Electronic Supplementary Information (ESI)

The long-range convergence of the energetic properties of the water monomer in bulk water at room temperature

Stuart J. Davie, Peter Maxwell, Paul L. A. Popelier*

Manchester Institute of Biotechnology (MIB), 131 Princess Street, Manchester M1 7DN, Great Britain

and

School of Chemistry, University of Manchester, Oxford Road, Manchester M13 9PL, Great Britain

Corresponding Author

paul.popelier@manchester.ac.uk, +44 161 3064511
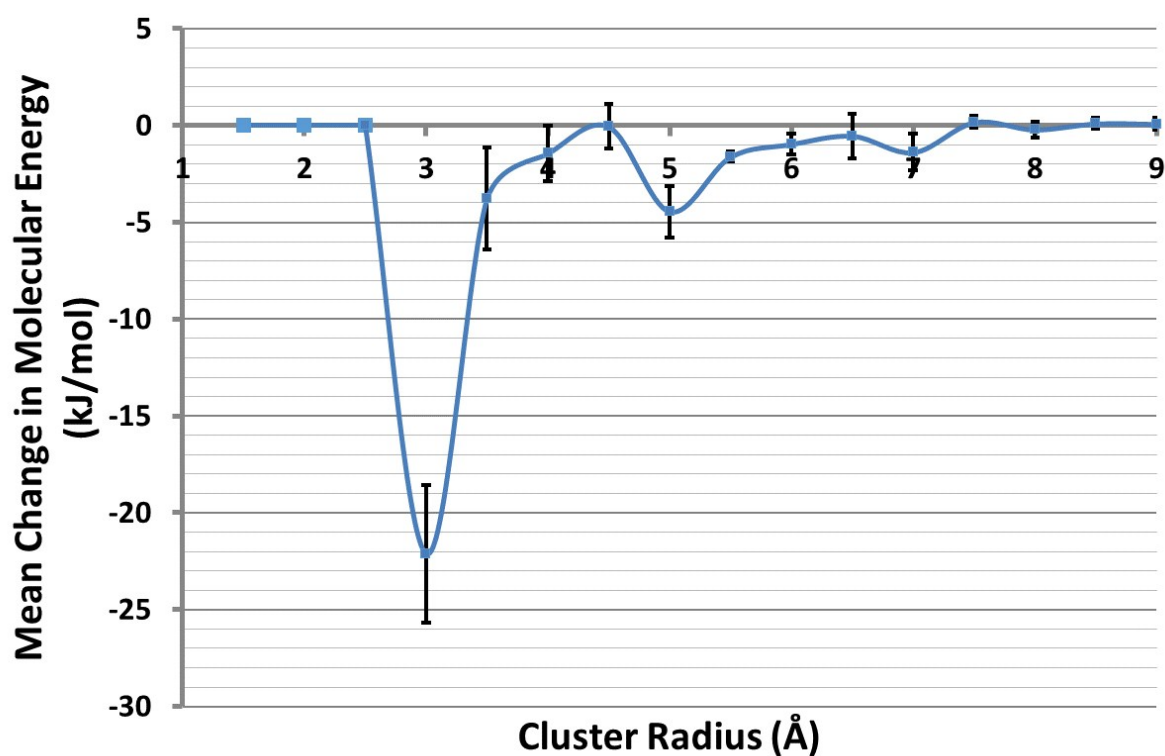
ENERGIES

