Table 39. SGI/Cray Y-MP Timings[a]

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

Method	Gaussian 90 (H)	Gaussian 92 (C)	MOLPRO (92.3)
Conv. RHF	2/22 (28)	3/27 (85)	2/14 (59)
Direct RHF	5/65 (80)	5/69 (169)	NA
RHF Gradient	15/37 (52)	12/35 (96)	39/53 (154)
RHF Hessian	225/247 (371)	186/213 (354)	NA
UHF	5/61 (67)	3/36 (314)	1/15 (68)
Conv. MP2	12/34 (38)	11/38 (93)	1/15 (62)
Direct MP2	57/79 (136)	37/64 (106)	NA
MP2 Gradient	92/126 (144)	86/124 (221)	NA
MP4(SDTQ)	280/334 (398)	227/254 (1085)	18/32 (151)
SDCI	28/329 (389)	25/281 (741)	1/22 (73)
CCSD	NA	37/435 (1883)	2/28 (105)
QCISD		28/305 (614)	1/26 (115)
CASSCF		56/533 (6313)[c]	1/18 (67)

Method	GAMESS-US 6/17/92	HONDO (8.3)	GAMESS-UK (2)
Conv. RHF		Not ported to a YMP	
Direct RHF			
RHF Gradient			
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2	NA		
MP2 Gradient	NA		
MP4(SDTQ)	NA		
SDCI			
CCSD	NA		
QCISD	NA		
CASSCF			

Table 39. SGI/Cray Y-MP Timings (cont.)

Method	**DISCO (1.82)**	**ACES II**
Conv. RHF		/13 (?)
Direct RHF		NA
RHF Gradient		29/42 (?)
RHF Hessian	NA	307/320 (?)
UHF	NA	14 (?)
Conv. MP2	NA	7/20 (?)
Direct MP2		NA
MP2 Gradient	NA	46/66 (?)
MP4(SDTQ)	NA	28/41 (?)
SDCI	NA	1/32 (?)
CCSD	NA	2/31 (?)
QCISD	NA	2/31 (?)
CASSCF	NA	NA

Table 39. SGI/Cray Y-MP 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)

Method	**Gaussian 90 (H)**	**Gaussian 92 (A)**	**MOLPRO (92.3)**
Conv. RHF			
Direct RHF			NA
RHF Gradient			
RHF Hessian			NA
UHF			
MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD	NA		
CASSCF			

Method	**GAMESS-US 6/17/92**	**HONDO (8.3)**	**GAMESS-UK (2)**
Conv. RHF		Not ported to a YMP	
Direct RHF			
RHF Gradient			
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2	NA		
MP2 Gradient	NA		
MP4(SDTQ)	NA		
SDCI			
CCSD	NA		
QCISD	NA		
CASSCF			

Method	**DISCO (1.82)**	**ACES II**
Conv. RHF		10/175 (?)
Direct RHF		NA
RHF Gradient		342/517 (?)
RHF Hessian	NA	6460/6635 (?)
UHF	NA	9/180 (?)
Conv. MP2	NA	91/266 (?)
Direct MP2		NA
MP2 Gradient	NA	697/963 (?)
MP4(SDTQ)	NA	283/458 (?)
SDCI	NA	16/398 (?)
CCSD	NA	23/425 (?)
QCISD	NA	20/390 (?)
CASSCF	NA	NA

Table 39. SGI/Cray Y-MP Timings (cont.)

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

Method	**Gaussian 90 (H)**	**Gaussian 92 (A)**	**MOLPRO (92.3)**
Conv. RHF		12/116 (630)	18/122 (635)
Direct RHF		21/252 (1099)	NA
RHF Gradient		54/170 (771)	
RHF Hessian		1620/1736 (2832)	NA
UHF			
MP2			4/126 (359)
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			3/142 (588)
CCSD	NA		
CASSCF			

Method	**GAMESS-US 6/17/92**	**HONDO (8.3)**	**GAMESS-UK (2)**
Conv. RHF		Not ported to a YMP	
Direct RHF			
RHF Gradient			
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2	NA		
MP2 Gradient	NA		
MP4(SDTQ)	NA		
SDCI			
CCSD	NA		
QCISD	NA		
CASSCF			

Method	**DISCO (1.82)**	**ACES II**
Conv. RHF		8/123 (?)
Direct RHF		NA
RHF Gradient		225/348 (?)
RHF Hessian	NA	2696/2819 (?)
UHF	NA	7/125 (?)
Conv. MP2	NA	32/155 (?)
Direct MP2		NA
MP2 Gradient	NA	455/610 (?)
MP4(SDTQ)	NA	106/229 (?)
SDCI	NA	6/208 (?)
CCSD	NA	8/207 (?)
QCISD	NA	7/196 (?)
CASSCF	NA	NA

Table 39. SGI/Cray Y-MP 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		80/2234 (4647)	
RHF Gradient			
RHF Hessian			NA
Conv. RHF		63/2589 (5392)	
Direct RHF		18/942 (1040)	
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD			
CASSCF			

Method	**GAMESS-US**	**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 39. SGI/Cray Y-MP 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 SCF step.

