**Impact of Non-Empirically Tuning the Range-Separation Parameter of Long-Range Corrected Hybrid Functionals on Ionization Potentials, Electron Affinities, and Fundamental Gaps**

Talapunur Vikramaditya,[[1]](#endnote-1) Jeng-Da Chai,[[2]](#endnote-2)\* and Shiang-Tai Lini\*

1. T. Vikramaditya, Shiang-Tai Lin

Computational Molecular Engineering Laboratory,Department of Chemical Engineering, National Taiwan University, Taipei 10617, Taiwan. [↑](#endnote-ref-1)
2. Jeng-Da Chai

Department of Physics, Center for Theoretical Physics, and Center for Quantum Science and Engineering, National Taiwan University, Taipei 10617, Taiwan.

**Supporting Information**

Table 1. CCSD(T)//ATZ IP, EA and FG evaluated employing ∆SCF approach

(30 compounds).

|  |  |  |  |
| --- | --- | --- | --- |
| **Compounds** | **IP** | **EA**  | **FG** |
| Butyl amine | 9.44 | -0.57 | 10.01 |
| Cyclohexyl amine | 9.3 | -0.53 | 9.83 |
| Dimethyl amine | 8.94 | -0.61 | 9.55 |
| Sec-Butyl amine | 9.31 | -0.56 | 9.87 |
| Butanol | 10.68 | -0.74 | 11.42 |
| Ethyleneglycol | 10.97 | -0.7 | 11.67 |
| Phenol | 9.2 | -0.49 | 9.69 |
| Quinol | 8.99 | -0.59 | 9.58 |
| 1-Butyne | 10.38 | -0.59 | 10.97 |
| Butadine | 9.22 | -0.78 | 10 |
| 1,4-Cyclohexadine | 9.08 | -0.79 | 9.87 |
| Benzene | 9.43 | -0.79 | 10.22 |
| Naphthalene | 8.23 | -0.63 | 8.86 |
| Acridine | 8.06 | 0.54 | 7.52 |
| Azulene | 7.54 | 0.41 | 7.13 |
| Furan | 9.05 | -0.83 | 9.88 |
| Thiophene | 9.39 | -0.77 | 10.16 |
| Pyridine | 9.73 | -0.74 | 10.47 |
| Indole | 7.93 | -0.38 | 8.31 |
| Quinoline | 8.77 | -0.59 | 9.36 |
| Carbazole | 7.78 | -0.36 | 8.14 |
| Benzonitrile | 9.89 | -0.32 | 10.21 |
| meta Cyano Benzonitrile | 10.41 | 0.52 | 9.89 |
| TCNE | 11.96 | 2.92 | 9.04 |
| Fumeronitrile | 11.41 | 0.88 | 10.53 |
| Benzoquinone | 10.17 | 1.47 | 8.7 |
| F4- Benzoquinone | 11.01 | 2.18 | 8.83 |
| Benzaldehyde | 9.85 | -0.06 | 9.91 |
| Maleic Anhydride | 11.21 | 0.94 | 10.27 |
| Pthalimide | 10.02 | 0.55 | 9.47 |

**Table 2. LC-ωPBE//ATZ IP, EA and FG evaluated employing ∆SCF approach with default range separation parameter (ω=0.40 bohr-1). (30 compounds).**

