

Introduction to Gaussian: Theory and Practice
Beijing, China
August 18 – August 22, 2014



Day 1: Monday, August 18, 2014

9:00	Opening remarks by Professor Wei-Hai Fang, Welcome & Introduction by workshop instructors
9:40	Potential Energy Surface
10:00	Geometry Optimization I: Min
10:30	Vibrational Spect & Thermo
11:00	Coffee Break
11:20	Geometry Optimization II: TS
11:50	Hartree-Fock
12:30	Basis Sets
1:00	Lunch
2:30	Lab

Day 2: Tuesday, August 19, 2014

9:00	Dynamics & Rxn Paths
9:30	Electron Correlation
10:20	DFT
11:00	Coffee Break
11:20	Semi-Empirical & MM
11:50	Wavefunction
12:20	Model Chemistry
1:00	Lunch
2:30	Lab

Day 3: Wednesday, August 20, 2014

9:00	ONIOM
9:50	Input Files I
10:20	Output
11:00	Coffee Break
11:20	NMR
11:50	Chiroptical Spect
12:30	Optical & UV Spectra
1:00	Lunch
2:30	Lab

Introduction to Gaussian: Theory and Practice
Beijing, China
August 18 – August 22, 2014



Day 4: Thursday, August 21, 2014

9:00	Solvation
9:30	SCF Conv. & Stability
10:10	Input Files II
11:00	Coffee Break
11:20	Utility Programs
12:00	CASSCF
1:00	Lunch
2:30	Lab

Day 5: Friday, August 22, 2014

9:00	PBC
9:30	Resources
10:30	Summary
11:10	Q & A