Unless otherwise noted all Cray Y-MP calculations were performed on a Y-MP/864 running Unicos 6.1 at the National Energy Research Supercomputer Center. Runs were made during off hours at interactive priorities.

G90 and ACES II timings were obtained on the Florida State University Supercomputer Center Y-MP/832 running Unicos 7.0.2. All FSU runs were made from a batch queue. Wall clock times for the FSU runs do not include queue wait time.

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 after the decimal point (7 - 8 digits in the density).

(b) The ethylene UHF calculation corresponded to 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.

(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.

Table 40. SGI/Cray Y-MP EL Timings[a]

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

Method	**Gaussian 92 (C)**	**Gaussian 92/DFT (F)**	**MOLPRO (92.3)**
Conv. RHF	10/96 (113)[b]		
Direct RHF	23/230 (226)[b]		NA
RHF Gradient	55/151 (194)[b]		
RHF Hessian	857/953 (1071)[b]		NA
UHF	11/131 (226)[b]		
Conv. MP2	71/167 (444)[b]		
Direct MP2	73/303 (698)[b]		NA
MP2 Gradient	400/567 (1270)[b]		NA
MP4(SDTQ)	860/956 (2857)[b]		
SDCI	112/1211 (1764)[b]		
CCSD	159/1847 (5517)[b]		
CCSD(T)	2591/2687 (7829)[b]		
QCISD	126/1358 (1805)[b]		
QCISD(T)	2073/2169 (5142)[b]		
CASSCF	129/2555 (6620)[b]		

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	NA		
MP2 Gradient	NA		
MP4(SDTQ)	NA		
SDCI			
CCSD	NA		
QCISD	NA		
CASSCF			

Table 40. SGI/Cray Y-MP EL 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.
All Cray YMP EL calculations were performed on a EL 4/512 (4 processor, 512 Mwords) running Unicos 7.0.5 mmd.2 at the Cray facilites in Eagan, Minnesota.
NA: not available wNAed to complete - not enough disk space.
FTC-unknown: Failed to complete for unknown reasons.
SCF calculations were converged to approximately 13 digits after the decimal point (7 - 8 digits in the density).

(b) Calculations run by Dr. Carlos Sosa of Cray Research.

Table 41. SGI/Cray C90 Timings[a]

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

Method	**Gaussian 92 (D)**	**Gaussian 92/DFT (F)**	**Gaussian 94 (C.3)**
Conv. RHF	2/21 (263)	1/9 (17)[g]	2/19 (55)
Direct RHF	3/33 (64)	4/37 (54)[g]	3/34 (76)
In-core RHF			1/11 (278)
RHF Gradient	19/40 (207)	9/18 (29)[g]	8/27 (81)
RHF Hessian	117/138 (278)	119/128 (170)[g]	106/125 (241)
UHF	5/63 (2682)	1/13 (21)[g]	2/23 (65)
Conv. MP2	13/34 (127)	10/19 (32)[g]	6/25 (51)
Direct MP2	12/45 (145)	6/43 (50)[g]	7/40 (68)
MP2 Gradient	51/85 (371)	28/47 (62)[g]	137/162 (446)
MP2 Hessian			374/399 (1118)
MP4(SDTQ)	150/171 (953)	100/109 (254)[g]	93/121 (859)
SDCI	18/203 (2329)	13/142 (227)[g]	11/118 (407)
CCSD	26/310 (3593)	20/225 (376)[g]	19/206 (1547)
CCSD(T)	442/463 (5893)	315/324 (674)[g]	343/362 (2241)
QCISD	16/177 (1031)	15/163 (276)[g]	13/147 (686)
QCISD(T)	312/333 (2552)	253/262 (415)[g]	305/324 (1833)
CASSCF	20/408 (963)	20/412 (451)[g]	23/472 (1782)
CAS-CI	NA	NA	NA
SVWN (LSD)	NA	4/23 (87)	13/105 (156)
BLYP (NLSD)	NA	4/22 (224)	15/119 (177)

