

## **Appendix B**

### **Iteration Count**

## Appendix B

### Iteration Count

Ethylene, 16 electrons,  $^1A_g$ , D<sub>2h</sub> point group, Basis Set=6-311++G\*\*  
(74 functions, 6-term d's)

Method	Gaussian 90 (H)	Gaussian 92 (C)	Gaussian 92/DFT
Conv. RHF	11	10	10
Direct RHF	12	15	15
RHF Gradient	11	10	10
RHF Hessian	11	10	10
UHF	13	12	12
Conv. MP2	11	11	11
Direct MP2	12	11	11
MP2 Gradient	11	11	11
MP4(SDTQ)	11	11	11
SDCI	11-SCF, 11-CI	10-SCF,10-CI	10-SCF,10-CI
CCSD	NA	10-SCF,11-CC	10-SCF,11-CC
QCISD	11-SCF,10-CI	10-SCF,10-CI	10-SCF,10-CI
CASSCF	9-CAS	10-SCF,19-MC	10-SCF,19-MC
CAS-CI	NA	NA	NA
SVWN	NA	NA	6
BLYP	NA	NA	5

Method	Gaussian 94 (B)	MOLPRO (94.3)
Conv. RHF	10	9
Direct RHF	11	NA
RHF Gradient	10	9
RHF Hessian	10	NA
UHF		15
Conv. MP2		9
Direct MP2		NA
MP2 Gradient		NA
MP4(SDTQ)		9
SDCI		9-SCF,7-CI
CCSD		9-SCF, 9-CC
QCISD		9-SCF,9-CI
CASSCF		9-SCF,4-CAS
CAS-CI		9-SCF,4-CAS,8-CI
SVWN		12
BLYP		12

Method	<b>GAMESS-US 6/17/92</b>	<b>HONDO (8.4)</b>	<b>GAMESS-UK (2)</b>
Conv. RHF	9	11	12
Direct RHF	9	11	
RHF Gradient	9	11	12
RHF Hessian	9	11	
UHF	10	14	
Conv. MP2	9	11	
Direct MP2	NA	NA	
MP2 Gradient	9	11	
MP4(SDTQ)	NA	11	
SDCI	9-SCF, 9-CI	11-SCF, 10-CI	
CCSD	NA	NA	
QCISD	NA	NA	
CASSCF	9-SCF, 10-CAS	11-SCF, 10-MC	

Method	<b>DISCO (1.82)</b>	<b>SUPERMOLECULE</b>	<b>ACES II</b>
Conv. RHF	13	14	17
Direct RHF	13	14	NA
RHF Gradient	13		
RHF Hessian	NA		
UHF	NA		
Conv. MP2	NA		
Direct MP2	13		NA
MP2 Gradient	13		
MP4(SDTQ)	NA		
SDCI	NA		14-CI
CCSD	NA		11-CC
QCISD	NA		11-CI
CASSCF	NA		NA

Method	<b>SPARTAN 3.0.1</b>
Conv. RHF	13
Direct RHF	16
RHF Gradient	13
RHF Hessian	
UHF	
Conv. MP2	
Direct MP2	NA
MP2 Gradient	NA
MP4(SDTQ)	NA
SDCI	NA
CCSD	NA
QCISD	NA
CASSCF	NA

Ethylene, 16 electrons,  $^1A_g$ , D<sub>2h</sub> point group, Basis Set=cc-pVTZ  
(116 functions, 7-term f's, 5-term d's)

Method	Gaussian 90 (H)	Gaussian 92 (C)	MOLPRO (92.3)
RHF	11	10	10
Direct RHF	13	10	NA
RHF Gradient	11	10	NA
RHF Hessian	11	10	NA
UHF	13	12	13
MP2	11	10	10
Direct MP2	13	10	NA
MP2 Gradient	11	10	NA
MP4(SDTQ)	11	10	10
SDCI	11-SCF, 11-CI	11-SCF, 11-CI	10-SCF, 7-CI
CCSD	NA	10-SCF, 11-CC	10-SCF, 8-CC
QCISD	11-SCF, 10-CI	11-SCF, 10-QCI	10-SCF, 9-QCI
CASSCF			10-SCF, 4 MC

