

INTRODUCTION

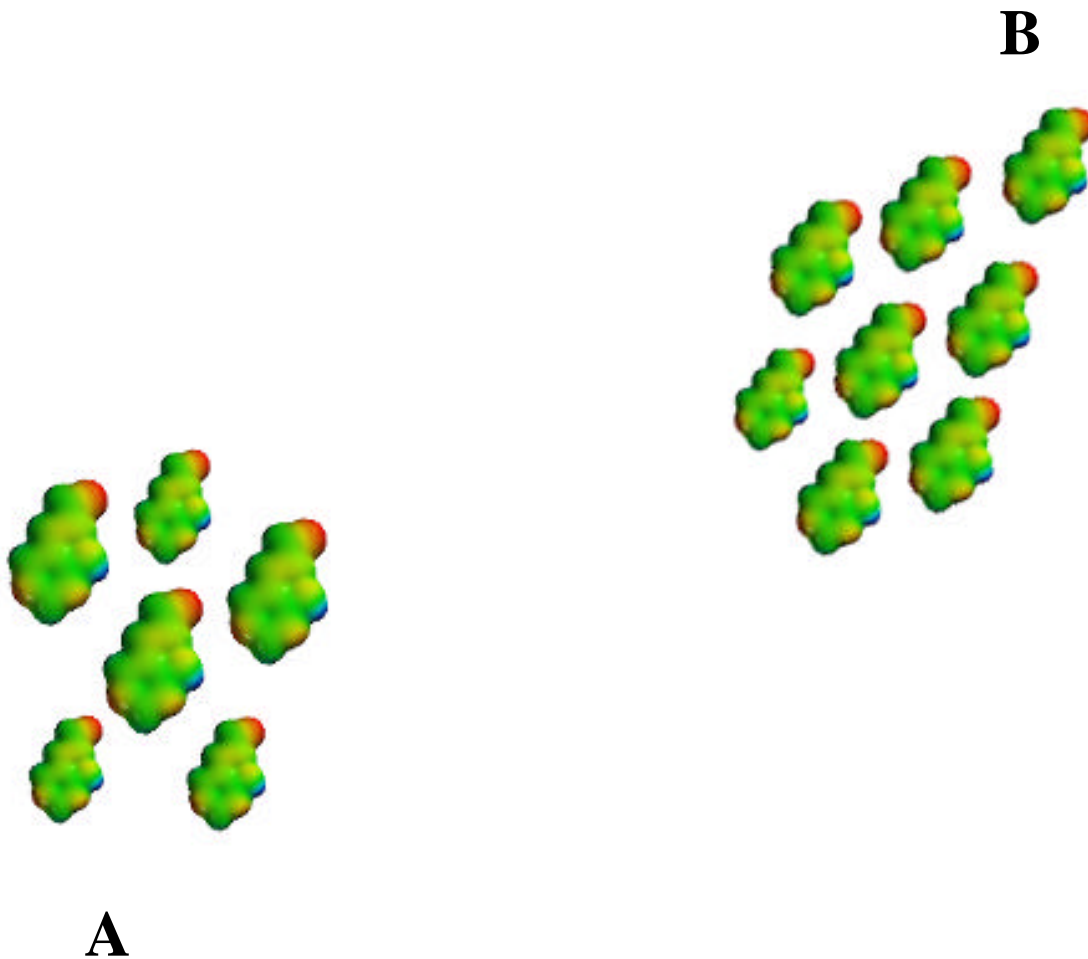


Figure 1. Charge Distributions A and B.

The classical N-body problem requires $O(N^2)$ calculations, thus as N grows the computational requirements quickly become overwhelming. Numerical techniques designed to deal with large N generally compute some kind of “average” for the charge distribution in A and B. And then use these “averages” to estimate the potential. One method that has shown good results for point charges is the Fast Multipole Method (FMM).

