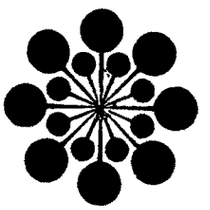

CHAPTER - 5

EVALUATION OF SPECTROSCOPIC CONSTANTS OF POLAR DIATOMIC MOLECULES ON GEP AND GLP FUNCTIONS

5.1 INTRODUCTION

We have described in Chapter 1 the criteria for testing the validity of a given potential function. Its merits and demerits are decided by testing it in two different ways:

i) By comparing its potential energy curve with the experimental RKRV curve and

ii) By calculating the various spectroscopic constants like α_e, $\omega_e x_e$ etc and comparing their values with the experimental results. However, the evaluation of correct values for these spectroscopic constants is only a necessary condition but not sufficient. A function which is satisfactory in producing the potential energy curve may not be so in evaluating α_e and $\omega_e x_e$. Further a function, which may be useful for calculating $\omega_e x_e$ may not be accurate in estimating α_e values.

By employing Varshni's method[1] one can obtain expressions for α_e and $\omega_e x_e$ after taking the derivatives of the function upto the fourth order, while in the case of higher order constants the fifth order derivative is also required. This means the results for these spectroscopic constants are found to be very sensitive to the form of potential function used in the calculations. This provides a sensitive method for checking the validity of a given potential energy function. This fact has been well considered in our GEP and GLP functions proposed in Section 4.3. The characteristic features of these functions are the parameters n and m involved in the repulsive type

terms. By suitably changing the values of n and m one can vary the forms of the two functions so as to get the most accurate $\alpha_e, \omega_e x_e$ and higher order spectroscopic constants.

In this Chapter, first we have obtained the expressions for the potential parameters relevant to the GEP and GLP functions. Then using these potential parameters we have derived expressions for α_e and $\omega_e x_e$. The higher order spectroscopic constants are related to α_e and $\omega_e x_e$ through the known relations in the literature.

5.2 EXPRESSIONS FOR SPECTROSCOPIC CONSTANTS

5.2.1 Using GEP Function

On GEP function the expressions for potential parameters are already derived and reported in Section 4.3.2 [eqs.(4.25), (4.30) and (4.31)] . Also the derivatives of first and second order are given by the eqs. (4.22) and (4.23). At $r=r_e$ the eq.(4.23) takes the form

$$U^{II}(r_e) = \frac{(-e^2/r_e^3)\left[\, r(n+1) + (m(m+2n+1)r_e^m/Q_1) + (m\, r_e^m/Q_1)^2 \right]}{(n+ m\, r_e^m/Q_1)} \quad .....(5.1)$$

Differentiating eq.(4.23) we can obtain the third and fourth order derivatives whose values at $r=r_e$ are found to be

$$U^{III}(r_e) = (e^2/r_e^4)\left[6(n+m\, r_e^m/Q_1) - \left[A' + (B' r_e^m/Q_1) + C'(r_e^m/Q_1)^2 + D'(r_e^m/Q_1)^3\right]\right] / (n+ m\, r_e^m/Q_1) \quad .....(5.2)$$

and

$$U^{IV}(r_e) = (-e^2/r_e^5)\left[24n+A'(n-3)+(ar_e^m/Q_1)+b(r_e^m/Q_1)^2 + d(r_e^m/Q_1)^3 + mD'(r_e^m/Q_1)^4\right]/(n+mr_e^m/Q_1) \quad .....(5.3)$$

where $a = m(A'+24)+ B'(m+n-3)$

$b = mB' +(2m + n -3)C'$

$d = mC' + (3m + n - 3)D'$

$A' = n(n - 1)(n - 2)$

$B' = m\left[n(n - 1)+(m + 2n - 1)(m + n -2)\right]$

$C' = 3m^2(m + n - 1)$

$D' = m^3$

and Q_1 is given by eq. (4.30) and by eq.(4.32) for n=0

Employing eqs.(5.1)-(5.2) the expressions for α_e and $\omega_e x_e$ are derived with the help of equations given by Varshni[1]

$$\alpha_e = (6B_e/\omega_e)\left[\left(U^{III}(r_e)/U^{II}(r_e)\right)(r_e/3)+1\right] \quad .....(5.4)$$

$$\omega_e x_e = \left(2.1078 \times 10^{-16}/\mu\right)\left[(5/3)\left(U^{III}(r_e)/U^{II}(r_e)\right)^2 - U^{IV}(r_e)/U^{II}(r_e)\right] \quad .....(5.5)$$

Using the eqs.(5.4)-(5.5), the expressions for higher order spectroscopic constants[13] are written as,

$$B_e = D_e\left[(8\omega_e x_e/\omega_e)-(5\alpha_e/B_e)-(\alpha_e^2\omega_e/24B_e^3)\right] \quad .....(5.6)$$

and

$$H_v=(2\ D_e/\ 3\ \omega_e^2)(\ 12\ B_e^2-\alpha_e\omega_e) \qquad .....(5.7)$$

5.2.2 Using GLP Function

The expressions for potential parameters on GLP function are already derived in Section 4.3.1 and are given by eqs.(4.17), (4.18). The first order derivative is given by eq.(4.14). Differentiating eq.(4.14) further with respect to internuclear distance r , derivatives up to fourth order are obtained. Their values at $r=r_e$ are expressed as

$$U^{II}(r_e) = \left[(-\ 1/r_e)+p\ q/s^2\right]\ 2\ e^2/r_e^2 \qquad .....(5.8)$$

