

Graphical User Interface	SpartanModel	Student V5	Spartan'10
Available Platforms:	Win/Mac	Win/Mac	Win/Mac/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 Spectra & Properties Database Access*	IR and H of F	•	•
Protein Databank Access	•	•	•
National Cancer Institute (CACTUS) Database Access	—	•	—
Automatic Tautomer Detection	—	—	•
Extraction of bound Ligands	—	—	•
Chemical Functional Descriptors	—	—	•
Reaction Calculator	—	•	•
Display molecules in multiple model styles	•	•	•
Display/Manipulation of structural models	•	•	•
Measures distance, angle, dihedrals	•	•	•
Normal-mode animations	•	•	•
Spreadsheet and Data Plots (2D & 3D)	—	2D Only	•
Ramachandron Plots	•	•	—
Molecular Alignment and scoring	—	•	•
Linear Regression Analysis	—	—	•
File Compatibility - Import/Export	SpartanModel	Student V5	Spartan'10
Spartan Files	import	•	•
SYBYL MOL and MOL2	—	•	•
PDB	import	•	•
MACROMODEL	—	•	•
MDL SKC, TGF, and SDF	—	•	•
SMILES	—	export	export
CIF	—	import	import
XYZ	—	•	•
JCAMP	—	•	•
ChemDraw (.CDX)	—	import	import
Graphics Export/Save as	SpartanModel	Student V5	Spartan'10
JPEG	—	•	•
PNG	•	•	•
BMP	—	win only	•
QuickTime Recording	—	•	Win/Mac
Tasks - Calculations	SpartanModel	Student V5	Spartan'10
Energies	•	•	•
Equilibrium Geometries	•	•	•
Transition State Geometries	—	•	•
Intrinsic Reaction Coordinate (IRC)	—	—	•
Conformation Distribution	—	—	•
Conformer Library	—	—	•
Energy Profiles	—	•	•
Similarity Analysis	—	—	•
Spectra Calculations	SpartanModel	Student V5	Spartan'10
Infrared/Raman	from DB	IR	•
UV/vis	—	—	•
NMR Chemical Shifts	—	•	•
HH Splitting	—	•	•

Properties	SpartanModel	Student V5	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	—	•	•
Mulliken Charges & Natural Charges	—	—	•
Electrostatic Fit Charges	•	•	•
Bond Orders	—	•	•
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 V5	Spartan'10
SYBYL	—	—	•
MMFF94	•	•	•
MMFF94(aq)	—	—	•
MNDO, MNDO(d)	—	—	•
AM1	—	—	•
RM1	—	—	•
PM3, PM3 Transition Metal Extensions	PM3/HF	to 75 atoms	•
Hartree Fock	PM3/HF	to 30 atoms	•
DFT local/BP/BLYP/B3LYP	—	B3LYP<30 atoms	•
DFT EDF1/EDF2/M06/_B97X-D	—	EDF2<30 atoms	•
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 Database	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	—	—	•
pseudopotentials for heavy elements	—	•	•

Graphical Models	SpartanModel	Student V5	Spartan'10
Orbital Energy 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 V5	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 V5	Spartan'10
Spartan Molecular Database (# molecules)	5000	5000	5000
Spartan Spectra & Properties Database (# molecules)	—	5000	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 Spectra & Properties Database (SSPD) includes more than 110,000 Molecules

Conformationally searched and optimized with the DFT EDF2 functional, and includes calculated IR spectra and proton and ¹³C NMR spectra and T1 heat of formation

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



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