Table 16. IBM RS/6000 591 Timings[a]

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

Method	**Gaussian 92/DFT (G)**	**Gaussian 94 (C)**	
Conv. RHF	1/11 (12)	1/13 (14)	
Direct RHF	3/28 (29)	3/31 (32)	
RHF Gradient	6/17 (19)	10/23 (25)	
RHF Hessian	93/104 (108)	80/93 (96)	
UHF	1/12 (14)	1/16 (18)	
Conv. MP2	11/22 (23)	6/19 (20)	
Direct MP2	12/40 (42)	7/38 (38)	
MP2 Gradient	48/70 (83)	95/114 (141)	
MP2 Hessian	511/533 (840)	1173/1186 (1323)	
MP4(SDTQ)	322/334 (382)	310/323 (337)	
SDCI	24/251 (254)	15/149 (152)	
CCSD	36/407 (916)	29/303 (355)	
CCSD(T)	696/707 (1224)	595/608 (649)	
QCISD	29/296 (330)	21/225 (240)	
QCISD(T)	584/595 (648)	551/564 (594)	
CASSCF	10/203 (821)	8/176 (277)	
CAS-CI	NA	NA	
SVWN (LSD)	3/18 (25)	10/77 (81)	
BLYP (NLSD)	3/16 (18)	14/110 (115)	

Method	**MOLPRO (94.8)**	**GAMESS-US 11/17/94**	**HONDO (8.3)**
Conv. RHF			
Direct RHF	NA		
RHF Gradient			
RHF Hessian	NA		
UHF			
Conv. MP2			
Direct MP2	NA	NA	NA
MP2 Gradient	NA	NA	NA
MP2 Hessian	NA	NA	
MP4(SDTQ)		NA	
SDCI			
CCSD		NA	NA
CCSD(T)		NA	
QCISD		NA	NA
QCISD(T)		NA	
CASSCF			
CAS-CI		NA	
SVWN (LSD)		NA	
BLYP (NLSD)		NA	

Table 16. IBM RS/6000 591 Timings (cont.)

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

Method	Gaussian 92/DFT (G)	Gaussian 94 (C)	
Conv. RHF		12/118 (126)	
Direct RHF		17/173 (182)	
RHF Gradient		61/179 (194)	
RHF Hessian		445/563 (594)	
UHF		11/132 (146)	
Conv. MP2		340/458 (499)	
Direct MP2			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
CCSD(T)			
QCISD			
QCISD(T)			
CASSCF			
SVWN (LSD)	NA		
BLYP (NLSD)	NA		

Method	MOLPRO (94.8)	GAMESS-US 7/17/93	HONDO (8.3)
Conv. RHF			
Direct RHF	NA		
RHF Gradient	NA		
RHF Hessian	NA		
UHF			
Conv. MP2			
Direct MP2	NA	NA	NA
MP2 Gradient	NA	NA	NA
MP4(SDTQ)		NA	
SDCI			
CCSD		NA	NA
CCSD(T)			
QCISD		NA	NA
QCISD(T)			
CASSCF			
SVWN (LSD)			
BLYP (NLSD)			

Table 16. IBM RS/6000 591 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)**	
Direct RHF	42/539 (558)		
RHF Gradient	216/755 (774)		
RHF Hessian	12790/13326 (13611)		
Conv. RHF			
Conv. MP2			
Direct MP2			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Method	**GAMESS-US 6/17/92**	**HONDO (8.1)**	**MOLPRO (92.3)**
Direct RHF			
RHF Gradient			
RHF Hessian			NA
Conv. RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Table 16. IBM RS/6000 591 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 (C)	MOLPRO (92.3)
Direct RHF	225/2925 (2940)		
RHF Gradient			
RHF Hessian			NA
Conv. RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD			
QCISD			
CASSCF			

Method	GAMESS-US 6/17/92	HONDO (8.1)	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 16. IBM RS/6000 591 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	9607/144105 (144820)	8474/127124 (127577)	
RHF Gradient			
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 (C)**		**MOLPRO (92.3)**
Direct RHF	2666/34659 (34862)		
RHF Gradient	14158/48817 (49108)		
RHF Hessian			NA
Conv. RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			
MP4(SDTQ)			

Table 16. IBM RS/6000 591 Timings (cont.)

(a) All times are in seconds. CPU times are the sum of the "user + system" contributions. Wall clock times are given in parentheses. For the iterative methods (RHF, UHF, SD-CI, QCISD and CASSCF) each entry consists of a trio of numbers: “CPU-time-per-teration/total-CPU (total-wall-clock)”. The "CPU-time-per-iteration" for the conventional SCF methods was defined as the total run time (integrals + SCF) divided by the number of iterations. These values are intended to facilitate comparison with direct HF methods. For other methods the leftmost entry corresponds to the incremental time for the method. For example, the MP2 entry preceding the slash is the total run time minus the time needed for the HF step.
Calculations were performed on a machine with 256 MB of memory and two 4.5 GB IBM F/W SCSI 2 disk running under AIX 4.1 with disk striping enabled. Release 4.1 of XLF Fortran was used for applications which had to be recompiled. Runs were made on an otherwise quiet system.
NA: not available with this program.
FTC-ND: Failed to complete - not enough disk space.
FTC-unknown: Failed to complete for unknown reasons.
SCF calculations were converged to approximately 15 digits after the decimal point (8 digits in the density).

(b) The ethylene UHF calculation treated the $\pi \rightarrow \pi^*$ ($^3B_{1u}$) state. The ethylene ground state is $^1A_{g.}$ MP2, MP4, CISD and QCISD calculations involved all electrons, i.e., there were no “core” electrons. The CAS configuration list contains 8 CSF’s in D_{2h} symmetry and was generated with 4 electrons in 4 orbitals (3_{ag}, $1b_{3u}$, $1b_{2g}$, $2b_{1u}$). This configuration list is sufficient to allow ethylene to dissociate into two singlet methylenes. The time reported includes the time required to compute the integrals and solve the CAS equations using the canonical RHF orbitals as the starting guess.
The default INDO initial guess used by Gaussian for ethylene's open shell calculations did not pick up the $\pi \rightarrow \pi^*$ $^3B_{1u}$ state. If the ordering of the initial guess orbitals was corrected using an ALTER command the calculation with Gaussian 90 died with a complaint that symmetry was being broken. Thus, it was necessary to run these calculations with the NOSYMM option, which ignored the available D_{2h} symmetry. Gaussian 92 fixed this problem with the UHF benchmark and it was run in full D_{2h} symmetry.