$$U^{III}(r_e)=(\ 2\ e^2/r^3)\left[(3/r_e)-(2\,p\ q^2/s^3)+\ 4p(q\ -\ H)/n\ s^2\right] \qquad .....(5.9)$$

$$U^{IV}(r_e) =(4\ e^2/r^4)\left[(-6/r_e)+(3\ p\ q^3/s^4)-(12\ p\ q(q-H)/n\ s^3)\right.$$
$$\left.+\ 2\ p(\ q\ -\ H)(4\ -\ n)/\ n^2\ s^2\right] \qquad .....(5.10)$$

where $p = (2\ G\ H)/n\ e^2$

$$q = (\ 2^{n-1}((4/n)+1)r_e^{4/n})+\ H$$

$$s = (2^{n-1}\ r_e^{4/n})+\ H$$

With the help of eqs(5.8)-(5.10), the expressions for α_e, $\omega_e x_e$ and higher order spectroscopic constants can be obtained as in the case of GEP function.

5.3 RESULTS AND DISCUSSION

In this section we present the calculated values of various spectroscopic constants using the eqs.(5.4)-(5.7) derived on GEP and GLP potentials as explained in Section 5.2. The necessary molecular data required in this connection have been taken from Refs.(2) and (3) and the same have been listed in Tables 5.1 for alkali halides and hydrides and heavy metal halide molecules. Appropriate computer programs have been written in BASIC so as to carry out fast and accurate evaluation of spectroscopic constants. These programs have been given in Tables 5.2 & 5.4. A WIPRO PC was employed to obtain the print outs of the calculated results.

5.3.1 Calculations of α_e Constants

a) ALKALI HALIDE MOLECULES

The estimated α_e values on different ionic potential functions for a number of alkali halide molecules are given in Table 5.6. A comparative study of the results shows that our GEP function with n=0 and m=1 yields an average error of $\pm$ 16.65 % which is comparable to the errors evaluated on potentials due to Gupta et al[4] and Hasan et al[5]. However, this error is found to be considerably large in comparison with those calculated on the potentials due to Sangachin and Bakshi[6], Harrison[7], Chaturvedi et al[8] and Shankar and Kumar[9].Our GLP function with n = 1 fails to evaluate accurate α_e values for alkali halides because the average % error comes out to be abnormally large.

b) ALKALI HYDRIDES

The calculated α_e values are listed in Table 5.7. The results show that the performance of our GEP function with n=0 and m=1 is found to be in agreement with that of the potential due to Varshni and Shukla.[10] In each case the average error comes out to be above $\pm$ 17 %, while GLP function with n =1 evaluates a larger % error. However, the potential functions due to Sangachin and Bakshi[6], Ali et al[11] and Hellmann[12] are found to yield more satisfactory results comparatively.

c) HEAVY METAL HALIDES

The calculated results for this group of molecules are tabulated in Table 5.7. We have reported only the results on GEP function for various combinations of n and m. The α_e values on GLP functions are found to be abnormally high leading to errors of the order of few hundred %. Hence these are not reported here. Further to our knowledge spectroscopic constants for heavy metal halide molecules have not been reported in the literature so far. Therefore a comparative study with our results has become difficult in this work. The reported values in Table 5.7 show that the GEP function with n=2 and m=2 proves to be a satisfactory potential in evaluating α_e values for heavy metal halides.

A final look at the Tables 5.6 and 5.7 shows that the GEP function with different n and m paired values is found to be more successful as compared to the GLP function with n=1.

5.3.2 Calculations of $\omega_e x_e$ Constants

a) ALKALI HALIDES

The vibration anharmonicity constants determined for this group of molecules are reported in Table 5.8. The performance of GEP function is seen to be comparatively satisfactory only for the combination n=0 and m=1. This GEP function estimates an average error of $\pm$ 19.87% which is better than that given by the potential due to Hasan et al[5]. However, compared to other potential functions listed in Table 5.8, the performance of the said GEP function is not an encouraging one. Similarly GEP function with n=1 evaluates considerably larger average error of about 68%.

b) ALKALI HYDRIDES

The relevant results are given in Table 5.9. In this case GLP function with n=1 and GEP with n=0 and m=1 determine average errors of the order of 12 to 15%. However, this accuracy is not satisfactory in comparison with the errors presented by other potential functions.

c) HEAVY METAL HALIDES

In Table 5.9 are given the $\omega_e x_e$ values calculated on GEP potential with two different combinations of n and m values. It is seen that with m=0.5 and n= -1 and -2 the GEP function evaluates errors of $\pm$ 35.63 and $\pm$ 9.93% respectively. To the best of our knowledge $\omega_e x_e$ constants for heavy metal halides are not reported

in the literature to this date. Therefore our calculations may perhaps be first of their kind. Our GLP function gives large % error values and hence the results are not reported in Table 5.9.

5.3.3 Calculations of Higher Order Spectroscopic Constants

The higher order spectroscopic constants have been reported in the literature by quite a few investigators. Further only the experimental data of rotational constants β_e compiled by Brummer and Karplus[14] is available in the literature.

a) ALKALI HALIDES

The calculated values of constants β_e and H_v are presented in Table 5.10. The GEP function with n=0 and m=1 is found to estimate reasonably accurate β_e values only for fluorides and chlorides of various alkali atoms. In certain cases the values come out to be positive as against negative experimental values. This is in contradiction with the results obtained by Hasan et al.[5] On the other hand the GLP function evaluates negative and high β_e values for all the alkali halides. Therefore this function is not suitable for calculations of β_e constants of alkali halides.

