Supporting information for: GW100: A Slater Type Orbital Perspective

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The following three tables contain additional information on the calculation we have performed. The first table contains the KS eigenvalues calculated with PBE, and the second and third table contain the quasi-particle energies at the aug-TZ3P and aug-QZ6P level of theory, respectively. They also list technical parameters which we have used in the calculations.

Table 1: PBE HOMO and LUMO energies at finite basis sets (all values in eV). TZ denotes aug-TZ3P and QZ denotes aug-QZ6P

| Name       | HOMO  | LUMO  |
|------------|-------|-------|
|            | TZ    | QZ    | TZ    | QZ    |
| 1 Helium   | $-15.76$ | $-15.76$ | $1.41$ | $0.34$ |
| 2 Neon     | $-13.36$ | $-13.35$ | $0.59$ | $-0.02$ |
| 3 Argon    | $-10.29$ | $-10.29$ | $0.29$ | $-0.28$ |
| 4 Krypton  | $-9.30$  | $-9.28$ | $-0.16$ | $-0.40$ |
| 5 Xenon    | $-8.30$  | $-8.29$ | $-0.30$ | $-0.43$ |
| 6 Hydrogen | $-10.39$ | $-10.38$ | $0.29$ | $0.26$ |
| 7 Lithiumdimer | $-3.23$ | $-3.22$ | $-1.79$ | $-1.79$ |
| 8 Sodiumdimer | $-3.13$ | $-3.13$ | $-1.78$ | $-1.78$ |
| 9 Sodiumtetramer | $-2.68$ | $-2.68$ | $-2.09$ | $-2.09$ |
| 10 Sodiumhexamer | $-2.99$ | $-2.99$ | $-1.89$ | $-1.89$ |
| 11 Dipotassium | $-2.56$ | $-2.56$ | $-1.61$ | $-1.61$ |
| 12 Dirubidium | $-2.44$ | $-2.44$ | $-1.54$ | $-1.54$ |
| 13 Nitrogen | $-10.27$ | $-10.27$ | $-1.96$ | $-1.96$ |
| 14 Phosphorusdimer | $-7.14$ | $-7.13$ | $-3.43$ | $-3.43$ |
| 15 Arsenicedimer | $-6.59$ | $-6.57$ | $-3.45$ | $-3.44$ |
| 16 Fluorine | $-9.46$  | $-9.45$ | $-5.82$ | $-5.80$ |
| 17 Chlorine | $-7.30$  | $-7.31$ | $-4.24$ | $-4.24$ |

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| Name                | HOMO  | LUMO  |
|---------------------|-------|-------|
|                     | TZ    | QZ    | TZ    | QZ    |
| 18 Bromine          | −6.86 | −6.85 | −4.48 | −6.46 |
| 19 Iodine           | −6.34 | −6.33 | −4.33 | −4.32 |
| 20 Methane          | −9.46 | −9.46 | −0.39 | −0.39 |
| 21 Ethane           | −8.16 | −8.16 | −0.44 | −0.45 |
| 22 Propane          | −7.76 | −7.76 | −0.48 | −0.49 |
| 23 Butane           | −7.58 | −7.58 | −0.49 | −0.50 |
| 24 Ethylene         | −6.78 | −6.78 | −1.07 | −1.07 |
| 25 Acetylene        | −7.20 | −7.20 | −0.42 | −0.42 |
| 26 Tetracarbon      | −7.27 | −7.26 | −6.12 | −6.11 |
| 27 Cyclopropane     | −7.05 | −7.05 | −0.34 | −0.36 |
| 28 Benzene          | −6.34 | −6.34 | −1.26 | −1.25 |
| 29 Cyclooctatetraene| −5.31 | −5.30 | −2.32 | −2.32 |
| 30 Cyclopentadiene  | −5.41 | −5.41 | −1.49 | −1.49 |
| 31 Vinyl fluoride   | −6.55 | −6.55 | −0.97 | −0.97 |
| 32 Vinyl chloride   | −6.44 | −6.44 | −1.43 | −1.44 |
| 33 Vinylbromide     | −5.86 | −5.85 | −1.37 | −1.37 |
| 34 Vinyl fluoride   | −6.10 | −6.09 | −1.71 | −1.70 |
| 35 Carbontetrafluoride| −10.43−10.41 | −0.42 | −0.43 |
| 36 Carbontetrachloride| −7.67−7.68 | −2.78 | −2.77 |
| 37 Carbontetrafluoride| −7.00−6.99 | −3.56 | −3.53 |
| 38 Carbontetrabromide| −6.29−6.28 | −4.29 | −4.28 |
| 39 Silane           | −8.53 | −8.52 | −0.47 | −0.49 |
| 40 Germane          | −8.38 | −8.37 | −0.67 | −0.68 |
| 41 Disilane         | −7.30 | −7.29 | −0.68 | −0.69 |
| 42 Pentasilane      | −6.59 | −6.58 | −1.68 | −1.67 |
| 43 Lithium hydride  | −4.36 | −4.36 | −1.62 | −1.64 |
| 44 Potassium hydride| −3.46 | −3.46 | −1.62 | −1.62 |
| 45 Borane           | −8.50 | −8.49 | −3.07 | −3.07 |
| 46 Diborane6        | −7.87 | −7.87 | −2.04 | −2.04 |
| 47 Ethane           | −6.19 | −6.18 | −0.74 | −0.75 |
| 48 Hydrogen azide   | −6.81 | −6.80 | −2.10 | −2.10 |
| 49 Phosphine        | −6.72 | −6.72 | −0.67 | −0.67 |
| 50 Arsine           | −6.73 | −6.74 | −0.77 | −0.77 |
| 51 Hydrogensulfide  | −6.30 | −6.30 | −0.86 | −0.87 |
| 52 Hydrogen fluoride| −9.66 | −9.65 | −0.97 | −0.97 |
| 53 Hydrogen chloride| −8.04 | −8.04 | −1.12 | −1.12 |
| 54 Lithium fluoride | −6.13 | −6.13 | −1.53 | −1.52 |
| 55 Magnesium fluoride| −8.30−8.30 | −2.58 | −2.58 |
| 56 Titanium fluoride| −10.45−10.44 | −4.19 | −4.19 |
| 57 Aluminum fluoride| −9.72−9.71 | −2.54 | −2.54 |
| 58 Fluoroborane     | −6.79 | −6.78 | −2.15 | −2.14 |
| 59 Sulfetetrafluoride| −8.25 | −8.24 | −2.97 | −2.96 |
| 60 Potassium bromide| −4.76 | −4.76 | −1.87 | −1.87 |
| 61 Gallium monochloride| −6.53−6.53 | −2.44 | −2.43 |
| 62 Sodium chloride  | −5.29 | −5.29 | −2.24 | −2.24 |
| 63 Magnesium chloride| −7.63−7.63 | −2.55 | −2.54 |
| 64 Aluminum triiodide| −6.72−6.71 | −2.71 | −2.71 |
| 65 Boron nitride    | −7.46 | −7.46 | −7.29 | −7.29 |
| 66 Hydrogen cyanide | −9.04 | −9.04 | −1.11 | −1.11 |
| 67 Phosphorous mononitride| −7.77−7.76 | −3.41 | −3.40 |
| 68 Hydrazene        | −5.30 | −5.30 | −0.96 | −0.96 |
| 69 Formaldehyde     | −6.28 | −6.27 | −2.71 | −2.71 |
| 70 Methanol         | −6.35 | −6.35 | −0.65 | −0.66 |

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| Name                  | HOMO | LUMO |
|----------------------|------|------|
|                      | TWZ  | TQZ  | TWZ  | TQZ  |
| Ethanol              | -6.16| -6.16| -0.67| -0.68|
| Acetaldehyde         | -5.98| -5.98| -2.16| -2.16|
| Ethoxethane          | -5.81| -5.80| -0.51| -0.53|
| Formic Acid          | -6.95| -6.94| -1.56| -1.56|
| Hydrogenperoxide     | -6.46| -6.45| -1.69| -1.68|
| Water                | -7.26| -7.25| -0.94| -0.93|
| Carbon dioxide       | -9.10| -9.09| -0.91| -0.95|
| Carbon disulfide     | -6.81| -6.80| -2.86| -2.86|
| Carbonoxysulfide     | -7.49| -7.48| -1.95| -1.95|
| Carbonoxyselenide    | -6.99| -6.98| -2.07| -2.07|
| Carbon monoxide      | -9.35| -9.34| -3.35| -3.35|
| Ozon                 | -7.96| -7.96| -6.16| -6.16|
| Sulfur dioxide       | -8.09| -8.08| -4.41| -4.40|
| Beryllium monoxide   | -6.14| -6.14| -4.81| -4.81|
| Magnesium monoxide   | -4.80| -4.80| -4.29| -4.29|
| Toluene              | -6.01| -6.01| -1.23| -1.23|
