## **Spartan ODYSSEY** (v.6) **Student Edition** (v.7) <u>Platforms</u> Windows Win 7 or newer Win 7 or newer macOS / OS X 10.8 or newer 10.9.5 or newer **3D Visualization** Styles (Wire, Ball&Spoke, Space Filling, etc.) 5 5 Models Side-by-Side 2-4 Any Number Via Edit→Select Via Properties Dialog Multiple Styles in Same Model Synchronize Side-by-Side Simulations N/A Selected Examples Any List of Models Scroll through Daisy-Chained Models Align Similar Molecules No Show Hydrogen Bonding, Show Dipoles **Show Idealized Lone Pair Positions** No Show Collisions, Show Reactive Events N/A Show Velocity Vectors, Show Trajectories N/A Emphasize H-Bonds/Dipoles/Collisions No Ribbons for Biopolymers **Chirality Labels Selected Models** Red-Green-Blue Color Scale (for Isosurfaces) ✓ Red-White-Blue Color Scale (for Isosurfaces) No **Custom Ranges for Property Maps** No Hyperlinkable from PowerPoint Export of JPG/PNG/BMP Images SMILES Export (EXPERT Setting) No Quicktime Recording No **Declare Custom Colors** Anaglyph Red-Blue Stereo **Changing Parameters** Change Bond Length, Graphically Driven In Build Mode Change Torsion Angle, Graphically Driven In Build Mode Set Bond Length, Numerical Entry No Set Bond Angle, Numerical Entry No Set Torsion Angle, Numerical Entry No Move Molecules Relative to Each Other In Build Mode N/A Change Temperature Change Simulation Cell Volume N/A **Change Numbers of Molecules** N/A Change Time Step (to Slow Down Motion) N/A

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Building New Models				
2D Sketcher 3D Entry-Level Builder	No ✓	<b>✓</b>		
3D Advanced/Inorganic Builder 3D Crystal Builder (Solids) 3D Disordered Phase Builder (Gases, Liquids)	✓ 52 Templates ✓	√ No No		
3D Peptide Builder 3D Nucleotide Builder	Simplified Simplified	<b>✓</b>		
Maximum Number of Atoms, General Maximum Number of Atoms, Crystal Builder	9,999 (per Atom Type) 1,500	No Limit N/A		
Chemical Validity Check Build with Clipboard Define Planes and Virtual Points	√ No No	No ✓ ✓		
Name Acyclic Organic Molecules Name Other Molecules IUPAC or Common Names (for Built-In Models) Add Arbitrary Labels	Any Molecule For Molecules in Database ✓	For Molecules in Database For Molecules in Database N/A No		
PDB File Import CACTUS Chemical Structure Lookup ChemDraw Import Spartan Database Search SMILES Import	Drag and Drop No Drag and Drop No Drag and Drop	By PDB ID By Name Integrated Integrated Drag and Drop		
New User Tutorials (for Building Models)	25 Built-In Lessons	PDF Files		
Mol	ecular Mechanics			
Find Local Energy Minimum Calculate Normal Modes Set Constraints Calculate Conformer Distribution	Single-Click No No No	Single-Click Yes (Job Submission) ✓ ✓		
Molecular Dynamics				
Start Interactive Simulation Control Simulation Speed with Slider Recommended Maximum Number of Atoms	Single-Click ✓ ~1,000	No N/A N/A		
Translational and Rotational Motion Intramolecular Vibrational Motion Periodic Boundaries for Condensed Phases	Always Yes (Unless Constrained) ✓	N/A Can Show Normal Modes No		

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Electronic Structure				
Calculate (from Quantum Mechanics) Semiempirical Model (PM3) Hartree-Fock Model DFT (B3LYP and EDF2) Moller-Plesset (MP2)	Single-Click (Always Followed by HF) Up to 30 Atoms No No	Job Submission Up to 75 Atoms Up to 30 Atoms Up to 30 Atoms Up to 20 Atoms		
Electron Density Isosurfaces Arbitrary Isovalue for Surfaces Polarity Maps (Electrostatic Potential Maps)	✓ No ✓	✓ ✓ ✓		
Atomic Orbitals Cross-Sections ("Slices") Molecular Orbitals Electrostatic Potentials, Spin Densities LUMO Maps, Ionization Potentials	Pre-Calculated Examples Pre-Calculated Examples Pre-Calculated Examples Pre-Calculated Examples No	✓ ✓ ✓		
Choice of Basis Set Inclusion of Solvent (Continuum Model) Control over Graphical Resolution Time Estimates (for Submitted Calculations)	No No No N/A	✓ ✓ ✓		
	Analysis			
Distances, Angles, and Torsion Angles Atomic/Molecular Properties Thermodynamic Properties Dynamic Properties QSAR Properties	✓ ✓ ✓ ✓ No	✓ ✓ ✓ N/A ✓		
Symmetry Detection (Point Groups) Extended Property List (EXPERT Setting) Orbital Energy Diagrams	No ✓ No	√ N/A √		
Integrated Spreadsheet Export to Excel	No N/A	<b>✓</b>		
XY Plots Linear Regression Polymial Fit Lorentzian Fit, Gaussian Fit, Other Fits Reciprocal and Logarithmic Axes Radial Distribution Function (EXPERT Setting) Ramachandran Plots Kinetic Energy/Speed Histograms	✓ ✓ ✓ No ✓ ✓ No ✓ ✓	✓ ✓ ✓ No No ✓		
IR Spectra NMR Spectra (Proton and C-13)	No No	<b>✓</b> ✓		

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Ch	emical Reactions			
Reaction Dynamics at Set Temperature Dynamic Equilibria Examine Reaction Profiles Find Transition States	Selected Examples Selected Examples Selected Examples No	No No ✓		
Integrated Content				
Prebuilt Models (Molecules, Bulk Samples)	> 3,000	No		
Quick Visuals (Demonstrations) Molecular Labs (Worksheets) Concepts & Applications (Essays and Models) Molecular Stockroom	> 120 > 120 > 160 ✓	No No No No		
New User Tutorials (for Operation of Program) Content Search Engine Wikipedia Access Periodic Table of the Elements	14 Built-In Lessons  ✓  Hyperlinks ✓	PDF Files N/A By Keyword No		
Listed Misconceptions (for Molecular Labs)  Comments (for Molecular Labs)	Instructor's Ed. <b>Only</b> ✓	N/A N/A		
Assessment Questions Google Forms Worksheet Questions Answer Key	> 1,200 Instructor's Ed. Only Instructor's Ed. Only	No N/A N/A		
Add Model Snapshots to Answers Annotation of Pages	<b>✓ ✓</b>	N/A N/A		
Customization of Questions Authoring Capability	Instructor's Ed. Only Instructor's Ed. Only	N/A N/A		
Japanese Language Content Spanish Language Content German Language Content	✓ ✓ ✓	No No No		