Perspectives On The POINT-DIPOLE *Approximation:* for the Prospective INTUITIVE-CHEMISTS' *Approaches*

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ADDRESSES FOR SOME OF THIS AUTHOR'S WEBPAGES WHERE MATERIALS RELEVANT TO THE TOPIC HERE ARE DOCUMENTED.

WebSite URL (I) *:* http://saravamudhan.tripod.com

Explaining the trends of Nuclear Shielding caused by Magnetic moments related to Susceptibilties

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WebSite URL (II): http://geocities.com/amudhan20012000/Confview.html
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ABSTRACT

A dipole by definition **[SHEET_2**] consists of two unlike poles but equal in magnitude (pole strength) separated by a finite distance '**d'**. When the point (where this dipole's effect is) being considered is located at such large distances 'R' from the dipole that **'d'** is negligible compared to **'R'** [d<< R(as in **SHEET_8 and 9**)], the point-dipole approximation is said to be valid. When **'R'** becomes nearly equal (comparable in magnitude) to **'d',** then the point dipole-approximation would not be reliable.

Then, by [1] hypothetically considering [**SHEET_10**]each of the poles to be made up of 'n' number of equally divided polestrengths and [2] placing each of this divided poles separated from the correspondingly divided unlike-pole, and, further , [3] this distance of separation being equal to **d' = d / n**, a set of 'n' smaller dipoles can be constructed all these dipoles being centered at the same Electrical Centre of Gravity as the original undivided, single dipole. The value of 'n' can be so chosen that the distances of separation **d'** is negligible compared to the value **R**. This would enable the point dipole approximation to be valid for each of the divided, smaller dipoles and their effect at a point at distance 'R' can be calculated. Since all the 'n' number of divided dipoles are identical their contributions will all be the same and having calculated the effect of one of the dipoles, the effect of 'n' dipoles can be obtained by a multiplication by 'n'[***A critical question 'n' or 'n^2'***]. This should yield the effect of the single dipole within the frame work of point dipole approximation. Does this mean that dividing and multiplying by 'n'[***or 'n^2'***] [***effectively the multiplication factor is '1' or 'n'***] makes it a valid description that which was originally not reliable ? This procedure would be providing an argument to say the same numerical values are reliable eventhough at the outset this result could have been discarded as unreliable.

Since this is an argument which can lead a chemist astray while trying to interpret the results, it is intended in this poster presentation to address this question in greater detail so as to enable a confident handling of the point-dipole approximation which is inevitably the beginners' approach in chemical contexts.

