|  |  |  |  |
| --- | --- | --- | --- |
| Methods | Absolute errors for each reaction ( kcal∙mol-1) | SD | MAEs for each reaction |
| 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) | 2.3 | 1.5 | 2.1 | 1.9 | 2.2 | 3.9 | 3.1 | 3.6 | 3.4 | 3.8 | 2.5 | 0.6 | 6.7 | 7.2 | 7.4 | 7.5 | 8.3 | 5.1 | 7.5 | 1.2 | 2.3 | 4.1 |
| B3LYP-D3/6-31+G(d) | 2.4 | 1.6 | 2.5 | 1.9 | 0.3 | 3.8 | 3.0 | 3.9 | 3.3 | 1.1 | 3.3 | 0.3 | 6.7 | 3.9 | 2.0 | 4.3 | 2.9 | 4.4 | 4.9 | 2.9 | 2.4 | 3.0 |
| B3LYP/6-311+G(d) | 2.1 | 1.1 | 1.5 | 2.0 | 2.0 | 3.9 | 2.9 | 3.3 | 3.8 | 3.8 | 2.6 | 0.3 | 7.6 | 7.7 | 8.0 | 7.9 | 8.9 | 6.5 | 7.8 | 0.3 | 2.1 | 4.2 |
| B3LYP-D3/6-311+G(d) | 2.2 | 1.1 | 1.8 | 2.0 | 1.3 | 3.9 | 2.8 | 3.5 | 3.7 | 0.4 | 3.4 | 0.0 | 7.7 | 4.4 | 2.6 | 4.7 | 3.5 | 5.8 | 5.3 | 4.4 | 2.2 | 3.2 |
| BLYP/6-311+G(d) | 2.6 | 1.5 | 2.0 | 2.7 | 2.6 | 3.3 | 2.2 | 2.7 | 3.4 | 3.3 | 3.3 | 1.7 | 8.3 | 8.6 | 9.0 | 9.4 | 10.6 | 9.3 | 12.4 | 2.8 | 2.6 | 5.1 |
| BLYP-D3/6-311+G(d) | 2.7 | 1.6 | 2.5 | 2.7 | 0.9 | 3.3 | 2.2 | 3.1 | 3.2 | 1.5 | 4.3 | 1.4 | 8.4 | 4.5 | 2.3 | 5.5 | 3.9 | 8.4 | 9.3 | 2.1 | 2.7 | 3.7 |
| BP86/6-311+G(d) | 1.1 | 0.5 | 0.4 | 1.8 | 1.3 | 2.6 | 4.8 | 4.8 | 6.1 | 5.6 | 0.9 | 0.5 | 10.8 | 2.8 | 3.2 | 3.7 | 5.1 | 5.5 | 8.2 | 2.2 | 1.1 | 3.6 |
| BP86-D3/6-311+G(d) | 1.2 | 0.6 | 0.9 | 1.8 | 0.2 | 2.6 | 1.9 | 2.3 | 3.1 | 1.2 | 1.8 | 3.0 | 8.0 | 0.9 | 2.9 | 0.1 | 1.2 | 4.7 | 5.3 | 6.7 | 1.2 | 2.5 |
| TPSS/6-311+G(d) | 2.4 | 1.5 | 1.7 | 2.9 | 2.7 | 4.2 | 3.3 | 3.5 | 4.6 | 4.5 | 3.0 | 0.5 | 7.4 | 3.3 | 3.7 | 4.1 | 5.2 | 4.0 | 6.4 | 2.4 | 2.4 | 3.6 |
| TPSS-D3/6-311+G(d) | 2.5 | 1.6 | 2.0 | 2.9 | 0.4 | 4.2 | 3.3 | 3.7 | 4.6 | 2.1 | 3.6 | 0.3 | 7.4 | 0.8 | 0.6 | 1.6 | 0.9 | 3.4 | 4.4 | 5.5 | 2.5 | 2.8 |
| BHandHLYP/6-311+G(d) | 2.1 | 1.2 | 1.8 | 1.6 | 1.7 | 5.2 | 4.3 | 4.9 | 4.7 | 4.8 | 3.2 | 2.7 | 6.8 | 7.5 | 7.4 | 6.8 | 7.4 | 4.8 | 3.2 | 2.3 | 2.1 | 4.2 |
