

b)

No (T):  
CCSD/CBS  
+DMRG

11.1

No CBS:  
CCSD(T)/TZ  
+DMRG

4.3

No DMRG:  
CCSD(T)/CBS

2.4

FiRE,  $c = 5a_0$

1.8

 $E - E_{\text{mean}} [\text{m}E_h]$ MAE vs. conventional best estimate [ $\text{m}E_h$ ]