|  |  |
| --- | --- |
| Methods | Errors for each reaction ( kcal∙mol-1) |
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |
| B3LYP/6-31+G(d) | 2.34 | 1.54 | 2.10 | 1.90 | 2.21 | 3.88 | 3.08 | 3.64 | 3.44 | 3.75 | 2.54 | -0.57 | 6.68 | 7.23 | 7.41 | 7.53 | 8.32 | 5.10 | 7.46 | -1.18 |
| B3LYP-D3/6-31+G(d) | 2.41 | 1.61 | 2.49 | 1.90 | -0.33 | 3.83 | 3.04 | 3.92 | 3.33 | 1.09 | 3.30 | -0.32 | 6.73 | 3.86 | 2.01 | 4.35 | 2.89 | 4.36 | 4.88 | 2.85 |
| B3LYP/6-311+G(d) | 2.14 | 1.05 | 1.45 | 2.01 | 1.97 | 3.94 | 2.86 | 3.26 | 3.81 | 3.78 | 2.63 | -0.29 | 7.65 | 7.74 | 8.03 | 7.90 | 8.89 | 6.53 | 7.85 | 0.35 |
| B3LYP-D3/6-311+G(d) | 2.20 | 1.12 | 1.85 | 2.00 | -1.25 | 3.90 | 2.82 | 3.54 | 3.70 | 0.44 | 3.39 | -0.04 | 7.70 | 4.37 | 2.64 | 4.72 | 3.46 | 5.79 | 5.26 | 4.37 |
| BLYP/6-311+G(d) | 2.61 | 1.53 | 1.99 | 2.69 | 2.63 | 3.31 | 2.22 | 2.68 | 3.38 | 3.32 | 3.33 | -1.72 | 8.34 | 8.60 | 8.97 | 9.41 | 10.64 | 9.28 | 12.45 | -2.82 |
| BLYP-D3/6-311+G(d) | 2.69 | 1.61 | 2.52 | 2.69 | 0.94 | 3.25 | 2.17 | 3.08 | 3.24 | 1.50 | 4.30 | -1.40 | 8.40 | 4.54 | 2.29 | 5.49 | 3.87 | 8.38 | 9.28 | 2.09 |
| BP86/6-311+G(d) | 1.12 | 0.48 | 0.43 | 1.77 | 1.27 | 2.62 | 4.81 | 4.76 | 6.10 | 5.59 | 0.89 | -0.50 | 10.81 | 2.80 | 3.25 | 3.70 | 5.05 | 5.54 | 8.24 | 2.20 |
| BP86-D3/6-311+G(d) | 1.19 | 0.56 | 0.91 | 1.76 | -0.23 | 2.57 | 1.94 | 2.29 | 3.14 | 1.15 | 1.77 | -3.03 | 8.04 | 0.94 | -2.91 | 0.10 | -1.16 | 4.72 | 5.34 | 6.73 |
| TPSS/6-311+G(d) | 2.42 | 1.52 | 1.72 | 2.87 | 2.69 | 4.19 | 3.29 | 3.49 | 4.64 | 4.46 | 3.00 | -0.53 | 7.36 | 3.30 | 3.75 | 4.07 | 5.23 | 4.00 | 6.36 | 2.38 |
| TPSS-D3/6-311+G(d) | 2.47 | 1.58 | 2.04 | 2.86 | 0.39 | 4.16 | 3.27 | 3.73 | 4.55 | 2.08 | 3.63 | -0.33 | 7.40 | 0.76 | -0.55 | 1.63 | 0.92 | 3.45 | 4.40 | 5.51 |
| BHandHLYP/6-311+G(d) | 2.07 | 1.22 | 1.76 | 1.57 | 1.70 | 5.16 | 4.32 | 4.86 | 4.67 | 4.80 | 3.19 | 2.67 | 6.78 | 7.45 | 7.41 | 6.76 | 7.37 | 4.79 | 3.16 | 2.28 |
| HF/6-311+G(d) | 3.34 | 2.42 | 3.96 | 2.71 | 3.14 | 7.42 | 6.51 | 8.04 | 6.80 | 7.23 | 7.10 | 8.48 | 5.65 | 15.46 | 14.70 | 13.44 | 13.69 | 11.19 | 8.73 | -6.63 |