Regarding the estimation of H_v values it is seen that GEP and GLP functions evaluate negative values in most of the cases as against those given by Hasan et al.[5]

When we compare the H_v values calculated on GEP function with those reported by Hasan et al[5] it is found that there is a

satisfactory agreement between individual H_v values for the halides of Na, K, Rb and Cs. In case of Li halides GEP function estimates considerably lower values than those calculated by Hasan et al.[5] On the GLP function, in general the H_v results are found to be considerably large when compared with other two potentials in the Table 5.10. Since experimentally H_v data is not available it is difficult to test the accuracy of evaluation by the individual functions.

b) AKLALI HYDRIDES

The higher spectroscopic constants for alkali hydrides are reported in Table 5.11. Since the experimental data on β_e and H_v is not available to our knowledge, it is difficult to compare the calculated values with some standards and to draw any conclusion regarding the merits and demerits of individual functions in the evaluation of higher order spectroscopic constants for alkali hydride molecules.

c) HEAVY METAL HALIDES

The β_e and H_v values calculated for this set of molecules on GEP function with n=-2 and m=0.5 are also listed in Table 5.11. These reported values would be first of their kind as experimental/theoretical data is not found in the literature.

5.4 SUMMARY

In the beginning we have obtained the expressions for the relevant potential parameters involved in the GEP and GLP functions.

Expressions for α_e, $\omega_e x_e$, β_e and H_v are reported for each type of functions. For the evaluation purpose computer programs have been developed and presented in separate Tables 5.2-5.4.

In the case of α_e values for alkali halides, the GEP function with n=0 and m=1 calculates satisfactory results, while GLP function with n=1 totally fails. This is more or less true in the case of alkali hydrides also. For heavy metal halides the GEP function with n=2 and m=2 once again proves to be successful, whereas the GLP function leads to abnormally high % errors. The GLP function with n=1 yields considerably large % errors in $\omega_e x_e$ values for alkali halides and heavy metal halides. But in the case of alkali hydrides the performance of this function is found to be comparatively satisfactory. On the other hand GEP function is found to evaluate consistent satisfactory $\omega_e x_e$ values for all the three types of ionic molecules considered in the present work.

Regarding the calculations of higher order spectroscopic constants it is seen that, in the case of alkali halides, the GEP function with n=0 and m=1, estimates reasonably accurate β_e values only for fluorides and chlorides. Also the H_v values on this function satisfactorily agree with those reported by Hasan et al.[5] However, GLP function with n=1 fails to give accurate results. In the case of alkali hydrides and heavy metal halides our reported values for β_e and H_v may be first of their kind in the absence of any reliable exprimental data.

TABLE 5.1

MOLECULAR DATA* USED IN THE CALCULATIONS

Molecule	μ (a.m.u.)	$\omega_e(cm^{-1})$	$\omega_e x_e(cm^{-1})$	$B_e(cm^{-1})$	$\alpha_e(cm^{-1})$	$r_e(\mathring{A})$	$D_e(10^{-7}cm^{-1})$
1	2	3	4	5	6	7	8
			ALKALI HALIDE MOLECULES				
LiF	5.1238103	910.34	7.929	1.3452576	0.0202868	1.563864	117.54
LiCl	5.8435744	643.31	4.5	0.7065222	0.0080096	2.020673	34.087
LiBr	6.4431916	563.1	3.5	0.555399	0.005644	2.170427	21.59
LiI	6.648441	498.1	3.3	0.443182	0.004090	2.391924	14.48
NaF	10.4021896	536	3.4	0.4369012	0.0045586	1.92594	11.6
NaCl	13.8706867	366	2.0	0.218063	0.0016248	2.36079	3.120
NaBr	17.803435	302	1.5	0.1512533	0.0009409	2.50203	1.553
NaI	19.463754	258	1.0	0.1178056	0.0006477	2.71145	0.973
KF	12.7712442	428	2.4	0.27993741	0.00233503	2.17145	4.834
KCl	18.4291764	281	1.3	0.1286347	0.0007899	2.66665	1.087
KBr	26.0849820	213	0.8	0.08122109	0.00041481	2.82078	0.4461
KI	29.8108348	186.53	0.574	0.06087473	0.00026776	3.04784	0.2594
RbF	15.5248345	376	1.9	0.210664	0.0015227	2.270333	2.683
RbCl	24.7685361	228	0.92	0.0876404	0.0004536	2.78673	0.4947
RbBr	40.902717	169.46	0.463	0.04752798	0.00018596	2.94474	0.14959
RbI	50.872801	138.51	0.335	0.3283293	0.00010946	3.17687	0.07380

Contd...118

(Contd.....Table 5.1

1	2	3	4	5	6	7	8
CsF	16.6223003	352.56	1.61	0.18436969	0.0011756	2.345351	2.0168
CsCl	27.6847083	214.17	0.731	0.07209149	0.00033756	2.90627	0.32675
CsBr	49.516045	149.66	0.374	0.03606925	0.00012401	3.07225	0.08380
CsI	64.917826	119.178	0.2505	0.02362735	0.000068263	3.31519	0.037146
			ALKALI HYDRIDE MOLECULES				
LiH	0.88123833	1405.65	23.20	7.5131	0.2132	1.5957	8617
NaH	0.96549966	1172.2	19.72	4.9012	0.1353	1.8874	3320
KH	0.98241434	983.6	14.3	3.412	0.081	1.242	1500
RbH	0.99600357	936.9	14.21	3.020	0.072	2.367	1230
CsH	1.00024037	891.0	12.9	2.7099	0.0579	2.4938	1130
			HEAVY METAL HALIDE MOLECULES				
TlF	17.3868727	477.3	2.3	0.223150163	0.00150385	2.084438	1.948
TlCl	29.875631	283.7	0.81	0.091397	0.0003979	2.484826	0.375
TlBr	58.014373	192.10	0.39	0.0423895	0.0001275	2.61819	0.083
TlI	78.378506	150.0	-	0.0271676	0.0000663	2.81367	0.036
InF	16.3028614	535.3	2.64	0.262324	0.0018797	1.985396	2.52
InCl	26.8097927	317.4	1.01	0.109058	0.0005178	2.401169	0.51

