Table 20. SGI Indigo 50/100 MHz R4000 Timings[a]

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

Method	**Gaussian 92 (E)**	**Gaussian 92/DFT**	**MOLPRO (94.3)**
Conv. RHF	4/43 (46)		8/72 (75)
Direct RHF	11/124 (137)		NA
RHF Gradient	38/81 (87)		78/150 (156)
RHF Hessian	626/669 (720)		NA
UHF	5/58 (64)		5/74 (77)
Conv. MP2	85/128 (138)		1/73 (77)
Direct MP2	88/212 (223)		NA
MP2 Gradient	310/438 (472)		NA
MP2 Hessian	3546/3674 (4214)		NA
MP4(SDTQ)	2665/2708 (3067)		76/148 (155)
SDCI	163/1676 (1811)		6/114 (121)
CCSD	278/3096 (4484)		9/154 (161)
CCSD(T)	5644/5687 (7244)		136/208 (219)
QCISD	211/2152 (2328)		7/134 (140)
QCISD(T)	4729/4772 (5340)		64/136 (141)
CASSCF	52/1024 (1084)		5/92 (99)
CAS-CI	NA		11/178 (181)[c]
SVWN (LDA)	NA		8/92 (117)[d]
BLYP (NLDA)	NA		10/118 (138)[f]

Method	**GAMESS-US 7/17/93**	**HONDO (8.3)**	**GAMESS-UK (2)**
Conv. RHF	2/27 (30)	Not ported to	
Direct RHF	12/153 (156)	an SGI	
RHF Gradient	45/72 (76)		
RHF Hessian	843/870 (875)		
UHF	3/46 (48)		
Conv. MP2	68/95 (98)		
Direct MP2	NA	NA	NA
MP2 Gradient	NA	NA	
MP2 Hessian	NA	NA	
MP4(SDTQ)	NA		NA
SDCI	60/547 (764)		
CCSD	NA	NA	NA
CCSD(T)	NA	NA	
QCISD	NA	NA	
QCISD(T)	NA	NA	
CASSCF	185/1874 (1933)		
CAS-CI			
SVWN (LDA)	NA		
BLYP (NLDA)	NA		

Table 20. SGI Indigo 50/100 MHz R4000 Timings (cont.)

Method	SUPERMOLECULE	ACES II (1.0)	SPARTAN 3.0.1
Conv. RHF		4/68 (71)	4/51 (76)[(c)]
Direct RHF		NA	17/270 (278)[(c)]
RHF Gradient		114/182 (196)	24/73 (77)
RHF Hessian	NA	672/740 (771)	NA
UHF	NA	4/72 (76)	
Conv. MP2	NA	10/78 (86)	
Direct MP2		NA	
MP2 Gradient	NA	183/261 (310)	NA
MP2 Hessian	NA	NA	
MP4(SDTQ)	NA	181/249 (288)	NA
SDCI	NA	11/221 (269)	NA
CCSD	NA	16/244 (279)	NA
CCSD(T)	NA	329/397 (457)	
QCISD	NA	13/208 (252)	NA
QCISD(T)	NA	296/364 (404)	
CASSCF	NA	NA	NA
SVWN (LDA)	NA	NA	NA
BLYP (NLDA)	NA	NA	NA

Table 20. SGI Indigo 50/100 MHz R4000 Timings (cont.)

Isobutene, 32 electrons, $^1A_1$ (C_{2v}), Basis Set=6-311++G**
(148 functions, 6-term d's)

Method	**Gaussian 92 (E)**	**Gaussian 92/DFT**	**MOLPRO (92.3)**
Conv. RHF	64/829 (1396)		
Direct RHF	169/2706 (2714)		NA
RHF Gradient	814/1643 (2220)		
RHF Hessian			NA
UHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			NA
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Method	**GAMESS-US 6/17/92**	**HONDO (8.3)**	**GAMESS-UK (2)**
Conv. RHF		not ported to	
Direct RHF		an SGI	
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 20. SGI Indigo 50/100 MHz R4000 Timings (cont.)