Method	**MOLPRO (94.1)**[f]	**GAMESS-US 6/17/92**	**GAMESS-UK (2)**
Conv. RHF	2/18 (46)	1/13 (73)	
Direct RHF	NA	8/98 (130)	
RHF Gradient	35/53 (150)	20/33 (185)	
RHF Hessian	NA	171/184 (1198)	
UHF	2/24 (77)	1/20 (242)	
Conv. MP2	1/19 (91)	26/47 (417)	
Direct MP2	NA	NA	
MP2 Gradient	NA	NA	
MP4(SDTQ)	20/38 (137)	NA	
SDCI	2/31 (128)	26/257 (1883)[c]	
CCSD	2/34 (108)	NA	
CCSD(T)	42/60 (217)		
QCISD	2/32 (242)	NA	
QCISD(T)	31/49 (162)		
CASSCF	1/23 (36)	278/279 (14763)[c]	
SVWN (LSD)	2/20 (81)[i]		
BLYP (NLSD)	FTC-unknown[j]		

Table 41. SGI/Cray C90 Timings (cont.)

Method	DISCO (1.82)	SUPERMOL. (1.08)	ACES II
Conv. RHF	1/19 (101)		
Direct RHF	3/37 (60)	1/20 (?)[k]	NA
RHF Gradient	31/50 (77)		
RHF Hessian	NA	NA	
UHF	NA	NA	
Conv. MP2	NA	NA	
Direct MP2	15/52 (76)		NA
MP2 Gradient	NA	NA	
MP4(SDTQ)	NA	NA	
SDCI	NA	NA	
CCSD	NA	NA	
CCSD(T)	NA	NA	
QCISD	NA	NA	
QCISD(T)	NA	NA	
CASSCF	NA	NA	NA
SVWN (LSD)	NA	NA	
BLYP (NLSD)	NA	NA	

Table 41. SGI/Cray C90 Timings (cont.)

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

Method	**Gaussian 92 (A)**	**Gaussian 92/DFT (F)**	**MOLPRO (92.3)**[f]
Conv. RHF	6/63 (138)	()[g]	8/80 (176)
Direct RHF	13/132 (152)		NA
RHF Gradient	27/90 (169)		NA
RHF Hessian	1019/1157 (1419)		NA
UHF	7/89 (297)		6/82 (283)
Conv. MP2	54/117 (336)		1/81 (156)
Direct MP2	54/186 (351)		NA
MP2 Gradient	291/408 (739)		NA
MP4(SDTQ)	774/837 (8334)		42/122 (368)
SDCI	104/1203 (2491)		2/93 (630)
CCSD	145/1655 (10101)		4/108 (479)
CCSD(T)			
QCISD	118/1242 (3749)		4/120 (517)
QCISD(T)			
CASSCF	FTC-ND		3/93 (501)

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	NA		
MP2 Gradient	NA		
MP4(SDTQ)	NA		
SDCI			
CCSD	NA		
CCSD(T)	NA		
QCISD	NA		
QCISD(T)	NA		
CASSCF			

Table 41. SGI/Cray C90 Timings (cont.)

Method	DISCO (1.82)	SUPERMOL. (1.08)	ACES II
Conv. RHF	3/263 (352)		
Direct RHF	34/339 (394)		NA
RHF Gradient	482/745 (1176)		
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
CCSD(T)	NA	NA	
QCISD			
QCISD(T)	NA	NA	
CASSCF			NA

Table 41. SGI/Cray C90 Timings (cont.)

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

Method	**Gaussian 92 (C)**	**Gaussian 92/DFT (F)**	**MOLPRO (92.3)**
Conv. RHF	14/135 (341)	5/49 (172)[g]	
Direct RHF	14/173 (269)	16/174 (184)[g]	NA
RHF Gradient		31/80 (167)[g]	
RHF Hessian		1688/1735 (1926)[g]	NA
UHF		8/99 (278)[g]	
Conv. MP2		66/115 (196)[g]	
Direct MP2		59/233 (248)[g]	NA
MP2 Gradient		296/411 (685)[g]	NA
MP4(SDTQ)		2899/2948 (6677)[g]	
SDCI			
CCSD		/2819 (7313)[g]	
QCISD		/2165 (2414)[g]	
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	NA		
MP2 Gradient	NA		
MP4(SDTQ)	NA		
SDCI			
CCSD	NA		
QCISD	NA		
CASSCF			

Table 41. SGI/Cray C90 Timings (cont.)

