# BLYP

| atom | energy | mult |
|---|---|---|
| H | -0.50 | 2 |
| C | -37.85 | 3 |
| N | -54.59 | 4 |
| O | -75.08 | 3 |
| F | -99.76 | 2 |
| S | -398.11 | 3 |
| Cl | -460.15 | 2 |
| Ti | -849.36 | 3 |
| V | -943.92 | 6 |
| Cr | -1044.46 | 7 |
| Mn | -1151.01 | 6 |
| Fe | -1263.66 | 5 |
| Co | -1382.77 | 2 |
| Ni | -1508.30 | 3 |
| Cu | -1640.58 | 2 |
| Zn | -1779.48 | 1 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| TiH | -849.95 | 4 | 101.27 | 116.40 | 15.13 |
| TiN | -904.16 | 2 | 91.65 | 112.10 | 20.45 |
| TiO | -924.72 | 3 | -6.50 | 13.70 | 20.20 |
| TiS | -1247.67 | 3 | 53.99 | 76.20 | 22.21 |
| TiF | -949.34 | 4 | -10.76 | -4.00 | 6.76 |
| TiF2 | -1049.35 | 3 | -147.27 | -164.50 | -17.23 |
| TiF3 | -1149.34 | 2 | -276.68 | -284.10 | -7.42 |
| TiCl | -1309.66 | 4 | 40.37 | 24.20 | -16.17 |
| TiCl2 | -1770.00 | 3 | -50.82 | -57.00 | -6.18 |
| TiCl3 | -2230.31 | 2 | -125.64 | -128.90 | -3.26 |

| | |
|---|---|
| mean error | 3.45 |
| abs error | 13.50 |
| rmsd | 15.02 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| V2 | -1887.97 | 3 | 162.89 | 187.40 | 24.51 |
| VH | -944.52 | 5 | 109.66 | 125.90 | 16.24 |
| VN | -998.72 | 3 | 103.73 | 121.00 | 17.27 |
| VO | -1019.27 | 4 | 15.47 | 30.50 | 15.03 |
| VS | -1342.21 | 4 | 74.29 | 80.40 | 6.11 |
| VF | -1043.89 | 5 | 5.12 | 0.70 | -4.42 |
| VCl | -1404.22 | 5 | 50.81 | 37.80 | -13.01 |
| VCl2 | -1864.54 | 4 | -29.21 | -51.60 | -22.39 |
| VCl3 | -2324.82 | 3 | -85.20 | -88.20 | -3.00 |

| | |
|---|---|
| mean error | 4.04 |
| abs error | 13.55 |
| rmsd | 15.37 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CrH | -1045.04 | 6 | 92.38 | 80.20 | -12.18 |
| CrN | -1099.21 | 4 | 105.09 | 120.70 | 15.61 |
| CrO | -1119.73 | 5 | 37.16 | 45.00 | 7.84 |
| CrO2 | -1195.03 | 3 | -42.17 | -18.00 | 24.17 |
| CrO3 | -1270.30 | 1 | -102.29 | -70.50 | 31.79 |
| CrOH | -1120.33 | 6 | 24.13 | 18.90 | -5.23 |
| Cr(OH)2 | -1196.23 | 5 | -68.29 | -78.10 | -9.81 |
| CrS | -1442.70 | 5 | 81.38 | 78.20 | -3.18 |

| | | | | | |
|---|---|---|---|---|---|
| CrF | -1144.40 | 6 | -2.77 | 3.10 | 5.87 |
| CrF2 | -1244.35 | 5 | -104.99 | -99.10 | 5.89 |
| CrF3 | -1344.29 | 4 | -200.29 | -199.80 | 0.49 |
| CrCl | -1504.74 | 6 | 37.66 | 31.00 | -6.66 |
| CrCl2 | -1965.02 | 5 | -19.16 | -28.10 | -8.94 |
| CrCl3 | -2425.29 | 4 | -64.69 | -67.70 | -3.01 |

| | |
|---|---|
| mean error | 3.05 |
| abs error | 10.05 |
| rmsd | 13.05 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| MnF | -1250.94 | 7 | -19.68 | -19.90 | -0.22 |
| MnF2 | -1350.91 | 6 | -136.06 | -126.20 | 9.86 |
| MnF3 | -1450.81 | 5 | -203.72 | -188.00 | 15.72 |
| MnCl | -1611.28 | 7 | 20.31 | 11.30 | -9.01 |
| MnCl2 | -2071.59 | 6 | -56.49 | -63.00 | -6.51 |
| MnH | -1151.58 | 5 | 75.56 | 64.20 | -11.36 |
| MnO | -1226.27 | 6 | 16.20 | 29.60 | 13.40 |
| MnOH | -1226.87 | 7 | 1.08 | 3.70 | 2.62 |
| MnS | -1549.25 | 6 | 53.59 | 63.30 | 9.71 |

| | |
|---|---|
| mean error | 2.69 |
| abs error | 8.71 |
| rmsd | 9.88 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Fe2 | -2527.50 | 7 | 85.32 | 172.40 | 87.08 |
| FeH | -1264.30 | 4 | 64.69 | 117.20 | 52.51 |
| FeO | -1338.98 | 5 | 8.13 | 61.10 | 52.97 |
| FeS | -1661.97 | 5 | 43.98 | 83.80 | 39.82 |
| Fe(OH)2 | -1415.50 | 6 | -104.96 | -79.00 | 25.96 |
| FeCO | -1377.10 | 3 | 8.98 | 63.90 | 54.92 |
| Fe(CO)2 | -1490.50 | 3 | -59.79 | 0.20 | 59.99 |
| Fe(CO)3 | -1603.89 | 3 | -121.25 | -55.80 | 65.45 |
| Fe(CO)4 | -1717.28 | 3 | -178.89 | -105.10 | 73.79 |
| FeF | -1363.65 | 4 | -25.54 | 11.40 | 36.94 |
| FeF2 | -1463.62 | 5 | -142.42 | -93.00 | 49.42 |
| FeF3 | -1563.52 | 6 | -208.58 | -196.20 | 12.38 |
| FeCl | -1723.98 | 4 | 17.23 | 49.50 | 32.27 |
| FeCl2 | -2184.30 | 5 | -61.66 | -32.80 | 28.86 |
| FeCl3 | -2644.54 | 6 | -94.00 | -60.60 | 33.40 |

| | |
|---|---|
| mean error | 47.05 |
| abs error | 47.05 |
| rmsd | 50.79 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CoH | -1383.38 | 3 | 80.25 | 110.70 | 30.45 |
| CoO | -1458.05 | 4 | 35.03 | 74.00 | 38.97 |
| CoF2 | -1582.67 | 4 | -104.97 | -87.50 | 17.47 |
| CoCl | -1843.06 | 3 | 36.67 | 50.30 | 13.63 |
| CoCl2 | -2303.37 | 4 | -34.19 | -22.60 | 11.59 |
| CoCl3 | -2763.60 | 5 | -60.13 | -39.10 | 21.03 |

| | |
|---|---|
| mean error | 22.19 |
| abs error | 22.19 |
| rmsd | 24.20 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Ni2 | -3016.80 | 3 | 77.17 | 156.70 | 79.53 |
| NiH | -1508.95 | 2 | 53.07 | 85.60 | 32.53 |
| NiO | -1583.61 | 3 | 18.67 | 75.00 | 56.33 |
| NiS | -1906.61 | 3 | 42.98 | 81.70 | 38.72 |
| Ni(OH)2 | -1660.12 | 3 | -92.36 | -60.80 | 31.56 |
| NiCO | -1621.77 | 1 | -9.86 | 35.10 | 44.96 |
| Ni(CO)2 | -1735.18 | 1 | -86.13 | -39.00 | 47.13 |
| Ni(CO)3 | -1848.57 | 1 | -144.95 | -92.70 | 52.25 |
| Ni(CO)4 | -1961.94 | 1 | -193.70 | -144.00 | 49.70 |
| NiF | -1608.27 | 2 | -16.81 | 17.50 | 34.31 |
| NiF2 | -1708.22 | 3 | -117.53 | -77.80 | 39.73 |
| NiCl | -1968.63 | 2 | 12.89 | 41.70 | 28.81 |
| CiCl2 | -2428.92 | 3 | -48.65 | -17.40 | 31.25 |
| | | | | | |
| mean error | 48.08 | | | | |
| abs error | 43.60 | | | | |
| rmsd | 45.62 | | | | |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Cu2 | -3281.23 | 1 | 114.21 | 113.80 | -0.41 |
| CuH | -1641.18 | 1 | 69.49 | 65.90 | -3.59 |
| CuO | -1715.78 | 2 | 67.07 | 76.50 | 9.43 |
| CuOH | -1716.43 | 1 | 17.80 | 28.70 | 10.90 |
| CuS | -2038.80 | 2 | 80.75 | 75.10 | -5.65 |
| CuF | -1740.49 | 1 | 3.44 | -3.20 | -6.64 |
| CuF2 | -1840.38 | 2 | -63.02 | -66.00 | -2.98 |
| CuCl | -2100.85 | 1 | 29.67 | 19.30 | -10.37 |
| CuCl2 | -2561.10 | 2 | -4.47 | -9.00 | -4.53 |
| | | | | | |
| mean error | -1.54 | | | | |
| abs error | 6.06 | | | | |
| rmsd | 6.94 | | | | |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Zn2 | -3558.96 | 1 | 65.04 | 57.70 | -7.34 |
| ZnF2 | -1979.29 | 1 | -113.11 | -118.90 | -5.79 |
| ZnCl | -2239.70 | 2 | 17.96 | 6.50 | -11.46 |
| ZnCl2 | -2699.99 | 1 | -46.82 | -63.50 | -16.68 |
| ZnO | -1854.62 | 1 | 56.21 | 52.80 | -3.41 |
| ZnS | -2177.64 | 1 | 70.19 | 48.70 | -21.49 |
| ZnH | -1780.01 | 2 | 65.50 | 62.90 | -2.60 |
| Zn(CH3) | -1819.29 | 2 | 56.94 | 26.00 | -30.94 |
| Zn(CH3)2 | -1859.19 | 1 | 26.76 | 12.90 | -13.86 |
| | | | | | |
| mean error | -12.62 | | | | |
| abs error | 12.62 | | | | |
| rmsd | 15.37 | | | | |

# MPWPW91

| atom | energy | mult |
|---|---|---|
| H | -0.50 | 2 |
| C | -37.84 | 3 |
| N | -54.59 | 4 |
| O | -75.08 | 3 |
| F | -99.75 | 2 |
| S | -398.13 | 3 |
| Cl | -460.17 | 2 |
| Ti | -849.41 | 5 |
| V | -943.99 | 6 |
| Cr | -1044.54 | 7 |
| Mn | -1151.04 | 6 |
| Fe | -1263.80 | 5 |
| Co | -1382.85 | 4 |
| Ni | -1508.41 | 3 |
| Cu | -1640.69 | 2 |
| Zn | -1779.60 | 1 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| TiH | -850.01 | 4 | 104.71 | 116.40 | 11.69 |
| TiN | -904.21 | 2 | 93.45 | 112.10 | 18.65 |
| TiO | -924.77 | 3 | -6.53 | 13.70 | 20.23 |
| TiS | -1247.74 | 3 | 52.03 | 76.20 | 24.17 |
| TiF | -949.39 | 4 | -11.74 | -4.00 | 7.74 |
| TiF2 | -1049.38 | 3 | -146.17 | -164.50 | -18.33 |
| TiF3 | -1149.37 | 2 | -275.92 | -284.10 | -8.18 |
| TiCl | -1309.75 | 4 | 33.38 | 24.20 | -9.18 |
| TiCl2 | -1770.10 | 3 | -54.41 | -57.00 | -2.59 |
| TiCl3 | -2230.43 | 2 | -132.50 | -128.90 | 3.60 |

| | |
|---|---|
| mean error | 4.78 |
| abs error | 12.43 |
| rmsd | 14.30 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| V2 | -1888.08 | 3 | 175.27 | 187.40 | 12.13 |
| VH | -944.58 | 5 | 115.48 | 125.90 | 10.42 |
| VN | -998.78 | 3 | 109.31 | 121.00 | 11.69 |
| VO | -1019.33 | 4 | 17.39 | 30.50 | 13.11 |
| VS | -1342.29 | 4 | 74.15 | 80.40 | 6.25 |
| VF | -1043.95 | 5 | 7.47 | 0.70 | -6.77 |
| VCl | -1404.31 | 5 | 51.50 | 37.80 | -13.70 |
| VCl2 | -1864.65 | 4 | -30.63 | -51.60 | -20.97 |
| VCl3 | -2324.95 | 3 | -88.95 | -88.20 | 0.75 |

| | |
|---|---|
| mean error | 1.43 |
| abs error | 10.64 |
| rmsd | 11.91 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CrH | -1045.12 | 6 | 97.82 | 80.20 | -17.62 |
| CrN | -1099.29 | 4 | 111.58 | 120.70 | 9.12 |
| CrO | -1119.80 | 5 | 41.68 | 45.00 | 3.32 |
| CrO2 | -1195.10 | 3 | -36.95 | -18.00 | 18.95 |
| CrO3 | -1270.37 | 1 | -98.89 | -70.50 | 28.39 |
| CrOH | -1120.41 | 6 | 27.04 | 18.90 | -8.14 |
| Cr(OH)2 | -1196.31 | 5 | -63.76 | -78.10 | -14.34 |
| CrS | -1442.79 | 5 | 83.23 | 78.20 | -5.03 |

| | | | | | |
|---|---|---|---|---|---|
| CrF | -1144.47 | 6 | 0.61 | 3.10 | 2.49 |
| CrF2 | -1244.41 | 5 | -99.15 | -99.10 | 0.05 |
| CrF3 | -1344.35 | 4 | -194.28 | -199.80 | -5.52 |
| CrCl | -1504.84 | 6 | 37.92 | 31.00 | -6.92 |
| CrCl2 | -1965.14 | 5 | -19.03 | -28.10 | -9.07 |
| CrCl3 | -2425.43 | 4 | -66.84 | -67.70 | -0.86 |

| | |
|---|---|
| mean error | -0.37 |
| abs error | 9.27 |
| rmsd | 12.06 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| MnF | -1251.02 | 7 | -60.18 | -19.90 | 40.28 |
| MnF2 | -1350.98 | 6 | -174.36 | -126.20 | 48.16 |
| MnF3 | -1450.87 | 5 | -240.33 | -188.00 | 52.33 |
| MnCl | -1611.39 | 7 | -22.76 | 11.30 | 34.06 |
| MnCl2 | -2071.72 | 6 | -100.50 | -63.00 | 37.50 |
| MnH | -1151.65 | 5 | 45.77 | 64.20 | 18.43 |
| MnO | -1226.35 | 6 | -22.40 | 29.60 | 52.00 |
| MnOH | -1226.96 | 7 | -39.88 | 3.70 | 43.58 |
| MnS | -1549.35 | 6 | 12.76 | 63.30 | 50.54 |

