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Verification of RPC Scheme with the help of the RPC's of some diatomic molecules

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ABSTRACT

Rules of RPC scheme are verified by drawing the reduced potential curves (RPC) of some diatomic molecules such as H_2, N_2, O_2, Al_2, Si_2, I_2, Nb_2, AlCl, BCl and MgS. RPC's of these molecules obey the rules of this scheme. Eventually RPC technique serves as a check on the experimental data of the diatomic molecules.

Introduction:

Reduced potential curve of a diatomic molecule is the graph of potential energy in reduced form versus inter-nuclear distance in reduced form. With the help of RPC's Jenc predicted the inaccuracies in 1) rotational analysis of Cl_2 [1] and 2) in the calculation of the RKR data of $a^3\Sigma^u_+$ state of Na_2 molecule [2]. Correct constants were derived later and these anomalies disappeared [3-5]. Eventually the RPC technique serves as a check on the experimental data.

With the help of RPC, dissociation energy of the ground state of KRb molecule was estimated by Jenc [6] which was to be in surprising agreement with the values reported in the literature [7]. Predictions of ground state potential of Te_2 molecule [8] on the basis of RPC method was also found.

Looking at the thrust in the RPC method, to check the accuracy in the molecular constants, determined experimentally, it was found necessary to apply it to the molecules

excluding the molecules verified by Jenc and verify the rules of RPC scheme.

Practical applications of RPC method:

1. Construction of reliable interatomic potential energy curve of the diatomic molecule for a sufficiently large range of inter-atomic distances.
2. Estimation of spectroscopic constants such as equilibrium inter-nuclear distance r_e, dissociation energy D_e, and force constant K_e.
3. Classification of empirical potential functions to approximate the inter-nuclear potentials.
4. Detection of errors in the experimentally determined values of spectroscopic constants and in the analysis of spectra.
5. Detection of perturbations.

Formulae used in RPC method:

The reduced quantities in RPC method are defined as follows.

$$u = U/D_e$$

$$\rho = \{ r-[1-\exp(-r/\rho_{ij})] \rho_{ij} \} / \{ r_e-[1-\exp(-r/\rho_{ij})] \rho_{ij} \} \quad \text{----------(2)}$$

where

$$\rho_{ij} = [r_e - (kD_e/k_e)^{1/2}] / [1-\exp(-r_e/\rho_{ij})] \quad \text{----------(3)}$$

$$k = 3.96$$

$$K_e = 4 \pi^2 c^2 \mu \omega_e^2 \quad \text{----------(4)}$$

All the symbols have their usual meaning.

For $0 \leq \rho_{ij} \leq r_e$

$\rho \geq 0$

$\rho = 0$ for $r = 0$

$\rho = 1$ for $r = r_e$

$\rho \rightarrow \infty$ for $r \rightarrow \infty$

$u \neq 0$ for $U \neq 0$

$u = 0$ for $U = 0$

$u \rightarrow \infty$ for $U \rightarrow \infty$

$u = -1$ for $U = -D_e$

The reduced coordinates of the minimum of the potential curves are $\rho = 1$ and $u = -1$. In figures ρ is always plotted against $(u+1)$ so that all the RPC now have (1,0) minimum.

Rules of RPC:

1. By definition the RPC's of different have a common (1,0) minimum
2. RPC's of different molecules never intersect.
3. The RPC's of different diatomic molecule with only slightly differing values of two atomic numbers, approximately coincide. The difference seem to decrease with increasing value of atomic numbers
4. The difference in the RPC's of molecules , the atomic numbers of which differ by more units, are more pronounced for light molecules and diminish rapidly with increase in atomic weights of constituent atoms.
5. A large change in only one of the atomic number of an atom constituting a diatomic molecule has considerably less pronounced effect than a much smaller change in both the atomic numbers.
6. In general the shape of the RPC turns slowly to the right around the minimum while becoming broader.
7. Rare gas molecules do not follow rule no 3, 5 and 6. The RPC's of rare gas molecules coincide approximately to each other and form the right hand boundary of the RPC region. The left hand boundary of this region is formed by the RPC of hydrogen molecule.
8. All RPC including excited states lie in the RPC region.
9. The approximate coincidence mentioned in rule 3 and 7 is very accurate in repulsive limb.

Verification of RPC method

Reduced potential curves of H_2, N_2, O_2, Al_2, Si_2, I_2, Nb_2, AlCl, BCl and MgS molecules are drawn using equations 1 to 4 and are presented in figures 1 to 11. The values of r_e, D_e, K_e used, are presented in table 1 along with the values of ?ij calculated. All the molecular parameters are taken from Huber [9].

