Dipole Moment

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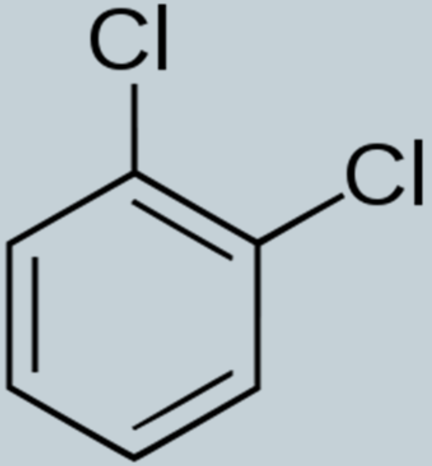
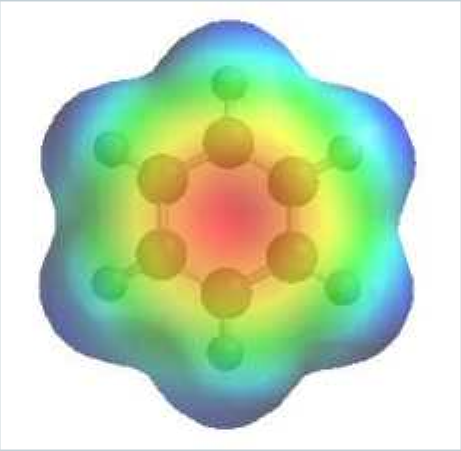
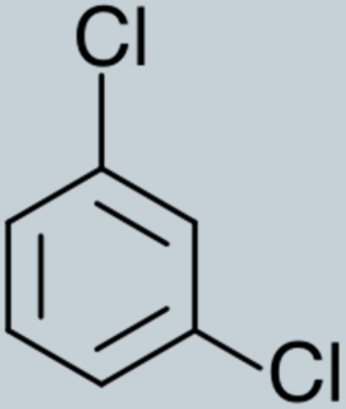






Purpose

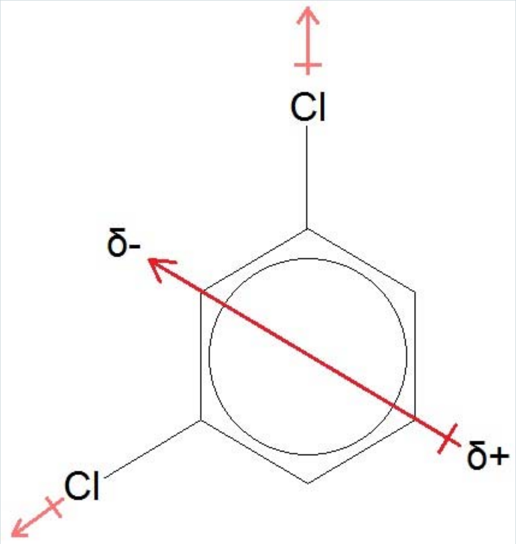
An inductor-capacitor (LC) circuit was used to measure the dipole moment of two polar molecules, Meta and Ortho-dichlorobenzene

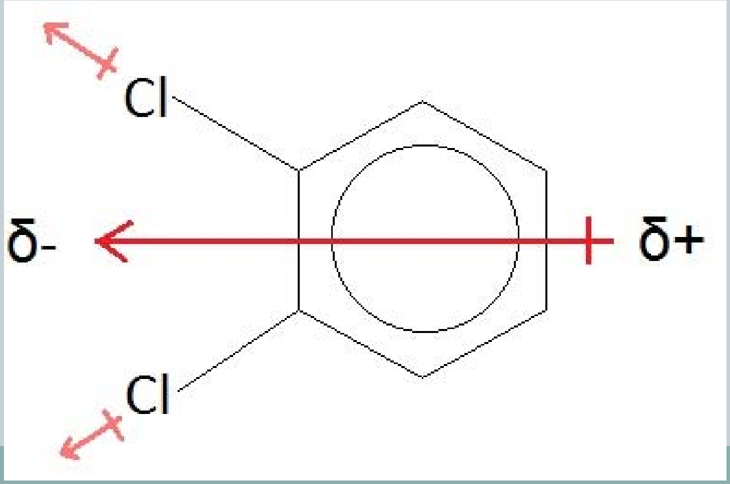
Uses:

- Polar versus non-polar solutions
- Solvent-solute interactions
- Net polarity and local polarity of molecules