The basic FMM formula (equation 0) is of the form,

$$\sum_{m=0} \sum_B B_m(P_k) \sum_A A_m(Q_j) . \quad (1)$$

This naturally leads to the following question. Does there exist an expression for the potential that has the following form:

$$\sum_{m=0} \sum_B B_m(P_k) \sum_A A_m(Q_j) . \quad (2)$$

Since chemistry deals with continuous charge distributions, a more appropriate form might be:

$$\sum_{m=0} \sum_B B_m(P_k) \sum_A A_m(Q_j) . \quad (2')$$

The advantage that the latter equations have over the former is that in the latter equations the sum/integral over B is independent of A. This should hopefully result in a more efficient method for computing distant interaction potentials.

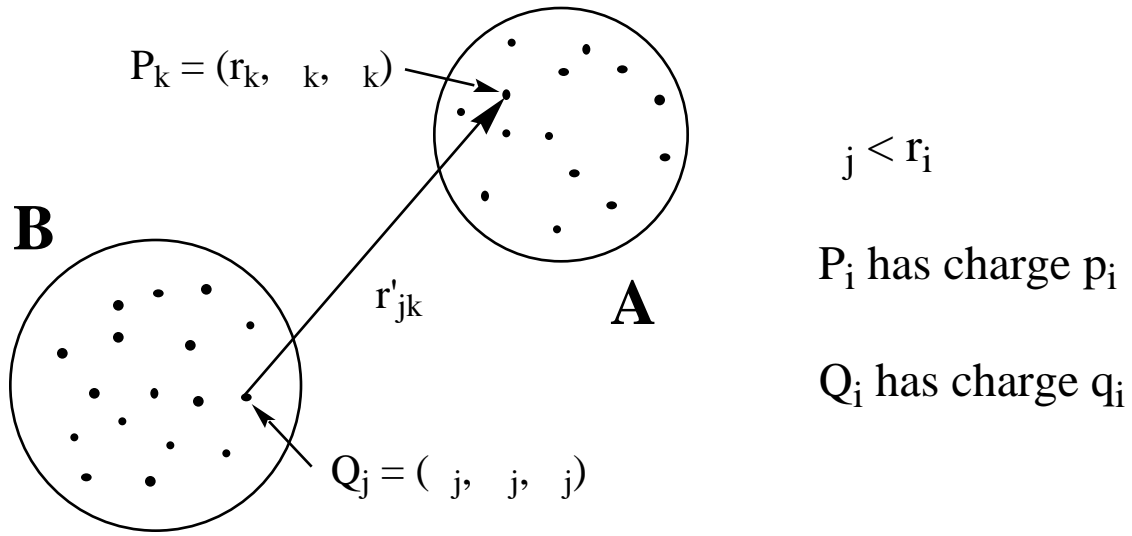


Figure 2. Definitions Concerning the Charge Distributions.

How the FMM achieves its asymptotic efficiency can be seen in the following formula for the interaction potential between charge distributions A and B.

$$Potential = \sum_{m=0}^{\infty} \sum_{i=1}^N \frac{q_i}{\rho_i^{m+1}} \left[\sum_{k=-m}^m Y_m^k A_m^k (\alpha_{j,\beta_j}) \right] \quad (0)$$

Where the Y_m^k are the spherical harmonic basis functions and

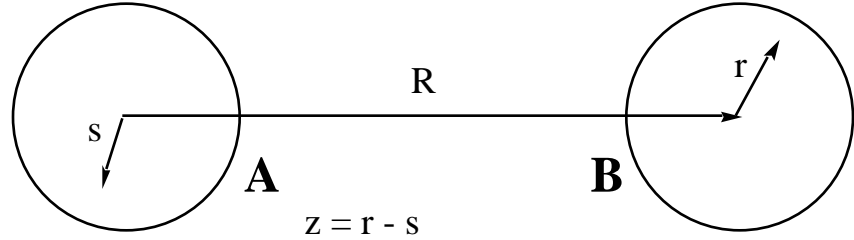
$$A_m^k = \sum_{j=1}^N p_j r_j^m y_m^{-k} (\theta_i, \phi_i).$$

The key feature of the above equation is that the values of the A_m^k are independent of the charges in B. This makes this equation asymptotically more efficient to evaluate than a straight forward pairwise calculation.

