ORCA로 ESP계산하는 방법

부제목 : 아닐린 화합물을 타겟으로 진행.

작성일자 : 2025 01 20

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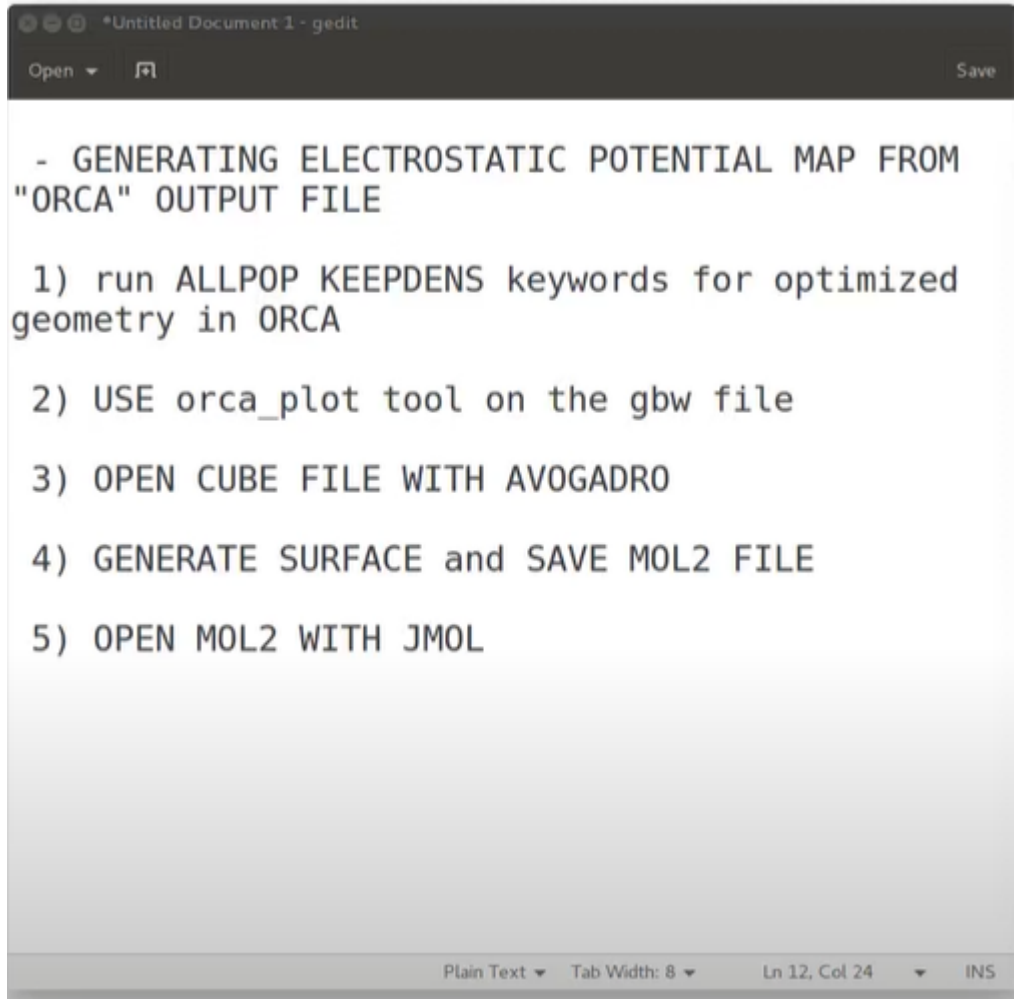
ORCA ESP calc Process

