Table 28. DEC AXP Model 300 Timings[a]

Ethylene, 16 electrons, $^1A_1$ (D_{2h}), Basis Set=6-311++G**
(74 functions, 6-term d's)[b]

Method	**Gaussian 92 (E)**	**Gaussian 92/DFT**	**MOLPRO (92.3)**
Conv. RHF	5/48 (59)		
Direct RHF	12/134 (139)		NA
RHF Gradient	48/96 (105)		
RHF Hessian	668/716 (737)		NA
UHF	5/63 (69)		
Conv. MP2	94/142 (152)		
Direct MP2	183/231 (247)		NA
MP2 Gradient	432/480 (493)		NA
MP4(SDTQ)	1737/1785 (1926)		
SDCI	168/1732 (2178)		
CCSD	3188/3236 (5168)		
CCSD(T)	4997/5054 (7374)		
QCISD	1920/1968 (2835)		
QCISD(T)	3777/3825 (6088)		
CASSCF	38/802 (824)		
CAS-CI	NA		
SVWN	NA		
BLYP	NA		

Method	**GAMESS-US 7/17/93**	**HONDO (8.3)**	**GAMESS-UK**
Conv. RHF	3/30 (35)		
Direct RHF			
RHF Gradient	41/69 (73)		
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2	NA	NA	
MP2 Gradient	NA	NA	
MP4(SDTQ)	NA		
SDCI			
CCSD	NA	NA	
QCISD	NA	NA	
CASSCF			

Table 28. DEC AXP Model 300 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)**
Direct RHF	224/2908 (2940)		
RHF Gradient	1392/4300 (4341)		
RHF Hessian	107483/110391 (111283)		NA
Conv. RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
CCSD(T)			
QCISD			
QCISD(T)			
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			

Table 28. DEC AXP Model 300 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 AXP 300 calculations were performed on a model 600 machine with 128 MB of memory, a 2 GB SCSI 2 disk running OSF/1version 1.3A with Release 3.3-342 of DEC 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 ($3a_g$, $1b_{3u}$, $1b_{2g}$, $2b_{1u}$). 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.

Table 29. DEC AXP Model 600 Timings[a]

Ethylene, 16 electrons, $^1A_1$ (D_{2h}), Basis Set=6-311++G**
(74 functions, 6-term d's)[b]

Method	**Gaussian 92 (E)**	**Gaussian 92/DFT**	**MOLPRO (92.3)**
Conv. RHF	2/23 (28)		
Direct RHF	4/65 (74)		NA
RHF Gradient	20/43 (52)		
RHF Hessian	312/335 (355)		NA
UHF	3/33 (38)		
Conv. MP2	42/65 (72)		
Direct MP2	42/107 (115)		NA
MP2 Gradient	105/216 (388)		NA
MP4(SDTQ)	822/845 (1003)		
SDCI	75/777 (1309)		
CCSD	120/1342 (3590)		
CCSD(T)	2016/2039 (3347)		
QCISD	89/910 (1679)		
QCISD(T)	1704/1727 (2509)		
CASSCF	25/456 (490)		

Method	**GAMESS-US 7/17/93**	**HONDO (8.3)**	**GAMESS-UK**
Conv. RHF	1/16 (31)		
Direct RHF			
RHF Gradient	23/39 (55)		
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2	NA	NA	
MP2 Gradient	NA	NA	
MP4(SDTQ)	NA		
SDCI			
CCSD	NA	NA	
CCSD(T)	NA		
QCISD	NA	NA	
QCISD(T)	NA		
CASSCF			

Table 29. DEC AXP Model 600 Timings (cont.)

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

Method	**Gaussian 92 (E)**	**Gaussian 92/DFT**	**MOLPRO (92.3)**
RHF	17/170 (493)		
Direct RHF	49/492 (639)		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 6/17/92**	**HONDO (8.1)**	**GAMESS-UK (2)**
Conv. RHF	unable to handle 5-term	unable to handle 5-term	unable to handle 5-term
Direct RHF	d's and 7-term f's.	d's and 7-term f's.	d's and 7-term f's.
RHF Gradient			
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
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 29. DEC AXP Model 600 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)**
Direct RHF	86/1123 (1165)		
RHF Gradient	482/1605 (1841)		
RHF Hessian	44682/45805 (46651)		NA
Conv. RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
CCSD(T)			
QCISD			
QCISD(T)			
CASSCF			

Method	**GAMESS-US 6/17/92**	**HONDO (8.1)**	**GAMESS-UK (2)**
Direct RHF			
RHF Gradient			
RHF Hessian			
Conv. RHF			
Conv. MP2			
Direct MP2			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

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

Table 29. DEC AXP Model 600 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 AXP 600 calculations were performed on a model 600 machine with 256 MB of memory, a 8 GB SCSI 2 disk running OSF/1version 1.3A with Release 3.3-342 of DEC 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.

