

ORCA로 ESP계산하는 방법

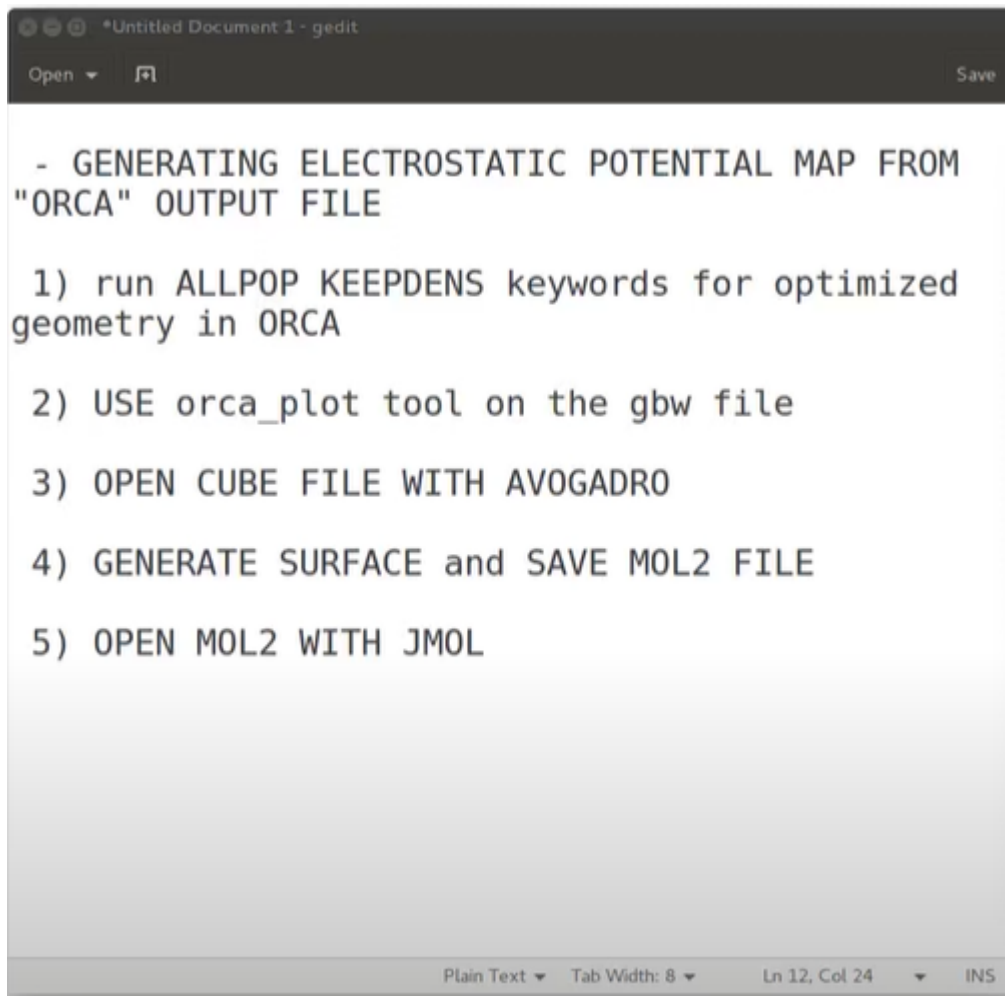
부제목 : 아닐린 화합물을 타겟으로 진행.