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

Method	**Gaussian 90 (H)**	**Gaussian 92 (C)**	**MOLPRO (92.3)**
Conv. RHF		39/542 (1505)	
Direct RHF		17/256 (945)	NA
RHF Gradient		24/564 (2115)	
RHF Hessian			NA
UHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)		14046 (60358)	
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	**SUPERMOL. (1.08)**	**ACES II**
Conv. RHF		
Direct RHF	?/679 (?)[k]	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 41 SGI/Cray C90 Timings (cont.)

Imidazole, 36 electrons, $^1A'$, 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		183/2560 (7763)	
Direct RHF		131/1962 (2227)	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	**SUPERMOL. (1.08)**	**ACES II**
Conv. RHF		
Direct RHF	?/7749 (?)[(k)]	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 41. SGI/Cray C90 Timings (cont.)

Isobutene, 32 electrons, 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		23/303 (627)	
Direct RHF			
RHF Gradient			
RHF Hessian			NA
UHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD			
CASSCF			

Method	**GAMESS-US**	**HONDO (8.1)**	**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			

Table 41. SGI/Cray C90 Timings (cont.)

Method	SUPERMOL. (1.08)	ACES II
Conv. RHF		
Direct RHF	?/348 (?)[k]	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 41. SGI/Cray C90 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 92 (D)**	**Gaussian 92 /DFT**	**MOLPRO (92.3)**
Conv. RHF	138/1655 (3104)		
Direct RHF	77/1006 (1318)		
RHF Gradient			
RHF Hessian			NA
UHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD			
CASSCF			

Method	**GAMESS-US**	**HONDO (8.1)**	**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			

Table 41. SGI/Cray C90 Timings (cont.)

Method	DISCO (1.82)	SUPERMOL. (1.08)	ACES II
Conv. RHF			
Direct RHF	215/2584 (4217)	?/3228 (?)	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 41. SGI/Cray C90 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			
RHF Gradient			
RHF Hessian			NA
Conv. RHF		57/2325 (17212)	
Direct RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD			
CASSCF			

Method	**GAMESS-US**	**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			

Table 41. SGI/Cray C90 Timings (cont.)

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

Method	Gaussian 90 (H)	Gaussian 92 (C)	Gaussian 94 (B)
Direct RHF		16/209 (638)	16/207 (254)
RHF Gradient		60/269 (677)	
RHF Hessian		13103/13312 (20935)	
Conv. RHF			
Conv. MP2			
Direct MP2		1428/1637 (1740)[e]	
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	SUPERMOL. (1.08)	MOLPRO (92.3)	ACES II
Conv. RHF			
Direct RHF	?/1224 (?)[k]		NA
RHF Gradient			
RHF Hessian	NA	NA	
UHF	NA		
Conv. MP2	NA		
Direct MP2		NA	NA
MP2 Gradient	NA		
MP4(SDTQ)	NA		
SDCI	NA		
CCSD	NA		
QCISD	NA		
CASSCF	NA		NA

Table 41. SGI/Cray C90 Timings (cont.)

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

Method	**Gaussian 90 (H)**	**Gaussian 92 (C)**	**Gaussian 94 (B)**
Direct RHF		85/1111 (1248)	84/1098 (1576)
RHF Gradient		317/1428 (1629)	
RHF Hessian		68140/69251 (107603)	
Direct MP2		17804/18915 (48001)[e]	
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD	NA		
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)**	**MOLPRO (92.3)**	**ACES II**
Direct RHF			NA
RHF Gradient			
RHF Hessian	NA	NA	
UHF	NA		
Direct MP2		NA	NA
MP2 Gradient	NA		
MP4(SDTQ)	NA		
SDCI	NA		
CCSD	NA		
QCISD	NA		
CASSCF	NA		NA

Table 41. SGI/Cray C90 Timings (cont.)

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

Method	**Gaussian 90 (H)**	**Gaussian 92 (C)**	**MOLPRO (92.3)**
Direct RHF		2541/40663 (53509)	
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 (8.3)**	**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 41. SGI/Cray C90 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.
Except where otherwise noted, all Cray C90 calculations were performed on a C90/16256 (16 processor, 256 Mwords) running Unicos 7.C at the National Energy Research Supercomputer Center.
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 after the decimal point (7 - 8 digits in the density).

