Table 6. Sun SPARCstation 2 Timings[a]

Ethylene, 16 electrons, ^1A_g (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	18 /196 (269)	12/122 (155)	23/203 (213)
Direct RHF	69/824 (881)	42/450 (464)	NA
RHF Gradient	193/389 (445)	126/248 (283)	1058/1261 (1292)
RHF Hessian	3123/3319 (3386)	2098/2220 (2313)	NA
UHF	54/697 (640)	16/188 (227)	14/215 (223)
Conv. MP2	526/722 (763)	250/372 (443)	14/217 (226)
Direct MP2	527/1351 (1374)	241/691 (706)	NA
MP2 Gradient	1756/2478 (2685)	816/1188 (1290)	NA
MP2 Hessian		8638/9010 (9187)	NA
MP4(SDTQ)	14276/14717 (17305)	10684/10806 (11784)	285/488 (497)
SDCI	968/11085 (15885)	457/4698 (5405)	23/362 (379)
CCSD	NA	709/7927 (15694)	31/485 (531)
CCSD(T)	NA	11781/11903 (16013)	
QCISD	1292/13358 (17406)	527/5396 (5828)	25/427 (441)
QCISD(T)	NA	7913/8035 (8115)	
CASSCF	434/4101 (6430)[c]	178/1660 (2092)	20/283 (298)
CAS-CI	NA	NA	33/548 (566)

Method	**GAMESS-US 6/17/92**	**HONDO (8.1)**	**GAMESS-UK (2)**
Conv. RHF	11 /132 (146)	12 /242 (277)	9/106 (124)
Direct RHF	48/626 (631)	62/1882 (1919)[e]	46/554 (566)
RHF Gradient	231/363 (369)	210/474 (491)	89/195 (223)
RHF Hessian	3301/3433 (4091)	2762/3026 (3340)	3649/3755 (3859)
UHF	14/214 (225)	16/429 (439)	
Conv. MP2	183/315 (334)	237/501 (530)	129/235 (255)
Direct MP2	NA	NA	NA
MP2 Gradient	NA	NA	386/621 (742)
MP4(SDTQ)	NA	5596/5860 (6309)	NA
SDCI	250/2380 (2941)[d]	351/3994 (4761)[d]	FTC-unknown
CCSD	NA	NA	NA
CCSD(T)	NA	NA	
QCISD	NA	NA	
QCISD(T)	NA	NA	
CASSCF	843/8569 (10261)[d]	519/5921 (7836)[d]	
CAS-CI			

Table 6. Sun SPARCstation 2 Timings (cont.)

Method	**DISCO (1.82)**	**ACES II**
Conv. RHF	21/268 (274)	
Direct RHF	106/1381 (1406)	NA
RHF Gradient	1124/1392 (1405)	
RHF Hessian	NA	
UHF	NA	
Conv. MP2	NA	
Direct MP2	1171/2573 (2581)	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	NA

Table 6. Sun SPARCstation 2 Timings (cont.)

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

Method	**Gaussian 90 (H)**	**Gaussian 92 (C)**	**MOLPRO (92.3)**
RHF	173/1900 (1945)	106/1057 (1170)	142/1415 (1510)
Direct RHF	689/8952 (10790)	327/3274 (3381)	NA
RHF Gradient	4186/6086 (6434)	1183/2240 (2365)	NA[i]
RHF Hessian	28789/30689 (30936)	16101/17158 (17510)	NA
UHF	182/2365 (2735)	119/1424 (2135)	112/1460 (1626)
Conv. MP2	6219/8119 (8274)	3576/4633 (4818)	40/1455 (1583)
Direct MP2	6366/15318 (14500)	3382/6656 (6730)	NA
MP2 Gradient	17284/25403 (27041)	8121/12754 (14189)	NA
MP4(SDTQ)	94140/99935 (218907)	76427/77484 (112614)	1154/2569 (2,808)
SDCI	5489/66171 (103905)	3723/42010 (49485)	82/1989 (2195)
CCSD	NA	53285/54342 (160825)	129/2449 (2613)
CCSD(T)			
QCISD	6380/69592 (115067)	5298/41340 (54032)	103/2339 (2628)
QCISD(T)			
CASSCF	FTC-ND	FTC-ND	33/1548 (1786)
CAS-CI			

Method	**GAMESS-US 6/17/92**	**HONDO (8.1)**	**GAMESS-UK (2)**
Conv. RHF	unable to handle 5-term	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.	d's and 7-term f's.
RHF Gradient			
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
CCSD(T)			
QCISD			
QCISD(T)			
CASSCF			
CAS-CI			

Table 6. Sun SPARCstation 2 Timings (cont.)

