Table 48. SGI 75 MHz R8000 PowerChallenge Timings for *Gaussian 92/DFT(Rev. G)*[a]

Benchmark	Basis	# Proc.'s	Wall Time	Speedup
18-crown-6, direct SCF	3-21G	1	382	1.0
		2	220	1.7
		3	180	2.1
		4	162	2.4
		5	155	2.5
18-crown-6, direct SCF	6-31G**	1	3014	1.0
		2	1643	1.8
		3	1181	2.6
		4	965	3.1
		5	837	3.6
		6	755	4.0
		7	712	4.2
		8	623	4.8
		9	594	5.1
		10	576	5.2
		11	566	5.3
18-crown-6, direct SCF+grad.	6-31G**	1	4514	1.0
		2	2427	1.9
		3	1736	2.6
		4	1390	3.2
		5	1172	3.9
		6	1014	4.5
		7	937	4.8
		8	871	5.2
		9	832	5.4
		10	791	5.7
		11	756	6.0
18-crown-6, direct SCF	aug-cc-pVDZ	1	159612	1.0
		2	79915	2.0
		3	54197	2.9
		4	43447	3.7
		5	38492	4.1
		10	19930	8.0
		12	17430	9.2

[a]All times are in seconds on a dedicated 12 processor PowerChallenge with 2.0 GB, 8-way interleaved memory under IRIX 6.1.

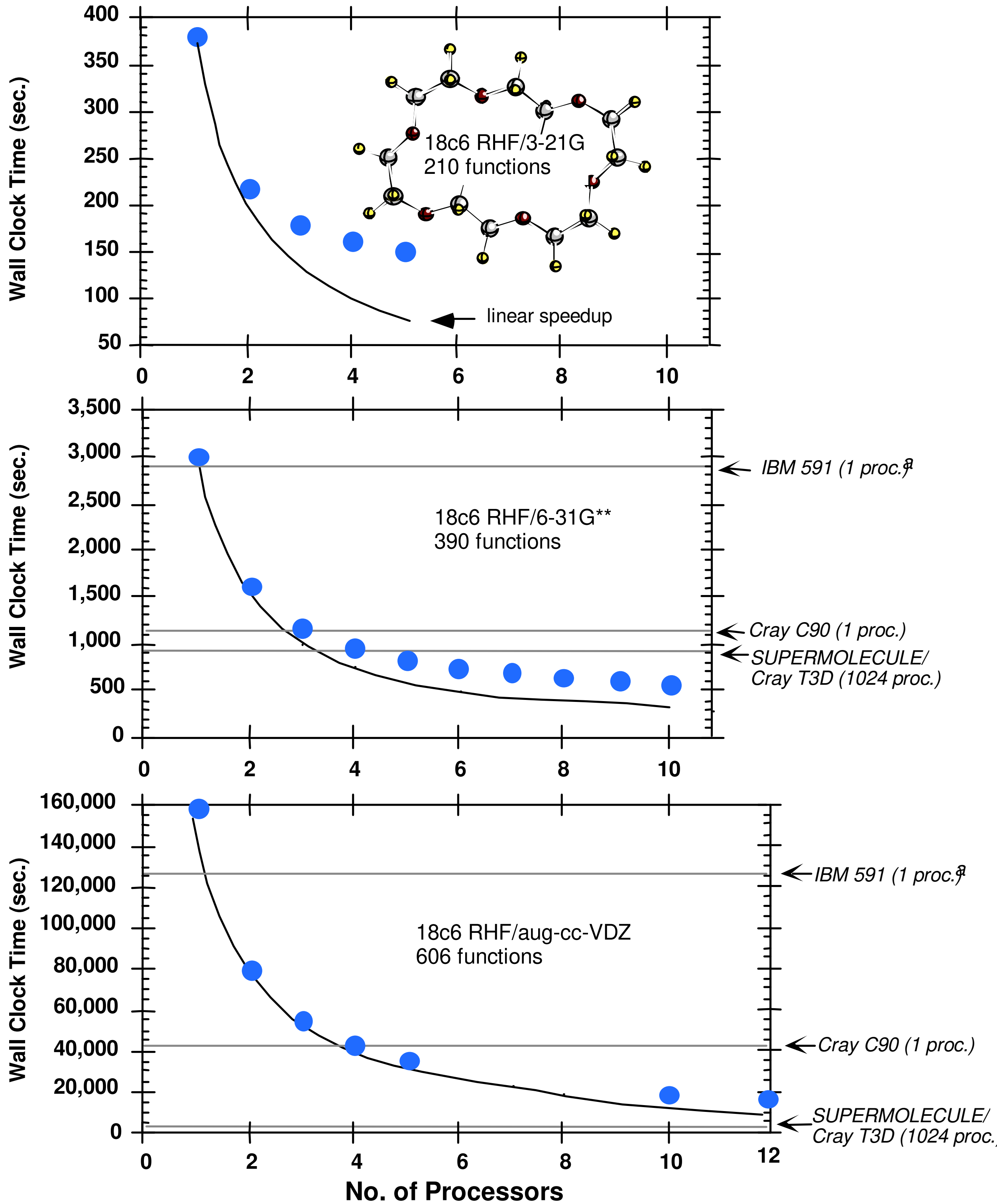

Figure 10. Wall clock times for direct Hartree-Fock calculations on an SGI PowerChallenge with 75 MHz processors. The IBM 591 times were estimated by assuming a 15% improvement over the model 590. SUPERMOLECULE times are based on runs conducted entirely on the T3D (i.e. nonheterogeneous). The fastest SUPERMOLECULE times were obtained in heterogeneous mode.

