}$ (%) |
|-------|---------------------------------|------------------|------------------|------------------|------------------|------------------|----------------|----------------|----------------|----------------|----------------|
| 22    |                                |                  |                  |                  |                  |                  |                 |                 |                 |                 |                 |
|   |      |      |      |      |      |      |      |      |      |      |
|---|------|------|------|------|------|------|------|------|------|------|
| 1 | 2.6100 | 3.2150 | 3.6250 | 3.9500 | 2.9708 | 3.1835 | 23.1 | 38.8 | 16.1 | 13.8 | 21.9 |
| 2 | 0.7254 | 0.8816 | 1.0518 | 0.8640 | 0.8468 | 0.8585 | 21.5 | 45.0 | 19.1 | 16.7 | 18.3 |
| 3 | 0.3276 | 0.3859 | 0.4808 | 0.3918 | 0.3814 | 0.3700 | 17.8 | 46.8 | 19.6 | 16.4 | 12.0 |
| 4 | 2.6943 | 3.5437 | 3.8631 | 3.1681 | 2.9890 | 3.5272 | 31.5 | 43.4 | 17.6 | 10.9 | 30.9 |
| 5 | 4.8000 | 4.4261 | 4.8800 | 4.0982 | 3.7199 | 4.3991 | 7.8  | 1.7  | 14.6 | 22.5 | 8.3  |
| 6 | 0.6079 | 0.7973 | 0.9169 | 0.7637 | 0.7016 | 0.7860 | 31.2 | 50.8 | 25.6 | 15.4 | 29.3 |
| 7 | 1.4920 | 1.9104 | 2.1026 | 1.7328 | 1.6202 | 1.8992 | 28.01| 40.9 | 16.1 | 8.6  | 27.3 |
| 8 | 2.1210 | 2.4911 | 2.9185 | 2.4660 | 2.2206 | 2.4423 | 17.4 | 37.6 | 16.3 | 4.7  | 15.5 |
| 9 | 1.8823 | 2.2354 | 2.5859 | 2.1712 | 1.9709 | 2.2002 | 18.8 | 37.4 | 15.3 | 4.7  | 16.9 |
| 10| 89.8800| 98.4446| 86.6965| 75.3269| 72.8732| 97.8364| 9.5  | 3.5  | 16.2 | 18.9 | 8.8  |
| 11| 120.6020| 152.4790| 126.4533| 148.9109| 117.6726| 150.6605| 26.4 | 4.9  | 23.5 | 2.4  | 24.9 |
| 12| 13.2883| 13.6250| 13.0016| 13.6854| 10.4741| 13.6117| 2.5  | 2.2  | 19.6 | 21.2 | 2.4  |
| 13| 9.8678 | 8.3081 | 8.8731 | 7.7068 | 6.7091 | 8.2869 | 15.8 | 10.0 | 21.9 | 32.0 | 16.0 |
| 14| 0.0826 | 0.0950 | 0.1209 | 0.09848| 0.09510| 0.8858 | 15.1 | 46.5 | 19.3 | 15.2 | 7.3  |
| 15| 0.1391 | 0.1678 | 0.2113 | 0.1721 | 0.1668 | 0.1581 | 20.6 | 51.9 | 23.7 | 19.9 | 13.6 |
| 16| 11.8410| 12.8083| 7.0028 | 5.9355 | 5.3070 | 11.9983| 8.2  | 40.9 | 49.8 | 55.1 | 1.3  |
| 17| 4.0000 | 2.6900 | 2.3960 | 2.0304 | 1.8202 | 2.6742 | 32.8 | 44.1 | 49.2 | 54.5 | 33.1 |
| 18| 2.4200 | 2.3130 | 2.3649 | 2.0126 | 1.7960 | 2.3124 | 4.4  | 2.3  | 16.8 | 25.7 | 4.4  |
| 19| 11.5008| 14.4758| 14.8287| 12.0728| 11.6615| 14.4715| 25.9 | 28.9 | 4.9  | 1.4  | 25.8 |
| 20| 14.0065| 16.8908| 17.7877| 14.5104| 13.8627| 16.8654| 20.6 | 26.9 | 3.6  | 1.0  | 20.4 |
| 21| 19.8513| 20.5039| 25.0369| 20.9516| 19.1156| 19.7470| 3.3  | 26.1 | 5.5  | 3.7  | 0.5  |
| 22| 10.6100| 12.5700| 15.4769| 12.7588| 11.9120| 12.0516| 18.4 | 45.8 | 20.2 | 12.3 | 13.6 |
| 23| 16.3040| 16.6684| 16.5940| 13.5247| 13.0900| 16.6683| 2.2  | 1.8  | 17.0 | 19.7 | 2.2  |
| 24| 14.0750| 16.1025| 16.9990| 13.5732| 13.1284| 16.0920| 14.4 | 20.7 | 3.6  | 6.7  | 14.3 |
| 25| 7.7000 | 9.4823 | 10.1317| 8.0125 | 7.7847 | 9.4755 | 23.1 | 31.6 | 4.1  | 1.1  | 23.1 |
| 26| 14.3240| 16.7209| 17.6615| 14.3895| 13.9912| 16.6926| 16.7 | 23.3 | 0.5  | 2.3  | 16.5 |
| 27| 13.8720| 16.5410| 17.9149| 14.6094| 13.9800| 16.4767| 19.2 | 29.1 | 5.3  | 0.8  | 18.7 |
| 28| 13.9490| 14.4239| 14.6521| 11.9894| 11.5933| 14.4221| 3.4  | 5.0  | 14.4 | 16.9 | 3.4  |
| 29| 14.1220| 17.4174| 18.9990| 15.4808| 14.8614| 17.3355| 23.3 | 34.5 | 9.6  | 5.2  | 22.7 |
| Average |   |   |   | 17.4 | 26.9 | 15.5 | 13.4 | 15.9 |