

Graphical User Interface	SpartanModel	Student V4	Spartan'10
Available Platforms:	Win/Mac	Win/Mac	Win/Mac and Linux
Organic Builder	—	✓	✓
Inorganic Builder	—	✓	✓
Peptide Builder	—	✓	✓
Nucleotide Builder	—	✓	✓
Sustituent Builder	—	—	✓
2-D Builder (Requires ChemDraw Access)	—	Win Only	Win Only
Automatic Transition State Guess	—	✓	✓
Transition State Library	—	✓	✓
Clipboard Access	—	✓	✓
Cambridge Structural Database Access	—	—	✓
Spartan Molecular Database Access*	IR and H of F	✓	✓
Protein Databank Access	✓	✓	✓
Automatic Tautomer Detection	—	—	✓
Extraction of bound Ligands	—	—	✓
Chemical Functional Descriptors	—	—	✓
Reaction Calculator	—	✓	✓
Display moolecules in multiple model styles	✓	✓	✓
Display/Manipulation of structural models	✓	✓	✓
Measures distance, angle, dihedrals	✓	✓	✓
Normal-mode animations	✓	✓	✓
Spreadsheet and Data Plots (2D & 3D)	—	2D Only	✓
Molecular Alignment and scoring	—	✓	✓
Linear Regression Analysis	—	—	✓
File Compatibility - Import/Export	SpartanModel	Student V4	Spartan'10
Spartan Files	import	✓	✓
SYBYL MOL and MOL2	—	✓	✓
PDB	import	✓	✓
MACROMODEL	—	import	✓
MDL SKC, TGF, and SDF	—	import	✓
SMILES	—	export	export
CIF	—	import	import
XYZ	—	import	✓
JCAMP	—	import	✓
ChemDraw (.CDX)	—	import	import
Graphics Export/Save as	SpartanModel	Student V4	Spartan'10
JPEG	—	✓	✓
PNG	✓	✓	✓
BMP	—	win only	✓
QuickTime Recording	—	✓	Win/Mac
Tasks - Calculations	SpartanModel	Student V4	Spartan'10
Energies	✓	✓	✓
Equilibrium Geometries	✓	✓	✓
Transition State Geometries	—	✓	✓
Intrinsic Reaction Coordinate (IRC)	—	—	✓
Conformation Distribution	—	—	✓
Conformer Library	—	—	✓
Energy Profiles	—	✓	✓
Similarity Analysis	—	—	✓
Spectra Calculations	SpartanModel	Student V4	Spartan'10
Infrared/Raman	from DB	IR	✓
UV/vis	—	—	✓
NMR Chemical Shifts	—	✓	✓
HH Splitting	—	✓	✓

Properties	SpartanModel	Student V4	Spartan'10
Weight, Area, Volume	✓	✓	✓
Solvation Energy SM5.4, SM5.0R	—	✓	✓
Solvation Energy SM8, SS(V)PE	—	—	✓
LogP	—	✓	✓
Polar Surface Area	✓	✓	✓
Polar Area from Electrostatic Potential Map	—	✓	✓
Muliken Charges	—	—	✓
Natural Charges	—	—	✓
Electrostatic Fit Charges	✓	✓	✓
Dipole Moments	✓	✓	✓
Higher Moments	—	—	✓
Polarizabilities	—	—	✓
Hyperpolarizabilities	—	—	✓
Electronegativity	—	✓	✓
Hardness	—	✓	✓
Q-minus and Q-plus	—	✓	✓
Molecular area and volume	—	✓	✓
Ovality	—	✓	✓
Enthalpy, entropy, free energy	—	✓	✓
HBA & HBD, +/- Ionizable Center Count	—	—	✓
Methods/Basis Sets	SpartanModel	Student V4	Spartan'10
SYBYL	—	—	✓
MMFF94	✓	✓	✓
MMFF94(aq)	—	—	✓
MNDO, MNDO(d)	—	—	✓
AM1	—	—	✓
RM1	—	—	✓
PM3, PM3 Transition Metal Extensions	—	to 75 atoms	✓
Hartree Fock	3-21G	to 30 atoms	✓
DFT local/BP/BLYP/B3LYP	—	B3LYP>30 atoms	✓
DFT EDF1/EDF2/M06/ωB97X-D	—	—	✓
DFT Slater-Dirac/Vokso-Wilk-Nusair	—	—	✓
DFT Perdew-Zunger/Wigner/Becke88/Gill96	—	—	✓
DFT Gilbert-Gill99/Lee-Yang-Parr/Perdew86	—	—	✓
DFT GGA91/BMK/M05/M05-2X	—	—	✓
DFT M06/M06-2X/M06-L/M06-HF	—	—	✓
Non-empirical GGA Functional PBE	—	—	✓
Customize Exchange and Correlation	—	—	✓
TDDFT	—	—	✓
MP2, MP3, MP4	—	MP2<20 atoms	✓
Resolution of the Identity - RI-MP2	—	—	✓
CCSD, CCSD(T), OD, OD(T)	—	—	✓
QCCSD, QCCSD(T)	—	—	✓
CIS, CISD	—	—	✓
QCIS, QCIS(D)	—	—	✓
Resolution of the Identity - RI-CIS(D)	—	—	✓
T1	from DB	from Database	✓
G2, G3, G3(MP2)	—	—	✓
Basis Sets:			
STO-3G	—	—	✓
3-21G	✓	✓	✓
6-31G, 6-31G*, 6-31G**, 6-31+G*	—	6-31G*	✓
6-311G*/6-311G**/6-311+G**/6-311++G**	—	6-311+G**	✓
6-311++G(2df,2p), cc-pVTZ	—	—	✓
additional and custom basis sets	—	—	✓
polarization and diffuse functions	—	✓	✓
dual basis sets	—	—	✓