Method	**DISCO (1.82)**	**ACES II**
Conv. RHF	201/2014 (2047)	
Direct RHF	516/5160 (5765)	NA
RHF Gradient	5988/11148 (11249)	
RHF Hessian	NA	
UHF	NA	
Conv. MP2	NA	
Direct MP2	6766/11944 (12643)	NA
MP2 Gradient	NA	
MP4(SDTQ)	NA	
SDCI	NA	
CCSD	NA	
QCISD	NA	
CASSCF	NA	NA

Table 6. Sun SPARCstation 2 Timings (cont.)

Ethylene, 16 electrons, $^{1}A_{g}$ (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 (A)**	**MOLPRO (92.3)**
Conv. RHF	205/2259 (2656)	167/1669 (2410)	337/3371 (3966)
Direct RHF	685/8221 (8363)	506/5563 (5726)	NA
RHF Gradient	3787/6046 (6417)	1949/3618 (4361)	
RHF Hessian	45569/47828 (49314)	32070/33739 (36165)	NA
UHF Total	248/3465 (4332)	205/2663 (4081)	
Conv. MP2	9171/11430 (13615)	4133/5802 (8016)	
Direct MP2	9012/17233 (17338)	3791/9354 (9469)	NA
MP2 Gradient	24919/36349 (39236)	12035/17838 (21081)	
MP4(SDTQ)	271564/278221 (363,794)	>18900 FTC-ND	
SDCI	>13300 FTC-ND(f)	FTC-ND	
CCSD	NA	FTC-ND	
QCISD	>14200 FTC-ND(f)	FTC-ND	
CASSCF	FTC-ND(g)	FTC-ND	

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

Table 6. Sun SPARCstation 2 Timings (cont.)

Method	**DISCO (1.82)**	**ACES II**
Conv. RHF	416/5411 (5827)	
Direct RHF	1178/15324 (15425)	NA
RHF Gradient	13798/19209 (19888)	
RHF Hessian	NA	
UHF	NA	
Conv. MP2	NA	
Direct MP2	16420/31744 (31844)	NA
MP2 Gradient	NA	
MP4(SDTQ)	NA	
SDCI	NA	
CCSD	NA	
QCISD	NA	
CASSCF	NA	NA

Table 6. Sun SPARCstation 2 Timings (cont.)

Imidazole, 36 electrons, $^1A'$ (C_s), Basis Set=6-311++G**
(143 functions, 6-term d's)

Method	**Gaussian 90 (H)**	**Gaussian 92 (C)**	**MOLPRO (92.3)**
Conv. RHF	764/11466 (13428)	260/3645 (6647)	645/9028 (8988)
Direct RHF	1454/29087 (29273)	917/13761 (13837)	NA
RHF Gradient	9187/11446 (13480)	4222/7867 (10920)	31171/40199 (44249)[h]
RHF Hessian	68176/70435 (75526)	47327/50972 (59925)	NA
UHF	505/12121 (15604)	370/8505 (16126)	
Conv. MP2	6993/18459 (21595)	5209/8854 (13324)	1125/10153 (14127)
Direct MP2	18182/47269 (47497)	8496/22257 (22412)	NA
MP2 Gradient	43303/61762 (71754)	19745/28639 (37539)	
MP4(SDTQ)	>28200 FTC-ND	FTC-ND	
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			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Table 6. Sun SPARCstation 2 Timings (cont.)

Method	DISCO (1.82)	ACES II
Conv. RHF	1241/11617 (12078)	
Direct RHF	4466/40197 (40428)	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 6. Sun SPARCstation 2 Timings (cont.)

Isobutene, 32 electrons, $^{1}A_{1}$ (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	239/3345 (4606)	158/2050 (3575)	
Direct RHF	647/16169 (16353)	408/6543 (6611)	NA
RHF Gradient	2534/5879 (7245)	1793/3843 (5384)	
RHF Hessian	91291/94636 (100117)	46678/48728 (53805)	NA
UHF	326/5541 (7369)	245/3913 (3505)	
Conv. MP2	14195/17540 (20158)	5590/7640 (11212)	
Direct MP2	14930/31100 (31897)	11893/13943 (14121)	NA
MP2 Gradient	FTC - unknown	18159/25799 (32020)	NA
MP4(SDTQ)	FTC-ND	FTC-ND	
SDCI	FTC-ND	FTC-ND	
CCSD	NA	FTC-ND	
QCISD	FTC-ND	FTC-ND	
CASSCF	FTC-ND	FTC-ND	

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			

Table 6. Sun SPARCstation 2 Timings (cont.)