In the figures presented RPC's of H_2, I_2 and N_2 are drawn. With these RPC's ,

the RPC's of other molecules are studied. Figure 1 shows the RPC's of H_2, N_2, O_2, Al_2, Si_2, and I_2. Figure 2 and 3 show the enlarged view of the left repulsive limb and the right attractive limb of the curves shown in figure 1. From these figures it can be seen that all the RPC's have common (1,0) minimum satisfying rule 1 of the RPC scheme. Further it is also observed that no RPC cross each other, satisfying rule 2.

To verify rule 3, molecules N2, O_2, Al_2 and Si_2 are selected. The difference in the atomic numbers of N_2 and O_2 and so also Al_2 and Si_2 is 1. N_2 and O_2 are lighter molecules as compared to Al_2 and Si_2 hence according to rule 3, RPC's of Al_2 and Si_2 should be more closer than that of N_2 and O_2. This is clearly revealed in figure 3. Figure 2, according to rule 9, shows coincidence of the RPC's of the molecules under study is very accurate.

To check rule 4, molecules H_2, Al_2, Cu_2 and Nb_2 are selected. The difference in their atomic numbers i.e. H_2 and Al_2 & Cu_2 and Nb_2 is 12. RPC's of these molecules are presented in figure 4. Figure 5 shows that repulsive limbs of all these molecules almost coincide. Figure 5 shows that the difference in the RPC's of lighter molecules H_2 and Al_2 is large as compared to the RPC's of heavier molecules Cu_2 and Nb_2. This satisfies rule 4 of the RPC scheme.

To check rule 5, molecules AlCl, BCl and MgS are selected. The atomic numbers of Al, B, Cl, Mg and S are 13, 5, 17, 12 and 16 respectively. In the pair of molecules AlCl and BCl, $Z_2^{Cl} = 17$ is constant, while $Z_1^{Al} - Z_1^{B} = 8$. In the pair of molecules AlCl and MgS, $Z_1^{AlCl} - Z_1^{MgS} = Z_2^{AlCl} - Z_2^{MgS} = 1$. According to rule 5 of the RPC scheme, RPC's of AlCl and BCl should lie closer than the RPC's of AlCl and MgS. This can be clearly seen from figures 6, 7 and 8. Confirming rule 5.

In figure 9 RPC's of H_2, N_2, O_2, Nb_2 and I_2 are drawn with the enlarged views of attractive and repulsive limbs in figure 10 and 11 respectively. RPC of H_2 forms the extreme left boundary and that of I_2 forms the extreme right boundary. RPC's of N_2, O_2 and Nb_2 lie in between these two. All the RPC's are arranged in the increasing order of the atomic numbers of the molecule. With increasing atomic number, RPC's turn to right while becoming broader. This rule 6 is found satisfied in almost every figure. Rule 7 and 8 too are found satisfied with the exception of RPC's of rare gas molecules and of excited

states.

Conclusion:

Rules of the RPC scheme are found to hold good as far as the RPC's of ground states of diatomic molecules are concerned. This method can be effectively used to check the accuracy of the molecular constants and / or the RKR data derived from these constants.

Acknowledgements:

Author thanks Dr. S H Behere, Dept. of Physics, Dr. B.A.M.U. Aurangabad and the college authorities for the encouragement.

Table 1 : Molecular parameters and ?ij calculated for different molecules.

Figure 1 : Reduced Potential Energy Curves of H_2, N_2, O_2, Al_2, Si_2, I_2 molecules.

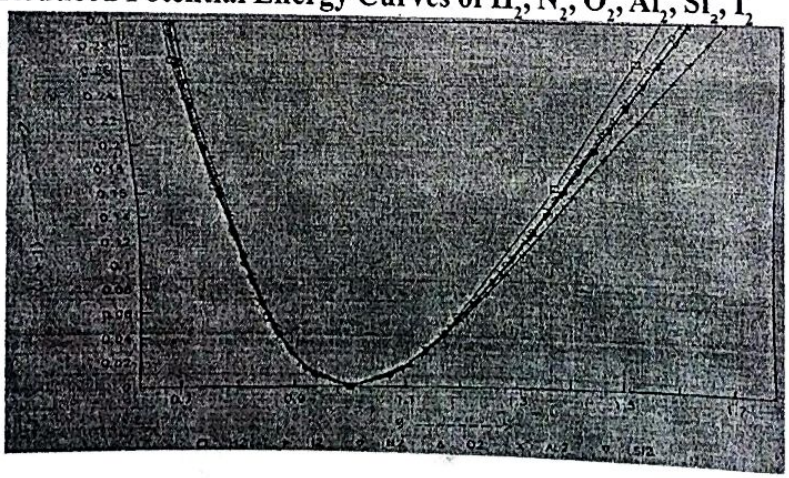


Figure 2 : Enlarged view of the repulsive limbs of Reduced Potential Energy Curves of H_2, N_2, O_2, Al_2, Si_2, I_2 molecules.