과정 요약



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

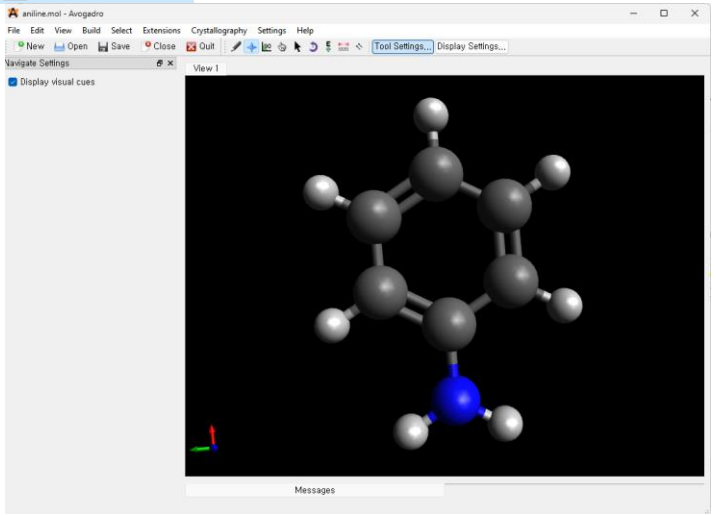
Step 1 : orca로 먼저 구조 파일을 최적화 한다.

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.

aniline.mol



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 populaton 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 자세한건 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>)