| | |
|---|---|
| mean error | 41.88 |
| abs error | 41.88 |
| rmsd | 43.13 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Fe2 | -2527.67 | 7 | 150.14 | 172.40 | 22.26 |
| FeH | -1264.38 | 4 | 100.43 | 117.20 | 16.77 |
| FeO | -1339.07 | 5 | 37.50 | 61.10 | 23.60 |
| FeS | -1662.07 | 5 | 71.71 | 83.80 | 12.09 |
| Fe(OH)2 | -1415.59 | 6 | -76.70 | -79.00 | -2.30 |
| FeCO | -1377.19 | 3 | 34.84 | 63.90 | 29.06 |
| Fe(CO)2 | -1490.59 | 3 | -42.92 | 0.20 | 43.12 |
| Fe(CO)3 | -1603.99 | 3 | -115.36 | -55.80 | 59.56 |
| Fe(CO)4 | -1717.39 | 3 | -183.32 | -105.10 | 78.22 |
| FeF | -1363.73 | 6 | 5.64 | 11.40 | 5.76 |
| FeF2 | -1463.70 | 5 | -112.80 | -93.00 | 19.80 |
| FeF3 | -1563.59 | 6 | -180.10 | -196.20 | -16.10 |
| FeCl | -1724.09 | 6 | 44.60 | 49.50 | 4.90 |
| FeCl2 | -2184.44 | 5 | -37.78 | -32.80 | 4.98 |
| FeCl3 | -2644.70 | 6 | -73.70 | -60.60 | 13.10 |

| | |
|---|---|
| mean error | 20.99 |
| abs error | 23.44 |
| rmsd | 31.37 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CoH | -1383.47 | 3 | 78.75 | 110.70 | 31.95 |
| CoO | -1458.14 | 4 | 30.61 | 74.00 | 43.39 |
| CoF2 | -1582.75 | 4 | -110.89 | -87.50 | 23.39 |
| CoCl | -1843.17 | 3 | 32.49 | 50.30 | 17.81 |
| CoCl2 | -2303.51 | 4 | -45.69 | -22.60 | 23.09 |
| CoCl3 | -2763.76 | 5 | -75.95 | -39.10 | 36.85 |

| | |
|---|---|
| mean error | 29.41 |
| abs error | 29.41 |
| rmsd | 30.71 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Ni2 | -3017.00 | 3 | 87.97 | 156.70 | 68.73 |
| NiH | -1509.06 | 2 | 60.16 | 85.60 | 25.44 |
| NiO | -1583.71 | 3 | 21.61 | 75.00 | 53.39 |
| NiS | -1906.73 | 3 | 43.11 | 81.70 | 38.59 |
| Ni(OH)2 | -1660.23 | 3 | -91.54 | -60.80 | 30.74 |
| NiCO | -1621.88 | 1 | -15.23 | 35.10 | 50.33 |
| Ni(CO)2 | -1735.30 | 1 | -99.45 | -39.00 | 60.45 |
| Ni(CO)3 | -1848.69 | 1 | -167.00 | -92.70 | 74.30 |
| Ni(CO)4 | -1962.07 | 1 | -225.68 | -144.00 | 81.68 |
| NiF | -1608.37 | 2 | -13.48 | 17.50 | 30.98 |
| NiF2 | -1708.32 | 3 | -115.24 | -77.80 | 37.44 |
| NiCl | -1968.76 | 2 | 13.79 | 41.70 | 27.91 |
| CiCl2 | -2429.07 | 3 | -51.97 | -17.40 | 34.57 |
| | | | | | |
| mean error | 53.74 | | | | |
| abs error | 47.27 | | | | |
| rmsd | 50.66 | | | | |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Cu2 | -3281.46 | 1 | 113.99 | 113.80 | -0.19 |
| CuH | -1641.29 | 1 | 71.27 | 65.90 | -5.37 |
| CuO | -1715.89 | 2 | 66.67 | 76.50 | 9.83 |
| CuOH | -1716.55 | 1 | 16.38 | 28.70 | 12.32 |
| CuS | -2038.93 | 2 | 77.42 | 75.10 | -2.32 |
| CuF | -1740.60 | 1 | 2.49 | -3.20 | -5.69 |
| CuF2 | -1840.49 | 2 | -64.66 | -66.00 | -1.34 |
| CuCl | -2100.99 | 1 | 25.38 | 19.30 | -6.08 |
| CuCl2 | -2561.26 | 2 | -11.84 | -9.00 | 2.84 |
| | | | | | |
| mean error | 0.44 | | | | |
| abs error | 5.11 | | | | |
| rmsd | 6.34 | | | | |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Zn2 | -3559.21 | 1 | 63.28 | 57.70 | -5.58 |
| ZnF2 | -1979.41 | 1 | -119.45 | -118.90 | 0.55 |
| ZnCl | -2239.85 | 2 | 10.77 | 6.50 | -4.27 |
| ZnCl2 | -2700.17 | 1 | -58.92 | -63.50 | -4.58 |
| ZnO | -1854.74 | 1 | 52.89 | 52.80 | -0.09 |
| ZnS | -2177.78 | 1 | 63.90 | 48.70 | -15.20 |
| ZnH | -1780.14 | 2 | 64.09 | 62.90 | -1.19 |
| Zn(CH3) | -1819.44 | 2 | 49.64 | 26.00 | -23.64 |
| Zn(CH3)2 | -1859.36 | 1 | 13.34 | 12.90 | -0.44 |
| | | | | | |
| mean error | -6.05 | | | | |
| abs error | 6.17 | | | | |
| rmsd | 9.79 | | | | |

# PBEPBE

| atom | energy | mult |
|---|---|---|
| H | -0.50 | 2 |
| C | -37.80 | 3 |
| N | -54.53 | 4 |
| O | -75.01 | 3 |
| F | -99.67 | 2 |
| S | -397.94 | 3 |
| Cl | -459.96 | 2 |
| Ti | -849.10 | 3 |
| V | -943.65 | 6 |
| Cr | -1044.19 | 7 |
| Mn | -1150.72 | 6 |
| Fe | -1263.41 | 5 |
| Co | -1382.44 | 2 |
| Ni | -1508.01 | 3 |
| Cu | -1640.23 | 2 |
| Zn | -1779.12 | 1 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| TiH | -849.70 | 4 | 104.27 | 116.40 | 12.13 |
| TiN | -903.85 | 2 | 89.46 | 112.10 | 22.64 |
| TiO | -924.40 | 3 | -9.33 | 13.70 | 23.03 |
| TiS | -1247.24 | 3 | 49.75 | 76.20 | 26.45 |
| TiF | -949.00 | 4 | -13.53 | -4.00 | 9.53 |
| TiF2 | -1048.91 | 3 | -149.59 | -164.50 | -14.91 |
| TiF3 | -1148.82 | 2 | -281.24 | -284.10 | -2.86 |
| TiCl | -1309.23 | 4 | 35.14 | 24.20 | -10.94 |
| TiCl2 | -1769.37 | 3 | -57.70 | -57.00 | 0.70 |
| TiCl3 | -2229.50 | 2 | -137.64 | -128.90 | 8.74 |

| | |
|---|---|
| mean error | 7.45 |
| abs error | 13.19 |
| rmsd | 15.52 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| V2 | -1887.44 | 3 | 165.06 | 187.40 | 22.34 |
| VH | -944.25 | 5 | 112.60 | 125.90 | 13.30 |
| VN | -998.40 | 3 | 103.41 | 121.00 | 17.59 |
| VO | -1018.93 | 4 | 12.27 | 30.50 | 18.23 |
| VS | -1341.78 | 4 | 69.58 | 80.40 | 10.82 |
| VF | -1043.54 | 5 | 3.42 | 0.70 | -2.72 |
| VCl | -1403.77 | 5 | 47.51 | 37.80 | -9.71 |
| VCl2 | -1863.91 | 4 | -36.23 | -51.60 | -15.37 |
| VCl3 | -2324.00 | 3 | -96.53 | -88.20 | 8.33 |

| | |
|---|---|
| mean error | 6.98 |
| abs error | 13.16 |
| rmsd | 14.31 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CrH | -1044.77 | 6 | 97.38 | 80.20 | -17.18 |
| CrN | -1098.89 | 4 | 108.42 | 120.70 | 12.28 |
| CrO | -1119.38 | 5 | 39.24 | 45.00 | 5.76 |
| CrO2 | -1194.61 | 3 | -41.99 | -18.00 | 23.99 |
| CrO3 | -1269.82 | 1 | -106.42 | -70.50 | 35.92 |
| CrOH | -1119.99 | 6 | 24.75 | 18.90 | -5.85 |
| Cr(OH)2 | -1195.82 | 5 | -68.61 | -78.10 | -9.49 |
| CrS | -1442.25 | 5 | 81.25 | 78.20 | -3.05 |

| | | | | | |
|---|---|---|---|---|---|
| CrF | -1144.04 | 6 | -1.00 | 3.10 | 4.10 |
| CrF2 | -1243.90 | 5 | -102.63 | -99.10 | 3.53 |
| CrF3 | -1343.75 | 4 | -199.73 | -199.80 | -0.07 |
| CrCl | -1504.29 | 6 | 36.29 | 31.00 | -5.29 |
| CrCl2 | -1964.38 | 5 | -22.44 | -28.10 | -5.66 |
| CrCl3 | -2424.46 | 4 | -72.06 | -67.70 | 4.36 |

| | |
|---|---|
| mean error | 3.10 |
| abs error | 9.75 |
| rmsd | 13.59 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| MnF | -1250.57 | 7 | -28.58 | -19.90 | 8.68 |
| MnF2 | -1350.45 | 6 | -144.36 | -126.20 | 18.16 |
| MnF3 | -1450.25 | 5 | -212.21 | -188.00 | 24.21 |
| MnCl | -1610.81 | 7 | 8.80 | 11.30 | 2.50 |
| MnCl2 | -2070.94 | 6 | -70.67 | -63.00 | 7.67 |
| MnH | -1151.29 | 5 | 77.23 | 64.20 | -13.03 |
| MnO | -1225.92 | 6 | 8.61 | 29.60 | 20.99 |
| MnOH | -1226.52 | 7 | -9.04 | 3.70 | 12.74 |
| MnS | -1548.80 | 6 | 44.07 | 63.30 | 19.23 |

| | |
|---|---|
| mean error | 11.24 |
| abs error | 14.14 |
| rmsd | 15.63 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Fe2 | -2526.90 | 7 | 148.02 | 172.40 | 24.38 |
| FeH | -1263.99 | 4 | 100.25 | 117.20 | 16.95 |
| FeO | -1338.61 | 5 | 36.14 | 61.10 | 24.96 |
| FeS | -1661.49 | 5 | 70.37 | 83.80 | 13.43 |
| Fe(OH)2 | -1415.06 | 6 | -80.63 | -79.00 | 1.63 |
| FeCO | -1376.69 | 3 | 29.42 | 63.90 | 34.48 |
| Fe(CO)2 | -1489.98 | 3 | -51.74 | 0.20 | 51.94 |
| Fe(CO)3 | -1603.27 | 3 | -128.14 | -55.80 | 72.34 |
| Fe(CO)4 | -1716.55 | 3 | -200.95 | -105.10 | 95.85 |
| FeF | -1363.25 | 6 | 4.79 | 11.40 | 6.61 |
| FeF2 | -1463.14 | 5 | -115.30 | -93.00 | 22.30 |
| FeF3 | -1562.95 | 6 | -185.02 | -196.20 | -11.18 |
| FeCl | -1723.49 | 6 | 43.73 | 49.50 | 5.77 |
| FeCl2 | -2183.63 | 5 | -40.35 | -32.80 | 7.55 |
| FeCl3 | -2643.69 | 6 | -78.41 | -60.60 | 17.81 |

| | |
|---|---|
| mean error | 25.65 |
| abs error | 27.14 |
| rmsd | 37.48 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CoH | -1383.06 | 3 | 82.09 | 110.70 | 28.61 |
| CoO | -1457.66 | 4 | 31.67 | 74.00 | 42.33 |
| CoF2 | -1582.17 | 4 | -110.53 | -87.50 | 23.03 |
| CoCl | -1842.55 | 3 | 35.61 | 50.30 | 14.69 |
| CoCl2 | -2302.68 | 4 | -45.32 | -22.60 | 22.72 |
| CoCl3 | -2762.73 | 5 | -77.13 | -39.10 | 38.03 |

| | |
|---|---|
| mean error | 28.24 |
| abs error | 28.24 |
| rmsd | 29.78 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Ni2 | -3016.13 | 3 | 132.79 | 156.70 | 23.91 |
| NiH | -1508.62 | 2 | 84.10 | 85.60 | 1.50 |
| NiO | -1583.20 | 3 | 43.81 | 75.00 | 31.19 |
| NiS | -1906.10 | 3 | 65.85 | 81.70 | 15.85 |
| Ni(OH)2 | -1659.65 | 3 | -71.67 | -60.80 | 10.87 |
| NiCO | -1621.33 | 1 | 4.20 | 35.10 | 30.90 |
| Ni(CO)2 | -1734.64 | 1 | -84.03 | -39.00 | 45.03 |
| Ni(CO)3 | -1847.92 | 1 | -155.94 | -92.70 | 63.24 |
| Ni(CO)4 | -1961.19 | 1 | -219.23 | -144.00 | 75.23 |
| NiF | -1607.85 | 2 | 9.60 | 17.50 | 7.90 |
| NiF2 | -1707.71 | 3 | -94.04 | -77.80 | 16.24 |
| NiCl | -1968.11 | 2 | 36.80 | 41.70 | 4.90 |
| CiCl2 | -2428.22 | 3 | -30.31 | -17.40 | 12.91 |
| | | | | | |
| mean error | 33.08 | | | | |
| abs error | 26.13 | | | | |
| rmsd | 34.05 | | | | |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Cu2 | -3280.54 | 1 | 112.62 | 113.80 | 1.18 |
| CuH | -1640.83 | 1 | 70.91 | 65.90 | -5.01 |
| CuO | -1715.36 | 2 | 64.75 | 76.50 | 11.75 |
| CuOH | -1716.02 | 1 | 14.16 | 28.70 | 14.54 |
| CuS | -2038.28 | 2 | 75.87 | 75.10 | -0.77 |
| CuF | -1740.06 | 1 | 1.06 | -3.20 | -4.26 |
| CuF2 | -1839.86 | 2 | -67.85 | -66.00 | 1.85 |
| CuCl | -2100.32 | 1 | 23.96 | 19.30 | -4.66 |
| CuCl2 | -2560.38 | 2 | -14.71 | -9.00 | 5.71 |
| | | | | | |
| mean error | 2.26 | | | | |
| abs error | 5.52 | | | | |
| rmsd | 7.09 | | | | |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Zn2 | -3558.24 | 1 | 62.77 | 57.70 | -5.07 |
| ZnF2 | -1978.76 | 1 | -121.82 | -118.90 | 2.92 |
| ZnCl | -2239.15 | 2 | 10.02 | 6.50 | -3.52 |
| ZnCl2 | -2699.27 | 1 | -61.35 | -63.50 | -2.15 |
| ZnO | -1854.19 | 1 | 51.29 | 52.80 | 1.51 |
| ZnS | -2177.11 | 1 | 62.63 | 48.70 | -13.93 |
| ZnH | -1779.65 | 2 | 64.37 | 62.90 | -1.47 |
| Zn(CH3) | -1818.90 | 2 | 47.16 | 26.00 | -21.16 |
| Zn(CH3)2 | -1858.77 | 1 | 7.79 | 12.90 | 5.11 |
| | | | | | |
| mean error | -4.20 | | | | |
| abs error | 6.32 | | | | |
| rmsd | 8.97 | | | | |