|  |  |  |  |
| --- | --- | --- | --- |
| **Compounds** | **IP** | **EA**  | **FG** |
| Butyl amine | 9.37 | -0.58 | 9.95 |
| Cyclohexyl amine | 9.22 | -0.57 | 9.79 |
| Dimethyl amine | 8.9 | -0.62 | 9.52 |
| Sec-Butyl amine | 9.28 | -0.59 | 9.87 |
| Butanol | 10.59 | -0.56 | 11.15 |
| Ethyleneglycol | 10.83 | -0.73 | 11.56 |
| Phenol | 9.16 | -0.53 | 9.69 |
| Quinol | 8.94 | -0.67 | 9.61 |
| 1-Butyne | 10.25 | -0.6 | 10.85 |
| Butadine | 9.1 | -0.79 | 9.89 |
| 1,4-Cyclohexadine | 9.03 | -0.81 | 9.84 |
| Benzene | 9.42 | -0.8 | 10.22 |
| Naphthalene | 8.31 | -0.43 | 8.74 |
| Acridine | 8.12 | 0.75 | 7.37 |
| Azulene | 7.35 | 0.78 | 6.57 |
| Furan | 9.03 | -0.81 | 9.84 |
| Thiophene | 9.42 | -0.79 | 10.21 |
| Pyridine | 9.67 | -0.89 | 10.56 |
| Indole | 8.01 | -0.38 | 8.39 |
| Quinoline | 8.82 | -0.02 | 8.84 |
| Carbazole | 7.84 | -0.39 | 8.23 |
| Benzonitrile | 9.94 | -0.09 | 10.03 |
| meta Cyano Benzonitrile | 10.49 | 0.78 | 9.71 |
| TCNE | 12.03 | 3.41 | 8.62 |
| Fumeronitrile | 11.41 | 1.26 | 10.15 |
| Benzoquinone | 10.67 | 1.74 | 8.93 |
| F4- Benzoquinone | 11.06 | 2.48 | 8.58 |
| Benzaldehyde | 9.8 | 0.15 | 9.65 |
| Maleic Anhydride | 11.63 | 1.23 | 10.4 |
| Pthalimide | 10.09 | 0.71 | 9.38 |

**Table 3. Tuned IP, EA evaluated employing ∆SCF approach using eq. 3 with LC-ωPBE//ATZ (30 compounds).**

|  |  |  |  |
| --- | --- | --- | --- |
| **Compounds** | **ω** | **IP** | **EA** |
| Butyl amine | 0.35 | 9.36 | -0.57 |
| Cyclohexyl amine | 0.33 | 9.18 | -0.55 |
| Dimethyl amine | 0.35 | 8.89 | -0.62 |
| Sec-Butyl amine | 0.34 | 9.26 | -0.58 |
| Butanol | 0.38 | 10.56 | -0.56 |
| Ethyleneglycol | 0.4 | 10.83 | -0.73 |
| Phenol | 0.28 | 9.11 | -0.5 |
| Quinol | 0.28 | 8.87 | -0.63 |
| 1-Butyne | 0.34 | 10.22 | -0.59 |
| Butadine | 0.31 | 9.06 | -0.78 |
| 1,4-Cyclohexadiene | 0.3 | 8.82 | -0.8 |
| Benzene | 0.28 | 9.38 | -0.78 |
| Naphthalene | 0.26 | 8.17 | -0.35 |
| Acridine | 0.24 | 7.89 | 0.82 |
| Azulene | 0.24 | 7.37 | 0.68 |
| Furan | 0.31 | 9.01 | -0.8 |
| Thiophene | 0.36 | 9.42 | -0.79 |
| Pyridine | 0.31 | 9.6 | -0.88 |
| Indole | 0.27 | 7.9 | -0.35 |
| Quinoline | 0.26 | 8.68 | 0.05 |
| Carbazole | 0.24 | 7.66 | -0.48 |
| Benzonitrile | 0.28 | 9.82 | -0.06 |
| meta Cyano Benzonitrile | 0.27 | 10.3 | 0.8 |
| TCNE | 0.3 | 11.76 | 3.36 |
| Fumeronitrile | 0.33 | 11.3 | 1.26 |
| Benzoquinone | 0.39 | 10.63 | 1.75 |
| F4- Benzoquinone | 0.3 | 10.8 | 2.49 |
| Benzaldehyde | 0.31 | 9.7 | 0.19 |
| Maleic Anhydride | 0.43 | 11.72 | 1.22 |
| Pthalimide | 0.3 | 10 | 0.76 |

