

Calculating information-theoretic quantities and some relevant quantities by Multiwfn

By Tian Lu (sobereva@sina.com)

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The information-theoretic quantities developed by Shubin Liu et al. is becoming more and more popular in predicting and understanding many chemical relevant problems, such as reactivity, regioselectivity, aromaticity, pK_a and so on. See [Acta Phys. -Chim. Sin., 32, 98 \(2016\)](#) and [WIREs Comput Mol Sci., e1461 \(2019\)](#) for reviews.

All the information-theoretic quantities can be easily calculated by Multiwfn program, which can be freely download at <http://sobereva.com/multiwfn>. This document will briefly illustrate how to calculate various information-theoretic and related quantities in Multiwfn, more information can be found in manual. The Multiwfn version corresponding to this document is the 3.7(dev) updated on 2020-Feb-24.

If you have any question about using Multiwfn, please feel free to post on Multiwfn official forum: <http://sobereva.com/wfnbbs>; while if you have question about concepts of information-theoretic quantities, please contact Prof. Shubin Liu (shubin@email.unc.edu).

Calculation of all of information-theoretic quantities need a file containing wavefunction information as input file. .mwfn, .wfn, .wfx, .fch, .molden, .gms can be used, see beginning of Chapter 4 of Multiwfn manual on how to generate them.

Calculation of Shannon entropy

Shannon entropy density is defined as

$$s_s(\mathbf{r}) = -\rho(\mathbf{r}) \ln \rho(\mathbf{r})$$

where ρ is electronic density. Integrating Shannon entropy density in a spatial region yields Shannon entropy of this region.

$s_s(\mathbf{r})$ corresponds to user-defined function 50 (see Section 2.7 of manual). Therefore, prior to calculation of Shannon entropy as exemplified below, you should first set "iuserfunc" in *settings.ini* file to 50.

Integral over the whole molecular space

```
examples\CH3NH2.wfn // An example input file
```

```
100 // Other function (Part 1)
```

```
4 // Integrate over the whole space
```

```
100 // User-defined function, which corresponds to Shannon entropy
```

Then you will see

```
Final result: 22.5021752870
```

That means $\int s_s(\mathbf{r}) d\mathbf{r}$ is 22.502175 a.u.

As mentioned in Section 3.100.4 of manual, this module calculates integral numerically, the accuracy is determined by number of radial and angular integration points; the higher the number,

the better the accuracy. The numbers of radial and angular parts are controlled by "radpot" and "sphpot" parameters in *settings.ini*. Since Shannon entropy varies relatively smooth, therefore the default number (75 for "radpot" and 434 for "sphpot") is adequate. However, if you want to gain better accuracy, you can increase the two values, and the cost will be correspondingly increased.

Integral over Becke atomic spaces

Definition of Becke atomic space can be found in Section 3.9.8 of manual. Shannon entropy can be calculated for individual atoms under Becke partition. The value for atom A is defined as $\int w_A(\mathbf{r})s_s(\mathbf{r})d\mathbf{r}$ with w_A being Becke's weighting function of A.

```
examples\CH3NH2.wfn // An example input file
15 // Fuzzy atomic space analysis
1 // Perform integration in fuzzy atomic spaces
100 // User-defined function, which now corresponds to Shannon entropy density
```

Then you can see:

Atomic space	Value	% of sum	% of sum abs
1(C)	5.72608486	25.446806	25.446806
2(H)	2.41939902	10.751845	10.751845
3(H)	2.41939902	10.751845	10.751845
4(H)	2.51276801	11.166778	11.166778
5(N)	5.15884315	22.925975	22.925975
6(H)	2.13284061	9.478375	9.478375
7(H)	2.13284061	9.478375	9.478375

Summing up above values: 22.50217529

Summing up absolute value of above values: 22.50217529

As can be seen, for example, the Shannon entropy of atom 2H under Becke partition is 2.419 a.u.

Since sum of weighting functions of all atoms is 1.0 everywhere, the sum of atomic Shannon entropies, namely 22.502, is exactly identical to the molecular Shannon entropy we obtained earlier using subfunction 4 of main function 100.

