Multiwfn quick start

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The Multiwfn manual is very detailedly written and well organized, however, it is relatively long. In order to make new users of Multiwfn quickly get started, here I provide a very short quick start document, which presents answers to a few frequently asked questions and basic guides on how to perform common tasks.

1. FAQ

- **Q: What analysis can Multiwfn do? What is the use of Multiwfn?**

A: Please check "Overview" page of Multiwfn website or Chapter 1 of Multiwfn manual.

- **Q: Where can I obtain latest Multiwfn program and manual?**

A: The Multiwfn official website is http://sobereva.com/multiwfn, all resources related to Multiwfn can be freely acquired from this site. I highly suggest you frequently check this site to update your Multiwfn to the latest version, since development and update of Multiwfn are very active.

- **Q: How to cite Multiwfn in most correct way?**

A: Check *How to cite Multiwfn.pdf* document in Multiwfn binary package.

- **Q: What should I do when I encounter problems in using Multiwfn?**

A: Please always pay attention to all prompts on screen and do not forget to check corresponding section of Multiwfn manual. If you are unable to easily find solution, please do not hesitate to post message on Multiwfn forum, the English forum is http://sobereva.com/wfnbbs, the Chinese forum is http://bbs.keinsci.com/wfn. Commonly, the developer Tian Lu checks these two forums every day and always timely replies questions.

- **Q: What is the smoothest and quickest way of learning Multiwfn?**

A: Reading Chapter 1, Sections 2.1-2.5 of Chapter 2, and then following the tutorials in Chapter 4. After that if you want to learn more about theoretical backgrounds and details of Multiwfn, then read Section 2.6-2.8 of Chapter 2 and Chapter 3. Note that the tutorials and examples given in Chapter 4 only cover most important and frequently used functions rather than all functions of Multiwfn. By the way, there is a Youtube channel of Multiwfn, in which there are a few video illustrations for special topics.

- **Q: How to install Multiwfn?**

A: Check Section 2.1.

- **Q: Which format of input file can be used?**

A: Check Section 2.3.

- **Q: How to generate input files for Multiwfn?**

A: Check beginning of Chapter 4. Almost all mainstream quantum chemistry codes can at least generate one kind of input file that supported by Multiwfn for wavefunction analysis purposes.

- **Q: Can Multiwfn analyze periodic systems?**

A: Yes, please check Section 2.9 of manual for detail.

- **Q: Why Multiwfn occasionally suddenly exits?**

A: Possible reasons:

(1) The format of input file is inappropriate for the present task. Please carefully check the corresponding section of the manual on the requirement of input file.

(2) The input file is problematic or incomplete. Please regenerate it or open it using text editor to check for abnormalities.

(3) Your operation steps are incorrect or the command you inputted is wrong and thus cannot be recognized. Please always carefully check prompts on screen, or try to reproduce the corresponding examples in the manual before using Multiwfn to study your system.

(4) Insufficient memory. If you are using Win32 version of Multiwfn, please change to the Win64 one. You can also try to increase "ompstacksize" in settings.ini. If you are using Linux version, please make sure you have properly configured your system according to Section 2.1.

(5) If your task relies on NBO output file and meantime diffuse functions are employed, remove diffuse functions and try again.

(6) Due to bug of Multiwfn. Please report it to developer on Multiwfn official forum.

- **Q: Why Multiwfn crashes under Linux and show error "Segmentation fault"?**

A: Commonly this is because you didn't strictly follow Section 2.1.2 to configure your system. If you are really unable to solve this problem, please use Windows version. If your input file is problematic, you may also encounter this problem.

- **Q: How to copy output of Multiwfn from console window to text file?**

A: See Section 5.4.

- **Q: How to run Multiwfn using command line mode? How to use Multiwfn process a batch of input files?**

A: See Sections 5.2 and 5.3.

- **Q: The console window cannot record all printed information, the older output was flushed out**

A: Increase buffer size of the console window so that the window can record more lines of output, see Sections 5.5.

- **Q: I don't understand meaning of each column of the text file outputted by Multiwfn**

A: Please carefully check prompts on screen. Bear in mind, when Multiwfn exports a file, the meaning of each column is always clearly shown.

- **Q: What is the unit of the data outputted by Multiwfn?**

A: Unless otherwise specified, all units are in atomic unit (a.u.). When Multiwfn exports a text file, the unit is always explicitly shown on screen.