DERIVATION OF MODIFIED FMM

In order to derive our modified FMM (i.e. eq. 2') we start with the following coordinate system.

Figure 3.
Definition of Local Coordinate System.



We would like to obtain a power series expansion for $|R+Z|^{-1}$ the reciprocal of the distance between a point in A and a point in B. We proceed as follows.

$$|R + z|^{-1} = |R|^{-1} \left(1 + \frac{2z \cdot R}{|R|^2} + \frac{|z|^2}{|R|^2} \right)^{-\frac{1}{2}}$$

Setting

$$x = \frac{2z \cdot R}{|R|^2} + \frac{|z|^2}{|R|^2}$$

and applying the appropriate expansion formula we get that $|R+Z|^{-1}$ has a power series expansion of the form:

$$|R + z|^{-1} = |R|^{-1} \left(1 + \sum_{n=1}^{\infty} a_n x^n \right)$$

whenever $|x| < 1$. With a little calculation it can be shown that

$$x^n = |R|^{-2n} \sum_{k=0}^n \binom{n}{k} 2^{n-k} \langle (\otimes^k I) \otimes (\otimes^{n-k} R), \otimes^{n+k} z \rangle$$

Where I is the 3 by 3 identity matrix, \otimes^k is the k-fold tensor product, and $\langle \cdot, \cdot \rangle$ is the inner product operator.

We can now write,

$$\frac{1}{|R+z|} = \frac{1}{|R|} \left(1 + \sum_{n=1}^{\infty} a_n \left[|R|^{-2n} \sum_{k=0}^n \binom{n}{k} 2^{n-k} \langle (\otimes^k I) \otimes (\otimes^{n-k} R), \otimes^{n+k} z \rangle \right] \right)$$

If we rearrange the terms above and introduce the following notation:

$$b_{j,k} = |R|^{-2j-1} a_j 2^{j-k} \binom{j}{k}, \quad A_{j,k} = (\otimes^k I) \otimes (\otimes^{j-k} R), \quad z = z(r, s)$$

we can write the above equation as

$$\frac{1}{|R+z|} = \frac{1}{|R|} + \sum_{m=1}^{\infty} \left\langle \sum_{k=0}^{\lfloor \frac{m}{2} \rfloor} b_{m-k,k} A_{m-k,k}, \otimes^m z(r, s) \right\rangle. \quad (3)$$

Where $\lfloor m/2 \rfloor$ is the greatest integer less than or equal to $m/2$. Thus the potential interaction between charge distributions **A** and **B** is

$$\begin{aligned} \int_{\mathbf{A}} \int_{\mathbf{B}} \frac{\rho(r) \sigma(s)}{|R+z(r, s)|} dr ds &= \frac{1}{|R|} \int_{\mathbf{A}} \int_{\mathbf{B}} \rho(r) \sigma(s) dr ds \\ &+ \int_{\mathbf{A}} \int_{\mathbf{B}} \rho(r) \sigma(s) \sum_{m=1}^{\infty} \left\langle \sum_{k=0}^{\lfloor \frac{m}{2} \rfloor} b_{m-k,k} A_{m-k,k}, \otimes^m z(r, s) \right\rangle dr ds \end{aligned}$$

This can be rewritten as

$$\begin{aligned} \int_{\mathbf{A}} \int_{\mathbf{B}} \frac{\rho(r) \sigma(s)}{|R+z(r, s)|} dr ds &= \frac{1}{|R|} \int_{\mathbf{A}} \int_{\mathbf{B}} \rho(r) \sigma(s) dr ds \\ &+ \sum_{m=1}^{\infty} \left\langle \sum_{k=0}^{\lfloor \frac{m}{2} \rfloor} b_{m-k,k} A_{m-k,k}, \int_{\mathbf{A}} \int_{\mathbf{B}} \rho(r) \sigma(s) (\otimes^m z(r, s)) dr ds \right\rangle \end{aligned}$$