# B3LYP

| atom | energy | mult |
|---|---|---|
| H | -0.50 | 2 |
| C | -37.86 | 3 |
| N | -54.60 | 4 |
| O | -75.10 | 3 |
| F | -99.77 | 2 |
| S | -398.13 | 3 |
| Cl | -460.16 | 2 |
| Ti | -849.36 | 3 |
| V | -943.91 | 4 |
| Cr | -1044.45 | 7 |
| Mn | -1151.00 | 6 |
| Fe | -1263.69 | 5 |
| Co | -1382.76 | 4 |
| Ni | -1508.31 | 3 |
| Cu | -1640.53 | 2 |
| Zn | -1779.45 | 1 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| TiH | -849.94 | 4 | 115.48 | 116.40 | 0.92 |
| TiN | -904.14 | 2 | 117.36 | 112.10 | -5.26 |
| TiO | -924.70 | 3 | 14.58 | 13.70 | -0.88 |
| TiS | -1247.66 | 3 | 68.92 | 76.20 | 7.28 |
| TiF | -949.34 | 4 | -0.56 | -4.00 | -3.44 |
| TiF2 | -1049.34 | 3 | -130.57 | -164.50 | -33.93 |
| TiF3 | -1149.33 | 2 | -251.69 | -284.10 | -32.41 |
| TiCl | -1309.67 | 4 | 46.25 | 24.20 | -22.05 |
| TiCl2 | -1770.03 | 3 | -44.28 | -57.00 | -12.72 |
| TiCl3 | -2230.34 | 2 | -112.22 | -128.90 | -16.68 |

| | |
|---|---|
| mean error | -11.92 |
| abs error | 13.56 |
| rmsd | 17.95 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| V2 | -1887.86 | 3 | 221.90 | 187.40 | -34.50 |
| VH | -944.51 | 5 | 112.75 | 125.90 | 13.15 |
| VN | -998.68 | 3 | 131.63 | 121.00 | -10.63 |
| VO | -1019.23 | 4 | 37.89 | 30.50 | -7.39 |
| VS | -1342.20 | 4 | 89.56 | 80.40 | -9.16 |
| VF | -1043.88 | 5 | 13.43 | 0.70 | -12.73 |
| VCl | -1404.23 | 5 | 53.37 | 37.80 | -15.57 |
| VCl2 | -1864.54 | 4 | -9.95 | -51.60 | -41.65 |
| VCl3 | -2324.84 | 3 | -70.30 | -88.20 | -17.90 |

| | |
|---|---|
| mean error | -15.15 |
| abs error | 18.07 |
| rmsd | 21.28 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CrH | -1045.03 | 6 | 95.19 | 80.20 | -14.99 |
| CrN | -1099.17 | 4 | 134.39 | 120.70 | -13.69 |
| CrO | -1119.69 | 5 | 59.27 | 45.00 | -14.27 |
| CrO2 | -1194.97 | 3 | 3.23 | -18.00 | -21.23 |
| CrO3 | -1270.21 | 1 | -27.50 | -70.50 | -43.00 |
| CrOH | -1120.32 | 6 | 30.87 | 18.90 | -11.97 |
| Cr(OH)2 | -1196.23 | 5 | -54.07 | -78.10 | -24.03 |
| CrS | -1442.68 | 5 | 92.69 | 78.20 | -14.49 |

| | | | | | |
|---|---|---|---|---|---|
| CrF | -1144.39 | 6 | 4.49 | 3.10 | -1.39 |
| CrF2 | -1244.34 | 5 | -90.87 | -99.10 | -8.23 |
| CrF3 | -1344.27 | 4 | -173.67 | -199.80 | -26.13 |
| CrCl | -1504.74 | 6 | 39.66 | 31.00 | -8.66 |
| CrCl2 | -1965.04 | 5 | -14.02 | -28.10 | -14.08 |
| CrCl3 | -2425.30 | 4 | -48.28 | -67.70 | -19.42 |

| | |
|---|---|
| mean error | -16.83 |
| abs error | 16.83 |
| rmsd | 19.36 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| MnF | -1250.93 | 7 | -13.46 | -19.90 | -6.44 |
| MnF2 | -1350.90 | 6 | -122.72 | -126.20 | -3.48 |
| MnF3 | -1450.78 | 5 | -173.54 | -188.00 | -14.46 |
| MnCl | -1611.29 | 7 | 22.06 | 11.30 | -10.76 |
| MnCl2 | -2071.61 | 6 | -52.07 | -63.00 | -10.93 |
| MnH | -1151.56 | 7 | 86.30 | 64.20 | -22.10 |
| MnO | -1226.23 | 6 | 41.15 | 29.60 | -11.55 |
| MnOH | -1226.87 | 7 | 7.93 | 3.70 | -4.23 |
| MnS | -1549.24 | 6 | 68.35 | 63.30 | -5.05 |

| | |
|---|---|
| mean error | -9.89 |
| abs error | 9.89 |
| rmsd | 11.37 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Fe2 | -2527.37 | 7 | 206.45 | 172.40 | -34.05 |
| FeH | -1264.27 | 4 | 105.63 | 117.20 | 11.57 |
| FeO | -1338.92 | 5 | 73.59 | 61.10 | -12.49 |
| FeS | -1661.93 | 5 | 95.58 | 83.80 | -11.78 |
| Fe(OH)2 | -1415.47 | 6 | -46.58 | -79.00 | -32.42 |
| FeCO | -1377.06 | 3 | 69.86 | 63.90 | -5.96 |
| Fe(CO)2 | -1490.45 | 3 | 19.91 | 0.20 | -19.71 |
| Fe(CO)3 | -1603.85 | 3 | -31.68 | -55.80 | -24.12 |
| Fe(CO)4 | -1717.23 | 1 | -67.46 | -105.10 | -37.64 |
| FeF | -1363.62 | 4 | 16.98 | 11.40 | -5.58 |
| FeF2 | -1463.57 | 5 | -79.00 | -93.00 | -14.00 |
| FeF3 | -1563.49 | 6 | -152.94 | -196.20 | -43.26 |
| FeCl | -1723.97 | 4 | 56.80 | 49.50 | -7.30 |
| FeCl2 | -2184.29 | 5 | -14.99 | -32.80 | -17.81 |
| FeCl3 | -2644.55 | 6 | -45.67 | -60.60 | -14.93 |

| | |
|---|---|
| mean error | -17.96 |
| abs error | 19.51 |
| rmsd | 22.74 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CoH | -1383.32 | 3 | 115.33 | 110.70 | -4.63 |
| CoO | -1457.99 | 4 | 75.47 | 74.00 | -1.47 |
| CoF2 | -1582.64 | 4 | -76.79 | -87.50 | -10.71 |
| CoCl | -1843.02 | 5 | 65.34 | 50.30 | -15.04 |
| CoCl2 | -2303.35 | 4 | -8.78 | -22.60 | -13.82 |
| CoCl3 | -2763.59 | 5 | -25.63 | -39.10 | -13.47 |

| | |
|---|---|
| mean error | -9.86 |
| abs error | 9.86 |
| rmsd | 11.08 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Ni2 | -3016.66 | 3 | 183.25 | 156.70 | -26.55 |
| NiH | -1508.91 | 2 | 92.69 | 85.60 | -7.09 |
| NiO | -1583.54 | 3 | 79.80 | 75.00 | -4.80 |
| NiS | -1906.55 | 3 | 96.35 | 81.70 | -14.65 |
| Ni(OH)2 | -1660.08 | 3 | -40.04 | -60.80 | -20.76 |
| NiCO | -1621.70 | 1 | 55.23 | 35.10 | -20.13 |
| Ni(CO)2 | -1735.12 | 1 | -8.51 | -39.00 | -30.49 |
| Ni(CO)3 | -1848.52 | 1 | -58.03 | -92.70 | -34.67 |
| Ni(CO)4 | -1961.90 | 1 | -97.29 | -144.00 | -46.71 |
| NiF | -1608.23 | 2 | 27.25 | 17.50 | -9.75 |
| NiF2 | -1708.18 | 3 | -68.09 | -77.80 | -9.71 |
| NiCl | -1968.60 | 2 | 50.31 | 41.70 | -8.61 |
| CiCl2 | -2428.90 | 3 | -2.73 | -17.40 | -14.67 |
| | | | | | |
| mean error | -22.87 | | | | |
| abs error | 19.12 | | | | |
| rmsd | 22.57 | | | | |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Cu2 | -3281.13 | 1 | 120.27 | 113.80 | -6.47 |
| CuH | -1641.13 | 1 | 73.16 | 65.90 | -7.26 |
| CuO | -1715.72 | 2 | 79.34 | 76.50 | -2.84 |
| CuOH | -1716.39 | 1 | 26.16 | 28.70 | 2.54 |
| CuS | -2038.76 | 2 | 86.35 | 75.10 | -11.25 |
| CuF | -1740.44 | 1 | 9.86 | -3.20 | -13.06 |
| CuF2 | -1840.33 | 2 | -48.18 | -66.00 | -17.82 |
| CuCl | -2100.82 | 1 | 30.55 | 19.30 | -11.25 |
| CuCl2 | -2561.06 | 2 | 12.61 | -9.00 | -21.61 |
| | | | | | |
| mean error | -9.89 | | | | |
| abs error | 10.46 | | | | |
| rmsd | 12.10 | | | | |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Zn2 | -3558.89 | 1 | 65.00 | 57.70 | -7.30 |
| ZnF2 | -1979.26 | 1 | -107.77 | -118.90 | -11.13 |
| ZnCl | -2239.68 | 2 | 15.99 | 6.50 | -9.49 |
| ZnCl2 | -2699.99 | 1 | -50.22 | -63.50 | -13.28 |
| ZnO | -1854.58 | 3 | 63.03 | 52.80 | -10.23 |
| ZnS | -2177.61 | 1 | 72.78 | 48.70 | -24.08 |
| ZnH | -1779.98 | 2 | 64.22 | 62.90 | -1.32 |
| Zn(CH3) | -1819.29 | 2 | 54.26 | 26.00 | -28.26 |
| Zn(CH3)2 | -1859.22 | 1 | 20.97 | 12.90 | -8.07 |
| | | | | | |
| mean error | -12.57 | | | | |
| abs error | 12.57 | | | | |
| rmsd | 14.88 | | | | |

# PBE1PBE

| atom | energy | mult |
|---|---|---|
| H | -0.50 | 2 |
| C | -37.81 | 3 |
| N | -54.54 | 4 |
| O | -75.02 | 3 |
| F | -99.67 | 2 |
| S | -397.97 | 3 |
| Cl | -459.99 | 2 |
| Ti | -849.14 | 5 |
| V | -943.69 | 6 |
| Cr | -1044.22 | 7 |
| Mn | -1150.76 | 6 |
| Fe | -1263.43 | 5 |
| Co | -1382.48 | 4 |
| Ni | -1508.01 | 3 |
| Cu | -1640.24 | 2 |
| Zn | -1779.14 | 1 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| TiH | -849.71 | 4 | 115.69 | 116.40 | 0.71 |
| TiN | -903.83 | 2 | 132.11 | 112.10 | -20.01 |
| TiO | -924.40 | 3 | 15.90 | 13.70 | -2.20 |
| TiS | -1247.29 | 3 | 66.16 | 76.20 | 10.04 |
| TiF | -949.02 | 4 | -2.37 | -4.00 | -1.63 |
| TiF2 | -1048.93 | 3 | -128.05 | -164.50 | -36.45 |
| TiF3 | -1148.82 | 2 | -246.92 | -284.10 | -37.18 |
| TiCl | -1309.29 | 4 | 40.27 | 24.20 | -16.07 |
| TiCl2 | -1769.47 | 3 | -50.16 | -57.00 | -6.84 |
| TiCl3 | -2229.62 | 2 | -119.41 | -128.90 | -9.49 |

| | |
|---|---|
| mean error | -11.91 |
| abs error | 14.06 |
| rmsd | 19.01 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| V2 | -1887.38 | 3 | 244.54 | 187.40 | -57.14 |
| VH | -944.28 | 5 | 118.20 | 125.90 | 7.70 |
| VN | -998.38 | 3 | 141.72 | 121.00 | -20.72 |
| VO | -1018.92 | 4 | 44.35 | 30.50 | -13.85 |
| VS | -1341.81 | 4 | 91.46 | 80.40 | -11.06 |
| VF | -1043.56 | 5 | 17.10 | 0.70 | -16.40 |
| VCl | -1403.84 | 5 | 53.16 | 37.80 | -15.36 |
| VCl2 | -1863.98 | 4 | -10.70 | -51.60 | -40.90 |
| VCl3 | -2324.12 | 3 | -71.43 | -88.20 | -16.77 |

| | |
|---|---|
| mean error | -20.50 |
| abs error | 22.21 |
| rmsd | 26.93 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CrH | -1044.79 | 6 | 101.50 | 80.20 | -21.30 |
| CrN | -1098.87 | 4 | 146.02 | 120.70 | -25.32 |
| CrO | -1119.37 | 5 | 68.79 | 45.00 | -23.79 |
| CrO2 | -1194.56 | 3 | 20.31 | -18.00 | -38.31 |
| CrO3 | -1269.71 | 1 | -3.73 | -70.50 | -66.77 |
| CrOH | -1120.01 | 6 | 37.26 | 18.90 | -18.36 |
| Cr(OH)2 | -1195.82 | 5 | -42.31 | -78.10 | -35.79 |
| CrS | -1442.30 | 5 | 95.83 | 78.20 | -17.63 |

| | | | | | |
|---|---|---|---|---|---|
| CrF | -1144.06 | 6 | 9.94 | 3.10 | -6.84 |
| CrF2 | -1243.91 | 5 | -80.97 | -99.10 | -18.13 |
| CrF3 | -1343.74 | 4 | -160.06 | -199.80 | -39.74 |
| CrCl | -1504.35 | 6 | 40.12 | 31.00 | -9.12 |
| CrCl2 | -1964.47 | 5 | -13.03 | -28.10 | -15.07 |
| CrCl3 | -2424.56 | 4 | -46.51 | -67.70 | -21.19 |

| | |
|---|---|
| mean error | -25.53 |
| abs error | 25.53 |
| rmsd | 29.56 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| MnF | -1250.60 | 7 | -18.52 | -19.90 | -1.38 |
| MnF2 | -1350.47 | 6 | -123.20 | -126.20 | -3.00 |
| MnF3 | -1450.24 | 5 | -167.84 | -188.00 | -20.16 |
| MnCl | -1610.89 | 7 | 12.59 | 11.30 | -1.29 |
| MnCl2 | -2071.04 | 6 | -61.71 | -63.00 | -1.29 |
| MnH | -1151.32 | 7 | 82.47 | 64.20 | -18.27 |
| MnO | -1225.91 | 6 | 42.43 | 29.60 | -12.83 |
| MnOH | -1226.55 | 7 | 3.87 | 3.70 | -0.17 |
| MnS | -1548.84 | 6 | 64.04 | 63.30 | -0.74 |