Integral over various Hirshfeld atomic spaces

Atomic Shannon entropy can also be calculated under Hirshfeld partition, whose definition is given in Section 3.9.1 of manual.

```
examples\CH3NH2.wfn // An example input file
15 // Fuzzy atomic space analysis
-1 // Select method for partitioning atomic space
3 // Hirshfeld partition based on built-in atomic densities in their isolated states (see
Appendix 3 of manual for detail)
1 // Perform integration in fuzzy atomic spaces
100 // User-defined function, which corresponds to Shannon entropy density
```

Note that in the study works of Shubin Liu's group, the atomic densities involved in Hirshfeld partition were calculated at the same level as molecular calculation, this is more physically sound. To do so, after selecting "-1 Select method for partitioning atomic space", you should "2 Hirshfeld", then input Gaussian keyword (e.g. M062X/6-31G*) so that Multiwfn can invoke Gaussian to generate .wfn file for various atoms. Alternatively, you can put previously generated atom .wfn files to the "atomwfn" subfolder in current folder, then Multiwfn will not invoke Gaussian but directly

utilize the .wfn files in this folder, see Section 3.7.3 of manual for detailed description.

Integral over various AIM atomic spaces

Atomic Shannon entropy can also be calculated under Hirshfeld partition, whose definition is given in Section 3.20.1 of manual.

```
examples\CH3NH2.wfn // An example input file
17 // Basin analysis
1 // Generate basins
1 // Using electron density to partition basins
2 // Medium quality grid (using better grid will result in more accurate result but the cost
will be evidently higher)
7 // Integrate real space functions in AIM basins with mixed type of grids
2 // Perform integration with exact refinement of basin boundary
100 // User-defined function, which corresponds to Shannon entropy density
```

The result is

Atom	Basin	Integral(a.u.)	Vol(Bohr ³)	Vol(rho>0.001)
1 (C)	4	3.55423261	139.320	62.508
2 (H)	7	2.98148375	416.107	49.830
3 (H)	3	2.98146942	407.684	49.830
4 (H)	5	3.10141618	521.925	52.506
5 (N)	2	5.97115311	533.046	111.602
6 (H)	6	1.94365108	373.757	33.192
7 (H)	1	1.94360005	365.697	33.192

Sum of above integrals: 22.47700621
Sum of basin volumes (rho>0.001): 392.660 Bohr³

Note that integration under AIM partition is quite sensitive to the grid spacing, therefore if your system is small and you can afford high cost, using more expensive "High quality grid" or even "Lunatic quality grid" is suggested if you want to obtain quite accurate result.

More information about basin analysis module can be found in Section 3.20 and Section 4.17 of manual.

Calculation of Fisher information and Ghosh-Berkowitz-Parr entropy

- Fisher information density: iuserfunc=51

$$i_F(\mathbf{r}) = |\nabla \rho(\mathbf{r})|^2 / \rho(\mathbf{r})$$

- Second Fisher information density: iuserfunc=52

$$i'_F(\mathbf{r}) = -\nabla^2 \rho(\mathbf{r}) \ln \rho(\mathbf{r})$$

- Ghosh-Berkowitz-Parr (GBP) entropy density: iuserfunc=53 and 54

$$s(\mathbf{r}) = (3/2)\rho(\mathbf{r})\{\lambda + \ln[t(\mathbf{r})/t_{TF}(\mathbf{r})]\}$$

See corresponding part of Section 2.7 of manual for introduction and details.

Integral over the whole space

The way of obtaining integral of above functions over the whole space is exactly the same as the case of Shannon entropy, you only need to modify "userfunc" before the calculation. Note that since second Fisher information density varies sharply in some regions, in order to accurately integrate it, you must set "radpot" and "sphpot" to large value, such as 400 and 2702, respectively, or even higher.

Note that in principle, integrating Fisher information density and Second Fisher information density over the whole space results in identical value.

Integral over atomic spaces

To calculate integral of these functions over atomic spaces partitioned in Becke or AIM way, you can use exactly the same procedure as the case of Shannon entropy, only "userfunc" should be changed to corresponding value.

If you need to calculate the integral under Hirshfeld partition, you should follow below steps

```
examples\CH3NH2.wfn // An example input file
```

```
15 // Fuzzy atomic space analysis
```

```
101 // Integrate a function over atomic spaces using Hirshfeld partition, but using molecular grid rather than atomic grid (the latter is used by option 1)
```

```
100 // User-defined function (depends on "userfunc" you set)
```

Since the Hirshfeld partition employed in option 101 relies on atom .wfn files, if you have not provide necessary ones in the "atomwfn" subfolder in current folder, Multiwfn will ask you to input Gaussian keyword used to calculate them and then invoke Gaussian.

