|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Methods | Reaction energies of 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) | -17.26 | -27.14 | -24.02 | -15.89 | -12.55 | 26.03 | 16.16 | 19.28 | 27.41 | 30.75 | -15.85 | 3.76 | -105.29 | 0.26 | -0.79 | -7.12 | -8.85 | -18.37 | -22.47 | 16.17 |
| B3LYP-D36-31+G(d) | -17.20 | -27.06 | -23.63 | -15.89 | -15.09 | 25.99 | 16.12 | 19.56 | 27.29 | 28.09 | -15.09 | 4.01 | -105.24 | -3.11 | -6.18 | -10.31 | -14.28 | -19.12 | -25.05 | 20.20 |
| B3LYP/6-311+G(d) | -17.47 | -27.63 | -24.66 | -15.78 | -12.78 | 26.10 | 15.94 | 18.90 | 27.78 | 30.78 | -15.76 | 4.05 | -104.32 | 0.77 | -0.16 | -6.75 | -8.29 | -16.95 | -22.08 | 17.69 |
| B3LYP-D3/6-311+G(d) | -17.40 | -27.55 | -24.27 | -15.79 | -16.01 | 26.05 | 15.90 | 19.18 | 27.66 | 27.44 | -15.00 | 4.30 | -104.27 | -2.60 | -5.56 | -9.94 | -13.71 | -17.69 | -24.67 | 21.72 |
| BLYP/6-311+G(d) | -16.99 | -27.15 | -24.13 | -15.10 | -12.13 | 25.46 | 15.30 | 18.32 | 27.35 | 30.32 | -15.07 | 2.61 | -103.63 | 1.63 | 0.78 | -5.25 | -6.53 | -14.20 | -17.48 | 14.53 |
| BLYP-D3/6-311+G(d) | -16.91 | -27.06 | -23.59 | -15.11 | -13.82 | 25.41 | 15.26 | 18.72 | 27.21 | 28.50 | -14.10 | 2.94 | -103.56 | -2.43 | -5.90 | -9.17 | -13.31 | -15.10 | -20.65 | 19.44 |
| BP86/6-311+G(d) | -18.48 | -28.19 | -25.68 | -16.02 | -13.49 | 24.77 | 17.89 | 20.40 | 30.06 | 32.59 | -17.51 | 3.84 | -101.16 | -4.16 | -4.94 | -10.96 | -12.12 | -17.94 | -21.69 | 19.55 |
| BP86-D3/6-311+G(d) | -18.41 | -28.12 | -25.21 | -16.03 | -14.99 | 24.72 | 15.02 | 17.93 | 27.11 | 28.15 | -16.62 | 1.30 | -103.93 | -7.91 | -11.10 | -14.55 | -18.33 | -18.76 | -24.59 | 24.08 |
| TPSS/6-311+G(d) | -17.18 | -27.15 | -24.40 | -14.92 | -12.07 | 26.35 | 16.38 | 19.13 | 28.61 | 31.46 | -15.39 | 3.81 | -104.61 | -3.67 | -4.44 | -10.59 | -11.94 | -19.48 | -23.57 | 19.72 |
| TPSS-D3/6-311+G(d) | -17.14 | -27.10 | -24.08 | -14.93 | -14.37 | 26.31 | 16.35 | 19.37 | 28.52 | 29.08 | -14.77 | 4.00 | -104.57 | -6.21 | -8.75 | -13.02 | -16.25 | -20.03 | -25.53 | 22.86 |
| BHandHLYP/6-311+G(d) | -17.54 | -27.46 | -24.36 | -16.22 | -13.06 | 27.32 | 17.40 | 20.50 | 28.64 | 31.80 | -15.20 | 7.01 | -105.19 | 0.49 | -0.78 | -7.89 | -9.80 | -18.69 | -26.77 | 19.63 |
| HF/6-311+G(d) | -16.27 | -26.26 | -22.16 | -15.08 | -11.62 | 29.58 | 19.59 | 23.68 | 30.76 | 34.23 | -11.29 | 12.82 | -106.32 | 8.49 | 6.51 | -1.22 | -3.49 | -12.29 | -21.20 | 10.72 |