(a) All times are in seconds. CPU times are the sum of the "user + system" contributions. Wall clock times are given in parentheses. For the iterative methods (RHF, UHF, SD-CI, QCISD and CASSCF) each entry consists of a trio of numbers: "CPU-time-per-teration/total-CPU (total-wall-clock)". The "CPU-time-per-iteration" for the conventional SCF methods was defined as the total run time (integrals + SCF) divided by the number of iterations. These values are intended to facilitate comparison with direct HF methods. For other methods the leftmost entry corresponds to the incremental time for the method. For example, the MP2 entry preceding the slash is the total run time minus the time needed for the preliminary HF step.
Unless otherwise noted all SGI Indigo calculations were performed on a 50 MHz R4000 machine with 112 MB of memory, a 1.2 GB SCSI 2 disk under IRIX version 5.2 with Release 4.0 of SGI 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 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 ($3a_g$, $1b_{3u}$, $1b_{2g}$, $2b_{1u}$). This configuration list is sufficient to allow ethylene to dissociate into two singlet methylenes. The time reported includes the time required to compute the integrals and solve the CAS equations using the canonical RHF orbitals as the starting guess.
The default INDO initial guess used by Gaussian for ethylene's open shell calculations did not pick up the $\pi \rightarrow \pi^*$ $^3B_{1u}$ state. If the ordering of the initial guess orbitals was corrected using an ALTER command the calculation with Gaussian 90 died with a complaint that symmetry was being broken. Thus, it was necessary to run these calculations with the NOSYMM option, which ignored the available D_{2h} symmetry. Gaussian 92 fixed this problem with the UHF benchmark and was run in full D_{2h} symmetry.

(c) Access to SPARTAN 3.0 was kindly provided by Dr. Susan Jackels. SPARTAN 3.0 does not have analytical second serivatives. However, it can compute the Hessian matrix using a finite differencing of first derivatives. For SPARTRAN the "user + system" CPU times were unavailable. The values listed correscpond to "user" CPU time only.

(d) MOLPRO can only compute the internally contracted CI wavefunction.

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

(f) 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.

Table 21. SGI Onyx 50/100 MHz R4400 Timings[a]

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

Method	Gaussian 92 (E)	Gaussian 92/DFT	MOLPRO (92.3)
Conv. RHF	4/40 (42)		Not ported to
Direct RHF	11/111 (122)		an SGI
RHF Gradient	39/79 (85)		
RHF Hessian	590/630 (638)		
UHF	5/57 (60)		
Conv. MP2	87/127 (133)		
Direct MP2	92/203 (208)		
MP2 Gradient	297/424 (452)		
MP4(SDTQ)	2504/2544 (2597)		
SDCI	153/1567 (1636)		
CCSD	253/2827 (3078)		
CCSD(T)	5222/5262 (5770)		
QCISD	194/1977 (2025)		
QCISD(T)			
CASSCF	54/1062 (1083)		

Method	GAMESS-US 8/17/92	HONDO (8.3)	GAMESS-UK (2)
Conv. RHF	3/31 (33)	Not ported to	
Direct RHF	14/184 (188)	an SGI	
RHF Gradient	52/83 (86)		
RHF Hessian	882/913 (932)		
UHF	3/48 (50)		
Conv. MP2	81/112 (143)		
Direct MP2	NA	NA	NA
MP2 Gradient	NA	NA	
MP4(SDTQ)	NA		NA
SDCI	514/545 (569)		
CCSD	NA	NA	NA
QCISD	NA	NA	
CASSCF	1943/1974 (2044)		

Table 21. SGI Onyx 50/100 MHz R4400 Timings (cont.)

Method	DISCO (1.82)	ACES II	TX90
Conv. RHF			7/86 (89)
Direct RHF		NA	
RHF Gradient			
RHF Hessian	NA		NA
UHF	NA		
Conv. MP2	NA		
Direct MP2		NA	NA
MP2 Gradient	NA		NA
MP4(SDTQ)	NA		NA
SDCI	NA		NA
CCSD	NA		NA
QCISD	NA		NA
CASSCF	NA	NA	

Table 21. SGI Onyx 50/100 MHz R4400 Timings

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

Method	**Gaussian 90 (H)**	**Gaussian 92 (E)**	**MOLPRO (93)**
RHF		31/314 (320)	
Direct RHF		94/942 (954)	NA
RHF Gradient		413/727 (741)	NA
RHF Hessian		5855/6169 (6243)	NA
UHF		33/398 (406)	
Conv. MP2		1357/1671 (1710)	
Direct MP2		1308/2251 (2333)	NA
MP2 Gradient			NA
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD			
CASSCF			

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

Table 21. SGI Onyx 50/100 MHz R4400 Timings (cont.)