Table 30. DEC AXP Model 800 Timings[a]

Ethylene, 16 electrons, $^1A_1$ (D_{2h}), Basis Set=6-311++G**
(74 functions, 6-term d's)[b]

Method	**Gaussian 92 (E)**	**Gaussian 92/DFT**	**MOLPRO (92.3)**
Conv. RHF	2/19 (22)[c]		
Direct RHF	3/51 (54)[c]		NA
RHF Gradient	16/35 (39)[c]		
RHF Hessian	248/267 (275)[c]		NA
UHF	2/28 (29)[c]		
Conv. MP2	33/52 (54)[c]		
Direct MP2	33/84 (86)[c]		NA
MP2 Gradient	117/169 (172)[c]		NA
MP4(SDTQ)	729/748 (819)[c]		
SDCI	58/601 (799)[c]		
CCSD	101/1132 (2038)[c]		
CCSD(T)			
QCISD	71/728 (1018)[c]		
QCISD(T)			
CASSCF	19/383 (392)[c]		
CAS-CI	NA	NA	
SVWN (LSD)	NA		
BLYP (NLSD)	NA		

Method	**GAMESS-US 7/17/93**	**HONDO (8.3)**	**GAMESS-UK**
Conv. RHF			
Direct RHF			
RHF Gradient			
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2	NA	NA	
MP2 Gradient	NA	NA	
MP4(SDTQ)	NA		
SDCI			
CCSD	NA	NA	
CCSD(T)	NA		
QCISD	NA	NA	
QCISD(T)	NA		
CASSCF			

Table 30. DEC AXP Model 800 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 AXP 600 calculations were performed on a model 800 machine with 128 MB of memory, a fast SCSI 2 disk (writeback cache enabled) running OSF/1version 1.3A with Release 3.3-342 of DEC 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) Calculations run by Mr. Bill DeSimone of Digital Equipment Corp. 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 Digital. This information is subject to change without notice and should not be construed as a commitment by Digital Equipment Corporation. Digital Equipment Corporation assumes no responsibility for any errors that may appear in this document.

Table 31. DEC AXP Model 900 Timings[a]

Ethylene, 16 electrons, $^1A_1$ (D_{2h}), Basis Set=6-311++G**
(74 functions, 6-term d's)[b]

Method	Gaussian 92 (E)	Gaussian 92/DFT	MOLPRO (92.3)
Conv. RHF	2/15 (16)[c]		
Direct RHF	3/38 (39)[c]		NA
RHF Gradient	11/26 (28)[c]		
RHF Hessian	193/208 (213)[c]		NA
UHF	2/21 (22)[c]		
Conv. MP2	26/41 (41)[c]		
Direct MP2	26/64 (65)[c]		NA
MP2 Gradient	94/135 (137)[c]		NA
MP4(SDTQ)	615/630 (693)[c]		
SDCI	50/518 (725)[c]		
CCSD	90/1008 (1905)[c]		
CCSD(T)			
QCISD	61/626 (919)[c]		
QCISD(T)			
CASSCF	15/301 (303)[c]		
CAS-CI	NA	NA	
SVWN (LSD)	NA		
BLYP (NLSD)	NA		

Method	GAMESS-US 7/17/93	HONDO (8.3)	GAMESS-UK
Conv. RHF			
Direct RHF			
RHF Gradient			
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2	NA	NA	
MP2 Gradient	NA	NA	
MP4(SDTQ)	NA		
SDCI			
CCSD	NA	NA	
CCSD(T)	NA		
QCISD	NA	NA	
QCISD(T)	NA		
CASSCF			

Table 31. DEC AXP Model 900 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 AXP 600 calculations were performed on a model 900 machine with 512 MB of memory, a fast SCSI 2 disk (writeback cache enabled) running OSF/1version 3.0 .
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 12 digits after the decimal point.

(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 Mr. Bill DeSimone of Digital Equipment Corp. 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 Digital. This information is subject to change without notice and should not be construed as a commitment by Digital Equipment Corporation. Digital Equipment Corporation assumes no responsibility for any errors that may appear in this document.

Table 32. DEC AlphaStation 600 5/266 Timings[a]

Ethylene, 16 electrons, $^1A_1$ (D_{2h}), Basis Set=6-311++G**
(74 functions, 6-term d's)[b]

Method	**Gaussian 92 (E)**	**Gaussian 92/DFT**	**MOLPRO (92.3)**
Conv. RHF	1/11 (32)		
Direct RHF	3/29 (34)		NA
RHF Gradient	10/21 (32)		
RHF Hessian	149/160 (178)		NA
UHF	2/21 (22)		
Conv. MP2			
Direct MP2	21/50 (56)		NA
MP2 Gradient			NA
MP4(SDTQ)			
SDCI			
CCSD			
CCSD(T)			
QCISD			
QCISD(T)			
CASSCF			
CAS-CI	NA	NA	
SVWN (LSD)	NA		
BLYP (NLSD)	NA		

Method	**GAMESS-US 7/17/93**	**HONDO (8.3)**	**GAMESS-UK**
Conv. RHF			
Direct RHF			
RHF Gradient			
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2	NA	NA	
MP2 Gradient	NA	NA	
MP4(SDTQ)	NA		
SDCI			
CCSD	NA	NA	
CCSD(T)	NA		
QCISD	NA	NA	
QCISD(T)	NA		
CASSCF			

Table 32. DEC AlphaStation 600 5/266 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.
All calculations were performed on a machine with 128 MB of memory, a standard SCSI disks running OSF/1version 3.0 .
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 12 digits after the decimal point.

(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.