Contd...119

* Ref.(2)

(Contd....Table 5.1)

1	2	3	4	5	6	7	8
InBr	47.480276	221.0	0.65	0.0548944	0.0001862	2.54318	0.135
InI	60.303194	177.1	0.4	0.036867	0.000104	2.75365	0.076
GaF	14.8932747	622.2	3.2	0.3595161	0.0028642	1.774369	5.0
GaCl	23.1990149	365.3	1.2	0.1499045	0.0007936	2.201690	1.01
GaBr	37.220586	263.0	0.81	0.081839	0.0003207	2.35248	0.320
GaI	44.666098	216.6	0.5	0.056934	0.000139	2.57467	0.157

* Ref.(2)

TABLE 5.2

COMPUTER PROGRAM TO CALCULATE α_e , wexe AND

HIGHER ORDER CONSTANTS USING GEP FUNCTION

```
10 'Gen.Exp  Potential I  proposed by Shri.V.M .Patil
20 'file Erot-vib
30 'Rotation vib. coupling const. & vib anharmonic const.
40 'M1=Mass,W=We,WX=WeXe,BE=Be,RC=αe,RE=re,DE=De,RC1=cal.αe
    WX1=cal.wexe,ERC1=% in αe ,EWX1=% in wexe,BE1= βe,HV=Hv
50 'ERC1=% in αe ,EWX1=% in wexe,BE1= βe,HV=Hv
60 INPUT M1,W,WX,BE,RC,RE,DE
70 PRINT "N","m
80 PRINT "rc1","erc1","wx1","ewx1","be1","hv
90 FOR N = -3 TO -1 STEP -1
100 FOR M =.5 TO 2 STEP .5
110 E1 =4.8E-10
120 KE=.Ø5888*M1*(W)^2
130 A=N*(KE*(RE)^3 + (N+1)*(E1)^2)/(E1)^2
140 B=M *(KE*(RE)^3+(2*N+M+1)*(E1)^2)*((RE)^M/(E1)^2)
150 L1=+B/(2*A)
160 L2 =-B/(2*A)
170 C=(M)^2*(RE)^(2*M)
180 Q=(((B)^2-4*A*C)^.5/(2*A))
190 Q1 =-L1 +Q
200 A1=N*(N-1)*(N-2)
210 B1=M*(N*(N-1)+(M+2*N-1)*(M+N-2))
220 C1=3*(M^2)*(M+N-1)
230 D1=M^3
240 P=M*(A1+24)+B1*(M+N-3)
250 U=M*B1+C1*(2*M+N-3)
260 S=C1*M+D1*(3*M+N-3)
270 T1=N*(N+1)+M*(M+2*N+1)*(RE^M/Q1)+(M^2)*(RE^M/Q1)^2
280 X1=-(6*N+(6*M-B1)*((RE^M)/Q1)-A1-C1*((RE^M)/Q1)^2-D1*
    ((RE^M)/Q1)^3)/(RE*T1)
290 Y1=(24*N+P*(RE^M/Q1)+A1*(N-3)+U*(RE^M/Q1)^2+S*
    (RE^M/Q1)^3+D1*(RE^M/Q1)^4)/(RE^2*T1)
300 RC1=-(6*BE^2)*((X1*RE/3)+1)/W
310 WX1=(2.1Ø78E-16)*((5*X1^2/3)-Y1)/M1
320 BE1=DE*((8*WX1/W)-(5*RC1/BE)-((RC1)^2*W/(24*BE^3)))
330 HV=((2*DE)/(3*W^2))*(12*BE^2-RC1*W)
340 ERC1=((RC1-RC)/RC)*1ØØ
350 EWX1=((WX1-WX)/WX)*1ØØ
360 PRINT N,M
370 PRINT RC1,ERC1,WX1,EWX1,BE1,HV
380 NEXT M
390 NEXT N
400 GOTO 60
410 END
```