| | |
|---|---|
| mean error | -6.57 |
| abs error | 6.57 |
| rmsd | 10.11 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Fe2 | -2526.83 | 7 | 216.39 | 172.40 | -43.99 |
| FeH | -1264.00 | 4 | 110.14 | 117.20 | 7.06 |
| FeO | -1338.59 | 5 | 68.75 | 61.10 | -7.65 |
| FeS | -1661.51 | 5 | 94.46 | 83.80 | -10.66 |
| Fe(OH)2 | -1415.04 | 6 | -43.04 | -79.00 | -35.96 |
| FeCO | -1376.67 | 5 | 68.24 | 63.90 | -4.34 |
| Fe(CO)2 | -1489.93 | 3 | 18.38 | 0.20 | -18.18 |
| Fe(CO)3 | -1603.20 | 3 | -36.64 | -55.80 | -19.16 |
| Fe(CO)4 | -1716.45 | 3 | -77.49 | -105.10 | -27.61 |
| FeF | -1363.26 | 4 | 18.66 | 11.40 | -7.26 |
| FeF2 | -1463.15 | 5 | -97.53 | -93.00 | 4.53 |
| FeF3 | -1562.94 | 6 | -152.22 | -196.20 | -43.98 |
| FeCl | -1723.54 | 6 | 54.57 | 49.50 | -5.07 |
| FeCl2 | -2183.70 | 5 | -22.86 | -32.80 | -9.94 |
| FeCl3 | -2643.79 | 6 | -56.05 | -60.60 | -4.55 |

| | |
|---|---|
| mean error | -15.12 |
| abs error | 16.66 |
| rmsd | 21.73 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CoH | -1383.04 | 3 | 119.21 | 110.70 | -8.51 |
| CoO | -1457.63 | 4 | 80.34 | 74.00 | -6.34 |
| CoF2 | -1582.17 | 4 | -75.79 | -87.50 | -11.71 |
| CoCl | -1842.59 | 5 | 57.83 | 50.30 | -7.53 |
| CoCl2 | -2302.76 | 4 | -20.90 | -22.60 | -1.70 |
| CoCl3 | -2762.81 | 5 | -33.91 | -39.10 | -5.19 |

| | |
|---|---|
| mean error | -6.83 |
| abs error | 6.83 |
| rmsd | 7.49 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Ni2 | -3016.07 | 3 | 179.90 | 156.70 | -23.20 |
| NiH | -1508.61 | 2 | 91.24 | 85.60 | -5.64 |
| NiO | -1583.16 | 3 | 79.21 | 75.00 | -4.21 |
| NiS | -1906.11 | 3 | 90.82 | 81.70 | -9.12 |
| Ni(OH)2 | -1659.63 | 3 | -41.68 | -60.80 | -19.12 |
| NiCO | -1621.28 | 1 | 49.93 | 35.10 | -14.83 |
| Ni(CO)2 | -1734.57 | 1 | -15.80 | -39.00 | -23.20 |
| Ni(CO)3 | -1847.85 | 1 | -69.58 | -92.70 | -23.12 |
| Ni(CO)4 | -1961.10 | 1 | -114.04 | -144.00 | -29.96 |
| NiF | -1607.84 | 2 | 23.14 | 17.50 | -5.64 |
| NiF2 | -1707.70 | 3 | -72.25 | -77.80 | -5.55 |
| NiCl | -1968.15 | 2 | 41.82 | 41.70 | -0.12 |
| CiCl2 | -2428.28 | 3 | -16.24 | -17.40 | -1.16 |

| | |
|---|---|
| mean error | -16.93 |
| abs error | 12.68 |
| rmsd | 15.91 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Cu2 | -3280.54 | 1 | 121.84 | 113.80 | -8.04 |
| CuH | -1640.82 | 1 | 76.67 | 65.90 | -10.77 |
| CuO | -1715.34 | 2 | 81.73 | 76.50 | -5.23 |
| CuOH | -1716.01 | 1 | 28.93 | 28.70 | -0.23 |
| CuS | -2038.30 | 2 | 84.43 | 75.10 | -9.33 |
| CuF | -1740.05 | 1 | 11.26 | -3.20 | -14.46 |
| CuF2 | -1839.84 | 2 | -45.98 | -66.00 | -20.02 |
| CuCl | -2100.36 | 1 | 26.93 | 19.30 | -7.63 |
| CuCl2 | -2560.44 | 2 | 4.26 | -9.00 | -13.26 |

| | |
|---|---|
| mean error | -9.88 |
| abs error | 9.88 |
| rmsd | 11.25 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Zn2 | -3558.27 | 1 | 63.66 | 57.70 | -5.96 |
| ZnF2 | -1978.77 | 1 | -110.48 | -118.90 | -8.42 |
| ZnCl | -2239.21 | 2 | 8.84 | 6.50 | -2.34 |
| ZnCl2 | -2699.36 | 1 | -61.71 | -63.50 | -1.79 |
| ZnO | -1854.20 | 3 | 60.76 | 52.80 | -7.96 |
| ZnS | -2177.15 | 1 | 67.91 | 48.70 | -19.21 |
| ZnH | -1779.67 | 2 | 63.34 | 62.90 | -0.44 |
| Zn(CH3) | -1818.93 | 2 | 50.36 | 26.00 | -24.36 |
| Zn(CH3)2 | -1858.81 | 1 | 14.50 | 12.90 | -1.60 |

| | |
|---|---|
| mean error | -8.01 |
| abs error | 8.01 |
| rmsd | 11.27 |

| atom | energy | mult |
|---|---|---|
| H | -0.50 | 2 |
| C | -37.84 | 3 |
| N | -54.58 | 4 |
| O | -75.07 | 3 |
| F | -99.73 | 2 |
| S | -398.07 | 3 |
| Cl | -460.10 | 2 |
| Ti | -849.28 | 3 |
| V | -943.82 | 6 |
| Cr | -1044.36 | 7 |
| Mn | -1150.93 | 6 |
| Fe | -1263.58 | 5 |
| Co | -1382.68 | 4 |
| Ni | -1508.24 | 3 |
| Cu | -1640.47 | 2 |
| Zn | -1779.39 | 1 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| TiH | -849.86 | 2 | 116.73 | 116.40 | -0.33 |
| TiN | -904.03 | 2 | 121.02 | 112.10 | -8.92 |
| TiO | -924.59 | 3 | 18.67 | 13.70 | -4.97 |
| TiS | -1247.52 | 3 | 69.77 | 76.20 | 6.43 |
| TiF | -949.21 | 4 | 4.18 | -4.00 | -8.18 |
| TiF2 | -1049.19 | 3 | -127.09 | -164.50 | -37.41 |
| TiF3 | -1149.14 | 2 | -250.52 | -284.10 | -33.58 |
| TiCl | -1309.53 | 2 | 46.60 | 24.20 | -22.40 |
| TiCl2 | -1769.83 | 3 | -46.33 | -57.00 | -10.67 |
| TiCl3 | -2230.09 | 2 | -118.35 | -128.90 | -10.55 |

| | |
|---|---|
| mean error | -13.06 |
| abs error | 14.34 |
| rmsd | 18.62 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| V2 | -1887.68 | 3 | 219.06 | 187.40 | -31.66 |
| VH | -944.42 | 5 | 111.60 | 125.90 | 14.30 |
| VN | -998.57 | 3 | 131.00 | 121.00 | -10.00 |
| VO | -1019.08 | 4 | 59.96 | 30.50 | -29.46 |
| VS | -1342.04 | 4 | 96.33 | 80.40 | -15.93 |
| VF | -1043.75 | 5 | 14.28 | 0.70 | -13.58 |
| VCl | -1404.08 | 5 | 48.94 | 37.80 | -11.14 |
| VCl2 | -1864.36 | 4 | -31.60 | -51.60 | -20.00 |
| VCl3 | -2324.59 | 3 | -82.44 | -88.20 | -5.76 |

| | |
|---|---|
| mean error | -13.69 |
| abs error | 16.87 |
| rmsd | 18.77 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CrH | -1044.94 | 6 | 94.82 | 80.20 | -14.62 |
| CrN | -1099.06 | 4 | 136.07 | 120.70 | -15.37 |
| CrO | -1119.57 | 5 | 59.61 | 45.00 | -14.61 |
| CrO2 | -1194.79 | 3 | 21.60 | -18.00 | -39.60 |
| CrO3 | -1270.03 | 1 | -30.15 | -70.50 | -40.35 |
| CrOH | -1120.20 | 6 | 30.17 | 18.90 | -11.27 |
| Cr(OH)2 | -1196.08 | 5 | -55.88 | -78.10 | -22.22 |
| CrS | -1442.54 | 5 | 88.01 | 78.20 | -9.81 |

| | | | | | |
|---|---|---|---|---|---|
| CrF | -1144.27 | 6 | 3.61 | 3.10 | -0.51 |
| CrF2 | -1244.18 | 5 | -93.56 | -99.10 | -5.54 |
| CrF3 | -1344.08 | 4 | -178.37 | -199.80 | -21.43 |
| CrCl | -1504.60 | 6 | 35.23 | 31.00 | -4.23 |
| CrCl2 | -1964.83 | 5 | -17.41 | -28.10 | -10.69 |
| CrCl3 | -2425.05 | 4 | -59.54 | -67.70 | -8.16 |

| | |
|---|---|
| mean error | -15.60 |
| abs error | 15.60 |
| rmsd | 19.39 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| MnF | -1250.81 | 7 | -7.82 | -19.90 | -12.08 |
| MnF2 | -1350.75 | 6 | -119.81 | -126.20 | -6.39 |
| MnF3 | -1450.60 | 5 | -171.31 | -188.00 | -16.69 |
| MnCl | -1611.14 | 7 | 24.98 | 11.30 | -13.68 |
| MnCl2 | -2071.42 | 6 | -55.44 | -63.00 | -7.56 |
| MnH | -1151.48 | 5 | 85.33 | 64.20 | -21.13 |
| MnO | -1226.12 | 6 | 48.16 | 29.60 | -18.56 |
| MnOH | -1226.76 | 7 | 13.78 | 3.70 | -10.08 |
| MnS | -1549.10 | 6 | 69.54 | 63.30 | -6.24 |

| | |
|---|---|
| mean error | -12.49 |
| abs error | 12.49 |
| rmsd | 13.50 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Fe2 | -2527.21 | 7 | 169.61 | 172.40 | 2.79 |
| FeH | -1264.17 | 6 | 97.15 | 117.20 | 20.05 |
| FeO | -1338.79 | 7 | 67.80 | 61.10 | -6.70 |
| FeS | -1661.80 | 5 | 70.46 | 83.80 | 13.34 |
| Fe(OH)2 | -1415.35 | 6 | -79.89 | -79.00 | 0.89 |
| FeCO | -1376.92 | 5 | 53.11 | 63.90 | 10.79 |
| Fe(CO)2 | -1490.29 | 3 | -4.37 | 0.20 | 4.57 |
| Fe(CO)3 | -1603.64 | 3 | -59.27 | -55.80 | 3.47 |
| Fe(CO)4 | -1716.99 | 3 | -108.83 | -105.10 | 3.73 |
| FeF | -1363.48 | 6 | 10.72 | 11.40 | 0.68 |
| FeF2 | -1463.43 | 5 | -102.02 | -93.00 | 9.02 |
| FeF3 | -1563.31 | 6 | -176.48 | -196.20 | -19.72 |
| FeCl | -1723.84 | 4 | 26.43 | 49.50 | 23.07 |
| FeCl2 | -2184.10 | 5 | -43.28 | -32.80 | 10.48 |
| FeCl3 | -2644.30 | 6 | -75.55 | -60.60 | 14.95 |

| | |
|---|---|
| mean error | 6.09 |
| abs error | 9.62 |
| rmsd | 11.92 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CoH | -1383.25 | 3 | 109.18 | 110.70 | 1.52 |
| CoO | -1457.86 | 4 | 90.31 | 74.00 | -16.31 |
| CoF2 | -1582.49 | 4 | -78.01 | -87.50 | -9.49 |
| CoCl | -1842.90 | 3 | 55.69 | 50.30 | -5.39 |
| CoCl2 | -2303.16 | 4 | -14.87 | -22.60 | -7.73 |
| CoCl3 | -2763.34 | 5 | -33.05 | -39.10 | -6.05 |

| | |
|---|---|
| mean error | -7.24 |
| abs error | 7.75 |
| rmsd | 8.98 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Ni2 | -3016.52 | 5 | 178.95 | 156.70 | -22.25 |
| NiH | -1508.84 | 2 | 92.42 | 85.60 | -6.82 |
| NiO | -1583.44 | 3 | 78.41 | 75.00 | -3.41 |
| NiS | -1906.43 | 3 | 92.03 | 81.70 | -10.33 |
| Ni(OH)2 | -1659.95 | 3 | -41.37 | -60.80 | -19.43 |
| NiCO | -1621.59 | 1 | 50.78 | 35.10 | -15.68 |
| Ni(CO)2 | -1734.97 | 1 | -14.51 | -39.00 | -24.49 |
| Ni(CO)3 | -1848.32 | 1 | -66.91 | -92.70 | -25.79 |
| Ni(CO)4 | -1961.66 | 1 | -109.48 | -144.00 | -34.52 |
| NiF | -1608.12 | 2 | 24.83 | 17.50 | -7.33 |
| NiF2 | -1708.04 | 3 | -70.80 | -77.80 | -7.00 |
| NiCl | -1968.48 | 2 | 44.93 | 41.70 | -3.23 |
| CiCl2 | -2428.70 | 3 | -2.01 | -17.40 | -15.39 |
| | | | | | |
| mean error | -18.08 | | | | |
| abs error | 15.05 | | | | |
| rmsd | 17.74 | | | | |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Cu2 | -3281.01 | 1 | 116.16 | 113.80 | -2.36 |
| CuH | -1641.06 | 1 | 72.81 | 65.90 | -6.91 |
| CuO | -1715.63 | 2 | 77.77 | 76.50 | -1.27 |
| CuOH | -1716.30 | 1 | 24.22 | 28.70 | 4.48 |
| CuS | -2038.64 | 2 | 81.78 | 75.10 | -6.68 |
| CuF | -1740.35 | 1 | 6.97 | -3.20 | -10.17 |
| CuF2 | -1840.20 | 2 | -50.06 | -66.00 | -15.94 |
| CuCl | -2100.70 | 1 | 24.88 | 19.30 | -5.58 |
| CuCl2 | -2560.90 | 2 | -2.40 | -9.00 | -6.60 |
| | | | | | |
| mean error | -5.67 | | | | |
| abs error | 6.67 | | | | |
| rmsd | 7.83 | | | | |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Zn2 | -3558.78 | 1 | 64.04 | 57.70 | -6.34 |
| ZnF2 | -1979.14 | 1 | -111.10 | -118.90 | -7.80 |
| ZnCl | -2239.57 | 2 | 13.45 | 6.50 | -6.95 |
| ZnCl2 | -2699.83 | 1 | -58.29 | -63.50 | -5.21 |
| ZnO | -1854.50 | 3 | 63.42 | 52.80 | -10.62 |
| ZnS | -2177.51 | 1 | 67.97 | 48.70 | -19.27 |
| ZnH | -1779.92 | 2 | 66.03 | 62.90 | -3.13 |
| Zn(CH3) | -1819.21 | 2 | 55.12 | 26.00 | -29.12 |
| Zn(CH3)2 | -1859.13 | 1 | 20.29 | 12.90 | -7.39 |
| | | | | | |
| mean error | -10.65 | | | | |
| abs error | 10.65 | | | | |
| rmsd | 13.22 | | | | |

