Densitizer

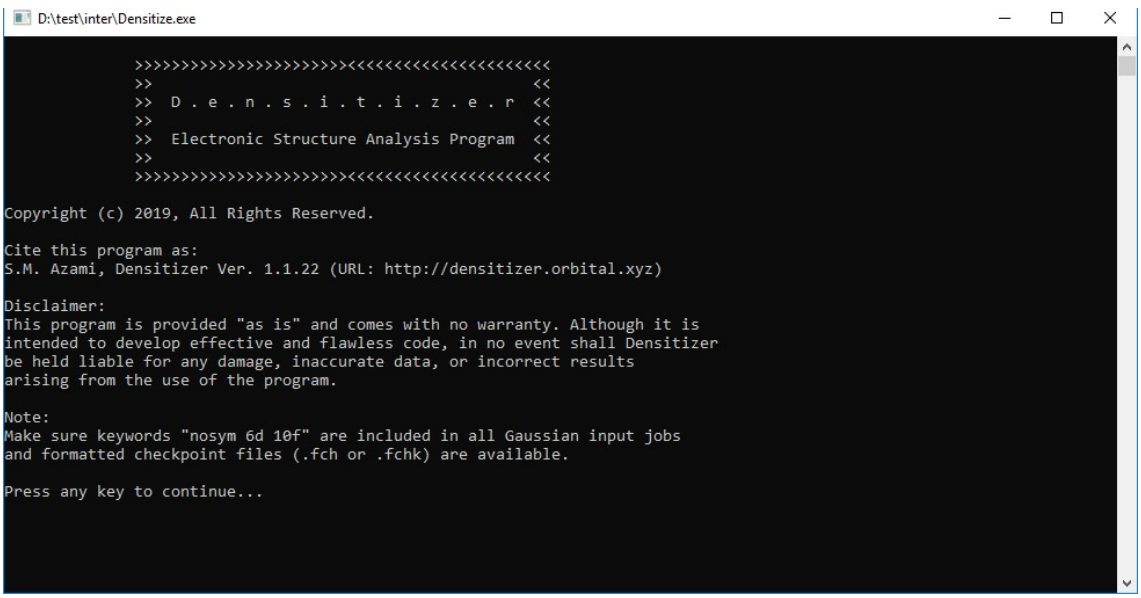
Electronic Structure Analysis Suite of Programs

User's Manual

Overview

Densitizer is an electronic structure analysis suite of programs which processes Gaussian's formatted checkpoint as input and provide quantum chemical information about the intra/intermolecular electronic structure. *Densitizer* possesses no graphical interface; instead, results are provided as two popular formats .fch and .wfn which enables the user to plot and visualize orbitals and electron density counter maps via many other programs such as GaussView, Multiwfn, AIMAll, AIM2000, etc. *Densitizer* requires no other code/software/platform to be installed on the system and is provided as a standalone executable bundled with manual and sample files in a single extractable .zip archive.

On the initial execution of *Densitizer*, the program displays welcome screen including several information about the program and disappears on keyboard hit:



```
              >>>>>>>>>>>>>>>>>>>>>><<<<<<<<<<<<<<<<<<<<<<
              >>                                        <<
              >>  D . e . n . s . i . t . i . z . e . r  <<
              >>                                        <<
              >>  Electronic Structure Analysis Program  <<
              >>                                        <<
              >>>>>>>>>>>>>>>>>>>>>><<<<<<<<<<<<<<<<<<<<<<

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Cite this program as:
S.M. Azami, Densitizer Ver. 1.1.22 (URL: http://densitizer.orbital.xyz)

Disclaimer:
This program is provided "as is" and comes with no warranty. Although it is
intended to develop effective and flawless code, in no event shall Densitizer
be held liable for any damage, inaccurate data, or incorrect results
arising from the use of the program.

Note:
Make sure keywords "nosym 6d 10f" are included in all Gaussian input jobs
and formatted checkpoint files (.fch or .fchk) are available.

Press any key to continue...
```
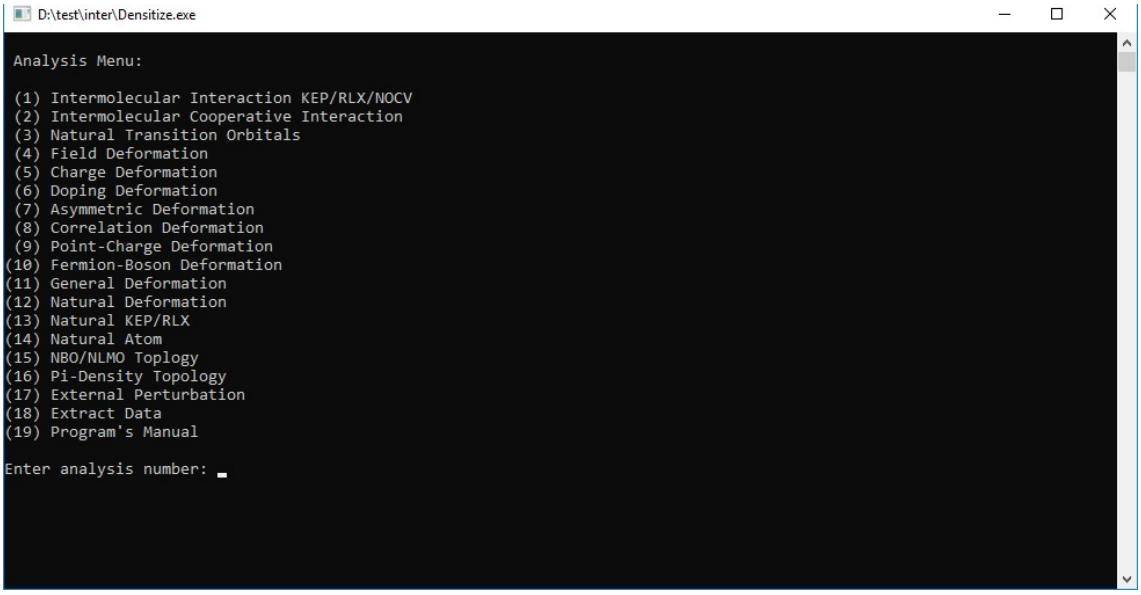

In the second screen, main analysis menu is displayed as below and user is required to input the number of analysis:


D:\test\inter\Densitize.exe
Analysis Menu:
(1) Intermolecular Interaction KEP/RLX/NOCV
(2) Intermolecular Cooperative Interaction
(3) Natural Transition Orbitals
(4) Field Deformation
(5) Charge Deformation
(6) Doping Deformation
(7) Asymmetric Deformation
(8) Correlation Deformation
(9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual
Enter analysis number:

Preparation of input files and running *Densitizer*

Densitizer requires formatted checkpoint file (.fch or .fchk) of Gaussian program as input which can be made via `formchk` utility of Gaussian. There is no difference between Windows or Linux versions of Gaussian, and *Densitizer* supports formatted checkpoints and outputs of two in Windows platform. User must include the following keywords in the route section of all jobs to make sure *Densitizer* does its work properly:

```
# nosym 6d 10f gfinput density
```

If user intend to analyze natural KEP/RLX, natural atom, and, NBO/NLMO topology, additional keywords are required in both route and NBO sections, and also a filename in which NBO results are present:

```
# nosym 6d 10f gfinput density pop=nboread
```

```
$NBO AONAO AONBO AONLMO $END
```

Densitizer accepts two types of NBO output. First way is direct use of NBO 3.0 program implemented in Gaussian. In this respect, the Gaussian input job looks like something like this:

```
%chk=water.chk
# nosym 6d 10f gfinput density pop=nboread

watertest

0 1
O                 -0.04480287    0.50179211    0.00000000
H                  0.91519713    0.50179211    0.00000000
H                 -0.36525745    1.40672794    0.00000000

$NBO AONAO AONBO AONLMO $END
```

Once *Densitizer* prompts to enter NBO filename, user specifies the Gaussian's output filename. Second way is to use external NBO program (e.g., GenNBO) via .47 archive file. In this respect, the Gaussian input job looks like something like this:

```
%chk=water.chk
# nosym 6d 10f gfinput density pop=nboread

Watertest

0 1
O                 -0.04480287    0.50179211    0.00000000
H                  0.91519713    0.50179211    0.00000000
H                 -0.36525745    1.40672794    0.00000000

$NBO ARCHIVE FILE=water $END
```

After Gaussian calculation, user should include these keywords in the .47 file (see NBO manual for more information):

```
$NBO AONAO AONBO AONLMO $END
```

Once *Densitizer* prompts to enter NBO filename, user specifies the NBO output filename generated by the external NBO program.

