Dipole Moment

CHRISS WESSEN
WASHINGTON STATE UNIVERSITY

[Chemical structures and diagrams related to dipole moments]
An inductor-capacitor (LC) circuit was used to measure the dipole moment of two polar molecules, Meta and Ortho-dichlorobenzene.

Uses:
- Polar versus non-polar solutions
- Solvent-solute interactions
- Net polarity and local polarity of molecules
• Differences in electron negativity cause electron density to be centered around one side of a molecule
• This causes the molecule to become polarized with a partial negative and partial positive charge
A capacitor can be used to measure this molecular polarization

- At time zero, metal plates have neutral charge
- At time zero+, metal plates are charged to the same voltage as the source
• Polar molecules present in the electric field of a capacitor orient themselves along that field
• The net charge at each plate is reduced by the presence of the partial charge of the polar molecule
• The source supplies more charge to compensate
• Net capacitance under polar solutions is larger than ambient conditions
By electrostatic theory

\[ D = \varepsilon E = \varepsilon_0 E + P \]  

Eq. 1

- D is the electric displacement
- E is the electric field strength
- \( \varepsilon \) is the electric permittivity
- \( \varepsilon_0 \) is the electric permittivity of air
- P is the polarization

Where \( \varepsilon \) is found with the dielectric constant \( \kappa \)

\[ \kappa = \frac{\varepsilon}{\varepsilon_0} \]  

Eq. 2

Substituting Eq. 2 into Eq. 1 yields

\[ \kappa E = E + \frac{1}{\varepsilon_0} P \]  

Eq. 3
F, the local electric field is a function of the electric field and the polarization

\[ F = E + \frac{1}{3 \varepsilon_0} P \]  \hspace{1cm} \text{Eq. 4}

Combining with Eq. 3 yields

\[ F = \left( \frac{\kappa + 2}{\kappa + 1} \right) \frac{1}{3 \varepsilon_0} P \]  \hspace{1cm} \text{Eq. 5}

This can be re-written to give the molar polarization \( P_M \) which has units of volume per mol

\[ P_M = \left( \frac{\kappa - 1}{\kappa + 2} \right) \frac{M}{\rho} \]  \hspace{1cm} \text{Eq. 6}

- \( M \) is the molar mass of solution
- \( \rho \) is the density of solution
Experimental

- Solutions of 1, 2, 3 and 4% Dichlorobenzene were made for both Meta and Ortho configurations, eight solutions total
- Capacitor cell was rinsed with 99.9% pure Benzene solution and were dried with compressed air
- Water jacket was installed with running water at 22.0 degrees C
- Empty cell was assembled, Hi and Lo frequency measurements were made
- 1% O-dichlorobenzene solution was poured into the cell until it was approximately ¾ths full
Experimental cont.

- Cell was reassembled and given 30 seconds for the solution to come to equilibrium temperature
- Three Hi and Lo frequency measurements were recorded
- Cell was emptied and rinsed with benzene solution and dried using compressed air
- Empty cell capacitance was measured again
- Process was repeated for each of the eight solutions
Experimental Setup
### Raw Data

<table>
<thead>
<tr>
<th>Compound</th>
<th>Mass dichlorobenzene</th>
<th>Mass Total</th>
<th>Clean</th>
<th>Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>M-dichlorobenzene</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1%</td>
<td>0.810</td>
<td></td>
<td>0.43091</td>
<td>0.43058</td>
</tr>
<tr>
<td>2%</td>
<td>1.638</td>
<td></td>
<td>0.41692</td>
<td>0.41644</td>
</tr>
<tr>
<td>3%</td>
<td>2.395 44.599</td>
<td></td>
<td>0.42228</td>
<td>0.4221</td>
</tr>
<tr>
<td>4%</td>
<td>3.197 44.747</td>
<td></td>
<td>0.4087</td>
<td>0.40841</td>
</tr>
<tr>
<td><strong>O-dichlorobenzene</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1%</td>
<td>0.800 43.914</td>
<td></td>
<td>0.41859</td>
<td>0.10504</td>
</tr>
<tr>
<td>2%</td>
<td>1.603 44.143</td>
<td></td>
<td>0.41659</td>
<td>0.40315</td>
</tr>
<tr>
<td>1%</td>
<td>0.795 44.033</td>
<td></td>
<td>0.41613</td>
<td>0.40247</td>
</tr>
<tr>
<td>2%</td>
<td>1.604 44.132</td>
<td></td>
<td>0.41613</td>
<td>0.40247</td>
</tr>
<tr>
<td>3%</td>
<td>2.407 44.590</td>
<td></td>
<td>0.41578</td>
<td>0.40233</td>
</tr>
<tr>
<td>4%</td>
<td>3.202 44.915</td>
<td></td>
<td>0.41578</td>
<td>0.40233</td>
</tr>
</tbody>
</table>
Calculations

