Wavefunction, Inc. © 1991-2024 - Spartan Comparison Chart Jan 2024

Graphical User Interface	Spartan'24	Student V9
Available Platforms:	**Win/Mac/Linux**	**Win/Mac**
Organic Builder	✓	✓
Inorganic Builder	✓	✓
Peptide Builder	✓	✓
Nucleotide Builder	✓	✓
Sustituent Builder	✓	—
Sketch (2-D) Builder	✓	✓
Chem Draw Builder (requires ChemDraw v. 12 or later)	**Win Only**	**Win Only**
Transition State Library	✓	✓
Clipboard Access	✓	✓
Cambridge Structural Database Access	✓	—
Spartan Spectra & Properties Database Access*	✓	✓
Protein Databank Access	✓	✓
NIST Infrared Database Access	✓	✓
Generate Isomers / Generate Tautomers	✓	**Isomers Only**
Extraction of bound Ligands	✓	—
Chemical Functional Descriptors	✓	—
Reactions Calculator	✓	✓
Experimental Data (input) menu	✓	—
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	**Spartan'24**	**Student V9**
All Spartan formats	✓	✓
SYBYL MOL and MOL2	✓	✓
PDB and standard XYZ file	✓	✓
MACROMODEL	✓	✓
MDL SKC, TGF, and SDF	✓	✓
InChI	✓	✓
SMILES	✓	✓
CIF	**import**	**import**
ChemDraw (.CDX)	**import**	**import**
JCAMP (.dx) or CSV for IR .CML for NMR	✓	✓
Export Spreadsheet as Excel, Open Document Spreadsheet or CSV	✓	✓
Graphics Export/Save As	**Spartan'24**	**Student V9**
JPEG	✓	✓
PNG	✓	✓
PNG - customize pixel size / resolution (Save Image As...)	✓	✓
BMP	✓	✓
Tasks - Calculations	**Spartan'24**	**Student V9**
Energies	**multi-core**	**multi-core**
Equilibrium Geometries	**multi-core**	**multi-core**
Transition State Geometries	**multi-core**	**multi-core**
Intrinsic Reaction Coordinate (IRC)	**multi-core**	—
Equilibrium Conformer	**multi-core**	**MMFF only**
Conformation Distribution	**multi-core**	**MMFF only**
NMR Spectrum (Boltzmann-weighted)	**multi-core**	—
SSPD Compatible calculaition (for adding to the database)	**multi-core**	—
Similiarity Library	✓	—
Energy Profiles	**multi-core**	**multi-core**
Similarity Analysis	✓	—
QSAR calculations	✓	✓
Thermodynamics and Vibrational Modes	✓	✓
Orbitals & Energies, Charges & Bond Orders	✓	✓