In order to convert our last equation into our desired form we must first convert

$$\int_{\mathbf{A}} \int_{\mathbf{B}} \rho(r) \sigma(s) (\otimes^m z(r, s)) dr ds$$

into an expression of multipoles. We give an example of how to accomplish this for the (a,b) tensor component of the m=2 term.

$$\begin{aligned} & \int_{\mathbf{A}} \int_{\mathbf{B}} \rho(r) \sigma(s) (\otimes^m z(r, s)) dr ds \\ &= \int_{\mathbf{A}} \int_{\mathbf{B}} \rho(r) \sigma(s) [(r_a - s_a)(r_b - s_b)] dr ds \\ &= \int_{\mathbf{A}} \int_{\mathbf{B}} \rho(r) \sigma(s) r_a r_b dr ds - \int_{\mathbf{A}} \int_{\mathbf{B}} \rho(r) \sigma(s) r_a s_b dr ds \\ & \quad - \int_{\mathbf{A}} \int_{\mathbf{B}} \rho(r) \sigma(s) s_a r_b dr ds + \int_{\mathbf{A}} \int_{\mathbf{B}} \rho(r) \sigma(s) s_a s_b dr ds \\ &= \left(\int_{\mathbf{B}} \sigma(s) ds \right) \left(\int_{\mathbf{A}} \rho(r) r_a r_b dr \right) - \left(\int_{\mathbf{B}} \sigma(s) s_b ds \right) \left(\int_{\mathbf{A}} \rho(r) r_a dr \right) \\ & \quad - \left(\int_{\mathbf{B}} \sigma(s) s_a ds \right) \left(\int_{\mathbf{A}} \rho(r) r_b dr \right) + \left(\int_{\mathbf{A}} \rho(r) dr \right) \left(\int_{\mathbf{B}} \sigma(s) s_a s_b ds \right) \end{aligned}$$

Once these type of calculations are carried out for the desired values of m, they can be inserted into equation 3. Then all that is left to do is to expand the inner product to get a multipole expansion of the desired form (i.e. eq. 2).

The multipole expansion (eq. 1) used in the FMM, while having good asymptotic behavior has a very high computational constant factor. However the FMM has a very simple but clever idea for reducing the computational constant. The basic idea is based on the fact that the size of the approximation error is directly related to the geometric size of the distribution and inversely related to the distance between the charge distributions. Thus as the distance increases we can collect nearby distributions together to form larger distributions. These larger distributions can then be used in eq.1, resulting in improved computational efficiency without an increase in the error.