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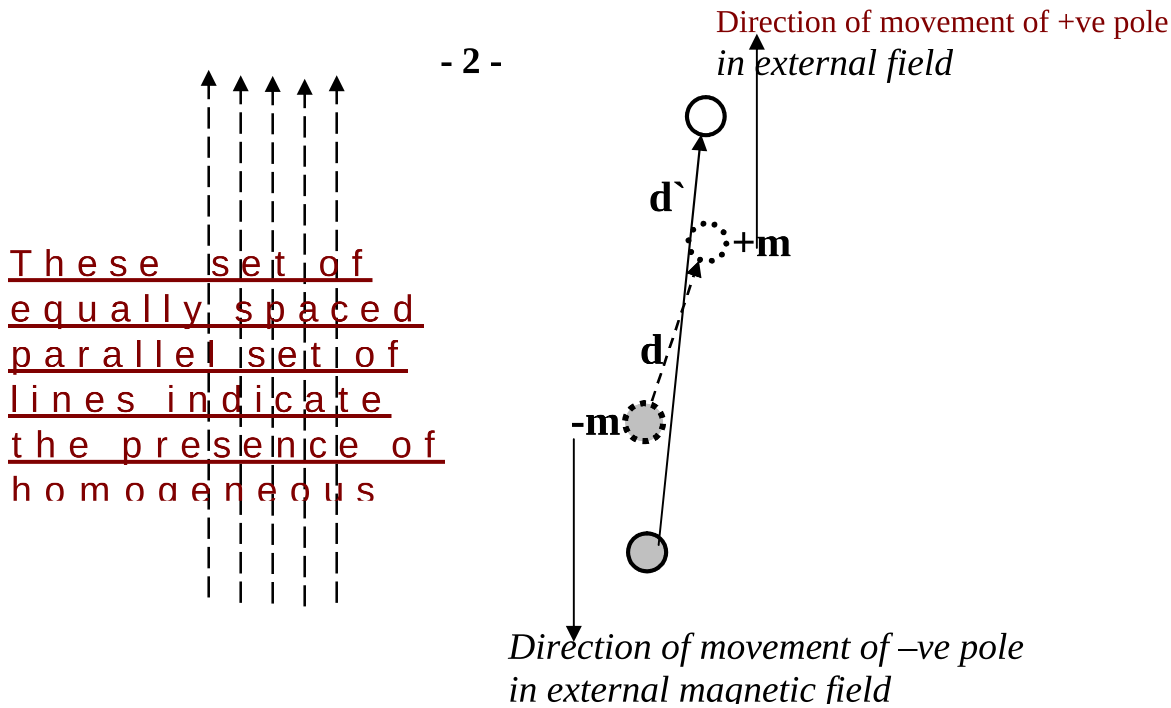
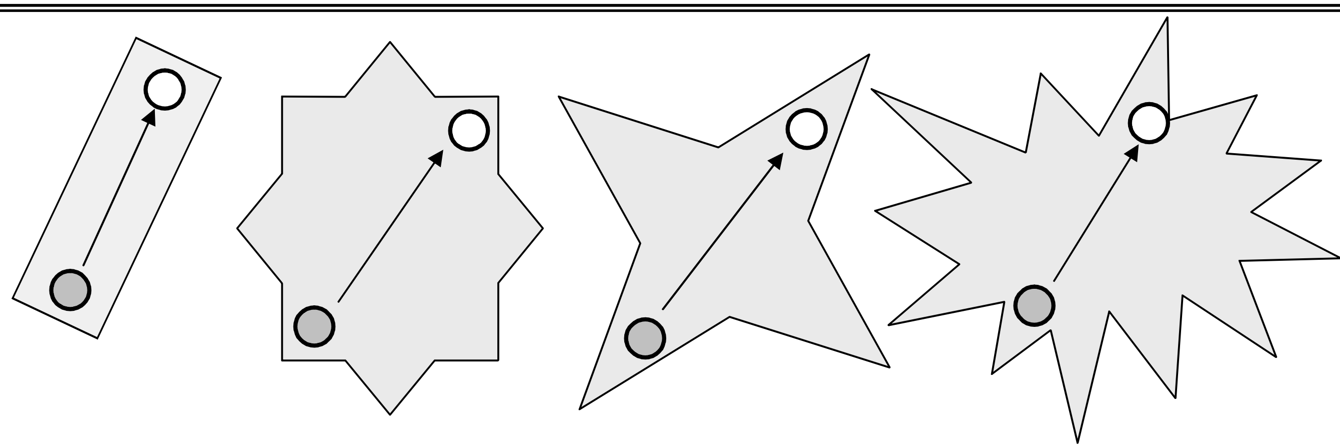


The two poles, equal in magnitude and oppsit in sign, are not held fixed in a non-flexible and hard frame-work. Hence in external fields the two poles can be moving independent of each other and hence the inter-pole distance d is not a constant. Thus the two poles cvnnot be said to be forming a "dipole" with a well defined value for the *"dipole moment".*



In the above set of illustration the pair of poles are held by non-flexible and hard FRAME-work and the inter-pole distance d cannot alter in presence of the external field. When a movement is required the two poles move together with fixed distance between them. When no trnslational motion can provide the rewuired change to the minimum potential energy situation, the minimization occurs by a rotation of the line (imaginary) connecting the two poles. This is said to align the "dipole" or the "Dipole moment" gets disposed along the direction of the external field.

"http://aravamudhan-s.ucoz.com/CRSI_NSC6_IITK.html"