**Table 4. Tuned EA, evaluated employing ∆SCF approach using eq. 4 with LC-ωPBE//ATZ (26 compounds).**

|  |  |  |
| --- | --- | --- |
| **Compounds** | **ω** | **EA** |
| Butyl amine | 0.11 | -0.42 |
| Cyclohexyl amine | 0.11 | -0.39 |
| Dimethyl amine | 0.11 | -0.45 |
| Sec-Butyl amine | 0.12 | -0.43 |
| Butanol | 0.11 | -0.40 |
| Ethyleneglycol | 0.39 | -0.73 |
| Phenol | 0.13 | -0.39 |
| Quinol | 0.18 | -0.54 |
| 1-Butyne | 0.11 | -0.43 |
| Butadine | 0.27 | -0.77 |
| Naphthalene | 0.24 | -0.33 |
| Acridine | 0.23 | 0.82 |
| Azulene | 0.23 | 0.67 |
| Thiophene | 0.36 | -0.79 |
| Indole | 0.21 | -0.32 |
| Quinoline | 0.25 | 0.05 |
| Carbazole | 0.23 | -0.47 |
| Benzonitrile | 0.26 | -0.05 |
| meta Cyano Benzonitrile | 0.25 | 0.81 |
| TCNE | 0.27 | 3.35 |
| Fumeronitrile | 0.3 | 1.27 |
| Benzoquinone | 0.29 | 1.81 |
| F4- Benzoquinone | 0.3 | 2.49 |
| Benzaldehyde | 0.27 | 0.21 |
| Maleic Anhydride | 0.31 | 1.26 |
| Pthalimide | 0.26 | 0.78 |

**Table 5. Tuned IP, EA, FG employing ∆SCF approach using eq. 5 with LC-ωPBE//ATZ (30 compounds).**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Compounds** | **ω** | **IP** | **EA**  | **FG** |
| Butyl amine | 0.35 | 9.36 | -0.57 | 9.93 |
| Cyclohexyl amine | 0.33 | 9.18 | -0.55 | 9.73 |
| Dimethyl amine | 0.35 | 8.89 | -0.62 | 9.51 |
| Sec-Butyl amine | 0.34 | 9.26 | -0.58 | 9.84 |
| Butanol | 0.38 | 10.56 | -0.56 | 11.12 |
| Ethyleneglycol | 0.4 | 10.83 | -0.73 | 11.56 |
| Phenol | 0.28 | 9.11 | -0.5 | 9.61 |
| Quinol | 0.28 | 8.87 | -0.63 | 9.5 |
| 1-Butyne | 0.34 | 10.22 | -0.59 | 10.81 |
| Butadine | 0.31 | 9.06 | -0.78 | 9.84 |
| 1,4-Cyclohexadiene | 0.3 | 8.82 | -0.8 | 9.62 |
| Benzene | 0.28 | 9.38 | -0.78 | 10.16 |
| Naphthalene | 0.25 | 8.15 | -0.34 | 8.49 |
| Acridine | 0.23 | 7.87 | 0.82 | 7.05 |
| Azulene | 0.23 | 7.38 | 0.67 | 6.71 |
| Furan | 0.31 | 9.01 | -0.8 | 9.81 |
| Thiophene | 0.36 | 9.42 | -0.79 | 10.21 |
| Pyridine | 0.31 | 9.6 | -0.88 | 10.48 |
| Indole | 0.27 | 7.9 | -0.35 | 8.25 |
| Quinoline | 0.26 | 8.68 | 0.05 | 8.63 |
| Carbazole | 0.23 | 7.65 | -0.47 | 8.12 |
| Benzonitrile | 0.28 | 9.82 | -0.06 | 9.88 |
| meta Cyano Benzonitrile | 0.27 | 10.3 | 0.8 | 9.5 |
| TCNE | 0.27 | 11.67 | 3.35 | 8.32 |
| Fumeronitrile | 0.33 | 11.3 | 1.26 | 10.04 |
| Benzoquinone | 0.39 | 10.63 | 1.75 | 8.88 |
| F4- Benzoquinone | 0.3 | 10.8 | 2.49 | 8.31 |
| Benzaldehyde | 0.3 | 9.69 | 0.19 | 9.5 |
| Maleic Anhydride | 0.43 | 11.72 | 1.22 | 10.5 |
| Pthalimide | 0.3 | 10 | 0.76 | 9.24 |

