AMPAC

Faster. Smarter. *Just better.*

Feature	AMPAC 9	MOPAC 2007
Graphical User Interface (GUI)		
Molecule Building / Viewing	▪	
Visual display of properties, surfaces, MOs	▪	
Animation of reaction coordinates and vibrations	▪	
Gaussian03 – shares common interface	▪	
Graphic images for publication	▪	
Submit and manage jobs from the GUI	▪	
Read pdb files and accurately complete hydrogens	▪	
Semiempirical Methods		
AM1, MNDO, MINDO3, PM3, MNDO/d, RM1, PM6	▪	▪
SAM1 (transition metals Fe and Cu), MNDOC	▪	
Geometry Optimization and SCF Convergence		
Automatic Heuristic SCF Convergence $^\Delta$	▪	
RHF/UHF	▪	▪
TRUSTE and TRUSTG geometry optimization $^\Delta$	▪	▪
Eigenvector Following (EF)	☆	▪
CHN and LTRD transition state location methods $^\Delta$	▪	
PATH, IRC for potential surfaces and reaction pathways	☆	▪
Reaction pathway definition	☆	▪
GRID 2D reaction pathway investigation	☆	▪
LFORCE for rapid characterization of TSs and minima	▪	
Sparse matrix method for large molecules	*	▪
Additional Methods		
Configuration Interaction (CI) $^\Delta$	☆	▪
Selected State Optimized CI $^\Delta$	▪	
Analytic CI Gradients and higher spin multiplicities (20) $^\Delta$	▪	
Simulated Annealing for Multiple Minima Searches	▪	
AMSOL Method for Solvated Molecules	▪	
COSMO Solvation Method	▪	▪
Tomasi Solvation Method		▪
Property Calculations		
Thermodynamic Properties	▪	▪
Unpaired Electron Spin Density	▪	▪
Population Analysis: Coulson / Mulliken / ESP	▪	▪
Non-linear Optical Properties	☆	▪
Polymers and solid states		▪
Limited molecular dynamics		▪
Compatibility and Support		
Fully Compatible with CODESSA™ QSAR Program	▪	
Multiple File formats for read/write (mol, mol2, G03, pdf, CIF)	▪	
Manual: new, fully updated and indexed in hypertext format	▪	
Updating and addition of new features regularly	▪	
Customer Support - knowledgeable and *available*	▪	
Generous site-licensing for academics	▪	

* Under active development.　　　　☆ Common feature enhanced and improved in AMPAC.

Δ AMPAC much faster and more reliable