| Ethylbenzene         | -6.01| -6.01| -1.16| -1.16|
| Hexafluorobenzene    | -6.66| -6.66| -2.22| -2.22|
| Phenol               | -5.64| -5.64| -1.37| -1.36|
| Aniline              | -5.03| -5.03| -1.12| -1.12|
| Pyridine             | -5.96| -5.95| -1.91| -1.90|
| Guanine              | -5.30| -5.29| -1.43| -1.43|
| Adenine              | -5.53| -5.53| -1.71| -1.71|
| Cytosine             | -5.73| -5.73| -2.07| -2.07|
| Thymine              | -6.06| -6.05| -2.29| -2.28|
| Uracil               | -6.29| -6.28| -2.45| -2.44|
| Urea                 | -5.94| -5.93| -1.01| -1.02|
| Silver dimer         | -4.75| -4.77| -2.75| -2.76|
| Silver dimer (ZORA)  | -5.21| -3.11|       |       |
| Copper dimer         | -4.78| -4.78| -2.94| -3.00|
| Copper cyanide       | -6.69| -6.72| -4.00| -4.04|

Table 2: IPs and EAs on the aug-TZ3P level of theory (in eV) and technical parameters used in the calculations: Number of grid points, number of orbitals and fit set (N = Normal, G = Good, VG = Very Good).
| Name                     | IP   | EA   | $N_o$ | $N_T$ | $N_{bas}$ | fit set |
|--------------------------|------|------|-------|-------|-----------|---------|
| Phosphorusdimer          | 9.88 | 0.38 | 20    | 20    | 96        | N       |
| Arsenicdimer             | 9.07 | 0.50 | 24    | 24    | 140       | N       |
| Fluorine                 | 14.62| -0.14| 17    | 17    | 80        | N       |
| Chlorine                 | 10.73| 0.33 | 21    | 21    | 96        | N       |
| Bromine                  | 9.91 | 0.90 | 24    | 24    | 140       | N       |
| Iodine                   | 9.01 | 1.28 | 27    | 29    | 200       | N       |
| Methane                  | 13.80| -0.97| 14    | 14    | 112       | VG      |
| Ethane                   | 12.23| -0.96| 15    | 15    | 188       | VG      |
| Propane                  | 11.64| -0.92| 15    | 15    | 264       | VG      |
| Buthane                  | 11.37| -0.89| 15    | 15    | 340       | VG      |
| Ethylene                 | 10.09| -2.12| 16    | 16    | 152       | VG      |
| Acetylene                | 10.83| -2.76| 16    | 16    | 116       | VG      |
| Tetracarbon              | 10.56| 2.27 | 19    | 19    | 160       | G       |
| Cyclopropane             | 10.39| -0.98| 16    | 16    | 228       | VG      |
| Benzene                  | 8.82 | -1.26| 17    | 17    | 348       | G       |
| Cyclooctatetraene        | 7.92 | -0.30| 18    | 18    | 464       | G       |
| Cyclopentadiene          | 8.13 | -1.17| 18    | 18    | 308       | G       |
| Vinylfluoride            | 9.98 | -2.21| 18    | 18    | 174       | G       |
| Vinylchloride            | 9.48 | -1.61| 20    | 20    | 182       | G       |
| Vinylbromide             | 8.76 | -1.50| 23    | 23    | 204       | N       |
| Vinylidolide             | 8.82 | -1.06| 27    | 32    | 234       | N       |
| Carbbontetrafluoride     | 15.10| -0.92| 16    | 16    | 200       | G       |
| Carbontetrachloride      | 10.68| -0.41| 20    | 20    | 232       | G       |
| Carbontetra bromide      | 9.64 | 0.62 | 24    | 24    | 320       | N       |
| Carbontetraiodide        | 8.63 | 1.64 | 27    | 31    | 440       | N       |
| Silane                   | 12.17| -0.92| 17    | 17    | 120       | VG      |
| Germane                  | 11.85| -1.00| 22    | 22    | 143       | G       |
| Disilane                 | 10.11| -0.93| 18    | 18    | 204       | G       |
| Pentasilane              | 8.73 | -0.39| 19    | 19    | 456       | G       |
| Lithiumhydride           | 5.98 | -0.02| 16    | 16    | 55        | N       |
| Potassiumhydride         | 4.83 | 0.06 | 23    | 23    | 76        | N       |
| Borane                   | 12.68| -0.48| 15    | 15    | 94        | G       |
| Diborane6                | 11.75| -1.07| 16    | 16    | 188       | G       |
| Amonia                   | 10.00| -0.93| 17    | 17    | 94        | G       |
| Hydrogenazide            | 10.16| -1.67| 16    | 16    | 138       | G       |
| Phosphine                | 9.99 | -0.84| 19    | 19    | 102       | G       |
| Arsine                   | 9.87 | -0.84| 22    | 22    | 124       | G       |
| Hydrogensulfide          | 9.73 | -0.94| 19    | 19    | 84        | N       |
| Hydrogenfluoride         | 14.88| -1.22| 16    | 16    | 58        | N       |
| Hydrogenchloride         | 11.81| -1.38| 19    | 19    | 66        | N       |
| Lithiumfluoride          | 9.80 | -0.08| 15    | 15    | 77        | N       |
| Magnesiumfluoride        | 12.16| 0.08 | 17    | 17    | 128       | N       |
| Titaniumfluoride         | 13.67| -0.89| 20    | 20    | 223       | N       |
| Aluminumtrifluoride      | 14.94| -0.21| 18    | 18    | 168       | G       |
| Fluoroborane             | 10.21| -1.49| 16    | 16    | 80        | N       |
| Sulfetetrafluoride       | 11.78| -0.73| 19    | 19    | 208       | G       |
| Potassiumbromide         | 7.24 | 0.23 | 24    | 24    | 128       | N       |
| Galliummonochloride      | 9.28 | -0.24| 24    | 24    | 119       | N       |
| Sodiumchloride           | 8.02 | 0.30 | 21    | 21    | 93        | N       |
| Magnesiumchloride        | 10.67| 0.27 | 19    | 19    | 144       | N       |
| Aluminumtrioiodide       | 9.17 | 0.39 | 27    | 30    | 348       | N       |
| Boronitrile             | 10.95| 3.09 | 24    | 24    | 80        | N       |
| Hydrogencyanide         | 13.01| -2.59| 14    | 14    | 98        | N       |
| Phosphorusmononitride    | 10.91| -0.16| 19    | 19    | 88        | N       |

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| Name         | IP   | EA    | $N_\omega$ | $N_T$ | $N_{bas}$ | fit set |
|--------------|------|-------|------------|-------|-----------|---------|
| Hydrazene    | 8.94 | -0.82 | 18         | 18    | 152       | G       |
| Formaldehyde | 10.13| -1.34 | 19         | 19    | 116       | G       |
