Table 44. Kendall Square Research 2 Wall Clock Timings for *GAMESS(US)*.[a]

Benchmark	Basis	# Proc.'s	SCF Time	Total Time	Speedup[b]
Ethylene	6-311++G**	5	70.8	76.3	5.0
		15	32.1	37.6	10.2
		30	23.7	30.0	12.7
		45	20.8	28.6	13.3
		60	20.0	29.0	13.1
Cis napthol	6-31+G*	5	11,655.4	11,732.2	5.0
		15	3,917.4	3,988.6	14.7
		30	2,181.6	2,253.1	26.0
		45	1,610.5	1,684.6	34.8
		60	1,417.9	1,494.7	39.3
18-crown-6	3-21G	5	2,525.9	2,730.9	5.0
		15	1,299.0	1,400.6	9.8
		30	858.0	960.0	14.2
		45	861.3	964.9	14.2
		60	718.1	826.2	16.5
	6-31G**	5	18,357.2	19,690.9	5.0
		15	7,720.1	9,001.8	10.9
		30	4,941.9	6,211.3	15.9
		45	4,027.1	5,320.0	18.5
		60	3,693.7	4,999.4	19.7
	aug-cc-pVDZ	5	114,251.4	115,613.7	5.0
		15	41,321.4	42,624.8	13.6
		30	25,066.1	26,358.6	21.9
		45	19,459.3	20,772.3	27.8
		60	18,029.5	19,354.6	29.9

[a]All times are in seconds. All runs are direct Hartree-Fock calculations.
[b]Total speedup assuming a speedup of 5.0 for five processors.

Table 45. Intel Paragon Timings for *GAMESS(US)*.[a]

Benchmark	Basis	# Proc.'s	SCF Time	Total Time	Speedup[b]
Ethylene	6-311++G**	5	84.2	95.7	5.0
		15	47.1	58.3	8.2
		30	30.9	42.9	11.2
		45	27.6	40.8	11.7
		60	27.7	40.8	11.7
Cis-napthol	6-31+G*	5	12,872.6	12,956.6	5.0
		15	4,498.1	4,576.4	14.2
		30	2,423.1	2,501.3	25.9
		45	1,726.3	1,806.6	35.9
		60	1,525.4	1,624.3	39.9
18-crown-6	3-21G	5	2,997.2	3,137.0	5.0
		15	1,262.7	1,400.5	11.0
		30	829.1	966.0	16.4
		45	685.3	822.8	19.1
		60	807.3	962.3	16.3
	6-31G**	5	19,089.6	20,536.0	5.0
		15	7,462.2	8,901.8	11.5
		30	4,566.2	6,008.7	17.1
		45	3,607.1	5,054.0	20.3
		60	3,803.9	5,378.1	19.1

[a] All times are in seconds. All runs are direct Hartree-Fock calculations.
[b] Total speedup assuming a speedup of 5.0 for five processors.

Table 46. Comparison of *GAMESS(US)* SCF Timings for the Best Benchmark Times on Three Systems.[a]

Benchmark	CRAY C90[b]	Intel Paragon		KSR 2	
Ethylene	92.8	27.7	(60 proc.)	20.0	(60 proc.)
Cis-napthol	16,751.5	1,525.4	(60 proc.)	1,417.9	(60 proc.)
18-crown-6 321G	5,758.0[c]	685.3	(45 proc.)	718.1	(60 proc.)
18-crown-6 6-31G**	31,269.2[d]	3,607.1	(45 proc.)	3,693.7	(60 proc.)
18-crown-6 aug-cc-pVDZ	152,630.8[e]	17,606.7	(45 proc.)[e]	18,029.5	(60 proc.)

[a]All times are in seconds.
[b]Single processor.
[c]For sake of comparison, the G92 direct HF total time for this run on a C90 is 209 CPU sec.
[d]For sake of comparison, the G92 direct HF total time for this run on a C90 is 1,111 CPU sec.
[e]Estimate based on KSR-2 timing.