- **Q: I can't find the file(s) exported by Multiwfn**

A: If Multiwfn doesn't explicitly ask you to input the path of the file for exporting, the file is always generated in current folder. The meaning of "current folder" has clearly been mentioned in page 2 of the manual.

- **Q: Electrostatic potential analysis (ESP) is slow for large systems**

A: Calculating ESP is significantly more expensive than calculating most other real space functions. If you are calculating ESP grid data (*e.g.* in main function 5, or in basin analysis module) I strongly suggest making Multiwfn invoke cubegen utility in Gaussian package to significantly speed up the calculation, see Section 5.7. However, for other kinds of ESP analysis, invoking cubegen will never bring benefit and is thus deprecated.

- **Q: Multiwfn failed to invoke Gaussian to perform calculation under Windows system with error "No executable for file l1.exe"**

A: See Appendix 1 of manual. You need to set up GAUSS_EXEDIR environment variable in your system.

- **Q: How to load a new file without rebooting Multiwfn?**

A: Return to main menu, input *r* (meaning “reload”).

- **Q: How to quit Multiwfn?**

A: Press Ctrl+C or directly close the window. If you want to exit gracefully, input *q* in the main function menu.

2. Which manual section should I read?

Below I will show you which manual section(s) should be read if you want to perform corresponding task. For brevity, "see Section x.x.x for introduction and Section y.y.y for example" will be abbreviated as "x.x.x (i); y.y.y (e)".

- **AIM analysis**

Topology analysis: 3.14 (i); 4.2 (e)
Plane map with critical points and bond paths: 3.5.5 (i); 4.4.6 (e)
Basin analysis for electron density: 3.20 (i); 4.17.1 (e)
Basin analysis for Source function: 4.17.5 (e)

- **ELF (electron localization function) and LOL (localized orbital locator) analysis**

Topology analysis: 3.14 (i); 4.2.2 (e)
Basin analysis for ELF: 3.20 (i); 4.17.2 (e)
Atom contributions to ELF basins: 4.17.7 (e)
Plotting as plane map: 4.4.2, 4.4.8, 4.4.9 (e), special case: 4.100.19 (e)
Plotting as isosurface map: 4.5.1, 4.5.3, 4.100.22 (e)
Spherically symmetric average ELF / LOL: 3.100.4 (i)
High ELF localization domain population and volume (HELP and HELV): 4.17.8 (i,e)

- **Visual analysis of weak interaction**

Non-covalent interaction (NCI) analysis: 3.23.1 (i,e); 4.20.1 (e).
Promolecular NCI analysis: 3.23.2 (i); 4.20.2 (e)
Averaged NCI analysis: 3.23.3 (i); 4.20.3 (e)
Topology analysis of IRI and RDG/NCI: 4.2.11 (e)
Domain analysis within NCI isosurfaces: 3.200.14 (i); 4.200.14.1 (e)
Independent gradient model (IGM) analysis: 3.23.5 (i); 4.20.10 (e)
IGM analysis based on Hirshfeld partition of molecular density (IGMH): 3.23.6 (i); 4.20.11 (e)
Modified IGM (mIGM) analysis: 3.23.10 (i); 4.20.12 (e)
Averaged mIGM (amIGM) analysis: 3.23.11 (i); 4.20.13 (e)
Interaction region indicator (IRI): 3.23.8 (i); 4.20.4 (e)
IRI descriptors: 3.200.14 (i); 4.200.14.4 (e)
Density overlap regions indicator (DORI) analysis: 3.23.4 (i); 4.20.5 (e)
Hirshfeld surface analysis: 3.15.5 (i); 4.12.5 and 4.12.6 (e)
Visualization of van der Waals potential: 3.23.7 (i), 4.20.6 (e)
Topology analysis of van der Waals potential: 4.2.10 (e)

- **Visualizing various kinds of orbitals as isosurface**

Isosurface map: 3.2 (i); 4.0 (e)
Plane map: 4.4.5 (e)
Exporting cube file for a batch of orbitals: 3.200.3 (i)

- **Evaluating various real space functions at a point**

3.3 (i); 4.1 (e)

- **Plotting various real space functions**

Curve map: 3.4 (i); 4.3 (e)

Plane map: 3.5 (i); 4.4 (e)

Isosurface map: 4.5 (e)

Radial distribution function: 3.200.5 (i); 4.200.5 (e)

- **Generate cube file of real space functions**

3.6 (i); 4.5 (e)