| Methanol     | 10.32| -1.05 | 18         | 18    | 152       | VG      |
| Ethanol      | 9.89 | -0.97 | 18         | 18    | 228       | VG      |
| Acetaldehyde | 9.36 | -1.43 | 19         | 19    | 192       | VG      |
| Ethoxyethane | 9.12 | -0.83 | 17         | 17    | 380       | VG      |
| Formalic Acid| 10.46| -2.12 | 18         | 18    | 156       | G       |
| Hydrogen peroxide | 10.69 | -2.38 | 18         | 18    | 116       | G       |
| Water        | 11.50| -1.02 | 18         | 18    | 76        | N       |
| Carbon dioxide | 13.05 | -1.03 | 17         | 17    | 120       | N       |
| Carbon disulfide | 9.42    | -0.17 | 19         | 19    | 136       | N       |
| Carbon oxysulfide | 10.62     | -1.52  | 19         | 19    | 128       | N       |
| Carbon oxyselenide | 9.88       | -1.25  | 24         | 24    | 151       | N       |
| Carbon monoxide | 13.23   | -1.16  | 18         | 18    | 80        | N       |
| Ozon         | 11.63 | 1.70  | 20         | 20    | 120       | N       |
| Sulfurdioxide | 11.61 | 0.58  | 20         | 20    | 128       | N       |
| Beryllium monoxide | 9.16    | 1.85   | 20         | 20    | 80        | N       |
| Magnesium monoxide | 6.76 | 1.55   | 23         | 23    | 88        | N       |
| Tuleone      | 8.48  | -1.15 | 18         | 18    | 424       | G       |
| Ethyl benzene | 8.33  | -1.17 | 17         | 17    | 500       | G       |
| Hexafluoro benzene | 9.26     | -0.46  | 17         | 17    | 480       | G       |
| Phenol       | 8.21  | -1.13 | 17         | 17    | 388       | G       |
| Aniline      | 7.49  | -1.30 | 18         | 18    | 406       | G       |
| Pyridine     | 8.82  | -0.77 | 16         | 16    | 330       | G       |
| Guanine      | 7.55  | -0.87 | 19         | 19    | 530       | VG      |
| Adenine      | 7.77  | -0.66 | 18         | 18    | 490       | G       |
| Cytosine     | 8.04  | -0.56 | 19         | 19    | 410       | G       |
| Thymine      | 8.51  | -0.36 | 19         | 19    | 468       | G       |
| Uracil       | 9.03  | -0.34 | 19         | 19    | 392       | VG      |
| Urea         | 8.99  | -0.64 | 18         | 18    | 232       | G       |
| Silver dimer | 6.99  | 0.70  | 27         | 31    | 178       | N       |
| Copper dimer | 7.13  | 0.64  | 24         | 24    | 126       | N       |
| Copper selenide | 9.58   | 1.08   | 24         | 24    | 143       | N       |
Table 3: IPs and EAs on the aug-QZ6P level of theory (in eV) and technical parameters used in the calculations: Number of grid points, number of orbitals and fit set (N = Normal, G = Good, VG = VeryGood).

| Name           | IP   | EA   | \(N_\omega\) | \(N_{\tau}\) | \(N\text{bas}\) | fit set |
|----------------|------|------|--------------|--------------|----------------|---------|
| 1 Helium       | 23.28| −0.84| 14           | 14           | 33             | N       |
| 2 Neon         | 20.08| −1.22| 19           | 19           | 68             | N       |
| 3 Argon        | 14.81| −0.82| 24           | 24           | 82             | N       |
| 4 Krypton      | 13.41| −0.75| 27           | 31           | 120            | N       |
| 5 Xenon        | 11.76| −0.68| 27           | 32           | 150            | N       |
| 6 Hydrogen     | 15.72| −0.90| 14           | 14           | 66             | N       |
| 7 Lithiumdimer | 4.90 | 0.43 | 18           | 18           | 128            | N       |
| 8 Sodiumdimer  | 4.79 | 0.50 | 24           | 24           | 146            | N       |
| 9 Sodiumtetramer| 4.19 | 0.92 | 24           | 24           | 292            | N       |
| 10 Sodiumhexamer| 4.24 | 0.95 | 24           | 24           | 438            | N       |
| 11 Dipotassium | 3.93 | 0.53 | 24           | 24           | 198            | N       |
| 12 Dirubidium  | 3.76 | 0.59 | 27           | 28           | 274            | N       |
| 13 Nitrogen    | 14.71| −2.54| 18           | 18           | 140            | N       |
| 14 Phosphorusdimer| 10.05| 0.49| 24           | 24           | 172            | N       |
| 15 Arsenicdimer| 9.28 | 0.74 | 24           | 24           | 238            | N       |
| 16 Fluorine    | 14.78| 0.15 | 21           | 21           | 140            | N       |
| 17 Chlorine    | 10.93| 0.56 | 24           | 24           | 174            | N       |
| 18 Bromine     | 10.15| 1.12 | 27           | 32           | 248            | N       |
| 19 Iodine      | 9.02 | 1.36 | 27           | 31           | 274            | N       |
| 20 Methane     | 13.84| −0.89| 17           | 17           | 196            | VG      |
| 21 Ethane      | 12.28| −0.88| 18           | 18           | 326            | VG      |
| 22 Propane     | 11.73| −0.83| 18           | 18           | 456            | VG      |
| 23 Butane      | 11.44| −0.81| 18           | 18           | 586            | VG      |
| 24 Ethylene    | 10.17| −2.03| 18           | 18           | 260            | VG      |
| 25 Acetylene   | 10.95| −2.65| 17           | 17           | 194            | VG      |
| 26 Tetracarbon | 10.63| 2.40 | 22           | 22           | 256            | G       |
| 27 Cyclopropane| 10.49| −0.88| 18           | 18           | 390            | VG      |
| 28 Benzene     | 8.92 | −1.14| 19           | 19           | 582            | G       |
| 29 Cyclooctetraene| 8.01 | −0.17| 20           | 20           | 776            | G       |
| 30 Cyclopentadiene| 8.25 | −1.07| 19           | 19           | 518            | G       |
| 31 Vinylfluoride| 10.09| −2.09| 20           | 20           | 297            | G       |
| 32 Vinylchloride| 9.62 | −1.49| 24           | 24           | 314            | G       |
| 33 Vinylbromide| 8.87 | −1.39| 27           | 32           | 351            | N       |
| 34 Viniliodide | 8.86 | −0.95| 27           | 32           | 372            | N       |