The reason to choose option 101 to use "molecular grid" algorithm rather than use option 1 to use "atom grid" algorithm as the Shannon entropy case is that these functions vary more sharply than Shannon entropy density and show oscillating behavior, and meantime Hirshfeld weighting function decays slow and thus more or less intrudes into region of neighbouring atoms, in this case atom grid is inadequate to integrate these functions in Hirshfeld atomic spaces with satisfactory accuracy.

You can also use option 101 to integrate Shannon entropy density in Hirshfeld atomic spaces, however the cost is higher than using option 1 while the result will not improve detectably.

Relative Shannon/Fisher entropy (Information gain)

The aim of this section is calculating variation of atomic entropies in molecular environment with respect to those in their isolated states.

Calculation under Hirshfeld partition

Under Hirshfeld partition, the atomic relative entropy is defined as follows

- Relative Shannon entropy: $\Delta S_S^A = \int \rho_A(\mathbf{r}) \ln \frac{\rho_A(\mathbf{r})}{\rho_A^0(\mathbf{r})} d\mathbf{r}$
- Relative Fisher entropy: $\Delta I_F^A = \int \rho_A(\mathbf{r}) \left| \frac{\nabla \rho_A(\mathbf{r})}{\rho_A(\mathbf{r})} - \frac{\nabla \rho_A^0(\mathbf{r})}{\rho_A^0(\mathbf{r})} \right|^2 d\mathbf{r}$

where $\rho_A(\mathbf{r}) = w_A^{\text{Hirshfeld}} \rho(\mathbf{r})$, while $\rho_A^0(\mathbf{r})$ is spherically averaged density of atom A in its isolated state.

To calculate them, set "ispecial" in *settings.ini* to 2, then input

examples\H2O.fch // An example

15 // Fuzzy atomic space analysis

99 // The function dedicated to calculate atomic relative entropy

This option needs atom .wfn files, therefore either you let Multiwfn invoke Gaussian to calculate them, or you provide them in "atomwfn" folder before the calculation. The atom .wfn files used in this example were generated at B3LYP/6-31G** level, which is in line with the .fch file.

The output is

Relative Shannon entropy and relative Fisher information w.r.t. its free-state

Atom	Rel.Shannon	Rel.Fisher(old)	Rel.Fisher(new)	
1(O)	0.36376828	-8.51171739	2.71756088	
2(H)	-0.08499355	0.92193512	2.84933172	
3(H)	-0.08499355	0.92193512	2.84933172	
Summing up above values:		0.19378119	-6.66784715	8.41622432

Shannon and Fisher information entropy of each atom

Atom	Shannon	Fisher	
1(O)	3.68373047	449.13298912	
2(H)	3.28735108	5.02996044	
3(H)	3.28735108	5.02996044	
Summing up above values:		10.25843264	459.19291000

1st and 2nd-order terms of each atom

Atom	1st	2nd
1(O)	0.30556183	0.06297363
2(H)	-0.15277893	0.13471499
3(H)	-0.15277893	0.13471499
Summing up above values:	0.00000396	0.33240360

In above output, the first part is the aforementioned atomic relative entropy. Please simply ignore the "Rel.Fisher(old)" terms, which are useless.

The second part of the above output is atomic Shannon and Fisher entropy calculated in below way (note that which is different to the "Integral over atomic spaces" mentioned earlier)

- Atomic Shannon entropy: $S_S^A = -\int \rho_A(\mathbf{r}) \ln \rho_A(\mathbf{r}) d\mathbf{r}$

- Atomic Fisher entropy: $I_F^A = \int \frac{|\nabla \rho_A(\mathbf{r})|^2}{\rho_A(\mathbf{r})} d\mathbf{r}$

The two terms in the third part of the above output is defined as follows

- 1st order term: $\Gamma^A = \int \rho_A x(\mathbf{r}) d\mathbf{r}$

- 2nd order term: $\zeta^A = \int \frac{\rho_A x(\mathbf{r})^2}{2} d\mathbf{r}$

where $x = \frac{\rho_A(\mathbf{r}) - \rho_A^0(\mathbf{r})}{\rho_A(\mathbf{r})}$.

Note that in order to acquire relatively accurate result, the "radpot" should be set to a value large than the default, 300 is high enough. It is suggested to set "sphpot" to a value larger than 974 (if you can afford high cost, sphpot=2030 is recommended).

