

## Partial Atomic Charge Derivation of small molecule

Partial atomic charge is very crucial for computing physical, chemical and biological properties, and reactivity of molecules. Through the information of the atomic charge in a given species, it is possible to predict the stability, solvation energetics of various molecules, and course of a particular reaction, determine its interaction with biological molecules and so on. The usefulness, notwithstanding, there is no direct method to determine the partial atomic charges from experiment. Also, there is no universally agreed upon best procedure for computing partial atomic charges. During the last few decades various methods have been developed to determine the partial atomic charges, but all these methods have their limitations.

**TPACM4:** Transferable Partial Atomic Charge Model – up to 4 bonds is used for deriving the partial atomic charges of small molecules for use in protein/DNA-ligand docking and scoring. The main idea of TPACM4 is based on a look up table of template fragments consisting of 4-bond paths around the atom being charged. This method overcomes the limitations of time complexity of assigning the partial atomic charges of a given molecule. The low value of average error against an experimentally/QM observable physico-chemical properties indicates the reliability comparable to the RESP/AM1BCC results. The structural input data for the TPACM4 is the pdb file format of small molecule.

### How to Use:

**Step 1: Provide the formal charge of the ligand.**

**Step 2: Upload the ligand molecule in pdb format on click on the Browse option.**

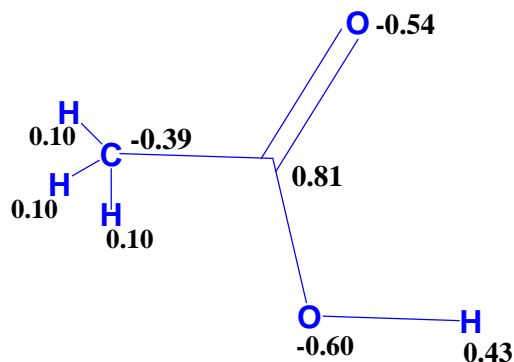
**Step 3: Then click on Submit.**

|   |                                      |  |
|---|--------------------------------------|--|
| Formal Charge   | <input type="text" value="0"/>       | <b>Provide the formal charge of the ligand</b> |
| Input PDB file  | <input type="text"/>                 | <input type="button" value="Browse..."/>       |
| <b>Upload the ligand molecule in pdb format on click on the Browse option</b> |                                      |  |
| <input type="button" value="Submit"/>   | <input type="button" value="Reset"/> | <b>Then click on Submit</b>                    |

Formal Charge of a molecule is the sum of the partial atomic charge of the molecule. It has to be an integer number. Say, for acetic acid the sum of the partial atomic charge of the molecule is zero. Therefore the formal charge of the molecule is zero. However for calculating the formal charge partial atomic charge concept is not required, it is first to see the valency (how many bonds are connected to the concerned atom) of each atom in a molecule. Then add the valency of all atoms to get the formal charge of the molecule.

| Element | Valency | Formal charge |
|---------|---------|---------------|
| C       | 4       | 0             |
| H       | 1       | 0             |
| N       | 3       | 0             |
| N       | 4       | 1             |
| N       | 2       | -1            |
| O       | 2       | 0             |
| O       | 3       | 1             |
| O       | 1       | -1            |
| S       | 2       | 0             |
| S       | 4       | 0             |
| S       | 6       | 0             |
| S       | 3       | 1             |
| S       | 5       | 1             |
| S       | 1       | -1            |
| P       | 3       | 0             |
| P       | 5       | 0             |
| P       | 4       | 1             |
| X       | 1       | 0             |

X is halogen atom



Acetic acid formal charge is zero here, because the formal charge of each atom is zero, therefore the sum of the partial atomic charge should be  $(-0.54+0.81-0.60-0.39+0.43+0.1+0.1+0.1)\approx 0$ .