**Table 9.** IBM PowerPC 250 Timings[a]

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

| Method | Gaussian 90 (J) | Gaussian 92 (C)[c] | MOLPRO (92.3) |
|---|---|---|---|
| Conv. RHF | | 4/38 (50) | 5/48 (52) |
| Direct RHF | | 12/126 (135) | NA |
| RHF Gradient | | 37/80 (112) | 82/130 (133) |
| RHF Hessian | | 631/669 (695) | NA |
| UHF Total | | 5/55 (62) | 4/56 (63) |
| Conv. MP2 | | 82/120 (131) | 12/59 (62) |
| Direct MP2 | | 88/214 (221) | NA |
| MP2 Gradient | | 325/445 (492) | NA |
| MP4(SDTQ) | | 1355/1393 (2034) | |
| SDCI | | 158/1583 (2237) | |
| CCSD | NA | 254/2833 (5769) | |
| CCSD(T) | | 4181/4219 (7155) | |
| QCISD | | 190/1904 (2801) | |
| QCISD(T) | | 3301/3339 (4236) | |
| CASSCF | | 42/845 (904) | |
| CAS-CI | | NA | |

| Method | GAMESS-US 6/17/92 | HONDO (8.3) | GAMESS-UK |
|---|---|---|---|
| Conv. RHF | 3/41 (43) | | |
| Direct RHF | 17/220 (223) | | |
| RHF Gradient | 68/109 (116) | | |
| RHF Hessian | | | |
| UHF | | | |
| Conv. MP2 | | | |
| Direct MP2 | NA | NA | |
| MP2 Gradient | NA | | |
| MP4(SDTQ) | NA | | |
| SDCI | | | |
| CCSD | NA | NA | |
| QCISD | NA | NA | |
| CASSCF | | | |

**Table 9.** IBM PowerPC 250 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.
Calculations were performed on a machine with 64 MB of memory and one 500 MB IBM disk running under AIX 3.2.5. A more 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 14 digits after the decimal point.

(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 was run in full $D_{2h}$ symmetry.
Gaussian 90 requires that RHF calculations which precede certain correlated methods be run in $C_1$ symmetry. This results in an increase in the ethylene SCF times from 196 seconds ($D_{2h}$) to 441 seconds ($C_1$) for the 6-311G** basis; from 1900 seconds ($D_{2h}$) to 5795 seconds ($C_1$) for the cc-pVTZ basis; from 1969 seconds ($D_{2h}$) to 6657 seconds ($C_1$) for the 6-311++G(3df,3pd) basis.

(c) Gaussian was compiled under version 2.0.2 of XLF Fortran and the executables were simply copied to the PowerPC. The latest version of XLF which was available on the PowerPC at the time of these benchmarks was version 2.3.0.13, but Gaussian had not been certified with it. Using MELDF, which could be compiled under both versions of the compiler, it is estimated that Gaussian run times would improve by 10 to 20% with the newer compiler.