If user include no file extension in the filename when *Densitizer* prompts to enter, *Densitizer* automatically searches for .fch and .fchk for formatted checkpoint, and .log, .out, .nbo for NBO results.

All examples of different analyses in the present manual are also located in the `samples` subdirectory of *Densitizer*'s installation directory and the user is encouraged to run the one which is related to his interest before going ahead.

Once *Densitizer* is run, it asks some questions related to filenames, etc., and when all required information for initialization of program are collected, Densitizer read matrices and shows message

```
Computing…
```

at the bottom of main window. After calculation of all requested analyses, message

```
-- Clear --
```

will appears at the bottom which means *Densitizer*'s work is terminated and the user can now close the window, safely.

Densitizer output files and visualization

Densitizer creates three type of files .fch, .wfn, plus a single .report.txt file as outputs. While .wfn includes electron density, .fch includes both electron density and molecular orbitals; and depending on data, the output .fch files may include one or both. Those .fch files which are directly located on the results directory, includes both electron density and molecular orbitals data, whiles those located in the "`num`" subdirectory, includes just electron density data.

In the present manual, GaussView is used for visualization of .fch, and AIM2000 for .wfn files. Although Multiwfn and AIMAll are also able to open and visualize .wfn files, they have some inconsistencies with negative electron density as it is common in deformation electron density maps. On the other hand, for absolute electron densities, these two softwares work and well support .wfn files. Since the data included in .fch and .wfn files differ with their ordinary uses, instructions of how to open, use, and visualize these files are given in the next pages.

In most of cases, *Densitizer* creates a text file `report.txt` in which eigenvelues of deformation density (components) are stored. These eigenvalues also exist in the corresponding .fch, where orbital energies are replaced by these eigenvalues and appears if user opens by an appropriate software.

General structure of report file

The .report.txt file is a text file beginning with program's information and followed by molecular related values on which Gaussian is calculations are performed, and is stored in the directory of output results:

```
form14.report.txt - Notepad
File  Edit  Format  View  Help

              >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
              >>                                          <<
              >>  D . e . n . s . i . t . i . z . e . r   <<
              >>                                          <<
              >>  Electronic Structure Analysis Program   <<
              >>                                          <<
              >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>

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Cite this program as:
S.M. Azami, Densitizer Ver. 1.1.14 (URL: http://densitizer.orbital.xyz)

Disclaimer:
This program is provided "as is" and comes with no warranty. Although
it is intended to develop effective and flawless code, in no event shall
Densitizer be held liable for any damage, incorrect data, or inaccurate
results arising from the use of the program.
==========================================================================
Molecular Formula             : H2CO
Charge                        : 0
Multiplicity                  : 1
Number of Atoms               : 4
Number of basis elements      : 60
Number of Primitive Gaussians : 90
Number of Total Electrons     : 16
Number of Alpha Electrons     : 8
Number of Beta  Electrons     : 8
Number of Fragments           : 0
Number of Subcomplexes        : 0
SCF Type                      : RHF

Molecular Coordinates:
-------------------------------------------
1   C     0.079909    -0.159817     0.000000
2   H     0.613072    -1.087522     0.000000
3   H    -0.990091    -0.159817     0.000000
4   O     0.706949     0.931233     0.000000
-------------------------------------------
```
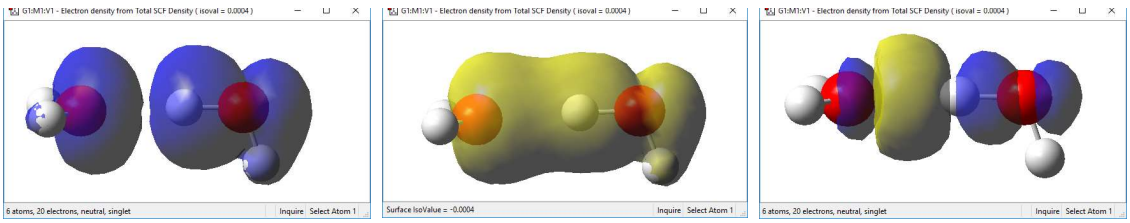
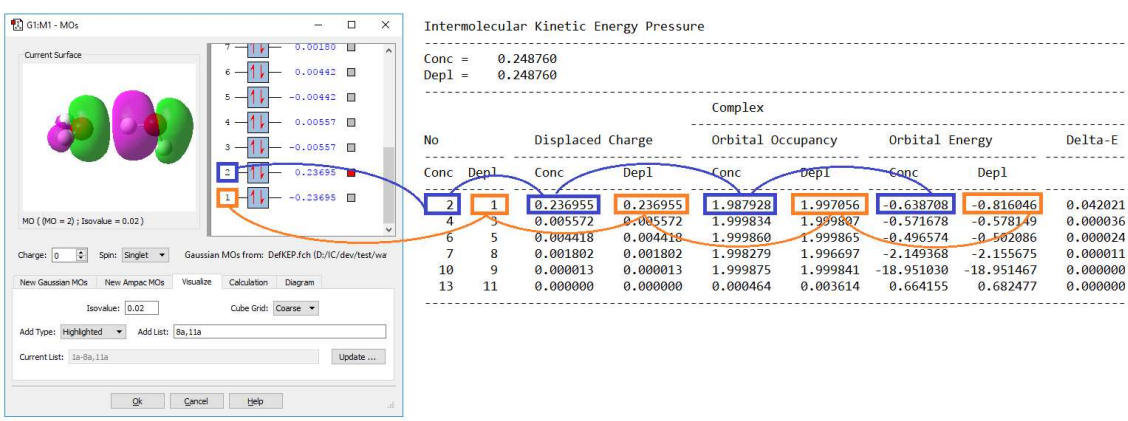

It follows by deformation density analysis of different phenomena as distinct sections, depending on the analysis requested by user. Each section is supplied by total concentration/depletion value, deformation orbital

(DO) number, displaced charge, orbital occupancies, energies, and stabilization (Delta-E) of DOs in complex and fragments. Each section begins with total concentration and depletion of charge due to its title. For example, below figure shows deformation density due to intermolecular kinetic energy pressure, where 0.248760 e is displaced. These values can be visualized with respect to the corresponding .fch which are different filenames for different analysis and will be discussed for each analysis, distinctly. As example, for intermolecular kinetic energy pressure, three files DefKEPConc.fch, DefKEPDepl.fch, DefKEP.fch, includes concentration, depletion, both concentration and depletion deformation densities, respectively:



DefKEPConc.fch DefKEPDepl.fch DefKEPDepl.fch

The first two columns, show the number of DO corresponding to depletion and concentration available in the other right columns and also to their number in GaussView orbital visualization window. Below figure shows these connections, clearly. Also, notice that the displaced charged values for each orbital is available in both report file, and right of the GaussView visualization window:



The rightest column is the stabilization energy (`Delta-E`) due to each DO with respect to its environment. In the above results, they are in the complex environment (see its subtitle).

