Table 10. IBM RS/6000 340 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 (J)**	**Gaussian 92 (E)**	**Gaussian 92/DFT (G)**
Conv. RHF	4/45 (49)	4/43 (74)	5/46 (75)
Direct RHF	15/175 (179)	12/131 (139)	13/133 (140)
RHF Gradient	43/88 (94)	37/80 (92)	36/82 (97)
RHF Hessian	487/532 (555)	547/590 (641)	530/576 (610)
UHF Total	12/152 (156)	5/58 (67)	5/60 (65)
Conv. MP2	72/117 (125)	71/114 (126)	67/113 (122)
Direct MP2	71/245 (254)	76/207 (215)	69/202 (211)
MP2 Gradient	273/390 (405)	271/385 (426)	
MP2 Hessian	NA	2713/2920 (3389)	
MP4(SDTQ)	1497/1613 (1898)	1351/1394 (2099)	
SDCI	154/1657 (3122)	133/1371 (2005)	
CCSD	NA	202/2270 (5340)	
CCSD(T)		3337/3380 (5900)	
QCISD	180/1913 (3719)	154/1579 (2542)	
QCISD(T)		2726/2769 (3624)	
CASSCF	58/520 (1023)[c]	57/1118 (1135)	
CAS-CI	NA	NA	
SVWN (LSD)	NA	NA	15/88 (94)
BLYP (NLSD)	NA	NA	16/79 (84)

Method	**MOLPRO (92.3)**	**MOLPRO (94.8)**	**HONDO (8.5)**
Conv. RHF	6/55 (91)	8/68 (74)	4/43 (48)
Direct RHF	NA	NA	18/197 (198)
RHF Gradient	71/130 (131)	72/140 (140)	31/74 (88)
RHF Hessian	NA	NA	171/214 (221)
UHF	4/58 (60)	5/70 (70)	4/60 (67)
Conv. MP2	2/57 (62)	1/69 (70)	8/51 (56)
Direct MP2	NA	NA	NA
MP2 Gradient	NA	NA	100/143 (154)
MP2 Hessian	NA	NA	NA
MP4(SDTQ)	54/109 (110)	37/105 (115)	1505/1548(1631)
SDCI	5/87 (88)	4/95 (97)	68/721 (881)
CCSD	6/113 (115)	6/119 (124)	NA
CCSD(T)		86/154 (156)	NA
QCISD	5/97 (99)	4/103 (105)	NA
QCISD(T)		80/148 (149)	NA
CASSCF	4/71 (73)	3/81 (83)	36/407 (423)
CAS-CI		10/150 (154)	NA
SVWN (LSD)		6/77 (79)	NA
BLYP (NLSD)		7/87 (88)	NA

Table 10. IBM RS/6000 340 Timings (cont.)

Method	**DISCO (1.82)**	**GAMESS-US 6/17/92**	**ACES II**
Conv. RHF	5/70 (73)	4/46 (55)	3/51 (63)
Direct RHF	21/298 (301)	18/229 (230)	NA
RHF Gradient	225/295 (300)	61/107 (112)	249/300 (620)
RHF Hessian	NA	324/370 (802)	549/600 (672)
UHF	NA	5/71 (86)	3/55 (67)
Conv. MP2	NA	66/112 (143)	13/64 (79)
Direct MP2	238/536 (539)	NA	NA
MP2 Gradient	NA	NA	49/113 (141)
MP2 Hessian	NA	NA	NA
MP4(SDTQ)	NA	NA	170/221 (266)
SDCI	NA	FTC - unknown	12/215 (294)
CCSD	NA	NA	18/248 (310)
CCSD(T)	NA	NA	330/381 (443)
QCISD	NA	NA	14/200 (260)
QCISD(T)	NA	NA	285/336 (394)
CASSCF	NA	277/2820 (4622)	NA
CAS-CI		NA	NA
SVWN (LSD)	NA	NA	NA
BLYP (NLSD)	NA	NA	NA

Table 10. IBM RS/6000 340 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	51/557 (620)	32/317 (340)	
Direct RHF	140/1817 (1927)	97/966 (982)	NA
RHF Gradient	695/1252 (1304)	336/653 (678)	
RHF Hessian	7355/7912 (7976)	5046/5363 (5471)	NA
UHF	50/654 (979)	36/432 (726)	
Conv. MP2		1041/1358 (1401)	
Direct MP2		203/2032 (2015)	NA
MP2 Gradient		2389/3747 (4031)	NA
MP4(SDTQ)		10503/10820 (28878)	
SDCI		1104/11365 (14147)	
CCSD	NA	1353/15197 (34939)	
QCISD		1121/11530 (15671)	
CASSCF		FTC - unknown	

