

Table 2: MB-UCB parameters for water

Multipoles									
Atom O		MDQ			MD				
q				-0.51966					-0.48660
μ_z				0.14279					-0.00245
Q_{xx}				0.56803					
Q_{yy}				-0.65906					
Q_{zz}				0.09103					
Atom H									
q				0.25983					0.24330
μ_x				-0.03859					-0.04508
μ_z				-0.05818					-0.24502
Q_{xx}				-0.01730					
Q_{yy}				-0.07631					
Q_{xz}				0.00007					
Q_{zz}				0.09361					
Polarizabilities									
Atom	α_{xx}	α_{xy}	α_{xz}	α_{yx}	α_{yy}	α_{yz}	α_{zx}	α_{zy}	α_{zz}
O	0.9412	-0.0007	-0.0061	-0.0007	0.9148	-0.0000	-0.0061	-0.0000	0.9417
H	0.2687	-0.0002	0.0938	-0.0002	0.1941	0.0005	0.0938	0.0005	0.2224
Charge penetration									
Atom	Z	α			β				
O	6	3.5000			3.1310				
O	1	3.3000			3.1780				
Charge transfer									
Atom	α^{ct}	b			d				
O	0.00219	0.59624			0.91593				
O	0.69555	0.05525			1.16358				
van der Waals									
Atom	Diameter (Å)	ϵ (kcal/mol)			H reduction factor				
O	3.5992	0.1416							
H	3.1409	0.0127			0.9100				