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REDUCED POTENTIAL CURVES FOR THE DIATOMIC HGCL, HGBR AND HGI MOLECULES

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ABSTRACT

The reduced potential curves (RPC) of the ground electronic states of HgCl, HgBr and HgI are constructed. These curves obey the rules of RPC scheme and also show similarity to respective RKR curves.

KEYWORDS: Potential energy curves, Reduced potential curves, diatomic molecules.

INTRODUCTION

Diatomic mercury halides HgX (X = Cl, Br and I) are used in laser. The experiment on photodissociation^[1] of HgX₂ vapour and electronbeam excitation^[2] of a mixture of Hg, Ar and halogen-bearing

hydrocarbons have shown that strong lasing action in the bound-state transitions B ${}^{2}\Sigma^{+}$ - X ${}^{2}\Sigma^{+}$ may be used in high-power lasers. Recently dissociation energies of HgCl, HgBr and HgI from potential energy curves reported by Bhartiya et al.^[3]

The potential energy curves are important in the studies of dissociation energies, Franck-Condon factors, chemical physics, laser physics etc. The potential functions can be drawn using RKR^[4-6] method, which is based on an experimental data. Recently Jenc and Brandt^[7] have developed a method of calculating potential energy curves, which is known as RPC. In the present study this method has been employed to construct the RPC's for the ground states of HgCl, HgBr and HgI molecules.

1. The reduced potential energy curves

The method suggested by Jenc and Brandt^[7] uses the RKR data. The reduced potential energy curves are drawn between two parameters namely ρ on X axis and u +1 on Y axis.

 $u = U/D_e$ where $U = \sum C_i (v + \frac{1}{2})^i$... (1)

 C_i are vibrational constants like $C_1 = \omega_{e_i}$, $C_2 = -\omega_e x_e$, $C_3 = \omega_e y_e$ etc. De is dissociation energy.

$$\rho = \frac{r - \left[1 - exp\left(-r / \rho_{ij}\right)\right]\rho_{ij}}{r_e - \left[1 - exp\left(-r / \rho_{ij}\right)\right]\rho_{ij}} \qquad \dots (2)$$

Where r_e is equillibrium inter-nuclear separation and ρ_{ij} can be calculated as follows,

$$\rho_{ij} = \frac{r_e - \left[\left(3.96 \right) D_e / \kappa_e \right]^{1/2}}{1 - exp \left(-r_e / \rho_{ij} \right)} \qquad \dots (3)$$

Where κ_e is a force constant.

The reduced quantities fulfill following conditions.

i)
$$\rho \ge 0$$

ii) $\rho = 0$ for $r = 0$
iii) $\rho = 1$ for $r = re$
iv) $\rho \rightarrow \infty$ for $r = \rightarrow \infty$
v) $u \le 0$ for $U \le 0$
vi) $u = 0$ for $U = 0$
vii) $u \rightarrow \infty$ for $U \rightarrow \infty$
viii) $u = -1$ for $U = -De$

2. Properties of RPC

- 1) The RPC's of different molecules never intersect.
- 2) The RPC's of diatomic molecules slightly differing in both atomic numbers coincide.
- 3) While keeping one atomic number constant a considerable change in the values of other effect than a relatively small change in the values of both atomic numbers. This fact is clear in the RPC's of heavy hydrides.
- 4) In general the shape of RPC turns slowly to the right around the minimum while becoming broader.
- 5) Rare gas molecules does not follow the rule number 2, 3 and 4. The RPC's of rare gas molecules coincide approximately to each other and form a right hand boundary of the admissible RPC region.
- 6) All RPC's including excited state lie in RPC region.
- The approximate coincidence mentioned in rule 2 and 5 is very accurate in repulsive limb.

It was found that deviations from the above rule in the RPC's of the diatomic molecules might appear suggesting the possible existence of perturbation in the state or because of erroneous extrapolation of the RKR potential.

3. Molecular Constants

The latest spectroscopic constants are used to construct RKR and RPC curves. The ρ_{ij} are calculated using expression (3). For the calculation of RKR curves, the vibrational as well as rotational constants are also needed which are listed in Table 1.

Constants	HgCl	HgBr	HgI
μ	29.807955	57.771192	77.935292
ω _e	298.973	188.249	126.071
ω _e X _e	2.15130	1.0359	1.2704
ω _e y _e	0.010112	-0.0015068	0.0159
ω _e Z _e	-0.00050562	-0.00024809	-
α _e	0.0007239	0.0003274	0.00018024
Be	0.09674	0.04345	0.02747
De	8350	5500	2750
r _e	2.4180	2.5916	2.80629
$ ho_{ij}$	3.668477	4.696022	6.224255
References	[3,8, 9]	[3,8,10]	[3, 8,10]

Table 1: Molecular constants of ground states of HgCl, HgBr and HgI molecules.

Note: All constants are in cm⁻¹ except r_e and ρ_{ij} , which are in Å and μ , is in amu.

4. Verification of RPC

The individual RKR and RPC of HgCl, HgBr and HgI are shown in Figs 1 (a,b,c and a', b', c') respectively. The RKR and RPCs of respective molecules have similarity. Secondly the combined RPCs of HgCl, HgBr and HgI which are shown in Fig. 2, the RPC of lighter molecule HgCl is in side where as the RPC of heavier molecule HgI is outside which is as expected.

The applications of RPC could be as follows.

- i) It can detect the errors in the construction of RKR.
- ii) It can be used to detect errors in molecular constants.
- iii) It can detect the errors in analysis of a spectrum due to perturbations or otherwise.

It is shown that the behavior of this group of chemically related molecules is fully in accord with the overall regularities observed for many other groups of diatomic molecules.^[11]



Fig. 1. The RKR of HgCl, HgBr and HgI molecules are shown in (a, b, and c) where as RPC are shown in (a', b', land c') respectively.



Fig 2: Combined RPC of ground states of HgCl, HgBr and HgI molecules.

6. CONCLUSION

The RPC scheme is verified for the ground states (X $^{2}\Sigma$) of HgCl, HgBr and HgI molecules. All the RPC's have common minima at (1,1) co-ordinate. Thus the rules are obeyed by RPCs. The RPC scheme seems to lead to a picture that might be called "a periodic system of diatomic molecules."

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