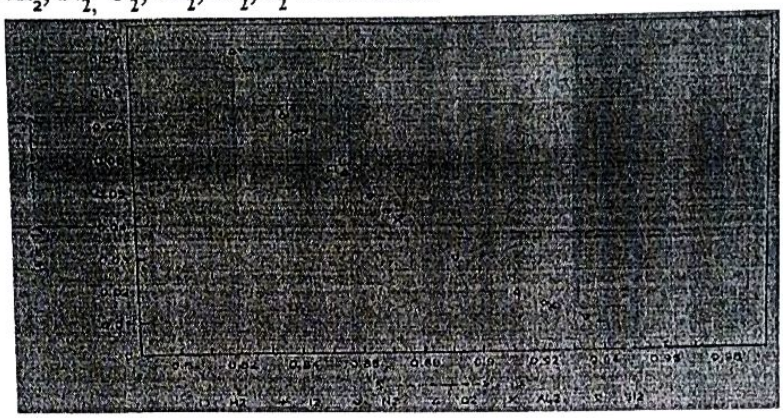


Figure 3 : Enlarged view of the attractive limbs of Reduced Potential Energy Curves of H_2, N_2, O_2, Al_2, Si_2, I_2 molecules.

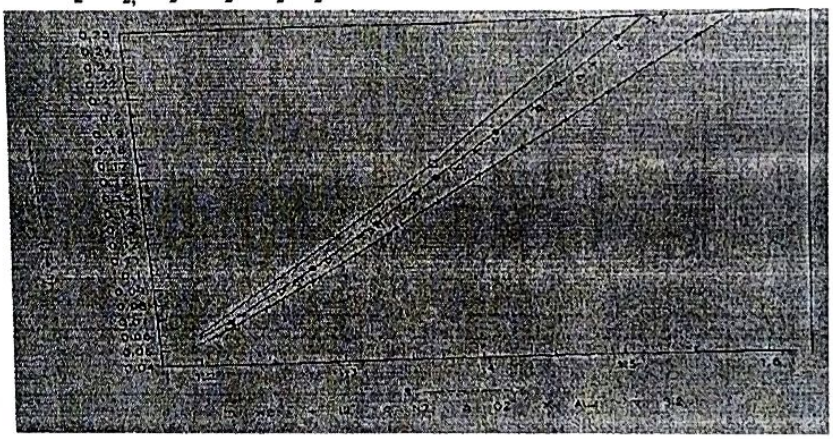


Figure 4 : Reduced Potential Energy Curves of H_2, N_2, Al_2, Cu_2, $Nb_2$and I_2 molecules.

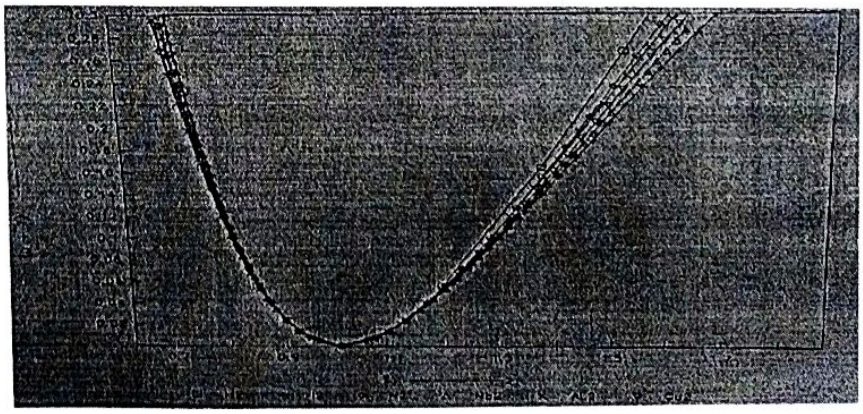


Figure 5 : Enlarged view of the attractive limbs of Reduced Potential Energy Curves of H_2, N_2, Al_2, Cu_2, $Nb_2$and I_2 molecules

