

## Benchmarking of various hardware using binary distributions of Gaussian 03 Revision C02

([http://www.gaussian.com/g\\_tech/g03\\_plat\\_c02.htm](http://www.gaussian.com/g_tech/g03_plat_c02.htm))

TEST397 – Valinomycin single point energy and force calculation at B3LYP/3-21G level

Stoichiometry: C<sub>54</sub>H<sub>90</sub>N<sub>6</sub>O<sub>18</sub>

882 basis functions, 1440 primitive gaussians, 882 cartesian basis functions, 600 electrons

SCF cycles: 15

|               | CPU              | MHz  | L2, Mb | nproc=1 | nproc=2 | nproc=3 | nproc=4 | nproc=5 | nproc=6 | nproc=7 | nproc=8 |
|---------------|------------------|------|--------|---------|---------|---------|---------|---------|---------|---------|---------|
| SGI O2k       | MIPS r10k - ip27 | 250  | 4096   | 0.16    | 0.28    | 0.36    | 0.52    | 0.60    | 0.70    | 0.81    | 1.00    |
| AMD           | XP2800+          | 2080 | 512    | 0.55    |         |         |         |         |         |         |         |
| AMD           | MP2800+          | 2133 | 512    | 0.47    | 0.84    |         |         |         |         |         |         |
| Intel         | P4               | 2600 | 512    | 0.58    |         |         |         |         |         |         |         |
| Intel         | Xeon 32 bit      | 2666 | 512    | 0.57    | 0.97    |         |         |         |         |         |         |
| AMD           | Opteron 246      | 1993 | 1024   | 0.73    | 1.34    |         |         |         |         |         |         |
| Intel         | Xeon EM64T       | 2993 | 1024   | 1.09    | 1.81    |         |         |         |         |         |         |
| SGI Altix 330 | Itanium 64bit    | 1500 | 1024   | 1.42    | 2.76    |         |         |         |         |         |         |
| Colfax 4wDC   | Opteron 880      | 2500 | 1024   | 0.87    | 1.61    | 2.34    | 2.90    | 3.67    | 4.26    | 5.70    | 6.28    |