**Table 6. LC-ωPBE//ADZ IP, EA and FG evaluated employing ∆SCF approach with default range separation parameter (ω=0.40 bohr-1). (30 compounds).**

|  |  |  |  |
| --- | --- | --- | --- |
| **Compounds** | **IP** | **EA** | **FG** |
| Butyl amine | 9.38 | -0.73 | 10.11 |
| Cyclohexyl amine | 9.22 | -0.71 | 9.93 |
| Dimethyl amine | 8.9 | -0.77 | 9.67 |
| Sec-Butyl amine | 9.29 | -0.74 | 10.03 |
| Butanol | 10.57 | -0.71 | 11.28 |
| Ethyleneglycol | 10.8 | -0.88 | 11.68 |
| Phenol | 9.13 | -0.67 | 9.8 |
| Quinol | 8.92 | -0.82 | 9.74 |
| 1-Butyne | 10.19 | -0.74 | 10.93 |
| Butadine | 9.04 | -1 | 10.04 |
| 1,4-Cyclohexadine | 8.99 | -1.03 | 10.02 |
| Benzene | 9.37 | -0.79 | 10.16 |
| Naphthalene | 8.27 | -0.4 | 8.67 |
| Acridine | 8.08 | 0.77 | 7.31 |
| Azulene | 7.32 | 0.8 | 6.52 |
| Furan | 8.99 | -1 | 9.99 |
| Thiophene | 9.42 | -1.32 | 10.74 |
| Pyridine | 9.68 | -0.88 | 10.56 |
| Indole | 7.97 | -0.49 | 8.46 |
| Quinoline | 8.77 | 0 | 8.77 |
| Carbazole | 7.81 | -0.48 | 8.29 |
| Benzonitrile | 9.89 | -0.07 | 9.96 |
| meta Cyano Benzonitrile | 10.44 | 0.8 | 9.64 |
| TCNE | 11.96 | 3.42 | 8.54 |
| Fumeronitrile | 11.34 | 1.28 | 10.06 |
| Benzoquinone | 10.67 | 1.77 | 8.9 |
| F4- Benzoquinone | 11.07 | 2.54 | 8.53 |
| Benzaldehyde | 9.79 | 0.18 | 9.61 |
| Maleic Anhydride | 11.61 | 1.27 | 10.34 |
| Pthalimide | 10.05 | 0.75 | 9.3 |

**Table 7. Tuned IP, EA, FG employing ∆SCF approach using eq. 5 with LC-ωPBE//ADZ (30 compounds).**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Compounds** | **ω** | **IP** | **EA** | **FG** |
| Butyl amine | 0.35 | 9.36 | -0.72 | 10.08 |
| Cyclohexyl amine | 0.33 | 9.18 | -0.69 | 9.87 |
| Dimethyl amine | 0.35 | 8.88 | -0.76 | 9.64 |
| Sec-Butyl amine | 0.34 | 9.26 | -0.72 | 9.98 |
| Butanol | 0.39 | 10.57 | -0.71 | 11.28 |
| Ethyleneglycol | 0.4 | 10.8 | -0.88 | 11.68 |
| Phenol | 0.28 | 9.08 | -0.62 | 9.7 |
| Quinol | 0.28 | 8.85 | -0.77 | 9.62 |
| 1-Butyne | 0.34 | 10.16 | -0.73 | 10.89 |
| Butadine | 0.3 | 9 | -0.86 | 9.86 |
| 1,4-Cyclohexadine | 0.3 | 8.78 | -1.01 | 9.79 |
| Benzene | 0.27 | 9.34 | -0.96 | 10.3 |
| Naphthalene | 0.27 | 8.1 | -0.59 | 8.69 |
| Acridine | 0.23 | 7.83 | 0.84 | 6.99 |
| Azulene | 0.23 | 7.34 | 0.69 | 6.65 |
| Furan | 0.31 | 8.97 | -0.99 | 9.96 |
| Thiophene | 0.37 | 9.41 | -1.32 | 10.73 |
| Pyridine | 0.31 | 9.61 | -0.87 | 10.48 |
| Indole | 0.27 | 7.86 | -0.45 | 8.31 |
| Quinoline | 0.26 | 8.64 | 0.06 | 8.58 |
| Carbazole | 0.23 | 7.62 | -0.46 | 8.08 |
| Benzonitrile | 0.28 | 9.78 | -0.04 | 9.82 |
| meta Cyano Benzonitrile | 0.27 | 10.25 | 0.81 | 9.44 |
| TCNE | 0.3 | 11.69 | 3.37 | 8.32 |
| Fumeronitrile | 0.33 | 11.23 | 1.28 | 9.95 |
| Benzoquinone | 0.39 | 10.64 | 1.78 | 8.86 |
| F4- Benzoquinone | 0.3 | 10.82 | 2.55 | 8.27 |
| Benzaldehyde | 0.3 | 9.67 | 0.21 | 9.46 |
| Maleic Anhydride | 0.43 | 11.7 | 1.26 | 10.44 |
| Pthalimide | 0.29 | 9.95 | 0.8 | 9.15 |