Total molecular energy

Figure ESI1. Mean change in total IQA molecular energy of a water monomer inside a water cluster (relative to the isolated monomer's energy, which is set to zero). Error bars represent ±1 standard deviation.
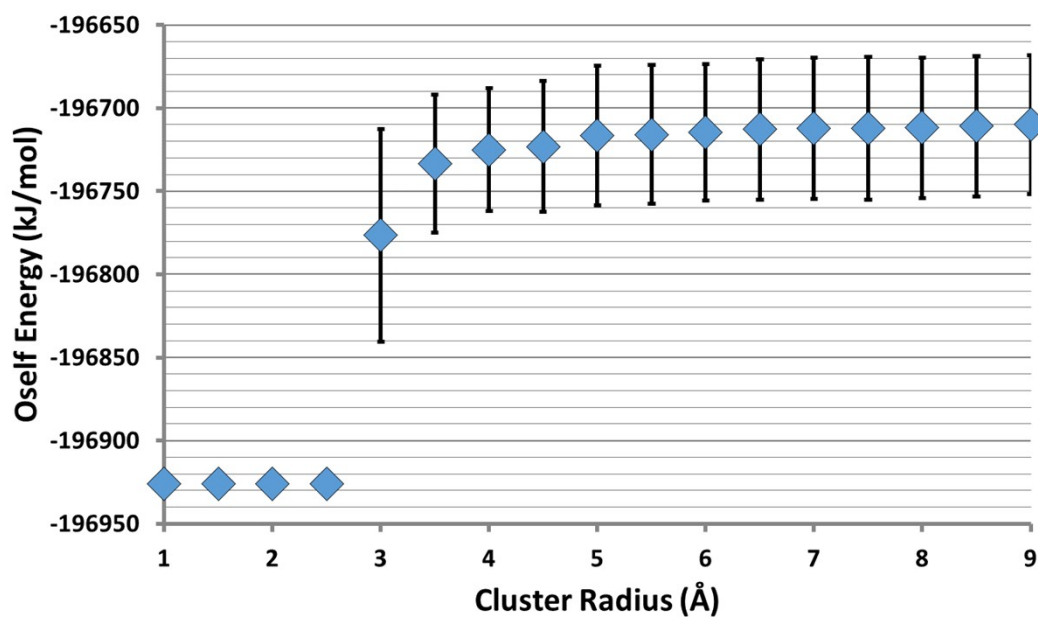
Atomic self-energy

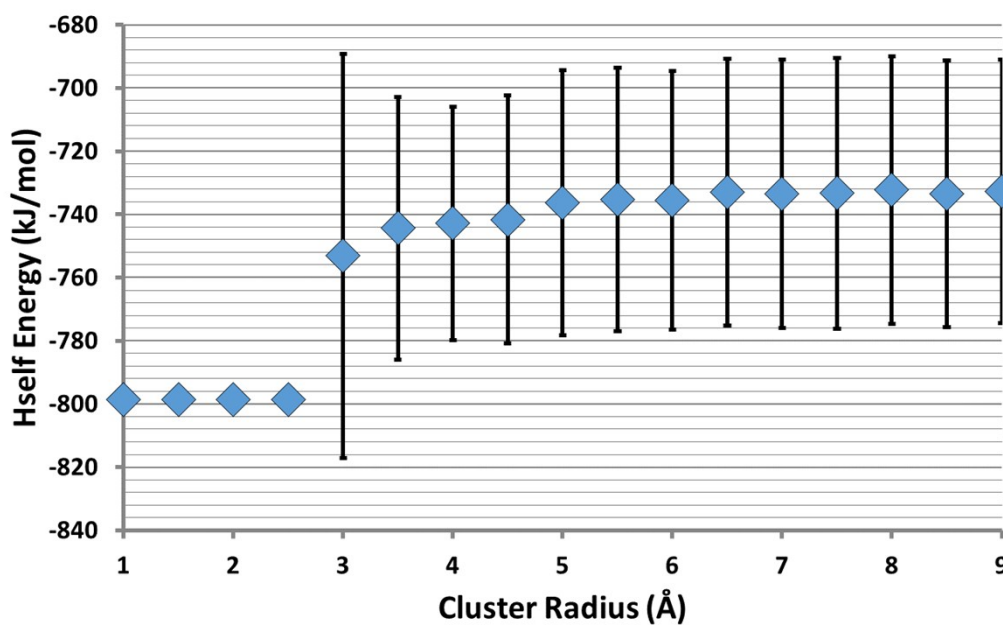**Figure ESI2**. Mean oxygen IQA self-energy. Error bars represent ±1 standard deviation.