| HF/aug-cc-pVDZ | -19.53 | -29.69 | -25.52 | -18.47 | -15.08 | 24.81 | 14.66 | 18.83 | 25.88 | 29.27 | -15.65 | 7.87 | -110.17 | 9.12 | 7.01 | -0.88 | -3.14 | -12.65 | -14.20 | 6.66 |
| HF/aug-cc-pVTZ | -20.14 | -29.99 | -25.69 | -18.79 | -15.41 | 24.69 | 14.85 | 19.15 | 26.05 | 29.42 | -15.79 | 7.84 | -109.48 | 11.50 | 9.45 | 1.57 | -0.59 | -11.72 | -13.11 | 5.91 |
| MP2/6-311+G(d) | -15.71 | -24.11 | -21.81 | -13.43 | -10.54 | 28.02 | 19.61 | 21.91 | 30.29 | 33.18 | -19.38 | 8.73 | -107.04 | -10.14 | -10.97 | -16.89 | -18.37 | -22.73 | -29.80 | 22.60 |
| MP2/aug-cc-pVDZ | -18.53 | -27.80 | -25.37 | -16.37 | -13.39 | 21.66 | 12.38 | 14.82 | 23.81 | 26.80 | -24.10 | 2.71 | -110.51 | -10.99 | -12.17 | -18.49 | -20.86 | -22.98 | -29.07 | 18.72 |
| MP2/aug-cc-pVTZ | -19.35 | -28.71 | -26.12 | -17.07 | -14.00 | 21.29 | 11.93 | 14.51 | 23.56 | 26.64 | -24.78 | 2.12 | -110.65 | -8.35 | -9.46 | -16.13 | -18.40 | -23.26 | -30.42 | 18.83 |
| SCS-MP2/aug-cc-pVDZ | -17.04 | -26.41 | -23.71 | -15.32 | -12.26 | 22.97 | 13.59 | 16.30 | 24.69 | 27.74 | -19.08 | 5.56 | -111.17 | -7.28 | -8.55 | -15.07 | -17.44 | -20.92 | -26.45 | 16.29 |
| SCS-MP2/aug-cc-pVTZ | -17.74 | -27.21 | -24.34 | -15.96 | -12.78 | 22.70 | 13.23 | 16.11 | 24.49 | 27.66 | -19.54 | 5.12 | -111.32 | -4.50 | -5.72 | -12.54 | -15.08 | -21.01 | -27.61 | 16.15 |
| CCSD(T)/aug-cc-pVDZ | -18.90 | -27.88 | -25.49 | -17.15 | -14.24 | 22.42 | 13.44 | 15.83 | 24.17 | 27.08 | -17.94 | 4.78 | -111.97 | -6.97 | -8.19 | -14.66 | -17.17 | -23.48 | -29.93 | 17.49 |
| CCSD(T)/aug-cc-pVTZ | -19.60 | -28.68 | -26.12 | -17.79 | -14.76 | 22.15 | 13.08 | 15.64 | 23.97 | 27.00 | -18.40 | 4.34 | -111.81 | -9.74 | -11.03 | -17.19 | -19.54 | -23.39 | -28.76 | 17.35 |
| SCCDFTB | -40.35 | -55.92 | -55.56 | -38.86 | -39.87 | 18.30 | 2.74 | 3.10 | 19.79 | 18.78 | -27.09 | -2.47 | -123.18 | -2.19 | -1.72 | -10.47 | -9.11 | -14.66 | -23.27 | 14.48 |
| PM3 | -41.38 | -55.77 | -54.46 | -45.16 | -44.79 | 17.62 | 3.23 | 4.53 | 13.84 | 14.21 | -30.09 | -9.75 | -118.28 | 6.42 | 5.55 | -4.24 | -4.40 | -14.13 | -21.54 | 8.95 |
| AM1 | -31.54 | -48.03 | -47.44 | -35.65 | -35.47 | 22.89 | 6.41 | 7.00 | 18.79 | 18.96 | -20.23 | 0.44 | -128.41 | 10.40 | 10.98 | -0.29 | -0.31 | -16.72 | -20.21 | 3.94 |