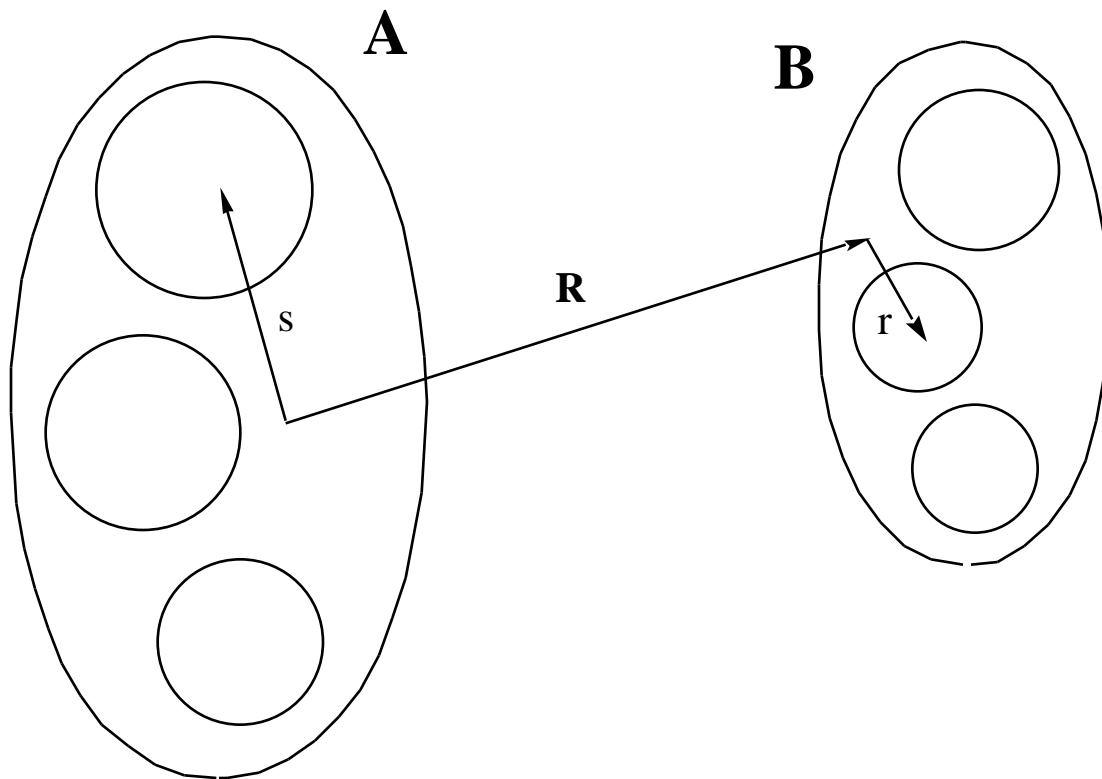


Figure 4. Formations of Aggregate Distributions from Small Distributions.

In order to be able to collect charge distributions into larger groups, three things are needed:

- 1) an appropriate data structure,
- 2) a method for combining distributions,
- 3) a good estimate of the error.

The FMM uses a multidimensional binary search tree known as an Octal tree to take care of item one. The Octal tree method as implemented in the FMM needs to be modified for continuous distributions. We will not discuss the necessary modifications. To accomplish item two we could simply add distributions together to form a large distribution. And then calculate the multipole moments for the new distribution. Assuming the multipole moments have already been computed, this would be a very inefficient approach. A more efficient approach is to find a method that uses the previously calculated multipole moments; which is what we do. The third item, a good error estimate, is needed in order to be able to determine how many distributions can be grouped together. The more distributions that can be grouped together; the more efficient the algorithm.

To illustrate how item two is calculated, we give an example that shows how two (i,j) quadrupole components are combined.

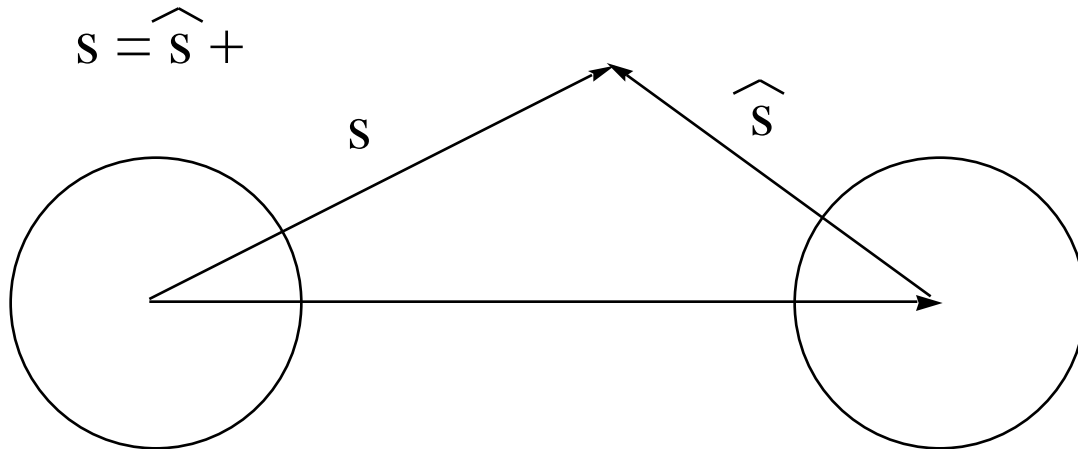


Figure 5. Coordinate System for Combination of Multipoles.