- **Atomic charge and population analysis**

Mulliken charges and population analysis: 3.9.3 (i); 4.7.0 (e)

Löwdin, SCPA: 3.9.4, 3.9.5 (i)

AIM charges: 3.9.12 (i); 4.7.11 and 4.17.1 (e)

ADCH (atomic dipole moment corrected Hirshfeld population): 3.9.9 (i); 4.7.2 (e)

Hirshfeld: 3.9.1 (i); 4.7.1 (e)

Hirshfeld-I: 3.9.13 (i); 4.7.4 (e)

CM5: 3.19.14 (i), 4.7.10 (e)

1.2*CM5: 4.7.10 (i,e)

Electronegativity Equalization Method (EEM): 3.9.15 (i); 4.7.5 (e)

CHELPG: 3.9.10 (i); 4.7.1 (e)

RESP (Restrained ElectroStatic Potential): 3.9.16 (i); 4.7.7 (e)

RESP2: 4.7.7.9 (i,e)

PEOE (Gasteiger): 3.9.16 (i); 4.7.9 (e)

MBIS: 3.9.18 (i)

- **Bond order analysis**

Laplacian bond order (LBO): 3.11.7 (i); 4.9.3 (e)

Mayer bond order: 3.11.1 (i); 4.9.1 (e)

Orbital occupancy-perturbed Mayer bond order 3.11.5 (i); 4.9.1 (e)

Multi-center bond order: 3.11.2 (i); 4.9.2 (e)

Wiberg bond order: 3.11.3 (i)

Decompose Wiberg bond order in NAO basis as atomic orbital pair contributions: 3.11.8 (i); 4.9.4 (e)

Mulliken bond order analysis and its decomposition: 3.11.4 (i); 4.9.5 (e)

Fuzzy bond order: 3.11.6 (i), 4.9.1 (e)

Bond order density (BOD) and natural adaptive orbital (NAdO) analyses: 3.200.20 (i), 4.200.20 (e)

Bond order alternation (BOA): 3.200.18 (i), 4.200.18 (e)

Intrinsic bond strength index (IBSI): 3.11.9 (i), 4.9.6 (e)

Delocalization index (DI) between AIM basins: 3.11.12 (i)

AV1245 index: 3.11.10 (i); 4.9.11 (e)

- **Density-of-state (DOS), photoelectron spectrum (PES) and COHP**

Total, partial, overlap DOS (TDOS, PDOS, OPDOS): 3.12.1 (i); 4.10.1 (e) and 4.10.3 (e)

Local DOS: 3.12.4 (i); 4.10.2 (e)

MO-PDOS: 4.10.5 (i,e)

Photoelectron spectrum based on Koopmans' theorem: 3.12.5 (i); 4.10.4 (e)

d-band center: 4.10.6 (e)

COHP: 3.12.6 (i), 4.10.7 (e)

- **Plotting IR, Raman, UV-Vis, ECD, VCD, ROA and NMR spectra**

IR, Raman, UV-Vis, ECD, VCD, ROA: 3.13 (i); 4.11 (e)

NMR: 3.13.5 (i); 4.11.10 (e)

Partial vibrational spectrum (PVS) and partial vibrational density-of-states (PVDOS): 3.13.6 (i); 4.11.12 (e)

Directional UV-Vis spectrum: 3.13.1 (i); 4.11.13 (e)

Predicting color based on UV-Vis spectrum: 3.12.7 (i); 4.11.14 (e)

- **Orbital composition analysis**

3.10 (i); 4.8 (e)

Analyzing π and lone pair compositions in an orbital: 4.100.22 (e) and 4.200.6.2 (e), respectively

Quantifying extent of spatial delocalization of orbitals via orbital delocalization index (ODI): 4.8.5 (i,e)

Quantifying extent of spatial delocalization of orbitals via spatial delocalization index (SDI): 3.200.19 (i); 4.200.19 (e)

- **Orbital localization and relevant analysis**

3.22 (i); 4.19 (e)

Oxidation state evaluation via LOBA method: 3.10.7 (i); 4.8.4 (e)

- **AdNDP (Adaptive natural density partitioning) analysis**

3.17 (i); 4.14 (e)

- **Charge decomposition analysis (CDA) and orbital interaction diagram**

3.19 (i); 4.16 (e)

- **Extended Transition State - Natural Orbitals for Chemical Valence (ETS-NOCV)**

3.26 (i); 4.23 (e)