Intermolecular Interaction Analysis

This analysis provides deformation density information of complex formation including kinetic energy pressure (KEP) due to Pauli repulsion (also known as steric effect), orbital relaxation (RLX), and natural orbitals for chemical valence (NOCV). In order to make Gaussian .gjf input jobs, fragments must be appeared continuously in the complex system and numbered as they exist in the complex. For example, below inputs show correct Gaussian jobs of water dimer, where xyz coordinates of two fragments are highlighted as blue and green.

Water dimer:

```
%chk=dimer.chk
# nosym 6d 10f

WaterDimer

0 1
 O                  -0.94320488   -2.68762673    0.00000000
 H                   0.01679512   -2.68762673    0.00000000
 H                  -1.26365946   -1.78269090    0.00000000
 O                  -1.74543284   -0.19446361    0.13175638
 H                  -1.95483880    0.43845606   -0.55901265
 H                  -1.82777487    0.22850095    0.98961462
```

Fragment 1:

```
%chk=dimer.chk
# nosym 6d 10f

Frag1

0 1
 O                  -0.94320488   -2.68762673    0.00000000
 H                   0.01679512   -2.68762673    0.00000000
 H                  -1.26365946   -1.78269090    0.00000000
```

Fragment 2:

```
%chk=dimer.chk
# nosym 6d 10f

Frag2

0 1
 O                  -1.74543284   -0.19446361    0.13175638
 H                  -1.95483880    0.43845606   -0.55901265
 H                  -1.82777487    0.22850095    0.98961462
```

Below examples show example for incorrect jobs:

Water dimer:

```
%chk=dimer.chk
# nosym 6d 10f

WaterDimer

0 1
 O                  -0.94320488   -2.68762673    0.00000000
 H                   0.01679512   -2.68762673    0.00000000
 O                  -1.74543284   -0.19446361    0.13175638
 H                  -1.95483880    0.43845606   -0.55901265
 H                  -1.26365946   -1.78269090    0.00000000
 H                  -1.82777487    0.22850095    0.98961462
```

Problem: One of the atoms of fragment #1 is located somewhere else.

Fragment 1:

```
%chk=dimer.chk
# nosym 6d 10f

Frag1

0 1
 O                  -1.74543284   -0.19446361    0.13175638
 H                  -1.95483880    0.43845606   -0.55901265
 H                  -1.82777487    0.22850095    0.98961462
```

Problem: Fragment's number does not match its order in the complex. While its title is fragment #1, the xyz coordinates belongs to fragment #2

Densitizer.exe	4/1/2019 7:25 AM	Application	3,316 KB
comp.fch	4/1/2019 7:36 AM	FCH File	77 KB
frag1.fch	4/1/2019 7:36 AM	FCH File	75 KB
frag2.fch	4/1/2019 7:36 AM	FCH File	75 KB
comp.gjf	4/1/2019 7:43 AM	GJF File	1 KB
frag1.gjf	4/1/2019 7:43 AM	GJF File	1 KB
frag2.gjf	4/1/2019 7:43 AM	GJF File	1 KB
comp.out	4/1/2019 7:44 AM	OUT File	12 KB
frag1.out	4/1/2019 7:44 AM	OUT File	14 KB
frag2.out	4/1/2019 7:44 AM	OUT File	14 KB
comp.chk	4/1/2019 7:36 AM	Recovered File Fra...	524 KB
frag1.chk	4/1/2019 7:36 AM	Recovered File Fra...	524 KB
frag2.chk	4/1/2019 7:36 AM	Recovered File Fra...	524 KB

If the .fch files due to water dimer available in the `samples` subdirectory are to be analyzed, the main screen should be something like this:

```
D:\test\inter\Densitize.exe

Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 1
Enter number of fragments: 2
Enter complex Gaussian formatted checkpoint (.fch or .fchk) filename    : comp
Enter Fragment #1 Gaussian formatted checkpoint (.fch or .fchk) filename: frag1
Enter Fragment #2 Gaussian formatted checkpoint (.fch or .fchk) filename: frag2
Enter foldername where results are to be stored: waterdimer
Reading data... 0 1 2
Reading matrices... 0 1 2

Computing...


 -- Clear --
```

num	4/1/2019 7:41 AM	File folder	
comp.fch	4/1/2019 7:36 AM	FCH File	77 KB
DefKEP.fch	4/1/2019 7:41 AM	FCH File	77 KB
DefKEPConc.fch	4/1/2019 7:41 AM	FCH File	77 KB
DefKEPDepl.fch	4/1/2019 7:41 AM	FCH File	77 KB
DefRLX.fch	4/1/2019 7:41 AM	FCH File	77 KB
DefRLXConc.fch	4/1/2019 7:41 AM	FCH File	77 KB
DefRLXDepl.fch	4/1/2019 7:41 AM	FCH File	77 KB
DefTOT.fch	4/1/2019 7:41 AM	FCH File	77 KB
DefTOTConc.fch	4/1/2019 7:41 AM	FCH File	77 KB
DefTOTDepl.fch	4/1/2019 7:41 AM	FCH File	77 KB
frag1.fch	4/1/2019 7:36 AM	FCH File	75 KB
frag2.fch	4/1/2019 7:36 AM	FCH File	75 KB
waterdimer.report.txt	4/1/2019 7:41 AM	Text Document	24 KB
DefKEP.wfn	4/1/2019 7:41 AM	WFN File	17 KB
DefRLX.wfn	4/1/2019 7:41 AM	WFN File	32 KB
DefTOT.wfn	4/1/2019 7:41 AM	WFN File	32 KB

Densitizer creates the three types of output files directly in the same directory, and puts numbered .fch files in `num` subdirectory, which are density of deformation orbitals, and also pairs of densities of deformation orbitals with positive and negative eigenvalues (symmetrically distributed in common). Filenames, analyses and what they store are shown in below table:

Filename	Analysis	Includes
`DefKEP.fch`	Kinetic energy pressure (steric)	Density\Orbital
`DefKEP.wfn`	Kinetic energy pressure (steric)	Density
`DefKEPnnnn.fch`	Kinetic energy pressure (steric)	Density
`DefKEPPairnnnn.fch`	Kinetic energy pressure (steric)	Density
`DefRLX.fch`	Orbital relaxation (NOCV)	Density\Orbital
`DefRLX.wfn`	Orbital relaxation (NOCV)	Density
`DefRLXnnnn.fch`	Orbital relaxation (NOCV)	Density
`DefRLXPairnnnn.fch`	Orbital relaxation (NOCV)	Density
`DefTOT.fch`	Total deformation density	Density\Orbital
`DefTOT.wfn`	Total deformation density	Density
`DefTOTnnnn.fch`	Total deformation density	Density
`DefTOTPairnnnn.fch`	Total deformation density	Density

The report file includes three sections for Intermolecular Kinetic Energy Pressure, Intermolecular Relaxation (NOCV), and, Total deformation density analyses.