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ORCA ESP calc Process

과정 요약



```
*Untitled Document 1 - gedit
Open Save

- GENERATING ELECTROSTATIC POTENTIAL MAP FROM
"ORCA" OUTPUT FILE

1) run ALLPOP KEEPDENS keywords for optimized
geometry in ORCA

2) USE orca_plot tool on the gbw file

3) OPEN CUBE FILE WITH AVOGADRO

4) GENERATE SURFACE and SAVE MOL2 FILE

5) OPEN MOL2 WITH JMOl

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```

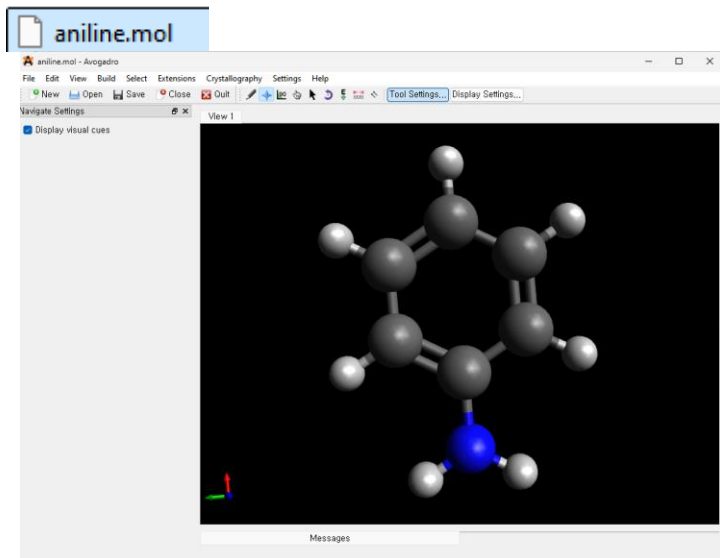
1. orca로 먼저 구조 파일을 최적화 한다.
ALLPOP / KEEPDENS 키워드를 사용해서 OPT계산을 진행한다.
2. orca_plot 명령으로 gpwfile을 처리
3. (2)번 과정에서 나온 .cube파일을 AVOGADRO를 통해 Open
4. Generate Surface 진행 및 .mol2 File로 save
5. jmol 소프트웨어에서 저장한 .mol2 File을 열고 ESP 확인

Step 1 : orca로 먼저 구조 파일을 최적화 한다.

구조 파일 확장자 변환 (.mol -> .xyz) 및 구조 최적화를 위한 orca .inp파일 만들기

1) 먼저 최적화할 구조 파일을 만들거나 가져와야 한다.

타겟으로 하는 물질을 pubchem3d와 같은 Database에서 찾아 구조파일을 얻는 방법이 가장 좋다.



위와 같이 Aniline물질의 .mol 3d구조 파일을 pubchem3d에서 다운받아 Avogadro 소프트웨어로 시각화 할 수 있다. 구조가 올바른 것을 확인했으므로 다음 단계로 진행한다.

2) 확장자 .xyz로 바꾸기

```
aniline.xyz
lsp32@celinux2:~$ obabel aniline.mol -O aniline.xyz
```

orca input을 만들기 위해 .xyz형식으로 변환한다

3) 확장자 .xyz로 바꾸기

ALLPOP / KEEPDENS 키워드를 사용해서 OPT DFT계산 인풋 파일을 만든다 (.inp)

```
C: > Users > PSID_PC_20 > Desktop > [00]Projects > [02]배터리DFT_KEIT
1  ! B3LYP def2-SVP OPT ALLPOP KEEPDENS
2
3  * xyz 0 1
4  N      -2.40460      0.00000      0.00050
5  C      -0.99410     -0.00020     -0.00030
6  C      -0.29690      1.20790     -0.00030
7  C      -0.29650     -1.20800     -0.00030
8  C       1.09800      1.20800      0.00010
9  C       1.09840     -1.20780      0.00010
10 C       1.79570      0.00020      0.00030
11 H      -0.82890      2.15580     -0.00030
12 H      -0.82830     -2.15610     -0.00020
13 H       1.64110      2.14860      0.00020
14 H       1.64170     -2.14820      0.00020
15 H       2.88180      0.00040      0.00060
16 H      -2.91090     -0.87550     -0.00050
17 H      -2.91070      0.87560     -0.00060
18  *
```

- B3LYP: DFT 계산을 위한 함수.
- def2-SVP: 기저 세트.
- OPT: 최적화 계산 수행.
- ALLPOP: 모든 전자 Population 분석 데이터를 출력.
- KEEPDENS: 계산 중 밀도를 유지.

* ALLPOP keyword

Output control			
NORMALPRINT	OUTPUT	PRINTLEVEL	Selects the normal output
MINIPRINT			Selects the minimal output
SMALLPRINT			Selects the small output
LARGEPRINT			Selects the large output
PRINTMOS	OUTPUT	Print[p.MOS]	Prints MO coefficients
NOPRINTMOS	OUTPUT		Suppress printing of MO coefficients
PRINTBASIS	OUTPUT	Print[p.basis]	Print the basis set in input format
PRINTGAP	OUTPUT	Print[p._homolumogap]	Prints the HOMO/LUMO gap in each SCF iteration. This may help to detect convergence problems
ALLPOP	OUTPUT	Print[...]	Turns on all population analysis
NOPOP			Turns off all population analysis

* KEEPDENS keyword

KEEPINTS	SCF	KEEPINTS	Keep two electron integrals on disk
NOKEEPINTS			Do not keep two electron integrals
KEEPDENS	SCF	KEEPDENS	Keep the density matrix on disk
NOKEEPDENS			Do not keep the density matrix
READINTS	SCF	READINTS	Reading of two electron integrals on
NOREADINTS			Reading of two electron integrals off
CHEAPINTS	SCF	USECHEAPINTS	Use the cheap integral feature in direct SCF calculations
NOCHEAPINTS			Turn that feature off

* 더 자세한 orca manual 자료 확인

https://www.afs.enea.it/software/orca/orca_manual_4_2_1.pdf

Step 1 : orca로 먼저 구조 파일을 최적화 한다.

|| orca를 이용한 구조 파일 최적화

1) orca input 파일을 orca로 실행한다

