

## Benchmarking of PC hardware using the official binary distribution of Gaussian 03 Revision E01 (OPT-900N)

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 Gaussian 03: AM64L-G03RevE.01 11-Sep-2007  
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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> (78 heavy atoms and 90 hydrogen atoms)  
 882 basis functions, 1440 primitive Gaussians, 882 Cartesian basis functions, 600 electrons

speed	Mellanox	Mellanox	Mellanox	TRSERVER	COW17	COW16	COW 5	COW21	COW 2A	COW14A	COW1
proc	iX5260	Opt 2382	iX5570	i7-920	Opt 8378	Opt 8220	Opt 880	Opt 246	EM64T	EM64T	PIII XN
speed	3.3 GHz	2.6 GHz	2.93 GHz	2.66 GHz	2.4 GHz	2.8 GHz	2.4 GHz	2 GHz	3 GHz	3 GHz	2.66 GHz
cache	6 MB	½ MB	8 MB	8MB L3	½ MB	1MB	1MB	1MB	1MB	1MB	½ MB
core	1x2	2x4	4x2	1x4 w/HT	4x4	4x2	4x2	2	2	2	2(4l)
mem	4GB	16GB	24GB	12GB	64 GB	16 GB	16 GB	1 GB	1 GB	2 GB	1 GB
os	Centos 5.0	RHES 5.1	RHES 5.3	SuSe 11.1	SuSe 11.0	Centos 5.0	SuSe 11.0	SuSe 10.3	SuSe 10.0	SuSe 9.1	RH 9.3
1	0.14	0.11	0.10	0.14	0.10	0.10	0.09	0.07	0.07	0.06	0.04 <sup>l</sup>
2	<b>0.25</b>	0.21	0.18	0.27	0.18	0.16	0.16	<b>0.13</b>	<b>0.13</b>	<b>0.11</b>	0.08 <sup>l</sup>
3		0.29	0.26	0.40	0.28	0.23	0.22				0.09 <sup>l</sup>
4		0.37	0.32	0.51	0.38	0.31	0.28				0.11 <sup>l</sup>
5		0.44	0.44	0.51	0.46	0.36	0.33				0.13 <sup>l</sup>
6		0.50	0.57	0.54	0.52	0.39	0.36				0.15 <sup>l</sup>
7		0.55	0.74	0.55	0.60	0.37	0.38				0.17 <sup>l</sup>
8		<b>0.60</b>	<b>0.85</b>	<b>0.56</b>	0.66	<b>0.45</b>	<b>0.42</b>				<b>0.20<sup>l</sup></b>
9					0.71						
10					0.75						
11					0.82						
12					0.85						
13					0.85						
14					0.94						
15					0.97						
16			1.10 <sup>l</sup>		<b>1.00</b>						

all data based on wall-clock time without any additional load 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: August 15, 2009  
 RK Szilagyi, Montana State University