The (i,j) quadrupole component for the combined distribution above is derived as follows,

$$\begin{aligned}
 \int \rho(s) s_i s_j ds &= \int \rho_1(s) s_i s_j ds + \int \rho_2(s) s_i s_j ds = \\
 &= \int \rho_1(s) s_i s_j ds + \int \rho_2(s) s_i s_j ds = \\
 &= \int \rho_1(s) s_i s_j ds + \int \rho_2(\hat{s} + \epsilon) (\hat{s}_i + \epsilon) (\hat{s}_j + \epsilon) d\hat{s} = \\
 &= \int \rho_1(s) s_i s_j ds + \int \sigma(\hat{s}) (\hat{s}_i + \epsilon) (\hat{s}_j + \epsilon) = \\
 &= \int \rho_1(s) s_i s_j ds + \int \sigma(\hat{s}) \hat{s}_i \hat{s}_j d\hat{s} + \epsilon_i \int \sigma(\hat{s}) \hat{s}_j d\hat{s} \\
 &\quad + \epsilon_j \int \sigma(\hat{s}) \hat{s}_i d\hat{s} + \epsilon_1 \epsilon_2 \int \sigma(\hat{s}) d\hat{s}.
 \end{aligned}$$

The latter expression is simply a linear combination of monopoles, dipoles, and quadrupoles.

To derive our error estimate (item 3) we use Taylor's remainder formula for $f(R_{r,s}) = |R + r - s|^{-1}$:

$$f(R_{r,s}) = f(R) + \sum_{n=1}^N \frac{1}{n!} \langle \nabla^n f(R), \otimes^n z(r,s) \rangle + \frac{1}{(N+1)!} \langle \nabla^{N+1} f(\zeta_{r,s}), \otimes^{N+1} z(r,s) \rangle \quad (4)$$

where $\zeta_{r,s} = R + t_{r,s}z(r,s)$ for some $t \in [0, 1]$.

The expression $\frac{1}{(N+1)!} \langle \nabla^{N+1} f(\zeta_{r,s}), \otimes^{N+1} z(r,s) \rangle$

is known as the remainder term. We will use this remainder term to derive our error estimate. By comparing equations (3) and (4) we conclude that

$$\begin{aligned} & \frac{1}{(N+1)!} \langle \nabla^{N+1} f(\zeta_{r,s}), \otimes^{N+1} z(r,s) \rangle \\ &= \sum_{k=0}^{\lfloor \frac{N+1}{2} \rfloor} c_k |R + t_{r,s}z(r,s)|^{-2N+2k-3} \langle A_k(t_{r,s}), \otimes^{N+1} z(r,s) \rangle. \end{aligned} \quad (5)$$

Where

$$c_k = a_{N+1-k} 2^{N+1-2k} \binom{N+1-k}{k}, \quad A_k(t) = (\otimes^k I) \otimes (\otimes^{N+1-2k} (R + t_{r,s}z(r,s)))$$

If we replace in equation (5) $|R + t_{r,s}z(r,s)|^{-2N+2k-3}$ with its power series expansion; then throw out all but the dominant term, and do a few other things, we get the following error estimate.

$$\left| \frac{1}{R} \right| \sum_{k=0}^{\lfloor \frac{N}{2} \rfloor} C_{N-k,k} \left\langle \otimes^{N-k} I, \otimes^{2N-2k} \frac{z}{|R|} \right\rangle t_{r,s}^{N-2k} \quad (6)$$

Since $|z| < |R|$, equation (6) is dominated by the $k = N/2$ term. Since we are looking for an estimate of the error, we will ignore all but the $k = N/2$ term and work with

$$\left| \frac{1}{R} \right| C_{N-\lfloor \frac{N}{2} \rfloor, \lfloor \frac{N}{2} \rfloor} \left\langle I, \otimes^2 \frac{z}{|R|} \right\rangle^{N-\lfloor \frac{N}{2} \rfloor} t_{r,s}^{N-2\lfloor \frac{N}{2} \rfloor} \quad (7)$$

Thus if N is odd (7) becomes,

$$\left| \frac{1}{R} \right| C_{\frac{N+1}{2}, \frac{N-1}{2}} \left\langle \otimes^{\frac{N+1}{2}} I, \otimes^{N+1} \frac{z}{|R|} \right\rangle t_{r,s}. \quad (8)$$

