

Graphical User Interface	06 Essential	Spartan'06
Available Platforms	Win / Mac	Mac / Windows / Linux
Organic Builder	✓	✓
Inorganic Builder	✓	✓
Peptide Builder	✓	✓
Nucleotide Builder	✓	✓
Substituent 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	✓	✓
Automatic Tautomer Detection	✓	✓
Extraction of bound Ligands	-	✓
Chemical Function Descriptors	-	✓
Display/manipulation of structural models	✓	✓
Measures geometries, areas, volumes	✓	✓
Normal-mode animations	✓	✓
Spreadsheet and Data Plots	✓	✓
Molecular Alignment	✓	✓
Linear Regression Analysis	✓	✓
File Compatibility - Import/Export	06 Essential	Spartan'06
SYBYL MOL and MOL2	✓	✓
PDB	✓	✓
MACROMODEL	✓	✓
MDL SKC, TGF, and SDF	✓	✓
SMILES	✓	✓
CIF files	✓	✓
XYZ files	✓	✓
File Compatibility - Save As/Export	06 Essential	Spartan'06
JPEG	✓	✓
PNG	✓	✓
BMP	✓	✓
PICT	-	-
AVI	Win only	Win only
QuickTime	-	-
Tasks	06 Essential	Spartan'06

Energies	✓	✓
Equilibrium Geometries	✓	✓
Transition State Geometries	✓	✓
Lowest Energy Conformer	✓	✓
Conformer Distribution	✓	✓
Energy Profiles	✓	✓
Thermochemistry Recipes	-	✓
Similarity Analysis	-	✓
Spectra Calculations	06 Essential	Spartan'06
Infrared	✓	✓
UV/vis	-	✓
NMR	-	✓
Properties	06 Essential	Spartan'06
Solvation Energy SM5.4a & SM50R	✓	✓
LogP	✓	✓
Polar Surface Area	✓	✓
Polar Area from ESP	-	✓
Muliken Charges	✓	✓
Natural Charges	✓	✓
Electrostatic-fit Charges	✓	✓
Dipole Moments	✓	✓
Higher Moments	-	✓
Polarizabilities	✓	✓
Hyperpolarizabilities	SE	✓
Electronegativity	✓	✓
Hardness	✓	✓
Q-minus and Q-plus	✓	✓
Molecular area and volume	✓	✓
Ovality	✓	✓
Enthalpy, entropy, free energy	✓	✓
HBA & HBD count	-	✓
Pos. & Neg. Ionizable Center count	-	✓
Methods/Basis Sets	06 Essential	Spartan'06
SYBYL	✓	✓
MMFF94	✓	✓
MMFF94aq	✓	✓
MNDO, MNDO(d)	✓	✓
AM1	✓	✓
PM3, PM3 Transition Metal Extensions	✓	✓
RM1	✓	✓
Hartree-Fock	✓	✓
DFT (local, BP, BLYP, EDF1, B3LYP)	-	✓

TDDFT (local, BP, BLYP, EDF1, B3LYP)	-	✓
MP2, MP3, MP4, LMP2	-	✓
Resolution of the Image - MP2 (RI-MP2)	-	✓
CCSD CCSD(T), OD, OD(T)	-	✓
QCCSD, QCCSD(T)	-	✓
CISD, CISD(T)	-	✓
QCISD, QCISD(T)	-	✓
T1	-	✓
G2, G3, G3(MP2)	-	✓
STO-3G	✓	✓
3-21G	✓	✓
6-31G*	✓	✓
6-311G*	✓	✓
cc-pVTZ	-	✓
Pseudopotentials	-	✓
Polarization functions	✓	✓
Diffuse Functions	✓	✓
Additional and Custom Basis Sets	-	✓
Dual Basis Sets	-	✓
Graphical Models	06 Essential	Spartan'06
Orbital surfaces, contours, maps	✓	✓
Density surfaces, and contours	✓	✓
Spin density surfaces and contours	✓	✓
Localized ionization potential maps	✓	✓
Graphical Models - Continued	06 Essential	Spartan'06
Electrostatic potential srfs/contours/maps	✓	✓
Emphasize Accessible Regions	✓	✓
Graphical animations	✓	✓
Ribbon Style Display for biopolymers	✓	✓
Defined planes	✓	✓
Display of hydrogen bonds	✓	✓
Additional Features	06 Essential	Spartan'06
Use of symmetry	✓	✓
Use of constraints and/or frozen atoms	✓	✓
Automatic inversion of chiral centers	✓	✓
Automatic on-screen centering	✓	✓
Cut/Paste Clipboard Access	✓	✓
Submit molecules as a single list	✓	✓
Remote submission capabilities	-	✓
Online Access to PDB (search by ID)	✓	✓
Experimental IR Spectra from NIST	✓	✓

Experimental UV/vis Spectra from NIST	–	✓
Experimental NMR Spectra from U. Cologne	–	✓
Spartan Molecular Database (SMD)	06 Essential	Spartan'06
Number of molecules	65,000	140,000
Hartree-Fock	3-21G / 6-31G*	3-21G/6-31G*
Hartree-Fock	3-21G / 6-31G*	6-311+G**
Density Functional Theory (EDF1)	–	6-31G*
Density Functional Theory (B3LYP)	–	6-31G*/6-311+G**
Moller Plesset (MP2)	–	6-31G*/6-311+G**
G3 (MP2)	IR	G3 (MP2)
Name Search	✓	✓
Formula, Isomer, Weight Search	✓	✓
Spectra	IR	IR, UV/Vis, NMR
Spartan Reaction Database	✓	✓

Spartan
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