| 35 Carbontetrafluoride| 15.24| −0.90| 19           | 19           | 344            | G       |
| 36 Carbontetracloride| 10.93| −0.21| 24           | 24           | 412            | G       |
| 37 Carbontetrahalide| 9.81 | 0.78 | 27           | 29           | 560            | N       |
| 38 Carbontetraiodide| 8.66 | 1.81| 27           | 32           | 644            | N       |
| 39 Silane      | 12.26| −0.83| 22           | 22           | 213            | VG      |
| 40 Germane     | 11.95| −0.77| 24           | 24           | 251            | G       |
| 41 Disilane    | 10.26| −0.85| 24           | 24           | 360            | G       |
| 42 Pentasilane | 8.88 | −0.26| 24           | 24           | 801            | G       |
| 43 Lithiumhydride| 6.21 | 0.01 | 14           | 14           | 97             | N       |
| 44 Potassiumhydride| 4.85 | 0.11| 24           | 24           | 132            | N       |
| 45 Borane      | 12.78| −0.39| 17           | 17           | 163            | G       |
| 46 Diborane6   | 11.83| −0.99| 18           | 18           | 326            | G       |
| 47 Amonia      | 10.12| −0.85| 19           | 19           | 169            | G       |
| 48 Hydrogenazide| 10.28| −1.55| 19           | 19           | 243            | G       |
| 49 Phosphine   | 10.12| −0.76| 24           | 24           | 185            | G       |

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| Name                   | IP   | EA   | $N_ω$ | $N_τ$ | $N_{bas}$ | fit set |
|------------------------|------|------|-------|-------|-----------|---------|
| Arsine                 | 10.06| -0.73| 24    | 24    | 218       | G       |
| Hydrogensulfide        | 9.90 | -0.85| 24    | 24    | 148       | N       |
| Hydrogenfluoride       | 14.99| -1.15| 19    | 19    | 103       | N       |
| Hydrogenchloride       | 12.06| -1.30| 24    | 24    | 120       | N       |
| Lithiumfluoride        | 9.90 | -0.06| 21    | 21    | 134       | N       |
| Magnesiumfluoride      | 12.27| 0.15 | 20    | 20    | 213       | N       |
| Titaniumfluoride       | 13.78| -0.48| 27    | 27    | 384       | N       |
| Aluminumtrifluoride    | 14.16| -0.10| 22    | 22    | 291       | G       |
| Fluoroborane           | 10.36| -1.38| 21    | 21    | 134       | N       |
| Sulfertetrafluoride    | 12.02| -0.55| 24    | 24    | 362       | G       |
| Potassiumbromide       | 7.50 | 0.27 | 27    | 32    | 223       | N       |
| Galliummonochloride    | 9.50 | -0.13| 24    | 24    | 206       | N       |
| Sodiumchloride         | 8.14 | 0.35 | 24    | 24    | 160       | N       |
| Magnesiumchloride      | 10.84| 0.44 | 24    | 24    | 247       | N       |
| Aluminumtriiodide      | 9.24 | 0.64 | 27    | 31    | 516       | N       |
| Borontritridioxide     | 10.95| 3.47 | 24    | 24    | 134       | N       |
| Hydrogencyanide        | 13.05| -2.48| 17    | 17    | 167       | N       |
| Phosphorusmononitride  | 10.99| -0.04| 24    | 24    | 156       | N       |
| Hydrazene              | 9.14 | -0.77| 19    | 19    | 272       | G       |
| Formaldehyde           | 10.26| -1.22| 21    | 21    | 195       | G       |
| Methanol               | 10.41| -0.95| 19    | 19    | 261       | VG      |
| Ethanol                | 10.01| -0.87| 20    | 20    | 391       | VG      |
| Acetaldehyde           | 9.46 | -1.32| 21    | 21    | 325       | VG      |
| Ethoxyethane           | 9.24 | -0.74| 20    | 20    | 651       | VG      |
| Formic Acid            | 10.61| -2.00| 20    | 20    | 260       | G       |
| Hydrogenperoxide       | 10.80| -2.25| 19    | 19    | 196       | G       |
| Water                  | 11.69| -0.96| 19    | 19    | 131       | N       |
| Carbon dioxide         | 13.17| -1.03| 19    | 19    | 194       | N       |
| Carbon disulfide       | 9.58 | -0.06| 24    | 24    | 228       | N       |
| Carbonoxysulfide       | 10.73| -1.40| 24    | 24    | 211       | N       |
| Carbonoxyselenide      | 10.08| -1.13| 24    | 24    | 248       | N       |
| Carbon monoxide        | 13.39| -1.04| 20    | 20    | 129       | N       |
| Ozon                   | 11.67| 1.83 | 23    | 23    | 195       | N       |
| Sulfur dioxide         | 11.71| 0.69 | 24    | 24    | 212       | N       |
| Beryllium monoxide     | 9.10 | 1.90 | 23    | 23    | 129       | N       |
| Magnesium monoxide     | 6.78 | 1.62 | 24    | 24    | 138       | N       |
| Toluene                | 8.58 | -1.05| 19    | 19    | 712       | G       |
| Ethylbenzene           | 8.46 | -1.05| 19    | 19    | 842       | G       |
| Hexafluorobenzene      | 9.44 | -0.29| 21    | 21    | 804       | G       |
| Phenol                 | 8.31 | -0.99| 20    | 20    | 647       | G       |
| Aniline                | 7.58 | -1.14| 20    | 20    | 685       | G       |
| Pyridine               | 8.96 | -0.64| 19    | 19    | 555       | G       |
| Guanine                | 7.64 | -0.71| 21    | 21    | 900       | VG      |
| Adenine                | 7.92 | -0.50| 20    | 20    | 835       | G       |
| Cytosine               | 8.20 | -0.40| 21    | 21    | 696       | G       |
| Thymine                | 8.65 | -0.20| 20    | 20    | 788       | G       |
| Uracil                 | 9.13 | -0.18| 21    | 21    | 658       | VG      |
| Urea                   | 9.10 | -0.58| 20    | 20    | 401       | G       |
| Silver dimer           | 7.02 | 0.78 | 27    | 31    | 284       | N       |
| Copper dimer           | 7.56 | 0.78 | 27    | 32    | 210       | N       |
| Coppercyanide          | 9.85 | 1.24 | 27    | 29    | 239       | N       |
Table 4: Ionization potentials and electron affinities for the subset of 250 molecules from the GW5000 database using TZ3P and QZ6P basis sets as well as complete basis set limit extrapolated values. All values are in eV.

