

Calculations

Spartan/Q-Chem | Gaussian

State: Ground

Total Charge: Neutral

Task: Equilibrium Geometry

Multiplicity: Singlet

Model: Semi-Empirical PM3

Start From: Initial geometry

Subject To: Constraints Frozen Atoms Symmetry

Compute: E. Solvation logP Frequencies Electrostatic Charges

Print: Orbitals & Energies Thermodynamics Vibration Modes Atomic Charges

Options: Converge

Cancel

SaveAs

Save