- **Electrostatic potential (ESP) analysis**

Various kinds of quantitative molecular surface analysis: 3.15 (i); 4.12.1 and 4.12.3 (e)

Plotting ESP colored vdW surface map: 4.A.13 (e)

Plotting plane map: 4.4.4 (e)

Topology analysis: 4.2.9 (e)

Basin analysis: 4.17.3 (e)

Predicting binding energy using ESP at nuclear position: 4.1.2 (i,e)

Plotting ESP minimum points with isosurface to reveal lone pairs: 4.17.4 (e)

Calculating area and average ESP value of σ-hole and π-hole: 4.12.10 (e)

Basin-like analysis on vdW surface for ESP: 4.12.11 (e)

- **Electron excitation analysis**

Comprehensive overview: 4.A.12

hole-electron analysis: 3.21.1 (i); 4.18.1 (e)

IFCT (InterFragment Charge Transfer) analysis, heat map of atom-atom charge transfer matrix:

3.21.8 (i); 4.18.8 (e)

Transition density and transition dipole moment density analysis: 3.21.1 (i); 4.18.2.1 (e)

Heat map of transition density matrix (TDM) and transition dipole moment density matrix: 3.21.2 (i); 4.18.2.2 and 4.18.2.3 (e)

Quantitative analysis for density difference grid data: 3.21.3 (i); 4.18.3 (e)

Δr and Λ indices: 3.21.4, 3.21.14 (i); 4.18.4 (e)

Natural transition orbitals (NTOs): 3.21.6 (i); 4.18.6 (e)

Wavefunction analysis for an excited state: 4.18.13 (e)

Transition dipole moments between excited states, excited state dipole moment: 3.21.5 (i)

Generating transition density matrix between ground state and excited states, as well as between two excited states: 3.21.9 (i); 4.18.2.3 (e)

Generating natural orbitals for transition density matrix: 3.21.9 (i); 4.18.9 (i)

Decomposing transition dipole moment as MO contributions: 3.21.10 (i); 4.18.10 (e)

Decomposing transition dipole moment as fragment, atom or basis function contributions: 3.21.11 (i); 4.18.11 (e)

TrEsp (transition charge from electrostatic potential) and exciton coupling: 4.A.9 (i,e)

Mulliken atomic transition charges: 3.21.12 (i)

Evaluating NBO contributions to electron excitation: 3.200.13 (i); 4.200.13.3 (e)

Ghost-hunter index: 3.21.7 (i); 4.18.1 (e)

Printing major MO transitions in all excited states: 3.21.15 (i,e)

Calculating charge-transfer spectrum (CTS): 3.21.16 (i), 4.18.16 (e)

Electron density polarization analysis based on electron excitations: 3.21.17 (i), 4.18.17 (e)

Calculating ECD/CPL dissymmetry factor (g) for chiral systems and visualizing transition electric/magnetic dipole moments: 3.21.18 (i), 4.18.18 (e)

- **Weak interaction analysis**

Comprehensive overview: 4.A.5

AIM topology study: 3.14 (i); 4.2 (e)

Various kinds of visual studies: See "Visual analysis of weak interaction" in present document

Simple energy decomposition or EDA-FF energy decomposition: See "Energy decomposition analysis" in present document

Plane or isosurface map of electron density difference between interacting monomers: 4.5.5 (e)

Plotting electrostatic potential (ESP) colored van der Waals (vdW) surface map and penetration graph of vdW surface of monomers: 4.A.13 (e)

Studying minima and maxima of ESP on vdW surface: 3.15 (i); 4.12.1 (e)

Quantitative evaluation of mutual penetration of vdW surfaces: 4.A.5 (i)

CVB index: 3.200.1 (i,e)

LOLIPOP (LOL Integrated Pi Over Plane): 3.100.14 (i); 4.200.14 (e)

$\Delta\Delta V_n$ index: 4.1.2 (i,e)

- **Predicting reactive site**

Overview: 4.A.4

ESP on vdW surface: 4.12.1 (e)

Average local ionization energy (ALIE) on vdW surface: 4.12.2 (e)

Local electron affinity and local electron attachment energy on molecular surface: 4.12.13 (e)

Manually calculating Fukui function and dual descriptor: 4.5.4 (e)

Manually calculating condensed Fukui function and condensed dual descriptor: 4.7.3 (e)

