

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

(http://www.gaussian.com/g_tech/g03_plat_c02.htm)

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

Stoichiometry: C₅₄H₉₀N₆O₁₈

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	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	0.81	1.65	2.46	2.99	3.49	3.91	4.57	5.04
ZT Group 8wDC	Engng Sample	2200	1024	0.98	1.77		3.26				4.32
Colfax 4wDC *	Opteron 8220	2800	1024	1.14	2.10	3.15	3.94	4.63	5.28	5.64	6.34

* using Gaussian03 Revision d01 (http://www.gaussian.com/g03_plat.htm)

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RK Szilagyi, Montana State University