Method	**GAMESS-US 6/17/92**	**HONDO (8.3)**	**GAMESS-UK (2)**
Conv. RHF	unable to handle 5-term	35/449 (505)	unable to handle 5-term
Direct RHF	d's and 7-term f's.	244/3181 (3192)	d's and 7-term f's.
RHF Gradient		551/1000 (1042)	
RHF Hessian		2798/3247 (3410)	
UHF			
Conv. MP2			
Direct MP2		NA	
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD		NA	
QCISD		NA	
CASSCF			

Table 10. IBM RS/6000 340 Timings (cont.)

Method	**DISCO (1.82)**	**ACES II**
Conv. RHF	119/1313 (1324)	
Direct RHF	111/1224 (1230)	NA
RHF Gradient	1509/2822 (2840)	
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 10. IBM RS/6000 340 Timings (cont.)

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

Method	**Gaussian 90 (J)**	**Gaussian 92 (A)**	**MOLPRO (92.3)**
Conv. RHF		50/496 (1313)	
Direct RHF			NA
RHF Gradient			
RHF Hessian			NA
UHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD			
CASSCF			

Method	**GAMESS-US 6/17/92**	**HONDO (8.3)**	**GAMESS-UK (2)**
Conv. RHF	unable to handle 5-term d's and 7-term f's.		unable to handle 5-term d's and 7-term f's.
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 10. IBM RS/6000 340 Timings (cont.)

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

Method	**Gaussian 90 (J)**	**Gaussian 92 (C)**	**MOLPRO (92.3)**
Conv. RHF	104/1559 (3286)	87/1215 (2860)	157/2202 (4699)
Direct RHF	282/5637 (5674)	270/4044 (4078)	NA
RHF Gradient	1137/2969 (4434)	1147/2362 (4010)	3154/5357 (7848)
RHF Hessian	10570/12129 (16973)	11774/12989 (17755)	NA
UHF	121/2902 (7204)	118/2718 (6870)	FTC-unknown
Conv. MP2	1349/2907 (4933)	1333/2548 (4470)	322/2524 (5364)
Direct MP2	2627/8264 (8307)	2364/6408 (6447)	NA
MP2 Gradient	2456/8093 (13027)		NA
MP4(SDTQ)			3516/5718 (8874)
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 10. IBM RS/6000 340 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			
Direct RHF		3154/44153 (44336)	NA
RHF Gradient			
RHF Hessian			NA
UHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD			
CASSCF			

Method	**GAMESS-US 6/17/92**	**HONDO (8.3)**	**GAMESS-UK (2)**
Conv. RHF		Not ported to a C90	
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 10. IBM RS/6000 340 Timings (cont.)

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

Method	**Gaussian 90 (J)**	**Gaussian 92 (C)**	**MOLPRO (92.3)**
Conv. UHF		128/3590 (9984)	
UHF Gradient		890/4480 (10886)	NA
UHF Hessian			
Conv. RHF		69/2821 (8126)	179/3552 (7921)
Direct RHF		156/8141 (8246)	
Conv. MP2		2775/5596 (11468)	FTC - unknown
Direct MP2			NA
MP2 Gradient			NA
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD			
CASSCF			

Method	**GAMESS-US 6/17/92**	**HONDO (8.3)**	**GAMESS-UK (2)**
Conv. UHF			
UHF Gradient			
UHF Hessian			
Conv. RHF			
Direct RHF			
Conv. MP2			
Direct MP2			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

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

Table 10. IBM RS/6000 340 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		55/712 (1601)	
Direct RHF		123/1971 (1993)	NA
RHF Gradient		493/1205 (2159)	
RHF Hessian		12121/12833 (15502)	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 10. IBM RS/6000 340 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		548/6574 (10655)	
Direct RHF		1301/16921 (16997)	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 (8.3)**	**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			
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 (1.83)**	**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 10. IBM RS/6000 340 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)
Conv. RHF		211/2536 (5435)	
Direct RHF		184/2389 (2419)	
Dir. RHF Grad.		1034/3424 (3451)	
Dir. RHF Hess.			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 10. IBM RS/6000 340 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	40821/653141 (653899)		
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 10. IBM RS/6000 340 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 64 MB of memory and two 2GB Cambex 6200-90 disks running under AIX 3.2 with Release 2.0 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 (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.
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.
The caffeine RHF calculation was on the cation state of the molecule.