(a) All times are in seconds. CPU times are the sum of the "user + system" contributions. Wall clock times are given in parentheses. For the iterative methods (RHF, UHF, SD-CI, QCISD and CASSCF) each entry consists of a trio of numbers: "CPU-time-per-teration/total-CPU (total-wall-clock)". The "CPU-time-per-iteration" for the conventional SCF methods was defined as the total run time (integrals + SCF) divided by the number of iterations. These values are intended to facilitate comparison with direct HF methods. For other methods the leftmost entry corresponds to the incremental time for the method. For example, the MP2 entry preceding the slash is the total run time minus the time needed for the preliminary HF step.
Unless otherwise noted all SGI Onyx calculations were performed on a single processor of a four processor 50/100 MHz R4400 machine with 512 MB of memory, a 2.4 GB SCSI 2 disk running IRIX version 5.1.1 with Release 4 of SGI Fortran. Runs were made on an otherwise quiet processor.
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.

Table 22. SGI Indigo 75/150 MHz R4400 Timings[a]

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

Method	**Gaussian 92 (E)**	**Gaussian 92/DFT**	**Gaussian 94 (B)**
Conv. RHF	3/27 (40)		4/40 (59)
Direct RHF	8/82 (105)		8/90 (100)
RHF Gradient	27/54 (66)		28/68 (85)
RHF Hessian	412/439 (463)		314/354 (396)
UHF	3/40 (47)		
Conv. MP2	59/86 (92)		
Direct MP2	60/142 (148)		
MP2 Gradient	214/300 (335)		
MP2 Hessian	2645/2731 (3292)		
MP4(SDTQ)	1805/1832 (2187)		
SDCI	108/1108 (1212)		
CCSD	188/2095 (3368)		
CCSD(T)	3830/3857 (5293)		
QCISD	139/1414 (1526)		
QCISD(T)	3164/3191 (3548)		
CASSCF	68/544 (1320)		
CAS-CI	NA		
SVWN (LDA)	NA		
BLYP (NLDA)	NA		

Method	**GAMESS-US 7/17/93**	**HONDO (8.3)**	**MOLPRO (94.3)**
Conv. RHF	2/19 (21)	Not ported to an SGI	6/51 (64)
Direct RHF	10/87 (95)		NA
RHF Gradient	33/53 (62)		48/101 (106)
RHF Hessian	619/639 (718)		NA
UHF	3/28 (30)		3/51 (52)
Conv. MP2	43/70 (75)		1/52 (56)
Direct MP2	NA	NA	NA
MP2 Gradient	NA	NA	NA
MP2 Hessian	NA	NA	NA
MP4(SDTQ)	NA		50/101 (104)
SDCI	42/402 (619)		4/76 (79)
CCSD	NA	NA	5/100 (105)
CCSD(T)	NA	NA	89/140 (144)
QCISD	NA	NA	4/87 (91)
QCISD(T)	NA	NA	127/199 (210)
CASSCF	136/1383 (1594)		4/64 (68)
CAS-CI	> 188[f]		8/124 (128)[c]
SVWN (LDA)	NA		5/61 (64)[d]
BLYP (NLDA)	NA		6/77 (80)[e]

Table 22. SGI Indigo 75/150 MHz R4400 Timings (cont.)

Method	SUPERMOLECULE	ACES II (1.0)	SPARTAN 3.0.1
Conv. RHF		4/68 (71)	
Direct RHF		NA	
RHF Gradient		114/182 (196)	
RHF Hessian	NA	672/740 (771)	NA
UHF	NA	4/72 (76)	
Conv. MP2	NA	10/78 (86)	
Direct MP2		NA	
MP2 Gradient	NA	183/261 (310)	NA
MP2 Hessian	NA	NA	NA
MP4(SDTQ)	NA	181/249 (288)	NA
SDCI	NA	11/221 (269)	NA
CCSD	NA	16/244 (279)	NA
CCSD(T)	NA	329/397 (457)	
QCISD	NA	13/208 (252)	NA
QCISD(T)	NA	296/364 (404)	
CASSCF	NA	NA	NA
CAS-CI	NA	NA	NA
SVWN (LDA)	NA	NA	NA
BLYP (NLDA)	NA	NA	NA

Table 22. SGI Indigo 75/150 MHz R4400 Timings (cont.)