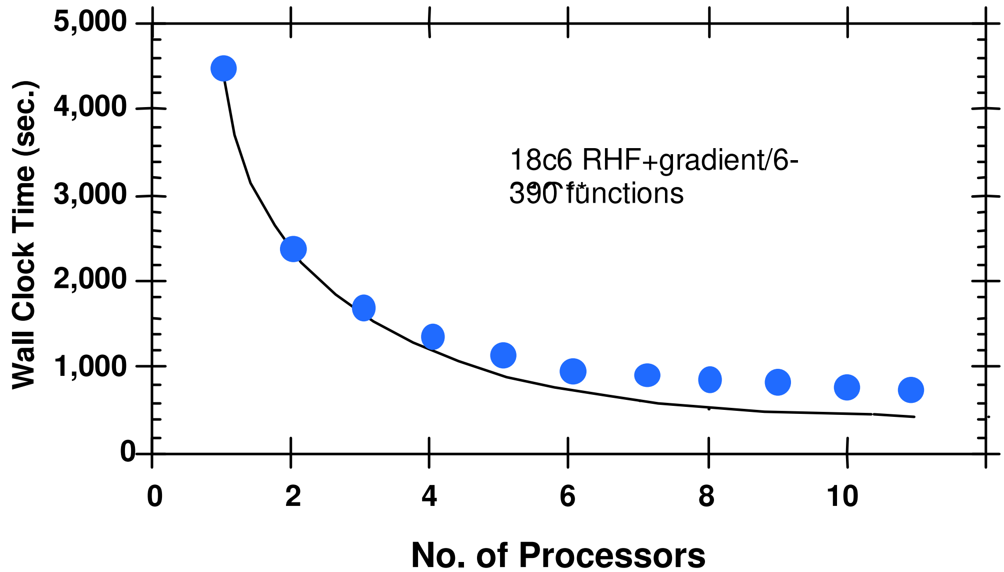

Figure 11. Wall clock times for direct Hartree-Fock + gradient calculations on an SGI PowerChallenge with 75 MHz R8000 processors.

Table 49. SGI 90 MHz R8000 PowerChallenge Timings for *Gaussian 92/DFT(Rev. G)*[(a)]

Benchmark	Basis	# Proc.'s	Wall Time (constant load)[b]	Speedup
18-crown-6, direct SCF + hessian	3-21G	1	13816	1.0
		2	7433	1.9
		3	5075	2.7
18-crown-6, direct SCF	aug-cc-pVDZ	1	143554	1.0
		2	75064	1.9
		4	40389	3.6
		8	21674	6.6
		10	18932	7.6

[(a)]All times are in seconds. Run on a 14 processor PowerChallenge with 1.2 GB, 4-way interleaved memory under IRIX 6.1.

[b]The system was operating under a constant load of 14 active jobs running on 14 processors to more closely simulate "real world" conditions.

Table 50. SGI 90 MHz R8000 PowerChallenge Timings for *Gaussian 94(Rev. C.2)*[a]

Benchmark	Basis	# Proc.'s	Wall Time (sec)	Speedup
18-crown-6, direct SCF	aug-cc-pVDZ	1	105,277	1.0
		4	29,462	3.6
		8	15,653	6.7
		12	11,433	9.2
		16	10,053	10.5
18-crown-6, direct SCF + gradient	aug-cc-pVDZ	1	131,489	1.0
		4	36,829	3.6
		8	19,722	6.7
		12	13,987	9.4
		16	12,261	10.7

[a]Run on two 16 processor PowerChallenges. One had 4.0 GB, 8-way interleaved memory and the other had 2.0 GB of 8-way interleaved memory. Both systems ran under IRIX 6.1. The amount of memory requested was 8 MW (1 Proc.), 24 MW (4 Proc.), 48 MW (8 Proc.), 72 MW (12 Proc.) and 96 MW (16 Proc.) for both the direct HF and direct HF + gradient runs. Calculations were run by Dr. Roberto Gomperts of Silicon Graphics, Inc.

Table 51. SGI 196 MHz R10000 Origin 2000 Timings for *Gaussian 94(Rev. D)*[a]

Benchmark	Basis	# Proc.'s	Wall Time (sec)	Speedup
18-crown-6, direct SCF	aug-cc-pVDZ	1	108,799	1.0
(606 basis functions)		4	29,450	3.7
		8	15,470	7.0
		12	10,861	10.0
		16	8,621	12.6
		20	7,433	14.6
		24	6,472	16.8
		28	5,897	18.5

[a]Run on a 32 processor Origin 2000. Calculations were run by Dr. Roberto Gomperts of Silicon Graphics, Inc.