Method	GAMESS-US 6/17/92	HONDO (8.3)	GAMESS-UK (2)
Conv. RHF	unable to handle	13	unable to handle
Direct RHF	5-term d's, 7-term f's	13	5-term d's, 7-term f's
RHF Gradient		13	
RHF Hessian		13	
UHF			
Conv. MP2			
Direct MP2		NA	
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD		NA	
QCISD		NA	
CASSCF			

Method	DISCO (1.82)	SUPERMOLECULE	ACES II
Conv. RHF	11	12	16
Direct RHF	11	12	NA
RHF Gradient	11		16
RHF Hessian	NA		16
UHF	NA		19
Conv. MP2	NA		
Direct MP2	11		NA
MP2 Gradient	NA		
MP4(SDTQ)	NA		
SDCI	NA		
CCSD	NA		11
QCISD	NA		11
CASSCF	NA		NA

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

Method	Gaussian 90 (H)	Gaussian 92 (A)	MOLPRO (92.3)
RHF	11	10	12
Direct RHF	12	11	NA
RHF Gradient	11	10	12
RHF Hessian	11	10	NA
UHF Total	14	13	
MP2	11	10	12
Direct MP2	12	11	NA
MP2 Gradient	11	10	NA
MP4(SDTQ)	11	10	12
SDCI	FTC-ND	FTC-ND	12-SCF, 6-CI
CCSD	NA	FTC-ND	12-SCF, 9-CC
QCISD	FTC-ND	FTC-ND	12-SCF, 9-QCI
CASSCF	FTC-ND	FTC-ND	12-SCF, 7-MC

Method	GAMESS-US	HONDO (8.3)	GAMESS-UK (2)
Conv. RHF	unable to handle		
Direct RHF	5-term d's		
RHF Gradient			
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2	NA	NA	
MP2 Gradient			
MP4(SDTQ)	NA		
SDCI			
CCSD	NA	NA	
QCISD	NA	NA	
CASSCF			

Method	DISCO (1.82)	ACES II
Conv. RHF	13	
Direct RHF	13	NA
RHF Gradient	13	
RHF Hessian	NA	
UHF	NA	
Conv. MP2	NA	
Direct MP2	13	NA
MP2 Gradient	NA	
MP4(SDTQ)	NA	
SDCI	NA	
CCSD	NA	
QCISD	NA	
CASSCF	NA	NA

Imidazole, 36 electrons,  $^1A'$ , Cs, Basis Set=6-311++G\*\*  
(143 functions, 6-term d's)

Method	Gaussian 90 (H)	Gaussian 92 (C)	MOLPRO (92.3)
Conv. RHF	15	14	14
Direct RHF	20	15	
RHF Gradient	15	14	
RHF Hessian	15	14	NA
UHF	24	23	
MP2	15	14	
Direct MP2	20	15	NA
MP2 Gradient	15	14	
MP4(SDTQ)	15	15	
SDCI	15-SCF	14-SCF	
CCSD	NA	14-SCF	
QCISD	15-SCF	14-SCF	
CASSCF	15-SCF	14-SCF	

Method	GAMESS-US	HONDO (8.3)	GAMESS-UK (2)
Conv. RHF			
Direct RHF			
RHF Gradient			
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2	NA	NA	
MP2 Gradient			
MP4(SDTQ)	NA		
SDCI			
CCSD	NA	NA	
QCISD	NA	NA	
CASSCF			

Method	DISCO (1.82)	ACES II
Conv. RHF	9	
Direct RHF	9	NA
RHF Gradient	9	
RHF Hessian	NA	
UHF	NA	
Conv. MP2	NA	
Direct MP2	9	NA
MP2 Gradient	NA	
MP4(SDTQ)	NA	
SDCI	NA	
CCSD	NA	
QCISD	NA	
CASSCF	NA	NA

Imidazole, 36 electrons,  $^1A'$ , Cs, Basis Set=cc-pVTZ  
(206 functions, 5-term d's, 7-term f's)

Method	Gaussian 90 (H)	Gaussian 92 (C)	MOLPRO (92.3)
Conv. RHF		14	
Direct RHF		15	
RHF Gradient			
RHF Hessian			NA
UHF			
MP2			
Direct MP2			NA
MP2 Gradient			NA
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD			
CASSCF			

