

Graphical User Interface	SpModel	Student V4	06 Essential	Spartan'08
Available Platforms:	Win/Mac	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	Win Only
Automatic Transition State Guess	—	✓	✓	✓
Transition State Library	—	✓	✓	✓
Clipboard Access	—	✓	✓	✓
Cambridge Structural Database Access	—	—	✓	✓
Spartan Molecular Database Access*	✓	✓	✓	✓
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 geometries, areas, volumes	✓	✓	✓	✓
Normal-mode animations	✓	✓	✓	✓
Spreadsheet and Data Plots (2D & 3D)	2D Only	2D Only	✓	✓
Molecular Alignment and scoring	—	✓	✓	✓
Linear Regression Analysis	—	—	✓	✓
Vector Algebra	—	—	—	✓
File Compatibility - Import/Export	SpModel	Student V4	06 Essential	Spartan'08
SYBYL MOL and MOL2	import	✓	✓	✓
PDB	import	import	✓	✓
MACROMODEL	import	import	✓	✓
MDL SKC, TGF, and SDF	import	import	✓	✓
SMILES	import	import	✓	✓
CIF	—	import	import	import
XYZ	—	import	✓	✓
JCAMP	—	import	—	✓
ChemDraw (.CDX)	—	import	—	✓
Graphics Export/Save as	SpModel	Student V4	06 Essential	Spartan'08
JPEG	—	✓	✓	✓
PNG	—	✓	✓	✓
BMP	capture	win only	win only	✓
QuickTime Recording	—	✓	—	Win/Mac
Tasks - Calculations	SpModel	Student V4	06 Essential	Spartan'08
Energies	—	✓	✓	✓
Equilibrium Geometries	mm or DB	✓	✓	✓
Transition State Geometries	—	✓	✓	✓
Lowest Energy Conformation	—	—	✓	✓
Conformation Distribution	—	—	✓	✓
Conformer Library	—	—	✓	✓
Energy Profiles	—	✓	✓	✓
Similarity Analysis	—	—	—	✓
Spectra Calculations	SpModel	Student V4	06 Essential	Spartan'08
Infrared/Raman	from DB	IR	IR	✓
UV/vis	—	—	—	✓
NMR Chemical Shifts	—	✓	—	✓
HH Splitting	—	✓	—	✓

Properties	SpModel	Student V4	06 Essential	Spartan'08
Solvation Energy SM5.4, SM5.0R	QM from DB	✓	✓	✓
Solvation Energy SM8, SS(V)PE	—	—	—	✓
LogP	—	✓	✓	✓
Polar Surface Area	—	✓	✓	✓
Polar Area from Electrostatic Potential Map	—	✓	✓	✓
Muliken Charges	—	—	✓	✓
Natural Charges	—	—	✓	✓
Electrostatic Fit Charges	from DB	✓	✓	✓
Dipole Moments	from DB	✓	✓	✓
Higher Moments	—	—	✓	✓
Polarizabilities	—	—	✓	✓
Hyperpolarizabilities	—	—	SE models	✓
Electronegativity	—	✓	✓	✓
Hardness	—	✓	✓	✓
Q-minus and Q-plus	—	✓	✓	✓
Molecular area and volume	—	✓	✓	✓
Ovality	—	✓	✓	✓
Enthalpy, entropy, free energy	—	✓	✓	✓
HBA & HBD, +/- Ionizable Center Count	—	—	—	✓
Methods/Basis Sets	SpModel	Student V4	06 Essential	Spartan'08
SYBYL	—	—	✓	✓
MMFF94	—	✓	✓	✓
MMFF94(aq)	—	—	✓	✓
MNDO, MNDO(d)	—	—	✓	✓
AM1	—	—	✓	✓
RM1	—	—	✓	✓
PM3, PM3 Transition Metal Extensions	—	to 75 atoms	✓	✓
Hartree Fock	3-21 from DB	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 Database	—	✓
G2, G3, G3(MP2)	—	—	—	✓
Basis Sets:				
STO-3G	—	—	✓	✓
3-21G	from DB	✓	✓	✓
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	SpModel	Student V4	06 Essential	Spartan'08
Orbital surface, contours, maps	—	✓	✓	✓
Density surfaces and contours	from DB	✓	✓	✓
vdW surfaces	from DB	—	✓	✓
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	SpModel	Student V4	06 Essential	Spartan'08
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	IR Only	✓
Experimental NMR access from U. Mainz	—	✓	—	✓
Plot NOESY and COSY plots	—	—	—	✓
Boltzmann Averaged NMR spectra	—	—	—	✓
Spartan Molecular Database*	SpModel	Student V4	06 Essential*	Spartan'08*
Included subset (# molecules)	5000	5000	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:**

Full Database includes 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



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