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 Direct RHF RHF Gradient RHF Hessian UHF Conv. MP2		Not ported to a YMP	
Direct MP2	NA		
MP2 Gradient	NA		
MP4(SDTO)	NA		
SDCI			
CCSD	NA		
OCISD	NA		
CASSCF			

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

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			NT A
Direct RHF			NA
RHF Gradient			NI A
			NA
MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTO)			
SDCI			
CCSD	NA		
CASSCF			
Method	GAMESS-US 6/17/92	HONDO (8.3)	GAMESS-UK (2)
Conv. DUE		Not norted to a VMD	
Direct RHF		Not ported to a TMF	
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		10/398 (?)	
OCISD		23/423 (?) 20/200 (?)	
CASSCE	ΝΔ	20/390 (?) NA	
	1111	1 11 1	

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)			2/142 (599)
SDCI	ΝA		3/142 (588)
CASSCE	INA		
Chibber			
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		
CCSD	NΔ		
OCISD	NA		
CASSCF	1 12 1		
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		6/208 (?) 8/207 (?)	
OCISD		0/207 (?) 7/106 (?)	
CASSCE	NA	NA	
~	1 1/ 1	1 1 Å Å	

Caffeine, C₈H₉O₂N₄, 101 electrons, C1, Basis Set=3-21G, (144 functions)

Method	Gaussian 90 (H)	Gaussian 92 (C)	MOLPRO (92.3)
UHE		80/2234 (4647)	
RHF Gradient		00/223+ (+0+7)	
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			
CASSCE			
CASSUL			

(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 $\pi \to \pi^*$ (${}^{3}B_{1u}$) state. The ethylene ground state is ${}^{1}A_{g}$. 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 (${}^{3}ag$, 1 ${}^{b}3u$, 1 ${}^{b}2g$, 2 ${}^{b}1u$). 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 $\pi \to \pi^* \, {}^3B_{1u}$ 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 ccpVTZ 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. The Gaussian CAS calculation using RHF canonical orbitals aborted with an error message saying

(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, ${}^{1}A_{g}$, 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			
KHF Hessian			
Conv MP2			
Direct MP2	NA		
MP2 Gradient	NA		
MP4(SDTQ)	NA		
SDCI			
CCSD	NA		
QCISD	NA		
CASSCF			

- (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.

Ethylene, 16 electrons, ¹ Ag, 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)
C DUE	2/19 (46)	1 (12 (72)	
Conv. RHF	2/18 (46) NA	1/13(73) 8/08(120)	
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	
QUISD(T)	31/49 (162)		
	1/23 (30)	278/279 (14763) ^(C)	
SVWN (LSD)	2/20 (81)(1)		
BLYP (NLSD)	FTC-unknown ^(J)		

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	

Method	Gaussian 92 (A)	Gaussian 92/DFT (F)	MOLPRO (92.3) ^(f)
Conv RHF	6/63 (138)	$O(\mathbf{g})$	8/80 (176)
Direct PHE	13/132 (152)	()(8)	NA
Dilect Kill [*]	27/00 (160)		NA NA
RHF Undelin	27/90(109) 1010/1157(1/10)		NA NA
	7/80 (207)		6/82 (283)
Conv. MD2	54/117(226)		$\frac{0}{82}(283)$
Direct MD2	54/117 (550)		1/81 (130) NA
MD2 Cradiant	201/408 (720)		INA NA
MP2 Gradient	291/408 (759)		NA 42/122 (268)
MP4(SDTQ)	1/4/857 (8554)		42/122 (508)
SDCI	104/1203 (2491)		2/93 (630)
CCSD	145/1655 (10101)		4/108 (479)
CCSD(1)	110/1040 (2740)		4/100 (517)
QCISD	118/1242 (3749)		4/120 (517)
QCISD(T)			
CASSCF	FIC-ND		3/93 (501)
Method	GAMESS-US 6/17/92	HONDO (8.3)	GAMESS-UK (2)
Conv. DHE		Not ported to a COO	
Direct BUE		Not ported to a C90	
DIFE Credient			
UHF Conv. MD2			
Direct MD2	NA		
MD2 Cradient	INA NA		
MP2 Gradient	INA NA		
MP4(SDTQ)	INA		
SDCI	NT A		
CC2D(1)			
QUISD	NA		
QCISD(T)	NA		
CASSCF			

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

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

Method	Gaussian 92 (C)	Gaussian 92/DFT (F)	MOLPRO (92.3)
Conv. PHF	14/135 (341)	5/40(170)(9)	
Direct DUE	14/172 (200)	5/49(1/2)(5)	NT A
Direct RHF	14/173 (209)	16/174 (184)(8)	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		
QUISD	NA		
CASSCF			