Figure ESI3. Mean hydrogen IQA self-energy. Error bars represent ±1 standard deviation.
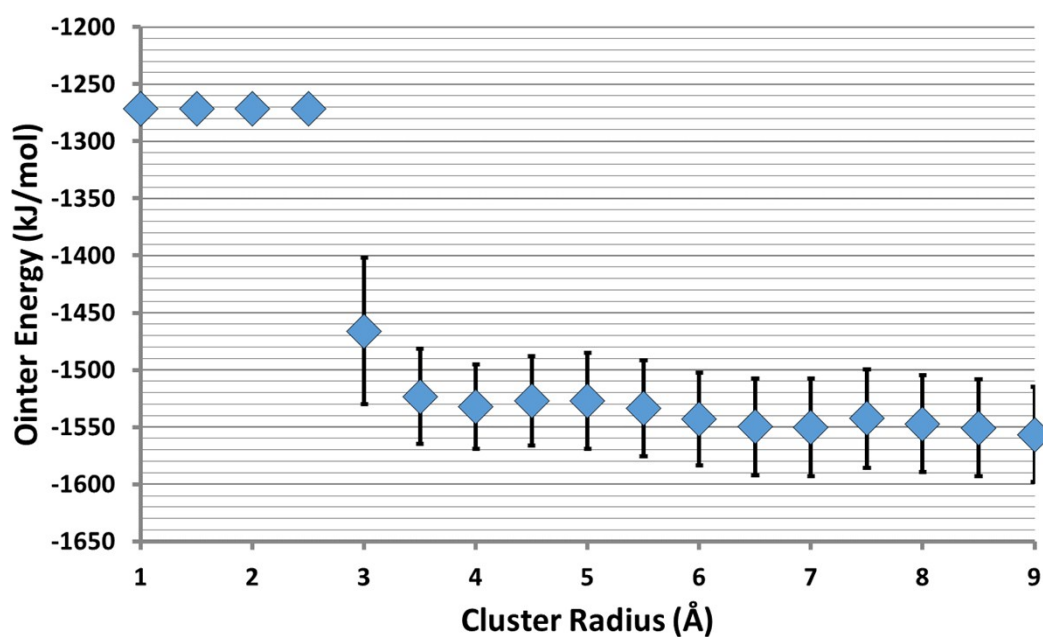
Atomic interaction energy

Figure ESI4. Mean oxygen IQA interaction energy. Error bars represent ±1 standard deviation.
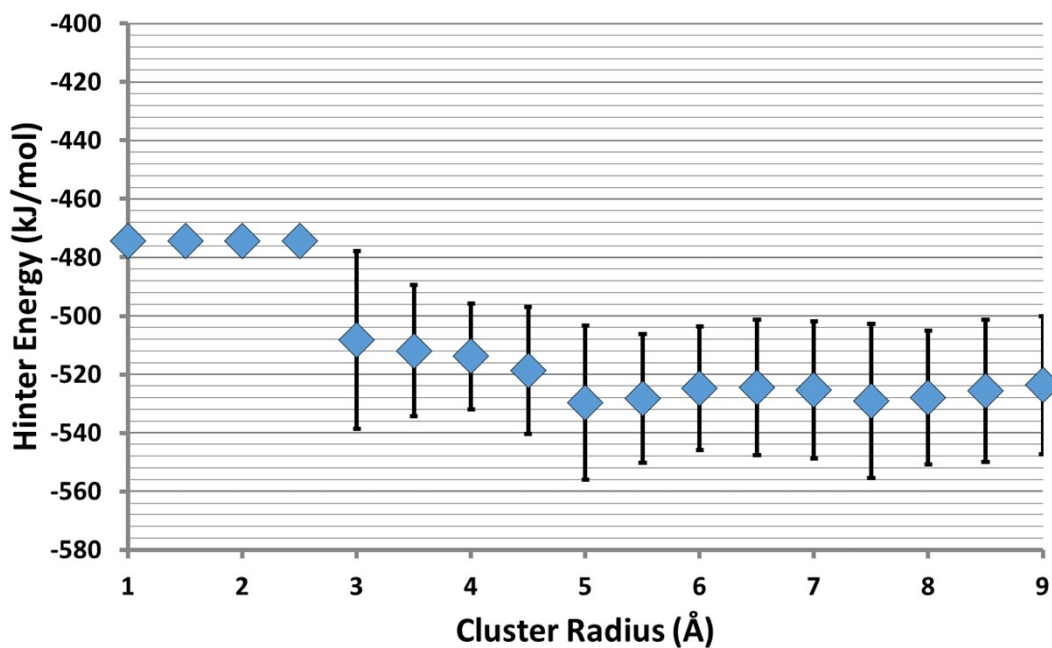

Figure ESI5. Mean hydrogen IQA interaction energy. Error bars represent ±1 standard deviation.