Frequency was used to measure the dielectric constant

\[ f = \frac{1}{2\pi \sqrt{LC}} \quad \rightarrow \quad C = \frac{1}{4\pi L f^2} \]

\[ C_{Hi} - C_{Lo} = \frac{1}{4\pi L} \left( \frac{1}{f_{Hi}^2} - \frac{1}{f_{Lo}^2} \right) \quad \rightarrow \quad \kappa = \frac{C_{Hi} - C_{Lo}}{(C_{Hi} - C_{Lo})_{air}} \]

Which simplifies to

\[ \kappa = \left( \frac{1}{f_{Hi}^2 - f_{Lo}^2} \right)_{\text{sample}} \left/ \left( \frac{1}{f_{Hi}^2 - f_{Lo}^2} \right)_{air} \right. \]
To find the molar polarization of the solution, Eq. 6 is modified to yield

$$P_M = X_1 P_{1M} + X_2 P_{2M} = \left( \frac{\kappa - 1}{\kappa + 2} \right) \frac{M_1 X_1 + M_2 X_2}{\rho}$$  \hspace{1cm} \text{Eq. 7}$$

- $X_1$ is the mole fraction of benzene
- $P_{1M}$ is the molar polarization of benzene
- $M_1$ is the molar mass of benzene
- $X_2$ is the mole fraction of dichlorobenzene
- $P_{2M}$ is the molar polarization of dichlorobenzene
- $M_2$ is the molar mass of dichlorobenzene
- $\rho$ is the density of solution
To find the molar polarization of the solute in solution, Eq. 7 is modified to

$$P_{2M}^0 = \frac{3M_1a}{(\kappa_1 + 2)^2 \rho_1} + \frac{\kappa_1 - 1}{(\kappa_1 + 2)^2 \rho_1} \left( \frac{M_2 - M_1b}{\rho_1} \right)$$  \hspace{1cm} \text{Eq. 8}$$

Where $\kappa_1$ is the dielectric constant of pure benzene, ‘$a$’ is the slope of the linearlized dielectric constant, and ‘$b$’ is the slope of the linearlized density.
Density and Dielectric Constant Versus Mole Fraction

$y = 3.628x + 2.159$
$R^2 = 0.944$

$y = 5.668x + 2.175$
$R^2 = 0.689$

$y = 0.601x + 0.872$
$R^2 = 0.962$

$y = 0.630x + 0.872$
$R^2 = 0.948$

Meta and ortho respectively. Red denotes ‘a’ values for Eq.8

$y = 3.628x + 2.159$
$R^2 = 0.944$

$y = 5.668x + 2.175$
$R^2 = 0.689$

Meta and ortho respectively. Red denotes ‘b’ values for Eq.8

$y = 0.601x + 0.872$
$R^2 = 0.962$

$y = 0.630x + 0.872$
$R^2 = 0.948$
This molar polarization in solution is the sum of the molar distortion polarization \( (P_{2d}^0) \) and the molar orientation polarization \( (P_{2\mu}^0) \)

\[
P_{2M}^0 = P_{2\mu}^0 - P_{2d}^0
\]

With

\[
P_{2d}^0 = \frac{n_2^2 - 1}{n_2^2 + 2 \rho_2} M_2
\]

Eq. 9

Eq. 10

- \( n_2 \) is the index of refraction for dichlorobenzene
- \( \rho_2 \) is the density of pure dichlorobenzene
Finally, the dipole moment ($\mu$) of the molecule is found with the equation

$$\mu = 12.8(\frac{P_0^0}{T})^{1/2}$$

Eq. 11

Where $T$ is the absolute temperature of the solution. This solution has units of Debye.
Vector Addition

Vector addition of electron negativity

$$\mu_{meta} = 2 \times 1.55 \cos(a)$$
$$a = 60^\circ$$

$$\mu_{ortho} = 2 \times 1.55 \cos(b)$$
$$b = 30^\circ$$
## Results and Error Analysis

### Summary of Results and Relative Error

<table>
<thead>
<tr>
<th>Dichlorobenzene</th>
<th>Vector Addition (D)</th>
<th>Experimental (D)</th>
<th>Literature (D)*</th>
<th>Percent Error Lit. vs. Exp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Meta</td>
<td>1.55</td>
<td>1.54</td>
<td>1.48</td>
<td>3.91</td>
</tr>
<tr>
<td>Ortho</td>
<td>2.68</td>
<td>1.96</td>
<td>2.16</td>
<td>9.04</td>
</tr>
</tbody>
</table>

*literature values were found for liquid dichlorobenzene from Kuzbassk Polytechnical Institute, 1969
Conclusion

- Error Considerations
  - Frequency readings
  - Solvent effects
  - Wet vs. dry air frequencies

- Improvements
  - Overall well designed experiment

- Questions?
Sources