Intermolecular Kinetic Energy Pressure

Conc = 0.248760
Depl = 0.248760

No		Displaced Charge		Complex Orbital Occupancy		Complex Orbital Energy		Delta-E
Conc	Depl	Conc	Depl	Conc	Depl	Conc	Depl	
2	1	0.236955	0.236955	1.987928	1.997056	-0.638708	-0.816046	0.042021
4	3	0.005572	0.005572	1.999834	1.999807	-0.571678	-0.578149	0.000036
6	5	0.004418	0.004418	1.999860	1.999865	-0.496574	-0.502086	0.000024
7	8	0.001802	0.001802	1.998279	1.996697	-2.149368	-2.155675	0.000011
10	9	0.000013	0.000013	1.999875	1.999841	-18.951030	-18.951467	0.000000
13	11	0.000000	0.000000	0.000464	0.003614	0.664155	0.682477	0.000000

Intermolecular Relaxation (NOCV)

Conc = 0.277086
Depl = 0.277086

No		Displaced Charge		Complex Orbital Occupancy		Complex Orbital Energy		Delta-E
Conc	Depl	Conc	Depl	Conc	Depl	Conc	Depl	
1	2	0.199769	0.199769	1.099885	0.900115	0.094817	0.218551	-0.024718
4	3	0.028553	0.028553	1.014277	0.985723	0.014049	0.030375	-0.000466
5	6	0.025722	0.025722	1.012861	0.987139	0.073741	0.090843	-0.000440
8	7	0.023041	0.023041	1.011520	0.988480	0.013157	0.028872	-0.000362
9	10	0.000000	0.000000	2.000000	2.000000	-0.736755	-14.778280	0.000000
11	12	0.000000	0.000000	2.000000	2.000000	-2.421961	-12.153795	0.000000
13	14	0.000000	0.000000	2.000000	2.000000	-1.252247	-11.779755	0.000000

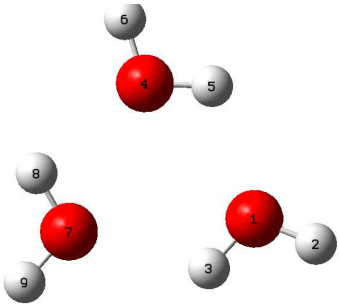
Total

Conc = 0.444501
Depl = 0.444501

No		Displaced Charge		Complex Orbital Occupancy		Complex Orbital Energy		Delta-E
Conc	Depl	Conc	Depl	Conc	Depl	Conc	Depl	
1	2	0.315207	0.270819	1.633414	1.672303	-0.294944	-0.499030	0.042178
4	3	0.066125	0.109467	1.480093	1.118790	-0.781850	-0.268414	-0.022317
6	5	0.026151	0.026661	1.052731	1.042357	0.054462	0.069419	-0.000427
8	7	0.023549	0.023595	1.036960	1.025610	0.005274	0.016534	-0.000266
10	9	0.012675	0.013898	1.133768	0.961496	-0.428145	-0.301279	-0.001240
11	13	0.000578	0.000062	1.933373	1.989478	-2.171720	-17.602562	-0.000167

These table continues horizontally to include the above information for fragments as well as complex.

Cooperative interaction analysis



Densitizer.exe	4/3/2019 8:51 AM	Application	3,317 KB
form.fch	4/3/2019 6:54 AM	FCH File	81 KB
form.gjf	4/3/2019 6:52 AM	GJF File	1 KB
form.out	4/3/2019 6:54 AM	OUT File	18 KB
form.chk	4/3/2019 6:54 AM	Recovered File Fra...	640 KB

D:\test\dens\Densitize.exe

```
Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 2
Enter number of fragments: 3
Enter overall complex  Gaussian formatted checkpoint (.fch or .fchk) filename: trimer
Enter Fragment   #1    Gaussian formatted checkpoint (.fch or .fchk) filename: frag1
Enter Fragment   #2    Gaussian formatted checkpoint (.fch or .fchk) filename: frag2
Enter Fragment   #3    Gaussian formatted checkpoint (.fch or .fchk) filename: frag3
Enter subcomplex #1-#2 Gaussian formatted checkpoint (.fch or .fchk) filename: dimer1
Enter subcomplex #1-#3 Gaussian formatted checkpoint (.fch or .fchk) filename: dimer2
Enter subcomplex #2-#3 Gaussian formatted checkpoint (.fch or .fchk) filename: dimer3
Enter foldername where results are to be stored: watertrimer
Reading data... 0 1 2 3 4 5 6
Reading matrices... 0 1 2 3 4 5 6

Computing...


 -- Clear --
```

Natural Transition Orbitals

```
D:\test\dens\Densitize.exe

 Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 3
Enter excited state ("density" keyword included) Gaussian formatted checkpoint (.fch or .fchk) filename: form
(1) Absorption
(2) Fluorescence
Enter choice: 1
Enter foldername where results are to be stored: form
Reading data... 0 1
Reading matrices... 0 1        1 file(s) moved.


Computing...


 -- Clear --
```

Field electron deformation orbitals

Densitizer.exe	4/3/2019 8:51 AM	Application	3,317 KB
ace.fch	4/3/2019 9:09 AM	FCH File	53 KB
ace100.fch	4/3/2019 9:09 AM	FCH File	53 KB
ace.gjf	4/3/2019 9:08 AM	GJF File	1 KB
ace100.gjf	4/3/2019 9:08 AM	GJF File	1 KB
ace.out	4/3/2019 9:09 AM	OUT File	11 KB
ace100.out	4/3/2019 9:09 AM	OUT File	12 KB
ace.chk	4/3/2019 9:09 AM	Recovered File Fra...	524 KB
ace100.chk	4/3/2019 9:09 AM	Recovered File Fra...	524 KB

D:\test\dens\Densitize.exe

```
 Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 4
Enter field-free    Gaussian formatted checkpoint (.fch or .fchk) filename: ace
Enter field-dressed Gaussian formatted checkpoint (.fch or .fchk) filename: ace100
Enter foldername where results are to be stored: ace
Reading data... 0 1
Reading matrices... 0 1

Computing...


 -- Clear --
```

Charge deformation

Densitizer.exe	4/3/2019 8:51 AM	Application	3,317 KB
cat.fch	4/3/2019 9:21 AM	FCH File	115 KB
cyc.fch	4/3/2019 9:22 AM	FCH File	115 KB
cat.gjf	4/3/2019 9:18 AM	GJF File	1 KB
cyc.gjf	4/3/2019 9:18 AM	GJF File	1 KB
cat.out	4/3/2019 9:21 AM	OUT File	20 KB
cyc.out	4/3/2019 9:19 AM	OUT File	20 KB
cat.chk	4/3/2019 9:21 AM	Recovered File Fra...	524 KB
cyc.chk	4/3/2019 9:22 AM	Recovered File Fra...	524 KB

D:\test\dens\Densitize.exe

```
Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 5
Enter neutral Gaussian formatted checkpoint (.fch or .fchk) filename: cyc
Enter charged Gaussian formatted checkpoint (.fch or .fchk) filename: cat
Enter foldername where results are to be stored: cyc
Reading data... 0 1
Reading matrices... 0 1

Computing...


 -- Clear --
```

Doping deformation

Densitizer.exe	4/3/2019 8:51 AM	Application	3,317 KB
cyc.fch	4/3/2019 9:46 AM	FCH File	159 KB
cycdope.fch	4/3/2019 9:46 AM	FCH File	159 KB
BCN.gjf	4/3/2019 9:35 AM	GJF File	1 KB
cyc.gjf	4/3/2019 9:43 AM	GJF File	5 KB
cycdope.gjf	4/3/2019 9:45 AM	GJF File	5 KB
BCN.out	4/3/2019 9:35 AM	OUT File	14 KB
cyc.out	4/3/2019 9:44 AM	OUT File	14 KB
cycdope.out	4/3/2019 9:46 AM	OUT File	14 KB
cyc.chk	4/3/2019 9:46 AM	Recovered File Fra...	568 KB
cycdope.chk	4/3/2019 9:46 AM	Recovered File Fra...	568 KB