Calculation under AIM partition

The atomic relative entropy under AIM partition is defined as follows

- Relative Shannon entropy: $\Delta S_S^A = \int_{\Omega_A} \rho(\mathbf{r}) \ln \frac{\rho(\mathbf{r})}{\rho_A^0(\mathbf{r})} d\mathbf{r}$
- Relative Fisher entropy: $\Delta I_F^A = \int_{\Omega_A} \rho(\mathbf{r}) \left| \frac{\nabla \rho(\mathbf{r})}{\rho(\mathbf{r})} - \frac{\nabla \rho_A^0(\mathbf{r})}{\rho_A^0(\mathbf{r})} \right|^2 d\mathbf{r}$

where Ω_A denotes spatial region of atomic basin of A.

To calculate them, set "ispecial" in *settings.ini* to 2, then input

examples\H2O.fch // An example

17 // Basin analysis

1 // Generate basin

1 // Use electron density to define basins (AIM basins)

3 // High quality grid

7 // Integrate atomic basins using mixed grid

2 // Exact refinement of basin boundary

Again, the calculation requires atom .wfn files. The atom .wfn files used in this example were generated at B3LYP/6-31G** level, which is in line with the .fch file.

The output is

Atom	Basin	Rel.Shannon	Rel.Fisher(old)	Rel.Fisher(new)
1 (O)	2	1.64507692	-2.44957044	3.50315721
2 (H)	3	-0.00468311	0.53831837	0.41502736
3 (H)	1	-0.00467728	0.53834346	0.41502352
Sum of relat_Shannon:		1.63571653		
Sum of relat_Fisher(old):			-1.37290861	
Sum of relat_Fisher(new):			4.33320809	

The "Rel.Fisher(old)" terms are meaningless and thus should be ignored.

Note that although computational cost even for small systems is high, you should not use "medium quality grid" instead to try to reduce cost, because these quantities are sensitive to grid quality.

Calculation of Rényi entropy

Molecular Rényi entropy

There are two forms of Rényi entropy:

Quadratic form: $-\log \int \rho^2(\mathbf{r}) d\mathbf{r}$

Cubic form: $-(1/2) \log \int \rho^3(\mathbf{r}) d\mathbf{r}$

To calculate them, set "ispecial" in settings.ini to 2, then input

examples\CH3NH2.wfn // An example input file

15 // Fuzzy atomic space analysis

102 // The option dedicated to calculate Rényi entropy

This option needs atom .wfn files, therefore either you let Multiwfn to invoke Gaussian to calculate them, or you provide them in "atomwfn" folder before the calculation.

The output of this example is

Atomic contribution to $\text{int}(\rho^2)$ and $\text{int}(\rho^3)$ under Hirshfeld partition:

Atom	Quadratic	Cubic
1(C)	3.11783284E+01	1.10191626E+03
2(H)	1.13656284E-01	1.06307257E-01
3(H)	1.13656284E-01	1.06307257E-01
4(H)	1.16619595E-01	2.89627389E-01
5(N)	5.18083517E+01	2.95270437E+03
6(H)	1.24221060E-01	2.35085090E-01
7(H)	1.24221060E-01	2.35085090E-01
Total	8.35790544E+01	4.05559304E+03

Molecular quadratic Rényi entropy: -1.92209745

Molecular cubic Rényi entropy: -1.80402718

As you can see, not only molecular value is outputted, but also $\int w_A^{\text{Hirshfeld}} \rho^2(\mathbf{r}) d\mathbf{r}$ and

$\int w_A^{\text{Hirshfeld}} \rho^3(\mathbf{r}) d\mathbf{r}$ of each atom are printed.

Molecular relative Rényi entropy

There are two forms of molecular relative Rényi entropy:

Quadratic form: $-\log \sum_A \int \rho_A^2(\mathbf{r}) / \rho_{A,0}(\mathbf{r}) d\mathbf{r}$

Cubic form: $-\log \sum_A \int \rho_A^3(\mathbf{r}) / \rho_{A,0}^2(\mathbf{r}) d\mathbf{r}$

where $\rho_A(\mathbf{r}) = w_A^{\text{Hirshfeld}} \rho(\mathbf{r})$, while $\rho_{A,0}(\mathbf{r})$ is spherically averaged density of atom A in its isolated state.