Method	GAMESS-US	HONDO (8.3)	GAMESS-UK (2)
Conv. RHF			
Direct RHF			
RHF Gradient			
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2	NA	NA	
MP2 Gradient			
MP4(SDTQ)	NA		
SDCI			
CCSD	NA	NA	
QCISD	NA	NA	
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

Isobutene, 32 electrons, C<sub>2v</sub>, Basis Set=6-311++G\*\*  
(148 functions, 6-term d's)

<u>Method</u>	<u>Gaussian 90 (H)</u>	<u>Gaussian 92 (C)</u>	<u>MOLPRO (92.3)</u>
Conv. RHF	14	13	
Direct RHF	25	16	NA
RHF Gradient	14	13	
RHF Hessian	14	13	NA
UHF	17		
Conv. MP2			
Direct MP2			NA
MP2 Gradient			NA
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD			
CASSCF			

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

<u>Method</u>	<u>DISCO (1.82)</u>	<u>ACES II</u>
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



Isobutene, 32 electrons, C<sub>2v</sub>, Basis Set=cc-pVTZ  
(232 functions, 5-term d's, 7-term f's)

<u>Method</u>	<u>Gaussian 90 (H)</u>	<u>Gaussian 92 (C)</u>	<u>MOLPRO (92.3)</u>
Conv. RHF		12	
Direct RHF	15	13	NA
RHF Gradient			
RHF Hessian			NA
UHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			NA
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD			
CASSCF			
<u>Method</u>	<u>GAMESS-US 6/17/92</u>	<u>HONDO (8.1)</u>	<u>GAMESS-UK (2)</u>
Conv. RHF			
Direct RHF			
RHF Gradient			
RHF Hessian			
UHF			
Conv. MP2			
Direct MP2	NA	NA	
MP2 Gradient			
MP4(SDTQ)	NA		
SDCI			
CCSD	NA	NA	
QCISD	NA	NA	
CASSCF			
<u>Method</u>	<u>DISCO (1.82)</u>	<u>ACES II</u>	
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	

Caffeine, C<sub>8</sub>H<sub>9</sub>O<sub>2</sub>N<sub>4</sub>, 101 electrons, C1, Basis Set=3-21G  
(144 functions)

<u>Method</u>	<u>Gaussian 90 (H)</u>	<u>Gaussian 92 (C)</u>	<u>MOLPRO (92.3)</u>
UHF	42	41	
UHF Gradient	42	41	
UHF Hessian	42	41	NA
Conv. RHF	41	53	18
Direct RHF			NA
Conv. MP2			
Direct MP2			NA
MP2 Gradient			NA
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD			
CASSCF			

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

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

Caffeine, C<sub>8</sub>H<sub>9</sub>O<sub>2</sub>N<sub>4</sub>, 101 electrons, C1, Basis Set=6-31G\*\*,  
(255 functions)

<u>Method</u>	<u>Gaussian 90 (H)</u>	<u>Gaussian 92 (C)</u>	<u>MOLPRO (92.3)</u>
Direct UHF	34	26	NA
RHF Gradient			
RHF Hessian			NA
ROHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			NA
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD			
CASSCF			

  

<u>Method</u>	<u>GAMESS-US</u>	<u>HONDO (8.1)</u>	<u>GAMESS-UK (2)</u>
Direct UHF			
RHF Gradient			
RHF Hessian			
ROHF			
Conv. MP2			
Direct MP2	NA	NA	
MP2 Gradient			
MP4(SDTQ)	NA		
SDCI			
CCSD	NA	NA	
QCISD	NA	NA	
CASSCF			

  

<u>Method</u>	<u>DISCO (1.82)</u>	<u>ACES II</u>
Direct UHF		
RHF Gradient		
RHF Hessian		
ROHF		
Conv. MP2		
Direct MP2	NA	NA
MP2 Gradient		
MP4(SDTQ)	NA	
SDCI		
CCSD	NA	NA
QCISD	NA	NA
CASSCF		

18-crown-6, C<sub>12</sub>H<sub>24</sub>O<sub>6</sub>, 144 electrons, C<sub>i</sub>, Basis Set=3-21G  
(210 functions)

