FCI quality energy for an (8e,957o) active space of H_2O in a cc-pV9Z basis set

I. INTRODUCTION

Table I.

	cc-pV2Z	cc-pV3Z	cc-pV4Z	cc-pV5Z	cc-pV6Z	cc-pV7Z	cc-pV8Z	cc-pV9Z	CBS
RHF	-76.026 77 88	-76.057 139 16	-76.064 804 29						
CCSD	-76.237 998 10	-76.324 545 75	-76.350 800 61						
CCSD(T)	-76.241 033 59	-76.332 192 23	-76.359 793 96						
CCSDT	-76.241 195 72	-76.332 268 49	-76.359 807 24						
CCSDT(Q)	-76.241 679 91	-76.332 623 49	-76.360 217 39						
CCSDTQ	-76.241 650 58	-76.332 587 70	-76.360 183 01						
CCSDTQ(P)	-76.241 665 00	-76.332 602 77	-76.360 189 48						
CCSDTQP	-76.241 665 92	-76.332 606 22	-76.360 198 47						
CCSDTQP(H)	-76.241 667 98	-76.332 606 77	-76.360 199 02						
CCSDTQPH	-76.241 668 32	-76.332 606 94	-76.360 199 19						
CCSDTQPH(S)	-76.241 668 38	-76.332 606 99(10)	-76.360 199 24						
CCSDTQPHS	-76.241 668 43	-76.332 607 05(10)	-76.360 199 29						
CCSDTQPHS(O)	-76.241 668 43	-76.332 607 05(01)	-76.360 199 30						
CCSDTQPHSO	-76.241 668 45	-76.332 607 07(10)	-76.360 199 31						

red are from CC(N)-CC(N-1) in 2Z,
[a]

[a] Uncertainties are just 1 in the next order of magnitude since differences can get larger in 3Z compared to 2Z but never by more than 10x