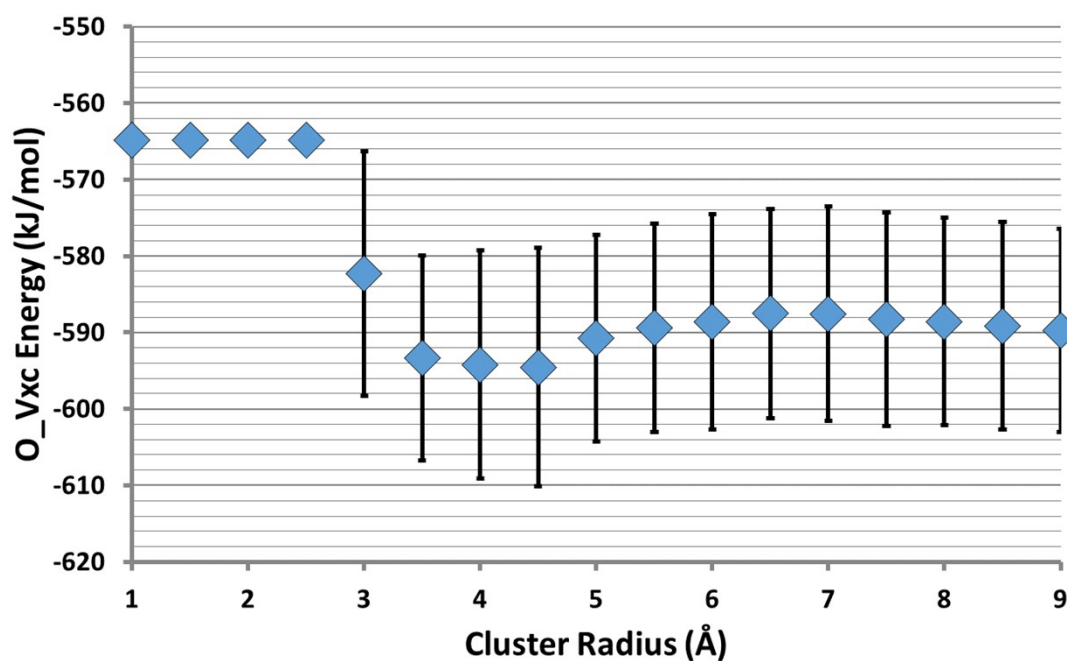# Atomic exchange energy

Figure ESI6. Mean oxygen IQA exchange-correlation energy. Error bars represent ±1 standard deviation.

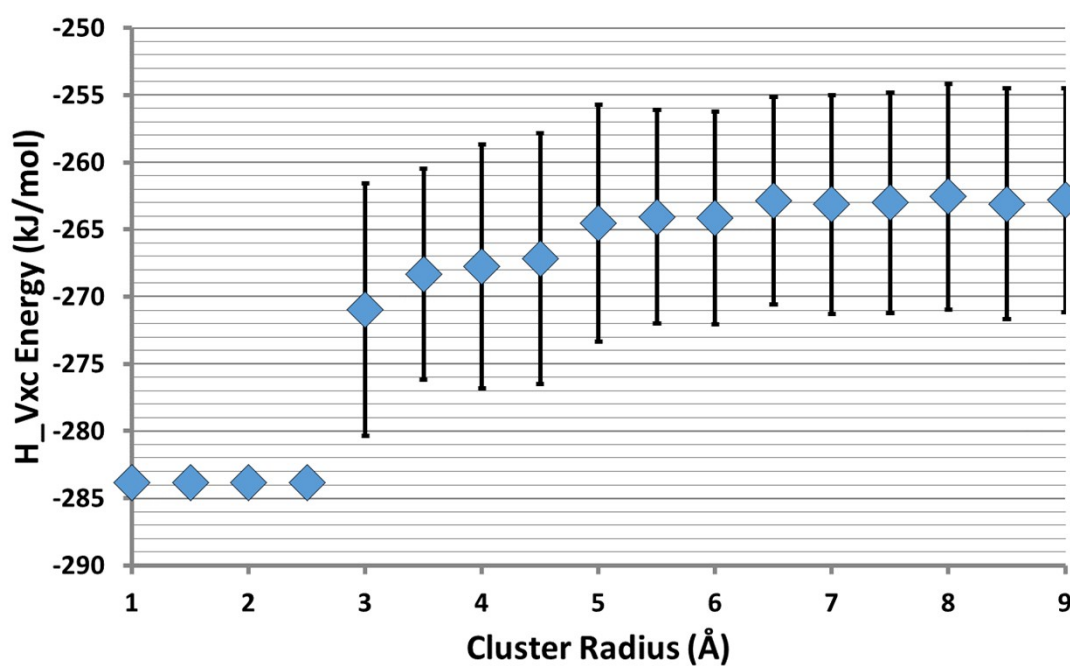**Figure ESI7**. Mean hydrogen IQA exchange-correlation energy. Error bars represent ±1 standard deviation.