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

Method	**Gaussian 92 (E)**	**Gaussian 92 /DFT**	**MOLPRO (92.3)**
Conv. RHF	138/1657 (3673)		
Direct RHF	120/1561 (1635)		
Dir. RHF Grad.	830/2346 (2445)		
Dir. RHF Hess.	64869/66430 (68907)		NA
Conv. RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Method	**GAMESS-US 7/17/93**	**HONDO (8.1)**	**GAMESS-UK (2)**
Direct RHF	378/6796 (6949)		
Dir. RHF Grad.			
Dir. RHF Hess.			
Conv. RHF			
Conv. MP2			
Direct MP2			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Method	**DISCO (1.82)**	**ACES II**
Direct UHF		NA
Dir. RHF Grad.		
Dir. RHF Hess.	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 22. SGI Indigo 75/150 MHz R4400 Timings (cont.)

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

Method	**Gaussian 92 (E)**	**Gaussian 92/DFT**	**MOLPRO (92.3)**
Direct RHF	1100/14298 (14968)		
RHF Gradient			
RHF Hessian			NA
Conv. RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Method	**GAMESS-US 7/17/93**	**HONDO (8.1)**	**GAMESS-UK (2)**
Direct RHF	1896/34133 (35455)		
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 22. SGI Indigo 75/150 MHz R4400 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	24560/392960 (393081)		
RHF Gradient			
RHF Hessian			NA
Conv. RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Method	**GAMESS-US 7/17/93**	**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 22. SGI Indigo 75/150 MHz R4400 Timings (cont.)

(a) All times are in seconds. CPU times are the sum of the "user + system" contributions. Wall clock times are given in parentheses. For the iterative methods (RHF, UHF, SD-CI, QCISD and CASSCF) each entry consists of a trio of numbers: "CPU-time-per-teration/total-CPU (total-wall-clock)". The "CPU-time-per-iteration" for the conventional SCF methods was defined as the total run time (integrals + SCF) divided by the number of iterations. These values are intended to facilitate comparison with direct HF methods. For other methods the leftmost entry corresponds to the incremental time for the method. For example, the MP2 entry preceding the slash is the total run time minus the time needed for the preliminary HF step.
Unless otherwise noted all SGI Indigo 75/150 MHz calculations were performed on a 1.2 GB SCSI 2 disk under IRIX version 5.2 with Release 4.0 of SGI Fortran. Runs were made on an otherwise quiet processor.
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.

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

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

(e) 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.

(f) GAMESS(US) was unable to perform a true CAS-CI calculation. The closest it could come was a so-called second order CI with a CAS. With this approach the total number of configurations is only 4688 whereas in the true CAS-CI there are over 100,000 configurations.

Table 23. SGI PowerChallenge 75 MHz R8000 Timings[a]

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

Method	**Gaussian 92 (G)**	**Gaussian 92/DFT**	**MOLPRO (94.3)**
Conv. RHF	1/13 (14)[c]		
Direct RHF	2/33 (34)[c]		
RHF Gradient	10/23 (24)[c]		
RHF Hessian	154/167 (171)[c]		
UHF	1/17 (18)[c]		
Conv. MP2	16/29 (31)[c]		
Direct MP2	17/50 (51)[c]		
MP2 Gradient	43/93 (96)[c]		
MP2 Hessian	711/740 (783)[c]		
MP4(SDTQ)	568/581 (592)[c]		
SDCI	32/336 (344)[c]		
CCSD	59/663 (751)[c]		
CCSD(T)	1189/1202 (1248)[c]		
QCISD	39/403 (414)[c]		
QCISD(T)	929/942 (965)[c]		
CASSCF	228/241 (293)[c]		
CAS-CI	NA		
SVWN (LDA)	NA		
BLYP (NLDA)	NA		

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

Table 23. SGI PowerChallenge 75 MHz R8000 Timings (cont.)

