# Benchmark timings for Intel Core i5-4670 @ 3.4GHz under Linux using one core

| Benchmark | CPU timings (Time, sec) | Wall clock timings (Time, sec) | Number of atoms | Number of CAO basis functions | Method / Property | Details / Comment |
|---|---|---|---|---|---|---|
| Aspirine  | 19.2 | 19.3 | 21 | 211 / def-SV(P) | Energy, Hartree-Fock | no symmetry, single-point energy Hartree-Fock calculation, 13 SCF iterations |
| Cp2Mo2As6  | 197 | 197 | 28 | 432 / def-SV(P) | Energy, Hartree-Fock | C2v symmetry, single-point energy Hartree-Fock calculation, 19 SCF iterations |
| Camphor  | 3120 | 3130 | 27 | 1005 / aug-cc-pVTZ | Energy, Hartree-Fock | no symmetry, single-point energy Hartree-Fock calculation, 3 SCF iterations |
| C28H15  | 13.5 | 14 | 43 | 450 / def-SV(P) | Energy, RI-DFT | C2v symmetry, unrestricted single-point energy RI-DFT (BP86) , 19 SCF iterations |
| Cd10Me  | 17.6 | 17.7 | 126 | 1400 / def-SV(P) | Energy, RI-DFT | T symmetry, single-point energy RI-DFT (BP86) , 15 SCF iterations |
| Cd20Se31 | 13.3 | 13.4 | 51 | 1605 / def-SV(P) | Energy, RI-DFT | Td symmetry, single-point energy RI-DFT (BP86) , 18 SCF iterations |

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|---|---|---|---|---|---|---|
|  | | | | | | SCF iterations |
| CoPH36As12  | 11.2 | 11.3 | 42 | 780 / SVP | Energy, RI-DFT | D3d symmetry, single-point energy RI-DFT (BP86) , 29 SCF iterations |
| ZnO Cluster | 359 | 360 | 207 | 1858 / SVP | Energy, RI-DFT | no symmetry, single-point energy RI-DFT (PBE), 27470 point charges, larger DFT grid size (m4) , 3 SCF iterations |
| CoPH36As12  | 3.3 | 3.4 | 42 | 780 / SVP | Gradient, RI-DFT | D3d symmetry, gradient RI-DFT (BP86) |
| Dodeca-Helicene  | 129 | 130 | 78 | 806 / def-SV(P) | Ex. State, TD-DFT (RPA) | C2 symmetry, UV/Vis one singlet excitation TDDFT (BP86) |
| Zn-porphyrin  | 98 | 98 | 37 | 588 / TZVP | Gradient, TD-DFT (RPA) | no symmetry, TDDFT gradient of a triplet state (BP86) |
| Ferrocene, vibrations  | 176 | 177 | 21 | 472 / def2-TZVP | vib. frequencies, DFT | D5h symmetry, vibrational frequencies/IR (DFT, BP86) |
| C35H36, vibration  | 1336 | 1341 | 71 | 597 / def-SV(P) | vib. frequencies, DFT | Td symmetry, vibrational frequencies/IR (DFT, BP86) |
| Fullerene C60, MP2 energy  | 192 | 196 | 60 | 2100 / cc-pVTZ | Energy, RI-MP2 | D2h symmetry, (RI-) MP2 energy |

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|---|---|---|---|---|---|---|
| Calicheamicin, MP2 energy  | 241 | 242 | 39 | 1069 / cc-pVTZ | Energy, RI-MP2 | no symmetry, (RI-) MP2 energy |
| Chlorophyll-a, MP2 energy  | 904 | 926 | 91 | 969 / cc-pVDZ | Energy, RI-MP2 | no symmetry, (RI-) MP2 energy |
| DMABN, CC2 excited state  | 125 | 129 | 21 | 855 / aug-cc-pVTZ | Ex. State, RI-CC2 | C2v symmetry, CC2 excitation energy |
| (H2O)40, MP2 energy  | 819 | 832 | 120 | 760 / 6-31G* | Energy, RI-MP2 | no symmetry, (RI-) MP2 energy |
| Cd10Me, geometry opt  | - | 549 | 126 | 1400 / SVP+SV(P) | Opt, RI-DFT | T symmetry, SVP for Cd and Se and SV(P) for P,C,H geometry opt RI-DFT (BP86), 25 cycles |
| Pd-Complex  | - | 603 | 60 | 736 / TZVP | Opt, RI-DFT | no symmetry, geometry opt RI-DFT (BP86), larger DFT grid (m4), 8 cycles |