D:\test\dens\Densitize.exe

```
 Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 6
Enter pure-structure  Gaussian formatted checkpoint (.fch or .fchk) filename: cyc
Enter doped-structure Gaussian formatted checkpoint (.fch or .fchk) filename: cycdope
Enter foldername where results are to be stored: cycdope
Reading data... 0 1
Reading matrices... 0 1

Computing...


 -- Clear --
```

Asymmetric deformation

Densitizer.exe	4/3/2019 8:51 AM	Application	3,317 KB
ace.fch	4/3/2019 10:00 AM	FCH File	53 KB
L.fch	4/3/2019 10:00 AM	FCH File	53 KB
R.fch	4/3/2019 10:00 AM	FCH File	53 KB
ace.gjf	4/3/2019 9:58 AM	GJF File	1 KB
L.gjf	4/3/2019 9:58 AM	GJF File	1 KB
R.gjf	4/3/2019 9:59 AM	GJF File	1 KB
ace.out	4/3/2019 9:59 AM	OUT File	11 KB
L.out	4/3/2019 9:59 AM	OUT File	11 KB
R.out	4/3/2019 9:59 AM	OUT File	11 KB
ace.chk	4/3/2019 10:00 AM	Recovered File Fra...	524 KB
L.chk	4/3/2019 10:00 AM	Recovered File Fra...	524 KB
R.chk	4/3/2019 10:00 AM	Recovered File Fra...	524 KB

D:\test\dens\Densitize.exe

```
 Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 7
Enter Gaussian formatted checkpoint of       Free    State (.fch or .fchk) filename: ace
Enter Gaussian formatted checkpoint of Left -Exposed State (.fch or .fchk) filename: L
Enter Gaussian formatted checkpoint of Right-Exposed State (.fch or .fchk) filename: R
Enter foldername where results are to be stored: aceasym
Reading data... 0 1 2
Reading matrices... 0 1 2

Computing...


 -- Clear --
```

Correlation deformation

Densitizer.exe	4/3/2019 10:10 AM	Application	3,317 KB
cyc.fch	4/3/2019 10:13 AM	FCH File	82 KB
cyc.gjf	4/3/2019 10:12 AM	GJF File	1 KB
cyc.out	4/3/2019 10:13 AM	OUT File	25 KB
cyc.chk	4/3/2019 10:13 AM	Recovered File Fra...	524 KB

D:\test\dens\Densitize.exe

```
 Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 8
Enter correlated-level Gaussian formatted checkpoint (.fch or .fchk) filename: cyc
Enter foldername where results are to be stored: cyccorr
Reading data... 0 1
Reading matrices... 0 1

Computing...


 -- Clear --
```

Point-Charge deformation

Densitizer.exe	4/3/2019 10:10 AM	Application	3,317 KB
form.fch	4/5/2019 11:27 PM	FCH File	53 KB
formpoint.fch	4/5/2019 11:27 PM	FCH File	53 KB
form.gjf	4/5/2019 11:25 PM	GJF File	1 KB
formpoint.gjf	4/5/2019 11:26 PM	GJF File	1 KB
form.out	4/5/2019 11:27 PM	OUT File	11 KB
formpoint.out	4/5/2019 11:27 PM	OUT File	13 KB
form.chk	4/5/2019 11:27 PM	Recovered File Fra...	524 KB
formpoint.chk	4/5/2019 11:27 PM	Recovered File Fra...	524 KB

D:\test\dens\Densitize.exe

```
 Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 9
Enter free-state      Gaussian formatted checkpoint (.fch or .fchk) filename: form
Enter polarized-state Gaussian formatted checkpoint (.fch or .fchk) filename: formpoint
Enter foldername where results are to be stored: formpoint
Reading data... 0 1
Reading matrices... 0 1

Computing...


 -- Clear --
```

Fermion-Boson deformation

G09w	4/5/2019 11:33 PM	File folder	
Densitizer.exe	4/3/2019 10:10 AM	Application	3,317 KB
water.fch	4/5/2019 11:33 PM	FCH File	28 KB
water.gjf	4/5/2019 11:32 PM	GJF File	1 KB
water.out	4/5/2019 11:32 PM	OUT File	11 KB
water.chk	4/5/2019 11:33 PM	Recovered File Fra...	524 KB

General deformation

Densitizer.exe	4/3/2019 10:10 AM	Application	3,317 KB
cycb3.fch	4/5/2019 11:47 PM	FCH File	175 KB
cychf.fch	4/5/2019 11:47 PM	FCH File	175 KB
cycb3.gjf	4/5/2019 11:44 PM	GJF File	1 KB
cychf.gjf	4/5/2019 11:45 PM	GJF File	1 KB
cycb3.out	4/5/2019 11:47 PM	OUT File	19 KB
cychf.out	4/5/2019 11:46 PM	OUT File	18 KB
cycb3.chk	4/5/2019 11:47 PM	Recovered File Fra...	592 KB
cychf.chk	4/5/2019 11:47 PM	Recovered File Fra...	592 KB

D:\test\dens\Densitize.exe

```
 Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 11
Enter initial-state Gaussian formatted checkpoint (.fch or .fchk) filename: cychf
Enter final-state   Gaussian formatted checkpoint (.fch or .fchk) filename: cycb3
Enter foldername where results are to be stored: cychfb3
Reading data... 0 1
Reading matrices... 0 1

Computing...


 -- Clear --
```

Natural Deformation

NBO 3.0 implemented in Gaussian:

Densitizer.exe	4/3/2019 10:10 AM	Application	3,317 KB
water.fch	4/6/2019 12:28 AM	FCH File	28 KB
water.gjf	4/6/2019 12:27 AM	GJF File	1 KB
water.out	4/6/2019 12:27 AM	OUT File	50 KB
water.chk	4/6/2019 12:28 AM	Recovered File Fra...	524 KB

D:\test\dens\Densitize.exe

```
Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 12
Enter Gaussian formatted checkpoint (.fch or .fchk) filename: water
Enter filename where NBO results are present: water
Enter two atom numbers for interatomic analysis separated by spaces
and terminated by 0 as end:
1 2
2 3
0
Enter foldername where results are to be stored: water
Reading data... 0
Reading matrices... 0

Computing...


 -- Clear --
```

NBO 5.0 or higher as external source:

WATERNBO5.47	4/6/2019 12:21 AM	47 File	43 KB
Densitizer.exe	4/3/2019 10:10 AM	Application	3,317 KB
GenNBO.exe	7/31/2004 5:36 PM	Application	2,371 KB
water.fch	4/6/2019 12:21 AM	FCH File	28 KB
water.gjf	4/6/2019 12:20 AM	GJF File	1 KB
nbodone.lst	4/6/2019 12:21 AM	LST File	1 KB
WATERNBO5.nbo	4/6/2019 12:21 AM	NBO File	14 KB
water.out	4/6/2019 12:21 AM	OUT File	26 KB
water.chk	4/6/2019 12:21 AM	Recovered File Fra...	524 KB

D:\test\dens\Densitize.exe

```
Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 12
Enter Gaussian formatted checkpoint (.fch or .fchk) filename: water
Enter filename where NBO results are present: waternbo5
Enter two atom numbers for interatomic analysis separated by spaces
and terminated by 0 as end:
1 2
2 3
0
Enter foldername where results are to be stored: waternbo5
Reading data... 0
Reading matrices... 0

Computing...


 -- Clear --
```

