FCI quality energy for H_2O with a frozen core in a cc-pV9Z basis set: 8 electrons in 957 spatial orbitals

I. INTRODUCTION

Table I.

	cc-pV2Z	cc-pV3Z	cc-pV4Z	cc-pV5Z	
RHF	-76.026 77 88	-76.057 139 16	-76.064 804 29	-76.067 059 74	-
CCSD	-76.237 998 10	-76.324 545 75	-76.350 800 61	-76.359 518 95	-
CCSD(T)	-76.241 033 59	-76.332 192 23	-76.359 793 96	-76.369 041 18	-
CCSDT	-76.241 195 72	-76.332 268 49	-76.359 807 24	-76.368 996 80	-
CCSDT(Q)	-76.241 679 91	-76.332 623 49	-76.360 217 39	-76.369 430 92	-
CCSDTQ	-76.241 650 58	-76.332 587 70	-76.360 183 01	-76.369 394 18	-
CCSDTQ(P)	-76.241 665 00	-76.332 602 77	-76.360 189 48	-76.369 400 65(ok, because difference is getting smaller noticeably)	-
CCSDTQP	-76.241 665 92	-76.332 606 22	-76.360 198 47	-76.369 409 64(500?)(not ok because difference got bigger)	-
CCSDTQP(H)	-76.241 667 98	-76.332 606 77	-76.360 199 02(200)	-76.369 410 19	-
CCSDTQPH	-76.241 668 32	-76.332 606 94	-76.360 199 19(220)[a]	-76.369 410 36	-
CCSDTQPH(S)	-76.241 668 38	-76.332 606 99(10)	-76.360 199 24(230)	-76.369 410 41	-
CCSDTQPHS	-76.241 668 43	-76.332 607 05(10)	-76.360 199 29(230)	-76.369 410 47	-
CCSDTQPHS(O)	-76.241 668 43	-76.332 607 05(01)	-76.360 199 30(221)	-76.369 410 47	-
CCSDTQPHSO	-76.241 668 45	-76.332 607 07(10)	-76.360 199 31(230)	-76.369 410 49	-

[b]   [c]

[a] can alex thom do it?
[b] 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. red are from CC(N)-CC(N-1) in 2Z,
[c] uncertainty of 200 comes from the fact that CCSDTQP(H)-CCSDTQP got smaller by 0.000001514664987 in 3z-2z, so could potentially get bigger by 2 uH from 3z to 4z. 20 comes from same argument but now it's 0.000000169944002 which is one order of magnitude smaller. Everything else is just simply adding uncertainties from previous column. Really should probably be sqrt(a^2 + b^2) but instead I did a+b for now.