| Name | TZ3P | IP | QZ6P | extra | TZ3P | EA | QZ6P | extra |
|------|------|----|------|-------|------|----|------|-------|
| 16   | 7.20 | 7.39 | 7.63 | −0.20 | 0.05 | 0.36 |
| 212  | 8.01 | 8.14 | 8.30 | 0.34  | 0.59 | 0.90 |
| 389  | 8.29 | 8.46 | 8.66 | 0.33  | 0.55 | 0.84 |
| 584  | 10.50| 10.43| 10.60| 1.44  | 1.65 | 1.92 |
| 964  | 8.16 | 8.22 | 8.30 | 0.27  | 0.50 | 0.78 |
| 1145 | 7.30 | 7.48 | 7.69 | 0.51  | 0.73 | 1.01 |
| 1304 | 8.58 | 8.70 | 8.86 | 1.27  | 1.44 | 1.65 |
| 1415 | 7.83 | 8.00 | 8.22 | −0.30 | −0.02| 0.33 |
| 1627 | 7.50 | 7.70 | 7.95 | 1.34  | 1.56 | 1.84 |
| 1761 | 8.05 | 8.24 | 8.48 | 0.12  | 0.35 | 0.65 |
| 1942 | 7.77 | 7.92 | 8.10 | −0.29 | −0.05| 0.24 |
| 2142 | 8.07 | 8.26 | 8.49 | 0.57  | 0.82 | 1.14 |
| 2403 | 7.14 | 7.32 | 7.54 | 0.65  | 0.86 | 1.12 |
| 2686 | 7.71 | 7.87 | 8.08 | 1.16  | 1.38 | 1.66 |
| 2869 | 8.58 | 8.71 | 8.86 | 0.80  | 1.00 | 1.25 |
| 3133 | 10.76| 10.90| 11.06| 1.51  | 1.74 | 2.03 |
| 3387 | 7.51 | 7.68 | 7.88 | 0.50  | 0.73 | 1.01 |
| 3793 | 8.71 | 8.88 | 9.08 | −0.06 | 0.20 | 0.53 |
| 4002 | 7.93 | 8.06 | 8.23 | 2.01  | 2.20 | 2.45 |
| 4257 | 8.23 | 8.32 | 8.45 | −0.10 | 0.17 | 0.54 |
| 4465 | 7.87 | 8.09 | 8.36 | 0.32  | 0.56 | 0.86 |
| 4727 | 7.73 | 7.92 | 8.16 | −0.18 | 0.07 | 0.37 |
| 4986 | 8.52 | 8.64 | 8.80 | −0.17 | 0.13 | 0.51 |
| 5179 | 7.16 | 7.34 | 7.58 | 0.83  | 1.07 | 1.37 |
| 5330 | 8.28 | 8.47 | 8.70 | 0.35  | 0.57 | 0.84 |
| 5760 | 10.49| 10.61| 10.75| 0.13  | 0.41 | 0.74 |
| 5948 | 6.73 | 6.91 | 7.14 | −0.10 | 0.17 | 0.49 |
| 6247 | 7.74 | 7.89 | 8.08 | −0.08 | 0.17 | 0.47 |
| 6527 | 8.48 | 8.65 | 8.87 | 1.00  | 1.23 | 1.53 |
| 6838 | 8.71 | 8.87 | 9.08 | −0.13 | 0.10 | 0.39 |
| 7071 | 7.37 | 7.53 | 7.72 | 0.17  | 0.40 | 0.68 |
| 7348 | 8.07 | 8.33 | 8.66 | −0.18 | 0.05 | 0.33 |
| 7474 | 8.14 | 8.32 | 8.54 | 0.45  | 0.68 | 0.96 |
| 7729 | 8.66 | 8.80 | 8.96 | 0.64  | 0.86 | 1.14 |
| 7902 | 8.04 | 8.26 | 8.52 | 0.07  | 0.35 | 0.70 |
| 8115 | 7.90 | 8.08 | 8.29 | 0.53  | 0.78 | 1.10 |
| 8314 | 8.88 | 9.06 | 9.27 | −0.26 | 0.01 | 0.34 |
| 8509 | 8.93 | 9.10 | 9.32 | 0.19  | 0.42 | 0.71 |
| 8740 | 7.93 | 8.12 | 8.36 | −0.02 | 0.26 | 0.62 |
| 9040 | 6.85 | 6.97 | 7.12 | −0.22 | −0.04| 0.19 |
| 9202 | 8.11 | 8.28 | 8.48 | 0.91  | 1.10 | 1.33 |
| 9538 | 8.36 | 8.55 | 8.79 | 1.27  | 1.48 | 1.73 |
| 9844 | 8.35 | 8.48 | 8.64 | 0.08  | 0.36 | 0.71 |
| 10214| 10.05| 10.20| 10.38| 2.06  | 2.25 | 2.48 |
| 10450| 7.64 | 7.79 | 7.97 | 0.05  | 0.30 | 0.60 |
| 10698| 9.21 | 9.41 | 9.65 | 0.54  | 0.78 | 1.08 |
| 10978| 7.17 | 7.35 | 7.57 | −0.10 | 0.15 | 0.46 |
| 11151| 7.89 | 8.05 | 8.25 | 0.55  | 0.77 | 1.05 |
| 11403| 11.14| 11.26| 11.41| −0.40 | −0.17| 0.12 |
| 11661| 8.33 | 8.43 | 8.56 | −0.18 | 0.07 | 0.37 |
| 12004| 7.39 | 7.58 | 7.81 | 0.15  | 0.39 | 0.70 |

Continued on next page
| Name  | TZ3P | IP QZ6P | extra | TZ3P | EA QZ6P | extra |
|-------|------|--------|-------|------|---------|-------|
| 12143 | 8.25 | 8.43   | 8.65  | 0.52 | 0.74    | 1.01  |
| 12405 | 7.89 | 8.03   | 8.20  | 0.13 | 0.37    | 0.66  |
| 12569 | 9.32 | 9.46   | 9.64  | 0.20 | 0.43    | 0.72  |
| 12919 | 7.51 | 7.72   | 7.97  | 0.18 | 0.42    | 0.73  |
| 13151 | 7.82 | 7.98   | 8.17  | -0.02| 0.21    | 0.49  |
| 13321 | 7.88 | 8.03   | 8.21  | 1.04 | 1.28    | 1.58  |
| 13505 | 7.49 | 7.66   | 7.88  | 0.17 | 0.41    | 0.70  |
| 13702 | 6.72 | 6.91   | 7.14  | -0.35| -0.06   | 0.30  |
| 13712 | 7.71 | 7.86   | 8.04  | 0.82 | 1.02    | 1.26  |
| 13722 | 7.85 | 8.05   | 8.30  | 0.29 | 0.52    | 0.80  |
| 13736 | 7.03 | 7.18   | 7.36  | 0.00 | 0.19    | 0.43  |
| 13760 | 7.17 | 7.33   | 7.54  | 0.19 | 0.46    | 0.80  |
| 14098 | 6.89 | 7.09   | 7.33  | 0.34 | 0.58    | 0.87  |