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

Method	**Gaussian 92 (E)**	**Gaussian 92 /DFT(G)**	**MOLPRO (92.3)**
Conv. RHF		70/842 (856)	
Direct RHF		29/376 (382)	
Dir. RHF Grad.		162/538 (551)	
Dir. RHF Hess.		15320/16162 (16365)	NA
Conv. RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Method	**GAMESS-US 7/17/93**	**HONDO (8.1)**	**GAMESS-UK (2)**
Direct RHF			
Dir. RHF Grad.			
Dir. RHF Hess.			
Conv. RHF			
Conv. MP2			
Direct MP2			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Method	**DISCO (1.82)**	**ACES II**
Direct UHF		NA
Dir. RHF Grad.		
Dir. RHF Hess.	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 23. SGI PowerChallenge 75 MHz R8000 Timings (cont.)

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

Method	**Gaussian 92 (E)**	**Gaussian 92/DFT(G)**	**MOLPRO (92.3)**
Direct RHF		230/2995 (3014)	
RHF Gradient		1461/4456 (4514)	
RHF Hessian		149603/152598 (152677)	NA
Conv. RHF			
Conv. MP2			
Direct MP2		147382/150377 (153925)[d]	NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Method	**GAMESS-US 7/17/93**	**HONDO (8.1)**	**GAMESS-UK (2)**
Direct RHF	1896/34133 (35455)		
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 23. SGI PowerChallenge 75 MHz R8000 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(G)	MOLPRO (92.3)
Direct RHF		9904/158471 (159612)	
RHF Gradient			
RHF Hessian			NA
Conv. RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Method	GAMESS-US 7/17/93	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 23. SGI PowerChallenge 75 MHz R8000 Timings (cont.)

(a) All times are in seconds. CPU times are the sum of the "user + system" contributions. Wall clock times are given in parentheses. For the iterative methods (RHF, UHF, SD-CI, QCISD and CASSCF) each entry consists of a trio of numbers: "CPU-time-per-teration/total-CPU (total-wall-clock)". The "CPU-time-per-iteration" for the conventional SCF methods was defined as the total run time (integrals + SCF) divided by the number of iterations. These values are intended to facilitate comparison with direct HF methods. For other methods the leftmost entry corresponds to the incremental time for the method. For example, the MP2 entry preceding the slash is the total run time minus the time needed for the preliminary HF step.
Unless otherwise noted all SGI PowerChallenge 75 MHz R8000 calculations were performed on a system with 4 R8000 processors and 256 MB of memory, SCSI 2 disk and IRIX version 6.0 with Fortran Release 6.0. Runs were made on an otherwise quiet processor.
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 ($3a_g$, $1b_{3u}$, $1b_{2g}$, $2b_{1u}$). 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.

(c) Calculations run by Rick Verbeck from Silicon Graphics, Inc. on a 2 processor system with 1 GB of semiconductor memory. Performance is highly dependent on configuration, application, and operating environment. No warranty of system performance is expressed or implied in this data which has been provided by SGI. This information is subject to change without notice and should not be construed as a commitment by Silicon Graphics, Inc. SGI assumes no responsibility for any errors that may appear in this document.

(d) This run was made using only 10 MW of memory. With successively larger amounts of memory the CPU time drops to 71,953 sec. (20 MW), 50,609 sec (30 MW) or 46,034 (40 MW).

Table 24. SGI PowerChallenge 90 MHz R8000 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 92/DFT (G)**	**Gaussian 94 (C)**	**MOLPRO (94.3)**
Conv. RHF	1/12 (114)[(b)]	2/15 (16)	
Direct RHF	3/28 (39)	3/32 (36)	NA
In-core RHF		2/19 (19)	NA
RHF Gradient	8/20 (111)	11/26 (29)	
RHF Hessian	154/166 (230)	110/125 (129)	NA
UHF	1/17 (360)	2/19 (22)	
Conv. MP2	18/30 (45)	6/21 (23)	
Direct MP2	14/42 (47)	7/39 (39)	NA
MP2 Gradient	50/80 (622)	31/52 (53)	NA
MP2 Hessian	624/654 (1076)	687/708 (750)	NA
MP4(SDTQ)	507/519 (741)	361/376 (396)	
SDCI	27/281 (298)	24/183 (257)	
CCSD	53/599 (894)	42/435 (713)	
CCSD(T)	1110/1129 (1360)	809/824 (1125)	
QCISD	38/393 (417)	25/268 (383)	
QCISD(T)	817/829 (866)	710/725 (847)	
CASSCF	10/203 (821)	12/262 (289)	
CAS-CI	NA	NA	
SVWN (LDA)	3/20 (187)	10/79 (80)	
BLYP (NLDA)	3/17 (18)	13/104 (107)	

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		

Table 24. SGI PowerChallenge 90 MHz R8000 Timings (cont.)