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

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 Direct RHF RHF Gradient RHF Hessian UHF		39/542 (1505) 17/256 (945) 24/564 (2115)	NA NA
Conv. MP2 Direct MP2 MP2 Gradient MP4(SDTQ)		14046 (60358)	NA
SDCI CCSD QCISD CASSCF	NA		
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		Not ported to a C90	
Method	SUPERMOL. (1.08)	ACES II	
Conv. RHF Direct RHF RHF Gradient	?/679 (?) ^(k)	NA	
RHF Hessian UHF Conv. MP2 Direct MP2	NA NA NA	NA	
MP2 Gradient MP4(SDTQ) SDCI CCSD	NA NA NA NA		
QCISD CASSCF	NA NA	NA	

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

Conv. RHF 183/2560 (7763) Direct RHF Interval 183/2560 (7763) Direct RHF Interval 131/1962 (2227) NA RHF Gradient NA HFF Gradient NA M2 Gradient MP2 M2 Gradient MP4 (SDTQ) SDC1 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 RHF P2 Gradient MP4 (SDTQ) SDC1 CCSD CASSCF Method SUPERMOL. (1.08) ACES II Conv. RHF Direct RHF $2/7749 (7)^{(k)}$ NA RHF Gradient RHF Hessian NA UHF NA Conv. RHF Direct RHF $2/7749 (7)^{(k)}$ NA RHF Gradient RHF Hessian NA UHF NA Conv. RHF Direct RHF NA Conv. RHF Direct RHF $2/7749 (7)^{(k)}$ NA RHF Gradient RHF Gradient RHF Gradient RHF Gradient RHF Gradient RHF Gradient RHF MA Direct MP2 NA Direct MP3 NA CSDS NA QCISD N	Method	Gaussian 90 (H)	Gaussian 92 (C)	MOLPRO (92.3)
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 CONV. RHF Not ported to a C90 Direct RHF RHF Gradient RHF Hessian UHF Conv. MP2 Direct RHF RHF Gradient RHF Hessian UHF Conv. MP2 Direct RP2 MP2 Gradient MP4(SDTQ) SDCI CCSD CASSCF CONV. RHF Not ported to a C90 Direct RHF RHF RHF Convert State S	Conv. RHF		183/2560 (7763)	
Arr Ordadient NA UHF conv. 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 Not ported to a C90 Direct RHF RHF Gradient RHF Gradient RHF Hessian UHF Conv. RP2 Direct MP2 MP2 Gradient Method SUPERMOL. (1.08) ACES II Conv. RHF Conv. RHF Direct RHF ?/7749 (?) ^(k) NA RHF Gradient RHF Gradient RHF Hessian NA Conv. RHF Direct RHF ?/7749 (?) ^(k) NA RHF Gradient RHF Hessian NA Conv. MP2 Direct MP2 Method SUPERMOL. (1.08) ACES II Conv. RHF Direct RHF ?/7749 (?) ^(k) NA RHF Gradient RHF Hessian NA Conv. MP2 NA Direct MP2 NA Conv. MP2 NA Conv. MP2 NA Conv. MP2 NA Conv. MP2 NA Conv. MP2 NA Conv. MP3 NA C	Direct RHF		131/1962 (2227)	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) Method GAMESS-US 6/17/92 HONDO (8.3) GAMESS-UK (2) Onv. RHF Direct RHF RHF Gradient RHF Gradient RHF Gradient MP4(SDTQ) SDCI COSD QCISD CASSCF Method SUPERMOL. (1.08) ACES II Conv. RHF Direct RHF 7/7749 (2)(k) NA RHF Gradient RHF Hessian NA UHF NA Conv. RHF Direct RHF 7/7749 (2)(k) NA RHF Gradient RHF Hessian NA UHF NA Conv. MP2 NA Direct MP3 NA Conv. MP2 NA Direct MP5 NA CONV. MP3 NA CONV. MP3 NA CONV. MP3 NA DIRECT MP3 NA	RHF Hessian			NA
Conv. MP2 Direct MP2 MP2 Gradient MP4(SDTQ) SDC1 CCSD 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 Gradient MP4 (SDTQ) SDC1 CCSD QCISD CASSCF Method SUPERMOL. (1.08) ACES II Conv. RHF Direct RHF pirect RHF	UHF			
