



$\delta_{\text{HF}} = 3.12$   
 $\delta_{\text{B3LYP}} = 3.09$

平均  
 $\delta_{\text{HF}} = 2.73$   
 $\delta_{\text{B3LYP}} = 2.68$

$\delta_{\text{HF}} = 1.94$   
 $\delta_{\text{B3LYP}} = 1.81$

$\delta_{\text{HF}} = 8.25$   
 $\delta_{\text{B3LYP}} = 8.11$

$\delta_{\text{HF}} = 3.09$   
 $\delta_{\text{B3LYP}} = 3.14$

$\delta_{\text{HF}} = 2.33$   
 $\delta_{\text{B3LYP}} = 2.18$

平均  
 $\delta_{\text{HF}} = 2.84$   
 $\delta_{\text{B3LYP}} = 2.82$