Step 2: orca_plot 명령으로 gpwfile을 처리

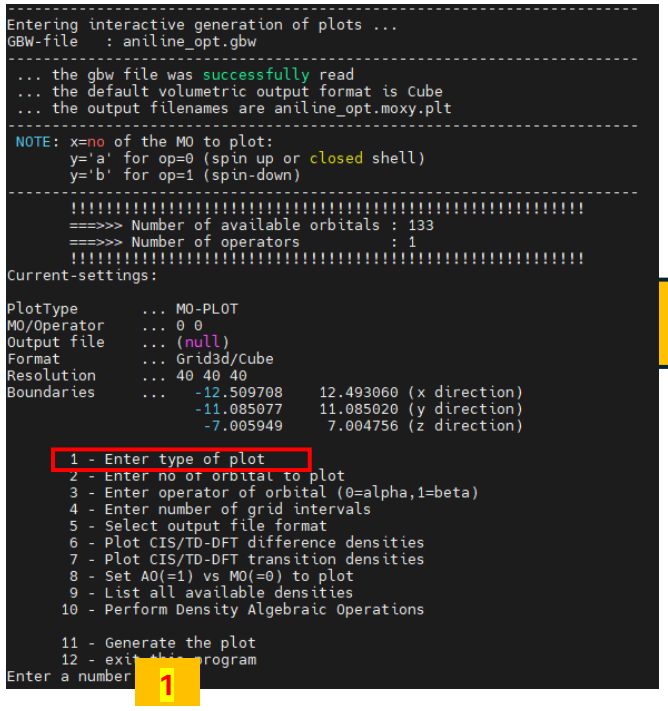
orca_plot으로 gpwfile을 처리 > .cube파일 생성

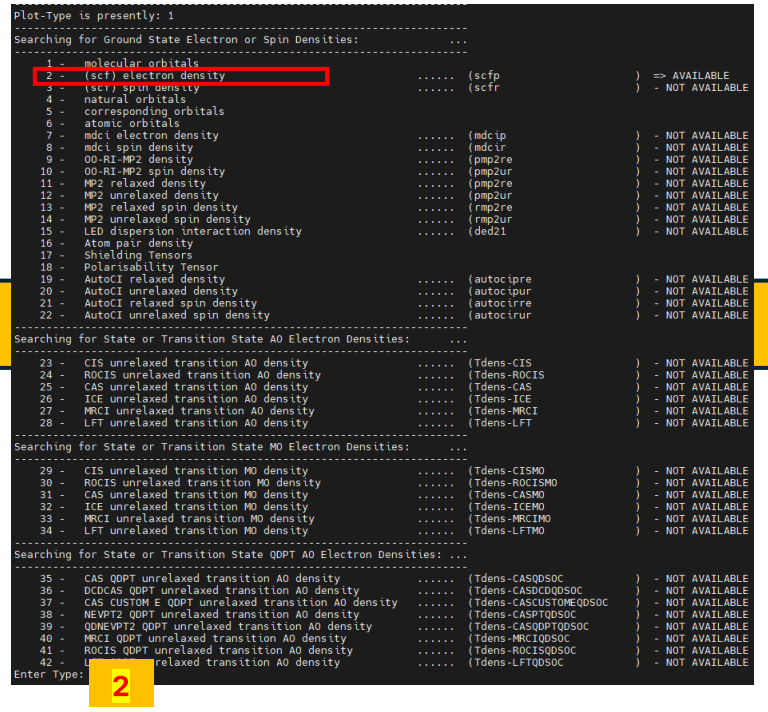
1) orca_plot 명령을 이용한 .cube 파일 생성

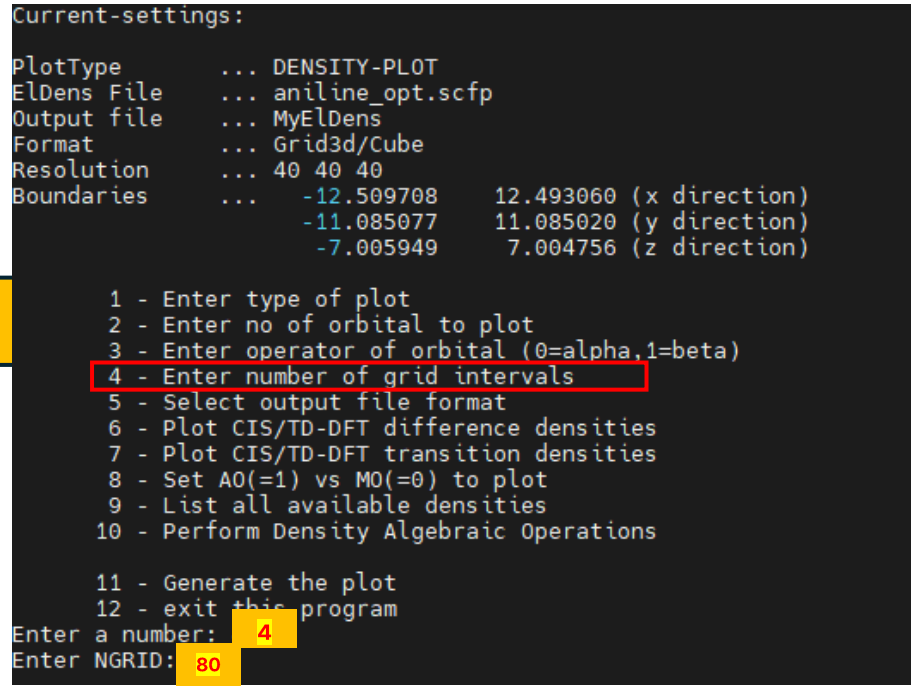
다음 명령을 이용해 gbw파일을 처리한다

```
orca_plot aniline_opt.gbw -i
```

