



A Brief Population Analysis on Polarized Water

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Non-polarized Water

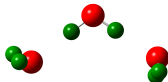
Polarized Water

第二章标题





Configuration I



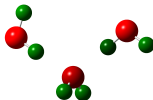
Atom charges	Mulliken	NPA	ESP(MK)
O	-0.642	-1.011	-0.877
H	0.295	0.486	0.449
H	0.274	0.483	0.379
dipole			

Table: Atomic charges on each atom of polarized water





Configuration II



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
dipole			

Table: Atomic charges on each atom of polarized water



Thank you!

Q&A

