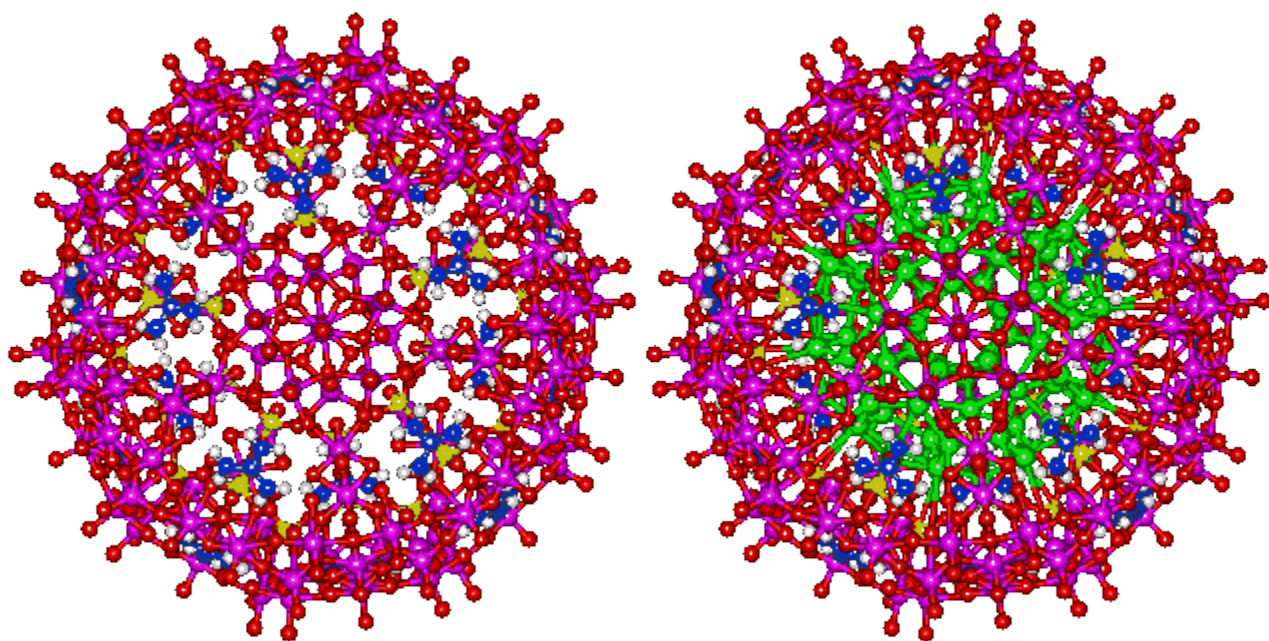


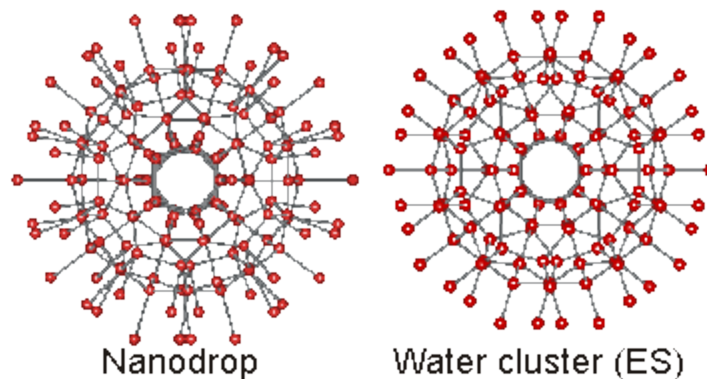
## Polyoxomolybdate and Aqueous Nanodrop



The water nanodrop consists of 100 water molecules inside a spherical polyoxomolybdate nanocapsule cluster  $\{(\text{Mo})\text{Mo}_5\}_{12}(\text{Mo}_2 \text{ spacer})_{30}$  [417]. The structure of the contained nanodrop may be modulated by changes in the surrounding molybdenum-based cluster [547]. The water molecules are held by ice-like hydrogen bonding with the attractive bond energies between of the 30 hydrogen bonds in the inner dodecahedron, the 50 hydrogen bonds in the inner two shells and all the hydrogen bonds in the outer shell of 60 water molecules calculated to be  $23.3 \text{ kJ mol}^{-1}$ ,  $29.7 \text{ kJ mol}^{-1}$  and  $28.9 \text{ kJ mol}^{-1}$  respectively [547]. The structure [417] is shown below with the interior  $\text{H}_2\text{O}$  oxygen atoms shown green on the right.

