MOPAC-derived descriptors

Summary

MOPAC (Molecular Orbital PACkage) is a semi-empirical quantum chemistry program by James Stewart.

Theory

MOPAC is a general-purpose semi-empirical molecular orbital package for the study of molecular structures and reactions. For details on MOPAC, see its manual and website of Stewart Computational Chemistry. OCHEM uses version 7.1 of MOPAC, which is still open source (later version are commercial).

Descriptors

OCHEM descriptors are calculated using the mopac@home project.

MOPAC-derived descriptors include both per-molecule descriptors (molecular descriptors) and per-atom descriptors (atomic descriptors).

Molecular descriptors

A block of basic descriptors is calculated. These include **TotalEnergy** Sum of the electronic and nuclear (core-core) energies.
ElectronicEnergy Electronic energy.
CoreRepulsion Nuclear energy (core-core repulsion.
FinalHeat The final heat of formation.
IonisationPotential The smallest energy required to remove an electron.
HomoEnergy The energy of the highest occupied molecular orbital.
LumoEnergy The energy of the lowest unoccupied molecular orbital.
DipolPointCharge Molecular dipole.
DipolHybrid Molecular dipole.
DipolSum Molecular dipole.
ElectronNuclear
ElectronElectron
ResonanceEnergy
ExchangeEnergy
ElectronElectronRepulsion
ElectronNuclearAttraction
NuclearNuclearRepulsion
TotalElectrostaticInteraction
PrincipalMomentsInertia Principal components as PrincipalMomentsInertiaA, PrincipalMomentsInertiaB, and PrincipalMomentsInertiaC .

Atomic descriptors

Atomic descriptors are grouped into net atomic charges and frontier electron theory descriptors. The latter include

Electrophilic frontier electron density
Nucleophilic frontier electron density
Electrophilic superdelocalizability
Nucleophilic superdelocalizability
Radial superdelocalizability
Atom self-polarizability

Frontier electron theory descriptors, in particular electrophilic superdelocalisability, have been successfully used to model acid dissociation constants (Tehan et al., 2002).

Options

Both molecular and atomic descriptors offer the option **use stereochemistry** --

For atomic descriptors, the **schema** determines for which atoms the descriptors are computed. The atom (called the center atom) is usually determined by an obligatory property, e.g., as in acid dissociation constants (pKa).

References

- MOPAC
- Kenichi Fukui, Teijiro Yonezawa, Chikayoshi Nagata: Theory of Substitution in Conjugated Molecules, Bulletin of the Chemical Society of Japan 27(7): 423-427, Chemical Society of Japan, 1954. *Frontier electron theory*
- Benjamin Tehan, Edward Lloyd, Margaret Wong, Will Pitt, John Montana, David Manallack, Emanuela Gancia: Estimation of pKa Using Semiempirical Molecular Orbital Methods. Part 1: Application to Phenols and Carboxylic Acids, Quantitative Structure-Activity Relationships 21(5): 457-472, Wiley, 2002.
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