TABLE 5.3
COMPUTER PROGRAM TO CALCULATE α_e , wexe AND

HIGHER ORDER CONSTANTS USING GEP FUNCTION

IN THE CASE OF n=Ø

```
1Ø 'Gen.Exp  Potential I  proposed by Shri.V.M .Patil
2Ø 'file Erot-vib
3Ø 'Rotation vib. coupling const. & vib anharmonic const.
4Ø 'M1=Mass,W=We,WX=WeXe,BE=Be,RC=αe,RE=re,DE=De,RC1=cal.αe
    WX1=cal.wexe,ERC1=% in αe ,EWX1=% in wexe,BE1=βe,HV=Hv
5Ø 'ERC1=% in αe ,EWX1=% in wexe,BE1= βe,HV=Hv
6Ø INPUT M1,W,WX,BE,RC,RE,DE
7Ø PRINT "N","m
8Ø PRINT "rc1","erc1","wx1","ewx1","be1","hv
9Ø N=Ø
1ØØ FOR M =.5 TO 2 STEP .5
11Ø E1 =4.8E-1Ø
12Ø KE=.Ø5888*M1*(W)^2
13Ø A=N*(KE*(RE)^3 + (N+1)*(E1)^2)/(E1)^2
14Ø B=M *(KE*(RE)^3+(2*N+M+1)*(E1)^2)*((RE)^M/(E1)^2)
15Ø L1=+B
17Ø C=(M)^2*(RE)^(2*M)
18Ø Q1=-C/L1
2ØØ A1=N*(N-1)*(N-2)
21Ø B1=M*(N*(N-1)+(M+2*N-1)*(M+N-2))
22Ø C1=3*(M^2)*(M+N-1)
23Ø D1=M^3
24Ø P=M*(A1+24)+B1*(M+N-3)
25Ø U=M*B1+C1*(2*M+N-3)
26Ø S=C1*M+D1*(3*M+N-3)
27Ø T1=N*(N+1)+M*(M+2*N+1)*(RE^M/Q1)+(M^2)*(RE^M/Q1)^2
28Ø X1=-(6*N+(6*M-B1)*((RE^M)/Q1)-A1-C1*((RE^M)/Q1)^2-D1*
    ((RE^M)/Q1)^3)/(RE*T1)
29Ø Y1=(24*N+P*(RE^M/Q1)+A1*(N-3)+U*(RE^M/Q1)^2+S*
    (RE^M/Q1)^3+D1*(RE^M/Q1)^4)/(RE^2*T1)
3ØØ RC1=-(6*BE^2)*((X1*RE/3)+1)/W
31Ø WX1=(2.1Ø78E-16)*((5*X1^2/3)-Y1)/M1
32Ø BE1=DE*((8*WX1/W)-(5*RC1/BE)-((RC1)^2*W/(24*BE^3)))
33Ø HV=((2*DE)/(3*W^2))*(12*BE^2-RC1*W)
34Ø ERC1=((RC1-RC)/RC)*1ØØ
35Ø EWX1=((WX1-WX)/WX)*1ØØ
36Ø PRINT N,M
37Ø PRINT RC1,ERC1,WX1,EWX1,BE1,HV
38Ø NEXT M
4ØØ GOTO 6Ø
41Ø END
```

TABLE 5.4

COMPUTER PROGRAM TO CALCULATE α_e, wexe AND

HIGHER OEDER CONSTANTS USING GLP FUNCTIONS

```
10 REM"File rot.vib"
20  REM" Gen Log.Potential proposed by Shri V.M.Patil"
30 REM"RC=cal.αe ","ERC=%.in αe","WX=cal.wexe","EWX=% in wexe"
40 REM"BE1= βe","HV=Hv","M=mass","W=we","WX1=wexe"
50 REM"B=Be","RC1= αe","RE=re","DE=De"
60 PRINT "G", "H"
70 PRINT  "n","RC","ERC"
80 PRINT "BE1",HV
90 PRINT "wx","ewx"
100 E1=4.8E-10
110 INPUT  M,W,WX1,B,RC1,RE,DE
120 KE =.05888*M*(W^2)
130 X=KE*RE+(E1/RE)^2
140 FOR N= -1 TO 2 STEP 1
150 Y =X/(X-4*(E1)^2/(N*(RE)^2))
160 G = N*(E1)^2*(1-Y)/(4*RE)
170 H= -2^(N-1)*(RE)^(4/N)/Y
180 P=(2*(G/E1)*(H/E1))/N
190 Q= 2^(N-1)*((4/N)+1)*(RE)^(4/N)+H
200 S=2^(N-1)*(RE)^(4/N)+H
210 T=4*(P*RE/S)*((Q-H)/S)
220 U=(P*RE/S)*(Q/S)
230 X3=-(3*N+T-(2*U*N*(Q/S)))/(N*RE*(1-U))
240 X4= 2*(-6*N^2+3*U*N^2*(Q/S)^2-12*N*U*((Q-H)/S)+(4-N)*
    (T/2))/((RE)^2*N^2*(U-1))
250 RC=-(6*(B)^2/W)*((RE*X3)/3+1)
260 WX=(2.1078E-16/M)*((5/3)*(X3)^2-X4)
270 BE1=DE*((8*WX/W)-(5*RC/B)-(RC^2*W)/(24*B^3))
280 HV=(2*DE/(3*W^2))*(12*B^2-RC*W)
290 ERC=((RC-RC1)/RC1)*100
300 EWX=((WX-WX1)/WX1)*100
310 PRINT G,H
320 PRINT N,RC,ERC
330 PRINT WX,EWX
340 PRINT  BE1,HV
350 NEXT N
360 GOTO  100
370 END
```

TABLE 5.5

CALCULATED VALUES OF POTENTIAL PARAMETERS IN THE PRESENT WORK FOR ALKALI HALIDE,HYDRIDE AND HEAVY METAL HALIDE MOLECULES

Molecule	GEP (n=0, m=1)		GLP (n=1)	
	$P_1(10^{-9})$	$Q_1(10^{-9})$	$G(10^{-12})$	$H(10^{-32})$
		ALKALI HALIDE MOLECULES		
LiF	1.12	- 2.54	- 12.81	- 1.34
LiCl	1.94	- 2.85	- 5.43	- 5.74
LiBr	2.22	- 2.95	- 4.54	- 8.19
LiI	2.93	- 3.08	- 3.47	-13.39
NaF	2.77	- 2.58	- 4.87	- 5.23
NaCl	4.51	- 2.86	- 3.01	-13.91
NaBr	5.32	- 2.94	- 2.63	-18.28
NaI	5.37	- 3.15	- 2.36	-25.60
KF	4.40	- 2.67	- 3.40	- 9.75
KCl	8.15	- 2.95	- 2.13	-25.44
KBr	6.09	- 3.21	- 2.15	-30.79
KI	10.67	- 3.21	- 1.68	-45.71
RbF	6.21	- 2 .65	- 2.84	-12.51
RbCl	8.29	- 3.06	- 2.01	-30.60
RbBr	11.90	- 3.07	- 1.70	-40.18
RbI	15.93	- 3.18	- 1.45	-56.57
CsF	7.48	- 2.66	- 2.58	-14.76
CsCl	16.94	- 2.92	- 1.60	-39.51
CsBr	20.12	- 3.01	- 1.44	-50.43
CsI	25.97	- 3.13	- 1.24	-70.38

