Table 13. IBM RS/6000 550 Timings[a]

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

Method	**Gaussian 90 (H)**	**Gaussian 92 (C)**	**MOLPRO (92.3)**
Conv. RHF	3/33 (45)	3/32 (65)	5/41 (115)
Direct RHF	11/125 (154)	8/93 (105)	NA
RHF Gradient	29/62 (74)	25/56 (80)	
RHF Hessian	340/373 (404)	347/378 (415)	NA
UHF	8/107 (115)	3/41 (46)	
Conv. MP2	48/81 (89)	47/78 (92)	
Direct MP2	48/173 (182)	47/140 (154)	NA
MP2 Gradient	180/261 (277)	174/252 (283)	NA
MP4(SDTQ)	1044/1128 (1596)	915/947 (1137)	
SDCI	92/1095 (1991)	86/891 (1442)	
CCSD	NA	141/1580 (4970)	
QCISD	112/1262 (2384)	107/1098 (2122)	
CASSCF	34/343 (652)[c]	45/888 (901)	

Method	**GAMESS-US 17/6/92**	**HONDO (8.3)**	**GAMESS-UK**
Conv. RHF			
Direct RHF			
RHF Gradient			
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2	NA	NA	
MP2 Gradient	NA	NA	
MP4(SDTQ)	NA		
SDCI			
CCSD	NA	NA	
QCISD	NA	NA	
CASSCF			

Method	**DISCO (1.82)**	**ACES II**
Conv. RHF		
Direct RHF		NA
RHF Gradient		
RHF Hessian	NA	
UHF	NA	
Conv. MP2	NA	
Direct MP2		NA
MP2 Gradient	NA	
MP4(SDTQ)	NA	
SDCI	NA	
CCSD	NA	
QCISD	NA	
CASSCF	NA	NA

Table 13. IBM RS/6000 550 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 preliminary HF step. Calculations were performed on a machine with 256 MB of memory and 2 GB of SCSI 1 disk running under AIX 3.2 with Release 2.0 of XLF Fortran. Runs were performed at interactive priority but the system had other jobs running.
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.
The default INDO initial guess used by Gaussian for ethylene's open shell calculations did not pick up the $\pi \rightarrow \pi^*$ $^3B_{1u}$ state. If the ordering of the initial guess orbitals was corrected using an ALTER command the calculation with Gaussian 90 died with a complaint that symmetry was being broken. Thus, it was necessary to run these calculations with the NOSYMM option, which ignored the available D_{2h} symmetry. Gaussian 92 fixed this problem with the UHF benchmark and was run in full D_{2h} symmetry.
Gaussian 90 requires that RHF calculations which precede certain correlated methods be run in C_1 symmetry. This results in an increase in the ethylene SCF times from 196 seconds (D_{2h}) to 441 seconds (C_1) for the 6-311G** basis; from 1900 seconds (D_{2h}) to 5795 seconds (C_1) for the cc-pVTZ basis; from 1969 seconds (D_{2h}) to 6657 seconds (C_1) for the 6-311++G(3df,3pd) basis.