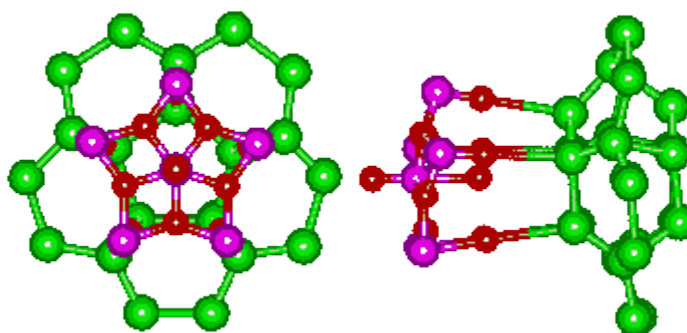


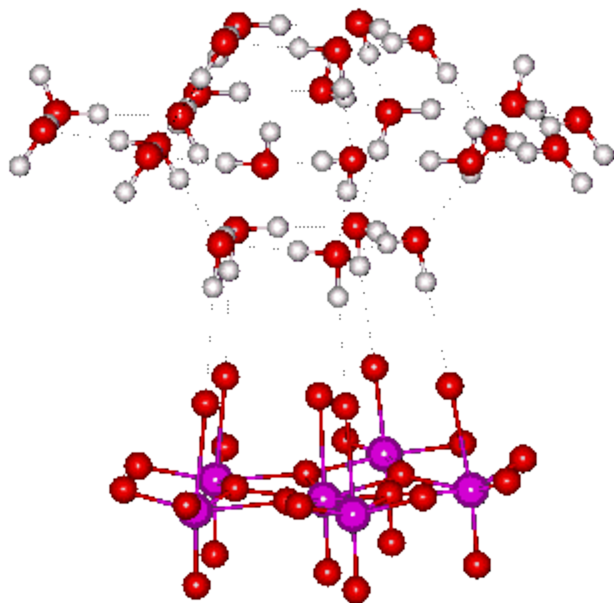
The inner four shells of ES, consisting of 160 water molecules (see below right), have been found in almost identical positions and orientations within the cavity-encapsulated icosahedral water nanodrop in the  $\{(\text{NH}_2)_3\text{C}\}_{20}\cdot\{(\text{Mo})\text{Mo}_5\text{O}_{21}(\text{H}_2\text{O})_6\}_{12}\cdot\{\text{Mo}_2\text{O}_4(\text{SO}_4)\}_{10}\cdot\{\text{Mo}_2\text{O}_4(\text{H}_2\text{PO}_2)\}_{20}\cdot 100\text{H}_2\text{O}$  cluster. The interactive structure of this cluster is available (Jmol) as is the water ES structure (Jmol).



