

## **Appendix C**

### **Molecular Energies (Hartrees)**

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### Molecular Energies (Hartrees)

#### Ethylene

Method	6-311++G**	cc-pVTZ	6-311++G(3df,3pd)
RHF	-78.056131	-78.064420	-78.063304
UHF	-77.927107	-77.751241	-77.752705
MP2	-78.387513	-78.429760	-78.444065
MP4	-78.427097	-78.469627	
SDCI	-78.386763	-78.422819	
CCSD	-78.416244	-78.455169	
CCSD(T)	-78.428374		
QCISD	-78.416770		
QCISD(T)	-78.428585		
CASSCF	-78.108478	-78.116214	
CAS-CI	-78.363768		
SVWN	-78.153807		
BLYP	-78.568261		

#### Isobutene

Method	6-311++G**	cc-pVTZ
RHF	-156.153387	-156.169067
UHF	-156.021366	
MP2	-156.830902	
MP4		
SDCI		
CCSD		
CASSCF		

#### Imidazole

Method	6-311++G**	cc-pVTZ
RHF	-224.874971	-224.896770
UHF	-224.714239	
MP2	-225.745074	
MP4		
SDCI		
CCSD		
CASSCF		

**Caffeine**

<u>Method</u>	<u>3-21G</u>	<u>6-31G**</u>
UHF	-671.906322	
RHF	-671.498350	
MP2	-672.902242	
MP4		
SDCI		
CCSD		
CASSCF		

<u>Method</u>	<u>3-21G</u>	<b>18-crown-6</b> <u>6-31G**</u>	<u>aug-cc-pVDZ</u>
RHF	-912.371076	-917.520266	-917.608365
UHF			
MP2		-920.281140	
MP4			
SDCI			
CCSD			
CASSCF			

<u>Method</u>	<u>6-31G**</u>	<b>s18-crown-6</b>
RHF	-1919.103358	
UHF		
MP2		
MP4		
SDCI		
CCSD		
CASSCF		