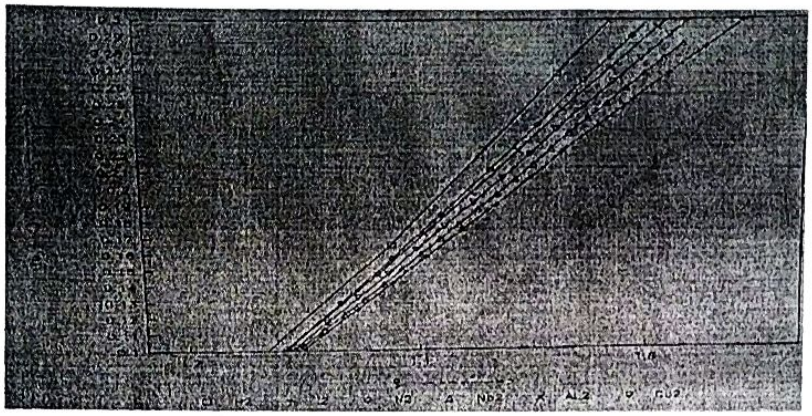


Figure 6 : Reduced Potential Energy Curves of H_2, I_2 ,N_2, AlCl, BCl and MgS molecules.

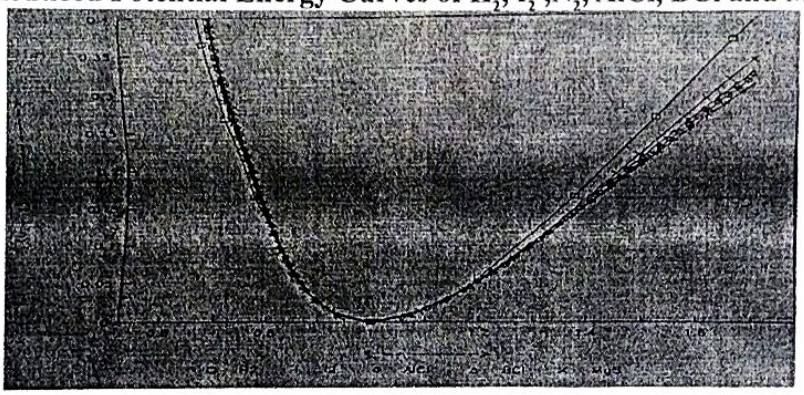


Figure 7 : Enlarged view of the attractive limbs of Reduced Potential Energy Curves of H_2, I_2 , N_2, AlCl, BCl and MgS molecules.

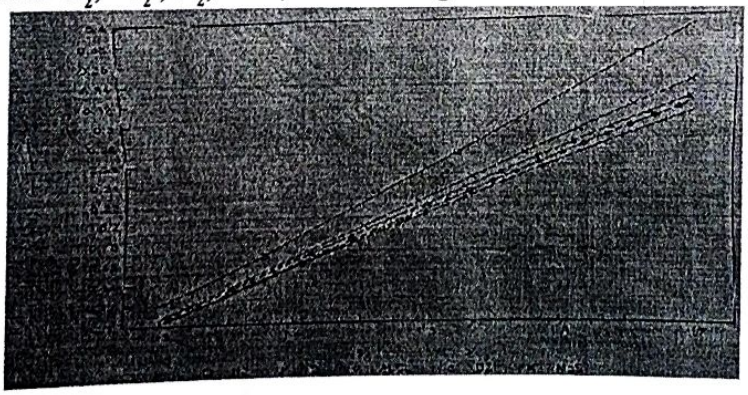


Figure 8 : Enlarged view of the repulsive limbs of Reduced Potential Energy Curves of H_2, I_2, N_2, AlCl, BCl and MgS molecules.

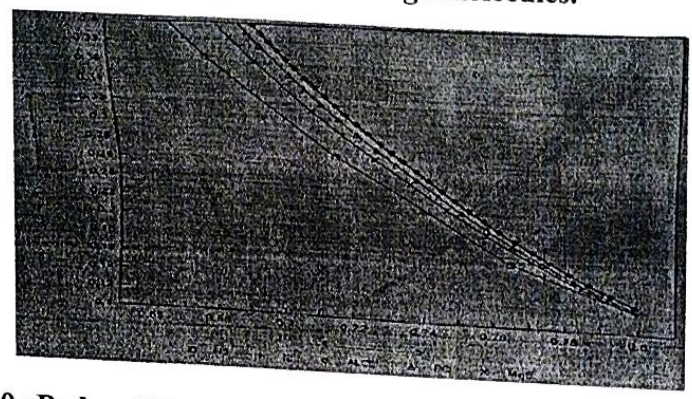


Figure 9 : Reduced Potential Energy Curves of H_2, I_2, N_2, O_2 and Nb_2 molecules.