**Table 8. HOMO, LUMO Energies and their gaps using default range separation parameter (0.40 bohr-1) employing LC-ωPBE//ATZ. (30 compounds).**

|  |  |  |  |
| --- | --- | --- | --- |
| **Compounds** | **-HOMO** | **-LUMO** | **Gap(L-H)** |
| Butyl amine | 9.62 | -0.76 | 10.38 |
| Cyclohexyl amine | 9.61 | -0.75 | 10.36 |
| Dimethyl amine | 9.14 | -0.77 | 9.91 |
| Sec-Butyl amine | 9.63 | -0.76 | 10.39 |
| Butanol | 10.67 | -0.74 | 11.41 |
| Ethyleneglycol | 10.82 | -0.76 | 11.58 |
| Phenol | 9.6 | -0.72 | 10.32 |
| Quinol | 9.37 | -0.7 | 10.07 |
| 1-Butyne | 10.52 | -0.77 | 11.29 |
| Butadine | 9.47 | -0.83 | 10.3 |
| 1,4-Cyclohexadine | 9.3 | -0.78 | 10.08 |
| Benzene | 9.86 | -0.77 | 10.63 |
| Naphthalene | 8.71 | -0.76 | 9.47 |
| Acridine | 8.52 | 0.31 | 8.21 |
| Azulene | 7.91 | 0.28 | 7.63 |
| Furan | 9.38 | -0.78 | 10.16 |
| Thiophene | 9.57 | -0.78 | 10.35 |
| Pyridine | 10.21 | -0.67 | 10.88 |
| Indole | 8.41 | -0.62 | 9.03 |
| Quinoline | 9.26 | -0.41 | 9.67 |
| Carbazole | 8.31 | -0.65 | 8.96 |
| Benzonitrile | 10.36 | -0.46 | 10.82 |
| meta Cyano Benzonitrile | 10.92 | 0.35 | 10.57 |
| TCNE | 12.33 | 2.99 | 9.34 |
| Fumeronitrile | 11.65 | 0.93 | 10.72 |
| Benzoquinone | 10.69 | 1.43 | 9.26 |
| F4- Benzoquinone | 11.35 | 2.18 | 9.17 |
| Benzaldehyde | 10.25 | -0.23 | 10.48 |
| Maleic Anhydride | 11.55 | 0.94 | 10.61 |
| Pthalimide | 10.65 | 0.32 | 10.33 |