| 14226 | 7.59 | 7.78   | 8.01  | -0.06| 0.18    | 0.48  |
| 14670 | 7.98 | 8.17   | 8.41  | 0.48 | 0.73    | 1.05  |
| 14979 | 8.66 | 8.85   | 9.08  | -0.24| 0.07    | 0.47  |
| 15273 | 7.35 | 7.50   | 7.68  | 0.01 | 0.25    | 0.54  |
| 15429 | 6.40 | 6.58   | 6.80  | 0.58 | 0.84    | 1.15  |
| 15634 | 8.29 | 8.46   | 8.67  | -0.27| -0.03   | 0.27  |
| 15938 | 7.85 | 8.00   | 8.18  | 0.08 | 0.36    | 0.71  |
| 16245 | 7.45 | 7.68   | 7.96  | -0.12| 0.14    | 0.47  |
| 16444 | 8.20 | 8.39   | 8.63  | 0.62 | 0.84    | 1.11  |
| 16704 | 6.21 | 6.37   | 6.58  | 0.93 | 1.16    | 1.45  |
| 16849 | 7.78 | 7.97   | 8.19  | 0.08 | 0.32    | 0.62  |
| 16982 | 7.66 | 7.81   | 8.02  | 0.11 | 0.31    | 0.57  |
| 17264 | 7.14 | 7.30   | 7.50  | 0.78 | 1.04    | 1.37  |
| 17502 | 8.37 | 8.53   | 8.73  | 0.40 | 0.64    | 0.95  |
| 17807 | 7.46 | 7.53   | 7.62  | -0.02| 0.16    | 0.39  |
| 18111 | 7.01 | 7.14   | 7.31  | 0.15 | 0.39    | 0.69  |
| 18255 | 8.65 | 8.79   | 8.97  | 0.96 | 1.20    | 1.49  |
| 18460 | 6.97 | 7.19   | 7.46  | 0.75 | 0.98    | 1.28  |
| 18611 | 8.54 | 8.69   | 8.88  | -0.28| -0.01   | 0.33  |
| 18825 | 7.18 | 7.35   | 7.58  | 0.47 | 0.71    | 1.02  |
| 19062 | 7.57 | 7.75   | 7.98  | -0.03| 0.23    | 0.57  |
| 19347 | 8.36 | 8.45   | 8.57  | 1.64 | 1.88    | 2.18  |
| 19664 | 8.57 | 8.76   | 9.00  | 0.69 | 0.98    | 1.34  |
| 19910 | 9.48 | 9.61   | 9.77  | 1.03 | 1.27    | 1.56  |
| 20065 | 7.90 | 8.06   | 8.26  | 0.58 | 0.80    | 1.08  |
| 20311 | 8.63 | 8.78   | 8.97  | -0.17| 0.08    | 0.38  |
| 20649 | 7.67 | 7.81   | 7.99  | -0.23| 0.01    | 0.29  |
| 20821 | 8.15 | 8.33   | 8.56  | 0.82 | 1.06    | 1.36  |
| 21105 | 8.06 | 8.24   | 8.46  | 1.96 | 2.16    | 2.41  |
| 21210 | 7.92 | 8.07   | 8.26  | 0.13 | 0.37    | 0.67  |
| 21361 | 8.24 | 8.38   | 8.56  | 1.20 | 1.42    | 1.69  |
| 21611 | 6.53 | 6.69   | 6.90  | 0.50 | 0.73    | 1.02  |
| 21895 | 9.28 | 9.42   | 9.59  | 0.03 | 0.25    | 0.52  |
| 22078 | 7.20 | 7.34   | 7.53  | 1.24 | 1.47    | 1.76  |
| 22407 | 8.66 | 8.81   | 9.00  | 1.19 | 1.42    | 1.70  |
| 22699 | 8.15 | 8.29   | 8.45  | 1.19 | 1.40    | 1.66  |
| 22875 | 7.39 | 7.58   | 7.83  | -0.17| 0.07    | 0.38  |
| 23028 | 8.66 | 8.79   | 8.96  | 0.39 | 0.60    | 0.86  |
| 23303 | 7.34 | 7.48   | 7.66  | 1.31 | 1.51    | 1.76  |
| 23652 | 7.86 | 8.02   | 8.23  | 0.17 | 0.42    | 0.72  |
| 23853 | 7.41 | 7.59   | 7.81  | 0.10 | 0.34    | 0.64  |
| 24031 | 6.23 | 6.40   | 6.62  | 0.11 | 0.37    | 0.70  |
| 24201 | 6.68 | 6.87   | 7.10  | -0.19| 0.06    | 0.36  |

Continued on next page
| Name | TZ3P | IP | QZ6P | extra | TZ3P | QZ6P | extra |
|------|------|----|------|-------|------|------|-------|
| 24419 | 8.52 | 8.69 | 8.92 | -0.17 | 0.08 | 0.40 |
| 24722 | 7.11 | 7.26 | 7.46 | 0.10 | 0.33 | 0.61 |
| 24951 | 7.36 | 7.52 | 7.73 | 0.22 | 0.47 | 0.78 |
| 25240 | 9.45 | 9.64 | 9.88 | -0.14 | 0.10 | 0.41 |
| 25412 | 7.74 | 7.83 | 8.04 | 0.47 | 0.71 | 1.00 |
| 25789 | 8.60 | 8.77 | 8.98 | 0.08 | 0.32 | 0.62 |
| 25995 | 7.21 | 7.39 | 7.61 | 0.01 | 0.25 | 0.55 |
| 26246 | 7.83 | 7.99 | 8.18 | 0.69 | 0.90 | 1.17 |
| 26458 | 7.58 | 7.75 | 7.97 | -0.04 | 0.21 | 0.51 |
| 26685 | 7.82 | 7.99 | 8.20 | 0.41 | 0.65 | 0.94 |
| 26821 | 7.93 | 8.07 | 8.24 | 0.12 | 0.36 | 0.66 |
| 27000 | 7.46 | 7.65 | 7.90 | -0.02 | 0.22 | 0.53 |
| 27374 | 7.80 | 7.95 | 8.13 | -0.08 | 0.16 | 0.46 |
| 27959 | 9.37 | 9.50 | 9.66 | 1.05 | 1.24 | 1.49 |
| 28001 | 7.81 | 8.00 | 8.23 | -0.08 | 0.20 | 0.53 |
| 28006 | 7.50 | 7.67 | 7.89 | 0.33 | 0.57 | 0.88 |
| 28162 | 7.23 | 7.33 | 7.54 | -0.01 | 0.15 | 0.35 |
| 28450 | 7.33 | 7.42 | 7.53 | 0.73 | 0.90 | 1.31 |
| 28674 | 8.08 | 8.23 | 8.41 | -0.08 | 0.18 | 0.51 |