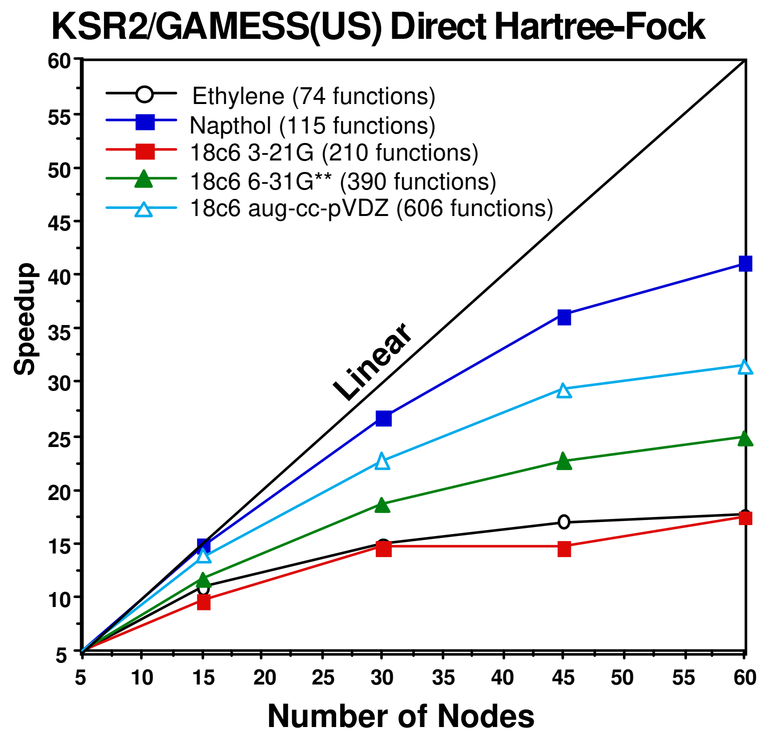

Figure 7. Speedup Curve for *GAMESS(US)* Running on the KSR-2. Page faults cause the larger basis calculations to deviate from ideal performance.

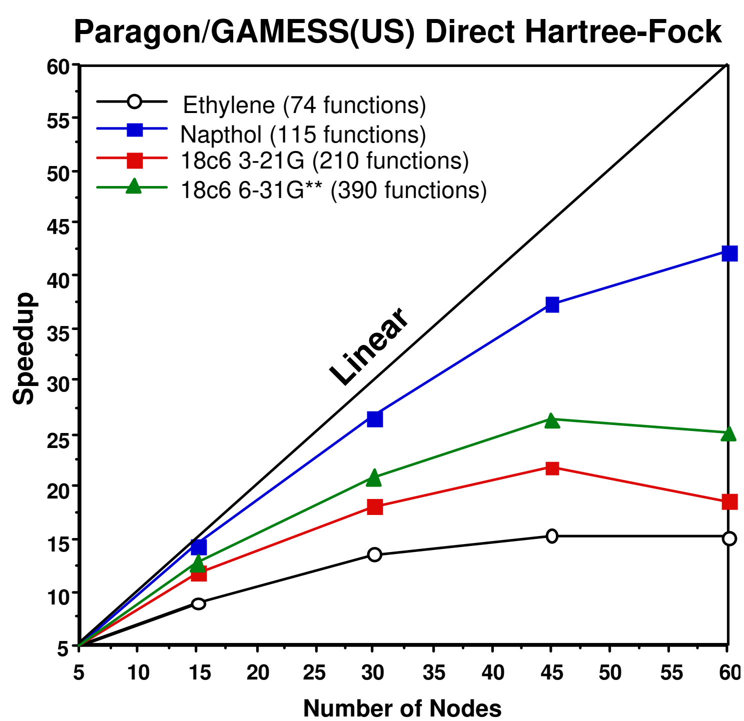

Figure 8. Speedup Curve for *GAMESS(US)* Running on the Intel Paragon. Page faults cause the larger basis calculations to deviate from ideal performance.

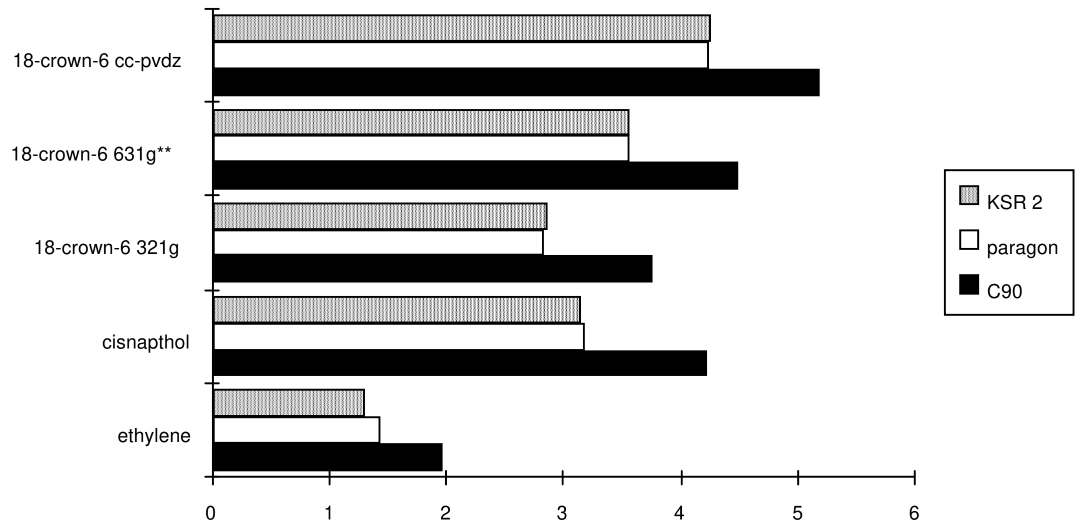

Figure 9. Log_{10}-based Timing Comparison for *GAMESS(US)* Running on the KSR-2, Intel Paragon and CRAY C90. This is a graphical representation of the data contained in Tables 32 and 33.