Table 12. IBM RS/6000 390 (w/o L2 cache) Timings[a]

Ethylene, 16 electrons, ^1A_g, (D_{2h}) Basis Set=6-311++G**
(74 basis functions, 6-term d's)[b]

Method	Gaussian 92/DFT (G)		
Conv. RHF	2/15 (20)		
Direct RHF	5/45 (68)		
RHF Gradient	15/30 (49)		
RHF Hessian	215/230 (252)		
UHF Total	2/20 (25)		
Conv. MP2	25/40 (47)		
Direct MP2	25/70 (77)		
MP2 Gradient	90/130 (160)		
MP2 Hessian	1066/1106 (1535)		
MP4(SDTQ)	514/529 (664)		
SDCI	10/110 (783)		
CCSD	78/878 (2413)		
CCSD(T)	1363/1378 (2880)		
QCISD	59/600 (1018)		
QCISD(T)	1083/1098 (1642)		
CASSCF	17/338 (933)		
CAS-CI	NA		
SVWN (LSD)	5/30 (35)		
BLYP (NLSD)	5/27 (41)		

Method	MOLPRO (94.8)	HONDO (8.5)	GAMESS(US)
Conv. RHF			
Direct RHF	NA		
RHF Gradient			
RHF Hessian	NA		
UHF			
Conv. MP2			
Direct MP2	NA		
MP2 Gradient	NA		
MP2 Hessian	NA		
MP4(SDTQ)			
SDCI			
CCSD			
CCSD(T)			
QCISD			
QCISD(T)			
CASSCF			
CAS-CI			
SVWN (LSD)			
BLYP (NLSD)			

Table 12. IBM RS/6000 390 (w/o L2 cache) Timings (cont.)

(a) All times are in seconds. CPU times are the sum of the "user + system" contributions. Wall clock times are given in parentheses. For the iterative methods (RHF, UHF, SD-CI, QCISD, and CASSCF), each entry consists of a trio of numbers: "CPU-time-per-teration/total-CPU (total-wall-clock)". The "CPU-time-per-iteration" for the conventional SCF methods was defined as the total run time (integrals + SCF) divided by the number of iterations. These values are intended to facilitate comparison with direct HF methods. For other methods the leftmost entry corresponds to the incremental time for the method. For example, the MP2 entry preceding the slash is the total run time minus the time needed for the HF.
Calculations were performed on a machine with 128 MB of memory and a 2 GB SCSI-2 disk running under AIX 3.2.5 with Release 3.0 of XLF Fortran. Runs were made on an otherwise quiet system.
NA: not available with this program.
FTC-ND: Failed to complete - not enough disk space.
FTC-unknown: Failed to complete for unknown reasons.
SCF calculations were converged to approximately 15 digits after the decimal point (8 digits in the density).

(b) The ethylene UHF calculation treated the $\pi \rightarrow \pi^*$ ($^3B_{1u}$) state. The ethylene ground state is ^1A_g. MP2, MP4, CISD and QCISD calculations involved all electrons, i.e., there were no "core" electrons. The CAS configuration list contains 8 CSF's in D_{2h} symmetry and was generated with 4 electrons in 4 orbitals ($3a_g$, $1b_{3u}$, $1b_{2g}$, $2b_{1u}$). This configuration list is sufficient to allow ethylene to dissociate into two singlet methylenes. The time reported includes the time required to compute the integrals and solve the CAS equations using the canonical RHF orbitals as the starting guess.