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

Method	Gaussian 94 (C)		MOLPRO (93)
RHF	15/151 (154)		
Direct RHF	17/171 (173)		NA
In-core RHF	15/152 (153)		NA
RHF Gradient			NA
RHF Hessian			NA
UHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			NA
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

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

Table 24. SGI PowerChallenge 90 MHz R8000 Timings (cont.)

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

Method	**Gaussian 94 (C)**		**MOLPRO (92.3)**
Conv. RHF	15/146 (153)		
Direct RHF	23/256 (268)		NA
In-core RHF	34/335 (338)		
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		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 24. SGI PowerChallenge 90 MHz R8000 Timings (cont.)

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

Method	**Gaussian 92 /DFT(G)**	**Gaussian 94 (C)**	**MOLPRO (92.3)**
Conv. RHF	61/728 (856)		
Direct RHF	25/320 (327)		
Dir. RHF Grad.	128/448 (467)		
Dir. RHF Hess.	13272/13591 (13816)		NA
Conv. RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Method	**GAMESS-US 7/17/93**	**HONDO (8.1)**	**GAMESS-UK (2)**
Direct RHF			
Dir. RHF Grad.			
Dir. RHF Hess.			
Conv. RHF			
Conv. MP2			
Direct MP2			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Method	**DISCO (1.82)**	**ACES II**
Direct UHF		NA
Dir. RHF Grad.		
Dir. RHF Hess.	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 24. SGI PowerChallenge 90 MHz R8000 Timings (cont)

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

Method	**Gaussian 92/DFT(G)**	**Gaussian 94(D)**	**MOLPRO (92.3)**
Direct RHF	201/2615 (2697)	197/2562 (2606)	
RHF Gradient		1170/3732 (3792)	
RHF Hessian			NA
Conv. RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Method	**GAMESS-US 7/17/93**	**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	**PS-GVB (2.3.2)**	**ACES II**
Direct RHF	1040/1097 (?)[d]	NA
RHF Gradient	677/1780 (1859)[d]	
RHF Hessian		
Direct RHF		
Conv. MP2		
Direct MP2		NA
MP2 Gradient		
MP4(SDTQ)		
SDCI		
CCSD		
QCISD		
CASSCF		NA

Table 24. SGI PowerChallenge 90 MHz R8000 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/DFT (G)**	**Gaussian 94 (C)**	**MOLPRO (92.3)**
Direct RHF	9483/142255 (143554)	6970/104547 (105277)	
RHF Gradient		26126/130709 (131489)	
RHF Hessian			NA
Conv. RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

s18-crown-6, $C_{34}H_{56}O_8$, 324 electrons, C_2, Basis Set=6-31G**
(910 functions)

Method	**Gaussian 94 (D)**	**PS-GVB (2.3.2)**	**MOLPRO (92.3)**
Direct RHF	2641/34329 (34384)	1033/11021 (?)[d]	
RHF Gradient	13323/47652 (48027)	5370/ 16651 (17195)[d]	
RHF Hessian			NA
Conv. RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			

Table 24. SGI PowerChallenge 90 MHz R8000 Timings (cont.)

(a) All times are in seconds. CPU times are the sum of the "user + system" contributions. Wall clock times are given in parentheses. For the iterative methods (RHF, UHF, SD-CI, QCISD and CASSCF) each entry consists of a trio of numbers: “CPU-time-per-teration/total-CPU (total-wall-clock)”. The "CPU-time-per-iteration" for the conventional SCF methods was defined as the total run time (integrals + SCF) divided by the number of iterations. These values are intended to facilitate comparison with direct HF methods. For other methods the leftmost entry corresponds to the incremental time for the method. For example, the MP2 entry preceding the slash is the total run time minus the time needed for the preliminary HF step.
Unless otherwise noted all SGI PowerChallenge 90 MHz R8000 calculations were performed on a system with 18 R8000 processors and 6 GB of memory, SCSI 2 disk and IRIX version 6.2 with Fortran Release 6.2. Runs were made on an otherwise quiet processor.
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 poor wall clock times were caused by a slow network connection to the Gaussian binaries.