Direct MP2 Method GAMESS-US 6/17/92 HONDO (8.3) GAMESS-UK (2) 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) SDC1 CCSD QCISD CASSCF Method SUPERMOL. (1.08) ACES II Conv. RHF Direct RHF ?/7749 (?) ^(k) NA RHF Gradient RHF Hessian NA UHF NA Conv. RHF Direct RHF ?/7749 (?) ^(k) NA RHF Gradient RHF Hessian NA UHF NA Conv. MP2 NA Direct MP2 NA Direct MP2 NA Direct MP2 NA Conv. MP2 NA Conv. MP2 NA Direct MP2 NA Conv. MP2 NA Direct MP2 NA Conv. MP3 NA COSD NA CCSD NA QCISD NA CCSD NA CCSD NA CCSD NA CCSD NA CCSD NA CCSD NA CCSD NA CCSD NA CCSD NA CASSCF NA NA	Conv. MP2			
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 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 MP3 NA Direct MP4 MP4(SDTQ) NA SDCI NA CCSD NA CCS	Direct MP2 MP2 Gradient			NA
SDCI CCSD NA QCISD CASSCF Method GAMESS-US 6/17/92 HONDO (8.3) GAMESS-UK (2) Not ported to a C90 Direct RHF RHF Gradient RHF Gradient MP4 (SDTQ) SDCI CCSD QCISD CASSCF Method SUPERMOL. (1.08) ACES II Conv. RHF Direct RHF ?/7749 (?)(k) NA RHF Gradient RHF Gradient RHF Hessian NA UHF NA Conv. MP2 NA Direct MP3 NA MP4 (SDTQ) NA SDCI NA CCSD NA	MP2 Gradient MP4(SDTO)			
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) SDC1 CCSD QCISD CASSCF Method SUPERMOL. (1.08) ACES II Conv. RHF Direct RHF ?/7749 (?)(k) NA RHF Gradient RHF Hessian RHF Hessian RHF Hessian RHF Gradient RHF Hassian NA UHF NA Conv. MP2 NA Direct MP2 NA Direct MP2 NA Direct MP2 NA Direct MP3 NA MP4(SDTQ) NA SDC1 CSD NA CCSD NA	SDCI			
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 RHF RHF Hessian UHF Conv. MP2 Direct MP2 MP4(SDTQ) SDC1 CCSD QCISD CASSCF Method Method SUPERMOL. (1.08) ACES II Conv. RHF Direct RHF ?/7749 (?) ^(k) NA RHF Gradient RHF Gradient RHF Gradient RHF NA UHF NA NP2 Gradient NA Pirect RHP NA NP2 Gradient NA MP2 Gradient NA MP2 Gradient NA MP2 Gradient NA QCISD NA QCISD NA MP2 Gradient NA MP2 Gradient NA QCISD NA QCISD NA QCISD NA QCISD <t< td=""><td>CCSD</td><td>NA</td><td></td><td></td></t<>	CCSD	NA		
Method GAMESS-US 6/17/92 HONDO (8.3) GAMESS-UK (2) Conv. RHF Not ported to a C90 Direct RHF NHF Gradient RHF Gradient RHF Hessian UHF Conv. MP2 Direct RP2 MP4 (SDTQ) SDC1 CCSD CCSD QCISD CASSCF Method Method SUPERMOL. (1.08) ACES II Conv. RHF Direct RHF ?/7749 (?)(k) NA RHF Gradient RHF Gradient RHF Hessian NA UHF NA Conv. RHF ?/7749 (?)(k) Direct RHF ?/7749 (?)(k) NA NA PUF Gradient NA RHF Hessian NA UHF NA Direct RHP NA Direct RHP NA Direct RHF ?/7749 (?)(k) NA NA Direct RHF NA COSD NA QCISD NA QCISD NA QCISD NA CASSCF NA	QCISD			
Method GAMESS-US 6/17/92 HONDO (8.3) GAMESS-UK (2) Conv. RHF Not ported to a C90 Direct RHF RHF Gradient RHF Bradient Not ported to a C90 UHF Onv. MP2 Direct MP2 Not ported to a C90 WP2 Gradient MP4(SDTQ) SDC1 CCSD CCSD QCISD Conv. RHF ?/7749 (?)(k) Direct RHF ?/7749 (?)(k) NA NA UHF NA Conv. MP2 NA Direct RHF ?/7749 (?)(k) Direct RHF ?/7749 (?)(k) NA NA UHF NA Conv. MP2 NA Direct RHF ?/7749 (?)(k) NA NA UHF NA Conv. MP2 NA Direct MP2 NA MP2 Gradient NA MP4(SDTQ) NA Direct MP2 NA QCISD	CASSCF			
Conv. RHF Not ported to a C90 Direct RHF RHF Gradient RHF flessian 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 UHF Conv. RHF Direct RHF ?/7749 (?) ^(k) NA UHF Conv. RHF Direct RHF ?/7749 (?) ^(k) NA UHF Conv. MP2 NA Direct MP2 NA QCISD NA QCISD NA QCISD NA QCISD NA QCISD NA QCISD NA <td>Method</td> <td>GAMESS-US 6/17/92</td> <td>HONDO (8.3)</td> <td>GAMESS-UK (2)</td>	Method	GAMESS-US 6/17/92	HONDO (8.3)	GAMESS-UK (2)