To calculate them, set "ispecial" in settings.ini to 2, then input

examples\CH3NH2.wfn // An example input file

15 // Fuzzy atomic space analysis

103 // The option dedicated to calculate relative Rényi entropy

Again, this option requires atom .wfn files

The output of this example is

Note: $\rho_A = w_A \rho(r)$ is density of A in molecule, ρ_{A0} is density of A in its free-state

Atom	$\text{int}(\rho_A^2/\rho_{A0})$	$\text{int}(\rho_A^3/\rho_{A0}^2)$
1(C)	6.21272104E+00	6.56578808E+00
2(H)	1.02090616E+00	1.14140140E+00

3(H)	1.02090616E+00	1.14140140E+00
4(H)	1.05071008E+00	1.18021008E+00
5(N)	7.60168678E+00	8.15127932E+00
6(H)	8.98354673E-01	9.51431599E-01
7(H)	8.98354673E-01	9.51431599E-01
Total	1.87036396E+01	2.00829435E+01

Molecular quadratic Rényi relative entropy: -1.27192612

Molecular cubic Rényi relative entropy: -1.30282737

As you can see, not only molecular relative Rényi entropy is outputted, but also

$\int \rho_A^2(\mathbf{r}) / \rho_{A,0}(\mathbf{r}) d\mathbf{r}$ and $\int \rho_A^3(\mathbf{r}) / \rho_{A,0}^2(\mathbf{r}) d\mathbf{r}$ of each atom are printed.

Note that to calculate relative Rényi entropy, the atom .wfn files must be generated at exactly the same level as molecular wavefunction.

A script of simultaneously calculating various information-theoretic quantities

If you want to simultaneously calculate Shannon entropy, Fisher information, Ghosh-Berkowitz-Parr entropy, relative Shannon/Fisher entropy, absolute and relative Rényi entropy, it is highly recommended to use the Bash shell script written by Bin Wang in Shubin Liu's group, which can be downloaded here: <http://sobereva.com/multiwfn/res/ITA0.6.sh>. This script automatically invokes Multiwfn to compute the quantities in turn. The usage of this script has been detailedly described at the beginning of this file.

Calculation of Hirshfeld charge

Simply enter main function 7 and choose option 1. See Section 3.9.1 for introduction of its definition and Section 4.7.1 of manual for practical example.

Strong covalent interaction (SCI)

SCI was defined in *J. Phys. Chem. A*, **122**, 3087 (2018) and further examined in *J. Mol. Model.*, **24**, 213 (2018). This function was shown to be very useful for identifying very strong covalent bonds.

SCI corresponds to user-defined function 37. Therefore, if you set "userfunc" in *settings.ini* to 37, and then follow examples in Sections 4.3, 4.4, 4.5 but select "100 User-defined function" as the function to be plotted, you will obtain curve map, plane map and isosurface map, respectively.

Only an example of generating cube file of SCI is explicitly given here:

```
examples\CH3NH2.wfn // An example input file
5 // Calculate grid data
100 // User-defined function, which now corresponds to SCI
2 // Medium quality grid
-1 // Visualize isosurface map (of course, this step can be skipped)
```



```
2 // Export data to Gaussian-type cube file in current folder
```

Now you have *userfunc.cub* in current folder, which contains grid data of SCI covering the molecule. Then you can use third-part softwares such as VMD, ChimeraX and GaussView to visualize isosurface map, you can also use VMD or GaussView to map the SCI onto molecular surface via different colors, see <http://sobereva.com/402> (in Chinese) for related example.

Calculation of information-theoretic aromaticity index

In *ACS Omega*, **3**, 18370 (2018) it is shown that arithmetic mean of some information-theoretic quantities of the atoms constituting a ring has good linear relationship with other widely accepted aromaticity indices. In fuzzy analysis module of Multiwfn there is a function dedicated to perform this kind of calculation, see Section 3.18.11 of Multiwfn manual for explanation.

Kinetic energy density (KED) and relevant quantities

Multiwfn supports a large number of kinetic energy density (KED), see end of Section 2.7 of manual for detailed introduction, and they are involved in the study *J. Chem. Phys.*, **150**, 204106 (2019). To study the KEDs, you should set "iuserfunc" in *settings.ini* to 1200, the employed KED is determined by "iKEDsel" in *settings.ini*. In addition, " $\nabla^2\rho$ /uservar" term will be added to the current KED if the "uservar" in *settings.ini* is not equal to 0.