Image (1) of the 2 images for this display

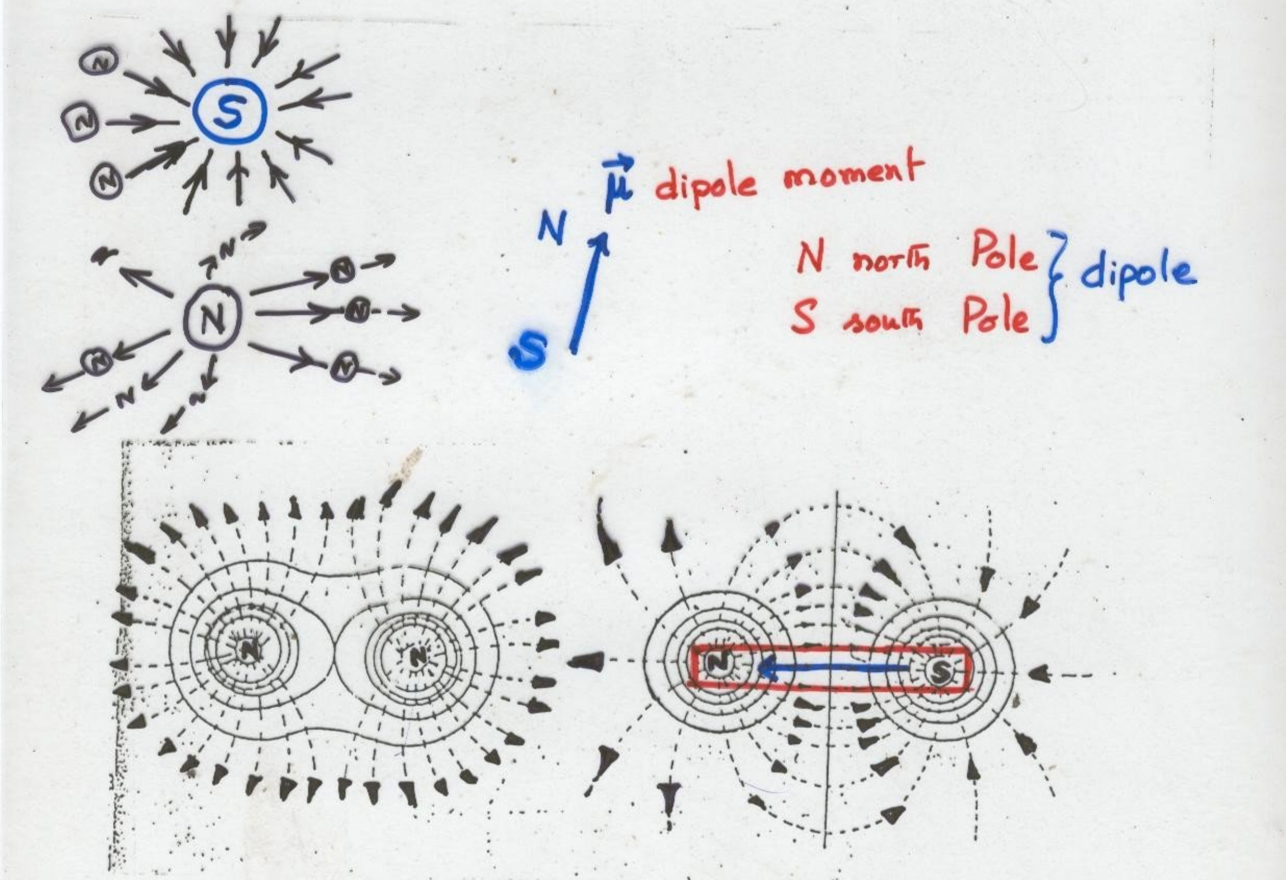


Image (2)

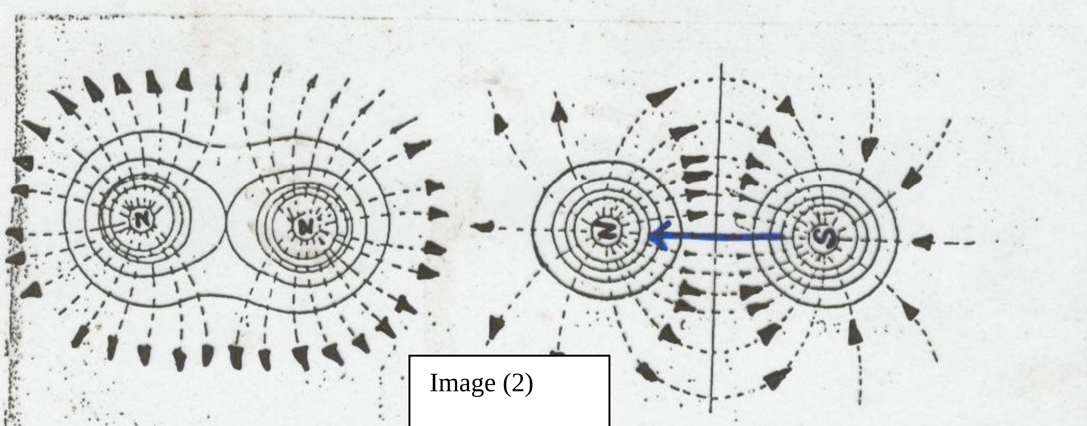
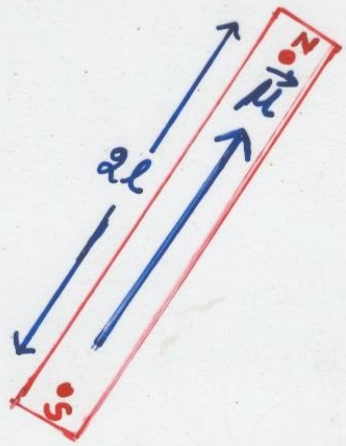