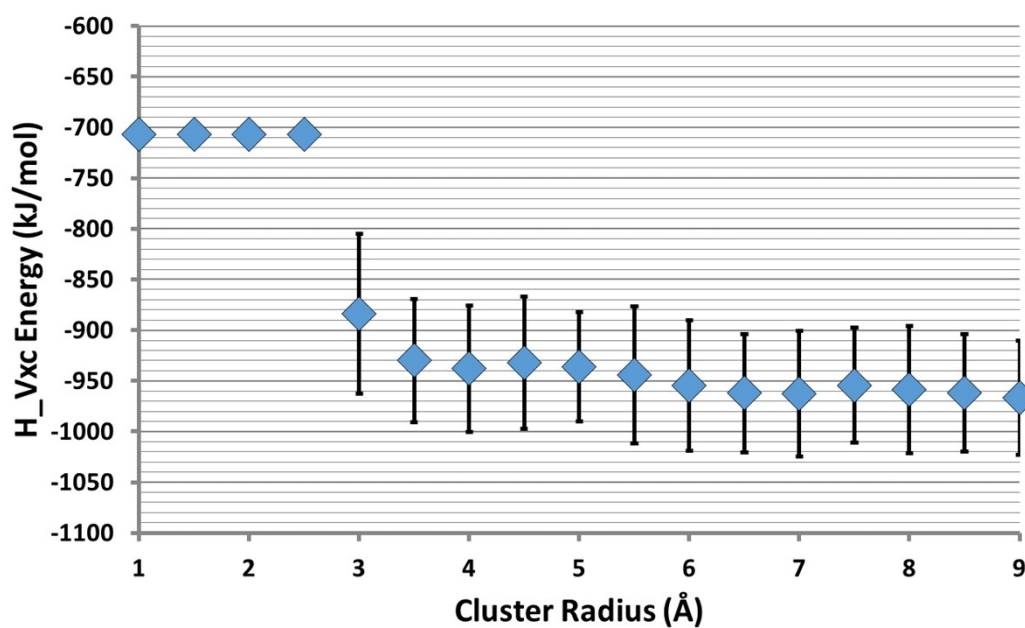# Atomic classical electrostatic energy

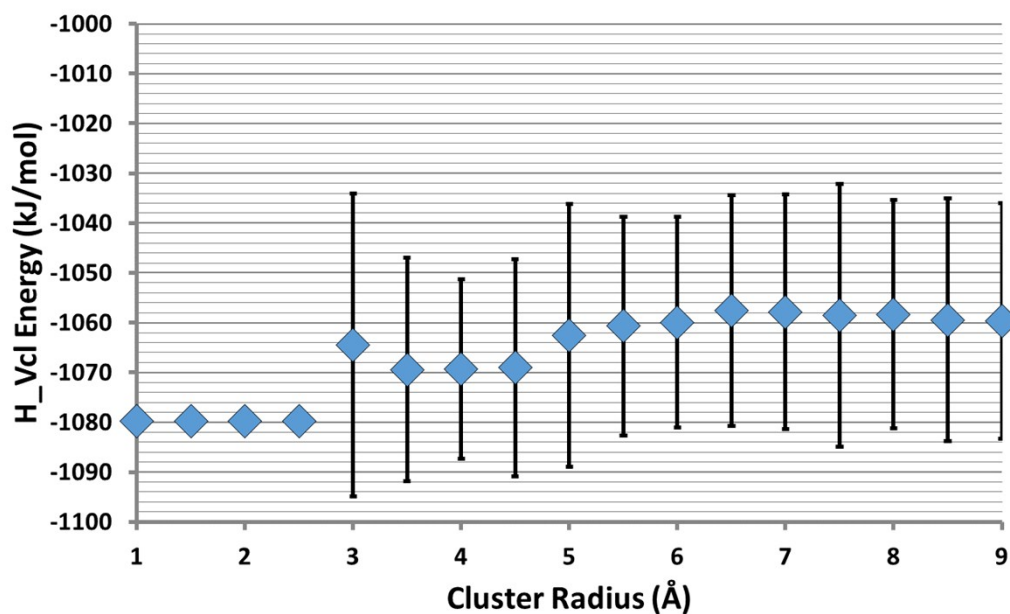**Figure ESI8**. Mean oxygen IQA classical electrostatic energy. Error bars represent ±1 standard deviation.