NBO/NLMO Topology

Densitizer.exe	4/3/2019 10:10 AM	Application	3,317 KB
eth.fch	4/6/2019 6:10 AM	FCH File	77 KB
eth.gjf	4/6/2019 6:10 AM	GJF File	1 KB
eth.out	4/6/2019 6:10 AM	OUT File	125 KB
eth.chk	4/6/2019 6:10 AM	Recovered File Fra...	524 KB

D:\test\dens\Densitize.exe

```
Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 15
Enter Gaussian formatted checkpoint (.fch or .fchk) filename: eth
Enter filename where NBO results are present: eth
Enter NBO/NLMO numbers for topological analysis separated by spaces
and terminated by 0 as end (-1 for all NBOs/NLMOs with occ. > 0.1):
3 4 0
Enter foldername where results are to be stored: eth
Reading data... 0
Reading matrices... 0

Computing...


 -- Clear --
```

Natural Transition Orbitals / Charge Deformation / Field Deformation

This analyses provides deformation orbitals, where the required .fch input files are as below. Note that the molecular geometry of second .fch must be frozen to that in the first .fch file.
Natural Transition Orbitals: Excited state.
Charge Deformation: Neutral and charged species.
Field Deformation: Relaxed molecule, and that exposed to external electric field.

Filenames, analyses and what they store for these three analyses are shown in below table:

Filename	Analysis	Includes
`NTO.fch`	Natural Transition Orbitals	Density\Orbital
`NTO.wfn`	Natural Transition Orbitals	Density
`NTOnnnn.fch`	Natural Transition Orbitals	Density
`NTOPairnnnn.fch`	Natural Transition Orbitals	Density
`CDO.fch`	Charge Deformation	Density\Orbital
`CDO.wfn`	Charge Deformation	Density
`CDOnnnn.fch`	Charge Deformation	Density
`CDOPairnnnn.fch`	Charge Deformation	Density
`EDO.fch`	Field Deformation	Density\Orbital
`EDO.wfn`	Field Deformation	Density
`EDOnnnn.fch`	Field Deformation	Density
`EDOPairnnnn.fch`	Field Deformation	Density

Block Deformation Analysis

This analysis provides deformation density information of complex

Natural KEP/RLX Analysis

This analysis provides deformation density information of complex

Natural Atom Analysis

This analysis provides deformation density information of complex

NBO/NLMO Topological Analysis

This analysis provides deformation density information of complex

Pi-Density Topology Analysis

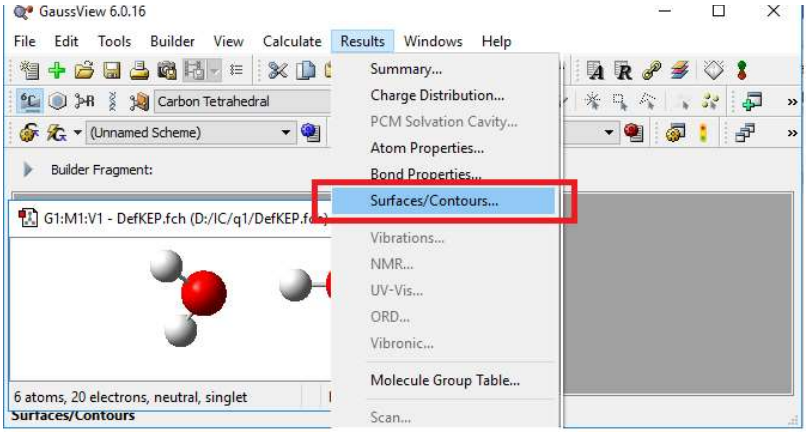
This analysis provides deformation density information of complex

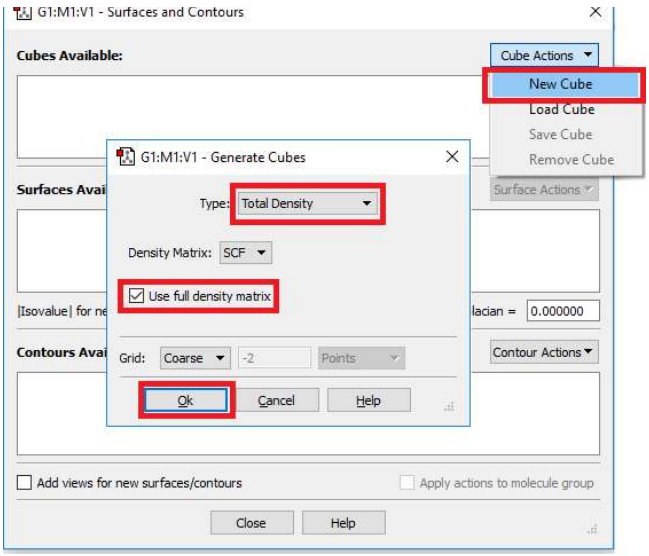
Extract Data

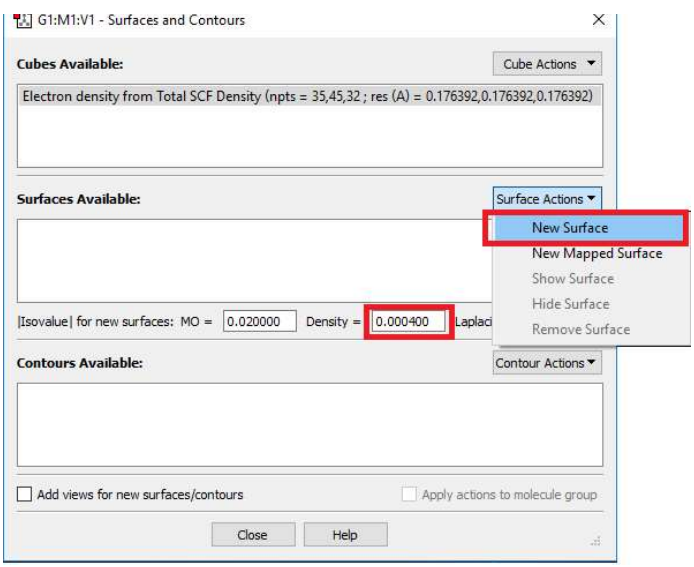
This analysis provides deformation density information of complex

