Table 17. HP 730 Timings[a]

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

Method	**Gaussian 90 (H)**	**Gaussian 92 (C)**	**MOLPRO (92.3)**
Conv. RHF	4/43 (93)		5/45 (60)
Direct RHF	12/172 (183)		NA
RHF Gradient	37/80 (138)		35/80 (94)
RHF Hessian	529/572 (716)		NA
UHF Total	10/136 (373)		3/47 (62)
Conv. MP2	75/118 (169)		2/47 (60)
Direct MP2	75/247 (256)		NA
MP2 Gradient	296/414 (541)		NA
MP4(SDTQ)	2500/2593 (4419)		54/99 (115)
SDCI	223/2320 (6470)		4/72 (85)
CCSD	NA		6/97 (115)
QCISD	252/2612 (7203)		4/83 (98)
CASSCF	FTC - unknown		3/58 (70)

Method	**GAMESS-US 17/6/92**	**HONDO (8.3)**	**GAMESS-UK**
Conv. RHF	5/55 (78)		
Direct RHF	13/176 (177)		
RHF Gradient	47/102 (120)		
RHF Hessian	936/991 (1206)		
UHF	6/92 (139)		
Conv. MP2	127/182 (217)		
Direct MP2	NA	NA	
MP2 Gradient	NA		
MP4(SDTQ)	NA		
SDCI	102/970 (1190)		
CCSD	NA	NA	
QCISD	NA	NA	
CASSCF	366/3350 (4694)		

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	

Table 17. HP 730 Timings (cont.)

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

Method	**Gaussian 90 (H)**	**Gaussian 92 (C)**	**MOLPRO (92.3)**
RHF	31/342 (541)		
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 17/6/92**	**HONDO (8.3)**	**GAMESS-UK (2)**
Conv. RHF	unable to handle 5-term		unable to handle 5-term
Direct RHF	d's and 7-term f's.		d's and 7-term f's.
RHF Gradient			
RHF Hessian			
UHF			
ROHF			
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	

Table 17. HP 730 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 64 MB of memory and two 1.3 GB fast differential SCSI 2 disks running under HP Fortran 9000, Release 8.05. 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).

Table 18. HP 735 Timings[a]

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

Method	Gaussian 92 (C)	Gaussian 92/DFT (G)	MOLPRO (93)
Conv. RHF	3/26 (34)	3/28 (53)	2/29 (30)[c]
Direct RHF	5/82 (89)	7/69 (79)	NA
RHF Gradient	28/54 (61)	23/51 (69)	18/47 (48)[c]
RHF Hessian	433/459 (482)	366/395 (440)	NA
UHF Total	4/44 (101)	3/37 (49)	
Conv. MP2	51/77 (87)	50/78 (95)	1/30 (31)[c]
Direct MP2	51/133 (139)	42/111 (123)	NA
MP2 Gradient	193/270 (306)	165/243 (303)	NA
MP2 Hessian		2006/2084 (3162)	
MP4(SDTQ)	1808/1834 (3921)	1206/1234 (1506)	28/57 (58)[c]
SDCI	128/1305 (1648)	110/1126 (1526)	2/39 (40)[c]
CCSD	238/2642 (6002)	222/2466 (4963)	3/55 (56)[c]
CCSD(T)	4577/4603 (6758)	3424/3452 (5741)	
QCISD	184/1838 (2252)	160/1629 (2114)	2/48 (49)[c]
QCISD(T)	3656/3682 (4272)	2766/2794 (3469)	
CASSCF	28/559 (577)	30/600 (3656)	2/37 (38)[c]
CAS-CI	NA	NA	
SVWN (LSD)		7/44 (54)	
BLYP (NLSD)		8/41 (49)	

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		
MP4(SDTQ)	NA		
SDCI			
CCSD	NA	NA	
QCISD	NA	NA	
CASSCF			

Table 18. HP 735 Timings (cont.)

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

Method	**Gaussian 90 (H)**	**Gaussian 92 (C)**	**MOLPRO (93)**
RHF		20/201 (207)	17/182 (189)[c]
Direct RHF		66/659 (677)	NA
RHF Gradient		253/454 (498)	NA
RHF Hessian		2811/3021 (3048)	NA
UHF		21/254 (276)	
Conv. MP2		905/1106 (1115)	3/185 (191)[c]
Direct MP2		862/1521 (1540)	NA
MP2 Gradient		2070/3176 (3497)	NA
MP4(SDTQ)		11779/11980 (23315)	130/312 (312)[c]
SDCI			7/224 (234)[c]
CCSD	NA		12/274 (294)[c]
QCISD			8/253 (263)[c]
CASSCF			6/205 (215)[c]

Method	**GAMESS-US 17/6/92**	**HONDO (8.3)**	**GAMESS-UK (2)**
Conv. RHF	unable to handle 5-term		unable to handle 5-term
Direct RHF	d's and 7-term f's.		d's and 7-term f's.
RHF Gradient			
RHF Hessian			
UHF			
ROHF			
Conv. MP2			
Direct MP2			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Table 18. HP 735 Timings (cont.)

