Table 14. IBM RS/6000 580 Timings[a]

Ethylene, 16 electrons, $^1A_1$ (D_{2h}), Basis Set=6-311++G**
(74 functions, 6-term d's)[b]

Method	**Gaussian 90 (J)**	**Gaussian 92 (C)**	**Gaussian 92/DFT**
Conv. RHF	2 /21 (27)	2/20 (41)	
Direct RHF	7/84 (90)	4/66 (69)	
RHF Gradient	19/40 (49)	16/39 (52)	
RHF Hessian	217/238 (260)	221/241 (257)	
UHF	5/63 (77)	2/27 (55)	
Conv. MP2	32/53 (60)	30/50 (59)	
Direct MP2	32/116 (123)	31/123 (126)	
MP2 Gradient	125/178 (190)	116/166 (177)	
MP4(SDTQ)	690/741 (1108)	620/640 (963)	
SDCI	67/738 (2681)	55/569 (897)	
CCSD	NA	101/1008 (3101)	
CCSD(T)		1572/1592 (3257)	
QCISD	89/886 (3357)	70/702 (1358)	
QCISD(T)		1275/1295 (2641)	
CASSCF		29/576 (596)	
CAS-CI	NA	NA	
SVWN (LSD)	NA	NA	
BLYP (NLSD)	NA	NA	

Method	**MOLPRO (92.3)**	**GAMESS-US 7/17/93**	**HONDO (8.3)**
Conv. RHF	3/24 (41)	1/17 (40)	
Direct RHF	NA		
RHF Gradient	28/52 (89)	27/44 (101)	
RHF Hessian	NA		
UHF	2/27 (44)		
Conv. MP2	1/25 (43)		
Direct MP2	NA	NA	NA
MP2 Gradient	NA	NA	NA
MP4(SDTQ)	23/47 (79)	NA	
SDCI	12/36 (62)		
CCSD	3/47 (80)	NA	NA
CCSD(T)			
QCISD	2/40 (45)	NA	NA
QCISD(T)			
CASSCF	2/31 (53)		
SVWN (LSD)			
BLYP (NLSD)			

Table 14. IBM RS/6000 580 Timings (cont.)

Method	**GAMESS-UK**	**DISCO (1.82)**	**ACES II**
Conv. RHF		3/33 (36)	
Direct RHF		11/140 (143)	NA
RHF Gradient		105/138 (146)	
RHF Hessian		NA	
UHF		NA	
Conv. MP2		NA	
Direct MP2			NA
MP2 Gradient		NA	
MP4(SDTQ)		NA	
SDCI		NA	
CCSD		NA	
CCSD(T)		NA	
QCISD		NA	
QCISD(T)		NA	
CASSCF		NA	NA
CAS-CI		NA	

Table 14. IBM RS/6000 580 Timings (cont.)

Ethylene, 16 electrons, ^1A_g, (D_{2h}), Basis Set=cc-pVTZ
(116 basis functions, 7-term f's, 5-term d's)[b]

Method	**Gaussian 90 (J)**	**Gaussian 92 (C)**	**MOLPRO (92.3)**
Conv. RHF			18/178 (190)
Direct RHF			NA
RHF Gradient			NA
RHF Hessian			NA
UHF			14/179 (191)
Conv. MP2			2/180 (191)
Direct MP2			NA
MP2 Gradient			NA
MP4(SDTQ)			89/267 (281)
SDCI			5/212 (228)
CCSD	NA		8/245 (261)
QCISD			6/231 (268)
CASSCF			4/192 (210)

Method	**GAMESS-US 6/17/92**	**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	**SUPERMOLECULE**	**ACES II**
Conv. RHF	31/369 (441)	
Direct RHF	60/723 (857)	NA
RHF Gradient	867/1236 (1425)	
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 14. IBM RS/6000 580 Timings (cont.)

Isobutene, 32 electrons, $^1A_1$ (C_{2v}), Basis Set=6-311++G**
(148 functions, 6-term d's)

Method	**Gaussian 90 (H)**	**Gaussian 92 (C)**	**MOLPRO (92.3)**
Conv. RHF		23/293 (793)	
Direct RHF			NA
RHF Gradient			
RHF Hessian			NA
UHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			NA
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD			
CASSCF			

Method	**GAMESS-US 6/17/92**	**HONDO (8.1)**	**GAMESS-UK (2)**
Conv. RHF			
Direct RHF			
RHF Gradient			
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2	NA	NA	NA
MP2 Gradient	NA	NA	
MP4(SDTQ)	NA		NA
SDCI			
CCSD	NA	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 14. IBM RS/6000 580 Timings (cont.)

Imidazole, 36 electrons, ^{1}A', Cs, Basis Set=cc-pVTZ
(206 functions, 5-term d's, 7-term f's)

Method	**Gaussian 90 (H)**	**Gaussian 92 (C)**	**MOLPRO (92.3)**
Conv. RHF		348/4878 (6836)	
Direct RHF		1347/20211 (20219)	NA
RHF Gradient		4964/9842 (15011)	
RHF Hessian		36968/41846 (74672)	NA
UHF			
Conv. MP2			
Direct MP2		20254/40473 (40615)	NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD			
CASSCF			

Method	**GAMESS-US 6/17/92**	**HONDO (8.3)**	**GAMESS-UK (2)**
Conv. RHF			
Direct RHF			
RHF Gradient			
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
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 14. IBM RS/6000 580 Timings (cont.)

18-crown-6, $C_{12}H_{24}O_6$, 144 electrons, C_i, Basis Set=aug-cc-pVDZ
(606 functions)

Method	**Gaussian 92 (E)**	**Gaussian 92/DFT**	**MOLPRO (92.3)**
Direct RHF	29181/437716 (438413)		
RHF Gradient			
RHF Hessian			NA
Conv. RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Method	**GAMESS-US 6/17/92**	**HONDO (8.3)**	**GAMESS-UK (2)**
Direct RHF			
RHF Gradient			
RHF Hessian			
Direct MP2			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
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 14. IBM RS/6000 580 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 step.
Calculations were performed on a machine with 256 MB of memory and one 2 GB IBM SCSI 2 disk running under AIX 3.2 with Release 2.3.5 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 $\pi \varnothing \pi^*$ ($^3B_{1u}$) 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 (3_{ag}, $1b_{3u}$, $1b_{2g}$, $2b_{1u}$). 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 $\pi \varnothing \pi^*$ $^3B_{1u}$ 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.

(c) The Gaussian CAS calculation using RHF canonical orbitals aborted with an error message saying that the initial guess resulted in a rotation of more than 45 degrees in one of the active orbitals.