(c) Run by Dr. Roberto Gomperts, Silicon Graphics Corporation.

(d) Run by Dr. James Anchell , Schrödinger, Inc. These runs made use of the pseudo-spectral approximation.

Table 25. SGI PowerChallenge 196 MHz R10000 Timings[a]

Ethylene, 16 electrons, $^{1}A_{g}$, 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	1/10 (15)		
Direct RHF	2/23 (26)		NA
In-core RHF	2/22 (22)		NA
RHF Gradient	10/20 (23)		
RHF Hessian	84/94 (101)		NA
UHF	1/16 (19)		
Conv. MP2	7/17 (20)		
Direct MP2	6/29 (31)		NA
MP2 Gradient	25/42 (50)		NA
MP2 Hessian	662/679 (741)		NA
MP4(SDTQ)	402/412 (460)		
SDCI	20/192 (377)		
CCSD	50/506 (1032)		
CCSD(T)	997/1007 (1675)		
QCISD	27/270 (392)		
QCISD(T)	720/730 (851)		
CASSCF	8/156 (185)		
CAS-CI	NA		
SVWN (LDA)	6/49 (49)		
BLYP (NLDA)	11/90 (91)		

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		

Table 25. SGI PowerChallenge 196 MHz R10000 Timings (cont)

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

Method	**Gaussian 94 (D)**		**MOLPRO**
Direct RHF	206/2683 (2985)		
RHF Gradient	1212/3895 (4264)		
RHF Hessian	149915/152598 (152677)		NA
Conv. RHF			
Conv. MP2			
Direct MP2	28499/31182 (31527)		NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Table 25. SGI PowerChallenge 196 MHz R10000 Timings (cont.)

(a) All times are in seconds. CPU times are the sum of the "user + system" contributions. Wall clock times are given in parentheses. For the iterative methods (RHF, UHF, SD-CI, QCISD and CASSCF) each entry consists of a trio of numbers: “CPU-time-per-teration/total-CPU (total-wall-clock)”. The "CPU-time-per-iteration" for the conventional SCF methods was defined as the total run time (integrals + SCF) divided by the number of iterations. These values are intended to facilitate comparison with direct HF methods. For other methods the leftmost entry corresponds to the incremental time for the method. For example, the MP2 entry preceding the slash is the total run time minus the time needed for the preliminary HF step.

Unless otherwise noted all SGI PowerChallenge 196 MHz R10000 calculations were performed on a system with 16 R8000 processors, 2 MB of L2 cache per processor and 6 GB of memory, SCSI 2 disk and IRIX version 6.2 with Fortran Release 6.2. Runs were made on an otherwise quiet processor.

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 poor wall clock times were caused by a slow network connection to the Gaussian binaries.

(c) Run by Dr. Roberto Gomperts, Silicon Graphics Corporation.

Table 26. SGI O2 174 MHz R10000 Timings[a]

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

Method	**Gaussian 94 (E.1)**		**MOLPRO (96.3)**
Conv. RHF	2/19 (28)		
Direct RHF	4/35 (41)		NA
In-core RHF	4/37 (54)		NA
RHF Gradient	13/32 (37)		
RHF Hessian	134/153 (177)		NA
UHF	2/24 (26)		
Conv. MP2	7/24 (26)		
Direct MP2	8/38 (40)		NA
MP2 Gradient	40/64 (67)		NA
MP2 Hessian	1125/1149 (1294)		NA
MP4(SDTQ)	699/716 (777)		
SDCI	39/368 (441)		
CCSD	105/1067 (1723)		
CCSD(T)	1923/1942 (2816)		
QCISD	67/689 (828)		
QCISD(T)	1466/1483 (1169)		
CASSCF	14/289 (515)		
CAS-CI	NA		
SVWN (LDA)	9/75 (82)		
BLYP (NLDA)	22/187 (222)		

Method	**GAMESS-US 7/17/93**	**HONDO (8.3)**	**GAMESS-UK (2)**
Conv. RHF		Not ported to an SGI	
Direct RHF			
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		

Table 26. SGI O2 174 MHz R10000 Timings (cont.)