Contd...124

(Contd....Table 5.5)

Molecule	GEP (n=0, m=1)		GLP (n=1)	
	$P_1(10^{-9})$	$Q_1(10^{-9})$	$G(10^{-12})$	$H(10^{-32})$
ALKALI HYDRIDE MOLECULES				
LiH	0.17	- 4.19	12.11	2.75
NaH	0.21	- 4.41	16.94	2.79
KH	0.25	- 4.73	39.12	1.78
RbH	0.28	- 4.76	262.87	0.29
CsH	0.31	- 4.85	- 62.75	-1.37

Contd....125

(Contd.....Table 5.5)

Molecule	GEP(n=-2, m=0.5)		GEP(n=-2, m=2)		GEP(n=2, m=2)	
	$P_1(10^{-20})$	$Q_1(10^{-6})$	$P_1(10^{-26})$	$Q_1(10^{-17})$	$P_1(10^{+5})$	$Q_1(10^{-17})$
	HEAVY METAL HALIDE MOLECULES					
TlF	1.269	-8.420	5.533	- 8.841	28.513	- 5.997
TlCl	2.492	-8.921	7.370	-12.231	18.721	- 8.377
TlBr	0.414	-10.288	5.153	-15.057	10.813	- 9.932
TlI	9.113	-8.876	10.845	-14.765	16.590	-10.322
InF	1.694	-8.051	5.681	- 7.876	35.457	- 5.377
InCl	3.086	-8.643	7.527	-11.274	21.877	- 7.756
InBr	4.733	-8.706	8.659	-12.406	19.935	- 8.593
InI	9.940	-8.728	10.079	-14.068	18.116	- 9.853
GaF	0.179	-8.732	3.163	- 7.105	31.616	- 4.637
GaCl	0.333	-9.461	4.294	-10.674	18.026	- 7.034
GaBr	0.451	-9.628	4.832	-12.019	15.524	- 7.962
GaI	1.487	-9.388	6.754	-13.527	14.959	- 9.168

TABLE 5.6

CALCULATED α_e (cm^{-1}) VALUES ON DIFFERENT POTENTIALS FOR ALKALI HALIDE MOLECULES

Molecule	Exptl*	GEP n=0, m=1	GLP n=1	Harrrison Potential	Chaturvedi et al	Shankar et al	Gupta et al	Hasan et al	Sangachin et al
1	2	3	4	5	6	7	8	9	10
LiF	0.0203	0.01856	0.03013	0.01095	0.01839	0.01616	0.01901	0.018066	0.02048
LiCl	0.00801	0.008854	0.01491	0.00798	0.00841	0.00793	0.00841	0.00645	0.00816
LiBr	0.0056	0.006534	0.01108	0.00571	0.00583	0.00582	0.00606	0.00571	0.00586
LiI	0.0041	0.005090	0.008688	0.00429	0.00421	0.00436	0.00454	0.00333	0.00425
NaF	0.0046	**0.**004337	0.00738	0.00438	0.00473	0.00403	0.00435	0.00438	0.00469
NaCl	0.0016	0.001800	0.003122	0.00161	0.00161	0.00151	0.00171	0.00154	0.00169
NaBr	0.00094	0.001089	0.001899	0.000899	0.00098	0.000882	0.00101	0.000915	0.000981
NaI	0.00065	0.0007850	0.001371	0.000660	0.00067	0.00069	0.000724	0.000728	0.000683
KF	0.0023	0.002488	0.004304	0.00221	0.00221	0.00202	0.00245	0.00289	0.00245
KCl	0.00079	0.0009149	0.001611	0.00077	0.00077	0.000767	0.000873	0.000787	0.000812
KBr	0.00042	0.0004642	0.0008135	0.000404	0.0004	0.000402	0.000448	0.000483	0.000435
KI	0.00027	0.0003273	0.0005804	0.000267	0.00026	0.000274	0.000306	0.000414	0.000281
RbF	0.0015	0.001714	0.002991	0.00149	0.00145	0.0013	0.00168	0.00126	0.00156

Contd...127

(Contd....Table 5.6)

1	2	3	4	5	6	7	8	9	10
RbCl	0.00045	0.0005282	0.0009311	0.00045	0.00048	0.000436	0.000516	0.000510	0.000484
RbBr	0.00019	0.0002248	0.0003982	0.000184	0.00019	0.000182	0.000211	0.000207	0.000201
RbI	0.00011	0.0001361	0.0002431	0.000108	0.00012	0.000111	0.000128	0.000168	0.000117
CsF	0.0012	0.001450	0.002542	0.00109	0.00117	0.000956	0.00142	0.000941	0.00122
CsCl	0.00034	0.0004230	0.0007549	0.00033	0.00034	0.000322	0.000393	0.000457	0.000368
CsBr	0.00012	0.0001560	0.0002794	0.000122	0.00013	0.000120	0.000142	0.000215	0.000139
CsI	0.000068	0.0000876	0.0001774	0.000065	0.000071	0.000068	0.0000796	0.0000818	0.000075
Average % errors		± 16.65	± 101.56	± 2.96	±4.03	±6.48	± 11.02	±20.75	± 5.27