Figure ESI9. Mean hydrogen IQA classical electrostatic energy. Error bars represent ±1 standard deviation.
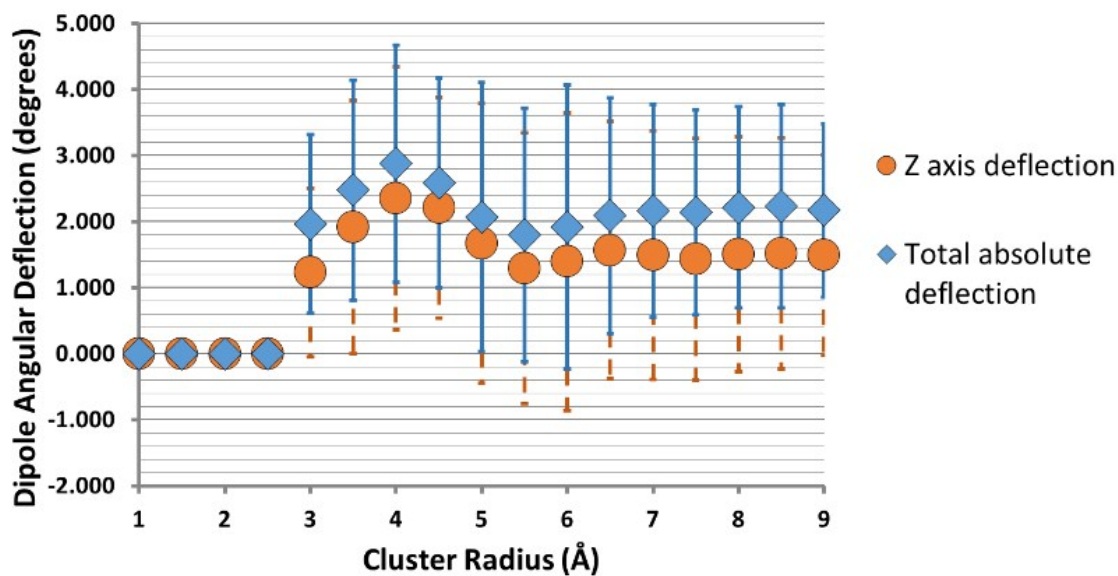
MULTIPOLE MOMENTS