Fully automatic calculation of all functions and quantities involved in the conceptual density functional theory (CDFT): 3.25 (i); 4.22.1 (e)

Fukui potential and dual descriptor potential: 4.22.4 (e)

Orbital weighted Fukui function and dual descriptor: 3.25.3 (i), 4.22.2 (e)

(Quasi-)degenerate Fukui function and dual descriptor as well as relevant quantities: 3.25.4 (i), 4.22.3 (e)

Bond dual descriptor: 3.25.1 (i); 4.22.5 (e)

Evaluating MO and NBO contributions to Fukui function: 3.200.13 (i); 4.200.13.1 and 4.200.13.2 (e)

Orbital overlap distance function: 4.12.8 (e)

- **Aromaticity analysis**

Comprehensive Overview: 4.A.3

Iso-chemical shielding surface (ICSS): 3.28.3 (i); 4.25.3 (e)

1-dimensional NICS curve map, integral NICS (INICS), FiPC-NICS: 3.28.13 (i); 4.25.13 (e)

2-dimensional NICS plane map: 3.28.14 (i); 4.25.14 (e)

HOMA and Bird indices: 3.28.6 (i); 4.25.6 (e)

HOMAc and HOMER indices: 3.28.7 (i)

Multi-center bond order (multi-center index, MCI): 3.11.2 (i); 4.9.2 (e)

AV1245 index: 3.11.10 (i); 4.9.11 (e)

Shannon aromaticity index (SA) and properties at ring critical point (RCP): 3.14.6 (i); 4.2.1 (e)

PDI: 3.18.6 (i); 4.15.2 (e)

FLU, FLU-π: 3.18.7 (i); 4.15.2 (e)

PLR: 3.18.9 (i); 4.15.2 (e)

ELF-σ, ELF-π: 4.4.9, 4.5.3, 4.100.22 (e)

Information-theoretic aromaticity index: 3.18.11 (i)

$NICS_{ZZ}$ for non-planar or tilted system: 3.28.4 (i)

- **Electronic density difference (EDD) analysis**

Plane and isosurface EDD maps between two fragments: 4.5.5 (e)

Between excited state and ground state: 4.18.3 (e)

Between two excited states: 4.18.13 (e)

Deformation density: 4.4.7 (e)

Basin analysis: 4.17.4 (e)

Charge displacement curve: 3.16.14 (i) and 4.13.6 (e)

- **Processing grid data**

Mathematical operation between grid data: 3.16.7 (i); 4.13.2 (e)

Screening specific regions: 3.16.9 and 3.16.10 (i); 4.13.4 (e)

Statistical analysis: 3.16.13 (i)

- **Electronic spin distribution analysis**

Spin density curve map: 4.3.1 (e)

Overview of spin population calculation: 4.A.2

- **Energy decomposition analysis**

sobEDA and sobEDAw energy decomposition: *J. Phys. Chem. A*, **127**, 7023 (2023) (i); http://sobereva.com/soft/sobEDA_tutorial.zip (e)

Energy decomposition based on forcefield (EDA-FF): 3.24.1 (i); 4.21.1 (e)

Analysis of atomic contributions to dispersion energy and dispersion energy: 3.24.4 (i); 4.21.4 (e)

Shubin Liu's energy decomposition (EDA-SBL): 3.24.2 (i); 4.21.2 (e)

Simple energy decomposition: 3.100.8 (i); 4.100.8 (e)

- **(Hyper)polarizability study**

Parsing output file of "polar" task of Gaussian, obtaining various quantities related to (hyper)polarizability and hyper-Rayleigh scattering (HRS) experiment: 3.27.1 (i); 4.24.1 (e)

Calculating (hyper)polarizability using sum-over-states (SOS) method: 3.27.2.1 (i); 4.24.2.1 (e)

Two-level and three-level analyses for first hyperpolarizability: 3.27.2.2 (i); 4.24.2.2 (e)

(Hyper)polarizability density and atomic contribution to (hyper)polarizability: 4.27.3 (i); 4.24.3 (e)

Unit sphere representation and vector representation of (hyper)polarizability: 3.27.5 (i), 4.24.5 (e)

Calculating atomic effective volume, atomic polarizability and C6 dispersion coefficient in a molecule: 3.18.12 (i), 4.15.4 (e)

- **Predicting properties of condensed phase**

3.15.1 (i); 4.12.7 (e)

- **Overlap analysis of wavefunction and geometry**

Intermolecular electron density overlap: 4.13.7 (e)