Isobutene, 32 electrons, $^1A_1$ (C_{2v}), Basis Set=cc-pVTZ
(232 functions, 5-term d's, 7-term f's)

Method	**Gaussian 90 (H)**	**Gaussian 92 (C)**	**MOLPRO (92.3)**
Conv. RHF			
Direct RHF	9384/140756 (142164)	4325/56227 (57012)	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	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			
Conv. MP2			
Direct MP2	NA	NA	NA
MP2 Gradient	NA	NA	
MP4(SDTQ)	NA		NA
SDCI			
CCSD	NA	NA	NA
QCISD	NA	NA	
CASSCF			

Table 6. Sun SPARCstation 2 Timings (cont.)

Caffeine, $C_8H_9O_2N_4$, 101 electrons, C1, Basis Set=3-21G, (144 functions)

Method	**Gaussian 90 (H)**	**Gaussian 92 (C)**	**MOLPRO (92.3)**
UHF	556/16112 (20580)	427/11950 (22529)	
UHF Gradient	4374/20486 (24869)	3150/15100 (26520)	
UHF Hessian	205561/221673 (240483)	135452/147402 (187180)	NA
Conv. RHF	291/12237 (18489)	216/8867 (33493)	
Direct RHF	837/34306 (34533)	512/27172 (27341)	NA
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)**
UHF			
RHF Gradient			
RHF Hessian			
Conv. RHF			
Direct RHF			
Conv. MP2			
Direct MP2			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

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

Table 6. Sun SPARCstation 2 Timings (cont.)

Caffeine, $C_8H_9O_2N_4$, 101 electrons, C1, Basis Set=6-31G**
(255 functions)

Method	**Gaussian 90 (H)**	**Gaussian 92 (C)**	**MOLPRO (92.3)**
Direct UHF	7126/242275 (245059)	5922/153966 (155815)	
RHF Gradient			
RHF Hessian			NA
Direct RHF			NA
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 UHF			
RHF Gradient			
RHF Hessian			
Direct RHF			
Direct MP2			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD	NA		
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 6. Sun SPARCstation 2 Timings (cont.)

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

Method	**Gaussian 90 (H)**	**Gaussian 92 (C)**	**MOLPRO (92.3)**
Direct RHF	905/12670 (12844)	569/7391 (7532)	
RHF Gradient	7724/20394 (20658)	3613/11004 (11222)	
RHF Hessian			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 6. Sun SPARCstation 2 Timings (cont.)

18-crown-6, $C_{12}H_{24}O_6$, 144 electrons, C_i, Basis Set=6-31G**
(390 functions)

Method	**Gaussian 90 (H)**	**Gaussian 92 (C)**	**MOLPRO (92.3)**
Direct RHF		5058/65758 (67217)	
RHF Gradient			
RHF Hessian			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 6. Sun SPARCstation 2 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 (C)**	**Gaussian 92/DFT**	**MOLPRO (92.3)**
Direct RHF	144321/2309143 (3210525)		
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 6. Sun SPARCstation 2 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-iteration/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.
Unless otherwise noted all SPARC 2 calculations were performed on a machine with 64 MB of memory, a 900 MB Seagate ST4766 disk and a 600 MB Fujitsu M2266 disk running under SunOS 4.1.1 with Release 1.4 of Sun Fortran. G90 was compiled with version 1.2 of the Fortran compiler because of problems encountered in getting it to run under 1.4. 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 7 - 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 CSFs 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 triplet methylenes. The time reported includes the time required to compute the integrals and solve the CAS equations using the canonical 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 that 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.
The caffeine RHF calculation was on the cation state of the molecule.

(c) The Gaussian CAS calculation using RHF canonical orbitals aborted with an error message saying that the initial guess was too poor. After massaging the initial guess, the calculation could be made to proceed, but the final energy was approximately 20 millihartrees too high. The total times reported have been increased by the amount necessary to perform a SCF calculation.

(d) GAMESS and HONDO could not do a combined RHF + SDCI or RHF + CAS in one job step. In order to make the total time comparable to what is reported for other programs, the time to perform the RHF calculation (exclusive of the 2-el. integral time) was simply added to the SDCI or CAS time.

(e) Failed to converge in 30 iterations. By iteration 11 the energy was within 10^{-7} hartree of the converged result, but the energy subsequently oscillated.

(f) This calculation died due to a lack of disk space in the middle of iteration 2. At that point the size of the "rwf" exceeded 900 MB, the size of the largest scratch partition available.

(g) The number of configurations in the SDCI calculations were 21,037 for 6-311++G** ethylene; 50,741 for cc-pVTZ ethylene.

(h) This MOLPRO calculation failed to produce correct gradients.

(i) The MOLPRO gradient integral package is unable to handle generally contracted basis sets.