**Table 9. HOMO, LUMO Energies and their gaps tuned using eq. 5 employing LC-ωPBE//ATZ. (30 compounds).**

|  |  |  |  |
| --- | --- | --- | --- |
| **Compounds** | **-HOMO** | **-LUMO** | **GAP(L-H)** |
| Butyl amine | 9.33 | -0.75 | 10.08 |
| Cyclohexyl amine | 9.18 | -0.73 | 9.91 |
| Dimethyl amine | 8.86 | -0.76 | 9.62 |
| Sec-Butyl amine | 9.28 | -0.75 | 10.03 |
| Butanol | 10.54 | -0.74 | 11.28 |
| Ethyleneglycol | 10.82 | -0.76 | 11.58 |
| Phenol | 9.11 | -0.68 | 9.79 |
| Quinol | 8.88 | -0.66 | 9.54 |
| 1-Butyne | 10.21 | -0.76 | 10.97 |
| Butadine | 9.08 | -0.81 | 9.89 |
| 1,4-Cyclohexadine | 8.82 | -0.75 | 9.57 |
| Benzene | 9.37 | -0.74 | 10.11 |
| Naphthalene | 8.12 | -0.36 | 8.48 |
| Acridine | 7.84 | 0.79 | 7.05 |
| Azulene | 7.33 | 0.68 | 6.65 |
| Furan | 9 | -0.76 | 9.76 |
| Thiophene | 9.42 | -0.78 | 10.2 |
| Pyridine | 9.62 | -0.65 | 10.27 |
| Indole | 7.89 | -0.58 | 8.47 |
| Quinoline | 8.69 | 0 | 8.69 |
| Carbazole | 7.61 | -0.49 | 8.1 |
| Benzonitrile | 9.83 | -0.12 | 9.95 |
| meta Cyano Benzonitrile | 10.3 | 0.72 | 9.58 |
| TCNE | 11.56 | 3.35 | 8.21 |
| Fumeronitrile | 11.29 | 1.15 | 10.14 |
| Benzoquinone | 10.63 | 1.45 | 9.18 |
| F4- Benzoquinone | 10.78 | 2.49 | 8.29 |
| Benzaldehyde | 9.65 | 0.08 | 9.57 |
| Maleic Anhydride | 11.73 | 0.86 | 10.87 |
| Pthalimide | 10.02 | 0.61 | 9.41 |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|   |   |   |   |   |   |
| **Compounds** | **ω=0.20** | **ω=0.30** | **ω=0.40** | **ω=0.50** | **ω=0.60** |
| Butyl amine | -0.65 | -0.73 | -0.76 | -0.77 | -0.77 |
| Cyclohexyl amine | -0.64 | -0.72 | -0.75 | -0.76 | -0.77 |
| Dimethyl amine | -0.67 | -0.75 | -0.77 | -0.79 | -0.79 |
| Sec-Butyl amine | -0.64 | -0.73 | -0.76 | -0.77 | -0.78 |
| Butanol | -0.63 | -0.71 | -0.74 | -0.76 | -0.76 |
| Ethyleneglycol | -0.64 | -0.73 | -0.76 | -0.78 | -0.78 |
| Phenol | -0.6 | -0.69 | -0.72 | -0.73 | -0.74 |
| Quinol | -0.58 | -0.67 | -0.7 | -0.71 | -0.72 |
| 1-Butyne | -0.66 | -0.74 | -0.77 | -0.78 | -0.79 |
| Butadine | -0.39 | -0.81 | -0.83 | -0.83 | -0.84 |
| 1,4-Cyclohexadine | -0.66 | -0.75 | -0.78 | -0.79 | -0.79 |
| Benzene | -0.67 | -0.75 | -0.77 | -0.78 | -0.79 |
| Naphthalene | -0.1 | -0.55 | -0.76 | -0.77 | -0.77 |
| Acridine | 0.93 | 0.53 | 0.31 | 0.17 | 0.08 |
| Azulene | 0.81 | 0.46 | 0.28 | 0.18 | 0.1 |
| Furan | -0.7 | -0.76 | -0.78 | -0.79 | -0.79 |
| Thiophene | -0.7 | -0.76 | -0.78 | -0.79 | -0.79 |
| Pyridine | -0.44 | -0.65 | -0.67 | -0.68 | -0.68 |
| Indole | -0.52 | -0.59 | -0.62 | -0.63 | -0.64 |
| Quinoline | 0.31 | -0.15 | -0.41 | -0.57 | -0.68 |
| Carbazole | -0.33 | -0.62 | -0.65 | -0.66 | -0.66 |
| Benzonitrile | 0.29 | -0.2 | -0.46 | -0.55 | -0.55 |
| meta Cyano Benzonitrile | 1.08 | 0.61 | 0.35 | 0.21 | 0.11 |
| TCNE | 3.24 | 3.24 | 2.99 | 3.24 | 3.24 |
| Fumeronitrile | 1.84 | 1.27 | 0.93 | 0.73 | 0.6 |
| Benzoquinone | 2.36 | 1.78 | 1.43 | 1.21 | 1.08 |
| F4- Benzoquinone | 3.01 | 2.49 | 2.18 | 1.99 | 1.87 |
| Benzaldehyde | 0.62 | 0.08 | -0.23 | -0.42 | -0.54 |
| Maleic Anhydride | 1.92 | 1.31 | 0.94 | 0.72 | 0.58 |
| Pthalimide | 1.12 | 0.61 | 0.32 | 0.14 | 0.03 |

