D.P. VIPRA COLLEGE BILASPUR

SESSION-2021-22

DEPARTMENT OF CHEMISTRY

PRESENTATION
ON

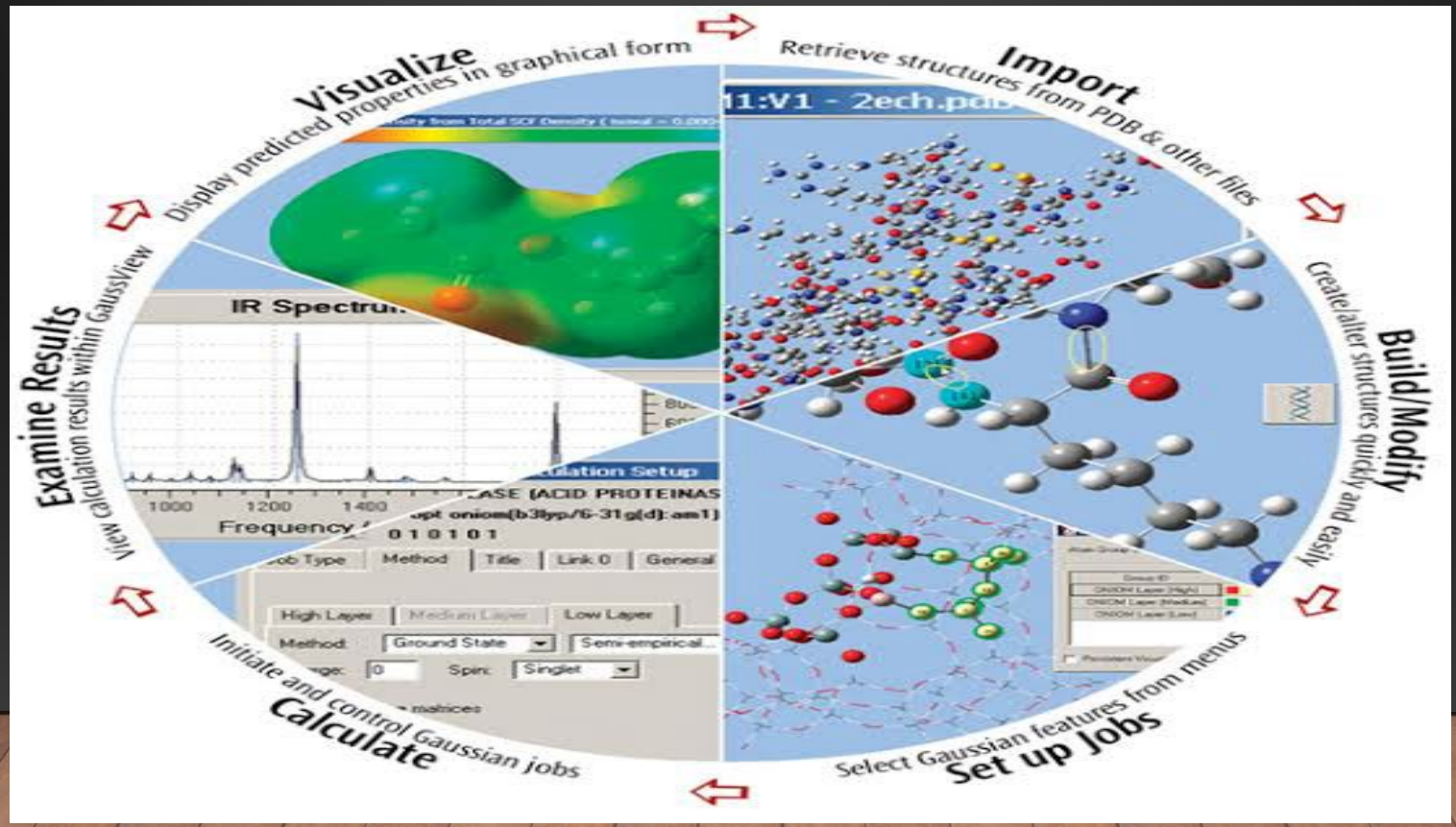
GAUSSIAN

HISTORY

- Gaussian is a general purpose computational chemistry software package initially released in 1970 by JOHN POPLE and his research group at Carnegie Melllon university as Gaussian 70.
- It has been continuously updated since then.
- The name originates from Pople's use of Gaussian orbitals to speed up molecular electronic structure calculations.

INTRODUCTION

- Gaussian is a general purpose ab initio electronic structure package that is capable of computing energies, geometries, vibrational frequencies, transition states, reaction paths of any compound.



Gaussian is used by chemists, chemical engineers, biochemists, physicists and others for research in established and emerging areas of chemical interest.

- There are two versions of Gaussian installed at SERC.

