Spherical Coordinates of the Icosahedral Water Clusters

Use of spherical coordinates is nicely applicable to symmetrical systems with molecules positioned on nested concentric spherical surfaces, such as the icosahedral water cluster. In place of the orthogonal x, y and z coordinates, r, θ (theta), and φ (phi) are used. The symbol r defines the distance from a central origin while θ and φ combine to define the direction. φ is the polar angle (from the z axis, latitude) and varies from 0° to 180°. θ is the azimuthal angle (in the xy plane, longitude) and varies between 0° to 360°.*

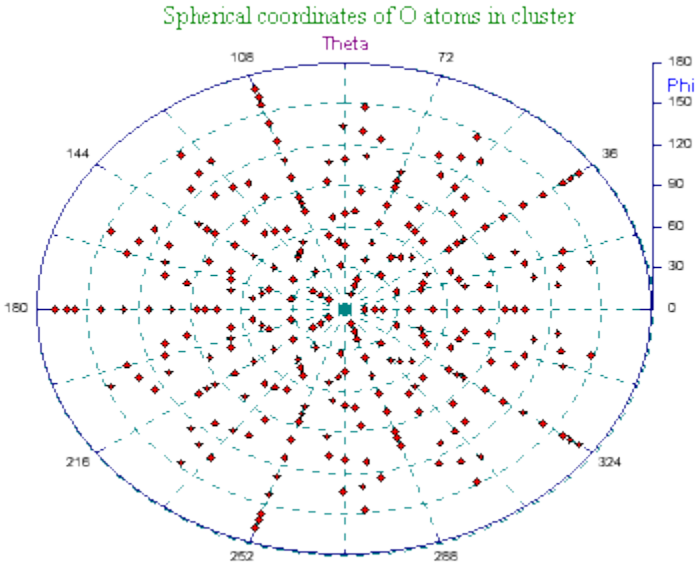

Figure 1. Spherical coordinates of the water oxygen atoms in icosahedral water clusters (ES). Radial values (r) are given on another page.

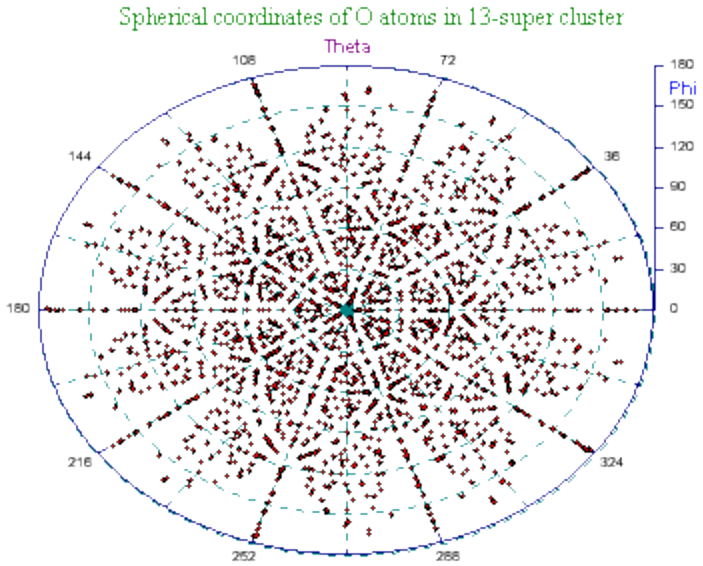

Figure 2. Spherical coordinates of the water oxygen atoms in a super cluster of 13 icosahedral water clusters (ES). Radial values (r) are given on another page.

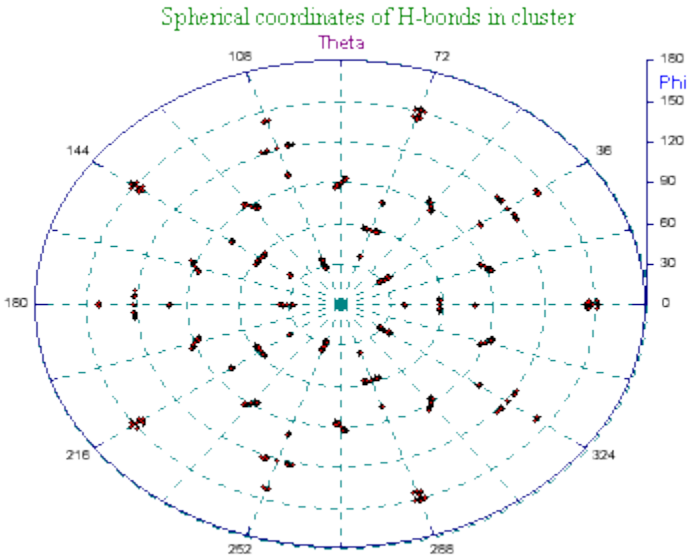

Figure 3. The hydrogen bonding angles of the water molecules in icosahedral water clusters (ES), given as spherical coordinates about their oxygen atoms.

* Conversion between (x, y, z) and (r, θ, φ) coordinate systems:

$r = \sqrt{(x^2+y^2+z^2)}$, $\theta = \arctan(y/x)$, $\varphi = \arccos(z/r)$

if x is positive and y is positive, $0° \le \theta \le 90°$

if x is negative and y is positive, $90° \leq \theta \leq 180°$

if x is negative and y is negative, $180° \leq \theta \leq 270°$

if x is positive and y is negative, $270° \leq \theta \leq 360°$

$x = r.\cos(\theta).\sin(\varphi)$, $y = r.\sin(\theta).\sin(\varphi)$, $z = r.\cos(\varphi)$

Source : http://www1.lsbu.ac.uk/water/spher.html