

Supplementary Materials: Statistical Significance of the Maximum Hardness Principle Applied to Some Selected Chemical Reactions

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Table S1. The Ionization Potential (I, eV) and Electron Affinity (A, eV) calculated at B3LYP/6-311++G(2df,3pd)/def2-QZVP and LC-BLYP/6-311++G(2df,3pd)/def2-QZVP levels for the molecules.

| Molecule | B3LYP/6-311++G(2df,3pd)/def2-QZVP | | LC-BLYP/6-311++G(2df,3pd)/def2-QZVP | |
|---|-----------------------------------|-----------------------|-------------------------------------|-----------------------|
| | Ionization Potential (I) | Electron Affinity (A) | Ionization Potential (I) | Electron Affinity (A) |
| CH ₃ F | 9.68 | 0.18 | 13.22 | -0.88 |
| CH ₄ (12.62) | 10.77 | 0.15 | 14.31 | -0.91 |
| CH ₂ F ₂ | 9.82 | 0.18 | 13.31 | -0.89 |
| CH ₃ OH | 7.76 | 0.34 | 11.26 | -0.81 |
| CH ₂ (OH) ₂ | 8.36 | 0.69 | 11.94 | -0.59 |
| FCH ₂ OH | 9.02 | 0.44 | 12.53 | -0.78 |
| CH ₃ NH ₂ | 6.66 | 0.30 | 9.96 | -0.84 |
| HOCH ₂ NH ₂ | 6.91 | 0.45 | 10.24 | -0.74 |
| CH ₂ (NH ₂) ₂ | 6.48 | 0.45 | 9.73 | -0.74 |
| FCH ₂ NH ₂ | 7.82 | 0.32 | 11.24 | -0.87 |
| SiH ₃ F | 9.64 | 0.69 | 12.95 | -1.04 |
| SiH ₂ F ₂ | 9.79 | 0.37 | 13.10 | -1.24 |
| SiH ₄ | 9.67 | 0.13 | 12.98 | -1.05 |
| CF ₂ Cl ₂ | 9.25 | 1.41 | 12.66 | -1.35 |
| CF ₄ | 12.39 | -0.20 | 16.25 | -1.60 |
| CCl ₄ | 8.87 | 2.11 | 12.19 | -0.97 |
| CHF ₃ | 11.26 | 0.14 | 14.86 | -0.92 |
| CH ₃ Cl | 8.26 | 0.45 | 11.60 | -0.81 |
| CH ₃ OCH ₃ | 7.23 | 0.22 | 10.60 | -0.88 |
| C(OCH ₃) ₄ | 7.74 | 0.15 | 11.24 | -0.87 |
| CF ₃ Cl | 9.84 | 0.73 | 13.43 | -1.47 |
| CH ₃ CH ₃ | 9.42 | 0.16 | 12.73 | -0.92 |
| C(CH ₃) ₄ | 8.78 | 0.31 | 12.06 | -0.83 |
| SiF ₄ | 12.53 | 0.82 | 16.40 | -0.91 |
| SiF ₃ H | 11.11 | 0.01 | 14.61 | -1.39 |
| Si(OCH ₃) ₄ | 7.83 | 0.23 | 11.26 | -0.85 |
| Me ₂ O | 7.23 | 0.22 | 10.60 | -0.88 |
| H ₂ O | 8.82 | 0.59 | 12.62 | -0.80 |
| H ₂ S | 7.32 | 0.54 | 10.57 | -0.79 |
| MeHS | 6.62 | 0.51 | 9.78 | -0.81 |
| (HS) ₂ S | 7.32 | 1.85 | 10.31 | -0.70 |
| HSSH | 6.23 | 1.85 | 10.47 | -0.79 |
| HSF | 7.29 | 2.22 | 10.54 | -0.54 |
| HOF | 9.12 | 2.04 | 12.79 | -0.76 |
| HOCl | 8.02 | 2.04 | 11.37 | -0.43 |
| Cl ₂ O | 8.10 | 3.87 | 11.35 | 0.58 |
| F ₂ O | 9.63 | 3.00 | 13.28 | -0.95 |
| NH ₃ | 7.47 | 0.42 | 10.94 | -0.86 |
| MeNH ₂ | 6.66 | 0.30 | 9.96 | -0.84 |
| Me ₂ NH | 6.19 | 0.25 | 9.41 | -0.85 |
| NMe ₃ | 5.95 | 0.27 | 9.11 | -0.85 |
| HMeC=CH ₂ | 7.14 | 0.20 | 10.32 | -0.91 |
| H ₂ C=CH ₂ | 7.69 | 0.29 | 10.98 | -1.08 |
| Me ₂ C=CH ₂ | 6.85 | 0.25 | 9.97 | -0.85 |

