Table1. The time saving results for CCSD iterations of ground state energy calculation in double- and mixed-precision are shown in the tables below. The calculations were running for water clusters consisting of 1 to 7 water molecules with 3-21g basis set. It is shown that the proposed mixed-precision method has comparable accuracy as double-precision calculation and can reach the expected time saving with the increasing system size. (*Accuracy column shows how many digits after the decimal places can the results match with PSI4 package.)

	Double-precision(dp)			Mixed-precision(mp)			Single-precision(sp)				
Number of H_2O	Time/s	Iterations	Accuracy*	Time /s	Iterations	Accuracy	Time /s	Iterations	Accuracy	Time savings (mp)	Time savings (sp)
2	2.69	15	6	1.64	15	6	1.52	15	5	0.609665	0.565056
3	23.28	16	6	13.14	16	6	11.57	16	4	0.564433	0.496993
4	122.95	16	6	61.97	15	5	60.47	15	2	0.504026	0.491826
5	428.63	17	6	239.43	17	6	209.77	17	5	0.558594	0.489396
6	1211.93	17	6	617.63	16	6	621.28	16	4	0.509625	0.512637
7	2790.41	17	6	1497.20	17	6	1432.02	17	4	0.536552	0.513193