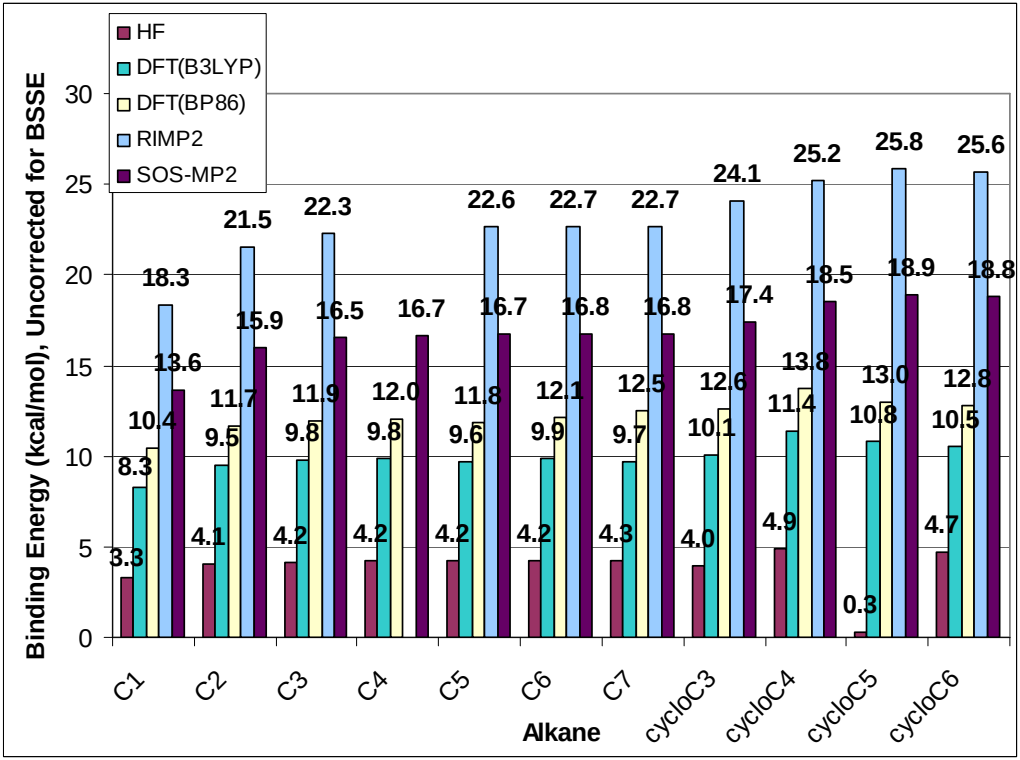
HF
DFT(B3LYP)
DFT(BP86)
RIMP2
SOS-MP2
Binding Energy (kcal/mol), Uncorrected for BSSE
0
5
10
15
20
25
30
3.3
8.3
10.4
18.3
13.6
4.1
9.5
11.7
21.5
15.9
4.2
9.8
11.9
22.3
16.5
4.2
9.8
12.0
16.7
4.2
9.6
11.8
22.6
16.7
4.2
9.9
12.1
22.7
16.8
4.3
9.7
12.5
22.7
16.8
4.0
10.1
12.6
24.1
17.4
4.9
11.4
13.8
25.2
18.5
0.3
10.8
13.0
25.8
18.9
4.7
10.5
12.8
25.6
18.8
C1
C2
C3
C4
C5
C6
C7
cycloC3
cycloC4
cycloC5
cycloC6
Alkane