

1.976  
1.922  
2.434      3.045  
1.951      2.812  
3.235  
2.743

Figure S1b

|              |              |              |              |              |              |
|--------------|--------------|--------------|--------------|--------------|--------------|
|              |              | <b>1.961</b> |              |              |              |
|              |              |              |              |              | <b>1.838</b> |
| <b>2.421</b> | <b>2.966</b> |              | <b>1.785</b> |              |              |
|              |              |              |              |              |              |
|              |              | <b>2.168</b> |              | <b>2.002</b> | <b>2.315</b> |
|              |              |              |              |              | <b>1.905</b> |

Figure S1c

|              |              |              |  |              |              |
|--------------|--------------|--------------|--|--------------|--------------|
|              |              | <b>1.974</b> |  |              |              |
|              |              |              |  | <b>1.897</b> | <b>1.908</b> |
|              | <b>1.942</b> | <b>2.404</b> |  |              |              |
| <b>2.814</b> |              |              |  |              |              |
|              |              |              |  |              |              |
| <b>3.092</b> |              |              |  |              |              |
|              | <b>2.712</b> |              |  |              |              |
|              |              |              |  |              |              |
|              |              |              |  | <b>1.977</b> | <b>2.419</b> |

Figure S1d

|              |              |              |              |              |
|--------------|--------------|--------------|--------------|--------------|
|              | <b>1.974</b> |              |              |              |
| 1.953        | <b>2.419</b> | <b>3.033</b> | <b>1.931</b> | <b>1.921</b> |
| <b>2.820</b> |              |              |              |              |
| <b>3.183</b> |              |              |              |              |
| <b>2.685</b> |              |              |              | <b>2.354</b> |
|              |              |              |              | <b>1.996</b> |

Figure S1e

|        |       |       |
|--------|-------|-------|
|        | 1.971 |       |
| 2.055  | .423  | 2.346 |
| 2.383  |       | 1.913 |
| 2.718* |       | 2.644 |
| 2.876  |       |       |

\* CI-HC

|       |       |
|-------|-------|
|       | 1.887 |
| 1.981 | 1.840 |
| 2.354 |       |

Figure S1f

|              |              |              |              |              |
|--------------|--------------|--------------|--------------|--------------|
|              |              | <b>1.974</b> |              |              |
|              |              | <b>3.100</b> | <b>2.373</b> |              |
|              | <b>1.965</b> |              |              | <b>1.906</b> |
| <b>2.830</b> |              |              | <b>1.924</b> |              |
|              |              |              |              |              |
| <b>2.907</b> |              |              |              |              |
|              | <b>2.683</b> |              |              | <b>2.267</b> |
|              |              |              |              | <b>1.985</b> |

Figure S1g

|              |              |               |
|--------------|--------------|---------------|
|              |              | <b>2.17</b>   |
|              | <b>2.574</b> | <b>1.793</b>  |
|              |              | <b>3.113</b>  |
| <b>2.219</b> | <b>2.483</b> | <b>2.363</b>  |
|              |              |               |
|              |              |               |
| <b>1.790</b> |              | <b>2.180</b>  |
|              |              |               |
|              | <b>2.561</b> |               |
|              |              | <b>2.890*</b> |
|              | <b>2.115</b> |               |

\* Br-HC

Figure S2

$\Delta H_{\text{B3LYP}}$  ( $\Delta G_{\text{B3LYP}}$ )  
 $\Delta H_{\text{MP2}}$  ( $\Delta G_{\text{MP2}}$ )  
 $\Delta H_{\text{MP2-AUG}}$  ( $\Delta G_{\text{MP2-AUG}}$ )

|                   |                      |
|-------------------|----------------------|
| 70.9 (-6.3)       | 188.9 (84.3)         |
| 72.6 (-4.5)       | 212.7 (108.1)        |
| <b>78.1 (0.9)</b> | <b>235.5 (130.9)</b> |

Figure S3

2,5-A

2,5-B

3,5