Dipole Moment

Figure ESI10. Deflection of the molecular dipole moment. Blue represents that absolute deflection with respect to the initial vector, while orange represents the deflection in the z-axis (i.e. out of the HOH plane). Error bars represent ±1 standard deviation.
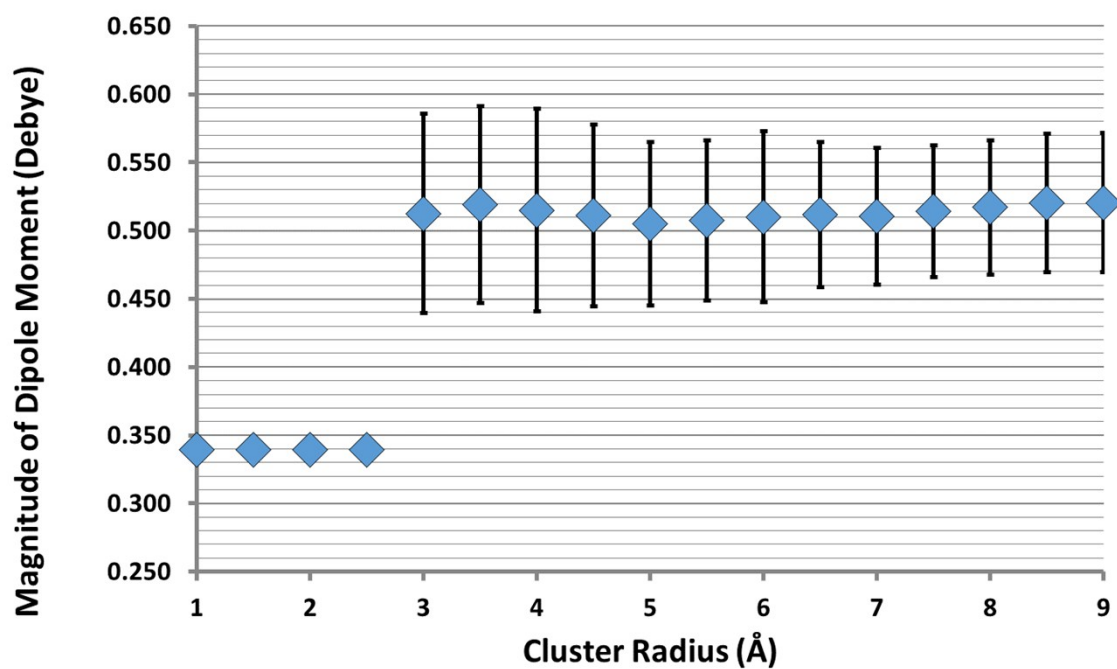
Figure ESI11. Mean magnitude of the dipole moment of the central oxygen atom. Error bars represent ±1 standard deviation.
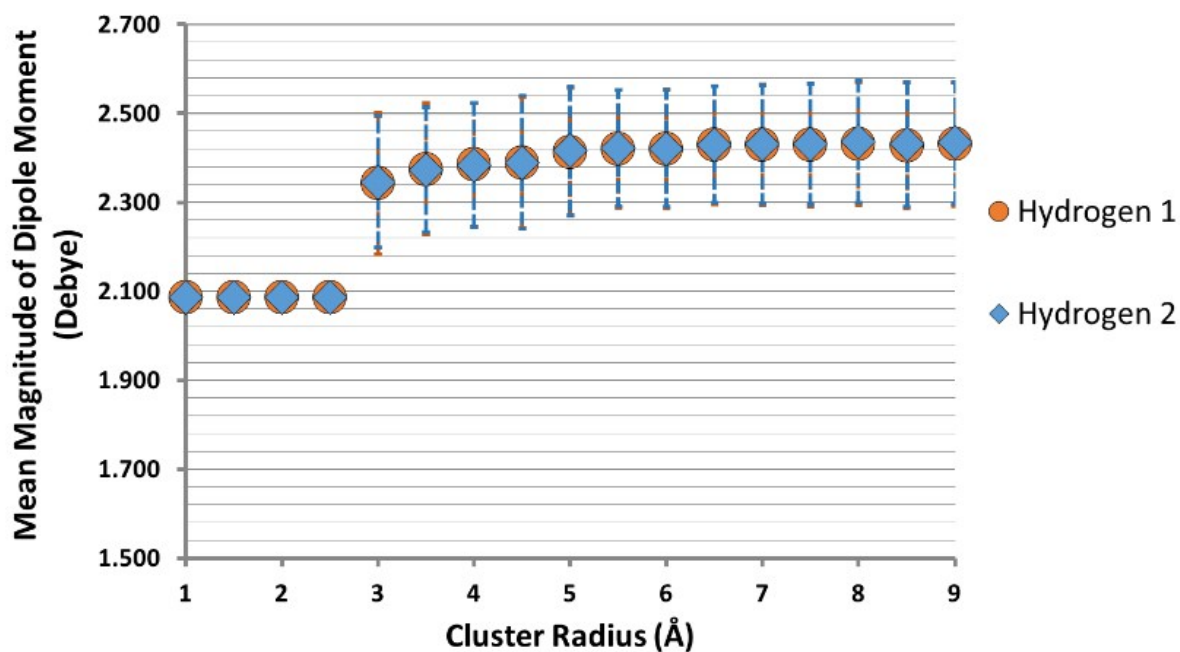

Figure ESI12. Mean magnitude of the dipole moment of the hydrogen atoms of the central molecule. Error bars represent ±1 standard deviation.
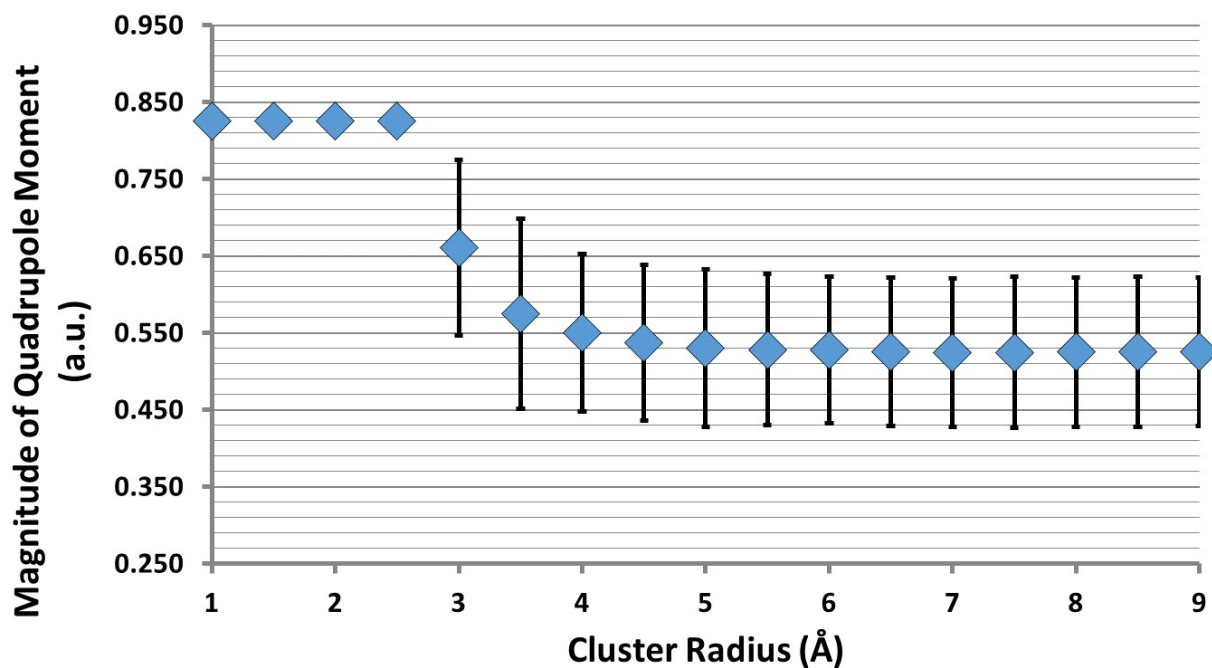
Quadrupole Moment