For example, we will calculate integral of Perdew-Wang 91 KED added by $\nabla^2\rho/4$ over the entire space and over various atomic spaces defined by Hirshfeld partition, we should set "iuserfunc" to 1200, set "iKEDsel" to 20, set "uservar" to 4, then input below commands

```
examples\CH3NH2.wfn // An example input file
15 // Fuzzy atomic space analysis
-1 // Select method for partitioning atomic space
3 // Hirshfeld partition based on built-in atomic densities in their isolated states (see
Appendex 3 of manual for detail)
1 // Perform integration in fuzzy atomic spaces
1200 // User-defined function, which now corresponds to Perdew-Wang 91 KED
```

Note that when "iKEDsel" is not equal to its default value (0), the Lagrangian kinetic energy density in electron localization function (ELF) and SCI will be replaced with corresponding KED. Therefore, via this feature you can examine influence of KED on character of these two functions.

For more information, please check KED part of Section 2.7 of manual.

Various "steric" functions

These functions correspond to different user-defined functions, as shown below. Expression and brief introduction are given in Section 2.7 of manual

- Steric energy density: iuserfunc=40.
- Steric potential: iuserfunc=41
- Steric charge: iuserfunc=42
- The magnitude of steric force: iuserfunc = 43

They can be studied in the same way as other real space functions in Multiwfn.

For example, we want to calculate integral of steric potential over the entire space and over each atomic space defined by Becke partition, so we set "iuserfunc" in *settings.ini* to 41, then input *examples\CH3NH2.wfn* // An example input file

15 // Fuzzy atomic space analysis

1 // Perform integration in fuzzy atomic spaces for a real space function (the default partition method is Becke)

100 // User-defined real space function, which now corresponds to steric potential

The result is

Atomic space	Value	% of sum	% of sum abs
1(C)	-0.6934965552D+02	17.836782	-17.836782
2(H)	-0.4282441383D+02	11.014470	-11.014470
3(H)	-0.4282441383D+02	11.014470	-11.014470
4(H)	-0.4420898486D+02	11.370583	-11.370583
5(N)	-0.1019875846D+03	26.231280	-26.231280
6(H)	-0.4380317175D+02	11.266207	-11.266207
7(H)	-0.4380317175D+02	11.266207	-11.266207

Summing up above values: -0.3888013961D+03
Summing up absolute value of above values: 0.3888013961D+03

No that since variation of steric charge and magnitude of steric force is much more sharp than steric potential, therefore before integrating them it is suggested to set "radpot" and "sphpot" in *settings.ini* to much larger values than default, for example, 300 and 2030, respectively.

Pauli potential/force/charge, quantum potential/force/charge and electrostatic force

They are defined as user-defined functions 60~67, see corresponding part of Section 2.7 of manual for introduction. They can be studied in Multiwfn in exactly the same way as other real space functions, therefore no example is explicitly given.

Shubin Liu's energy decomposition analysis

The energy decomposition analysis method proposed by Shubin Liu decomposes total molecular energy as follow

$$E = E_{\text{steric}} + E_{\text{electrostatic}} + E_{\text{quantum}}$$

where $E_{\text{quantum}} = E_{\text{pauli}} + E_{\text{XC}}$.

In Multiwfn, all above terms as well as many intermediate quantities can be printed, for example:

Electronic kinetic energy (ET): 79.359221 Hartree
Weizsacker kinetic energy (TW): 64.213411 Hartree
Interelectronic Coulomb repulsion energy (EJ): 80.308594 Hartree

Internuclear Coulomb repulsion energy (ENuc): 42.220921 Hartree
Nuclear-electronic Coulomb attraction energy (EV): -268.644374 Hartree
Energy without electronic correlation (ET+EV+EJ+ENuc): -66.755638 Hartree
Exchange correlation energy (Ex): -12.388347 Hartree
Coulomb correlation energy (Ec): -0.719998 Hartree
Pauli kinetic energy (ET-TW): 15.145810 Hartree

----- EDA-SBL energy decomposition terms:

E_steric: 64.213411 Hartree
E_electrostatic: -146.114859 Hartree
E_quantum: 2.037465 Hartree

E_total: -79.863983 Hartree

See Section 3.24.2 of manual for introduction of this method and Section 4.21.2 for example.