If N is even (7) becomes,

$$\left| \frac{1}{R} \right| C_{\frac{N}{2}, \frac{N}{2}} \left\langle \otimes^{\frac{N}{2}} I, \otimes^N \frac{z}{|R|} \right\rangle \quad (9)$$

Equation 8 is of little practical value. Equation 9 represents an error estimate in terms of previously computed multipole moments for even ordered expansions. We will therefore restrict ourselves to even ordered expansions. From a computational point of view, this is not a major drawback. Evaluating $N+1$ terms when N terms are sufficient results in greater accuracy. This greater accuracy should allow for larger aggregates of distributions; which in turn will reduce the computational cost. Thus cancelling out a major portion of the inefficiency produced by going to $N+1$.

CONCLUSION

The Multipole expansion derived above has several interesting features:

- 1) it has linear to near linear scaling,
- 2) it has an error estimate,
- 3) it satisfies equation 2'.

Item (1) (along with the appropriate data base) is the minimal requirement for a fast multipole algorithm. Item (2), the error estimate is a bit different than most error estimates in that it can also be used as a correction term. Item (3) is new to the FMM world and has some interesting consequences. Because of (3) we need only calculate the multipole moments of our basic distributions. Once this is done we can translate, rotate, and combine these moments to generate new moments, without any further integration. Thus avoiding costlier integral evaluations.

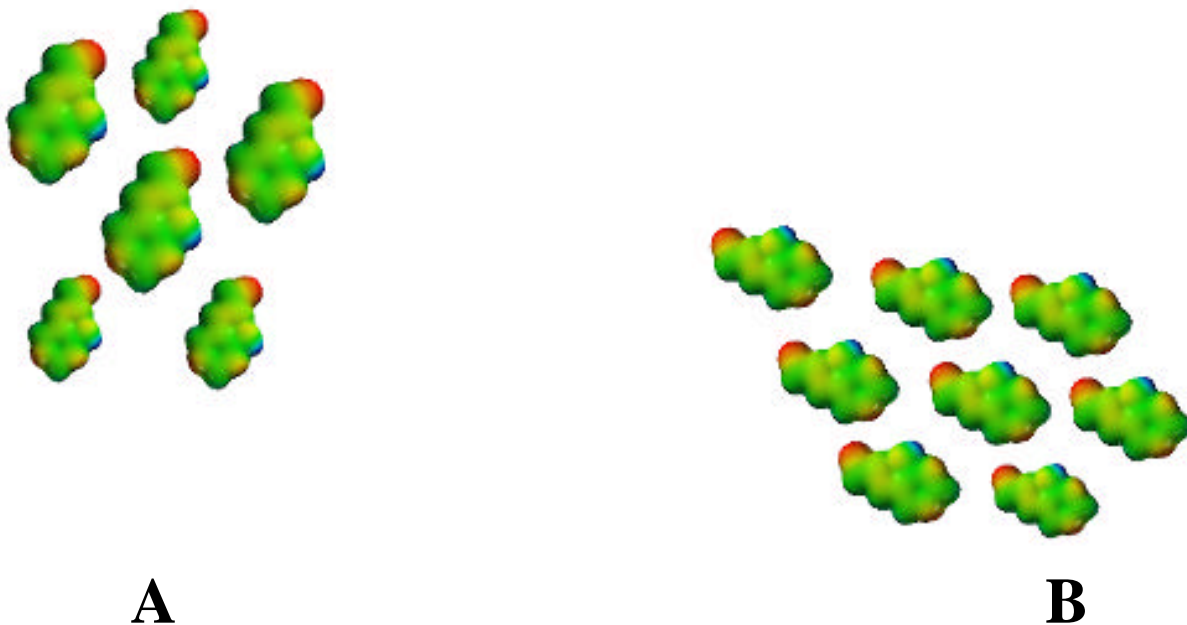


Figure 6. Translated and Rotated Charge Distributions.