A Brief Population Analysis on Polarized Water

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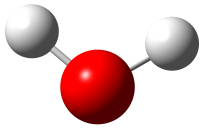
Contents

Non-polarized Water

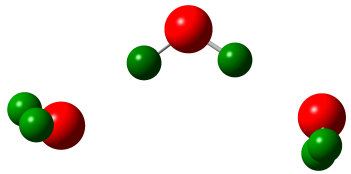


Atom charges	Mulliken	NPA	ESP(MK)
O	-0.603	-0.936	-0.724
H	0.302	0.468	0.362
H	0.302	0.468	0.362

Table: Atomic charges (a.u.) on each atom of non-polarized water

All results are calculated under M06-2X/def2-QZVP with Gaussian16.

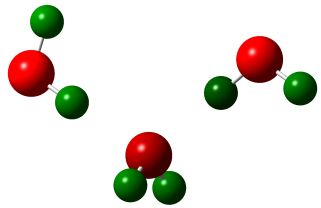
Case I – Polarized by Another 2 Water Molecule



Atom charges	Mulliken	NPA	ESP(MK)
O	-0.642	-1.011	-0.877
H	0.295	0.486	0.449
H	0.274	0.483	0.379

Table: Atomic charges (a.u.) on each atom of polarized water, Case I

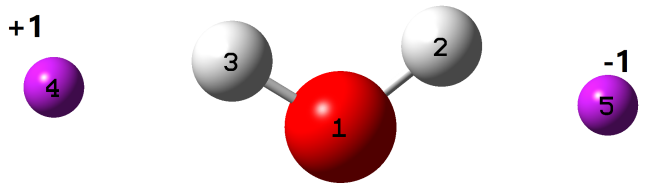
Case II – Polarized by Another 2 Water Molecule



Atom charges	Mulliken	NPA	ESP(MK)
O	-0.655	-0.950	-0.550
H	0.353	0.496	0.358
H	0.352	0.495	0.341

Table: Atomic charges (a.u.) on each atom of polarized water, Case II

Case III – Polarized by Background Charges



Atom charges	Mulliken	NPA	ESP(MK)
O	-0.365	-0.787	-0.523
H	0.720	0.647	0.725
H	-0.354	0.139	-0.202

Table: Atomic charges (a.u.) on each atom of polarized water, Case III

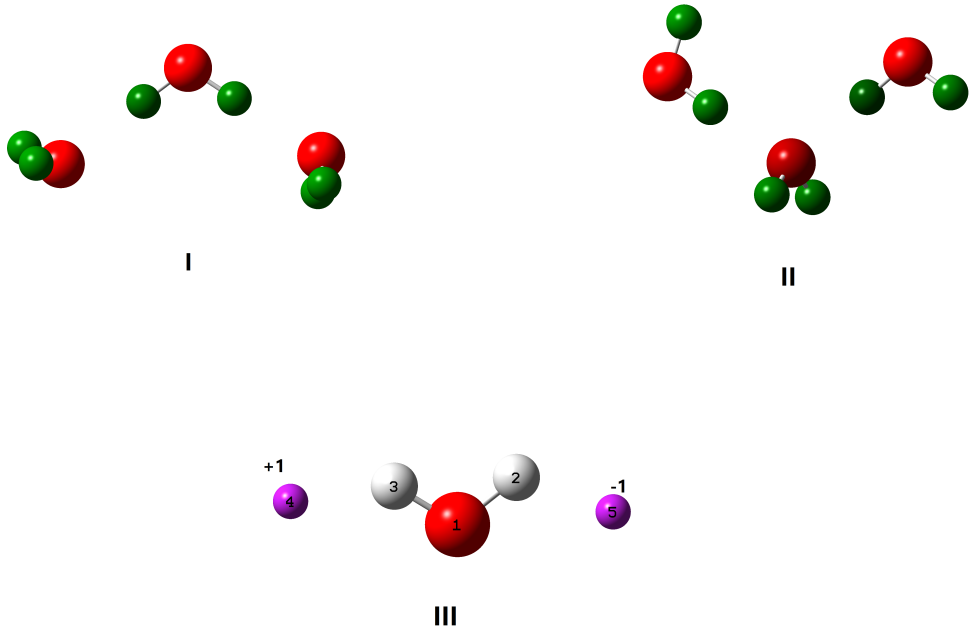
Case IV – Solvated Water

Atom charges	Mulliken	NPA	ESP(MK)
O	-0.640	-0.950	-0.763
H	0.320	0.475	0.381
H	0.320	0.475	0.381

Table: Atomic charges (a.u.) on each atom of water in cyclohexane solvent (PCM model)

The results show that water molecule is a little bit more polarized in cyclohexane.

Summary



Atom	non-polarized	I	II	III	IV
O	0	-0.153	0.174	0.201	-0.039
H	0	0.087	-0.004	0.363	0.019
H	0	0.017	-0.021	-0.564	0.019

Table: changes of ESP charges on each atom (set non-polarized results as zero)

Thank You