Appendix 1

Visualization of Deformation Density by GaussView

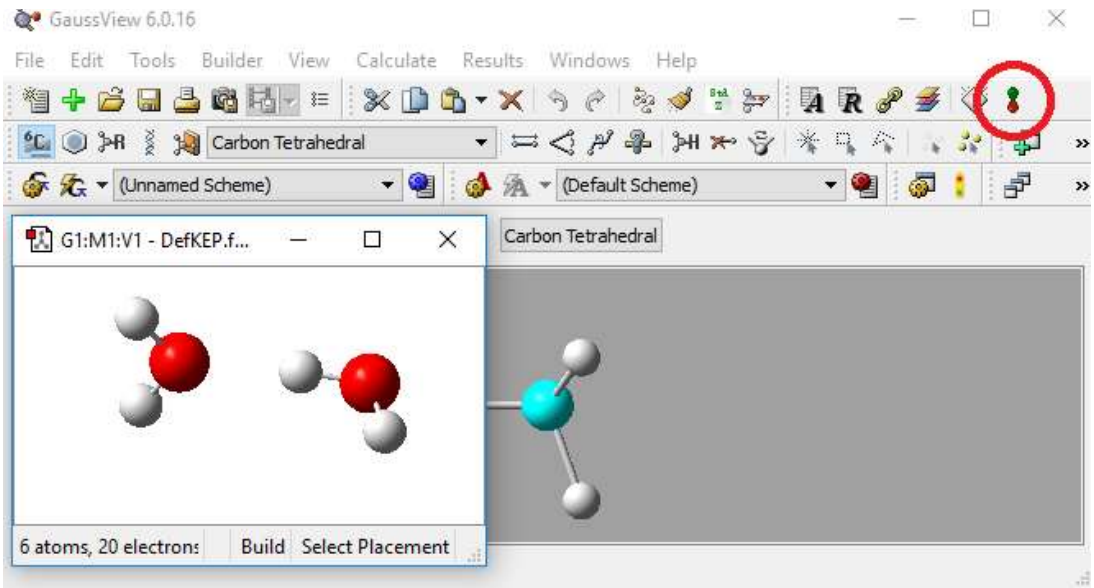


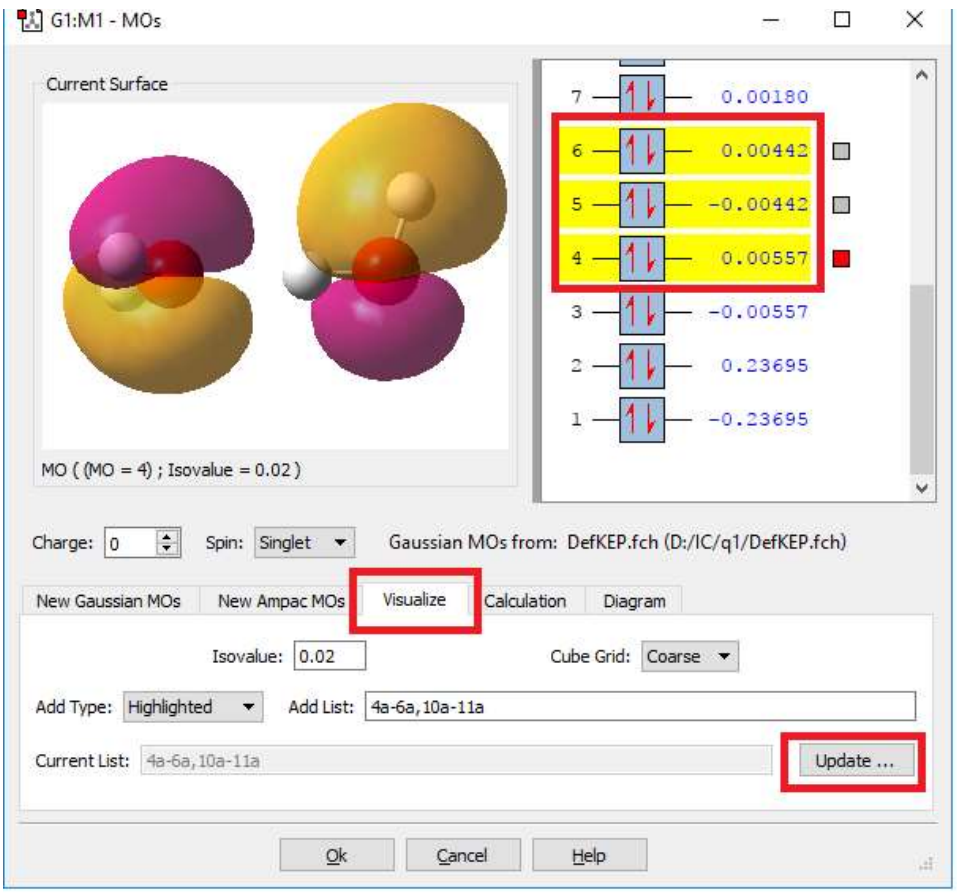




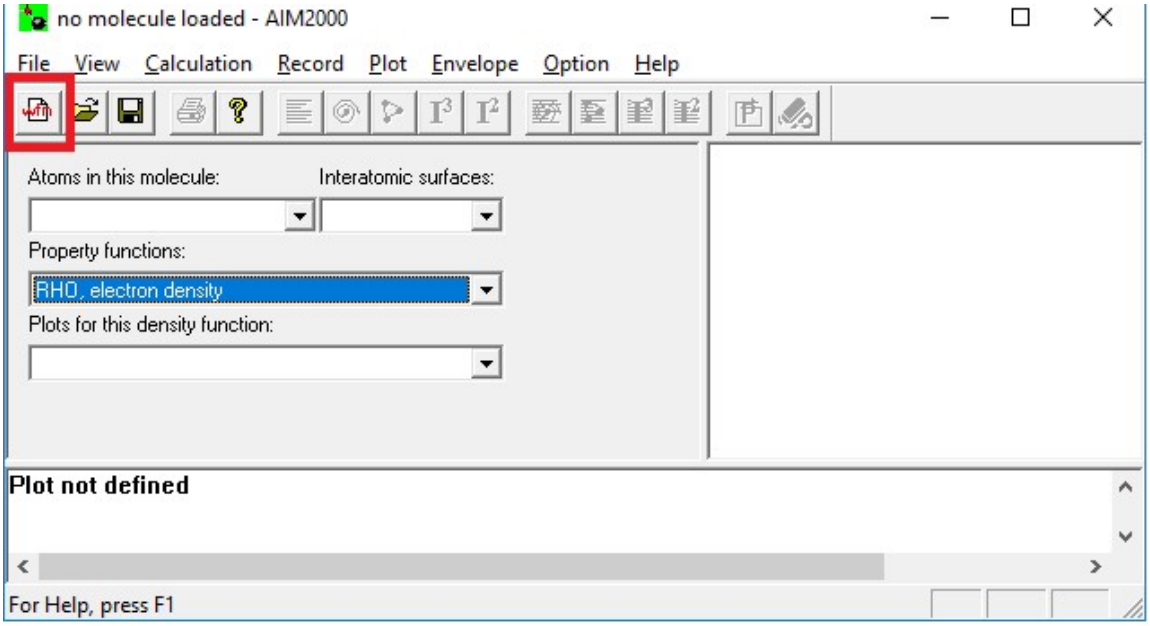
Appendix 2

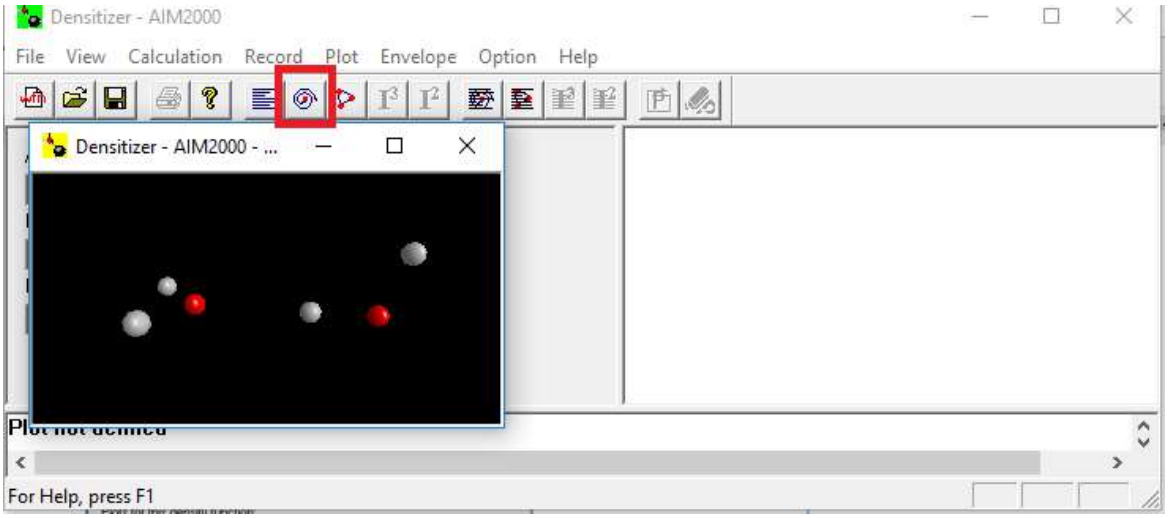
Visualization of Deformation Orbitals/NBOs/NLMOs by GaussView