Table 7. Sun SPARCstation 10/41 Timings[(a)]

Ethylene, 16 electrons, ^1A_g (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		6/56 (61)	10/88 (91)
Direct RHF		17/198 (207)	NA
RHF Gradient		57/113 (124)	461/549 (569)
RHF Hessian		1049/1105 (1141)	NA
UHF		7/84 (157)	10/89 (93)
Conv. MP2		101/157 (167)	6/94 (97)
Direct MP2		112/310 (334)	NA
MP2 Gradient		393/550 (658)	NA
MP2 Hessian		4850/5007 (5990)	NA
MP4(SDTQ)		4537/4593 (5382)	285/207 (222)
SDCI		200/2055 (3015)	10/157 (173)
CCSD	NA	340/3802 (9638)	14/211 (228)
CCSD(T)		5653/5709 (5826)	
QCISD		225/2306 (3672)	11/186 (197)
QCISD(T)		3388/3444 (3529)	
CASSCF		FTC-ND	9/123 (130)
CAS-CI	NA	NA	14/238 (242)

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
CCSD(T)			
QCISD	NA	NA	
QCISD(T)			
CASSCF			
CAS-CI			

Table 7. Sun SPARCstation 10/41 Timings (cont.)

Method	**DISCO (1.86)**	**ACES II**
Conv. RHF	8/111 (118)	
Direct RHF	40/545 (555)	NA
RHF Gradient	449/560 (568)	
RHF Hessian	NA	
UHF	NA	
Conv. MP2	NA	
Direct MP2	665/1210 (1227)	NA
MP2 Gradient	NA	
MP4(SDTQ)	NA	
SDCI	NA	
CCSD	NA	
QCISD	NA	
CASSCF	NA	NA

Table 7. Sun SPARCstation 10/41 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 (C)**	**Gaussian 92/DFT**	**MOLPRO (92.3)**
Direct RHF	62450/999206 (1000340)		
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 7. Sun SPARCstation 10/41 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-iteration/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.
Unless otherwise noted all SPARC 10 calculations were performed on a machine with 64 MB of memory, a 900 MB Seagate ST4766 disk and a 600 MB Fujitsu M2266 disk running under SunOS 4.1.1 with Release 1.4 of Sun Fortran.
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 13 digits following the decimal point (7 - 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 CSFs 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 triplet 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 that 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 was too poor. After massaging the initial guess, the calculation could be made to proceed, but the final energy was approximately 20 millihartrees too high. The total times reported have been increased by the amount necessary to perform a SCF calculation.

(d) GAMESS and HONDO could not do a combined RHF + SDCI or RHF + CAS in one job step. In order to make the total time comparable to what is reported for other programs, the time to perform the RHF calculation (exclusive of 2-el. integral time) was simply added to the SDCI or CAS time.

(e) Failed to converge in 30 iterations. By iteration 11 the energy was within 10^{-7} hartree of the converged result, but the energy subsequently oscillated.

(f) This calculation died due to a lack of disk space in the middle of iteration 2. At that point the size of the "rwf" exceeded 900 MB, the size of the largest scratch partition available.

(g) The number of configurations in the SDCI calculations were 21,037 for 6-311++G** ethylene; 50,741 for cc-pVTZ ethylene.

(h) This MOLPRO calculation failed to produce correct gradients.

(i) The MOLPRO gradient integral package is unable to handle generally contracted basis sets.

Table 8. Sun 167 MHz UltraSPARC1 Timings[a]

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

Method	**Gaussian 94 (D.3)**		**MOLPRO (96.3)**
Conv. RHF	2/17 (18)		
Direct RHF	5/45 (47)		NA
In-core RHF	5/49 (51)		NA
RHF Gradient	16/33 (43)		
RHF Hessian	159/176 (195)		NA
UHF	2/22 (24)		
Conv. MP2	5/27 (38)		
Direct MP2	10/55 (58)		NA
MP2 Gradient	53/70 (79)		NA
MP2 Hessian	1329/1346 (1704)		NA
MP4(SDTQ)	1628/1645 (1867)		
SDCI	27/264 (625)		
CCSD	54/559 (2245)		
CCSD(T)	2186/2203 (3678)		
QCISD	35/366 (916)		
QCISD(T)	2059/2076 (2941)		
CASSCF	15/317 (895)		
CAS-CI	NA		
SVWN (LDA)	16/124 (139)		
BLYP (NLDA)	34/274 (293)		

Method	**GAMESS-US 7/17/93**	**HONDO (8.3)**	**GAMESS-UK (2)**
Conv. RHF		Not ported to	
Direct RHF		an SGI	
In-core RHF	NA		
RHF Gradient			
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2	NA	NA	NA
MP2 Gradient	NA	NA	
MP2 Hessian	NA	NA	
MP4(SDTQ)	NA		NA
SDCI			
CCSD	NA	NA	NA
CCSD(T)	NA	NA	
QCISD	NA	NA	
QCISD(T)		NA	
CASSCF	185/1874 (1933)		
CAS-CI			
SVWN (LDA)	NA		
BLYP (NLDA)	NA		