Theory

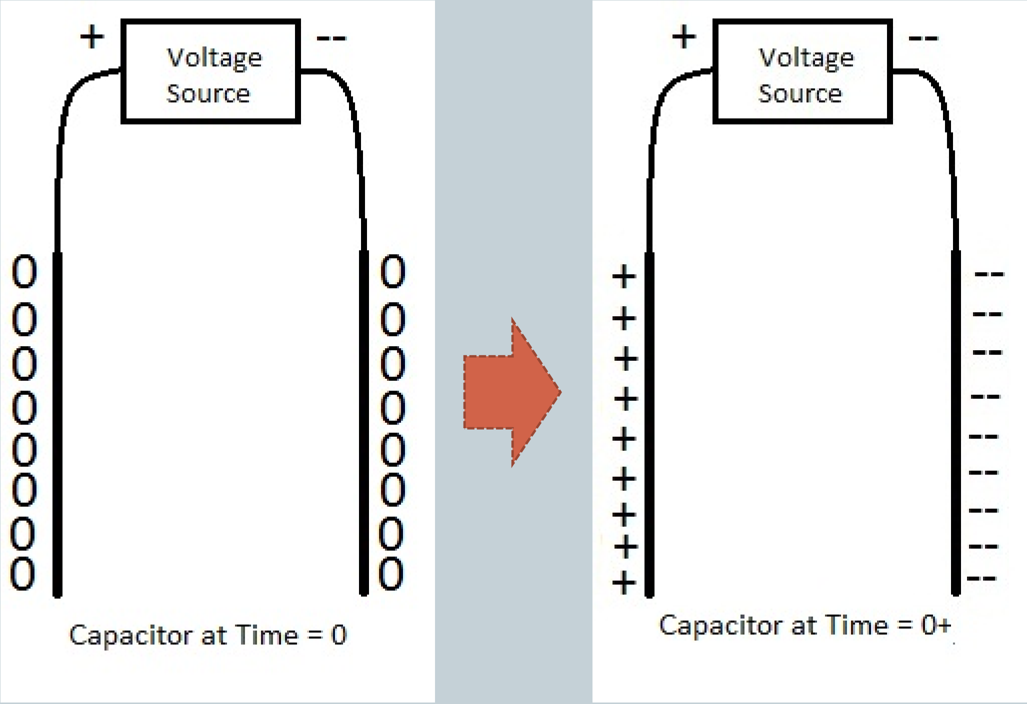
•Differences in electron negativity cause electron density to be centered around one side of a molecule
•This causes the molecule to become polarized with a partial negative and partial positive charge





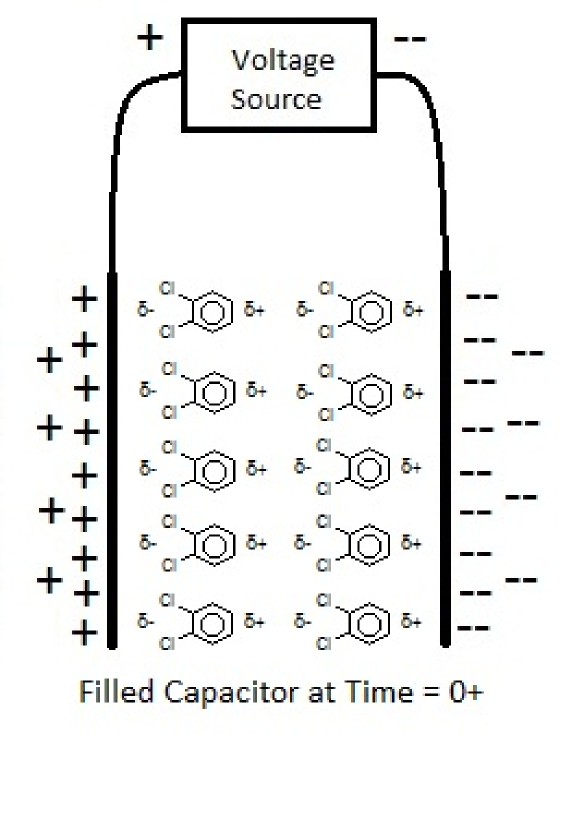
Theory cont.

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

Theory cont.



- 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

Theory cont.