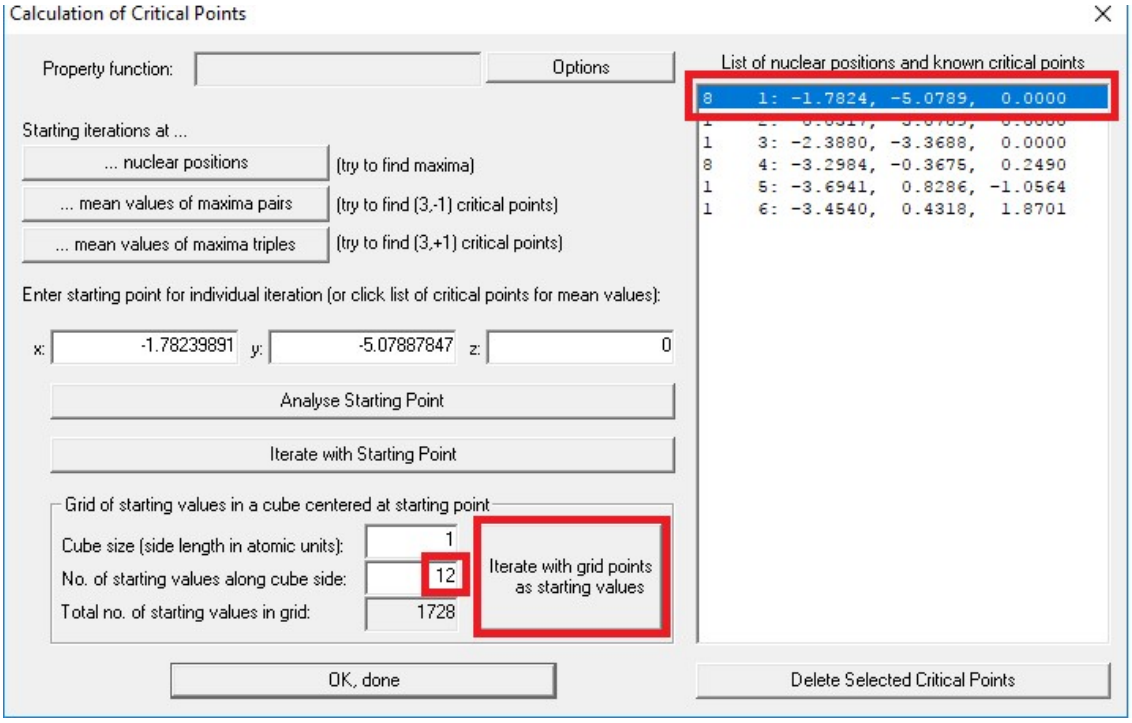


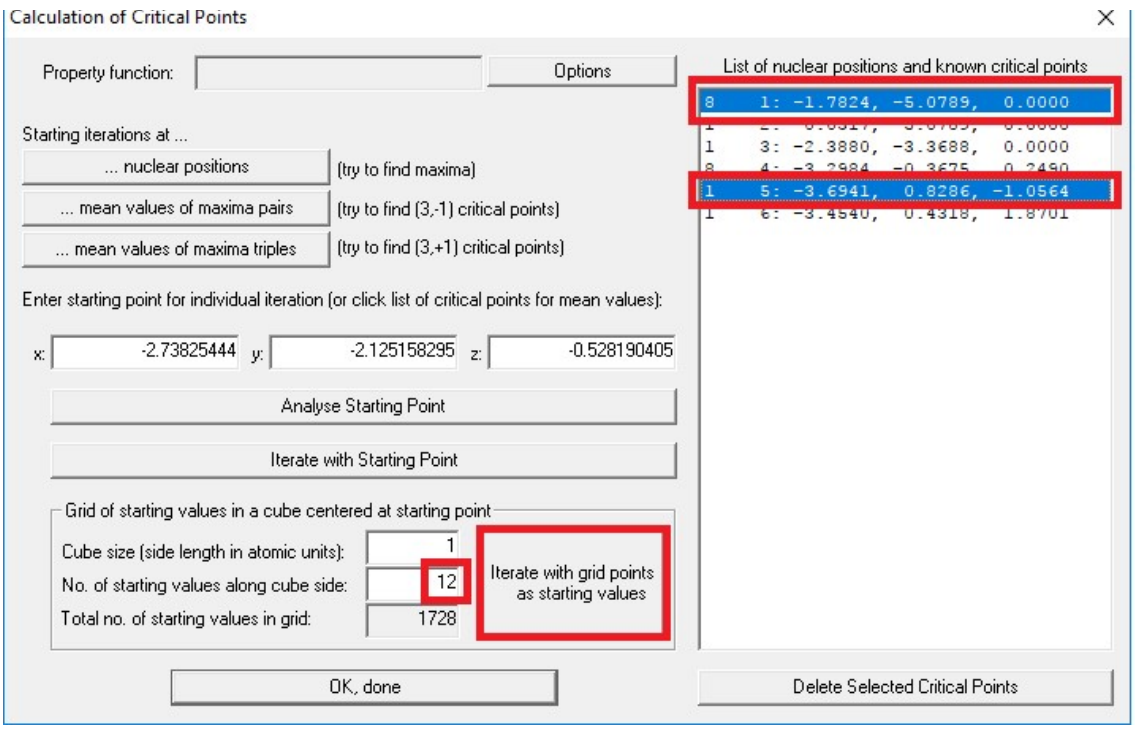


AIM2000: Topological analysis






Calculation of Critical Points
Property function:
Options
List of nuclear positions and known critical points
8 1: -1.7824, -5.0789, 0.0000
1 3: -2.3880, -3.3688, 0.0000
8 4: -3.2984, -0.3675, 0.2490
1 5: -3.6941, 0.8286, -1.0564
1 6: -3.4540, 0.4318, 1.8701
Starting iterations at ...
... nuclear positions
(try to find maxima)
... mean values of maxima pairs
(try to find (3,-1) critical points)
... mean values of maxima triples
(try to find (3,+1) critical points)
Enter starting point for individual iteration (or click list of critical points for mean values):
x: -1.78239891
y: -5.07887847
z: 0
Analyse Starting Point
Iterate with Starting Point
Grid of starting values in a cube centered at starting point
Cube size (side length in atomic units): 1
No. of starting values along cube side: 12
Total no. of starting values in grid: 1728
Iterate with grid points as starting values
OK, done
Delete Selected Critical Points


Calculation of Critical Points
Property function:
Options
List of nuclear positions and known critical points
8 1: -1.7824, -5.0789, 0.0000
1 3: -2.3880, -3.3688, 0.0000
1 5: -3.6941, 0.8286, -1.0564
Starting iterations at ...
... nuclear positions
(try to find maxima)
... mean values of maxima pairs
(try to find (3,-1) critical points)
... mean values of maxima triples
(try to find (3,+1) critical points)
Enter starting point for individual iteration (or click list of critical points for mean values):
x: -2.73825444
y: -2.125158295
z: -0.528190405
Analyse Starting Point
Iterate with Starting Point
Grid of starting values in a cube centered at starting point
Cube size (side length in atomic units): 1
No. of starting values along cube side: 12
Total no. of starting values in grid: 1728
Iterate with grid points as starting values
OK, done
Delete Selected Critical Points