Intermolecular van der Waals surface penetration: 4.A.13 (e)

Overlap integral between Alpha and Beta orbitals of a system and estimating $<S^2>$: 3.100.5 (i)

Intrasystem orbital superposition and centroid distance: 3.100.11 (i)

Intermolecular orbital overlap integral: 3.100.15 (i); 4.100.15 (e)

Correspondence between orbitals in two wavefunctions, overlap integral and superposition between orbitals in single or two wavefunctions: 3.200.6 (i); 4.200.6 (e)

- **Geometry structure analysis**

Measuring diameter and length/width/height: 3.100.21 (i); 4.100.21.1 (e)

Calculating molecular planarity parameter (MPP) and span of deviation from plane (SDP): 3.100.21 (i); 4.100.21.2, 4.100.21.3 (i,e)

Visualizing molecular cavities and calculating their volumes: 4.200.14.2 (e)

Calculating cavity diameter of molecules and crystals, as well as graphically representing it as sphere: 3.100.21 (i); 4.100.21.4 (e)

van der Waals volume (Monte Carlo method): 3.100.3 (i)

van der Waals volume (Marching Tetrahedron method): 4.12.1 (e)

Area of van der Waals surface of whole system or individual fragments: 4.12.9 (e)

Interatomic connectivity and atomic coordination number: 3.100.9 (i,e)

Average bond length and average coordinate number: 3.200.9 (i)

Bond length alternation (BLA), bond angle and dihedral alternations: 3.200.18 (i), 4.200.18 (e)

Kinetic diameter: 4.12.12 (e)

Viewing free regions and calculating free volume in a cell: 3.300.1 (i), 4.300.1 (e)

Plot surface distance projection map: 3.300.8 (i), 4.300.8 (e)

- **Electronic correlation analysis**

Visual study of Fermi hole and Coulomb hole: 4.3.2 (e)

Localization index (LI) and delocalization index (DI): 3.18.5 (i); 4.15.1, 4.17.1 (e)

Odd electron density: 4.A.6 (i,e)

Fractional occupation number weighted electron density (FOD) and local electron correlation functions: 4.A.7 (i,e)

- **Overview of all methods supported by Multiwfn for studying chemical bonds**

4.A.11

- **Others**

Biorthogonalization analysis for unrestricted orbitals: 3.100.12 (i); 4.100.12 (e)

Visualizing atomic electric dipole and quadrupole moments: 4.15.5 (e)

Valence electron density analysis: 4.6.2 (e)

Simulating scanning tunneling microscope (STM) image: 3.300.4 (i), 4.300.4 (e)

File format conversion and yield input file of quantum chemistry codes: 3.100.2 (i)

Integrating a function over the whole space, examination of difference of a real space function between two wavefunction files: 3.100.4 (i,e)

Detecting π orbitals and setting their/others occupation numbers, evaluating π composition of a given set of orbitals: 3.100.22 (i); 4.100.22, 4.5.3, 4.4.9 (e)

Yoshizawa's electron transmission route analysis: 3.100.18 (i); 4.100.18 (e)

Calculating atomic and bond dipole moments in Hilbert space: 3.200.2 (i)

Calculating atomic, fragment or system electric dipole/quadruple/octopole moments numerically: 3.18.3 (i); 4.15.3 (e)

Calculating system electric dipole/quadruple/octopole/hexadecapole moments and electronic spatial extent $<r^2>$ based on analytical integrals: 3.300.5 (i), 4.300.5 (e)

Outputting various kinds of integral between orbitals: 3.200.10 (i)

Outputting Coulomb and exchange integrals between two orbitals: 3.200.17 (i,e)

Calculating center, the first and second moments, radius of gyration, and spatial extent $<r^2>$ of a real space function: 3.200.11 (i,e)

Calculating energy index (EI) or bond polarity index (BPI): 3.200.12 (i); 4.200.12 (e)

Generating natural orbitals, natural spin orbitals and spin natural orbitals: 3.200.16 (i,e)

Geometry operation on the present system: 3.300.7 (i)

Determining Fermi level: 3.300.9 (i,e)

Fitting sphericalized atomic radial density as multiple STOs or GTFs: 3.300.2 (i), 4.300.2 (e)

Generating Gaussian input file with initial guess combined from fragment wavefunctions: 3.100.8 (i); 4.100.8 (e)

Monitoring SCF convergence process of Gaussian: 3.100.6 (i)