# TPSSTPSS

| atom | energy | mult |
|---|---|---|
| H | -0.50 | 2 |
| C | -37.86 | 3 |
| N | -54.61 | 4 |
| O | -75.10 | 3 |
| F | -99.77 | 2 |
| S | -398.13 | 3 |
| Cl | -460.17 | 2 |
| Ti | -849.36 | 5 |
| V | -943.92 | 6 |
| Cr | -1044.46 | 7 |
| Mn | -1150.99 | 6 |
| Fe | -1263.68 | 5 |
| Co | -1382.71 | 2 |
| Ni | -1508.30 | 3 |
| Cu | -1640.51 | 2 |
| Zn | -1779.39 | 1 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| TiH | -849.95 | 4 | 108.05 | 116.40 | 8.35 |
| TiN | -904.17 | 2 | 102.32 | 112.10 | 9.78 |
| TiO | -924.74 | 3 | -0.23 | 13.70 | 13.93 |
| TiS | -1247.69 | 3 | 52.76 | 76.20 | 23.44 |
| TiF | -949.35 | 4 | -7.65 | -4.00 | 3.65 |
| TiF2 | -1049.37 | 3 | -143.57 | -164.50 | -20.93 |
| TiF3 | -1149.37 | 2 | -270.79 | -284.10 | -13.31 |
| TiCl | -1309.69 | 4 | 37.62 | 24.20 | -13.42 |
| TiCl2 | -1770.05 | 3 | -57.59 | -57.00 | 0.59 |
| TiCl3 | -2230.39 | 2 | -133.88 | -128.90 | 4.98 |

| | |
|---|---|
| mean error | 1.71 |
| abs error | 11.24 |
| rmsd | 13.20 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| V2 | -1887.95 | 3 | 179.35 | 187.40 | 8.05 |
| VH | -944.52 | 5 | 108.99 | 125.90 | 16.91 |
| VN | -998.73 | 3 | 114.02 | 121.00 | 6.98 |
| VO | -1019.27 | 4 | 23.98 | 30.50 | 6.52 |
| VS | -1342.23 | 4 | 74.76 | 80.40 | 5.64 |
| VF | -1043.90 | 5 | 7.77 | 0.70 | -7.07 |
| VCl | -1404.25 | 5 | 48.11 | 37.80 | -10.31 |
| VCl2 | -1864.59 | 4 | -33.91 | -51.60 | -17.69 |
| VCl3 | -2324.89 | 3 | -91.64 | -88.20 | 3.44 |

| | |
|---|---|
| mean error | 1.39 |
| abs error | 9.18 |
| rmsd | 10.30 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CrH | -1045.04 | 6 | 92.56 | 80.20 | -12.36 |
| CrN | -1099.22 | 4 | 117.30 | 120.70 | 3.40 |
| CrO | -1119.73 | 5 | 46.33 | 45.00 | -1.33 |
| CrO2 | -1195.04 | 3 | -25.61 | -18.00 | 7.61 |
| CrO3 | -1270.33 | 1 | -80.40 | -70.50 | 9.90 |
| CrOH | -1120.34 | 6 | 29.15 | 18.90 | -10.25 |
| Cr(OH)2 | -1196.26 | 5 | -58.21 | -78.10 | -19.89 |
| CrS | -1442.71 | 5 | 82.60 | 78.20 | -4.40 |

| | | | | | |
|---|---|---|---|---|---|
| CrF | -1144.41 | 6 | 0.54 | 3.10 | 2.56 |
| CrF2 | -1244.37 | 5 | -98.39 | -99.10 | -0.71 |
| CrF3 | -1344.31 | 4 | -190.65 | -199.80 | -9.15 |
| CrCl | -1504.76 | 6 | 35.55 | 31.00 | -4.55 |
| CrCl2 | -1965.07 | 5 | -22.61 | -28.10 | -5.49 |
| CrCl3 | -2425.35 | 4 | -68.77 | -67.70 | 1.07 |

| | |
|---|---|
| mean error | -3.11 |
| abs error | 6.62 |
| rmsd | 8.39 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| MnF | -1250.94 | 7 | -27.31 | -19.90 | 7.41 |
| MnF2 | -1350.92 | 6 | -140.55 | -126.20 | 14.35 |
| MnF3 | -1450.82 | 5 | -204.61 | -188.00 | 16.61 |
| MnCl | -1611.30 | 7 | 7.51 | 11.30 | 3.79 |
| MnCl2 | -2071.63 | 6 | -71.27 | -63.00 | 8.27 |
| MnH | -1151.56 | 5 | 73.68 | 64.20 | -9.48 |
| MnO | -1226.27 | 6 | 15.48 | 29.60 | 14.12 |
| MnOH | -1226.88 | 7 | -4.78 | 3.70 | 8.48 |
| MnS | -1549.26 | 6 | 45.42 | 63.30 | 17.88 |

| | |
|---|---|
| mean error | 9.05 |
| abs error | 11.15 |
| rmsd | 12.02 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Fe2 | -2527.43 | 7 | 158.95 | 172.40 | 13.45 |
| FeH | -1264.27 | 4 | 96.63 | 117.20 | 20.57 |
| FeO | -1338.97 | 5 | 44.01 | 61.10 | 17.09 |
| FeS | -1661.96 | 5 | 74.15 | 83.80 | 9.65 |
| Fe(OH)2 | -1415.51 | 6 | -69.07 | -79.00 | -9.93 |
| FeCO | -1377.09 | 3 | 51.12 | 63.90 | 12.78 |
| Fe(CO)2 | -1490.53 | 3 | -14.67 | 0.20 | 14.87 |
| Fe(CO)3 | -1603.96 | 3 | -76.11 | -55.80 | 20.31 |
| Fe(CO)4 | -1717.37 | 1 | -128.03 | -105.10 | 22.93 |
| FeF | -1363.63 | 6 | 6.76 | 11.40 | 4.64 |
| FeF2 | -1463.62 | 5 | -110.43 | -93.00 | 17.43 |
| FeF3 | -1563.52 | 6 | -173.42 | -196.20 | -22.78 |
| FeCl | -1723.98 | 6 | 43.56 | 49.50 | 5.94 |
| FeCl2 | -2184.33 | 5 | -39.39 | -32.80 | 6.59 |
| FeCl3 | -2644.59 | 6 | -72.25 | -60.60 | 11.65 |

| | |
|---|---|
| mean error | 9.68 |
| abs error | 14.04 |
| rmsd | 15.21 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CoH | -1383.33 | 3 | 76.08 | 110.70 | 34.62 |
| CoO | -1458.02 | 4 | 32.41 | 74.00 | 41.59 |
| CoF2 | -1582.65 | 4 | -113.47 | -87.50 | 25.97 |
| CoCl | -1843.04 | 3 | 26.83 | 50.30 | 23.47 |
| CoCl2 | -2303.38 | 4 | -52.22 | -22.60 | 29.62 |
| CoCl3 | -2763.63 | 5 | -78.86 | -39.10 | 39.76 |

| | |
|---|---|
| mean error | 32.50 |
| abs error | 32.50 |
| rmsd | 33.19 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Ni2 | -3016.67 | 3 | 153.71 | 156.70 | 2.99 |
| NiH | -1508.90 | 2 | 88.51 | 85.60 | -2.91 |
| NiO | -1583.56 | 3 | 58.84 | 75.00 | 16.16 |
| NiS | -1906.57 | 3 | 76.33 | 81.70 | 5.37 |
| Ni(OH)2 | -1660.10 | 3 | -52.80 | -60.80 | -8.00 |
| NiCO | -1621.74 | 1 | 30.89 | 35.10 | 4.21 |
| Ni(CO)2 | -1735.19 | 1 | -41.03 | -39.00 | 2.03 |
| Ni(CO)3 | -1848.61 | 1 | -97.55 | -92.70 | 4.85 |
| Ni(CO)4 | -1962.01 | 1 | -145.38 | -144.00 | 1.38 |
| NiF | -1608.23 | 2 | 18.99 | 17.50 | -1.49 |
| NiF2 | -1708.19 | 3 | -82.13 | -77.80 | 4.33 |
| NiCl | -1968.60 | 2 | 44.06 | 41.70 | -2.36 |
| CiCl2 | -2428.92 | 3 | -22.79 | -17.40 | 5.39 |

| | |
|---|---|
| mean error | 2.89 |
| abs error | 4.73 |
| rmsd | 6.04 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Cu2 | -3281.09 | 1 | 113.38 | 113.80 | 0.42 |
| CuH | -1641.11 | 1 | 67.95 | 65.90 | -2.05 |
| CuO | -1715.72 | 2 | 69.15 | 76.50 | 7.35 |
| CuOH | -1716.38 | 1 | 19.47 | 28.70 | 9.23 |
| CuS | -2038.75 | 2 | 76.87 | 75.10 | -1.77 |
| CuF | -1740.43 | 1 | 2.93 | -3.20 | -6.13 |
| CuF2 | -1840.34 | 2 | -63.70 | -66.00 | -2.30 |
| CuCl | -2100.81 | 1 | 23.74 | 19.30 | -4.44 |
| CuCl2 | -2561.08 | 2 | -13.91 | -9.00 | 4.91 |

| | |
|---|---|
| mean error | 0.58 |
| abs error | 4.29 |
| rmsd | 5.09 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Zn2 | -3558.79 | 1 | 62.85 | 57.70 | -5.15 |
| ZnF2 | -1979.23 | 1 | -119.44 | -118.90 | 0.54 |
| ZnCl | -2239.64 | 2 | 8.08 | 6.50 | -1.58 |
| ZnCl2 | -2699.96 | 1 | -62.63 | -63.50 | -0.87 |
| ZnO | -1854.55 | 1 | 56.05 | 52.80 | -3.25 |
| ZnS | -2177.58 | 1 | 62.61 | 48.70 | -13.91 |
| ZnH | -1779.93 | 2 | 58.25 | 62.90 | 4.65 |
| Zn(CH3) | -1819.25 | 2 | 44.47 | 26.00 | -18.47 |
| Zn(CH3)2 | -1859.19 | 1 | 4.12 | 12.90 | 8.78 |

| | |
|---|---|
| mean error | -3.25 |
| abs error | 6.36 |
| rmsd | 8.65 |

# TPSSKCIS

| atom | energy | mult |
|---|---|---|
| H | -0.50 | 2 |
| C | -37.86 | 3 |
| N | -54.61 | 4 |
| O | -75.10 | 3 |
| F | -99.78 | 2 |
| S | -398.16 | 3 |
| Cl | -460.20 | 2 |
| Ti | -849.41 | 5 |
| V | -943.98 | 6 |
| Cr | -1044.52 | 7 |
| Mn | -1151.05 | 6 |
| Fe | -1263.72 | 3 |
| Co | -1382.82 | 4 |
| Ni | -1508.38 | 3 |
| Cu | -1640.60 | 2 |
| Zn | -1779.49 | 1 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| TiH | -850.00 | 4 | 109.83 | 116.40 | 6.57 |
| TiN | -904.23 | 2 | 96.60 | 112.10 | 15.50 |
| TiO | -924.80 | 3 | -3.40 | 13.70 | 17.10 |
| TiS | -1247.78 | 3 | 51.71 | 76.20 | 24.49 |
| TiF | -949.42 | 4 | -9.21 | -4.00 | 5.21 |
| TiF2 | -1049.44 | 3 | -145.38 | -164.50 | -19.12 |
| TiF3 | -1149.45 | 2 | -273.38 | -284.10 | -10.72 |
| TiCl | -1309.79 | 4 | 32.28 | 24.20 | -8.08 |
| TiCl2 | -1770.17 | 3 | -56.81 | -57.00 | -0.19 |
| TiCl3 | -2230.53 | 2 | -133.25 | -128.90 | 4.35 |

| | |
|---|---|
| mean error | 3.51 |
| abs error | 11.13 |
| rmsd | 13.29 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| V2 | -1888.07 | 3 | 175.21 | 187.40 | 12.19 |
| VH | -944.58 | 5 | 111.33 | 125.90 | 14.57 |
| VN | -998.79 | 3 | 108.52 | 121.00 | 12.48 |
| VO | -1019.34 | 4 | 20.38 | 30.50 | 10.12 |
| VS | -1342.32 | 4 | 73.59 | 80.40 | 6.81 |
| VF | -1043.97 | 5 | 6.80 | 0.70 | -6.10 |
| VCl | -1404.34 | 5 | 48.67 | 37.80 | -10.87 |
| VCl2 | -1864.71 | 4 | -33.49 | -51.60 | -18.11 |
| VCl3 | -2325.04 | 3 | -91.16 | -88.20 | 2.96 |

| | |
|---|---|
| mean error | 2.67 |
| abs error | 10.47 |
| rmsd | 11.34 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CrH | -1045.10 | 6 | 94.85 | 80.20 | -14.65 |
| CrN | -1099.28 | 4 | 111.50 | 120.70 | 9.20 |
| CrO | -1119.80 | 5 | 42.87 | 45.00 | 2.13 |
| CrO2 | -1195.12 | 3 | -32.25 | -18.00 | 14.25 |
| CrO3 | -1270.40 | 1 | -89.88 | -70.50 | 19.38 |
| CrOH | -1120.40 | 6 | 28.11 | 18.90 | -9.21 |
| Cr(OH)2 | -1196.32 | 5 | -60.59 | -78.10 | -17.51 |
| CrS | -1442.80 | 5 | 81.81 | 78.20 | -3.61 |

| | | | | | |
|---|---|---|---|---|---|
| CrF | -1144.48 | 6 | -0.23 | 3.10 | 3.33 |
| CrF2 | -1244.44 | 5 | -100.16 | -99.10 | 1.06 |
| CrF3 | -1344.40 | 4 | -194.24 | -199.80 | -5.56 |
| CrCl | -1504.85 | 6 | 36.23 | 31.00 | -5.23 |
| CrCl2 | -1965.19 | 5 | -22.02 | -28.10 | -6.08 |
| CrCl3 | -2425.50 | 4 | -68.65 | -67.70 | 0.95 |

| | |
|---|---|
| mean error | -0.82 |
| abs error | 8.01 |
| rmsd | 9.98 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| MnF | -1251.01 | 7 | -26.88 | -19.90 | 6.98 |
| MnF2 | -1351.00 | 6 | -140.77 | -126.20 | 14.57 |
| MnF3 | -1450.91 | 5 | -206.29 | -188.00 | 18.29 |
| MnCl | -1611.39 | 7 | 9.22 | 11.30 | 2.08 |
| MnCl2 | -2071.75 | 6 | -69.15 | -63.00 | 6.15 |
| MnH | -1151.62 | 5 | 74.87 | 64.20 | -10.67 |
| MnO | -1226.34 | 6 | 13.04 | 29.60 | 16.56 |
| MnOH | -1226.95 | 7 | -4.72 | 3.70 | 8.42 |
| MnS | -1549.35 | 6 | 45.23 | 63.30 | 18.07 |