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







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 AO(=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: 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 AO(=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: 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 AO(=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 12
```

Step 2: orca_plot 명령으로 gpwfile을 처리

orca_plot으로 gpwfile을 처리 > .cube파일 생성

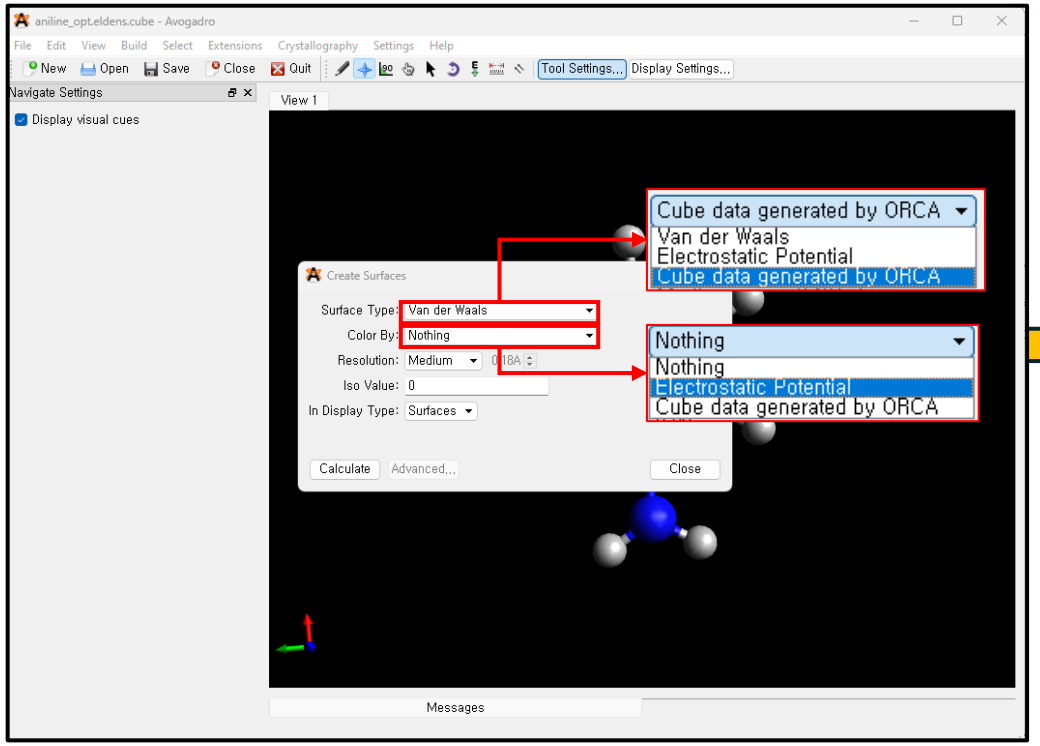
위 과정을 잘 따랐다면 아래와 같이 .cube파일이 있을 것이다.