```
(base) [yongsang@ga04 20250120_A]$ orca aniline_opt.inp > aniline_opt.out
(base) [yongsang@ga04 20250120_A]$ ls
aniline_opt.bibtex      aniline_opt.densitiesinfo  aniline_opt.gbw  aniline_opt.opt  aniline_opt.property.txt  aniline_opt.xyz
aniline_opt.densities  aniline_opt.engrad         aniline_opt.inp  aniline_opt.out  aniline_opt_trj.xyz
```

** 구조 파일 복잡도에 따라 시간이 다소 걸릴 수 있다.

(시간을 단축하고자 한다면 Parallel 기능을 이용해보자 – manual 참조 <PAL키워드>)

orca_plot으로 gpwfile을 처리 > .cube파일 생성

다음 명령을 이용해 qbw파일을 처리한다

```
orca_plot aniline_opt.gbwh -i
```

아래와 같은 command line UI가 나오며 필요한 번호를 입력해 설정을 바꾼다.
ESP를 위한 설정은 다음 사진들을 따라오면 된다.

```

Entering interactive generation of plots ...
GBW-file      : aniline_opt.gbw
-----
... the gbw file was successfully read
... the default volumetric output format is Cube
... the output filenames are aniline_opt.moxy.plt
-----
NOTE: x=no of the MO to plot:
      y='a' for op=0 (spin up or closed shell)
      y='b' for op=1 (spin-down)
-----
=====
====>>> Number of available orbitals : 133
====>>> Number of operators          : 1
=====
Current-settings:

PlotType      ... MO-PLOT
MO/Operator   ... 0 0
Output file   ... (null)
Format        ... Grid3d/Cube
Resolution    ... 40 40 40
Boundaries     ... -12.509708      12.493060 (x direction)
               ... -11.085077      11.085020 (y direction)
               ... -7.005949       7.004756 (z direction)
-----
1 - Enter type of plot
2 - Enter no or orbital to plot
3 - Enter operator of orbital (0=alpha,1=beta)
4 - Enter number of grid intervals
5 - Select output file format
6 - Plot CIS/TD-DFT difference densities
7 - Plot CIS/TD-DFT transition densities
8 - Set A0(=1) vs MO(=0) to plot
9 - List all available densities
10 - Perform Density Algebraic Operations