<u>Method</u>	<u>Gaussian 90 (H)</u>	<u>Gaussian 92 (C)</u>	<u>Gaussian 94 (B)</u>
Direct RHF		13	13
RHF Gradient		13	
RHF Hessian			
Conv. RHF			
Conv. MP2			
Direct MP2			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD			
CASSCF			
<u>Method</u>	<u>GAMESS-US</u>	<u>HONDO (8.1)</u>	<u>GAMESS-UK (2)</u>
Direct RHF			
RHF Gradient			
RHF Hessian			
Conv. RHF			
Conv. MP2			
Direct MP2	NA	NA	
MP2 Gradient			
MP4(SDTQ)	NA		
SDCI			
CCSD	NA	NA	
QCISD	NA	NA	
CASSCF			
<u>Method</u>	<u>DISCO (1.82)</u>	<u>MOLPRO (92.3)</u>	<u>ACES II</u>
Direct RHF			
RHF Gradient			
RHF Hessian			
Conv. RHF			
Conv. MP2			
Direct MP2	NA		NA
MP2 Gradient			
MP4(SDTQ)	NA		
SDCI			
CCSD	NA		NA
QCISD	NA		NA
CASSCF			

18-crown-6, C<sub>12</sub>H<sub>24</sub>O<sub>6</sub>, 144 electrons, C<sub>i</sub>, Basis Set=6-31G\*\*  
(390 functions)

Method	Gaussian 90 (H)	Gaussian 92 (C)	
Direct RHF		13	13
RHF Gradient		13	
RHF Hessian			
Conv. RHF			
Conv. MP2			
Direct MP2			
MP2 Gradient			
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD			
CASSCF			

  

Method	GAMESS-US	HONDO (8.1)	GAMESS-UK (2)
Direct RHF	18		
RHF Gradient			
RHF Hessian			
Conv. RHF			
Conv. MP2			
Direct MP2	NA	NA	
MP2 Gradient			
MP4(SDTQ)	NA		
SDCI			
CCSD	NA	NA	
QCISD	NA	NA	
CASSCF			

  

Method	DISCO (1.82)	MOLPRO (92.3)	ACES II
Direct RHF			NA
RHF Gradient			
RHF Hessian			
Conv. RHF			
Conv. MP2	NA		
Direct MP2			NA
MP2 Gradient	NA		
MP4(SDTQ)	NA		
SDCI	NA		
CCSD	NA		
QCISD	NA		
CASSCF			

18-crown-6, C<sub>12</sub>H<sub>24</sub>O<sub>6</sub>, 144 electrons, C<sub>i</sub>, Basis Set=aug-cc-pVDZ  
(606 functions)

<u>Method</u>	<u>Gaussian 92 (C)</u>	<u>Gaussian 94 (C)</u>	<u>MOLPRO (92.3)</u>
Direct RHF	16	16	NA
RHF Gradient			
RHF Hessian			NA
Conv. RHF			
Conv. MP2			
Direct MP2			NA
MP2 Gradient			NA
MP4(SDTQ)			
SDCI			
CCSD	NA		
QCISD			
CASSCF			

  

<u>Method</u>	<u>GAMESS-US</u>	<u>HONDO (8.1)</u>	<u>GAMESS-UK (2)</u>
Direct RHF			
RHF Gradient			
RHF Hessian			
Conv. RHF			
Conv. MP2			
Direct MP2	NA	NA	
MP2 Gradient			
MP4(SDTQ)	NA		
SDCI			
CCSD	NA	NA	
QCISD	NA	NA	
CASSCF			

s18-crown-6, C<sub>34</sub>H<sub>56</sub>O<sub>8</sub>, 324 electrons, C<sub>2</sub>, Basis Set=6-31G\*\*  
(910 functions)

<u>Method</u>	<u>Gaussian 94 (D)</u>	<u>MOLPRO</u>
Direct RHF	13	NA
RHF Gradient		
RHF Hessian		NA
Conv. RHF		
Conv. MP2		
Direct MP2		NA
MP2 Gradient		NA
MP4(SDTQ)		
SDCI		
CCSD	NA	
QCISD		
CASSCF		