```
(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.densitiesinfo
-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
```

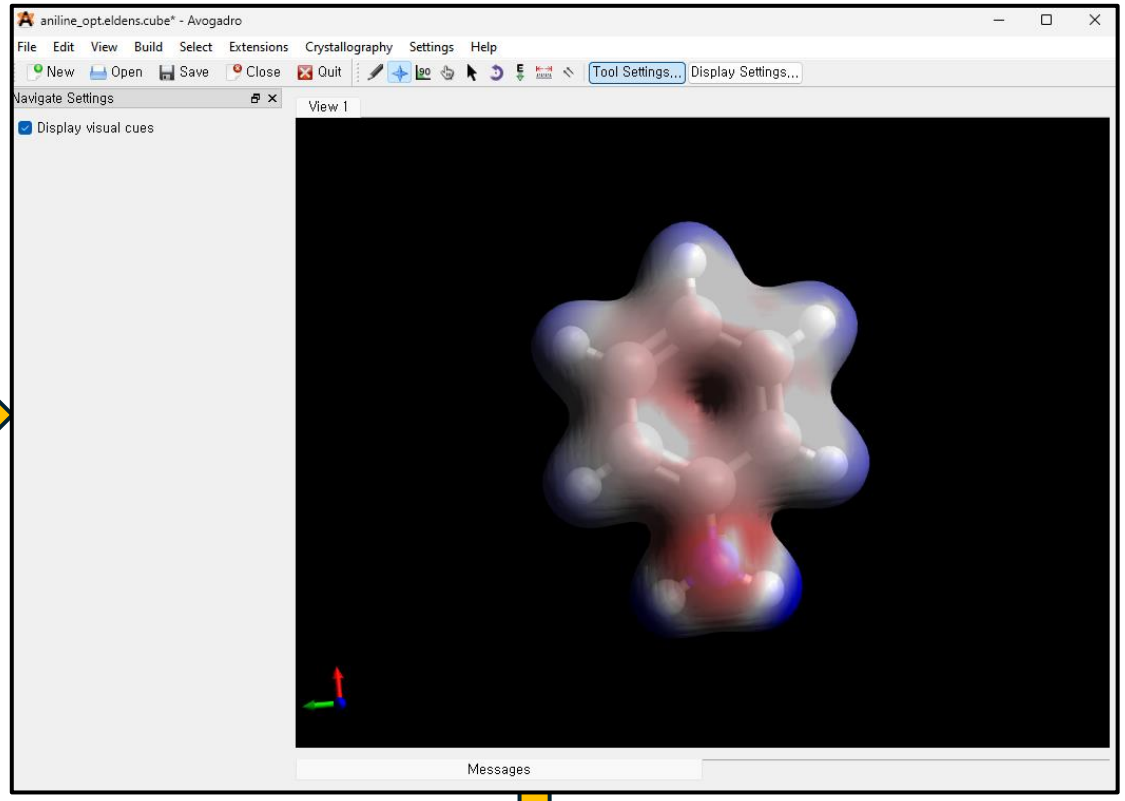
Step 3 & 4 : .cube파일을 AVOGADRO를 통해 Open

Avogadro를 통해 Open & Create Surfaces 진행

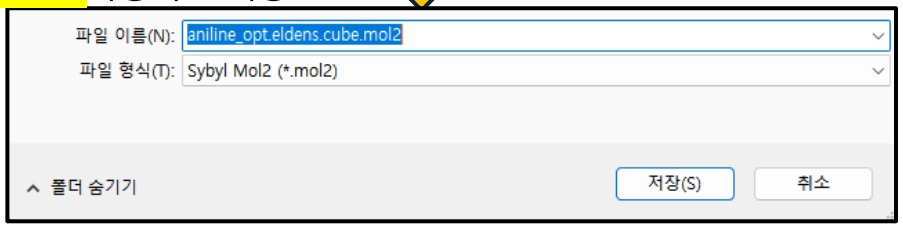