Spectra Calculations	Spartan'24	Student V9
Infrared/Raman	✓	**IR Only**
UV/vis	✓	✓
NMR Chemical Shifts	✓	✓
Calculated HH Splitting	✓	**Emiprical only**
Display of COSY, HSQC, & HMBC NMR Plots	✓	—
Properties	**Spartan'24**	**Student V9**
Weight, Area, Volume	✓	✓
Solvation Energy SM5.4, SM5.0R, SM8, SM12, SMD	✓	**SM5.4, SM5.0R**
Solvation Energy C-PCM, SS(V)PE	✓	**C-PCM only**
Orbitals & Energies, Charges & Bond Orders	✓	✓
Neural Network Estimated Energies	✓	—
Enthalpy, Entropy, Gibbs Free Energy	✓	✓
Heat Capacity & Zero Point Energy	✓	✓
LogP	✓	✓
QSAR Routines (& QSAR Tab in Properties dialogue)	✓	✓
Polar Surface Area	✓	✓
Polar Area from Electrostatic Potential Map	✓	✓
Mulliken Charges & Natural Charges	✓	**Output Summary**
Electrostatic Fit Charges	✓	✓
Bond Orders	✓	✓
Dipole Moments	✓	✓
Higher Moments	✓	—
Polarizabilities	✓	✓
Hyperpolarizabilities	✓	—
Electronegativity	✓	✓
Hardness	✓	✓
Q-minus and Q-plus	✓	✓
Ovality	✓	✓
HBA & HBD, +/- Ionizable Center Count	✓	✓
Methods/Basis Sets	**Spartan'24**	**Student V9**
SYBYL	✓	—
MMFF94	✓	✓
MMFF94(aq)	✓	—
Neural Network: Corrected MMFF (to wB97X-V/6-311+G(2df,2p)//MMFF	✓	—
MNDO, MNDO(d)	✓	—
AM1	✓	—
RM1	✓	—
PM3, PM3 Transition Metal Extensions	✓	**up to 75 atoms**
PM6	✓	—
Hartree Fock	✓	**up to 30 atoms**
GGA: B86PW91, BLYP, BPW91, B97-D2, SOGGA11, PBE-D3, VV10	✓	—
GH-GGA: B3LYP, B3LYP-D3, EDF2, B3PW91, MPW3LYP, SOGA11-X	✓	**B3LYP, EDF2,**
RSH-GGA: ωB97X-D, ωB97X-V, ωB97X, CAM-B3LYP, N12-SX, LC-VV10	✓	**and ωB97X-D**
mGGA: B97M-V, M06-L, BMK, M11-L, TPSS-D3	✓	**up to 30 atoms**
GH-mGGA: M06-2X, M06, M08-HX, M08-SO, MPW1B95	✓	—
RSH-mGGA: M11, ωB97M-V, MN12-SX	✓	—
Additional functionals	✓	—
Customize Exchange and Correlation	✓	—
Neural Network: Est. DFT ωB97X-D/6-31G* [Geometries only]	✓	—
Neural Network: Est. DFT ωB97X-V, ωB97M-V, ωB97M(2) [Energies only]	✓	—
TDDFT	✓	—
CIS, CISD, QCIS, QCIS(D)	✓	—
RI-MP2, MP2, MP3, MP4	✓	**MP2 up to 20 atoms**
CCSD, CCSD(T), OD, OD(T)	✓	—
QCCSD, QCCSD(T)	✓	—
CIS, CISD, QCIS, QCIS(D)	✓	—
Resolution of the Identity - RI-CIS(D)	✓	—
T1	✓	**up to 20 atoms**
G3, G3(MP2), G4, G4(MP2)	✓	—
G3elect, G3(MP2)elect, G4elect, G4(MP2)elect	✓	—

Basis Sets	Spartan'24	Student V9
Pople 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(2df,2p)	✓	**6-311+G****
Dunning basis sets: cc-pVDZ, cc-pVTZ, cc-pVQZ	✓	—
aug-cc-pVDZ, aug-cc-pVTZ, aug-cc-pVQZ	✓	—
Alrichs/Weigend basis sets: def2-SV(p), def2-SVP, def2-SVPD	✓	—
def2-TZVP, def2-TZVPPD, def2-QZVP, def2-QZVPPD	✓	—
Additional polarization and diffuse functions	✓	—
Dual basis sets	✓	**used in T1**
pseudopotentials for heavy elements	✓	✓
Graphical Models	**Spartan'24**	**Student V9**
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	✓	✓
Emphasize Accessible Regions	✓	✓
Graphical Animations	✓	✓
Ribbon Style Display for biopolymers	✓	✓
Defined points, plains	✓	✓
Chemical Function Descriptors	✓	—
Hydrogen bonds	✓	✓
Additional Features	**Spartan'24**	**Student V9**
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	✓	✓
Remote Submission Capabilities	✓	—
Experimental IR & UV/vis access via NIST	✓	✓
Experimental NMR access from NMR Shift DB	✓	✓
Boltzmann Weighted NMR spectra	✓	—
Import 2D NMR spectra (image)	✓	—
Remote Submission to Spartan'24	✓	—
Included Computational Server (receives remotely submitted jobs)	✓	—
Included Databases*	**Spartan'24**	**Student V9**
Spartan Spectra & Properties Database (# molecules)	**>317,000**	**≈ 6000**
Name Search	✓	✓
Structure / Substructure Search	✓	**Structure Only**
Formula Search	✓	—
Weight Search	✓	—
Isomer Search	✓	—
Substituent directed searching	✓	—
Searching by IR Spectra	✓	—
Spartan Reaction Database	✓	—
Spartan IR Database	✓	—
Regression Analysis from SSPD	✓	—