Ethylene, 16 electrons, ^1A_g (D_{2h}), Basis Set=6-311++G(3df,3pd)
(150 functions, 5-term d', 7-term f's)[b]

Method	**Gaussian 90 (H)**	**Gaussian 92 (C)**	**MOLPRO (93)**
RHF			37/445 (467)[c]
Direct RHF			NA
RHF Gradient			NA
RHF Hessian			NA
UHF			
Conv. MP2			7/452 (474)[c]
Direct MP2			NA
MP2 Gradient			NA
MP4(SDTQ)			332/777 (788)[c]
SDCI			18/552 (582)[c]
CCSD	NA		29/702 (757)[c]
QCISD			20/621 (655)[c]
CASSCF			9/509 (517)[c]

Method	**GAMESS-US 17/6/92**	**HONDO (8.3)**	**GAMESS-UK (2)**
Conv. RHF	unable to handle 5-term		unable to handle 5-term
Direct RHF	d's and 7-term f's.		d's and 7-term f's.
RHF Gradient			
RHF Hessian			
UHF			
ROHF			
Conv. MP2			
Direct MP2			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Table 18. HP 735 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 64 MB of memory and fast-wide SCSI 2 disks running under HP Fortran 9000, Release 9.01. 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 (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 $\pi \rightarrow \pi^*$ $^3B_{1u}$ 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.

(c) Run by Prof. Joachim Werner, Universitat Bielefeld, Bielefeld Germany. The machine had 176 MB of memory and fast, wide HP-C3035T SCSI 2 disks configured as a software disk-striped array (4x1GB). These calculations were performed with a preliminary version of MOLPRO93.

Table 19. HP 735/125 Timings[a]

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

Method	**Gaussian 92 (C)**	**Gaussian 92/DFT (G)**	**MOLPRO (94)**
Conv. RHF	2/21 (26)	2/22 (30)	3/23 (26)
Direct RHF	6/67 (82)	5/54 (57)	NA
RHF Gradient	23/44 (51)	18/40 (49)	17/40 (40)
RHF Hessian	362/383 (398)	290/312 (332)	NA
UHF Total	3/31 (41)		2/25 (25)
Conv. MP2	44/65 (70)		25/48 (49)
Direct MP2	45/112 (118)		NA
MP2 Gradient	167/232 (252)		NA
MP4(SDTQ)	1441/1462 (1573)		25/48 (49)
SDCI	106/1085 (1183)		2/35 (40)
CCSD	192/2136 (3680)		3/46 (46)
CCSD(T)	3667/3688 (5296)		45/68 (76)
QCISD	152/1539 (1686)		2/40 (44)
QCISD(T)	2932/2953 (3186)		41/64 (68)
CASSCF	25/491 (1690)		2/30 (31)
SVWN (LSD)	NA		3/30 (35)
BLYP (NLSD)	NA		3/33 (38)

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		
MP4(SDTQ)	NA		
SDCI			
CCSD	NA	NA	
QCISD	NA	NA	
CASSCF			

Table 19. HP 735/125 Timings (cont.)

18-crown-6, $C_{12}H_{24}O_6$, 144 electrons, C_i, Basis Set=3-21G
(210 functions)

Method	**Gaussian 92 (C)**	**Gaussian 92/DFT**	**MOLPRO (92.3)**
Direct RHF	108/1405 (1447)		
RHF Gradient	722/2127 (2156)		
RHF Hessian	57020/58425 (60159)		NA
Conv. RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD			
CASSCF			

Method	**GAMESS-US 6/17/92**	**HONDO (8.1)**	**GAMESS-UK (2)**
Direct RHF			
RHF Gradient			
RHF Hessian			
Conv. RHF			
Conv. MP2			
Direct MP2			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

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

Table 19. HP 735/125 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 64 MB of memory and fast-wide SCSI 2 disks running under HP Fortran 9000, Release 9.01. Runs were made on an otherwise quiet system. Due to problems with getting Gaussian 92 to compile and run correctly under HP f77 version 9.0, these benchmarks utilizied binaries created under an earlier release of the compiler.
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

(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 (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 $\pi \rightarrow \pi^*$ $^3B_{1u}$ 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.