|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Methods | For all 20 reactions | | | | | For proton transfer reaction (R1-13) | | | | | For non-proton transfer reaction (R14-20) | | | | |
| MAE | SD | LAE | Rxn No. | *R2* | MAE | SD | LAE | Rxn No. | *R2* | MAE | SD | LAE | Rxn No. | *R2* |
| CCSD(T)/aug-cc-pVTZ | 0.00 | 0.00 | 0.00 | - | 1.000 | 0.00 | 0.00 | 0.00 | - | 1.000 | 0.00 | 0.00 | 0.00 | - | 1.000 |
| CCSD(T)/aug-cc-pVDZ | 0.87 | 0.95 | 2.83 | 15 | 0.999 | 0.42 | 0.23 | 0.80 | 2 | 0.999 | 1.70 | 1.22 | 2.83 | 15 | 0.988 |
| MP2/aug-cc-pVTZ | 1.16 | 1.36 | 6.39 | 11 | 0.997 | 1.20 | 1.67 | 6.39 | 11 | 0.997 | 1.08 | 0.51 | 1.48 | 20 | 0.996 |
| SCS-MP2/aug-cc-pVDZ | 1.34 | 1.01 | 3.48 | 19 | 0.999 | 1.41 | 0.86 | 2.57 | 1 | 0.999 | 1.21 | 1.30 | 3.48 | 19 | 0.998 |
| SCS-MP2/aug-cc-pVTZ | 1.45 | 0.78 | 2.48 | 15 | 0.996 | 1.06 | 0.64 | 1.98 | 5 | 0.999 | 2.16 | 0.45 | 2.48 | 15 | 0.975 |
| MP2/aug-cc-pVDZ | 1.75 | 1.58 | 5.71 | 11 | 0.997 | 1.28 | 1.41 | 5.71 | 11 | 0.997 | 2.61 | 1.61 | 4.02 | 14 | 0.996 |
| BP86-D3/6-311+G(d) | 2.53 | 2.16 | 8.04 | 13 | 0.994 | 2.20 | 1.97 | 8.04 | 13 | 0.996 | 3.13 | 2.53 | 6.73 | 20 | 0.982 |
| TPSS-D3/6-311+G(d) | 2.79 | 1.88 | 7.40 | 13 | 0.997 | 2.96 | 1.87 | 7.40 | 13 | 0.997 | 2.46 | 1.99 | 5.51 | 20 | 0.997 |
| B3LYP-D3/6-31+G(d) | 2.98 | 1.56 | 6.73 | 13 | 0.996 | 2.64 | 1.72 | 6.73 | 13 | 0.997 | 3.60 | 1.03 | 4.88 | 19 | 0.990 |
| B3LYP-D3/6-311+G(d) | 3.23 | 1.89 | 7.70 | 13 | 0.986 | 2.61 | 1.97 | 7.70 | 13 | 0.997 | 4.37 | 1.06 | 5.79 | 18 | 0.993 |
| TPSS/6-311+G(d) | 3.56 | 1.61 | 7.36 | 13 | 0.955 | 3.25 | 1.71 | 7.36 | 13 | 0.997 | 4.15 | 1.30 | 6.36 | 19 | 0.988 |
| BP86/6-311+G(d) | 3.60 | 2.79 | 10.81 | 13 | 0.991 | 3.16 | 3.10 | 10.81 | 13 | 0.993 | 4.40 | 2.07 | 8.24 | 19 | 0.996 |
| BLYP-D3/6-311+G(d) | 3.69 | 2.44 | 9.28 | 19 | 0.994 | 2.91 | 1.89 | 8.40 | 13 | 0.997 | 5.13 | 2.80 | 9.28 | 19 | 0.994 |
| MP2/6-311+G(d) | 3.92 | 2.00 | 6.53 | 7 | 0.993 | 4.83 | 1.50 | 6.53 | 7 | 0.997 | 2.22 | 1.73 | 5.25 | 20 | 0.996 |
| B3LYP/6-31+G(d) | 4.10 | 2.48 | 8.32 | 17 | 0.986 | 2.90 | 1.49 | 6.68 | 13 | 0.998 | 6.32 | 2.47 | 8.32 | 17 | 0.927 |
| BHandHLYP/6-311+G(d) | 4.20 | 2.14 | 7.45 | 14 | 0.990 | 3.44 | 1.76 | 6.78 | 13 | 0.997 | 5.60 | 2.19 | 7.45 | 14 | 0.936 |
| B3LYP/6-311+G(d) | 4.21 | 2.91 | 8.89 | 17 | 0.977 | 2.83 | 1.82 | 7.65 | 13 | 0.997 | 6.75 | 2.91 | 8.89 | 17 | 0.941 |
| BLYP/6-311+G(d) | 5.10 | 3.57 | 12.45 | 19 | 0.977 | 3.06 | 1.70 | 8.34 | 13 | 0.997 | 8.88 | 2.97 | 12.45 | 19 | 0.926 |
| HF/aug-cc-pVDZ | 5.94 | 6.09 | 16.09 | 14 | 0.933 | 1.72 | 1.13 | 3.54 | 12 | 0.998 | 13.76 | 2.22 | 16.09 | 14 | 0.533 |
| HF/aug-cc-pVTZ | 6.69 | 6.91 | 18.47 | 14 | 0.916 | 1.91 | 1.06 | 3.51 | 12 | 0.998 | 15.56 | 2.81 | 18.47 | 14 | 0.411 |
| HF/6-311+G(d) | 7.83 | 4.02 | 15.46 | 14 | 0.962 | 5.60 | 2.18 | 8.48 | 12 | 0.997 | 11.98 | 3.27 | 15.46 | 14 | 0.655 |
| SCCDFTB | 11.56 | 8.36 | 29.44 | 3 | 0.863 | 14.57 | 8.97 | 29.44 | 3 | 0.958 | 5.98 | 2.14 | 8.82 | 18 | 0.944 |
| PM3 | 12.01 | 6.54 | 21.32 | 5 | 0.835 | 10.97 | 7.39 | 21.32 | 5 | 0.977 | 13.95 | 4.43 | 19.18 | 15 | 0.362 |
| AM1 | 14.58 | 7.82 | 30.03 | 5 | 0.786 | 16.55 | 9.06 | 30.03 | 5 | 0.947 | 10.92 | 2.34 | 13.74 | 15 | 0.660 |