| | |
|---|---|
| mean error | 8.94 |
| abs error | 11.31 |
| rmsd | 12.57 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Fe2 | -2527.58 | 7 | 116.09 | 172.40 | 56.31 |
| FeH | -1264.34 | 4 | 77.68 | 117.20 | 39.52 |
| FeO | -1339.04 | 5 | 21.51 | 61.10 | 39.59 |
| FeS | -1662.06 | 5 | 53.48 | 83.80 | 30.32 |
| Fe(OH)2 | -1415.58 | 6 | -90.15 | -79.00 | 11.15 |
| FeCO | -1377.17 | 3 | 24.28 | 63.90 | 39.62 |
| Fe(CO)2 | -1490.61 | 3 | -46.11 | 0.20 | 46.31 |
| Fe(CO)3 | -1604.05 | 3 | -111.86 | -55.80 | 56.06 |
| Fe(CO)4 | -1717.47 | 3 | -173.14 | -105.10 | 68.04 |
| FeF | -1363.71 | 6 | -13.08 | 11.40 | 24.48 |
| FeF2 | -1463.70 | 5 | -130.88 | -93.00 | 37.88 |
| FeF3 | -1563.61 | 6 | -193.83 | -196.20 | -2.37 |
| FeCl | -1724.08 | 6 | 24.78 | 49.50 | 24.72 |
| FeCl2 | -2184.46 | 5 | -57.69 | -32.80 | 24.89 |
| FeCl3 | -2644.75 | 6 | -90.04 | -60.60 | 29.44 |

| | |
|---|---|
| mean error | 35.06 |
| abs error | 35.38 |
| rmsd | 39.13 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CoH | -1383.41 | 3 | 99.30 | 110.70 | 11.40 |
| CoO | -1458.10 | 4 | 52.19 | 74.00 | 21.81 |
| CoF2 | -1582.75 | 4 | -91.47 | -87.50 | 3.97 |
| CoCl | -1843.15 | 3 | 49.02 | 50.30 | 1.28 |
| CoCl2 | -2303.51 | 4 | -28.25 | -22.60 | 5.65 |
| CoCl3 | -2763.80 | 5 | -54.77 | -39.10 | 15.67 |

| | |
|---|---|
| mean error | 9.96 |
| abs error | 9.96 |
| rmsd | 12.25 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Ni2 | -3016.85 | 3 | 154.11 | 156.70 | 2.59 |
| NiH | -1508.98 | 2 | 90.64 | 85.60 | -5.04 |
| NiO | -1583.65 | 3 | 57.68 | 75.00 | 17.32 |
| NiS | -1906.69 | 3 | 76.72 | 81.70 | 4.98 |
| Ni(OH)2 | -1660.19 | 3 | -52.84 | -60.80 | -7.96 |
| NiCO | -1621.83 | 1 | 25.87 | 35.10 | 9.23 |
| Ni(CO)2 | -1735.29 | 1 | -50.72 | -39.00 | 11.72 |
| Ni(CO)3 | -1848.71 | 1 | -111.56 | -92.70 | 18.86 |
| Ni(CO)4 | -1962.12 | 1 | -163.37 | -144.00 | 19.37 |
| NiF | -1608.32 | 2 | 19.15 | 17.50 | -1.65 |
| NiF2 | -1708.29 | 3 | -81.37 | -77.80 | 3.57 |
| NiCl | -1968.72 | 2 | 45.31 | 41.70 | -3.61 |
| CiCl2 | -2429.05 | 3 | -15.00 | -17.40 | -2.40 |
| | | | | | |
| mean error | 7.90 | | | | |
| abs error | 8.33 | | | | |
| rmsd | 10.41 | | | | |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Cu2 | -3281.28 | 1 | 114.88 | 113.80 | -1.08 |
| CuH | -1641.20 | 1 | 70.53 | 65.90 | -4.63 |
| CuO | -1715.82 | 2 | 68.61 | 76.50 | 7.89 |
| CuOH | -1716.48 | 1 | 19.46 | 28.70 | 9.24 |
| CuS | -2038.87 | 2 | 77.86 | 75.10 | -2.76 |
| CuF | -1740.53 | 1 | 3.28 | -3.20 | -6.48 |
| CuF2 | -1840.44 | 2 | -63.12 | -66.00 | -2.88 |
| CuCl | -2100.93 | 1 | 25.37 | 19.30 | -6.07 |
| CuCl2 | -2561.23 | 2 | -11.42 | -9.00 | 2.42 |
| | | | | | |
| mean error | -0.48 | | | | |
| abs error | 4.83 | | | | |
| rmsd | 5.49 | | | | |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Zn2 | -3558.99 | 1 | 63.52 | 57.70 | -5.82 |
| ZnF2 | -1979.35 | 1 | -118.59 | -118.90 | -0.31 |
| ZnCl | -2239.77 | 2 | 9.69 | 6.50 | -3.19 |
| ZnCl2 | -2700.12 | 1 | -59.65 | -63.50 | -3.85 |
| ZnO | -1854.65 | 1 | 54.93 | 52.80 | -2.13 |
| ZnS | -2177.71 | 1 | 63.52 | 48.70 | -14.82 |
| ZnH | -1780.03 | 2 | 61.86 | 62.90 | 1.04 |
| Zn(CH3) | -1819.34 | 2 | 48.21 | 26.00 | -22.21 |
| Zn(CH3)2 | -1859.27 | 1 | 12.06 | 12.90 | 0.84 |
| | | | | | |
| mean error | -5.61 | | | | |
| abs error | 6.02 | | | | |
| rmsd | 9.30 | | | | |

# BB95

| atom | energy | mult |
|---|---|---|
| H | -0.50 | 2 |
| C | -37.84 | 3 |
| N | -54.59 | 4 |
| O | -75.08 | 3 |
| F | -99.76 | 2 |
| S | -398.15 | 3 |
| Cl | -460.20 | 2 |
| Ti | -849.47 | 3 |
| V | -944.04 | 6 |
| Cr | -1044.61 | 7 |
| Mn | -1151.16 | 6 |
| Fe | -1263.87 | 5 |
| Co | -1382.96 | 4 |
| Ni | -1508.55 | 3 |
| Cu | -1640.81 | 2 |
| Zn | -1779.73 | 1 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| TiH | -850.06 | 4 | 105.35 | 116.40 | 11.05 |
| TiN | -904.28 | 2 | 87.32 | 112.10 | 24.78 |
| TiO | -924.83 | 3 | -10.59 | 13.70 | 24.29 |
| TiS | -1247.82 | 3 | 48.99 | 76.20 | 27.21 |
| TiF | -949.45 | 4 | -14.01 | -4.00 | 10.01 |
| TiF2 | -1049.45 | 3 | -150.56 | -164.50 | -13.94 |
| TiF3 | -1149.45 | 2 | -283.35 | -284.10 | -0.75 |
| TiCl | -1309.83 | 4 | 36.19 | 24.20 | -11.99 |
| TiCl2 | -1770.22 | 3 | -55.96 | -57.00 | -1.04 |
| TiCl3 | -2230.59 | 2 | -136.18 | -128.90 | 7.28 |

| | |
|---|---|
| mean error | 7.69 |
| abs error | 13.23 |
| rmsd | 16.00 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| V2 | -1888.23 | 3 | 159.64 | 187.40 | 27.76 |
| VH | -944.64 | 5 | 114.20 | 125.90 | 11.70 |
| VN | -998.85 | 3 | 102.60 | 121.00 | 18.40 |
| VO | -1019.39 | 4 | 11.52 | 30.50 | 18.98 |
| VS | -1342.39 | 4 | 69.54 | 80.40 | 10.86 |
| VF | -1044.02 | 5 | 4.34 | 0.70 | -3.64 |
| VCl | -1404.41 | 5 | 48.55 | 37.80 | -10.75 |
| VCl2 | -1864.78 | 4 | -34.03 | -51.60 | -17.57 |
| VCl3 | -2325.12 | 3 | -94.80 | -88.20 | 6.60 |

| | |
|---|---|
| mean error | 6.93 |
| abs error | 14.03 |
| rmsd | 15.65 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CrH | -1045.18 | 6 | 96.84 | 80.20 | -16.64 |
| CrN | -1099.36 | 4 | 105.42 | 120.70 | 15.28 |
| CrO | -1119.87 | 5 | 36.33 | 45.00 | 8.67 |
| CrO2 | -1195.18 | 3 | -48.76 | -18.00 | 30.76 |
| CrO3 | -1270.45 | 1 | -116.39 | -70.50 | 45.89 |
| CrOH | -1120.47 | 6 | 23.45 | 18.90 | -4.55 |
| Cr(OH)2 | -1196.37 | 5 | -70.93 | -78.10 | -7.17 |
| CrS | -1442.89 | 5 | 80.21 | 78.20 | -2.01 |

| | | | | | |
|---|---|---|---|---|---|
| CrF | -1144.55 | 6 | -2.11 | 3.10 | 5.21 |
| CrF2 | -1244.49 | 5 | -105.17 | -99.10 | 6.07 |
| CrF3 | -1344.43 | 4 | -203.96 | -199.80 | 4.16 |
| CrCl | -1504.94 | 6 | 36.83 | 31.00 | -5.83 |
| CrCl2 | -1965.28 | 5 | -22.89 | -28.10 | -5.21 |
| CrCl3 | -2425.60 | 4 | -72.94 | -67.70 | 5.24 |

| | |
|---|---|
| mean error | 5.70 |
| abs error | 11.62 |
| rmsd | 16.66 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| MnF | -1251.10 | 7 | -27.13 | -19.90 | 7.23 |
| MnF2 | -1351.07 | 6 | -144.83 | -126.20 | 18.63 |
| MnF3 | -1450.96 | 5 | -215.08 | -188.00 | 27.08 |
| MnCl | -1611.49 | 7 | 11.83 | 11.30 | -0.53 |
| MnCl2 | -2071.86 | 6 | -68.16 | -63.00 | 5.16 |
| MnH | -1151.73 | 5 | 75.78 | 64.20 | -11.58 |
| MnO | -1226.43 | 6 | 7.27 | 29.60 | 22.33 |
| MnOH | -1227.03 | 7 | -7.68 | 3.70 | 11.38 |
| MnS | -1549.46 | 6 | 43.30 | 63.30 | 20.00 |

| | |
|---|---|
| mean error | 11.08 |
| abs error | 13.77 |
| rmsd | 16.06 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Fe2 | -2527.85 | 7 | 131.89 | 172.40 | 40.51 |
| FeH | -1264.46 | 4 | 91.97 | 117.20 | 25.23 |
| FeO | -1339.16 | 5 | 29.08 | 61.10 | 32.02 |
| FeS | -1662.19 | 5 | 63.30 | 83.80 | 20.50 |
| Fe(OH)2 | -1415.67 | 6 | -86.57 | -79.00 | 7.57 |
| FeCO | -1377.28 | 3 | 21.84 | 63.90 | 42.06 |
| Fe(CO)2 | -1490.68 | 3 | -58.55 | 0.20 | 58.75 |
| Fe(CO)3 | -1604.08 | 3 | -133.87 | -55.80 | 78.07 |
| Fe(CO)4 | -1717.48 | 1 | -207.52 | -105.10 | 102.42 |
| FeF | -1363.82 | 4 | -0.47 | 11.40 | 11.87 |
| FeF2 | -1463.79 | 5 | -121.52 | -93.00 | 28.52 |
| FeF3 | -1563.69 | 6 | -191.66 | -196.20 | -4.54 |
| FeCl | -1724.22 | 4 | 34.46 | 49.50 | 15.04 |
| FeCl2 | -2184.59 | 5 | -43.92 | -32.80 | 11.12 |
| FeCl3 | -2644.89 | 6 | -82.07 | -60.60 | 21.47 |

| | |
|---|---|
| mean error | 32.71 |
| abs error | 33.31 |
| rmsd | 42.72 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CoH | -1383.56 | 3 | 87.38 | 110.70 | 23.32 |
| CoO | -1458.24 | 4 | 35.49 | 74.00 | 38.51 |
| CoF2 | -1582.86 | 4 | -105.39 | -87.50 | 17.89 |
| CoCl | -1843.31 | 3 | 37.12 | 50.30 | 13.18 |
| CoCl2 | -2303.67 | 4 | -37.88 | -22.60 | 15.28 |
| CoCl3 | -2763.96 | 5 | -70.36 | -39.10 | 31.26 |

| | |
|---|---|
| mean error | 23.24 |
| abs error | 23.24 |
| rmsd | 24.94 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Ni2 | -3017.22 | 3 | 131.89 | 156.70 | 24.81 |
| NiH | -1509.16 | 2 | 83.02 | 85.60 | 2.58 |
| NiO | -1583.82 | 3 | 41.33 | 75.00 | 33.67 |
| NiS | -1906.87 | 3 | 63.58 | 81.70 | 18.12 |
| Ni(OH)2 | -1660.33 | 3 | -73.12 | -60.80 | 12.32 |
| NiCO | -1621.99 | 1 | 2.35 | 35.10 | 32.75 |
| Ni(CO)2 | -1735.41 | 1 | -84.87 | -39.00 | 45.87 |
| Ni(CO)3 | -1848.80 | 1 | -155.60 | -92.70 | 62.90 |
| Ni(CO)4 | -1962.18 | 1 | -217.59 | -144.00 | 73.59 |
| NiF | -1608.48 | 2 | 9.86 | 17.50 | 7.64 |
| NiF2 | -1708.43 | 3 | -95.31 | -77.80 | 17.51 |
| NiCl | -1968.90 | 2 | 36.61 | 41.70 | 5.09 |
| CiCl2 | -2429.25 | 3 | -29.98 | -17.40 | 12.58 |
| | | | | | |
| mean error | 34.07 | | | | |
| abs error | 26.88 | | | | |
| rmsd | 34.34 | | | | |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Cu2 | -3281.70 | 1 | 111.87 | 113.80 | 1.93 |
| CuH | -1641.41 | 1 | 69.57 | 65.90 | -3.67 |
| CuO | -1716.01 | 2 | 64.10 | 76.50 | 12.40 |
| CuOH | -1716.67 | 1 | 12.79 | 28.70 | 15.91 |
| CuS | -2039.07 | 2 | 75.61 | 75.10 | -0.51 |
| CuF | -1740.72 | 1 | -0.53 | -3.20 | -2.67 |
| CuF2 | -1840.62 | 2 | -68.93 | -66.00 | 2.93 |
| CuCl | -2101.14 | 1 | 23.90 | 19.30 | -4.60 |
| CuCl2 | -2561.44 | 2 | -13.69 | -9.00 | 4.69 |
| | | | | | |
| mean error | 2.93 | | | | |
| abs error | 5.48 | | | | |
| rmsd | 7.33 | | | | |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Zn2 | -3559.46 | 1 | 64.32 | 57.70 | -6.62 |
| ZnF2 | -1979.54 | 1 | -122.23 | -118.90 | 3.33 |
| ZnCl | -2240.00 | 2 | 12.47 | 6.50 | -5.97 |
| ZnCl2 | -2700.36 | 1 | -58.66 | -63.50 | -4.84 |
| ZnO | -1854.87 | 1 | 49.93 | 52.80 | 2.87 |
| ZnS | -2177.94 | 1 | 62.05 | 48.70 | -13.35 |
| ZnH | -1780.25 | 2 | 65.51 | 62.90 | -2.61 |
| Zn(CH3) | -1819.54 | 2 | 51.99 | 26.00 | -25.99 |
| Zn(CH3)2 | -1859.45 | 1 | 15.51 | 12.90 | -2.61 |
| | | | | | |
| mean error | -6.20 | | | | |
| abs error | 7.58 | | | | |
| rmsd | 10.49 | | | | |