11 - Generate the plot
12 - exit this program

Enter a number 1

```

```

Plot-Type is presently: 1
-----
Searching for Ground State Electron or Spin Densities:
-----
  1 - molecular orbitals
  2 - (scf) electron density ..... (scfp) ) => AVAILABLE
  3 - (scf) spin density ..... (scfr) ) - NOT AVAILABLE
  4 - natural orbitals
  5 - corresponding orbitals
  6 - atomic orbitals
  7 - mdc1 electron density ..... (mdc1p) ) - NOT AVAILABLE
  8 - mdc1 spin density ..... (mdc1r) ) - NOT AVAILABLE
  9 - 00-RI-MP2 density ..... (pmp2re) ) - NOT AVAILABLE
 10 - 00-RI-MP2 spin density ..... (pmp2ur) ) - NOT AVAILABLE
 11 - MP2 relaxed density ..... (pmp2re) ) - NOT AVAILABLE
 12 - MP2 unrelaxed density ..... (pmp2ur) ) - NOT AVAILABLE
 13 - MP2 relaxed spin density ..... (pmp2re) ) - NOT AVAILABLE
 14 - MP2 unrelaxed spin density ..... (pmp2ur) ) - NOT AVAILABLE
 15 - LED dispersion interaction density ..... (ded21) ) - NOT AVAILABLE
 16 - Atom pair density
 17 - Shielding Tensors
 18 - Polarizability Tensor
 19 - AutoCI relaxed density ..... (autoc1pr) ) - NOT AVAILABLE
 20 - AutoCI unrelaxed density ..... (autoc1ur) ) - NOT AVAILABLE
 21 - AutoCI relaxed spin density ..... (autoc1re) ) - NOT AVAILABLE
 22 - AutoCI unrelaxed spin density ..... (autoc1ur) ) - NOT AVAILABLE
-----
Searching for State or Transition State AO Electron Densities:
-----
 23 - CIS unrelaxed transition AO density ..... (Tdens-CIS) ) - NOT AVAILABLE
 24 - ROCIS unrelaxed transition AO density ..... (Tdens-ROCIS) ) - NOT AVAILABLE
 25 - CAS unrelaxed transition AO density ..... (Tdens-CAS) ) - NOT AVAILABLE
 26 - ICE unrelaxed transition AO density ..... (Tdens-ICE) ) - NOT AVAILABLE
 27 - MC1 unrelaxed transition AO density ..... (Tdens-MC1) ) - NOT AVAILABLE
 28 - LFT unrelaxed transition AO density ..... (Tdens-LFT) ) - NOT AVAILABLE
-----
Searching for State or Transition State MO Electron Densities:
-----
 29 - CIS unrelaxed transition MO density ..... (Tdens-CISMO) ) - NOT AVAILABLE
 30 - ROCIS unrelaxed transition MO density ..... (Tdens-ROCISMO) ) - NOT AVAILABLE
 31 - CAS unrelaxed transition MO density ..... (Tdens-CASMO) ) - NOT AVAILABLE
 32 - ICE unrelaxed transition MO density ..... (Tdens-ICEMO) ) - NOT AVAILABLE
 33 - MC1 unrelaxed transition MO density ..... (Tdens-MC1MO) ) - NOT AVAILABLE
 34 - LFT unrelaxed transition MO density ..... (Tdens-LFTMO) ) - NOT AVAILABLE
-----
Searching for State or Transition State QDPT AO Electron Densities:
-----
 35 - CAS QDPT unrelaxed transition AO density ..... (Tdens-CASQDSC) ) - NOT AVAILABLE
 36 - DDCAS QDPT unrelaxed transition AO density ..... (Tdens-CASQDQDSC) ) - NOT AVAILABLE
 37 - CAS CUSTOM QDPT unrelaxed transition AO density ..... (Tdens-CASCUSTOMQDSC) ) - NOT AVAILABLE
 38 - NEVP72 QDPT unrelaxed transition AO density ..... (Tdens-CASQPTQDSC) ) - NOT AVAILABLE
 39 - QDNEVP72 QDPT unrelaxed transition AO density ..... (Tdens-CASQDPTQDSC) ) - NOT AVAILABLE
 40 - MC1 QDPT unrelaxed transition AO density ..... (Tdens-MC1QDSC) ) - NOT AVAILABLE
 41 - ROCIS QDPT unrelaxed transition AO density ..... (Tdens-ROCISQDSC) ) - NOT AVAILABLE
 42 - LFT QDPT unrelaxed transition AO density ..... (Tdens-LFTQDSC) ) - NOT AVAILABLE
-----
Enter Type: 2

```

```
Current-settings:

PlotType      ... DENSITY-PLOT
ElDens File   ... aniline_opt.scfp
Output file    ... MyElDens
Format        ... Grid3d/Cube
Resolution    ... 40 40 40
Boundaries     ... -12.509708    12.493060 (x direction)
               ... -11.085077    11.085020 (y direction)
               ... -7.005949     7.004756 (z direction)

1 - Enter type of plot
2 - Enter no of orbital to plot
3 - Enter operator of orbital (0=alpha,1=beta)
4 - Enter number of grid intervals
5 - Select output file format
6 - Plot CIS/TD-DFT difference densities
7 - Plot CIS/TD-DFT transition densities
8 - Set A0(=1) vs MO(=0) to plot
9 - List all available densities
10 - Perform Density Algebraic Operations

11 - Generate the plot
12 - exit this program

Enter a number: 4
Enter NGRID: 80
```

Step 2: orca_plot 명령으로 gpwfile을 처리

|| orca_plot으로 gpwfile을 처리 > .cube파일 생성

...이어서

```
Current-settings:
PlotType      ... DENSITY-PLOT
ElDens File   ... aniline_opt.scfp
Output file    ... MyElDens
Format        ... Grid3d/Cube
Resolution    ... 80 80 80
Boundaries    ... -12.509708 12.493060 (x direction)
               ... -11.085077 11.085020 (y direction)
               ... -7.005949  7.004756 (z direction)