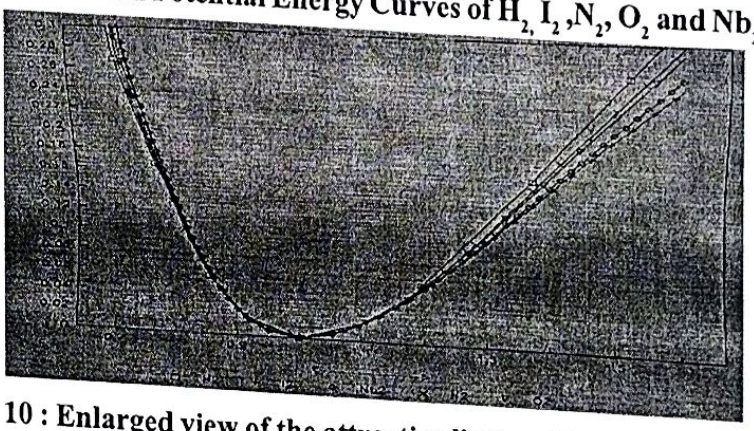


Figure 10 : Enlarged view of the attractive limbs of Reduced Potential Energy Curves of H_2, I_2, N_2, O_2 and Nb_2 molecules.

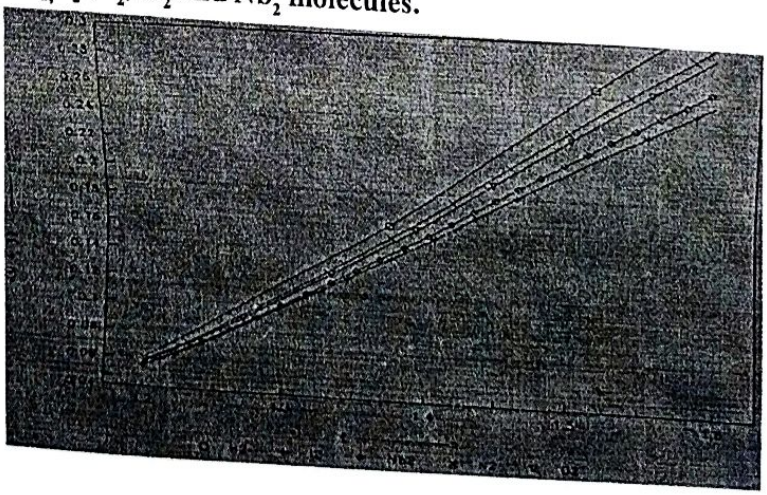
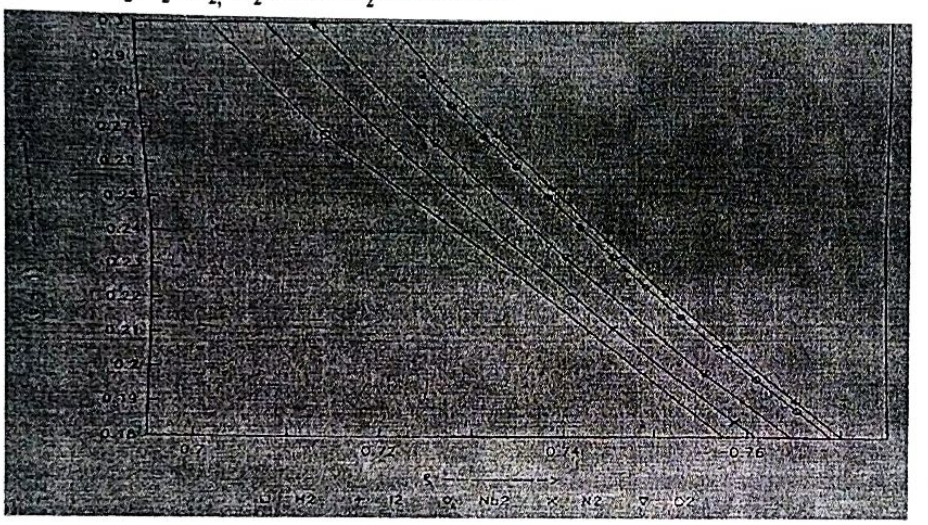


Figure 11 : Enlarged view of the repulsive limbs of Reduced Potential Energy Curves of H_2, I_2 ,N_2, O_2 and Nb_2 molecules.



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