# B1B95

| atom | energy | mult |
|---|---|---|
| H | -0.50 | 2 |
| C | -37.84 | 3 |
| N | -54.59 | 4 |
| O | -75.07 | 3 |
| F | -99.75 | 2 |
| S | -398.16 | 3 |
| Cl | -460.20 | 2 |
| Ti | -849.44 | 3 |
| V | -944.02 | 6 |
| Cr | -1044.57 | 7 |
| Mn | -1151.14 | 6 |
| Fe | -1263.83 | 5 |
| Co | -1382.91 | 4 |
| Ni | -1508.47 | 3 |
| Cu | -1640.72 | 2 |
| Zn | -1779.66 | 1 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| TiH | -850.02 | 4 | 115.49 | 116.40 | 0.91 |
| TiN | -904.20 | 2 | 121.05 | 112.10 | -8.95 |
| TiO | -924.72 | 1 | 46.81 | 13.70 | -33.11 |
| TiS | -1247.78 | 3 | 66.47 | 76.20 | 9.73 |
| TiF | -949.40 | 4 | -2.75 | -4.00 | -1.25 |
| TiF2 | -1049.38 | 3 | -128.69 | -164.50 | -35.81 |
| TiF3 | -1149.34 | 2 | -248.20 | -284.10 | -35.90 |
| TiCl | -1309.80 | 4 | 41.01 | 24.20 | -16.81 |
| TiCl2 | -1770.19 | 3 | -49.33 | -57.00 | -7.67 |
| TiCl3 | -2230.55 | 2 | -118.56 | -128.90 | -10.34 |

| | |
|---|---|
| mean error | -13.92 |
| abs error | 16.05 |
| rmsd | 20.72 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| V2 | -1888.04 | 3 | 241.25 | 187.40 | -53.85 |
| VH | -944.60 | 5 | 117.55 | 125.90 | 8.35 |
| VN | -998.75 | 3 | 142.02 | 121.00 | -21.02 |
| VO | -1019.31 | 4 | 43.69 | 30.50 | -13.19 |
| VS | -1342.33 | 4 | 90.69 | 80.40 | -10.29 |
| VF | -1043.96 | 5 | 16.00 | 0.70 | -15.30 |
| VCl | -1404.37 | 5 | 53.19 | 37.80 | -15.39 |
| VCl2 | -1864.72 | 4 | -11.52 | -51.60 | -40.08 |
| VCl3 | -2325.06 | 3 | -72.02 | -88.20 | -16.18 |

| | |
|---|---|
| mean error | -19.66 |
| abs error | 21.52 |
| rmsd | 25.88 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CrH | -1045.14 | 6 | 100.95 | 80.20 | -20.75 |
| CrN | -1099.26 | 4 | 147.23 | 120.70 | -26.53 |
| CrO | -1119.78 | 5 | 68.50 | 45.00 | -23.50 |
| CrO2 | -1195.02 | 3 | 18.52 | -18.00 | -36.52 |
| CrO3 | -1270.23 | 1 | -4.94 | -70.50 | -65.56 |
| CrOH | -1120.41 | 6 | 36.01 | 18.90 | -17.11 |
| Cr(OH)2 | -1196.28 | 5 | -44.65 | -78.10 | -33.45 |
| CrS | -1442.78 | 3 | 127.52 | 78.20 | -49.32 |

| | | | | | |
|---|---|---|---|---|---|
| CrF | -1144.48 | 6 | 8.95 | 3.10 | -5.85 |
| CrF2 | -1244.40 | 5 | -83.35 | -99.10 | -15.75 |
| CrF3 | -1344.30 | 4 | -163.04 | -199.80 | -36.76 |
| CrCl | -1504.90 | 6 | 40.11 | 31.00 | -9.11 |
| CrCl2 | -1965.23 | 5 | -13.76 | -28.10 | -14.34 |
| CrCl3 | -2425.53 | 4 | -47.27 | -67.70 | -20.43 |

| | |
|---|---|
| mean error | -26.78 |
| abs error | 26.78 |
| rmsd | 31.06 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| MnF | -1251.04 | 7 | -15.71 | -19.90 | -4.19 |
| MnF2 | -1350.99 | 6 | -121.96 | -126.20 | -4.24 |
| MnF3 | -1450.83 | 5 | -167.17 | -188.00 | -20.83 |
| MnCl | -1611.46 | 7 | 16.44 | 11.30 | -5.14 |
| MnCl2 | -2071.83 | 6 | -58.62 | -63.00 | -4.38 |
| MnH | -1151.69 | 7 | 85.50 | 64.20 | -21.30 |
| MnO | -1226.34 | 6 | 45.54 | 29.60 | -15.94 |
| MnOH | -1226.98 | 7 | 6.60 | 3.70 | -2.90 |
| MnS | -1549.40 | 6 | 66.34 | 63.30 | -3.04 |

| | |
|---|---|
| mean error | -9.11 |
| abs error | 9.11 |
| rmsd | 11.74 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Fe2 | -2527.63 | 7 | 218.73 | 172.40 | -46.33 |
| FeH | -1264.40 | 4 | 109.57 | 117.20 | 7.63 |
| FeO | -1339.03 | 5 | 78.45 | 61.10 | -17.35 |
| FeS | -1662.10 | 5 | 93.97 | 83.80 | -10.17 |
| Fe(OH)2 | -1415.55 | 6 | -43.53 | -79.00 | -35.47 |
| FeCO | -1377.15 | 3 | 70.89 | 63.90 | -6.99 |
| Fe(CO)2 | -1490.51 | 3 | 20.83 | 0.20 | -20.63 |
| Fe(CO)3 | -1603.87 | 3 | -33.63 | -55.80 | -22.17 |
| Fe(CO)4 | -1717.21 | 3 | -73.01 | -105.10 | -32.09 |
| FeF | -1363.74 | 4 | 18.07 | 11.40 | -6.67 |
| FeF2 | -1463.66 | 5 | -77.98 | -93.00 | -15.02 |
| FeF3 | -1563.56 | 6 | -151.47 | -196.20 | -44.73 |
| FeCl | -1724.15 | 4 | 54.78 | 49.50 | -5.28 |
| FeCl2 | -2184.52 | 5 | -21.74 | -32.80 | -11.06 |
| FeCl3 | -2644.81 | 6 | -53.23 | -60.60 | -7.37 |

| | |
|---|---|
| mean error | -18.25 |
| abs error | 19.26 |
| rmsd | 23.58 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CoH | -1383.47 | 3 | 117.27 | 110.70 | -6.57 |
| CoO | -1458.11 | 4 | 80.73 | 74.00 | -6.73 |
| CoF2 | -1582.74 | 4 | -75.89 | -87.50 | -11.61 |
| CoCl | -1843.22 | 5 | 60.68 | 50.30 | -10.38 |
| CoCl2 | -2303.59 | 4 | -16.70 | -22.60 | -5.90 |
| CoCl3 | -2763.86 | 5 | -31.66 | -39.10 | -7.44 |

| | |
|---|---|
| mean error | -8.10 |
| abs error | 8.10 |
| rmsd | 8.38 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Ni2 | -3016.99 | 3 | 181.60 | 156.70 | -24.90 |
| NiH | -1509.07 | 2 | 90.69 | 85.60 | -5.09 |
| NiO | -1583.68 | 3 | 80.05 | 75.00 | -5.05 |
| NiS | -1906.75 | 3 | 90.96 | 81.70 | -9.26 |
| Ni(OH)2 | -1660.19 | 3 | -41.44 | -60.80 | -19.36 |
| NiCO | -1621.83 | 1 | 51.16 | 35.10 | -16.06 |
| Ni(CO)2 | -1735.21 | 1 | -13.46 | -39.00 | -25.54 |
| Ni(CO)3 | -1848.57 | 1 | -66.06 | -92.70 | -26.64 |
| Ni(CO)4 | -1961.91 | 1 | -109.26 | -144.00 | -34.74 |
| NiF | -1608.38 | 2 | 22.74 | 17.50 | -5.24 |
| NiF2 | -1708.30 | 3 | -72.06 | -77.80 | -5.74 |
| NiCl | -1968.82 | 2 | 41.85 | 41.70 | -0.15 |
| CiCl2 | -2429.15 | 3 | -13.90 | -17.40 | -3.50 |
| | | | | | |
| mean error | -18.52 | | | | |
| abs error | 13.94 | | | | |
| rmsd | 17.61 | | | | |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Cu2 | -3281.51 | 1 | 121.14 | 113.80 | -7.34 |
| CuH | -1641.31 | 1 | 75.59 | 65.90 | -9.69 |
| CuO | -1715.89 | 2 | 82.41 | 76.50 | -5.91 |
| CuOH | -1716.55 | 1 | 27.90 | 28.70 | 0.80 |
| CuS | -2038.98 | 2 | 84.62 | 75.10 | -9.52 |
| CuF | -1740.61 | 1 | 9.89 | -3.20 | -13.09 |
| CuF2 | -1840.47 | 2 | -42.04 | -66.00 | -23.96 |
| CuCl | -2101.06 | 1 | 26.43 | 19.30 | -7.13 |
| CuCl2 | -2561.34 | 2 | -0.06 | -9.00 | -8.94 |
| | | | | | |
| mean error | -9.42 | | | | |
| abs error | 9.60 | | | | |
| rmsd | 11.30 | | | | |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Zn2 | -3559.31 | 1 | 64.82 | 57.70 | -7.12 |
| ZnF2 | -1979.43 | 1 | -110.75 | -118.90 | -8.15 |
| ZnCl | -2239.93 | 2 | 10.90 | 6.50 | -4.40 |
| ZnCl2 | -2700.29 | 1 | -60.25 | -63.50 | -3.25 |
| ZnO | -1854.77 | 3 | 63.42 | 52.80 | -10.62 |
| ZnS | -2177.86 | 1 | 67.49 | 48.70 | -18.79 |
| ZnH | -1780.18 | 2 | 64.56 | 62.90 | -1.66 |
| Zn(CH3) | -1819.47 | 2 | 54.16 | 26.00 | -28.16 |
| Zn(CH3)2 | -1859.37 | 1 | 20.31 | 12.90 | -7.41 |
| | | | | | |
| mean error | -9.95 | | | | |
| abs error | 9.95 | | | | |
| rmsd | 12.75 | | | | |

# TPSS1KCIS

| atom | energy | mult |
|---|---|---|
| H | -0.50 | 2 |
| C | -37.86 | 3 |
| N | -54.61 | 4 |
| O | -75.10 | 3 |
| F | -99.77 | 2 |
| S | -398.15 | 3 |
| Cl | -460.19 | 2 |
| Ti | -849.40 | 5 |
| V | -943.96 | 6 |
| Cr | -1044.50 | 7 |
| Mn | -1151.04 | 6 |
| Fe | -1263.73 | 5 |
| Co | -1382.80 | 4 |
| Ni | -1508.34 | 3 |
| Cu | -1640.57 | 2 |
| Zn | -1779.47 | 1 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| TiH | -849.98 | 4 | 113.32 | 116.40 | 3.08 |
| TiN | -904.19 | 2 | 111.48 | 112.10 | 0.62 |
| TiO | -924.75 | 3 | 8.83 | 13.70 | 4.87 |
| TiS | -1247.74 | 3 | 59.99 | 76.20 | 16.21 |
| TiF | -949.38 | 4 | -3.94 | -4.00 | -0.06 |
| TiF2 | -1049.39 | 3 | -134.70 | -164.50 | -29.80 |
| TiF3 | -1149.38 | 2 | -256.52 | -284.10 | -27.58 |
| TiCl | -1309.75 | 4 | 40.02 | 24.20 | -15.82 |
| TiCl2 | -1770.13 | 3 | -52.83 | -57.00 | -4.17 |
| TiCl3 | -2230.48 | 2 | -124.01 | -128.90 | -4.89 |

| | |
|---|---|
| mean error | -5.75 |
| abs error | 10.71 |
| rmsd | 14.96 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| V2 | -1887.97 | 3 | 212.28 | 187.40 | -24.88 |
| VH | -944.55 | 5 | 113.00 | 125.90 | 12.90 |
| VN | -998.74 | 3 | 126.50 | 121.00 | -5.50 |
| VO | -1019.29 | 4 | 34.86 | 30.50 | -4.36 |
| VS | -1342.28 | 4 | 83.45 | 80.40 | -3.05 |
| VF | -1043.93 | 5 | 12.40 | 0.70 | -11.70 |
| VCl | -1404.31 | 5 | 50.44 | 37.80 | -12.64 |
| VCl2 | -1864.65 | 4 | -15.02 | -51.60 | -36.58 |
| VCl3 | -2324.99 | 3 | -79.51 | -88.20 | -8.69 |

| | |
|---|---|
| mean error | -10.50 |
| abs error | 13.37 |
| rmsd | 16.85 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CrH | -1045.08 | 6 | 97.09 | 80.20 | -16.89 |
| CrN | -1099.23 | 4 | 131.14 | 120.70 | -10.44 |
| CrO | -1119.75 | 5 | 57.93 | 45.00 | -12.93 |
| CrO2 | -1195.03 | 3 | -0.73 | -18.00 | -17.27 |
| CrO3 | -1270.28 | 1 | -38.89 | -70.50 | -31.61 |
| CrOH | -1120.37 | 6 | 33.85 | 18.90 | -14.95 |
| Cr(OH)2 | -1196.27 | 5 | -48.53 | -78.10 | -29.57 |
| CrS | -1442.76 | 5 | 89.99 | 78.20 | -11.79 |

| | | | | | |
|---|---|---|---|---|---|
| CrF | -1144.44 | 6 | 5.37 | 3.10 | -2.27 |
| CrF2 | -1244.39 | 5 | -89.05 | -99.10 | -10.05 |
| CrF3 | -1344.32 | 4 | -173.60 | -199.80 | -26.20 |
| CrCl | -1504.82 | 6 | 38.41 | 31.00 | -7.41 |
| CrCl2 | -1965.15 | 5 | -16.86 | -28.10 | -11.24 |
| CrCl3 | -2425.44 | 4 | -55.47 | -67.70 | -12.23 |

| | |
|---|---|
| mean error | -15.35 |
| abs error | 15.35 |
| rmsd | 17.36 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| MnF | -1250.98 | 7 | -21.09 | -19.90 | 1.19 |
| MnF2 | -1350.95 | 6 | -129.28 | -126.20 | 3.08 |
| MnF3 | -1450.83 | 5 | -183.01 | -188.00 | -4.99 |
| MnCl | -1611.36 | 7 | 12.03 | 11.30 | -0.73 |
| MnCl2 | -2071.72 | 6 | -63.54 | -63.00 | 0.54 |
| MnH | -1151.60 | 7 | 79.59 | 64.20 | -15.39 |
| MnO | -1226.29 | 6 | 30.97 | 29.60 | -1.37 |
| MnOH | -1226.91 | 7 | 1.92 | 3.70 | 1.78 |
| MnS | -1549.31 | 6 | 56.65 | 63.30 | 6.65 |

