Table 33. Intel 486 DX/2 50 MHz Timings[a]

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

Method	**Gaussian 92 (E)**
Conv. RHF	44/(442)[b]
Direct RHF	80/(1203)[b]
RHF Gradient	447/(889)[b]
RHF Hessian	6171/(6613)[b]
UHF	58/(693)[b]
Conv. MP2	1371/(1813)[b]
Direct MP2	

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 (E)**
Conv. RHF	370/(3695)[b]
Direct RHF	1030/(10301)[b]
RHF Gradient	4198/(7893)[b]
RHF Hessian	39606/(43301)[b]
UHF	
Conv. MP2	
Direct MP2	

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

Method	**Gaussian 92 (E)**
Conv. RHF	721/(7211)[b]
Direct RHF	
RHF Gradient	5901/(13112)[b]
RHF Hessian	
UHF	
Conv. MP2	

Table 33. Intel 486 DX/2 50 MHz Timings (cont.)

(a) All times are in seconds. CPU times were not available. Total 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: “Wall-time-per-iteration/total-CPU (total-wall-clock)”. The "Wall-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.

(b) Run by Didier Vandervken, Catalytica Inc., on a 486 DX/2 with 16 MB of memory and 100 MB of available scratch disk under Microsoft Windows 3.1.

Table 34. Intel 486 DX/2 66 MHz Timings[a]

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

Method	**Gaussian 92 (E)**
Conv. RHF	31/(314)[b]
Direct RHF	62/(923)[b]
RHF Gradient	355/(669)[b]
RHF Hessian	4728/(5042)[b]
UHF	42/(503)[b]
Conv. MP2	1090/(1404)[b]
Direct MP2	3028/(3951)[b]

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 (E)**
Conv. RHF	286/(2860)[b]
Direct RHF	807/(8069)[b]
RHF Gradient	3268/(6128)[b]
RHF Hessian	30492/(33352)[b]
UHF	
Conv. MP2	
Direct MP2	

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

Method	**Gaussian 92 (E)**
Conv. RHF	552/(5520)[b]
Direct RHF	
RHF Gradient	4636/(10156)[b]
RHF Hessian	65078/(70598)[b]
UHF	609/(7917)[b]
Conv. MP2	

Table 34. Intel 486 DX/2 66 MHz Timings (cont.)

(a) All times are in seconds. CPU times were not available. Total 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: "Wall-time-per-iteration/total-CPU (total-wall-clock)". The "Wall-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.

(b) Run by Didier Vandervken, Catalytica Inc., on a 486 DX/2 with 16 MB of memory and 100 MB of available scratch disk under Microsoft Windows 3.1.

Table 35. Intel Pentium 133 MHz Timings[a]

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

Method	**Gaussian 94W (B)**
Conv. RHF	11/(112)
Direct RHF	28/(281)
RHF Gradient	130/(242)
RHF Hessian	960/(1076)
UHF	15/(180)
Conv. MP2	47/(159)
Direct MP2	97/(378)
Conv. MP4	3662/(3774)

(a) All times are in seconds. CPU times were not available. Total 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: "Wall-time-per-iteration/total-CPU (total-wall-clock)". The "Wall-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. Calculations were run on a Gateway P5-133 with 32 MB of memory and a 2GB disk drive under Microsoft Windows 95.

Table 36. Intel Pentium 166 MHz Timings[a]

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

Method	**Gaussian 94W (B)**
Conv. RHF	9/(90)
Direct RHF	23/(225)
RHF Gradient	104/(194)
RHF Hessian	772/(862)
UHF	12/(144)
Conv. MP2	37/(127)
Direct MP2	77/(302)
Conv. MP4	2934/(3024)

(a) All times are in seconds. CPU times were not available. Total 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: "Wall-time-per-iteration/total-CPU (total-wall-clock)". The "Wall-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. Calculations were run on a Gateway P5-166 with 32 MB of memory and a 2GB disk drive under Microsoft Windows 95.

Table 37. Intel Pentium 200 MHz Timings[a]

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

Method	**Gaussian 94W (B)**
Conv. RHF	8/(79)
Direct RHF	20/(191)
RHF Gradient	86/(165)
RHF Hessian	654/(733)
UHF	12/(144)
Conv. MP2	23/(102)
Direct MP2	64/(255)
Conv. MP4	2491/(2576)

(a) All times are in seconds. CPU times were not available. Total 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: "Wall-time-per-iteration/total-CPU (total-wall-clock)". The "Wall-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. Calculations were run on a Gateway P5-200 with 32 MB of memory and a 2GB disk drive under Microsoft Windows 95.