Figure ESI13. Mean magnitude of the quadrupole moment of the oxygen atom of the central molecule. Error bars represent ±1 standard deviation.
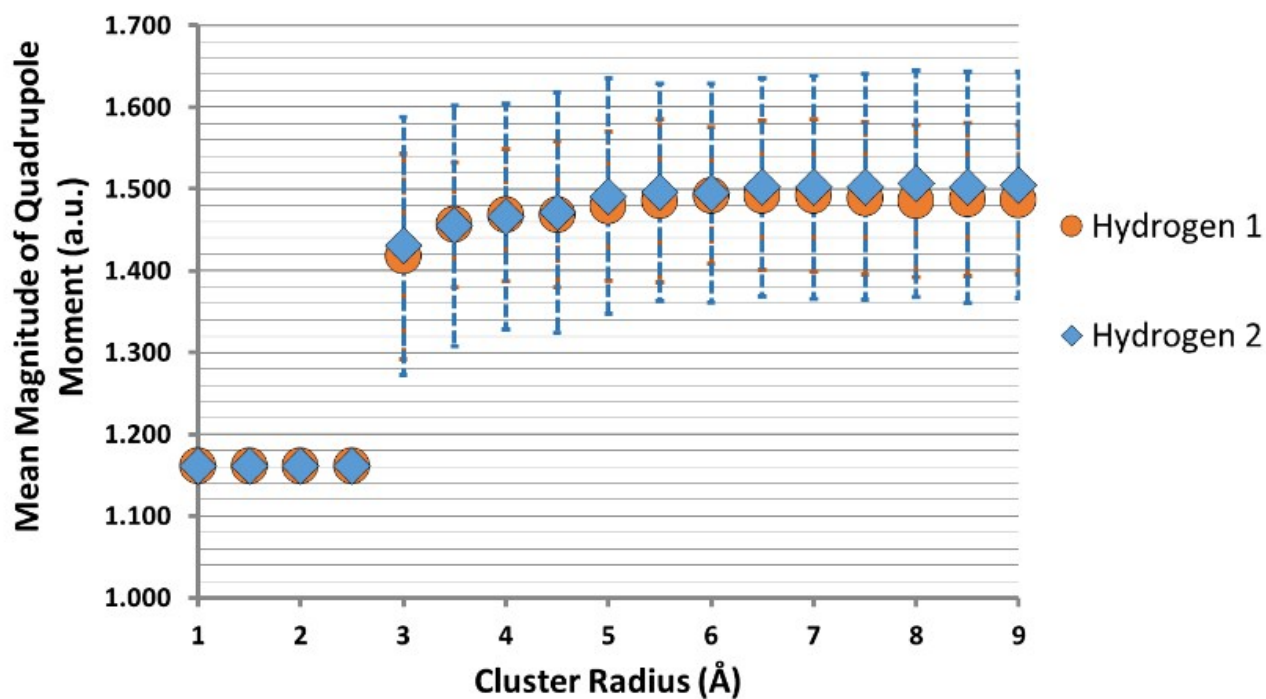

Figure ESI14. Mean magnitude of the quadrupole moment of the hydrogen atoms of the central molecule. Error bars represent ±1 standard deviation.