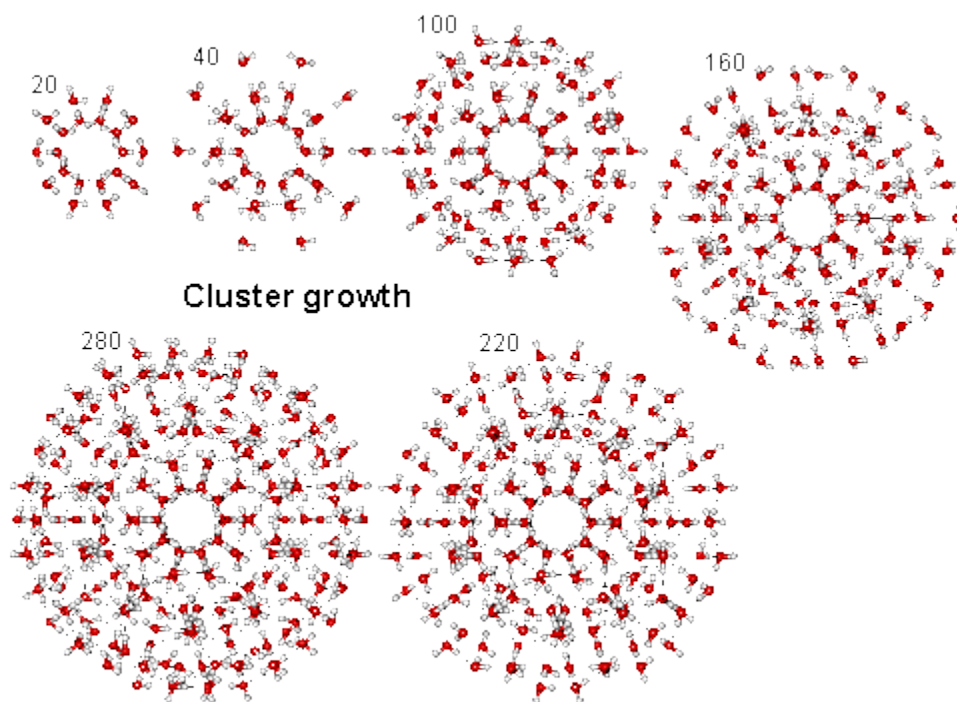
Shell	Nanodrop		Water cluster	
	Molecules	nm	Molecules	nm
1	20 H <sub>2</sub> O	0.38-0.40	20 H <sub>2</sub> O	0.39
2	20 H <sub>2</sub> O	0.65-0.68	20 H <sub>2</sub> O	0.66
3	60 H <sub>2</sub> O	0.76-0.79	60 H <sub>2</sub> O	0.79
4	60 O/H <sub>2</sub> O	1.06-1.07	60 H <sub>2</sub> O	1.06

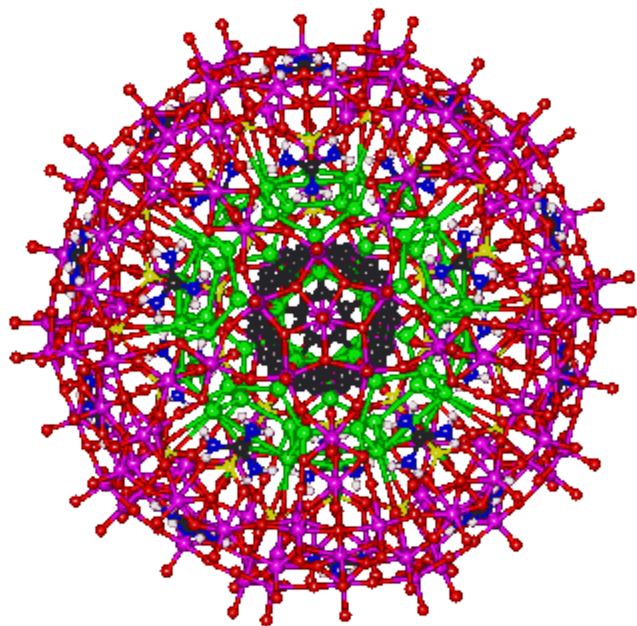
The linkage of water molecules (O-atoms shown green) to the pentagonal (Mo<sup>VI</sup>)Mo<sup>VI</sup><sub>5</sub> groups (Mo violet, O red) in the nanocapsule is shown below left. Five hydrogen-bonded links form between pentagonal boxes of water molecules (H<sub>2</sub>O)<sub>25</sub> in the nanodrop and each of twelve such groups. The full water molecules are shown on the right with the protons placed randomly.





The growth of the clustering is shown below, where the clustering up to 160 molecules of water is as within both the nanodrop and icosahedral water (*ES*) cluster whereas the larger clusters are found in *ES* only.





The structuring of the water inside the  $\{(Mo)Mo_5\}_{12}(Mo_2 \text{ spacer})_{30}$  nanocapsule and outside the  $C_{60}$  fullerene are easily matched and allows the possibility of containing a  $C_{60}$  fullerene within the nanodrop, as shown opposite. This cluster has not been found or even described until now, but is thought quite possible when considering the high solubility of both materials and the mechanism of formation of the nanocapsule. The interactive structure of this cluster is available ([Jmol](#)).

Source: <http://www1.lsbu.ac.uk/water/nano2.html>