CBP Summer School

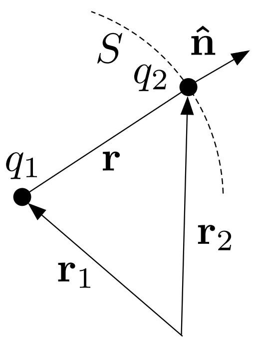
5 - 16 August, 2024

Physics Department, ASU

Lecture 8

Charge and dipole moment

Coulomb Law



Gauss law

$$\epsilon_0 E \times S = q_1, \quad S = 4\pi r^2$$

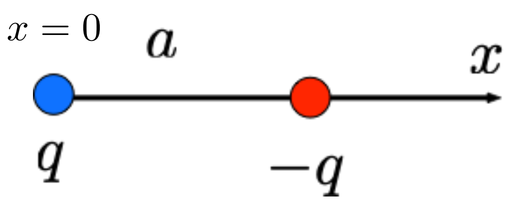
Field

$$E = \frac{q_1}{4\pi\epsilon_0 r^2}$$

Force

$$F = q_2 E = \frac{q_1 q_2}{4\pi\epsilon_0 r^2}$$

Field of two charges



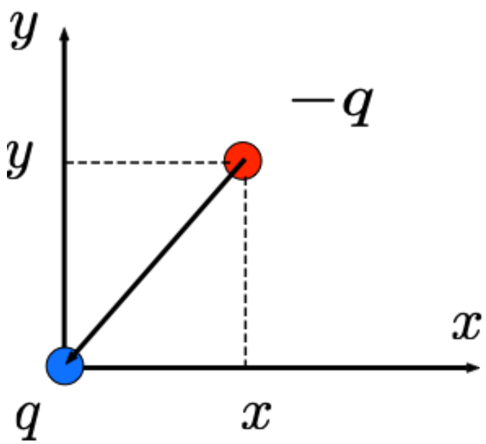
$$E(x) = \frac{q}{4\pi\epsilon_0 x} - \frac{q}{4\pi\epsilon_0 (x-a)}$$

$$E(x) \simeq -\frac{qa}{4\pi\epsilon_0 x^2}$$

$$E(x) \simeq \frac{M}{4\pi\epsilon_0 x^2}, \quad \boxed{M = -qa}$$

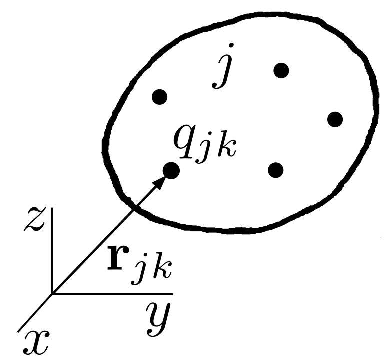
dipole moment

Dipole moment (2D/3D)



$$M_x = -qx$$

$$M_y = -qy$$



Dipole moment is directed from "minus" to "plus"

General definition

$$\mathbf{M} = M_x\hat{\mathbf{x}} + M_y\hat{\mathbf{y}} + M_z\hat{\mathbf{z}} = \sum_k q_k \mathbf{r}_k$$

Dipole moment direction

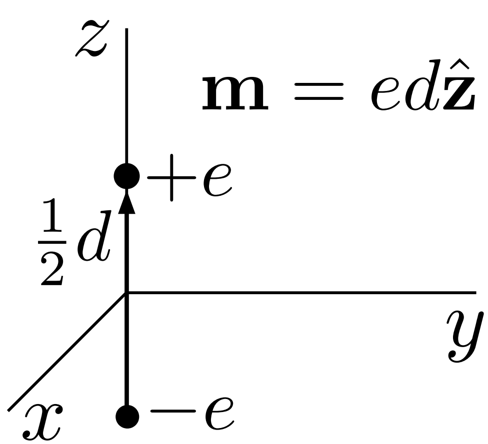
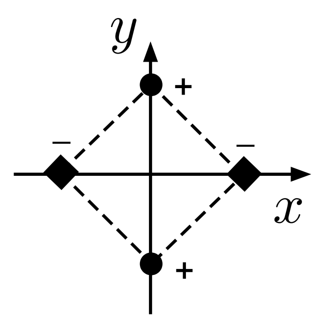


Table 2.1 Molecular multipoles and diameters

Molecule	m, D[a]	Q, D×Å[b]	m^*	Q^*	σ_s, Å[a]
Water	1.83	2.96	1.85	1.10	2.87
Methanol	2.87	5.7	1.93	1.04	3.77
Acetonitrile	3.92	1.8	2.29	0.06	4.14
Benzene	0	8.69	0	0.45	5.27



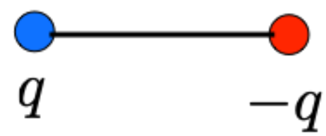
Quadrupole: two oppositely directed dipole moments

Dipole moment (units)