(a) All times are in seconds. CPU times are the sum of the "user + system" contributions. Wall clock times are given in parentheses. For the iterative methods (RHF, UHF, SD-CI, QCISD and CASSCF) each entry consists of a trio of numbers: “CPU-time-per-teration/total-CPU (total-wall-clock)”. The "CPU-time-per-iteration" for the conventional SCF methods was defined as the total run time (integrals + SCF) divided by the number of iterations. These values are intended to facilitate comparison with direct HF methods. For other methods the leftmost entry corresponds to the incremental time for the method. For example, the MP2 entry preceding the slash is the total run time minus the time needed for the preliminary HF step.
Unless otherwise noted all SGI PowerChallenge 196 MHz R10000 calculations were performed on a system with 16 R8000 processors, 2 MB of L2 cache per processor and 6 GB of memory, SCSI 2 disk and IRIX version 6.2 with Fortran Release 6.2. Runs were made on an otherwise quiet processor.
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 poor wall clock times were caused by a slow network connection to the Gaussian binaries.

(c) Run by Dr. Roberto Gomperts, Silicon Graphics Corporation.

Table 27. SGI Origin 2000 196 MHz R10000 Timings[a]

Ethylene, 16 electrons, $^{1}A_{g}$, 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	1/9 (9)		
Direct RHF	2/21 (22)		NA
In-core RHF	2/15 (15)		NA
RHF Gradient	7/16 (17)		
RHF Hessian	75/84 (85)		NA
UHF	1/11 (12)		
Conv. MP2	5/14 (14)		
Direct MP2	6/29 (31)		NA
MP2 Gradient	20/34 (35)		NA
MP2 Hessian	505/519 (532)		NA
MP4(SDTQ)	250/259 (267)		
SDCI	13/127 (141)		
CCSD	30/306 (365)		
CCSD(T)	581/590 (651)		
QCISD	21/195 (222)		
QCISD(T)	470/479 (508)		
CASSCF	6/136 (144)		
CAS-CI	NA		
SVWN (LDA)	6/46 (46)		
BLYP (NLDA)	10/79 (79)		

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			
CAS-CI			
SVWN (LDA)	NA		
BLYP (NLDA)	NA		

Table 27. SGI Origin 2000 196 MHz R10000 Timings (cont.)

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

Method	**Gaussian 94 (G)**	**Gaussian 94**	**MOLPRO (97)**
Direct RHF	179/2333 (2349)		
Dir. RHF Grad.	1096/3429 (3452)		
Dir. RHF Hess.	133791/136124 (137038)		NA
Conv. RHF			
Conv. MP2			
Direct MP2	25383/27716 (27897)[b]		NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

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

Method	**Gaussian 94(D)**		**MOLPRO**
Direct RHF	6760/101394 (102203)		
RHF Gradient	24998/126392 (127249)		
RHF Hessian			NA
Conv. RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Table 27. SGI Origin 2000 196 MHz R10000 Timings (cont.)

s18-crown-6, $C_{34}H_{56}O_8$, 324 electrons, C_2, Basis Set=6-31G**
(910 functions)

Method	**Gaussian 94 (D)**	**PS-GVB (2.3.2)**	**MOLPRO**
Direct RHF	2250/29250 (29573)		
RHF Gradient			
RHF Hessian			NA
Conv. RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			

(a) All times are in seconds. CPU times are the sum of the "user + system" contributions. Wall clock times are given in parentheses. For the iterative methods (RHF, UHF, SD-CI, QCISD and CASSCF) each entry consists of a trio of numbers: "CPU-time-per-teration/total-CPU (total-wall-clock)". The "CPU-time-per-iteration" for the conventional SCF methods was defined as the total run time (integrals + SCF) divided by the number of iterations. These values are intended to facilitate comparison with direct HF methods. For other methods the leftmost entry corresponds to the incremental time for the method. For example, the MP2 entry preceding the slash is the total run time minus the time needed for the preliminary HF step.
Unless otherwise noted all SGI Origin 2000 196 MHz R10000 calculations were performed on a system with 16 R8000 processors, 4 MB of L2 cache per processor and 8 GB of memory, UltrSCSI disk (striped 3 ways) and IRIX version 6.4 with Fortran Release 6.4. Runs were made on an otherwise quiet processor.
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) This run was made using only 10 MW of memory. With larger amounts of memory the Wall time drops to 16,107 sec. (20 MW), 12923 sec. (40 MW) and 11870 sec. (80 MW) and 11462 sec. (160 MW).