Fig. 3.10

Fig. 3.11



strength of north pole = m
strength of South pole = m

MAGNETIC DIPOLE MOMENT = $\vec{\mu}$

$\vec{\mu}$ POINTS from S to N INSIDE THE BAR MAGNET

magnitude $|\vec{\mu}| = 2\ell m$

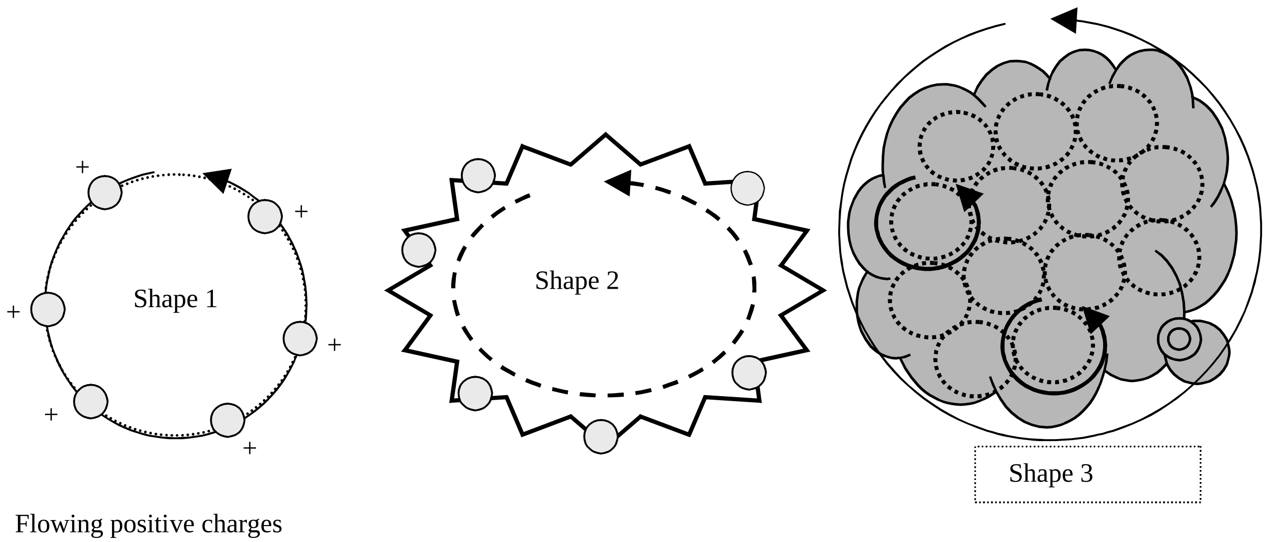
All the magnetic field effect representations can be done by simply considering the magnetic dipole moment vector $\vec{\mu}$ instead of picturising the bar magnet with its north pole and south pole.

Thus $\vec{\mu}$ represents the dipole characteristics.

"http://aravamudhan-s.ucoz.com/CRSI_NSC6_IITK.html"

While explaining the presence of a **"dipole moment"** by considering the poles which, depending on the context, the poles may be the "electrical (positive and negative) charges" or the ["magnetic charges"] magnetic "north" and "south" poles. In either case a dipole moment can be defined: in the former case it would be *electrical dipole moment* and in the latter case it would be *magnetic dipole moment*

In the case of flowing electrical charges, the current thus flowing can cause a magnetic field, which can be associated with the flow characteristics and the amount of the electrical charges. The magnetic field thus arising can be calculated and the direction of the field determined. This can be the attribute "dipolemoment" for the flowing charge systems.



In each of the above cases a magnetic moment can be attributed for the charge flow. In the case of SHAPE 3 the charge cloud is depicted. The total charge cloud can be considered as small, charged, volume elements inside the charge cloud. These volume elements each can be attributed a small dipole moment and the total dipole moment associated with currents in the charge cloud can be obtained by a vector addition of the individual elemental dipole moments.

IF THE PARTICLE UNDERGOING A ROTATIONAL MOTION ALSO HAS AN ELECTRICAL CHARGE, THEN THE ROTATIONAL MOTION OF THE CHARGE — i.e., a flowing charge — WILL PRODUCE A MAGNETIC FIELD.

IT IS WELL KNOWN THAT IF A CURRENT 'I' FLOWS THROUGH A CIRCULAR COIL AND IF THE AREA OF THE CIRCLE IS 'A', THEN THE MAGNETIC FIELD PRODUCED IS GIVEN BY $\mu = IA$

and the magnetic field is at the center of the circle.