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 Gradient RHF Hessian NA UHF NA Conv. MP2 NA Direct MP3 NA MP4(SDTQ) NA SDCI NA CCSD NA QCISD NA CASSCF NA NA	Conv. RHF		Not ported to a C90	
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 Gradient RHF Hessian NA UHF NA Conv. MP2 NA Direct MP3 NA Direct MP4 NA COSD NA SDCI NA SDCI NA SDCI NA SDCI NA SDCI NA SDCI NA SDCI NA CSD NA CASSCF NA NA	Direct RHF		I	
RHF Hessian UHF Conv. MP2 Direct MP2 MP2 Gradient MP4(SDTQ) SDC1 CCSD QCISD CASSCF <u>Method</u> 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 Direct MP2 NA Direct MP2 NA Direct MP2 NA MP4(SDTQ) NA SDC1 NA CCSD NA QCISD NA QCISD NA QCISD NA CASSCF NA NA	RHF Gradient			
UHF Conv. MP2 Direct MP2 MP2 Gradient MP4(SDTQ) SDC1 CCSD QCISD CASSCF <u>Method</u> 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 Direct MP2 NA Direct MP2 NA MP2 Gradient NA MP4(SDTQ) NA SDC1 NA CCSD NA QCISD NA QCISD NA QCISD NA CASSCF NA NA	RHF Hessian			
Conv. M12Direct MP2MP2 GradientMP4(SDTQ)SDCICCSDQCISDCASSCFMethodSUPERMOL. (1.08)ACES IIConv. RHFDirect RHF $?/7749 (?)^{(k)}$ NARHF GradientRHF HessianRHFOnv. MP2NADirect MP2NADirect MP2NADirect MP2NADirect MP2NADirect MP2NAQCISDNAQCISDNACoSDNACOSDNACASSCFNANANA168	Conv 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 MP3 NA MP4(SDTQ) NA SDCI NA CCSD NA QCISD NA CASSCF NA NA	Direct MP2			
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 Direct MP2 NA Direct MP2 NA Direct MP2 NA SDCI NA SDCI NA SDCI NA CCSD NA QCISD NA CASSCF NA NA	MP2 Gradient			
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 Direct MP2 NA Direct MP2 NA SDCI NA SDCI NA SDCI NA SDCI NA CCSD NA CCSD NA CCSD NA CCSD NA CCSD NA	MP4(SDTQ)			
Method SUPERMOL. (1.08) ACES II Method SUPERMOL. (1.08) ACES II Conv. RHF Direct RHF ?/7749 (?) ^(k) Direct RHF ?/7749 (?) ^(k) NA RHF Gradient RHF NA RHF Hessian NA NA UHF NA NA Direct MP2 NA NA Direct MP2 NA NA SDCI NA SDCI VA NA CCSD QCISD NA CASSCF NA NA NA	SDCI			
Method SUPERMOL. (1.08) ACES II Conv. RHF Direct RHF ?/7749 (?) ^(k) NA RHF Gradient RHF Hessian NA UHF NA Onv. MP2 Direct MP2 NA Direct MP2 NA Direct MP2 NA QCISD NA QCISD NA CASSCF NA	CCSD			
MethodSUPERMOL. (1.08)ACES IIConv. RHF Direct RHF?/7749 (?)(k)NARHF Gradient RHF HessianNAVAUHFNAVAConv. MP2NANADirect MP2NANAMP2 GradientNAMP4(SDTQ)NASDCINAQCISDNACASSCFNANA	CASSCF			
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	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	11101100			
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	Conv. RHF			
RHF GradientRHF HessianNAUHFNAConv. MP2NADirect MP2NAMP2 GradientNAMP4(SDTQ)NASDCINACCSDNAQCISDNACASSCFNANANA	Direct RHF	?/7749 (?) ^(k)	NA	
RHF HessianNAUHFNAConv. MP2NADirect MP2NAMP2 GradientNAMP4(SDTQ)NASDCINACCSDNAQCISDNACASSCFNANANA168	RHF Gradient	N7.4		
OHFNAConv. MP2NADirect MP2NAMP2 GradientNAMP4(SDTQ)NASDCINACCSDNAQCISDNACASSCFNANANA168	KHF Hessian	NA		
Direct MP2NAMP2 GradientNAMP4(SDTQ)NASDCINACCSDNAQCISDNACASSCFNANANA168	Conv MP2	NA		
MP2 GradientNAMP4(SDTQ)NASDCINACCSDNAQCISDNACASSCFNANANA	Direct MP2	14/1	NA	
MP4(SDTQ) NA SDCI NA CCSD NA QCISD NA CASSCF NA NA 168	MP2 Gradient	NA		
SDCI NA CCSD NA QCISD NA CASSCF NA NA 168	MP4(SDTQ)	NA		
CCSD NA QCISD NA CASSCF NA NA 168	SDCI	NA		
CASSCF NA NA 168	CCSD	NA		
168	QUISD CASSCE	NA NA	N۸	
100			168	