Avogadro로 .cube를 열고 상단리본 > Extensions > Create Surfaces 선택



위와 같은 화면이 나올것이다.



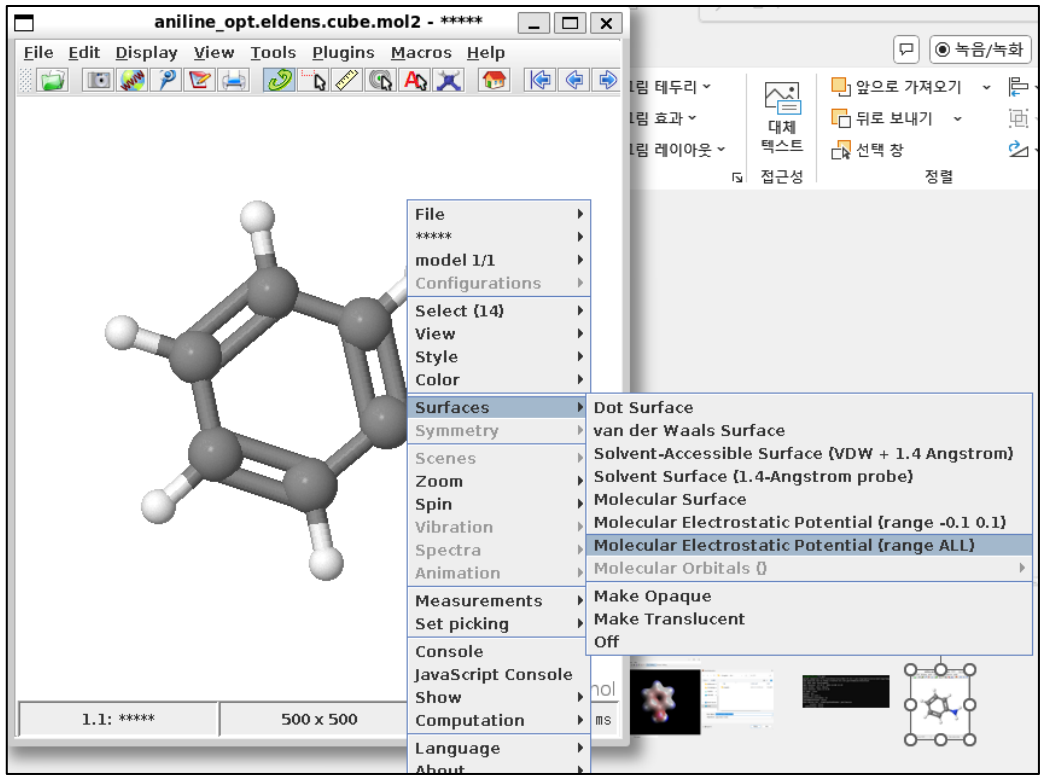
그리고 .mol2 확장자로 저장!

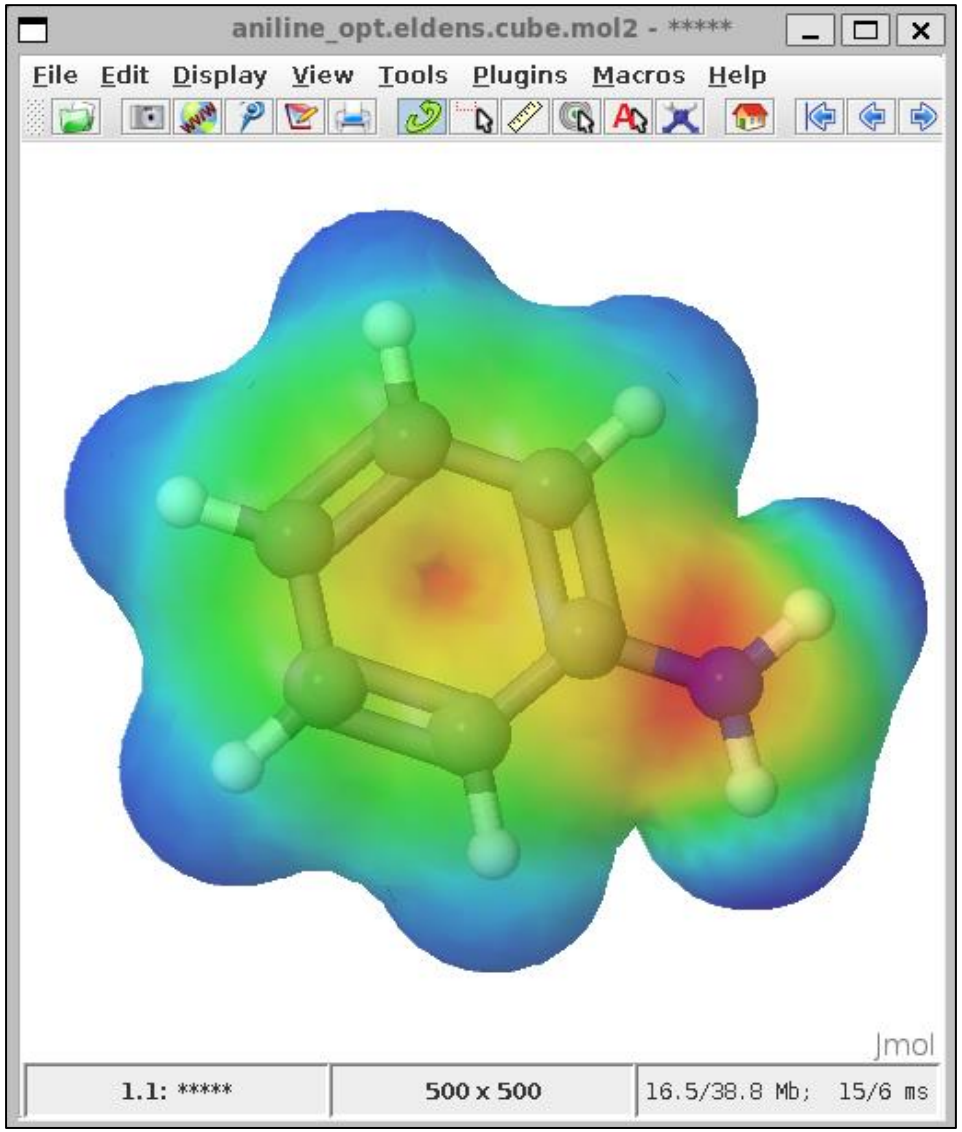


Step 5: jmol 소프트웨어에서 저장한 .mol2 File을 열고 ESP 확인

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

유투브 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/