# Partial Molar Volume Calculation

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November 10, 2015

The partial molar volume is given by the apparent volume in this calculation. Voloshin et. al. use $V_{app} = V_{int} + V_{hyd} - \frac{N_{hyd}}{\rho_0}$, where $V_{int}$ is the voronoi volume of the protein, $V_{hyd}$ is the volume of first hydration shell, $N_{hydr}$ is the number of waters in the first hydration shell, and $\rho 0$ is the number density of bulk water.[1]

The Voronoi polyhedra program calculates the volume of every atom in the box. The Voronoi polyhedra volume of the polymer ($VP_{int}$) was calculated by summing all of the volumes for each atom in the polymer. The Voronoi polyhedra volume of the first hydration shell ($VP_{hyd}$) was calculated by summing all of the volume for each atom in the first hydration shell. The Voronoi polyhedra of the bulk waters ($\frac{N_{hyd}}{\rho_0} = VP_b$) was averaged. The average volume was then multiplied by the number of atoms in the first hydration shell. This was so the Voronoi polyhedra volume of the first hydration shell and bulk water was for the same number of waters.

The Partial Molar Volume = $VP_{int}$ + $VP_{hyd}$ - $VP_b$.

**The Code for calculating the PMV:**

```
def partialMolarVolume(self):
       ### calculate the average volume of a bulk water molecule ###
       bulkVolume =0
       bulkCount =0
       for i in range(0, len(self.Shells)):
              if( self.Shells[i] == 'B'):
                   bulkVolume += self.Volume[i]
                   bulkCount +=1
       #### get the average volume of a single water in bulk
       avgbulkVolume = bulkVolume/(bulkCount*1.0)
       ## use the avgBulkVolume and multiply by the number of waters in first shell
       ## this gives the bulk volume for a number of waters (N)
       NbulkVolume = avgbulkVolume * self.firstShellCount

       ### calculate the partial molar volume using equation from Voloshin paper
       PMV =  (self.polymerVolume + self.firstShellVolume - NbulkVolume )
       self.PMV = PMV
       self.__printToFile("PMV.dat",PMV)
```

# References


(1) Voloshin, V. P.; Medvedev, N. N.; Smolin, N.; Geiger, A.; Winter, R. *J. Phys. Chem. B* **2015**, *119*, 1881–1890.