| | |
|---|---|
| mean error | -1.03 |
| abs error | 3.97 |
| rmsd | 5.99 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Fe2 | -2527.48 | 7 | 185.81 | 172.40 | -13.41 |
| FeH | -1264.31 | 4 | 100.31 | 117.20 | 16.89 |
| FeO | -1338.97 | 5 | 68.66 | 61.10 | -7.56 |
| FeS | -1662.00 | 5 | 87.08 | 83.80 | -3.28 |
| Fe(OH)2 | -1415.53 | 6 | -62.19 | -79.00 | -16.81 |
| FeCO | -1377.11 | 5 | 60.85 | 63.90 | 3.05 |
| Fe(CO)2 | -1490.52 | 3 | 3.03 | 0.20 | -2.83 |
| Fe(CO)3 | -1603.92 | 3 | -51.88 | -55.80 | -3.92 |
| Fe(CO)4 | -1717.31 | 1 | -94.74 | -105.10 | -10.36 |
| FeF | -1363.66 | 4 | 12.13 | 11.40 | -0.73 |
| FeF2 | -1463.65 | 5 | -104.23 | -93.00 | 11.23 |
| FeF3 | -1563.53 | 6 | -159.82 | -196.20 | -36.38 |
| FeCl | -1724.04 | 4 | 47.75 | 49.50 | 1.75 |
| FeCl2 | -2184.41 | 5 | -36.26 | -32.80 | 3.46 |
| FeCl3 | -2644.69 | 6 | -60.82 | -60.60 | 0.22 |

| | |
|---|---|
| mean error | -3.91 |
| abs error | 8.79 |
| rmsd | 12.70 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CoH | -1383.37 | 3 | 103.05 | 110.70 | 7.65 |
| CoO | -1458.04 | 4 | 68.92 | 74.00 | 5.08 |
| CoF2 | -1582.68 | 4 | -81.49 | -87.50 | -6.01 |
| CoCl | -1843.10 | 5 | 56.53 | 50.30 | -6.23 |
| CoCl2 | -2303.46 | 4 | -19.96 | -22.60 | -2.64 |
| CoCl3 | -2763.73 | 5 | -40.13 | -39.10 | 1.03 |

| | |
|---|---|
| mean error | -0.18 |
| abs error | 4.77 |
| rmsd | 5.28 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Ni2 | -3016.75 | 3 | 161.17 | 156.70 | -4.47 |
| NiH | -1508.94 | 2 | 86.67 | 85.60 | -1.07 |
| NiO | -1583.58 | 3 | 68.00 | 75.00 | 7.00 |
| NiS | -1906.63 | 3 | 82.03 | 81.70 | -0.33 |
| Ni(OH)2 | -1660.12 | 3 | -46.05 | -60.80 | -14.75 |
| NiCO | -1621.76 | 1 | 40.21 | 35.10 | -5.11 |
| Ni(CO)2 | -1735.18 | 1 | -26.22 | -39.00 | -12.78 |
| Ni(CO)3 | -1848.58 | 1 | -79.14 | -92.70 | -13.56 |
| Ni(CO)4 | -1961.97 | 1 | -122.73 | -144.00 | -21.27 |
| NiF | -1608.27 | 2 | 18.70 | 17.50 | -1.20 |
| NiF2 | -1708.22 | 3 | -77.35 | -77.80 | -0.45 |
| NiCl | -1968.67 | 2 | 40.46 | 41.70 | 1.24 |
| CiCl2 | -2429.00 | 3 | -17.62 | -17.40 | 0.22 |

| | |
|---|---|
| mean error | -7.37 |
| abs error | 6.42 |
| rmsd | 9.27 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Cu2 | -3281.20 | 1 | 119.64 | 113.80 | -5.84 |
| CuH | -1641.16 | 1 | 73.46 | 65.90 | -7.56 |
| CuO | -1715.76 | 2 | 77.44 | 76.50 | -0.94 |
| CuOH | -1716.42 | 1 | 26.35 | 28.70 | 2.35 |
| CuS | -2038.82 | 2 | 82.56 | 75.10 | -7.46 |
| CuF | -1740.48 | 1 | 8.57 | -3.20 | -11.77 |
| CuF2 | -1840.37 | 2 | -51.49 | -66.00 | -14.51 |
| CuCl | -2100.89 | 1 | 27.05 | 19.30 | -7.75 |
| CuCl2 | -2561.17 | 2 | -4.26 | -9.00 | -4.74 |

| | |
|---|---|
| mean error | -6.47 |
| abs error | 6.99 |
| rmsd | 8.06 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Zn2 | -3558.93 | 1 | 64.00 | 57.70 | -6.30 |
| ZnF2 | -1979.29 | 1 | -112.71 | -118.90 | -6.19 |
| ZnCl | -2239.74 | 2 | 9.50 | 6.50 | -3.00 |
| ZnCl2 | -2700.08 | 1 | -59.51 | -63.50 | -3.99 |
| ZnO | -1854.61 | 3 | 59.44 | 52.80 | -6.64 |
| ZnS | -2177.67 | 1 | 66.38 | 48.70 | -17.68 |
| ZnH | -1780.00 | 2 | 61.66 | 62.90 | 1.24 |
| Zn(CH3) | -1819.31 | 2 | 49.27 | 26.00 | -23.27 |
| Zn(CH3)2 | -1859.23 | 1 | 14.24 | 12.90 | -1.34 |

| | |
|---|---|
| mean error | -7.46 |
| abs error | 7.74 |
| rmsd | 10.56 |

# BB1K

| atom | energy | mult |
|---|---|---|
| H | -0.50 | 2 |
| C | -37.84 | 3 |
| N | -54.59 | 4 |
| O | -75.07 | 3 |
| F | -99.74 | 2 |
| S | -398.16 | 3 |
| Cl | -460.20 | 2 |
| Ti | -849.44 | 3 |
| V | -944.00 | 6 |
| Cr | -1044.55 | 7 |
| Mn | -1151.12 | 6 |
| Fe | -1263.81 | 5 |
| Co | -1382.89 | 4 |
| Ni | -1508.44 | 3 |
| Cu | -1640.68 | 2 |
| Zn | -1779.62 | 1 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| TiH | -850.01 | 4 | 118.06 | 116.40 | -1.66 |
| TiN | -904.15 | 2 | 149.82 | 112.10 | -37.72 |
| TiO | -924.68 | 3 | 62.40 | 13.70 | -48.70 |
| TiS | -1247.76 | 3 | 75.82 | 76.20 | 0.38 |
| TiF | -949.38 | 4 | 3.82 | -4.00 | -7.82 |
| TiF2 | -1049.35 | 3 | -117.93 | -164.50 | -46.57 |
| TiF3 | -1149.30 | 2 | -231.88 | -284.10 | -52.22 |
| TiCl | -1309.79 | 4 | 44.74 | 24.20 | -20.54 |
| TiCl2 | -1770.19 | 3 | -45.76 | -57.00 | -11.24 |
| TiCl3 | -2230.54 | 2 | -110.11 | -128.90 | -18.79 |

| | |
|---|---|
| mean error | -24.49 |
| abs error | 24.57 |
| rmsd | 31.07 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| V2 | -1887.95 | 5 | 278.71 | 187.40 | -91.31 |
| VH | -944.59 | 5 | 118.72 | 125.90 | 7.18 |
| VN | -998.71 | 3 | 159.82 | 121.00 | -38.82 |
| VO | -1019.27 | 4 | 58.00 | 30.50 | -27.50 |
| VS | -1342.30 | 4 | 98.89 | 80.40 | -18.49 |
| VF | -1043.94 | 5 | 20.24 | 0.70 | -19.54 |
| VCl | -1404.36 | 5 | 53.75 | 37.80 | -15.95 |
| VCl2 | -1864.71 | 4 | -9.95 | -51.60 | -41.65 |
| VCl3 | -2325.04 | 3 | -63.79 | -88.20 | -24.41 |

| | |
|---|---|
| mean error | -30.05 |
| abs error | 31.65 |
| rmsd | 39.38 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CrH | -1045.12 | 6 | 102.57 | 80.20 | -22.37 |
| CrN | -1099.22 | 4 | 162.49 | 120.70 | -41.79 |
| CrO | -1119.74 | 5 | 81.86 | 45.00 | -36.86 |
| CrO2 | -1194.96 | 3 | 48.11 | -18.00 | -66.11 |
| CrO3 | -1270.12 | 1 | 47.13 | -70.50 | -117.63 |
| CrOH | -1120.38 | 6 | 41.05 | 18.90 | -22.15 |
| Cr(OH)2 | -1196.25 | 5 | -34.75 | -78.10 | -43.35 |
| CrS | -1442.79 | 7 | 111.33 | 78.20 | -33.13 |

| | | | | | |
|---|---|---|---|---|---|
| CrF | -1144.45 | 6 | 13.29 | 3.10 | -10.19 |
| CrF2 | -1244.37 | 5 | -75.63 | -99.10 | -23.47 |
| CrF3 | -1344.25 | 4 | -146.67 | -199.80 | -53.13 |
| CrCl | -1504.89 | 6 | 40.85 | 31.00 | -9.85 |
| CrCl2 | -1965.22 | 5 | -12.37 | -28.10 | -15.73 |
| CrCl3 | -2425.51 | 4 | -37.52 | -67.70 | -30.18 |

| | |
|---|---|
| mean error | -37.57 |
| abs error | 37.57 |
| rmsd | 46.30 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| MnF | -1251.02 | 7 | -11.72 | -19.90 | -8.18 |
| MnF2 | -1350.95 | 6 | -113.71 | -126.20 | -12.49 |
| MnF3 | -1450.78 | 5 | -148.02 | -188.00 | -39.98 |
| MnCl | -1611.45 | 7 | 17.21 | 11.30 | -5.91 |
| MnCl2 | -2071.82 | 6 | -56.62 | -63.00 | -6.38 |
| MnH | -1151.67 | 7 | 85.88 | 64.20 | -21.68 |
| MnO | -1226.30 | 6 | 60.76 | 29.60 | -31.16 |
| MnOH | -1226.96 | 7 | 11.71 | 3.70 | -8.01 |
| MnS | -1549.38 | 6 | 74.18 | 63.30 | -10.88 |

| | |
|---|---|
| mean error | -16.07 |
| abs error | 16.07 |
| rmsd | 19.78 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Fe2 | -2527.54 | 7 | 257.46 | 172.40 | -85.06 |
| FeH | -1264.37 | 4 | 115.97 | 117.20 | 1.23 |
| FeO | -1338.98 | 5 | 95.90 | 61.10 | -34.80 |
| FeS | -1662.07 | 5 | 104.44 | 83.80 | -20.64 |
| Fe(OH)2 | -1415.51 | 6 | -31.50 | -79.00 | -47.50 |
| FeCO | -1377.11 | 5 | 88.75 | 63.90 | -24.85 |
| Fe(CO)2 | -1490.43 | 5 | 54.03 | 0.20 | -53.83 |
| Fe(CO)3 | -1603.78 | 3 | 11.05 | -55.80 | -66.85 |
| Fe(CO)4 | -1717.10 | 3 | -19.70 | -105.10 | -85.40 |
| FeF | -1363.70 | 4 | 24.19 | 11.40 | -12.79 |
| FeF2 | -1463.62 | 5 | -68.72 | -93.00 | -24.28 |
| FeF3 | -1563.50 | 6 | -137.34 | -196.20 | -58.86 |
| FeCl | -1724.13 | 6 | 58.08 | 49.50 | -8.58 |
| FeCl2 | -2184.50 | 5 | -18.59 | -32.80 | -14.21 |
| FeCl3 | -2644.79 | 6 | -44.05 | -60.60 | -16.55 |

| | |
|---|---|
| mean error | -36.86 |
| abs error | 37.03 |
| rmsd | 45.59 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| CoH | -1383.43 | 5 | 124.10 | 110.70 | -13.40 |
| CoO | -1458.05 | 4 | 100.34 | 74.00 | -26.34 |
| CoF2 | -1582.69 | 4 | -66.17 | -87.50 | -21.33 |
| CoCl | -1843.20 | 5 | 61.59 | 50.30 | -11.29 |
| CoCl2 | -2303.57 | 4 | -14.08 | -22.60 | -8.52 |
| CoCl3 | -2763.82 | 5 | -18.05 | -39.10 | -21.05 |

| | |
|---|---|
| mean error | -16.99 |
| abs error | 16.99 |
| rmsd | 18.13 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Ni2 | -3016.88 | 3 | 204.17 | 156.70 | -47.47 |
| NiH | -1509.03 | 2 | 94.02 | 85.60 | -8.42 |
| NiO | -1583.61 | 3 | 96.67 | 75.00 | -21.67 |
| NiS | -1906.70 | 3 | 101.73 | 81.70 | -20.03 |
| Ni(OH)2 | -1660.14 | 3 | -31.56 | -60.80 | -29.24 |
| NiCO | -1621.76 | 1 | 73.60 | 35.10 | -38.50 |
| Ni(CO)2 | -1735.12 | 1 | 18.84 | -39.00 | -57.84 |
| Ni(CO)3 | -1848.46 | 1 | -25.39 | -92.70 | -67.31 |
| Ni(CO)4 | -1961.79 | 1 | -60.09 | -144.00 | -83.91 |
| NiF | -1608.33 | 2 | 27.52 | 17.50 | -10.02 |
| NiF2 | -1708.25 | 3 | -66.06 | -77.80 | -11.74 |
| NiCl | -1968.78 | 2 | 43.43 | 41.70 | -1.73 |
| CiCl2 | -2429.04 | 3 | 36.89 | -17.40 | -54.29 |

| | |
|---|---|
| mean error | -41.60 |
| abs error | 34.78 |
| rmsd | 42.64 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Cu2 | -3281.42 | 1 | 124.80 | 113.80 | -11.00 |
| CuH | -1641.27 | 1 | 77.97 | 65.90 | -12.07 |
| CuO | -1715.83 | 2 | 88.44 | 76.50 | -11.94 |
| CuOH | -1716.50 | 1 | 33.98 | 28.70 | -5.28 |
| CuS | -2038.93 | 2 | 87.25 | 75.10 | -12.15 |
| CuF | -1740.56 | 1 | 13.75 | -3.20 | -16.95 |
| CuF2 | -1840.42 | 2 | -40.45 | -66.00 | -25.55 |
| CuCl | -2101.02 | 1 | 26.82 | 19.30 | -7.52 |
| CuCl2 | -2561.30 | 2 | 3.82 | -9.00 | -12.82 |

| | |
|---|---|
| mean error | -12.81 |
| abs error | 12.81 |
| rmsd | 13.93 |

| molecule | enthalpies | mult | HOF(theo) | HOF(exp) | error(e-t) |
|---|---|---|---|---|---|
| Zn2 | -3559.24 | 1 | 64.90 | 57.70 | -7.20 |
| ZnF2 | -1979.38 | 1 | -106.45 | -118.90 | -12.45 |
| ZnCl | -2239.90 | 2 | 9.66 | 6.50 | -3.16 |
| ZnCl2 | -2700.26 | 1 | -61.71 | -63.50 | -1.79 |
| ZnO | -1854.73 | 3 | 65.62 | 52.80 | -12.82 |
| ZnS | -2177.82 | 1 | 69.72 | 48.70 | -21.02 |
| ZnH | -1780.15 | 2 | 63.82 | 62.90 | -0.92 |
| Zn(CH3) | -1819.43 | 2 | 54.71 | 26.00 | -28.71 |
| Zn(CH3)2 | -1859.33 | 1 | 21.22 | 12.90 | -8.32 |

| | |
|---|---|
| mean error | -10.71 |
| abs error | 10.71 |
| rmsd | 13.83 |