| HF/6-311+G(d) | 3.3 | 2.4 | 4.0 | 2.7 | 3.1 | 7.4 | 6.5 | 8.0 | 6.8 | 7.2 | 7.1 | 8.5 | 5.6 | 15.5 | 14.7 | 13.4 | 13.7 | 11.2 | 8.7 | 6.6 | 3.3 | 7.8 |
| HF/aug-cc-pVDZ | 0.1 | 1.0 | 0.6 | 0.7 | 0.3 | 2.7 | 1.6 | 3.2 | 1.9 | 2.3 | 2.8 | 3.5 | 1.8 | 16.1 | 15.2 | 13.8 | 14.0 | 10.8 | 15.7 | 10.7 | 0.1 | 5.9 |
| HF/aug-cc-pVTZ | 0.5 | 1.3 | 0.4 | 1.0 | 0.7 | 2.5 | 1.8 | 3.5 | 2.1 | 2.4 | 2.6 | 3.5 | 2.5 | 18.5 | 17.6 | 16.2 | 16.6 | 11.8 | 16.8 | 11.4 | 0.5 | 6.7 |
| MP2/6-311+G(d) | 3.9 | 4.6 | 4.3 | 4.4 | 4.2 | 5.9 | 6.5 | 6.3 | 6.3 | 6.2 | 1.0 | 4.4 | 4.9 | 3.2 | 2.8 | 2.2 | 1.2 | 0.8 | 0.1 | 5.2 | 3.9 | 3.9 |
| MP2/aug-cc-pVDZ | 1.1 | 0.9 | 0.7 | 1.4 | 1.4 | 0.5 | 0.7 | 0.8 | 0.2 | 0.2 | 5.7 | 1.6 | 1.5 | 4.0 | 4.0 | 3.8 | 3.7 | 0.5 | 0.9 | 1.4 | 1.1 | 1.7 |
| MP2/aug-cc-pVTZ | 0.3 | 0.0 | 0.0 | 0.7 | 0.8 | 0.9 | 1.2 | 1.1 | 0.4 | 0.4 | 6.4 | 2.2 | 1.3 | 1.4 | 1.3 | 1.5 | 1.2 | 0.2 | 0.5 | 1.5 | 0.3 | 1.2 |
| SCS-MP2/aug-cc-pVDZ | 2.6 | 2.3 | 2.4 | 2.5 | 2.5 | 0.8 | 0.5 | 0.7 | 0.7 | 0.7 | 0.7 | 1.2 | 0.8 | 0.3 | 0.4 | 0.4 | 0.3 | 2.6 | 3.5 | 1.1 | 2.6 | 1.3 |
| SCS-MP2/aug-cc-pVTZ | 1.9 | 1.5 | 1.8 | 1.8 | 2.0 | 0.5 | 0.2 | 0.5 | 0.5 | 0.7 | 1.1 | 0.8 | 0.6 | 2.5 | 2.5 | 2.1 | 2.1 | 2.5 | 2.3 | 1.2 | 1.9 | 1.4 |
| CCSD(T)/aug-cc-pVDZ | 0.7 | 0.8 | 0.6 | 0.6 | 0.5 | 0.3 | 0.4 | 0.2 | 0.2 | 0.1 | 0.5 | 0.4 | 0.2 | 2.8 | 2.8 | 2.5 | 2.4 | 0.1 | 1.2 | 0.1 | 0.7 | 0.9 |
| CCSD(T)/aug-cc-pVTZ | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| SCCDFTB | 20.7 | 27.2 | 29.4 | 21.1 | 25.1 | 3.9 | 10.3 | 12.5 | 4.2 | 8.2 | 8.7 | 6.8 | 11.2 | 4.8 | 6.5 | 4.2 | 8.1 | 8.8 | 6.7 | 2.9 | 20.7 | 11.6 |
| PM3 | 21.8 | 27.1 | 28.3 | 27.4 | 30.0 | 4.5 | 9.9 | 11.1 | 10.1 | 12.8 | 11.7 | 14.1 | 6.3 | 13.4 | 13.7 | 10.4 | 12.8 | 9.4 | 8.4 | 8.4 | 21.8 | 12.0 |
| AM1 | 11.9 | 19.4 | 21.3 | 17.9 | 20.7 | 0.7 | 6.7 | 8.6 | 5.2 | 8.0 | 1.8 | 3.9 | 16.4 | 17.4 | 19.2 | 14.4 | 16.9 | 6.8 | 9.7 | 13.4 | 11.9 | 14.6 |