



Scientific Computing & Modelling



ADF Timings (mins) on 4 and 8 CPUs of a QS16-2600C-O64D QuantumCube™

molecule - job description	Basis (#AOs)	4 CPUs	8 CPUs
CO on 2-layer Pt slab - relativistic BAND	DZP (158)	10.5	6.0
(H ₂ O) ₃₀ – response properties	DZ (360)	14.2	7.5
VON ₄ C ₃₆ H ₄₄ - ESR and g-tensor, ZORA	DZ (436)	12.4	7.0
ZrN ₁₂ C ₃₆ H ₂₀ - dynamic hyperpolarizability	DZP (747)	9.0	5.5
C ₁₂₈ H ₃₂ - carbon nanotube, 10 excitations	DZ (1088)	14.5	9.2
C ₁₄ O ₈ H ₂₃ - GGA geom. opt., 1 cycle	DZP (401)	2.3	1.4
PtOP ₃ C ₅₅ H ₄₅ - GGA geom. opt., 1 cycle	DZP (1021)	30	17
W(CO) ₆ - frequencies, ZORA, all-electron	TZ2P (419)	48	26
FeSO ₆ N ₁₃ C ₅₆ H ₇₉ - single-point, BLYP	DZ (794)	80	44

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8- OR 16-CPU QUANTUMCUBE™ COMPLETE WITH ALL LINUX UTILITIES, PQS, SQM and the PQS GUI and with ADF/BAND and the ADF/BAND GUIs preinstalled

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QS16-2200C-O64D + ADF/BAND (1 year academic license) \$20,245

(ask for non-academic pricing; offer valid through 1 July 2007)

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