| 28988 | 7.56 | 7.77 | 8.03 | 0.15 | 0.43 | 0.78 |
| 29288 | 9.34 | 9.43 | 9.55 | -0.09 | 0.20 | 0.57 |
| 29484 | 7.88 | 8.07 | 8.30 | 0.42 | 0.67 | 0.97 |
| 29738 | 7.84 | 8.00 | 8.22 | -0.17 | 0.08 | 0.40 |
| 30014 | 6.81 | 6.98 | 7.20 | 0.91 | 1.16 | 1.47 |
| 30240 | 7.10 | 7.30 | 7.55 | -0.19 | 0.06 | 0.37 |
| 30510 | 6.64 | 6.86 | 7.13 | 0.10 | 0.37 | 0.71 |
| 30647 | 7.72 | 7.86 | 8.04 | 0.01 | 0.26 | 0.58 |
| 30833 | 7.59 | 7.78 | 8.01 | 0.75 | 0.97 | 1.23 |
| 31114 | 7.56 | 7.75 | 7.99 | 0.25 | 0.49 | 0.78 |
| 31332 | 7.79 | 7.94 | 8.14 | 0.24 | 0.49 | 0.81 |
| 31529 | 7.69 | 7.87 | 8.08 | -0.22 | -0.03 | 0.19 |
| 31853 | 7.67 | 7.74 | 7.83 | 0.69 | 0.85 | 1.06 |
| 32294 | 6.55 | 6.76 | 7.03 | 1.36 | 1.61 | 1.91 |
| 32571 | 8.97 | 9.10 | 9.27 | -0.09 | 0.18 | 0.52 |
| 32947 | 7.09 | 7.20 | 7.33 | 0.62 | 0.82 | 1.06 |
| 33146 | 9.04 | 9.18 | 9.35 | -0.08 | 0.16 | 0.46 |
| 33372 | 7.48 | 7.61 | 7.75 | -0.19 | 0.02 | 0.29 |
| 33531 | 7.43 | 7.57 | 7.74 | 0.29 | 0.52 | 0.80 |
| 33692 | 8.40 | 8.56 | 8.77 | 0.42 | 0.67 | 0.99 |
| 34005 | 7.40 | 7.58 | 7.81 | 0.08 | 0.36 | 0.70 |
| 34307 | 7.42 | 7.61 | 7.84 | 0.97 | 1.23 | 1.56 |
| 34564 | 6.52 | 6.72 | 6.96 | 0.42 | 0.68 | 1.00 |
| 34913 | 7.08 | 7.24 | 7.45 | 0.28 | 0.52 | 0.84 |
| 35225 | 7.99 | 8.12 | 8.29 | -0.23 | 0.06 | 0.43 |
| 35442 | 6.91 | 7.07 | 7.27 | 0.53 | 0.78 | 1.11 |
| 35790 | 7.20 | 7.37 | 7.58 | 0.16 | 0.46 | 0.82 |
| 36205 | 8.35 | 8.50 | 8.70 | 0.72 | 0.96 | 1.26 |
| 36515 | 7.76 | 7.98 | 8.26 | 0.35 | 0.60 | 0.92 |
| 36735 | 7.15 | 7.33 | 7.55 | 1.10 | 1.34 | 1.64 |
| 37128 | 8.40 | 8.55 | 8.74 | 1.94 | 2.11 | 2.32 |
| 37381 | 8.17 | 8.31 | 8.48 | -0.26 | -0.02 | 0.28 |
| 37765 | 9.23 | 9.36 | 9.51 | -0.06 | 0.16 | 0.43 |
| 38018 | 7.08 | 7.27 | 7.51 | 0.14 | 0.40 | 0.72 |
| 38315 | 8.49 | 8.66 | 8.87 | 0.41 | 0.64 | 0.93 |
| 38639 | 6.41 | 6.58 | 6.79 | 0.07 | 0.32 | 0.63 |
| 38920 | 6.89 | 7.06 | 7.26 | 0.69 | 0.94 | 1.24 |

Continued on next page
| Name  | TZ3P | IP QZ6P | extra | TZ3P | EA QZ6P | extra |
|-------|------|--------|-------|------|---------|-------|
| 39175 | 6.59 | 6.79   | 7.05  | 0.02 | 0.29    | 0.62  |
| 39418 | 7.94 | 8.12   | 8.34  | 0.66 | 0.91    | 1.21  |
| 39685 | 7.75 | 7.92   | 8.14  | 0.82 | 1.02    | 1.27  |
| 39917 | 7.80 | 7.93   | 8.09  | −0.19| 0.06    | 0.36  |
| 40143 | 7.87 | 8.08   | 8.34  | 0.66 | 0.91    | 1.22  |
| 40494 | 7.88 | 8.04   | 8.26  | 0.39 | 0.61    | 0.90  |
| 40764 | 8.44 | 8.56   | 8.70  | 1.73 | 1.96    | 2.25  |
| 40978 | 8.71 | 8.89   | 9.12  | −0.38| −0.15   | 0.14  |
| 41377 | 8.24 | 8.38   | 8.57  | 0.13 | 0.40    | 0.74  |
| 41571 | 6.44 | 6.62   | 6.85  | 0.55 | 0.83    | 1.17  |
| 41897 | 7.69 | 7.90   | 8.15  | 0.65 | 0.77    | 0.93  |
| 42090 | 7.54 | 7.74   | 7.99  | 0.15 | 0.42    | 0.75  |
| 42424 | 7.82 | 8.03   | 8.29  | −0.23| 0.05    | 0.40  |
| 42754 | 7.95 | 7.24   | 7.96  | 0.94 | 0.70    | 1.01  |
| 42908 | 7.20 | 7.40   | 7.96  | 0.25 | 0.49    | 0.80  |
| 43000 | 6.59 | 6.70   | 6.85  | 0.83 | 1.01    | 1.24  |
| 43385 | 7.30 | 7.47   | 7.68  | 0.49 | 0.73    | 1.04  |
| 43634 | 7.76 | 7.96   | 8.21  | 0.20 | 0.45    | 0.74  |
| 43905 | 7.45 | 7.66   | 7.93  | 0.07 | 0.31    | 0.62  |
| 44205 | 7.17 | 7.23   | 7.31  | 0.28 | 0.40    | 0.56  |
| 44586 | 6.15 | 6.31   | 6.51  | 0.57 | 0.78    | 1.04  |
| 44870 | 8.15 | 8.33   | 8.57  | −0.03| 0.22    | 0.53  |
| 45218 | 8.04 | 8.22   | 8.45  | 0.23 | 0.42    | 0.66  |
| 45485 | 7.91 | 8.10   | 8.35  | 1.13 | 1.37    | 1.67  |
| 45666 | 8.63 | 8.76   | 8.92  | −0.12| 0.14    | 0.47  |
| 45995 | 7.67 | 7.88   | 8.15  | 0.26 | 0.52    | 0.84  |
| 46362 | 8.57 | 8.72   | 8.91  | −0.20| 0.03    | 0.32  |
