各分子のDFT計算に要した時間

時間は1コアあたりに換算した値である。

|  |  |
| --- | --- |
| **Log File Name** | **Total Job CPU Time** |
| 1\_1\_1 | 0 days 6 hours 44 minutes 39.4 seconds |
| 1\_2\_1 | 0 days 20 hours 7 minutes 37.6 seconds |
| 1\_2\_3 | 5 days 21 hours 38 minutes 43.6 seconds |
| 1\_3\_1 | 0 days 6 hours 10 minutes 30.6 seconds |
| 1\_3\_3 | 1 days 13 hours 55 minutes 44.6 seconds |
| 1\_4\_1 | 0 days 23 hours 47 minutes 29.5 seconds |
| 1\_4\_3 | 2 days 14 hours 43 minutes 59.3 seconds |
| 1\_5\_1 | 0 days 12 hours 51 minutes 43.6 seconds |
| 1\_5\_3 | 8 days 16 hours 58 minutes 42.4 seconds |
| 1\_6\_1 | 0 days 8 hours 52 minutes 0.0 seconds |
| 1\_6\_3 | 1 days 22 hours 59 minutes 13.5 seconds |
| 1\_7\_1 | 0 days 10 hours 37 minutes 20.7 seconds |
| 1\_7\_3 | 2 days 8 hours 19 minutes 27.9 seconds |
| 1\_8\_1 | 0 days 10 hours 11 minutes 7.1 seconds |
| 1\_8\_3 | 1 days 23 hours 41 minutes 20.5 seconds |
| 1\_9\_1 | 0 days 10 hours 36 minutes 3.1 seconds |
| 1\_9\_3 | 2 days 12 hours 20 minutes 39.0 seconds |
| 1\_10\_1 | 0 days 5 hours 4 minutes 40.3 seconds |
| 1\_10\_3 | 1 days 7 hours 52 minutes 47.8 seconds |
| 1\_11\_1 | 0 days 4 hours 18 minutes 39.5 seconds |
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| 1\_16\_1 | 0 days 9 hours 33 minutes 11.5 seconds |
| 1\_16\_3 | 2 days 3 hours 57 minutes 18.8 seconds |
| 1\_18\_1 | 0 days 12 hours 17 minutes 26.3 seconds |
| 1\_18\_3 | 2 days 8 hours 1 minutes 12.2 seconds |
| 1\_19\_1 | 0 days 12 hours 57 minutes 45.4 seconds |
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| 1\_25\_1 | 0 days 7 hours 55 minutes 23.5 seconds |
| 1\_25\_3 | 1 days 14 hours 31 minutes 45.5 seconds |
| 3\_1\_1 | 0 days 8 hours 17 minutes 6.1 seconds |
| 3\_1\_3 | 1 days 1 hours 40 minutes 58.5 seconds |
| 3\_2\_1 | 0 days 18 hours 40 minutes 3.3 seconds |
| 3\_2\_3 | 5 days 13 hours 50 minutes 55.0 seconds |
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| 23\_4\_1 | 1 days 9 hours 10 minutes 25.8 seconds |
| 23\_4\_3 | 3 days 5 hours 58 minutes 50.8 seconds |
| 23\_5\_1 | 0 days 20 hours 4 minutes 43.5 seconds |
| 23\_5\_3 | 4 days 21 hours 23 minutes 53.4 seconds |
| 23\_6\_1 | 0 days 18 hours 39 minutes 0.1 seconds |
| 23\_6\_3 | 2 days 1 hours 27 minutes 10.5 seconds |
| 23\_7\_1 | 0 days 15 hours 0 minutes 18.2 seconds |
| 23\_7\_3 | 2 days 16 hours 50 minutes 3.1 seconds |
| 23\_8\_1 | 0 days 13 hours 7 minutes 27.5 seconds |
| 23\_8\_3 | 2 days 7 hours 22 minutes 1.3 seconds |
| 23\_10\_1 | 0 days 9 hours 8 minutes 17.4 seconds |
| 23\_10\_3 | 2 days 20 hours 18 minutes 4.9 seconds |
| 23\_11\_1 | 0 days 7 hours 39 minutes 33.9 seconds |
| 23\_11\_3 | 1 days 22 hours 59 minutes 53.6 seconds |
| 23\_12\_1 | 0 days 14 hours 8 minutes 51.9 seconds |
| 23\_12\_3 | 2 days 7 hours 34 minutes 39.1 seconds |
| 23\_13\_1 | 0 days 10 hours 10 minutes 45.4 seconds |
| 23\_13\_3 | 1 days 15 hours 39 minutes 37.9 seconds |
| 23\_14\_1 | 0 days 15 hours 32 minutes 3.0 seconds |
| 23\_14\_3 | 5 days 20 hours 6 minutes 31.1 seconds |
| 23\_15\_1 | 0 days 7 hours 52 minutes 59.1 seconds |
| 23\_15\_3 | 1 days 22 hours 9 minutes 30.1 seconds |
| 23\_16\_1 | 0 days 13 hours 8 minutes 19.2 seconds |
| 23\_16\_3 | 2 days 15 hours 37 minutes 47.8 seconds |
| 23\_17\_3 | 3 days 0 hours 52 minutes 16.7 seconds |
| 23\_18\_1 | 1 days 0 hours 0 minutes 9.6 seconds |
| 23\_18\_3 | 1 days 17 hours 15 minutes 45.1 seconds |
| 23\_19\_1 | 0 days 21 hours 11 minutes 56.7 seconds |
| 23\_19\_3 | 3 days 2 hours 52 minutes 44.5 seconds |
| 23\_20\_1 | 0 days 15 hours 28 minutes 54.5 seconds |
| 23\_20\_3 | 4 days 3 hours 2 minutes 49.4 seconds |
| 23\_21\_1 | 0 days 18 hours 57 minutes 3.6 seconds |
| 23\_22\_1 | 0 days 16 hours 0 minutes 42.8 seconds |
| 23\_22\_3 | 2 days 17 hours 41 minutes 26.3 seconds |
| 23\_23\_1 | 0 days 19 hours 15 minutes 59.4 seconds |
| 23\_23\_3 | 2 days 20 hours 57 minutes 36.1 seconds |
| 23\_24\_1 | 0 days 11 hours 54 minutes 31.4 seconds |
| 23\_24\_3 | 3 days 12 hours 58 minutes 29.2 seconds |
| 23\_25\_1 | 0 days 12 hours 30 minutes 58.4 seconds |
| 23\_25\_3 | 2 days 4 hours 11 minutes 15.4 seconds |