Graphical Models	SpartanModel	Student V4	Spartan'10
Molecular Orbital Diagram	✓	—	✓
Orbital surface, contours, maps	—	✓	✓
Density surfaces and contours	—	✓	✓
vdW surfaces	—	—	✓
Spin density surfaces and contours	—	✓	✓
Local ionization potential maps	—	✓	✓
ESP surfaces, contours, maps	ESP Map	✓	✓
Emphasize Accessible Regions	—	✓	✓
Graphical Animations	✓	✓	✓
Ribbon Style Display for biopolymers	✓	✓	✓
Defined points, plains	✓	✓	✓
Chemical Function Descriptors	—	—	✓
Hydrogen bonds	✓	✓	✓
Additional Features	SpartanModel	Student V4	Spartan'10
Automatic use of symmetry	—	✓	✓
Use of constraints and/or frozen atoms	—	✓	✓
Automatic inversion of chiral centers	✓	✓	✓
Automatic inversion of absolute chirality	✓	✓	✓
Automatic filling of open valences w/ H's	✓	✓	✓
Screen centering	✓	✓	✓
Cut/Paste Clipboard Access	Graphics	✓	✓
Remote Submission Capabilities	—	—	✓
Experimental IR & UV/vis access via NIST	—	IR Only	✓
Experimental NMR access from EBI	—	✓	✓
Draw NOESY, COSY, DEPT, HSQC, HMBC plots	—	—	✓
Boltzmann Averaged NMR spectra	—	—	✓
Included Databases*	SpartanModel	Student V4	Spartan'10
Spartan Molecular Database (# molecules)	5000	5000	5000
Spartan Spectra & Properties Database (# molecules)	—	—	5000
Name Search	✓	✓	✓
Substructure Search	—	—	✓
Formula Search	—	—	✓
Weight Search	—	—	✓
Isomer Search	—	—	✓
Substituent directed searching	—	—	✓
Searching by IR Spectra	—	—	✓
Spartan Reaction Database	—	—	✓
Spartan IR Database	—	—	✓

***Available for purchase:**

**Spartan Molecular Database includes (SMD) more than 150,000 Molecules
calculated at up to 10 theoretical Models**

Calculated Spectra: >40k IR spectra, >15 NMR spectra and >2k UV/vis spectra

T1 Thermochemical Database of ~ 40,000 molecules

Spartan Infrared Database of ~30,000 small molecules

**Spartan Spectra & Properties Database (SSPD) includes
more than 72,000 conformationally searched molecules
optimized with Density Functional Theory model EDF2
and including: T1 Heat of formation, IR and NMR
spectra, atomic and molecular properties**



Wavefunction, Inc.
18401 Von Karman, Suite 370
Irvine, CA 92612
www.wavefun.com