

	ODYSSEY (v.6)	Spartan Student Edition (v.8)
Platforms		
Windows	Win 7 or newer	Win 8.1 or newer
macOS / OS X	10.10 or newer	10.12.6 or newer
Parallel Processing	2 Threads (Simulate/Visualize)	Up to 16 Cores
3D Visualization		
Styles (Wire, Ball&Spoke, Space Filling, etc.)	5	5
Models Side-by-Side	2 (Some Examples: up to 5)	Any Number
Multiple Styles in Same Model	Via Edit→Select	Via Properties Dialog
Synchronize Side-by-Side Simulations	✓	N/A
Scroll through Daisy-Chain Models	Selected Examples	Any List of 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	✓
Color Scale (for Isosurfaces)	✓	✓
Choice of Green or White for Neutral	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
Change Temperature	✓	N/A
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 Models		
2D Sketcher	No	✓
3D Entry-Level Builder	✓	✓
3D Advanced/Inorganic Builder	✓	✓
3D Crystal Builder (Solids)	52 Templates	No
3D Disordered Phase Builder (Gases, Liquids)	✓	No
3D Peptide Builder	Simplified	✓
3D Nucleotide Builder	Simplified	✓
3D to 2D Conversion	No	✓
Maximum Number of Atoms, General	9,999 (per Atom Type)	No Limit
Maximum Number of Atoms, Crystal Builder	1,500	N/A
Chemical Validity Check	✓	No
Build with Clipboard	No	✓
Define Planes and Virtual Points	No	✓
Name Acyclic Organic Molecules	Any Molecule	For Molecules in Database
Name Other Molecules	For Molecules in Database	For Molecules in Database
IUPAC or Common Names (for Built-In Models)	✓	N/A
Add Arbitrary Labels	✓	No
PDB File Import	Drag and Drop	By PDB ID
CACTUS Chemical Structure Lookup	No	By Name
ChemDraw Import	Drag and Drop	Integrated
Spartan Database Search	No	Integrated
SMILES Import	Drag and Drop	Drag and Drop
Build Tutorials	28 Integrated Lessons	Organic Molecules (PDF Files)
Molecular Mechanics		
Find Local Energy Minimum	Single-Click	Single-Click
Calculate Normal Modes	No	Yes (Job Submission)
Set Constraints	No	✓
Calculate Conformer Distribution	No	✓
Molecular Dynamics		
Start Interactive Simulation	Single-Click	No
Control Simulation Speed with Slider	✓	N/A
Recommended Maximum Number of Atoms	~1,000	N/A
Translational and Rotational Motion	Always	N/A
Intramolecular Vibrational Motion	Yes (Unless Constrained)	Can Show Normal Modes
Periodic Boundaries for Condensed Phases	✓	No

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Electronic Structure		
Calculate (from Quantum Mechanics)	Single-Click	Job Submission
Semiempirical Model (PM3)	(Always Followed by HF)	Up to 75 Atoms
Hartree-Fock Model	Up to 30 Atoms	Up to 30 Atoms
DFT (ω B97X-D, EDF2, B3LYP)	No	Up to 30 Atoms
Møller-Plesset (MP2)	No	Up to 20 Atoms
T1 thermochemical recipe	No	Up to 20 Atoms
Electron Density Isosurfaces	✓	✓
Arbitrary Isovalue for Surfaces	No	✓
Polarity Maps/Electrostatic Potential Maps	✓	✓
Atomic Orbitals	Pre-Calculated Examples	✓
Cross-Sections ("Slices")	Pre-Calculated Examples	✓
Molecular Orbitals	Pre-Calculated Examples	✓
Electrostatic Potentials, Spin Densities	Pre-Calculated Examples	✓
LUMO Maps, Ionization Potentials	No	✓
Choice of Basis Set	No	✓
Inclusion of Solvent (Continuum Model)	No	✓
Control over Graphical Resolution	No	✓
Time Estimates (for Submitted Calculations)	N/A	✓
Chemical Reactions		
Reaction Dynamics at Set Temperature	Selected Examples	No
Dynamic Equilibria	Selected Examples	No
Examine Reaction Profiles	Selected Examples	✓
Search Transition State Library	No	✓
Reaction Energy Calculations from ΔH° & ΔG°	No	✓
Analysis and Plots		
Distances, Angles, and Torsion Angles	✓	✓
Atomic/Molecular Properties	✓	✓
Thermodynamic Properties	✓	✓
Dynamic Properties	✓	N/A
QSAR Properties	No	✓
Symmetry Detection (Point Groups)	No	✓
Extended Property List (EXPERT Setting)	✓	N/A
Orbital Energy Diagrams	No	✓
Bond Orders	No	✓
Volume, Area	✓	✓
Polar Surface Area, Ovality, Log P	No	✓

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Analysis and Plots (Cont'd)		
Tabular Data Display	Property Table	Spreadsheet
Export to Excel	N/A	✓
IR Spectra	No	✓
NMR Spectra (Proton and C-13)	No	✓
XY Plots	✓	✓
Linear Regression	✓	✓
Polynomial Fit	✓	✓
Lorentzian Fit, Gaussian Fit, Other Fits	No	✓
Reciprocal and Logarithmic Axes	✓	No
Radial Distribution Function (EXPERT Setting)	✓	No
Ramachandran Plots	No	✓
Kinetic Energy/Speed Histograms	✓	N/A
Chemistry Teaching Content		
Prebuilt Models (Molecules, Bulk Samples)	> 3,000	No
Spectra and Properties Database	No	> 6,000 Molecules
Demonstrations	> 50 Integrated Lessons	No
Labs	> 110 Integrated Lessons	41 (PDF Files)
Miscellaneous Topics	> 130 Integrated Lessons	13 (PDF Files)
Molecular Stockroom	✓	No
New User Tutorials	28 Integrated Lessons	11 (PDF Files)
Content Search	✓	N/A
Wikipedia Access	Through Hyperlinks	By Name Search
ChemSpider Access	No	By Name Search
PDB Access	No	✓
Periodic Table of the Elements	✓	No
Lists of Misconceptions	<i>Instructor's Ed. Only</i>	N/A
Comments	✓	N/A
Assessment Questions	> 1,200	No
Answer Key	<i>Instructor's Ed. Only</i>	N/A
Add Model Snapshots to Answers	✓	N/A
Annotation of Pages	✓	N/A
Customization of Questions	<i>Instructor's Ed. Only</i>	N/A
Authoring Capability	<i>Instructor's Ed. Only</i>	N/A
Japanese Language Content	✓	No
Spanish Language Content	✓	No
German Language Content	✓	No