| HF/aug-cc-pVDZ | 0.07 | -1.01 | 0.59 | -0.68 | -0.32 | 2.66 | 1.58 | 3.18 | 1.91 | 2.27 | 2.75 | 3.54 | 1.80 | 16.09 | 15.20 | 13.78 | 14.04 | 10.83 | 15.73 | -10.68 |
| HF/aug-cc-pVTZ | -0.54 | -1.31 | 0.43 | -1.00 | -0.65 | 2.54 | 1.77 | 3.51 | 2.08 | 2.42 | 2.60 | 3.50 | 2.49 | 18.47 | 17.64 | 16.23 | 16.58 | 11.76 | 16.82 | -11.44 |
| MP2/6-311+G(d) | 3.90 | 4.57 | 4.30 | 4.36 | 4.22 | 5.86 | 6.53 | 6.27 | 6.32 | 6.18 | -0.99 | 4.40 | 4.93 | -3.17 | -2.78 | -2.24 | -1.20 | 0.75 | 0.13 | 5.25 |
| MP2/aug-cc-pVDZ | 1.08 | 0.88 | 0.75 | 1.42 | 1.37 | -0.49 | -0.70 | -0.83 | -0.15 | -0.20 | -5.71 | -1.63 | 1.46 | -4.02 | -3.98 | 3.83 | -3.69 | 0.49 | 0.86 | 1.38 |
| MP2/aug-cc-pVTZ | 0.26 | 0.03 | -0.01 | 0.72 | 0.76 | -0.86 | -1.15 | -1.13 | -0.40 | -0.36 | -6.39 | -2.22 | 1.32 | -1.38 | -1.27 | -1.48 | -1.22 | 0.21 | -0.49 | -1.48 |
| SCS-MP2/aug-cc-pVDZ | 2.57 | 2.27 | 2.41 | 2.47 | 2.50 | 0.82 | 0.51 | 0.66 | 0.72 | 0.74 | -0.68 | 1.22 | 0.80 | -0.31 | -0.36 | -0.42 | -0.27 | 2.56 | 3.48 | -1.06 |
| SCS-MP2/aug-cc-pVTZ | 1.86 | 1.47 | 1.78 | 1.83 | 1.98 | 0.55 | 0.15 | 0.46 | 0.52 | 0.66 | -1.14 | 0.78 | 0.64 | 2.47 | 2.48 | 2.12 | 2.09 | 2.47 | 2.32 | -1.20 |
| CCSD(T)/aug-cc-pVDZ | 0.71 | 0.80 | 0.63 | 0.64 | 0.52 | 0.27 | 0.36 | 0.19 | 0.20 | 0.08 | 0.46 | 0.44 | 0.16 | -2.77 | -2.83 | -2.54 | -2.36 | 0.09 | 1.17 | -0.14 |
| CCSD(T)/aug-cc-pVTZ | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| SCCDFTB | -20.75 | -27.24 | -29.44 | -21.07 | -25.11 | -3.85 | -10.34 | -12.54 | -4.17 | -8.22 | -8.70 | -6.80 | -11.22 | 4.77 | 6.47 | 4.19 | 8.06 | 8.82 | 6.66 | -2.87 |
| PM3 | -21.77 | -27.09 | -28.35 | -27.37 | -30.03 | -4.53 | -9.85 | -11.11 | -10.13 | -12.79 | -11.69 | -14.09 | -6.31 | 13.39 | 13.74 | 10.41 | 12.77 | 9.35 | 8.39 | -8.39 |
| AM1 | -11.94 | -19.35 | -21.32 | -17.86 | -20.71 | 0.74 | -6.67 | -8.64 | -5.18 | -8.04 | -1.84 | -3.89 | -16.44 | 17.36 | 19.18 | 14.37 | 16.86 | 6.76 | 9.72 | -13.41 |