By electrostatic theory

$$D = \varepsilon E = \varepsilon_0 E + P$$ Eq. 1

- D is the electric displacement
- E is the electric field strength
- ε is the electric permittivity
- ε_o is the electric permittivity of air
- P is the polarization

Where ε is found with the dielectric constant κ

$$\kappa = \frac{\varepsilon}{\varepsilon_0}$$ Eq. 2

Substituting Eq. 2 into Eq. 1 yields

$$\kappa E = E + \frac{1}{\varepsilon_0} P$$ Eq. 3

Theory cont.

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

$$F = E + \frac{1}{3\varepsilon_0}P \qquad \text{Eq. 4}$$

Combining with Eq. 3 yields

$$F = \left(\frac{\kappa + 2}{\kappa + 1}\right)\frac{1}{3\varepsilon_0}P \qquad \text{Eq. 5}$$

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

$$P_M = \left(\frac{\kappa - 1}{\kappa + 2}\right)\frac{M}{\rho} \qquad \text{Eq. 6}$$

- M is the molar mass of solution
- ρ is the density of solution

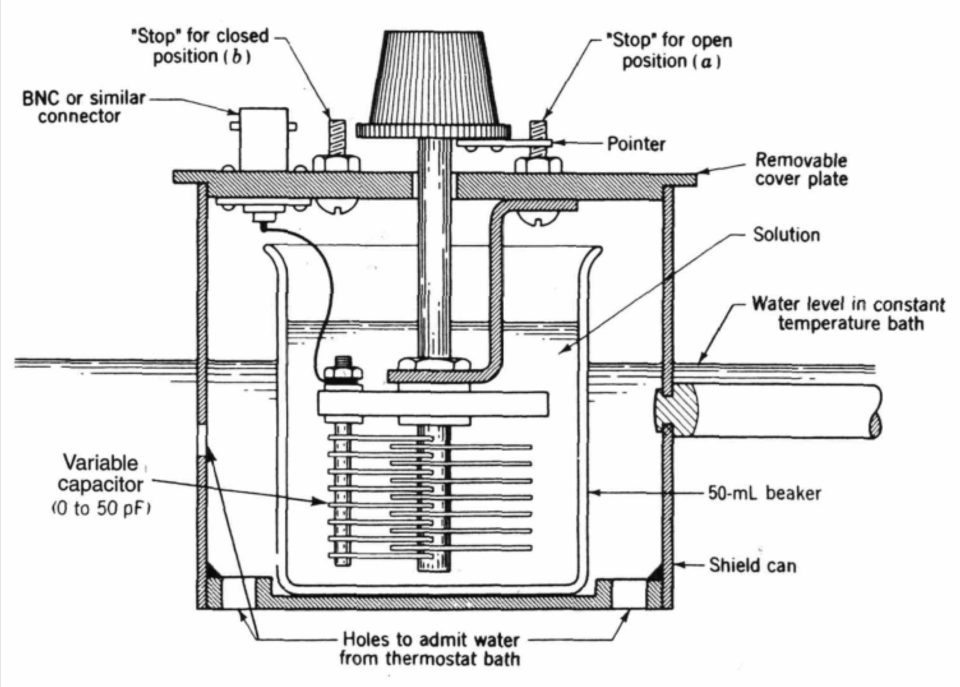
Experimental

- 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

		Mass			Clean			Solution		
		Mass dichloro benzene	Mass Total		1	2	3	1	2	3
M-dichlorobenzene	1%	0.810		*f* hi	0.43091	0.43058	0.4303	0.42483	0.42451	
				f low	0.41692	0.41644	0.41615	0.3958	0.39564	
	2%	1.638		*f* hi	0.42228	0.4221	0.42192	0.41819	0.41801	
				f low	0.4087	0.40841	0.4084	0.38945	0.38952	
	3%	2.395	44.599	*f* hi	0.41859			0.41507	0.41498	0.41489
				f low	0.10504			0.387	0.38658	0.3865
	4%	3.197	44.747	*f* hi	0.41659			0.41322	0.41319	0.41259
				f low	0.40315			0.38452	0.38452	0.38453
	1%	0.800	43.914	*f* hi	0.416			0.41316	0.41316	0.41317
				f low	0.40247			0.38549	0.3855	0.38551
	2%	1.603	44.143	*f* hi	0.41613			0.41339	0.41336	0.41337
				f low	0.40264			0.38567	0.38566	0.38565
O-dichlorobenzene	1%	0.795	44.033	*f* hi	0.41578			0.41257	0.4126	0.41259
				f low	0.40233			0.38452	0.38452	0.38453
	2%	1.604	44.132	*f* hi	0.41993			0.41668	0.41663	0.41662
				f low	0.40628			0.38803	0.38806	0.38801
	3%	2.407	44.590	*f* hi	0.41941			0.41641	0.4164	0.41641
				f low	0.40572			0.38758	0.38757	0.38759
	4%	3.202	44.915	*f* hi	0.41586			0.41241	0.41243	0.41243
				f low	0.40236			0.38226	0.38226	0.38228

