0.002 0.83 H - 0.369.4 1.2 1.7 0.26 0.97 He - 3.2 5.9 0.58 5.6 3.1 4.1 7.3 Li - 4.3 0.13 3.3 0.079 2.3 1.9 6.2 1.1 Be -

B -

C -

N -

6.5 9 7.8 10 12 9 9 1.7 7.6 3.3 11 7.3 4.8 6.6 1.9 2.8 5.7 4.9 9.5 2.9 3.3 0.2 2.1 9.1 3.9 4.1 5.6 0.56 0.51 1.7 6.7 0.79 11

Ionization energies error

12

10

8

error [kcal/mol]

abs.

1.4

0.11

10

8.6 0.52 4.2 4.9 0.1 0 -2.4 8.1 7.1 2.2 2.2 1.4 4.2 6.2 F - 3.8 2.2 3.4 2.1 1.4 Ne - 0.92 4.6 3.6 0.045 1.5 0.49 3.5 2 9.8 Na - 4.5 1.5 0.4 4.1 0.21 0.025 7.3 3.3 9.8 4.3 6.1 0.57 1.8 0.83 2.9 2.5 10 Mg - 1.2 5 Al -1 1.8 4.3 2 2.3 1.7 0.24 1.8 0.52 3.8 3 6.2 1.1 2.7 Si - 0.86 3.4 1.9 P - 0.760.73 3.3 3.9 4.3 1.8 1.5 0.33 3.5 S - 0.0792.6 0.5 0.66 0.17 0.014 2 0.014 2.5

1.2 0.23 CI - 0.26 0.61 0.92 0.28 1.6 3.2 4.4 0.2 0.23 4.9 Ar - 0.51.2 1.1 2 2.7 2 3 MAE - 3.1 3.4 3.7 3.1 2 3.4 2.5 5.8 B3LYP. SCAN PBE **AM05** 90W **MOD-B3LYP B97** M08-HX SOGGA11