|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Methods | Mean signed errors | SD | Minimum errors | Rxn No. | Maximum errors | Rxn No. |
| B3LYP/6-31+G(d) | 3.9 | 2.8 | -1.2 | 17 | 8.3 | 20 |
| B3LYP-D3/6-31+G(d) | 2.9 | 1.7 | -0.3 | 13 | 6.7 | 5 |
| B3LYP/6-311+G(d) | 4.2 | 3.0 | -0.3 | 13 | 8.9 | 12 |
| B3LYP-D3/6-311+G(d) | 3.1 | 2.1 | -1.3 | 13 | 7.7 | 5 |
| BLYP/6-311+G(d) | 4.6 | 4.2 | -2.8 | 19 | 12.4 | 20 |
| BLYP-D3/6-311+G(d) | 3.5 | 2.6 | -1.4 | 19 | 9.3 | 12 |
| BP86/6-311+G(d) | 3.5 | 2.9 | -0.5 | 13 | 10.8 | 12 |
| BP86-D3/6-311+G(d) | 1.8 | 2.8 | -3.0 | 13 | 8.0 | 12 |
| TPSS/6-311+G(d) | 3.5 | 1.7 | -0.5 | 13 | 7.4 | 12 |
| TPSS-D3/6-311+G(d) | 2.7 | 2.0 | -0.6 | 13 | 7.4 | 15 |
| BHandHLYP/6-311+G(d) | 4.2 | 2.1 | 1.2 | 14 | 7.5 | 2 |
| HF/6-311+G(d) | 7.2 | 5.2 | -6.6 | 14 | 15.5 | 20 |
| HF/aug-cc-pVDZ | 4.7 | 7.2 | -10.7 | 14 | 16.1 | 20 |
| HF/aug-cc-pVTZ | 5.2 | 8.2 | -11.4 | 14 | 18.5 | 20 |
| MP2/6-311+G(d) | 2.9 | 3.4 | -3.2 | 7 | 6.5 | 14 |
| MP2/aug-cc-pVDZ | -0.4 | 2.4 | -5.7 | 16 | 3.8 | 11 |
| MP2/aug-cc-pVTZ | -0.8 | 1.6 | -6.4 | 13 | 1.3 | 11 |
| SCS-MP2/aug-cc-pVDZ | 1.0 | 1.3 | -1.1 | 19 | 3.5 | 20 |
| SCS-MP2/aug-cc-pVTZ | 1.2 | 1.1 | -1.2 | 18 | 2.5 | 20 |
| CCSD(T)/aug-cc-pVDZ | -0.2 | 1.3 | -2.8 | 19 | 1.2 | 15 |
| CCSD(T)/aug-cc-pVTZ | 0.0 | 0.0 | 0.0 | - | 0.0 | - |
| SCCDFTB | -7.7 | 12.2 | -29.4 | 18 | 8.8 | 3 |
| AM1 | -7.8 | 14.9 | -30.0 | 14 | 13.7 | 5 |
| PM3 | -3.5 | 13.5 | -21.3 | 15 | 19.2 | 3 |