  Gaussian 16

  Gaussian 09

  Gaussian 03

SERC – STRUCTURAL ENGINEERING RESEARCH CENTRE

Gaussian 16

Major New Features:

- *TD frequencies, TS optimizations & IRC*
- *EOMCC optimizations*
- *Anharmonic vibrational spectroscopy*
- *Vibronic spectroscopy*

Performance Enhancements:

- *Support for GPUs*
- *Optimized memory algorithm to avoid I/O during CCSD iterations*
- *Enhancements to GEDIIS opt. algorithm*
- *CASSCF: Improvements in CI for ≥10x10*

Challenging Calculation:

- *GFP: reaction path on excited state PES*

ONIOM(TD B3LYP:Amber) IRC SCRF

Gaussian 09

Major New Features:

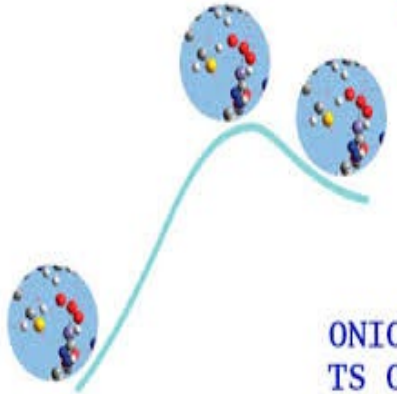
- *ONIOM IRC & frequencies*
- *TD-DFT optimizations, EOMCC energies*
- *IEFPCM solvation for all properties*
- *Anharmonic frequencies, FCHT analysis*

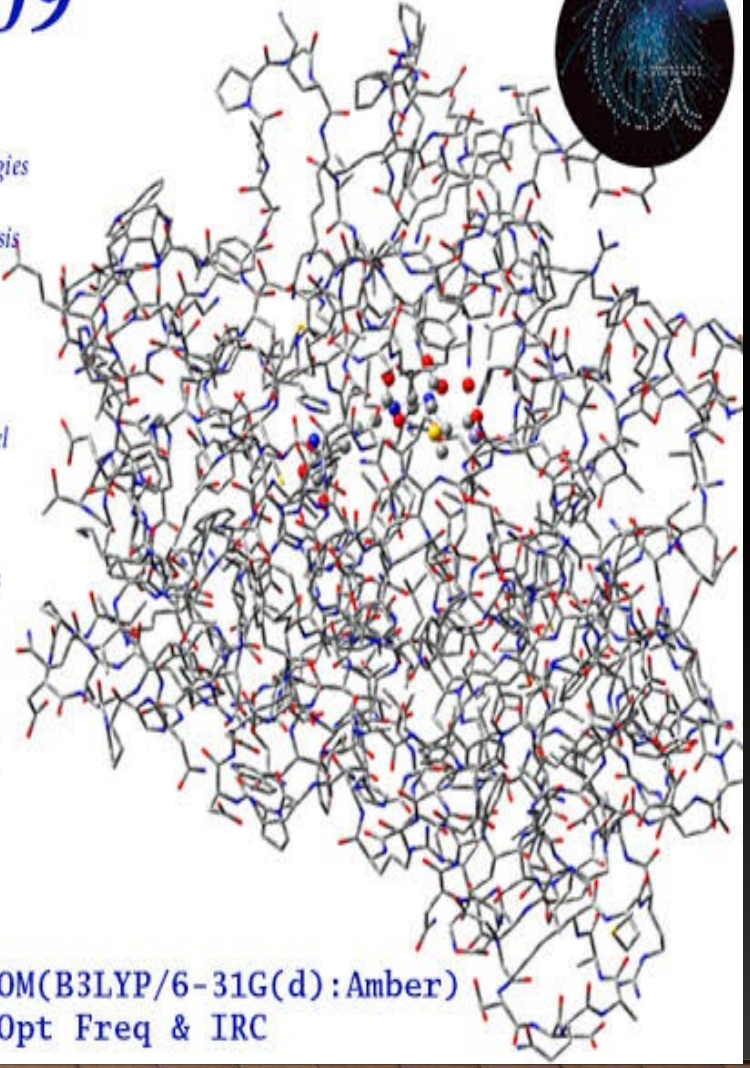
Performance Enhancements:

- *Optimizations for large molecules*
- *New IRC algorithm*
- *Large frequency calculations in parallel*

Challenging Calculation:

- *Isopenicillin N synthase reaction paths*





ONIOM(B3LYP/6-31G(d):Amber)
TS Opt Freq & IRC

LIST OF VERSIONS OF GAUSSIAN

- GAUSSIAN 70
- GAUSSIAN 76
- GAUSSIAN 80
- GAUSSIAN 82
- GAUSSIAN 86
- GAUSSIAN 88
- GAUSSIAN 90
- GAUSSIAN 92
- GAUUSIAN 92/DFT
- GAUSSIAN 94
- GAUSSIAN 98
- GAUSSIAN 03
- GAUSSIAN 09
- GAUSSIAN 16

BASICS OF GAUSSIAN

- Starting from the basic laws of quantum mechanics, Gaussian predicts the energies, molecular structures, and vibrational frequencies of molecular systems, along with numerous molecular properties derived from these basic computation types.
- It can be used to study molecules and reactions under a wide range of conditions, including both stable species and compounds which are difficult or impossible to observe experimentally such as short-lived intermediates and transition structures.

- Several reserach groups from various departments in Institute use Gaussian package for doing advanced electronic structure theory calculations. These calculations can be used for predicting various properties of atoms, molecules, radicals, ions, weakly and strongly bound complexes, etc.
- Other groups use Gaussain to calculate the equillibrium structure and infrared and Raman frequencies and intensities. Some use it to calculate enthalpies of formation of various chemical species. It is especially useful if experimental data are not available. Enthalpy of reactions can be determined.

THANK YOU