Calculations

Frequency was used to measure the dielectric constant

$$f = \frac{1}{2\pi\sqrt{LC}} \longrightarrow C = \frac{1}{4\pi L f^2} \longrightarrow$$

$$C_{Hi} - C_{Lo} = \frac{1}{4\pi L}\left(\frac{1}{f_{Hi}^2 - f_{Lo}^2}\right) \longrightarrow \kappa = \frac{C_{Hi} - C_{Lo}}{(C_{Hi} - C_{Lo})_{air}}$$

Which simplifies to

$$\kappa = {\left(\frac{1}{f_{Hi}^2 - f_{Lo}^2}\right)_{sample}} \Big/ {\left(\frac{1}{f_{Hi}^2 - f_{Lo}^2}\right)_{air}}$$

Calculations cont.

To find the molar polarization of the solution, Eq. 6 is modified to yield

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

- 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
- ρ is the density of solution

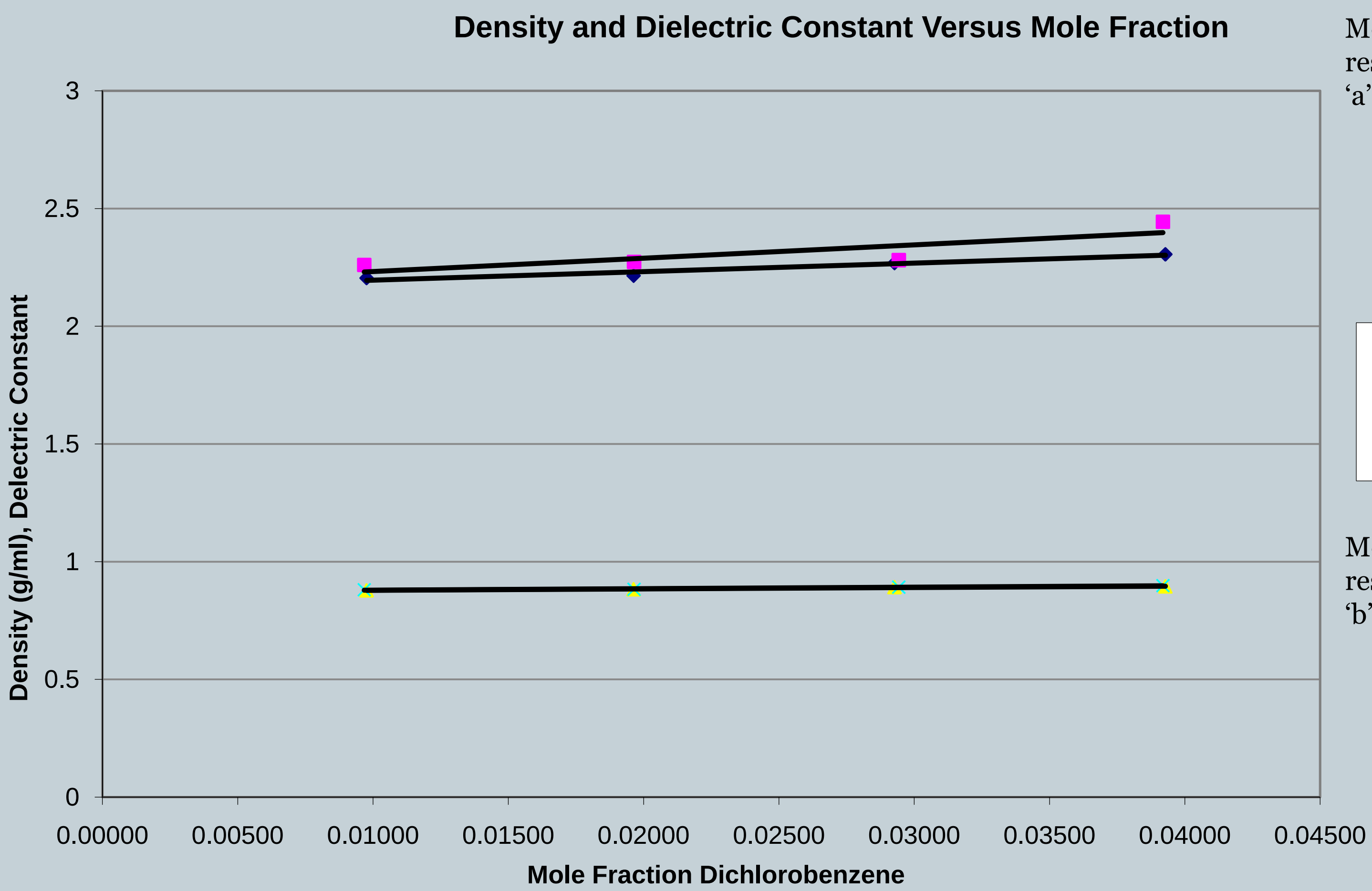
Calculations cont.

