

Benchmarking of various hardware using the Gaussian 03 Revision E01 using the official binary distribution

Gaussian 03: AM64L-G03RevE.01 11-Sep-2007

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

Stoichiometry: C₅₄H₉₀N₆O₁₈ (78 heavy atoms and 90 hydrogens)

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

speed	COW17	COW16	COW 5	COW 9	COW 2A	COW14A	COW1
proc	Opt 8378	Opt 8220	Opt 880	Opt 246	EM64T	EM64T	PIII XN
speed	2.4 GHz	2.8 GHz	2.4 GHz	2 GHz	3 GHz	3 GHz	2.66 GHz
core	4×4	4×2	4×2	2	2	2	2(4l)
mem	64 GB	16 GB	16 GB	1 GB	1 GB	2 GB	1 GB
os	SuSe 11.0	Centos 5.0	SuSe 11.0	SuSe 10.3	SuSe 10.0	SuSe 9.1	RH 9.3
1	0.10	0.10	0.09	0.07	0.07	0.06	0.04
2	0.18	0.16	0.16	0.13	0.13	0.11	0.08
3	0.28	0.23	0.22				0.09
4	0.38	0.31	0.28				0.11
5	0.46	0.36	0.33				0.13
6	0.52	0.39	0.36				0.15
7	0.60	0.37	0.38				0.17
8	0.66	0.45	0.42				0.20
9	0.71						
10	0.75						
11	0.82						
12	0.85						
13	0.85						
14	0.94						
15	0.97						
16	1.00						

all data based on wall-clock time without any load additional to minimal OS processes
core: number of processors per box × number of cores per processor; l indicates out-of-box parallelization via Linda

Last updated: January 19, 2009
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