**Table 10. Negative LUMO energies at various range separation parameters (0.20, 0.30, 0.40, 0.50, 0.60 bohr-1) with LC-ωPBE//ATZ. (30 compounds).**

**Table 11. Default and tuned (ω) based on eq. 5 IP, EA and FG (∆SCF) of LC-BLYP//ATZ. (30 compounds).**

|  |  |  |  |
| --- | --- | --- | --- |
|   | **Default ω** |  | **Tuned ω** |
|   | **IP** | **EA** | **FG** |   | **IP** | **EA** | **FG** |
| Butyl amine | 9.4 | -0.66 | 10.06 |   | 9.37 | -0.64 | 10.01 |
| Cyclohexyl amine | 9.25 | -0.65 | 9.9 |   | 9.19 | -0.61 | 9.8 |
| Dimethyl amine | 9.73 | -0.61 | 10.34 |   | 9.6 | -0.59 | 10.19 |
| Sec-Butyl amine | 9.33 | -0.66 | 9.99 |   | 9.29 | -0.63 | 9.92 |
| Butanol | 10.71 | -0.64 | 11.35 |   | 10.59 | -0.62 | 11.21 |
| Ethyleneglycol | 11.22 | -0.68 | 11.9 |   | 11.22 | -0.68 | 11.9 |
| Phenol | 9.19 | -0.61 | 9.8 |   | 9.14 | -0.55 | 9.69 |
| Quinol | 8.97 | -0.53 | 9.5 |   | 8.91 | -0.66 | 9.57 |
| 1-Butyne | 10.33 | -0.68 | 11.01 |   | 10.29 | -0.65 | 10.94 |
| Butadine | 9.15 | -0.76 | 9.91 |   | 9.15 | -0.95 | 10.1 |
| 1,4-Cyclohexadine | 9.09 | -0.69 | 9.78 |   | 8.87 | -0.65 | 9.52 |
| Benzene | 9.45 | -0.69 | 10.14 |   | 9.45 | -0.88 | 10.33 |
| Naphthalene | 8.34 | -0.68 | 9.02 |   | 8.15 | -0.37 | 8.52 |
| Acridine | 8.15 | 0.66 | 7.49 |   | 7.83 | 0.78 | 7.05 |
| Azulene | 7.35 | 0.72 | 6.63 |   | 7.38 | 0.63 | 6.75 |
| Furan | 9.1 | -0.7 | 9.8 |   | 9.09 | -0.68 | 9.77 |
| Thiophene | 9.42 | -0.7 | 10.12 |   | 9.43 | -0.69 | 10.12 |
| Pyridine | 9.73 | -0.57 | 10.3 |   | 9.68 | -0.9 | 10.58 |
| Indole | 8.04 | -0.48 | 8.52 |   | 7.9 | -0.42 | 8.32 |
| Quinoline | 8.85 | -0.1 | 8.95 |   | 8.68 | 0.02 | 8.66 |
| Carbazole | 7.87 | -0.49 | 8.36 |   | 7.67 | -0.51 | 8.18 |
| Benzonitrile | 9.99 | -0.43 | 10.42 |   | 9.83 | -0.09 | 9.92 |
| meta Cyano Benzonitrile | 10.56 | 0.72 | 9.84 |   | 10.3 | 0.76 | 9.54 |
| TCNE | 12.19 | 3.39 | 8.8 |   | 11.73 | 3.32 | 8.41 |
| Fumeronitrile | 11.52 | 1.21 | 10.31 |   | 11.32 | 1.24 | 10.08 |
| Benzoquinone | 10.94 | 1.7 | 9.24 |   | 10.5 | 1.79 | 8.71 |
| F4- Benzoquinone | 11.28 | 2.51 | 8.77 |   | 10.89 | 2.53 | 8.36 |
| Benzaldehyde | 9.91 | 0.1 | 9.81 |   | 9.72 | 0.19 | 9.53 |
| Maleic Anhydride | 11.89 | 1.21 | 10.68 |   | 11.59 | 1.26 | 10.33 |
| Pthalimide | 10.17 | 0.68 | 9.49 |   | 10 | 0.77 | 9.23 |