1 - Enter type of plot
2 - Enter no of orbital to plot
3 - Enter operator of orbital (0=alpha,1=beta)
4 - Enter number of grid intervals
5 - Select output file format
6 - Plot CIS/TD-DFT difference densities
7 - Plot CIS/TD-DFT transition densities
8 - Set A0(=1) vs M0(=0) to plot
9 - List all available densities
10 - Perform Density Algebraic Operations

11 - Generate the plot
12 - exit this program
Enter a number: 5
```

```
Enter a number: 5
File-Format is presently: 7
1 - 2D  Origin format
2 - 2D  HPGL format
3 - 2D  Gnuplot binary format
4 - 2D  Gnuplot ascii format
5 - 3D  Grid data binary (Fortran number format!)
6 - 3D  Grid data ASCII
7 - 3D  Gaussian cube
8 - 3D  simple format
Enter Format: 7
```

```
Current-settings:
PlotType      ... DENSITY-PLOT
ElDens File   ... aniline_opt.scfp
Output file    ... MyElDens
Format        ... Grid3d/Cube
Resolution    ... 80 80 80
Boundaries    ... -12.509708 12.493060 (x direction)
               ... -11.085077 11.085020 (y direction)
               ... -7.005949  7.004756 (z direction)

1 - Enter type of plot
2 - Enter no of orbital to plot
3 - Enter operator of orbital (0=alpha,1=beta)
4 - Enter number of grid intervals
5 - Select output file format
6 - Plot CIS/TD-DFT difference densities
7 - Plot CIS/TD-DFT transition densities
8 - Set A0(=1) vs M0(=0) to plot
9 - List all available densities
10 - Perform Density Algebraic Operations

11 - Generate the plot
12 - exit this program
Enter a number: 11
```

```
Calling PlotGrid3d with ATOM=A,B=0,0
Entering PlotGrid3d with Plottype =2
*** PLOTTING FINISHED ***
Output file: aniline_opt.eldens.cube
-----
Current-settings:
PlotType      ... DENSITY-PLOT
ElDens File   ... aniline_opt.scfp
Output file    ... aniline_opt.eldens.cube
Format        ... Grid3d/Cube
Resolution    ... 80 80 80
Boundaries    ... -12.509708 12.493060 (x direction)
               ... -11.085077 11.085020 (y direction)
               ... -7.005949  7.004756 (z direction)

1 - Enter type of plot
2 - Enter no of orbital to plot
3 - Enter operator of orbital (0=alpha,1=beta)
4 - Enter number of grid intervals
5 - Select output file format
6 - Plot CIS/TD-DFT difference densities
7 - Plot CIS/TD-DFT transition densities
8 - Set A0(=1) vs M0(=0) to plot
9 - List all available densities
10 - Perform Density Algebraic Operations

11 - Generate the plot
12 - exit this program
Enter a number: 12
```

Step 2: orca_plot 명령으로 gpwfile을 처리

|| orca_plot으로 gpwfile을 처리 > .cube파일 생성

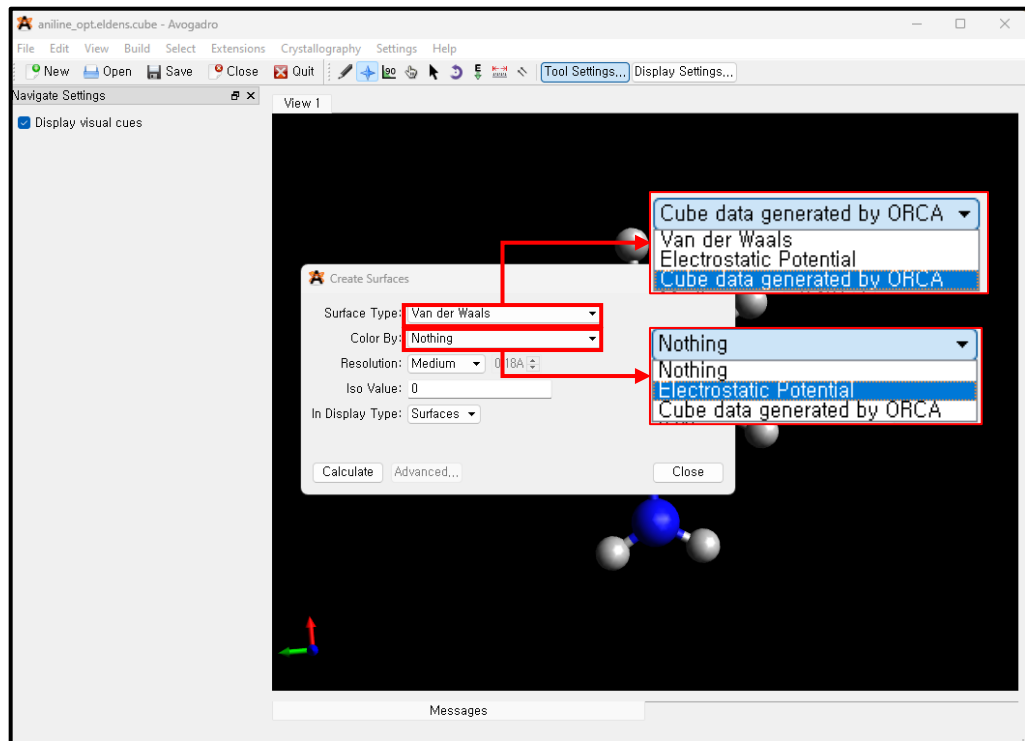
위 과정을 잘 따랐다면 아래와 같이 .cube파일이 있을 것이다.