Isobutene, 32 electrons, C _{2v} , Basis Set=6-311++0	G**,
(148 functions, 6-term d's)	

Method	Gaussian 90 (H)	Gaussian 92 (C)	MOLPRO (92.3)
Conv. RHF Direct RHF		23/303 (627)	
RHF Gradient			
RHF Hessian			NA
UHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI	NT A		
OCISD	NA		
CASSCE			
CASSEI			
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)			
MP4(SDTQ) SDCI			
MP4(SDTQ) SDCI CCSD OCISD			

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

Isobutene, 32 electrons, ${}^{1}A_{1}$ (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 Direct RHF	138/1655 (3104) 77/1006 (1318)		
RHF Gradient RHF Hessian UHF			NA
Direct MP2 MP2 Gradient MP4(SDTQ) SDCI			NA
CCSD QCISD CASSCF	NA		
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		Not ported to a C90	

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

Caffeine, C ₈ H ₉ O ₂ N ₄ ,	101 electrons, C	1, Basis Set=3-21G,
(144 functions)		

Method	Gaussian 90 (H)	Gaussian 92 (C)	MOLPRO (92.3)
UHF RHF Gradient RHF Hessian Conv. RHF Direct RHF		57/2325 (17212)	NA
Conv. MP2 Direct MP2 MP2 Gradient MP4(SDTQ) SDCI			NA
CCSD QCISD CASSCF	NA		
Method	GAMESS-US	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		Not ported to a C90	

18-crown-6, C₁₂H₂₄O₆, 144 electrons, C_i, Basis Set=3-21G (210 functions)^(e)

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

18-crown-6, C₁₂H₂₄O₆, 144 electrons, C_i, Basis Set=6-31G** (390 functions)^(e)

Method	Gaussian 90 (H)	Gaussian 92 (C)	Gaussian 94 (B)
Direct RHF RHF Gradient RHF Hessian Direct MP2 MP2 Gradient MP4(SDTQ) SDCI CCSD QCISD	NA	85/1111 (1248) 317/1428 (1629) 68140/69251 (107603) 17804/18915 (48001) ^(e)	84/1098 (1576)
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 RHF Gradient			NA
RHF Hessian	NA	NA	
UHF Direct MP2	NA	NA	NΛ
MP2 Gradient	NA	NA	NA
MP4(SDTO)	NA		
SDCI	NA		
CCSD	NA		
OCISD	NA		
CASSCF	NA		NA

18-crown-6, C₁₂H₂₄O₆, 144 electrons, C_i, Basis Set=aug-cc-pVDZ (606 functions)

Method	Gaussian 90 (H)	Gaussian 92 (C)	MOLPRO (92.3)
Direct RHF RHF Gradient		2541/40663 (53509)	
RHF Hessian Conv. RHF			NA
Direct MP2 MP2 Gradient MP4(SDTQ)			NA
SDCI CCSD QCISD CASSCF	NA		
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 RHF Gradient		NA	
RHF Hessian	NA		
UHF Conv. MD2	NA NA		
Direct MP2	INA	NΔ	
MP2 Gradient	NA		
MP4(SDTO)	NA		
SDCI	NA		
CCSD	NA		
QCISD	NA		
CASSCF	NA	NA	

(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 $\pi \to \pi^*$ (${}^{3}B_{1u}$) state. The ethylene ground state is ${}^{1}A_{g}$. 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 N³.
- (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, ${}^{1}A_{g}$, 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)			
DI VD (NI CD)			

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

Method	Gaussian 94 (D.4)		
	$\langle 1 \rangle$		
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)			
CCSD			
CCSD(T)			
OCISD			
OCISD(T)			
CASSCF			
SVWN (LSD)			
BLYP (NLSD)			

- (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.