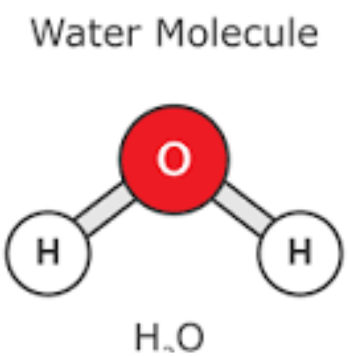
$[M] = \text{charge} \times \text{distance}$

Debye units

$$a = 1\ \text{Å} = 10^{-10}\ \text{m}$$

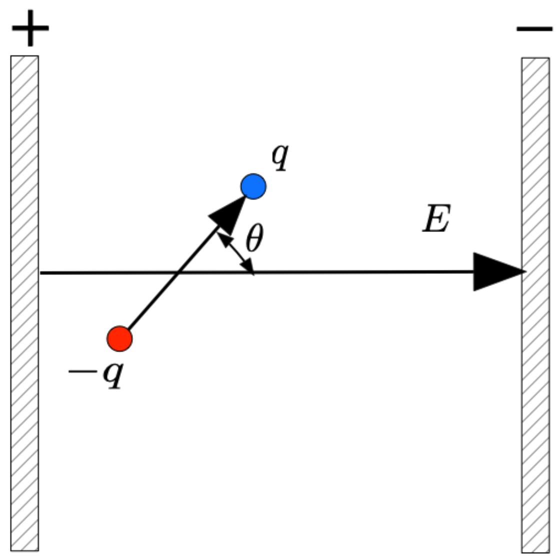


$$M = 4.8\ \text{D}$$



$M = 1.87\ \text{D}$

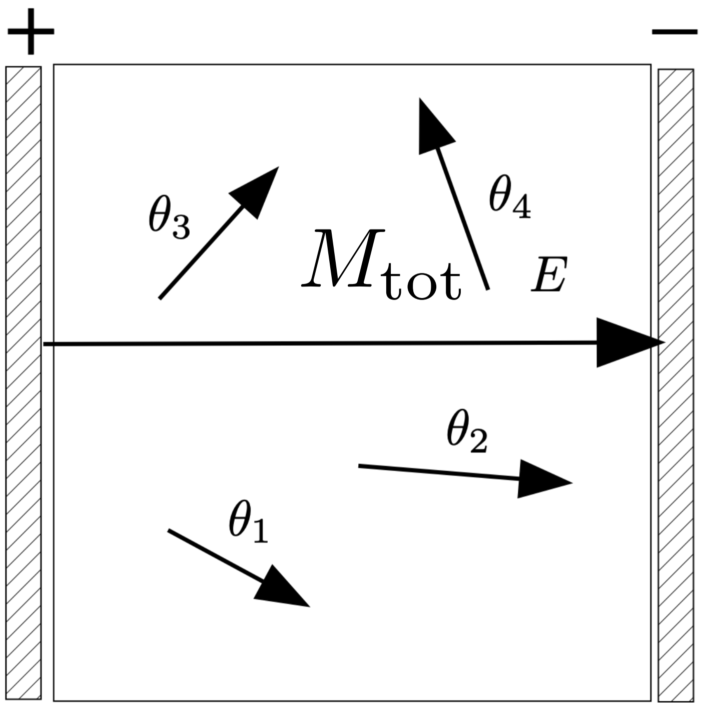
Dipole moment: Interaction with the field



$$U = -ME\cos\theta$$

$$\langle U\rangle = -ME\langle\cos\theta\rangle$$

Polarization of a sample

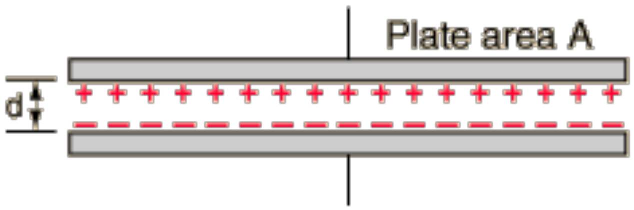


$$\langle \cos\theta \rangle \simeq \frac{ME}{3}$$

$$\langle M \rangle \simeq \frac{M^2 E}{3}$$

Measuring capacitance gives access to the molecular dipole moment

Capacitance



$$C = \frac{\varepsilon A}{d} = \frac{k\varepsilon_0 A}{d}$$

$$C(\omega) \propto k(\omega)$$

Frequency-dependent dielectric constant

Dipole moments of proteins

Determined from dielectric spectra of protein solutions:

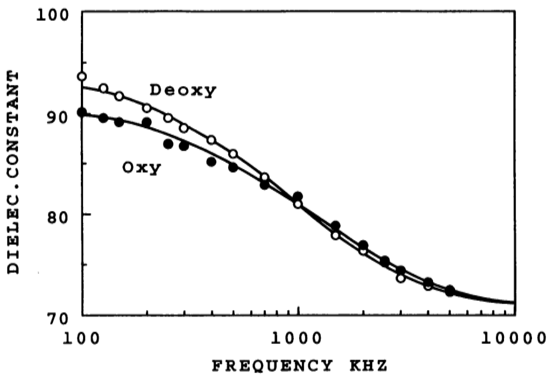


FIGURE 2 The frequency dependence of the dielectric constant of deoxy HbA (*open circles*) and oxy HbA (*filled circles*).