* Ref.(2)

TABLE 5.7

CALCULATED $\alpha_e(cm^{-1})$ VALUES ON DIFFERENT POTENTIALS FOR

A) ALKALI HYDRIDE MOLECULES

Molecule	Exptl *	GEP n=0, m=1	GLP n=1	Sangachin et al	Ali et al	Hellmann et al
LiH	0.2132	0.1367	0.157	0.24	0.2333	0.2023
NaH	0.1353	0.0984	0.133	0.14	0.1297	0.1237
KH	0.081	0.0712	0.104	0.07	0.0826	0.00826
RbH	0.072	0.0640	0.0566	0.08	0.0715	0.0726
CsH	0.0579	0.0578	0.0830	0.06	0.0630	0.0646
Average % errors		±17.27	±28.41	±8.87	±4.99	±5.61

B) HEAVY METAL HALIDE MOLECULES

Molecule	Exptl *	GEP		
		n= -2, m=0.5	n=-2, m=2	n=2, m=2
TlF	15.0385	22.34	18.96	16.53
TlCl	3.979	6.455	5.50	4.84
TlBr	1.275	2.123	1.82	1.62
TlI	0.663	1.138	0.979	0.877
InF	18.797	27.969	23.81	20.89
InCl	5.178	8.312	7.10	6.27
InBr	1.862	3.077	2.64	2.32

Contd...129

(Contd....Table 5.7)

Molecule	Exptl *	GEP		
		n=-2, m=0.5	n=-2, m=2	n=2, m=2
InI	1.040	1.784	1.53	1.37
GaF	28.642	40.603	33.86	28.39
GaCl	7.936	12.28	10.28	8.72
GaBr	3.207	4.564	4.32	3.68
GaI	1.390	3.195	2.71	2.36
Averge % errors		±63.65	±41.0	±27.5

* Ref.(2)

TABLE 5.8

CALCULATED $\omega_e x_e (cm^{-1})$ VALUES ON DIFFERENT POTENTIALS FOR ALKALI HALIDE MOLECULES

Molecule	Exptl *	GEP n=0, m=1	GLP n=1	Harrison Pot.	Chaturvedi et al	Shankar et al	Gupta et al	Hasan et al	Sangachin et al
1	2	3	4	5	6	7	8	9	10
LiF	7.929	8.025	11.15	7.99	7.96	7.95	7.967	6.652	8.21
LiCl	4.5	5.379	7.55	4.41	4.70	5.22	4.893	2.987	4.89
LiBr	3.5	4.471	6.28	4.10	3.69	4.83	3.978	3.339	3.97
LiI	3.3	3.931	5.532	3.51	3.51	3.75	3.353	1.704	3.54
NaF	3.4	3.612	5.08	3.75	3.68	3.61	3.526	3.729	3.98
NaCl	2.0	2.135	3.011	1.91	1.62	2.04	1.931	1.556	1.93
NaBr	1.5	1.557	2.196	1.26	1.31	1.49	1.354	1.241	1.35
NaI	1.0	1.237	1.744	1.10	1.09	1.21	1.091	1.037	1.09
KF	2.4	2.670	3.766	1.36	2.28	2.23	2.535	3.177	2.54
KCl	1.3	1.471	2.073	1.20	2.29	1.27	1.331	1.089	1.33
KBr	0.8	0.884	1.246	0.80	0.81	0.85	0.855	0.967	0.8
KI	0.574	0.755	1.063	0.62	0.62	0.67	0.675	1.078	0.66

Contd...131

(Contd.....Table 5.8)

1	2	3	4	5	6	7	8	9	10
RbF	1.9	2.196	3.097	1.72	1.85	1.66	2.073	1.192	2.07
RbCl	0.92	1.015	1.430	0.85	0.91	0.88	0.983	0.948	0.98
RbBr	0.463	0.606	0.853	0.49	0.49	0.51	0.546	0.506	0.55
RbI	0.335	0.444	0.623	0.35	0.37	0.37	0.398	0.600	0.38
CsF	1.61	2.016	2.842	1.59	1.64	1.56	1.938	0.887	1.93
CsCl	0.731	0.968	1.360	0.73	0.76	0.71	0.849	1.103	0.84
CsBr	0.374	0.506	0.709	0.37	0.39	0.38	0.434	0.868	0.43
CsI	0.2505	0.351	0.482	0.26	0.28	0.27	0.307	0.441	0.31
Average % erros		$\pm$19.87	$\pm$68.38	$\pm$5.49	$\pm$10.03	$\pm$8.64	$\pm$10.53	$\pm$39.22	$\pm$10.74

* Ref.(2)

TABLE 5.9

CALCULATED $\omega_e x_e (cm^{-1})$ VALUES ON DIFFERENT POTENTIALS FOR

A) ALKALI HYDRIDE MOLECULES

Molecule	Exptl	GEP n=0, m=1	GLP n=1	Sangachin et al	Ali et al	Hellmann Pot.	VS Pot.
LiH	23.20	18.39	23.57	23.8	22.52	21.13	25.58
NaH	19.72	15.1880	19.80	20.9	16.80	16.81	19.04
KH	14.3	12.832	17.08	15.5	13.48	13.85	15.12
RbH	14.21	12.367	16.62	15.4	12.72	13.23	14.26
CsH	12.9	11.848	16.04	13.4	12.12	12.60	13.46
Average % errors		+15.02	±12.57	±5.84	±7.07	±7.20	±4.82

Contd...133

(Contd....Table 5.9)