```
(base) [yongsang@ga04 a]$ ls -l
total 8840
-rw-rw-r-- 1 yongsang yongsang 3372 2025-01-20 10:26 aniline_opt.bibtex
-rw-rw-r-- 1 yongsang yongsang 283024 2025-01-20 10:26 aniline_opt.densities
-rw-rw-r-- 1 yongsang yongsang 1838 2025-01-20 10:26 aniline_opt.densities.info
-rw-rw-r-- 1 yongsang yongsang 7258576 2025-01-20 10:49 aniline_opt.eldens.cube
-rw-rw-r-- 1 yongsang yongsang 1747 2025-01-20 10:26 aniline_opt.engrad
-rw-rw-r-- 1 yongsang yongsang 1145200 2025-01-20 10:26 aniline_opt.gbw
-rw-rw-r-- 1 yongsang yongsang 758 2025-01-20 10:25 aniline_opt.inp
-rw-rw-r-- 1 yongsang yongsang 22547 2025-01-20 10:26 aniline_opt.opt
-rw-rw-r-- 1 yongsang yongsang 229699 2025-01-20 10:26 aniline_opt.out
-rw-rw-r-- 1 yongsang yongsang 56829 2025-01-20 10:26 aniline_opt.property.txt
-rw-rw-r-- 1 yongsang yongsang 4314 2025-01-20 10:26 aniline_opt_trj.xyz
-rw-rw-r-- 1 yongsang yongsang 1111 2025-01-20 10:26 aniline_opt.xyz
-rw-rw-r-- 1 yongsang yongsang 11644 2025-01-20 10:41 out.out
```

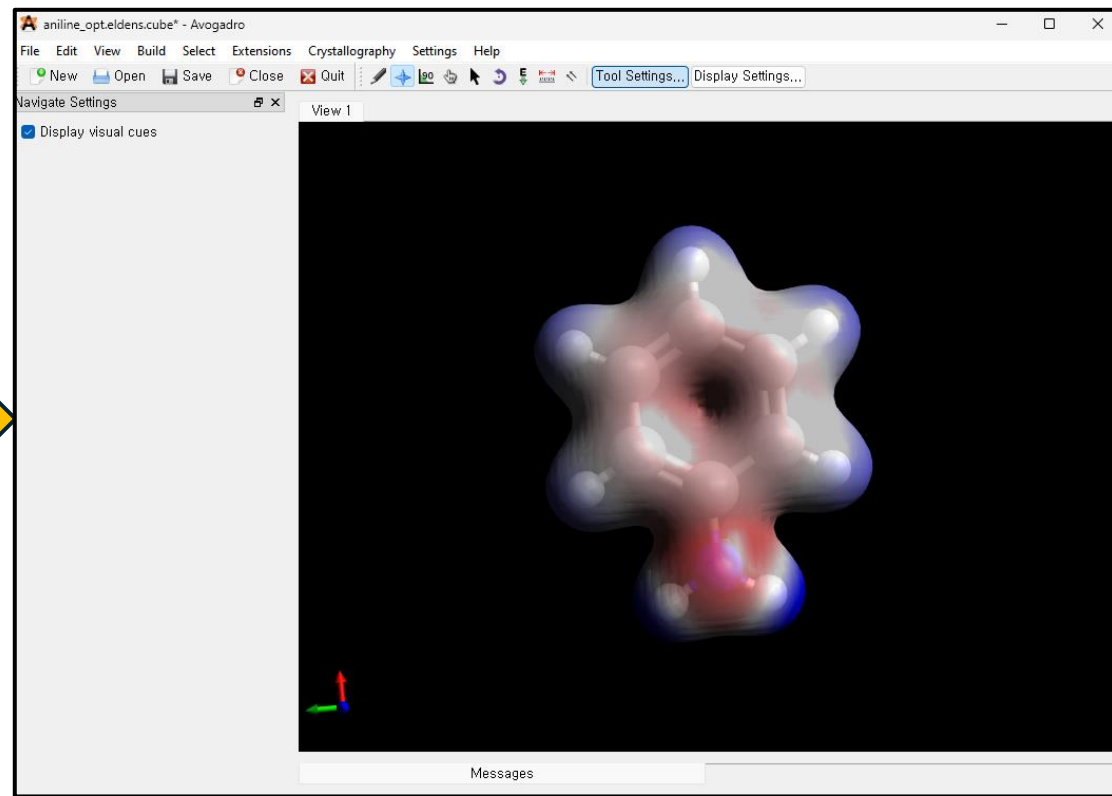
Step 3 & 4 : .cube파일을 AVOGADRO를 통해 Open

Avogadro를 통해 Open & Create Surfaces 진행

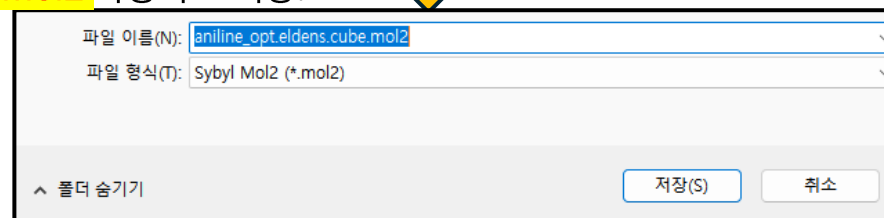
Avogadro로 .cube를 열고 상단리본 > Extensions > **Create Surfaces** 선택



위와 같은 화면이 나올것이다.



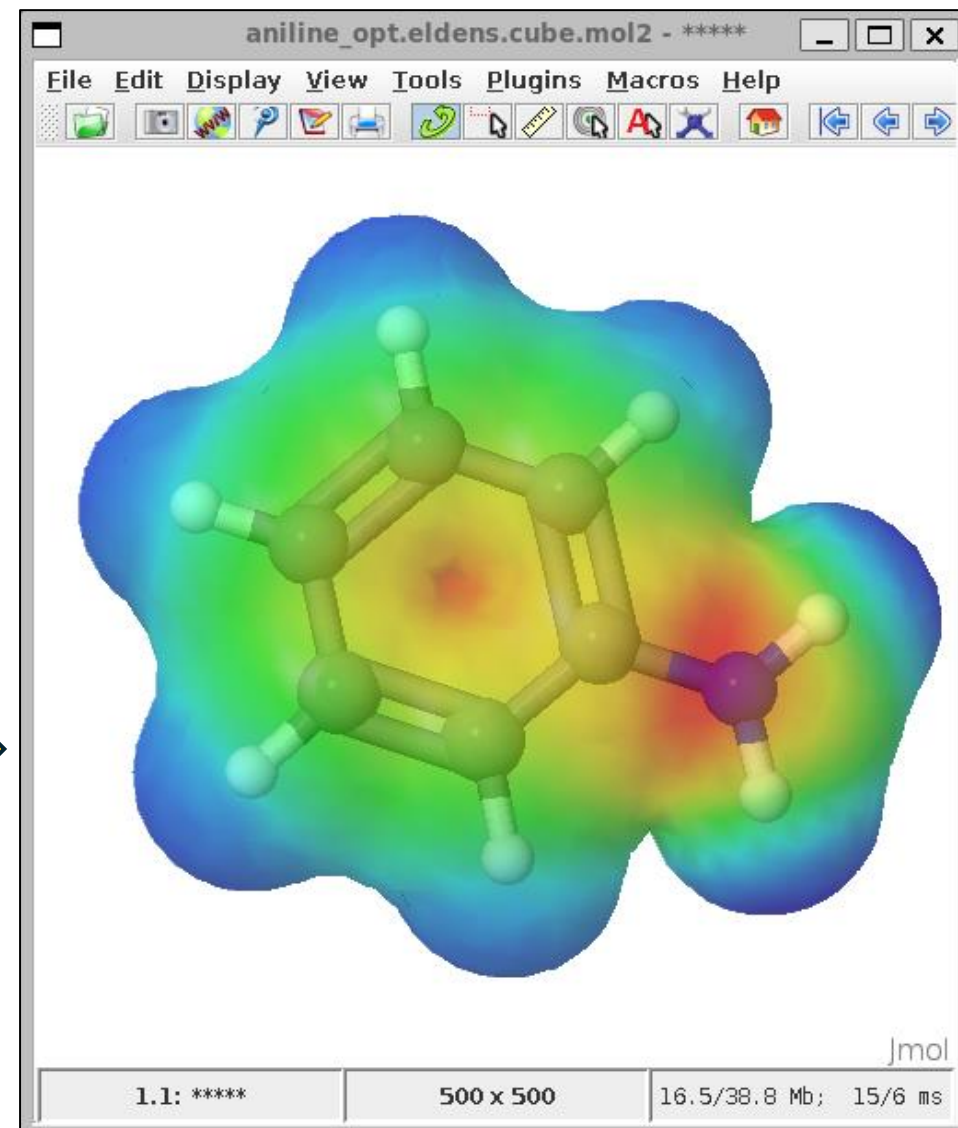
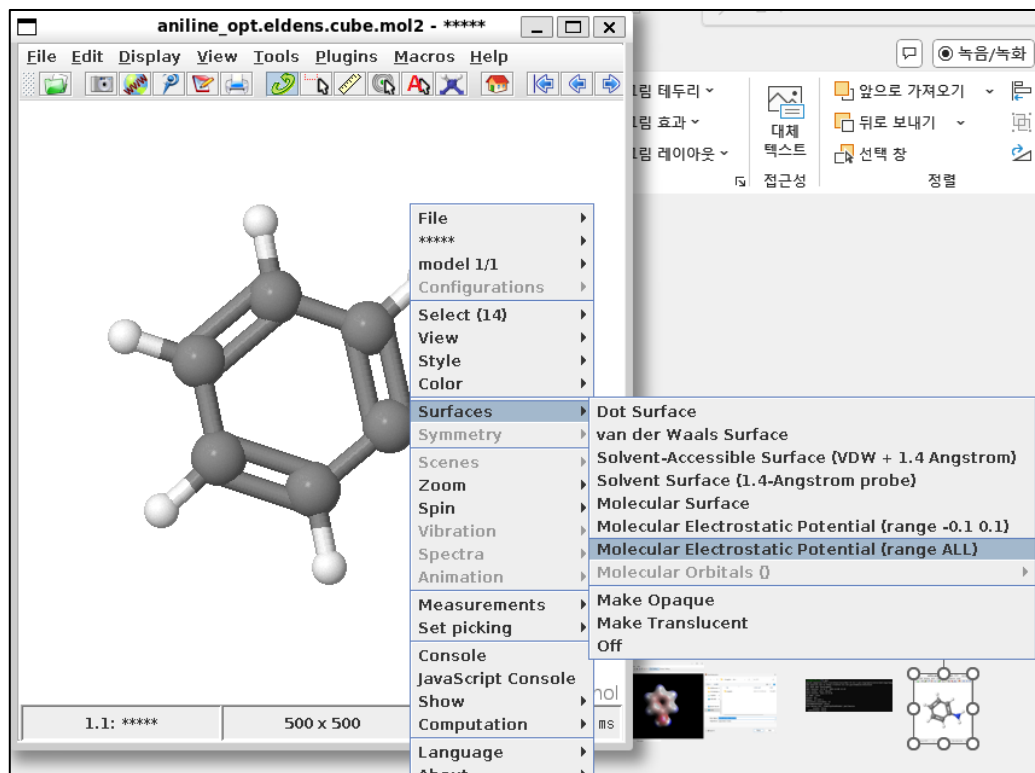
그리고 **.mol2** 확장자로 저장!



Step 5: jmol 소프트웨어에서 저장한 .mol2 File을 열고 ESP 확인

jmol 소프트웨어로 ESP그리기

```
lsp32@celinux2:~$ jmol
splash_image=jar:file:/usr/share/java/Jmol-14.32.3.jar!/org/openscience/jmol/app/imag
CIR resolver set to https://cactus.nci.nih.gov/chemical/structure
(C) 2015 Jmol Development
Jmol Version: 14.32.3 2021-12-08 13:29
java.vendor: Java: Ubuntu
java.version: Java 11.0.25
os.name: Linux
Access: ALL
memory: 23.3/67.1
processors available: 12
useCommandThread: false
User macros dir: /home/dydtkddhkdwk/.jmol/macros
exists: false
isDirectory: false
```



참고 자료

유튜브 영상

<https://www.youtube.com/watch?v=jEpUQZiVOUw>

참고 글

<https://www.henriquecastro.info/2022/03/17/plotting-molecular-electrostatic-potential-surfaces-meps-with-orca/>