POTENTIAL ENERGY CURVES OF THE GROUND STATES OF BeCl, CP & AIO

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Abstract:

The AIO molecule has astrophysical significance as it is observed in Mira stars. Moreover grenades used in warfare also contain aluminum and when fired the chemiluminescence shows the bands of AIO. The ground state of AIO i.e. X₂Σ⁺.Other molecule chosen viz BeCl and CP are isoelectronic to AIO. The reduced potential energy curves (RPC) of these molecules are computed and it is shown that these curves obey the rules of RPC.

1. Introduction:

In our program to study the AIO molecule through Fourier Transform Spectroscopy[1,2,3], besides the experimental work to study the perturbations, it was also thought to compute the potential energy curves which are of prime importance in the calculation of Dissociation energy, Franck-Condon factors, r-centroids [4] etc. The method suggested by Jenc to draw the RPC [5] is novel in nature as these curves are not plotted as per conventional RKR curves but with different variables but they are similar to RKR curves.

2. The Reduced Potential Energy Curves:

A novel method of constructing the potential energy curves uses the RKR data to construct the potential energy curves. The name reduced comes because the two parameters in which curves is plotted are not same as of other conventional potential functions in which potential energy U is in (cm⁻¹) and internuclear separation r is in A₀ units. On the other hand in the present method, the curve is plotted between two variables u and ρ which are as follows,
\[ u = U/De \quad \text{and} \]

\[
\rho = \frac{r - \left[1 - \exp\left(-\frac{r}{\rho_{ij}}\right)\right]_{ij}}{r_e - \left[1 - \exp\left(-\frac{r_e}{\rho_{ij}}\right)\right]_{ij}} \quad \ldots \quad (1)
\]

Where \( De \) is dissociation energy, \( U \) is a potential energy for any specific \( v \) calculated by the expression.

\[ U = \Sigma C_i (v + \frac{1}{2})^i \quad \ldots \quad (2) \]

\[ C_1 = \omega_e, C_2 = -\omega_{exe}, C_3 = \omega_{eye} \text{ etc.} \quad \ldots \quad (3) \]

The \( r_e \) is equilibrium internuclear separation. The constant \( \rho_{ij} \) can be calculated from the equation.

\[ \rho_{ij} = \frac{r_e - [(3.96) D_e/\kappa_e]^{\frac{1}{2}}}{1 - \exp(-r_e/\rho_{ij})} \quad \ldots \quad (4) \]

In this equation \( \rho_{ij} \) appears to either side of the equation, so a computer programme was made to solve this equation. \( \kappa_e \) is a force constant. The curve is plotted between \( \rho \) and \( u+1 \).

For \( 0 \leq \rho_{ij} < r_e \). The reduced quantities fulfill the following conditions:

i) \( \rho \geq 0 \) \quad \ldots \quad (5)

ii) \( \rho = 0 \text{ for } r = 0 \) \quad \ldots \quad (6)

iii) \( \rho = 1 \text{ for } r = r_e \) \quad \ldots \quad (7)

iv) \( \rho \to \infty \text{ for } r \to \infty \) \quad \ldots \quad (8)

v) \( u \leq 0 \text{ for } U \leq 0 \) \quad \ldots \quad (9)

vi) \( u = 0 \text{ for } U = 0 \) \quad \ldots \quad (10)

vii) \( u \to \infty \text{ for } U \to \infty \) \quad \ldots \quad (11)

viii) \( u = -1 \text{ for } U = -D_e \) \quad \ldots \quad (12)

The usual RKR curves are necessary for these RPC. The ‘r’ values obtained in RKR i.e turning points are introduced in the calculations of RPC. But before that it is worthwhile to understand the theory of RPC. The parameter \( u \) is defined as \( U/De \) where \( U \) is \( G(v) \) for different \( v \). The different \( G(v) \)’s are the vibrational term values of anharmonic oscillator calculated using standard formula[4]

\[ G(v) = \omega_e (v + \frac{1}{2}) \square \omega_{xe} (v + \frac{1}{2})^2 + \cdots \quad \ldots \quad (13) \]
where \( \nu \) is a vibrational quantum number, \( \omega_c \) is the harmonicity constant and \( x_c \) is an anharmonicity constant.

3. Rules Obeyed by RPC’s:

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 do 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.
7) 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.

4. Molecular Constants and RPC:

The latest molecular constants of these molecules known to authors are chosen and they are summarized in Table 1 nearly 80% of the RKR is traced by RKR curves for each molecule. For comparison purpose the RKR potential energy curves and RPC of respective molecules are shown side by side in figures 1 to 3 (a & b) respectively for BeCl, CP and AlO molecules. For the sake of brevity the energies calculated are not shown, only graphical result are shown in these figures.
Table 1: Spectroscopic constants of the ground states of BeCl, CP and AlO molecules

<table>
<thead>
<tr>
<th>Constants/Parameter</th>
<th>BeCl</th>
<th>CP</th>
<th>AlO</th>
</tr>
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<tbody>
<tr>
<td>μ</td>
<td>7.16766</td>
<td>8.65116</td>
<td>10.04191</td>
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<tr>
<td>ω_e</td>
<td>846.7</td>
<td>1239.67</td>
<td>979.524</td>
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<td>ω_e x_e</td>
<td>4.85</td>
<td>6.86</td>
<td>7.036</td>
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<tr>
<td>ω_e y_e</td>
<td>--</td>
<td>--</td>
<td>-0.00106</td>
</tr>
<tr>
<td>α_e</td>
<td>0.0069</td>
<td>0.00597</td>
<td>0.00593</td>
</tr>
<tr>
<td>Be</td>
<td>0.7285</td>
<td>0.7986</td>
<td>0.64165</td>
</tr>
<tr>
<td>De</td>
<td>28249</td>
<td>41913</td>
<td>42992</td>
</tr>
<tr>
<td>re</td>
<td>1.7971</td>
<td>1.5622</td>
<td>1.618</td>
</tr>
<tr>
<td>References</td>
<td>[6]</td>
<td>[6]</td>
<td>[1-3]</td>
</tr>
</tbody>
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Note: All constants are in cm⁻¹ except r_e, which is in Å and μ is in amu

Results and Discussion:

The RPCs, show similarity with RKR; although RKR curves are plotted amongst potential energies versus inter-nuclear separation, where as RPC’s are plotted u+1 versus ρ. The calculation of these quantities are already discussed.

Secondly the rules of RPC are obeyed by these molecules. These curves don’t cross each other. This is clear from fig.4. Thirdly, although BeCl and CP are isoelectronic their reduced masses are different and are in increasing order for BeCl, CP and AlO respectively. The RPC’s also appear in this order.
Acknowledgement:

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Fig. 2.a: RKR Potential energy curves for CP molecule (ground state)

Fig. 2.b: RPC of CP (ground state)

Fig. 3.a: RKR Potential energy curves for AIO molecule (ground state)

Fig. 3.b: RPC of AIO (ground state)
Fig. 4.: RPC of BeCl, CP and AIO (Ground State)
References:


