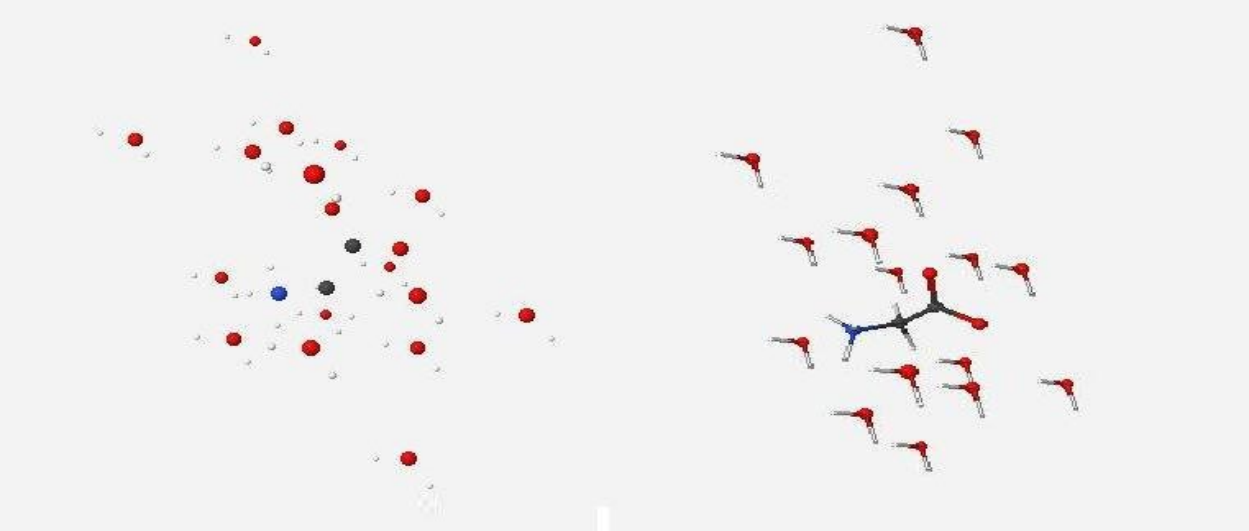
Illustration of a MOLECULAR CLUSTER



The Chemical "Molecule" itself would appear as a cluster of atoms, if the bonds connecting the atoms are not drawn. These atoms of a molecule can be placed at such distances from each other so that no interactions are possible among these atoms. This would appear simply as a cluster of atoms and remain so. If a Geometrical Optimization is carried out with the tools of Computational Chemistry, then the resulting stable structure due to the minimization of energy for the system of interacting atoms would be a molecule for which bond connectivity can be assigned to call it a molecule which has an independent stable existence; and not merely a cluster of atoms.

Having the possibility to realize Molecular systems from Cluster of atoms, it may be natural to enquire further what would happen if a cluster of molecules are subjected to the same kind of Geometrical Optimization. Then it is question of Molecular clusters resulting in a optimized stable system.

The approach in this presentation falls under this category of investigation with the tools of Computational Chemistry.

In the picture above find that on the left hand side, there are no bonds drawn and the entire system seems well described as a cluster of atoms. On the right hand side for the same set of atoms (in the same relative disposition on the Left), the bonds have been drawn and it would be possible to recognize a Glycine molecule at the center and surrounded by water molecules. Possible differences are due to the differences in the perspectives arising while displaying using the visualization tool (structure editor).

Such a cluster of molecules with or without bonds drawn can be submitted as input to a Computational Chemistry Software and would result in the optimized disposition for the molecules in the cluster. These programs require the only atomic coordinates as input and the molecular cluster can be treated as cluster of atoms and the calculations would proceed. Caution must be exercised if any symmetry specifications are required at the input stage.

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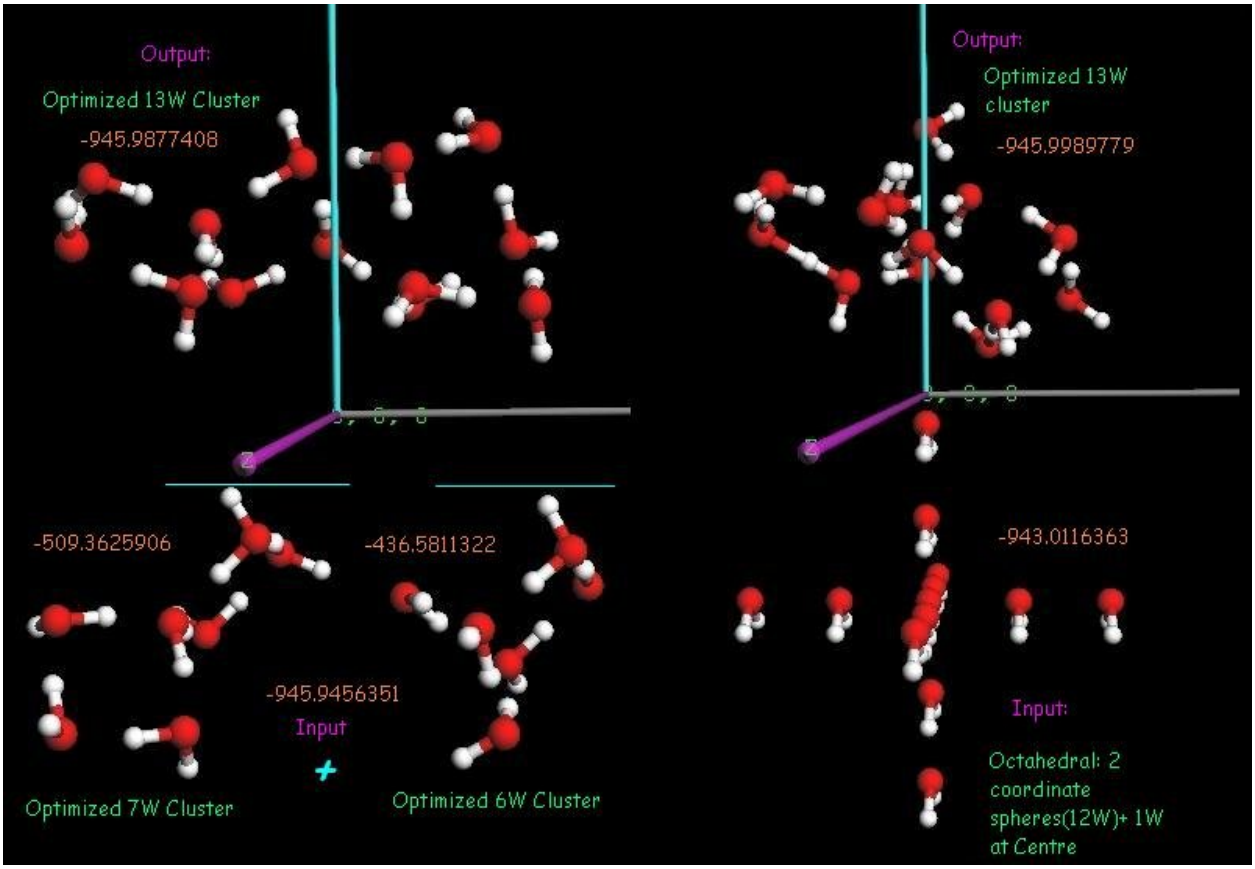

Above Left:

Two clusters of water molecules one with 6 water molecules and another with 7 water molecules have been initially optimized separately. Thus optimized clusters are put together to form a larger cluster of 13 water molecules. And this system of two (optimized clusters) when subjected to Geometrical Optimization results in an optimized cluster of 13water molecules. Relevant energy data are given above. The details of the actual quantum chemical method chosen is not given above since at this moment this may be a detail which can be deferred.

Above Right:

A 13 water molecules-cluster with the constituent molecules arranged with a well defined symmetrical order was subjected to the same Geometrical Optimization as for the system on the left.

The resulting Optimized molecular cluster of 13 molecules is also displayed with the comparable data.

This illustration is mainly for noting the possible queries which can arise from such an approach.

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