Table 38. Fujitsu VPP300 Timings[a]

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

Method	**Gaussian 92 (D)**	**Gaussian 92/DFT**	**MOLPRO (92.3)**
Conv. RHF	1/11 (54)[b]		
Direct RHF	3/32 (121)[b]		NA
RHF Gradient	7/18 (39)[b]		
RHF Hessian	110/111 (151)[b]		NA
UHF	1/15 (43)[b]		
Conv. MP2	7/18 (73)[b]		
Direct MP2	7/39 (77)[b]		NA
MP2 Gradient	35/46 (371)[b]		NA
MP4(SDTQ)	99/110 (390)[b]		
SDCI	17/167 (225)[b]		
CCSD	20/223 (906)[b]		
CCSD(T)			
QCISD	18/176 (243)[b]		
QCISD(T)			
CASSCF	26/232 (506)[b]		

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

Method	**Gaussian 92 (D)**	**Gaussian 92/DFT**	**MOLPRO (92.3)**
Conv. RHF	4/38 (136)[b]		
Direct RHF	11/120 (286)[b]		NA
RHF Gradient	28/66 (221)[b]		
RHF Hessian	899/937 (3376)[b]		NA
UHF	4/58 (222)[b]		
Conv. MP2	45/83 (192)[b]		
Direct MP2	45/165 (216)[b]		NA
MP2 Gradient	135/218 (503)[b]		NA
MP4(SDTQ)	698/736 (1699)[b]		
SDCI	130/1304 (2942)[b]		
CCSD	129/1424 (1805)[b]		
CCSD(T)			
QCISD	122/1219 (2893)[b]		
QCISD(T)			
CASSCF	159/1421 (1582)[b]		

Table 38. Fujitsu VPP300 Timings (contd)

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

Method	Gaussian 92/DFT (G)		
Conv. RHF	60/782 (884)[b]		
Direct RHF	14/183 (184)[b]		
RHF Gradient	62/245 (792)[b]		
RHF Hessian	7114/7297 (11290)[b]		
Direct MP2	1124/1307 (1340)[b,c]		

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

Method	Gaussian 92/DFT (G)		
Direct RHF	74/956 (1838)[b]		
RHF Gradient	316/1272 (1480)[b]		
Direct MP2	13644/14600 (24701)[b,d]		

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

Method	Gaussian 92/DFT (G)		
Direct RHF	2605/41674 (71741)[b]		
RHF Gradient	4867/46541 (59116)[b]		

(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-iteration/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 Fujitsu VPP300 calculations were run on a multiuser system with 1 processor and 512 MB of memory. Thus, wall clock times will vary widely.
NA: not available with this program.
FTC-ND: Failed to complete - not enough disk space.
FTC-unknown: Failed to complete for unknown reasons.

(b) Run by Brian L. Hammond, Computational Research Division, Fujitsu America, Inc. In-core timings for the 6-311++G** ethylene RHF, gradient and Hessian are 8 sec, 16 sec. and 61 sec. respectively in 5 Mwords of memory.

(c) This time drops to 724 sec. with 10 MW of memory.

(d) This time drops to 5968 sec. with 30 MW of memory.