B) HEAVY METAL HALIDE MOLECULES

Molecule	Exptl	GEP	
		n=-1, m=0.5	n=-2, m=0.5
TlF	2.3	1.355	2.27
TlCl	0.81	0.557	0.944
TlBr	0.39	0.259	0.447
TlI	-	0.166	0.290
InF	2.64	1.598	2.698
InCl	1.01	0.667	1.135
InBr	0.65	0.986	0.577
InI	0.4	0.226	0.394
GaF	3.2	2.133	3.442
GaCl	1.2	0.895	1.456
GaBr	0.81	0.543	0.84
GaI	0.5	0.346	0.578
Average % errors		±35.63	±9.93

TABLE 5.10

CALCULATED VALUES OF β_e AND H_v ON DIFFERENT POTENTIALS FOR ALKALI HALIDE MOLECULES

Molecule	$\beta_e(10^{-8})$				$H_v(10^{-11})$		
	Exptl *	GEP n=0, m=1	GLP n=1	Hasan † et al	GEP n=0. m=1	GLP n=1	Hasan † et al
1	2	3	4	5	6	7	8
LiF	- 12.44	- 4.458	- 33.07	- 14.21	+ 4.557	- 5.399	+ 7.206
LiCl	- 1.9013	- 0.594	- 9.708	- 4.16	+ 0.161	- 1.978	+ 0.766
LiBr	-	- 0.248	- 5.876	- 1.91	+ 0.0102	- 1.152	+ 0.205
LiI	-	- 0.069	- 3.934	- 1.79	- 0.695	- 0.766	+ 0.281
NaF	- 0.070	- 0.088	- 2.686	+ 0.12	- 0.0092	- 0.488	- 0.227
NaCl	- 0.0834	+ 0.0195	- 0.627	- 0.15	- 0.137	- 0.0888	- 0.0000669
NaBr	- 0.0497	+ 0.0142	- 0.275	- 0.00794	- 0.00619	- 0.0339	- 0.000390
NaI	- 0.0047	+ 0.00958	- 0.160	- 0.0217	- 0.00351	- 0.0182	- 0.00209
KF	- 0.0233	+ 0.0217	- 1.040	- 0.303	- 0.0219	- 0.159	- 0.0497
KCl	- 0.00834	+ 0.0188	- 0.194	- 0.0349	- 0.00537	- 0.0233	- 0.00280

Contd.....135

(Contd.....Table 5.10)

1	2	3	4	5	6	7	8
KBr	- 0.0002	+ 0.00477	- 0.0635	+ 11.50	- 0.00129	- 0.00617	- 0.00168
KI	+ 0.00043	+ 0.00475	- 0.0355	+ 0.0307	- 0.000824	- 0.00317	- 0.00183
RbF	- 0.0366	+ 0.0306	- 0.539	- 0.197	- 0.0141	- 0.0749	+ 0.00511
RbCl	+ 0.00233	+ 0.00768	- 0.0750	- 0.00019	- 0.00179	- 0.00762	- 0.00168
RbBr	+ 0.0005	+ 0.00265	- 0.0180	- 0.00065	- 0.000377	- 0.0014	- 0.000285
RbI	+ 0.000527	+ 0.00136	- 0.00789	+ 0.00654	- 0.000152	- 0.000532	- 0.000709
CsF	+ 0.0300	+ 0.0305	- 0.395	- 0.157	- 0.0112	- 0.0528	+ 0.00350
CsCl	+ 0.005	+ 0.00848	- 0.0494	+ 0.0174	- 0.00134	- 0.00471	- 0.00175
CsBr	+ 0.00002	+ 0.00181	- 0.00939	+ 0.0135	- 0.000193	- 0.000654	- 0.000474
CsI	+ 0.00025	+ 0.00080	- 0.00261	+ 0.00243	- 0.000065	- 0.00019	- 0.0000686

* Ref.(2)

† Ref.(5)

TABLE 5.11

CALCULATED VALUES OF β_e AND H_v ON DIFFERENT POTENTIALS FOR ALKALI HYDRIDE AND HEAVY METAL HALIDE MOLECULES

A) ALKALI HYDRIDE MOLECULES

Molecule	$B_e(10^{-8})$					$H_v(10^{-11})$	
	AH*	Hellmann	VS	GEP n=0, m=1	GLP n=1	GEP n=0, m=1	GLP n=1
LiH	- 3046	- 1802	- 3408	+ 958.87	+ 2258	14108	13271
NaH	- 882	- 652	- 1058	- 26.493	- 257.6	2784.4	2133
KH	- 328	- 279	- 413	- 77.40	359.5	720.39	390.3
RbH	- 224	- 202	- 290	76.18	361.85	462.13	185.1
CsH	- 163	- 152	+ 215	- 75.43	377.92	346.78	89.62

* Ref.(11)

Contd....137

(Contd....Table 5.11)

B) HEAVY METAL HALIDE MOLECULES

Molecule	$\beta_e(10^{-9})$ On GEP n= -2, m=0.5	$H_v(10^{-13})$ On GEP n=-2, m=0.5
TlF	- 4.0718	- 2.671
TlCl	- 0.5676	- 0.2575
TlBr	- 0.0926	- 0.0289
TlI	- 0.00343	- 0.00877
InF	- 5.710	- 0.394
InCl	- 0.0844	- 0.4086
InBr	- 0.167	- 0.0587
InI	- 0.0841	- 0.0247
GaF	-10.703	- 8.397
GaCl	- 1.604	- 0.9034
GaBr	- 0.1984	- 0.1223
GaI	- 0.184	- 0.0676

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