Oxygen Atomic Charge in H_2O

Mulliken Population Analysis,
HF/STO-3G structure, C_{2v} sym.

Theoretical Method	Rel. CPU	q(O)	Basis Functions
Hartree-Fock + Pople Basis Sets			
HF/STO-3G	1.00	-0.331	[2s1p,1s]
HF/3-21G	1.00	-0.705	[3s2p,2s]
HF/6-31G(d)	1.16	-0.853	[3s2p1d,2s]
HF/6-31G(d,p)	1.21	-0.675	[3s2p1d,2s1p]
HF/6-31+G(d,p)	1.23	-0.727	[4s3p1d,2s1p]
HF/6-31++G(d,p)	1.23	-0.704	[4s3p1d,3s1p]
Hartree-Fock + cc-Basis Sets			
HF/cc-pVDZ	1.16	-0.333	[3s2p1d,2s1p]
HF/aug-cc-pVDZ	1.35	-0.360	[4s3p2d,3s2p]
HF/cc-pVTZ	2.00	-0.490	[4s3p2d1f,3s2p1d]
HF/aug-cc-pVTZ	13.5	-0.485	[5s4p3d2f,4s3p2d]
HF/cc-pVQZ	35.6	-0.543	[5s4p3d2f1g,4s3p2d1f]
Becke3LYP + cc-Basis Sets			
B3LYP/cc-pVDZ	2.49	-0.277	[3s2p1d,2s1p]
B3LYP/aug-cc-pVDZ	3.05	-0.211	[4s3p2d,3s2p]
B3LYP/cc-pVTZ	4.56	-0.447	[4s3p2d1f,3s2p1d]
B3LYP/aug-cc-pVTZ	16.7	-0.405	[5s4p3d2f,4s3p2d]
B3LYP/cc-pVQZ	38.3	-0.508	[5s4p3d2f1g,4s3p2d1f]