(b) The ethylene UHF calculation corresponded to 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.
The caffeine RHF calculation was on the cation state of the molecule.

(c) 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.

(d) The 18-crown-6 MP2 calculations did not treat the carbon and oxygen core electrons.

(e) By increasing the amount of memory for Gaussian 92 MP2 calculations on 18-crown-6 it was possible to reduce the CPU time to 836 sec. for the 3-21G basis (4 MW to 10 MW) and 7782 sec. for the 6-31G** basis (10 MW to 30 MW).

(f) MOLPRO ran in YMP mode.

(g) A fully direct MP2 gradient calculation for 6-31G** 18-crown-6 requires approximately 61 MW of memory, since the fully direct algorithm scales as N^3.

(h) Run on the C90 at the Minnesota Supercomputer Center by Dr. Carlos Sosa of Cray Research, Inc.

(i) MOLPRO did not use the same SVWN functional as Gaussian 92/DFT.

(j) This run died for reasons which are unknown. Because MOLPRO does not use the same angular integration grid as Gaussian 92/DFT, the SBLYP energy produced by MOLPRO differed by ~ 0.01 E_h.

(k) Run by Dr. Martin Feyereisen of Cray Research, Inc.

Table 42. SGI/Cray J90 Timings[a]

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

Method	Gaussian 94 (D)		
Conv. RHF	6/61 (112)		
Direct RHF	11/111 (161)		
In-core RHF	4/43 (93)		
RHF Gradient	30/91 (157)		
RHF Hessian	321/382 (587)		
UHF	6/72 (142)		
Conv. MP2	17/78 (145)		
Direct MP2	19/130 (193)		
MP2 Gradient	387/465 (882)		
MP2 Hessian	1285/1415 (2189)		
MP4(SDTQ)	384/445 (1097)		
SDCI	40/425 (1140)		
CCSD	65/708 (3646)		
CCSD(T)	1233/1294 (4946)		
QCISD	47/532 (1425)		
QCISD(T)	1093/1154 (2449)		
CASSCF	FTC (unknown)		
CAS-CI	NA		
SVWN (LSD)	39/313 (348)		
BLYP (NLSD)	47/372 (416)		

Method	MOLPRO (94.1)[f]	GAMESS-US 6/17/92	GAMESS-UK (2)
Conv. RHF			
Direct RHF	NA		
RHF Gradient			
RHF Hessian	NA		
UHF			
Conv. MP2			
Direct MP2	NA	NA	
MP2 Gradient	NA	NA	
MP4(SDTQ)		NA	
SDCI			
CCSD		NA	
CCSD(T)			
QCISD		NA	
QCISD(T)			
CASSCF			
SVWN (LSD)			
BLYP (NLSD)			

Table 42. SGI/Cray J90 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.
Except where otherwise noted, all Cray J90 calculations were performed on a 32 processor, 1 GW (8 GB) machinerunning Unicos 9.0 at the National Energy Research Supercomputer Center.

Table 43. SGI/Cray T90 Timings[a]

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

Method	Gaussian 94 (D.4)		
Conv. RHF	2/15 (62)[b]		
Direct RHF	3/26 (72)[b]		
In-core RHF	1/9 (79)		
RHF Gradient	7/22 (91)[b]		
RHF Hessian	63/78 (178)[b]		
UHF	2/21 (68)		
Conv. MP2	4/19 (73)[b]		
Direct MP2	5/31 (79)[b]		
MP2 Gradient	95/114 (213)		
MP2 Hessian	290/309 (736)		
MP4(SDTQ)	66/81 (124)[b]		
SDCI	8/89 (175)[b]		
CCSD	14/159 (469)		
CCSD(T)	183/198 (265)[b]		
QCISD	7/87 (532)		
QCISD(T)	177/192 (319)[b]		
CASSCF	16/340 (369)[b]		
CAS-CI	NA		
SVWN (LSD)	8/81 (170)		
BLYP (NLSD)	9/93 (196)		

Method	MOLPRO (96)	GAMESS-US 6/17/92	GAMESS-UK (2)
Conv. RHF			
Direct RHF			
RHF Gradient			
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
CCSD(T)			
QCISD			
QCISD(T)			
CASSCF			
SVWN (LSD)			
BLYP (NLSD)			

Table 43. SGI/Cray T90 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.
All Cray T90 calculations were performed on a 32 processor, 1 GW machinerunning Unicos 9.0 at the Cray.

(b) Calculations run by Dr. Carlos Sosa of Cray Research, Inc.