| 46610 | 8.42 | 8.59   | 8.81  | 0.01 | 0.30    | 0.67  |
| 46821 | 6.97 | 7.14   | 7.35  | 0.71 | 0.94    | 1.22  |
| 46991 | 8.69 | 8.81   | 8.97  | 0.47 | 0.72    | 1.03  |
| 47200 | 7.04 | 7.65   | 7.77  | 0.32 | 0.57    | 0.87  |
| 47575 | 7.68 | 7.87   | 8.12  | 0.54 | 0.80    | 1.13  |
| 47797 | 7.10 | 7.32   | 7.59  | 0.46 | 0.73    | 1.06  |
| 47960 | 5.93 | 6.17   | 6.47  | 1.15 | 1.39    | 1.70  |
| 48162 | 8.03 | 8.18   | 8.36  | 0.81 | 1.06    | 1.37  |
| 48399 | 7.68 | 7.86   | 8.08  | 0.91 | 1.13    | 1.40  |
| 48653 | 7.49 | 7.65   | 7.84  | 1.29 | 1.50    | 1.75  |
| 48947 | 6.89 | 7.09   | 7.35  | −0.10| 0.14    | 0.44  |
| 49106 | 7.64 | 7.81   | 8.01  | 0.66 | 0.91    | 1.22  |
| 49471 | 6.01 | 6.19   | 6.42  | 1.46 | 1.70    | 2.00  |
| 49946 | 7.66 | 7.83   | 8.03  | 0.26 | 0.50    | 0.80  |
| 50224 | 8.39 | 8.55   | 8.75  | 0.35 | 0.61    | 0.95  |
| 50401 | 7.72 | 7.91   | 8.14  | −0.14| 0.10    | 0.41  |
| 50771 | 7.76 | 7.91   | 8.09  | −0.08| 0.16    | 0.45  |
| 51045 | 7.49 | 7.70   | 7.97  | −0.07| 0.14    | 0.39  |
| 51317 | 6.98 | 7.18   | 7.43  | 0.40 | 0.66    | 0.98  |
| 51639 | 7.67 | 7.83   | 8.02  | 1.04 | 1.25    | 1.51  |
| 51981 | 8.30 | 8.45   | 8.64  | 0.21 | 0.46    | 0.78  |
| 52259 | 8.23 | 8.41   | 8.62  | 0.48 | 0.76    | 1.10  |
| 52590 | 6.50 | 6.69   | 6.92  | 0.69 | 0.82    | 0.98  |
| 52978 | 8.17 | 8.33   | 8.52  | −0.40| −0.15   | 0.15  |
| 53229 | 8.52 | 8.65   | 8.81  | 0.16 | 0.47    | 0.86  |
| 53566 | 9.70 | 9.77   | 9.86  | −0.41| −0.15   | 0.16  |
| 53842 | 8.08 | 8.22   | 8.40  | 0.96 | 1.17    | 1.43  |
| 54009 | 7.61 | 7.78   | 8.00  | −0.27| −0.02   | 0.30  |
| 54233 | 7.60 | 7.77   | 7.97  | −0.24| 0.00    | 0.31  |

Continued on next page
| Name  | TZ3P | IP QZ6P | extra | TZ3P | EA QZ6P | extra |
|-------|------|---------|-------|------|---------|-------|
| 54412 | 8.48 | 8.62    | 8.80  | 0.89 | 1.10    | 1.36  |
| 54680 | 7.16 | 7.41    | 7.72  | -0.04| 0.21    | 0.52  |
| 54908 | 6.95 | 7.15    | 7.39  | 1.60 | 1.80    | 2.06  |
| 55110 | 8.31 | 8.49    | 8.73  | -0.10| 0.15    | 0.45  |
| 55259 | 7.57 | 7.73    | 7.93  | 0.66 | 0.87    | 1.13  |
| 55516 | 8.98 | 9.12    | 9.31  | 0.19 | 0.42    | 0.72  |
| 55803 | 8.93 | 9.09    | 9.29  | 0.64 | 0.87    | 1.14  |
| 56050 | 8.72 | 8.86    | 9.04  | -0.18| 0.07    | 0.39  |
| 56219 | 8.67 | 8.88    | 9.14  | 0.58 | 0.81    | 1.10  |
| 56406 | 7.22 | 7.39    | 7.60  | 0.46 | 0.70    | 0.98  |
| 56584 | 9.88 | 9.99    | 10.14 | 1.05 | 1.26    | 1.52  |
| 56782 | 8.59 | 8.72    | 8.87  | 0.13 | 0.37    | 0.65  |
| 57147 | 7.10 | 7.28    | 7.49  | 0.37 | 0.59    | 0.87  |
| 57383 | 9.26 | 9.37    | 9.50  | 1.02 | 1.22    | 1.46  |
| 57610 | 7.95 | 8.11    | 8.31  | -0.27| 0.01    | 0.35  |
| 57896 | 7.59 | 7.68    | 7.80  | 0.54 | 0.76    | 1.04  |
| 58206 | 6.85 | 7.02    | 7.24  | 0.60 | 0.83    | 1.12  |
| 58443 | 8.82 | 8.96    | 9.13  | -0.24| 0.01    | 0.34  |
| 58653 | 9.14 | 9.30    | 9.49  | 0.09 | 0.32    | 0.61  |
| 58846 | 8.03 | 8.15    | 8.30  | -0.01| 0.23    | 0.53  |
| 59124 | 7.06 | 7.23    | 7.43  | 1.14 | 1.33    | 1.57  |
| 59304 | 9.51 | 9.60    | 9.71  | 1.41 | 1.58    | 1.78  |
| 59631 | 7.32 | 7.47    | 7.65  | 0.58 | 0.80    | 1.06  |
| 59849 | 8.58 | 8.76    | 8.99  | -0.04| 0.21    | 0.51  |
| 60181 | 7.80 | 7.95    | 8.13  | 0.74 | 0.97    | 1.25  |
| 60360 | 8.46 | 8.69    | 8.95  | 0.44 | 0.66    | 0.92  |
| 60545 | 7.77 | 7.95    | 8.18  | 0.13 | 0.36    | 0.64  |
| 60749 | 7.67 | 7.82    | 8.01  | 0.78 | 1.01    | 1.31  |
| 60961 | 7.86 | 7.97    | 8.10  | 0.97 | 1.19    | 1.46  |
| 61133 | 7.17 | 7.35    | 7.56  | 0.13 | 0.35    | 0.63  |
| 61346 | 7.74 | 7.90    | 8.11  | -0.05| 0.21    | 0.54  |