**Table 12.** **Default and tuned (ω) based on eq. 5 IP, EA and FG (∆SCF) of ωB97XD//ATZ. (30 compounds).**

|  |  |  |  |
| --- | --- | --- | --- |
|   |   **Default ω**  |   |   **Tuned ω**  |
|   | **IP** | **EA** | **FG** |   | **IP** | **EA** | **FG** |
| Butyl amine | 9.29 | -0.64 | 9.93 |   | 9.41 | -0.64 | 10.05 |
| Cyclohexyl amine | 9.12 | -0.63 | 9.75 |   | 9.22 | -0.63 | 9.85 |
| Dimethyl amine | 8.82 | -0.69 | 9.51 |   | 9.72 | -0.6 | 10.32 |
| Sec-Butyl amine | 9.17 | -0.65 | 9.82 |   | 9.27 | -0.65 | 9.92 |
| Butanol | 10.51 | -0.63 | 11.14 |   | 10.64 | -0.62 | 11.26 |
| Ethyleneglycol | 10.57 | -0.69 | 11.26 |   | 11.28 | -0.69 | 11.97 |
| Phenol | 9.01 | -0.59 | 9.6 |   | 9.06 | -0.59 | 9.65 |
| Quinol | 8.78 | -0.7 | 9.48 |   | 8.83 | -0.63 | 9.46 |
| 1-Butyne | 10.11 | -0.65 | 10.76 |   | 10.25 | -0.65 | 10.9 |
| Butadine | 8.92 | -0.99 | 9.91 |   | 9.02 | -0.98 | 10 |
| 1,4-Cyclohexadine | 8.72 | -0.71 | 9.43 |   | 8.88 | -0.7 | 9.58 |
| Benzene | 9.28 | -0.83 | 10.11 |   | 9.34 | -0.69 | 10.03 |
| Naphthalene | 8.06 | -0.5 | 8.56 |   | 8.08 | -0.49 | 8.57 |
| Acridine | 7.81 | 0.67 | 7.14 |   | 7.79 | 0.66 | 7.13 |
| Azulene | 7.28 | 0.54 | 6.74 |   | 7.27 | 0.52 | 6.75 |
| Furan | 8.88 | -0.68 | 9.56 |   | 8.98 | -0.68 | 9.66 |
| Thiophene | 9.34 | -0.68 | 10.02 |   | 9.45 | -0.67 | 10.12 |
| Pyridine | 9.56 | -1.01 | 10.57 |   | 9.62 | -0.54 | 10.16 |
| Indole | 7.8 | -0.44 | 8.24 |   | 7.86 | -0.44 | 8.3 |
| Quinoline | 9.27 | -0.1 | 9.37 |   | 9.5 | -0.53 | 10.03 |
| Carbazole | 7.61 | -0.63 | 8.24 |   | 7.59 | -0.64 | 8.23 |
| Benzonitrile | 9.72 | -0.2 | 9.92 |   | 9.78 | -0.18 | 9.96 |
| meta Cyano Benzonitrile | 10.22 | 0.67 | 9.55 |   | 10.27 | 0.68 | 9.59 |
| TCNE | 11.61 | 3.25 | 8.36 |   | 11.76 | 3.3 | 8.46 |
| Fumeronitrile | 11.1 | 1.15 | 9.95 |   | 11.31 | 1.19 | 10.12 |
| Benzoquinone | 10.24 | 1.69 | 8.55 |   | 10.72 | 1.71 | 9.01 |
| F4- Benzoquinone | 10.7 | 2.35 | 8.35 |   | 10.87 | 2.39 | 8.48 |
| Benzaldehyde | 9.87 | 0.06 | 9.81 |   | 9.68 | 0.08 | 9.6 |
| Maleic Anhydride | 11.2 | 1.11 | 10.09 |   | 11.72 | 1.17 | 10.55 |
| Pthalimide | 10.1 | 0.63 | 9.47 |   | 10.15 | 0.64 | 9.51 |

 [↑](#endnote-ref-2)