To find the molar polarization of the solute in solution, Eq. 7 is modified to

$$P_{2M}^{0} = \frac{3M_1 a}{(\kappa_1 + 2)^2 \rho_1} + \frac{\kappa_1 - 1}{(\kappa_1 + 2)^2 \rho_1}\left(M_2 - \frac{M_1 b}{\rho_1}\right) \qquad \text{Eq. 8}$$

Where κ_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



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

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

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

- Dielectric Constant (M)
- Dielectric Constant (O)
- Density (M)
- Density (O)

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

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

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

Calculations cont.

This molar polarization in solution is the sum of the molar distortion polarization (P_{2d}^{o}) and the molar orientation polarization ($P_{2\mu}^{o}$)

$$P_{2M}^{0} = P_{2\mu}^{0} - P_{2d}^{0}$$ Eq. 9

With

$$P_{2d}^{0} = \frac{n_2^2 - 1}{n_2^2 + 2}\frac{M_2}{\rho_2}$$ Eq. 10

- n_2 is the index of refraction for dichlorobenzene
- ρ_2 is the density of pure dichlorobenze

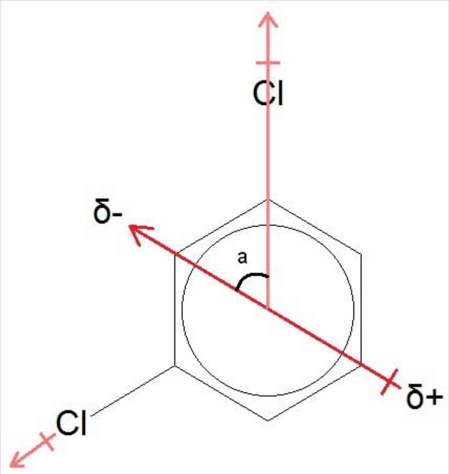
Calculations cont.

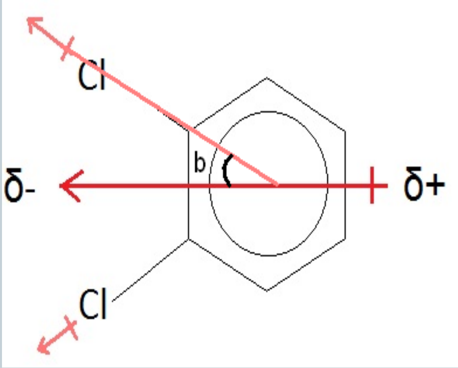
Finally, the dipole moment (μ) of the molecule is found with the equation

$$\mu = 12.8\left(P_{2\mu}^{0}T\right)^{1/2}$$ Eq. 11

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

Vector Addition





Vector addition of electron negativity

$$\mu_{meta} = 2 * 1.55\cos(a)$$

$$a = 60°$$

$$\mu_{ortho} = 2 * 1.55\cos(b)$$

$$b = 30°$$

Results and Error Analysis

Summary of Results and Relative Error

Dichloro-benzene	Vector Addition (D)	Experimental(D)	Literature (D)*	Percent Error Lit. vs. Exp.
Meta	1.55	1.54	1.48	3.91
Ortho	2.68	1.96	2.16	9.04

*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

Kuzbassk Polytechnical Institute. Translated from Izvestiya Vysshikh Uchebnykh Zavedenii Fizika, Vol. 12, No. 1, pp. 144-147, January, 1969.

Shoemaker, Garland and Nibler. *Experiments in Physical Chemistry 8th ed*. McGraw-Hill, New York, NY, 2003.