| | | | | |
|------------------------------------|-------|------|-------|-------|
| F ₂ C=CF ₂ | 7.53 | 0.19 | 10.82 | -1.29 |
| HFC=CF ₂ | 7.60 | 0.23 | 10.88 | -1.00 |
| H ₂ C=CF ₂ | 7.65 | 0.15 | 10.95 | -0.99 |
| Cl ₂ C=CCl ₂ | 7.20 | 1.38 | 10.15 | -1.21 |
| HCIC=CCl ₂ | 7.41 | 0.67 | 10.53 | -0.93 |
| H ₂ C=CCl ₂ | 7.44 | 1.01 | 10.53 | -0.97 |
| Me ₂ Hg | 6.81 | 0.42 | 9.96 | -0.83 |
| Cl ₂ Hg | 8.70 | 2.85 | 11.95 | 0.07 |
| MeHgCl | 8.04 | 1.25 | 11.46 | -0.57 |
| COS | 8.45 | 1.21 | 11.50 | -1.13 |
| CO ₂ | 10.48 | 0.52 | 14.01 | -1.01 |
| CS ₂ | 7.62 | 2.24 | 10.36 | -0.13 |
| CH ₂ =C=CH ₂ | 7.53 | 0.13 | 10.72 | -0.97 |
| CH ₂ =C=O | 6.95 | 1.29 | 10.11 | -0.91 |
| COF ₂ | 10.20 | 0.94 | 13.90 | -1.19 |
| COCl ₂ | 9.04 | 2.06 | 12.37 | -0.82 |
| CH ₂ CS | 6.44 | 2.43 | 9.30 | -0.19 |
| Me ₂ S | 6.09 | 0.27 | 9.16 | -0.88 |
| Me ₂ CH ₂ | 8.99 | 0.18 | 12.23 | -0.92 |
| CH ₂ Cl ₂ | 8.55 | 0.87 | 11.83 | -0.82 |
| CH ₂ I ₂ | 7.17 | 2.28 | 10.03 | -0.28 |
| CH ₃ I | 7.08 | 1.31 | 10.09 | -0.66 |
| CHCl ₃ | 8.68 | 1.49 | 11.98 | -0.90 |
| H ₂ CO | 7.66 | 1.72 | 11.04 | -0.91 |
| Me ₂ CO | 7.03 | 0.78 | 10.44 | -0.70 |
| HMeCO | 7.33 | 1.08 | 10.71 | -0.79 |
| ClMeCO | 8.42 | 1.44 | 11.66 | -0.73 |
| HOI | 7.16 | 3.11 | 10.18 | 0.35 |
| SiH ₃ Cl | 8.81 | 0.69 | 12.08 | -1.09 |
| SiH ₃ NH ₂ | 7.21 | 0.53 | 10.48 | -0.86 |
| SiH ₃ PH ₂ | 7.40 | 0.49 | 10.29 | -0.85 |
| SiH ₃ SiH ₃ | 8.18 | 0.28 | 11.16 | -0.97 |
| SiH ₃ CH ₃ | 8.99 | 0.32 | 12.32 | -0.88 |
| SiH ₃ I | 7.48 | 1.23 | 10.45 | -0.87 |
| CH ₃ PH ₂ | 6.99 | 0.47 | 9.94 | -0.81 |
| NH ₂ F | 8.05 | 0.54 | 11.46 | -0.77 |
| NHF ₂ | 8.86 | 0.47 | 12.26 | -0.80 |
| NF ₃ | 10.22 | 0.23 | 13.65 | -2.57 |
| HCOOH | 8.40 | 0.65 | 11.92 | -0.97 |
| HC(OH) ₃ | 8.55 | 0.44 | 12.04 | -0.79 |