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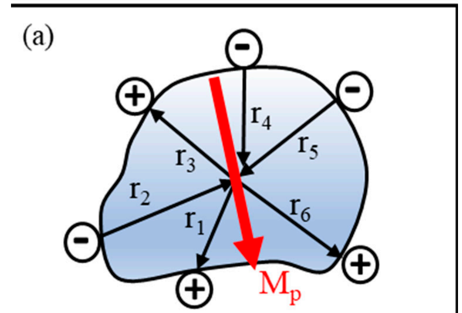
Table I Calculated and Measured Dipole Moments of Small Globular Proteins by Previous and Present Investigators[a]

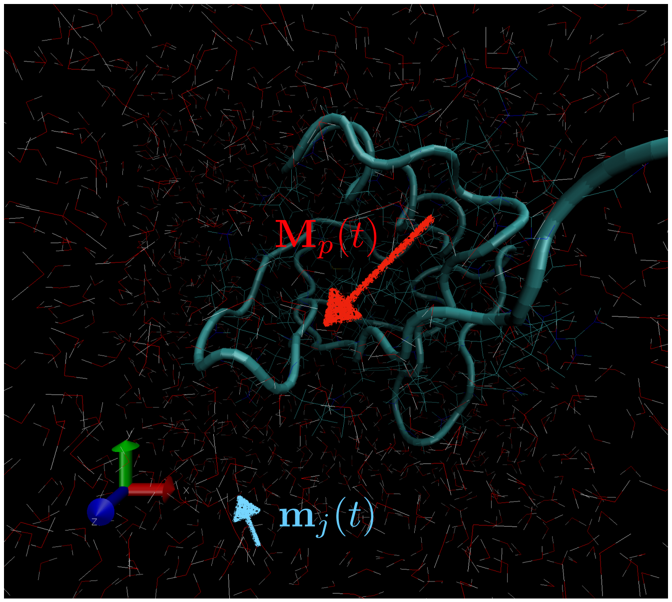
		Calculated (D)			
Name	M_W	Charge	Core	Total	Measured (D)
MBN[b]	17,000	170	0	170	167
MBN[c]		165	−10	155	200
CHP[d]				450	460
HBN[e]	64,000			527	523
HBN (α)	16,000	235	0	235	183[f]
CYT	13,000	310	−20	290	<u>235</u>
RNS	13,700	481	−80	401	<u>280</u>
					336[g]
LYZ	14,300	111	89	200	<u>122</u>
PB2	13,000	103	87	190	<u>141</u>
CPA	34,000	408	87	495	<u>637</u>
SBT	27,500	508	−58	450	<u>341</u>
TRP	23,000	356	0	356	<u>271</u>
CNA	102,000	187	103	290	<u>411</u>

[a] MBN: myoglobin; CHP: chymotrypsin; HBN: hemoglobin; HBN (α): hemoglobin α-chain; See text for other abbreviations. Underlined numbers are present experimental results. All other calculated values are by Barlow et al.[8]
[b] Schlect.[5]
[c] South et al.[6]
[d] Antociewicz et al.[7]
[e] Orttung.[4]
[f] Schlecht.[12]
[g] Keefe et al.[14]



$$M_p = qr_1 - qr_2 + qr_3 - qr_4 - qr_5 + qr_6$$

Dipole moment from simulations



Water dipole moment:

$$\mathbf{M}_w = \sum_j \mathbf{m}_j$$

Total dipole moment:

$$\mathbf{M}(t) = \mathbf{M}_w(t) + \mathbf{M}_p(t)$$

Trajectories of dipole moments

dipole_Protein.txt

beginning

-72.32307	-261.07138	13.07575
-64.55422	-257.60294	15.53045
-63.23687	-256.88925	21.38829
-67.56758	-264.98047	28.10897
-80.99371	-260.86780	26.57924
-77.44994	-253.50862	16.25313
-68.57877	-252.95900	23.41817
-72.65784	-246.52350	17.25969
-67.69681	-258.09607	27.07245
-67.09357	-252.15392	22.68427
-68.38203	-260.96970	19.96119
-71.49563	-255.51492	23.89831
-69.50024	-259.36267	18.69661

M_{px} M_{py} M_{pz}

end

-7.30663	-225.66634	73.71140
-22.62328	-225.72734	59.02941
-16.40680	-237.61035	51.90017
-23.35577	-234.72319	61.03447
-20.83559	-230.39952	56.91902
-21.63265	-232.50279	48.50206
-16.91199	-232.57957	63.22918
-15.88881	-234.83217	60.24128
-27.30851	-211.33237	71.88264
-30.86135	-213.10197	54.54554
-43.03381	-222.53931	53.81201
-39.69813	-228.07710	59.36641
-32.20247	-231.82474	59.64364
-25.81162	-210.24622	54.32720

Dipole moment does not change much on 500 ps of the trajectory

Complete characterization of the dynamics requires time correlation function