

C60-malonic ester 구조 제작

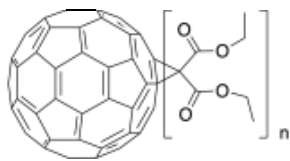
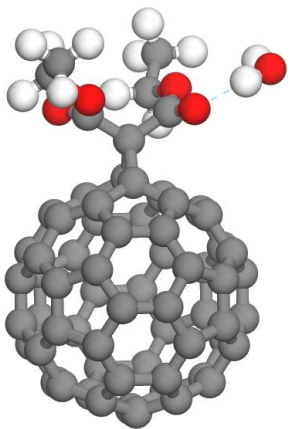
부제목 : 3d Structure DB에서 구조 파일 가져와서 진행하기

작성일자 : 2025 01 21

작성자 : 안용상

실험 개요

실험 배경



C60-malonic ester derivative

KETI 황치현 박사님에게 C60-malonic ester를 대상으로한 몇 가지 양자화학 계산 작업을 받았다. 해야할 작업들은 다음과 같다.

1. C60-malonic ester에 슈퍼_옥사이드 라디칼을 여러 흡착사이트에 붙여보며 흡착에너지를 확인하는 것
2. HOMO와 LUMO를 구하는 것

이를 달성하기 위해 가장 먼저 필요한 것은 C60-malonic ester의 구조 파일이다.

이를 만드는 것이 이번 실험의 목적이다.

간략한 실험 목적 및 계획

C60-malonic ester의 구조 파일을 만드는 것이 이번 실험의 목적이다.

3D 에디터로 비슷하게 만들 수 있지만 반드시 구조 최적화가 필요하다.


이번 실험의 목적은 구조 최적화가 완료된 C60 - malonic ester를 구하고, 가능한 계산량이라면 전자밀도 계산과 함께 ESP도 확인한다

1. 초기 구조 파일 준비:
2. 구조 러프하게 합치기:
3. 파일 변환:
4. 구조 최적화 by Orca:
5. orca_plot으로 .gbw파일 처리 후 .cube파일 생성
6. Generate Surface
7. Jmol로 ESP 확인

목표 아웃풋

확장자	설명
.gbw	orca output중 하나
.xyz	최종 구조 최적화 완료된 구조 파일
.cube	ESP 정보가 담긴 파일
.mol2	jmol로 ESP를 보기위한 파일

풀러렌 구하기 (chemtube3d)



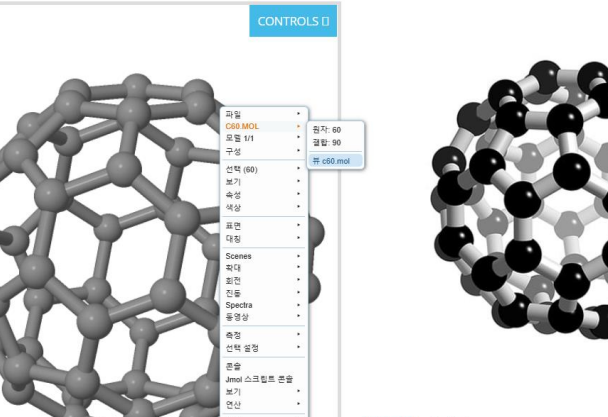
ChemTube3D

fullerene

Home Organic Inorganic Structure and Bonding A Level Polymers 360° Lab Safety News Periodic Table

ChemTube3D contains interactive 3D chemistry animations and structures, with supporting information, for students studying some of the most important topics in advanced school chemistry and university

C₆₀ – Buckminsterfullerene



CONTROLS

- 파일
- C60 MOL
- 모형 1/1
- 구성
- 선택 (60)
- 보기
- 축소
- 확대
- 회전
- 이동
- Spectra
- 물결장
- 속성
- 선택 설정
- 문열
- Jmol 스크립트 불러오기
- 보기
- 연산
- 언어
- 정보...

원자: 60
결합: 90
[C60 mol]

★★★★★ 4,4 (66)

How useful was this page?

The screenshot displays the Avogadro molecular editor interface. The title bar indicates the file is 'c60 (2).mol'. The menu bar includes File, Edit, View, Build, Select, Extensions, Crystallography, Settings, and Help. The toolbar contains icons for New, Open, Save, Close, Quit, and various navigation tools. The left sidebar shows 'Navigate Settings' and a checked 'Display visual cues' option. The main 3D view, labeled 'View 1', shows a complex organic molecule with a central cage-like structure and several side chains, rendered in a ball-and-stick model. A small 3D coordinate system is visible in the bottom left of the view. A 'Messages' panel is located at the bottom of the interface.


malonic ester 구하기 (pubchem 3d)

SEARCH FOR

malonic ester

Treating this as a text search.

BEST MATCH



DIETHYL MALONATE; 105-53-3; Diethyl propanedioate; Ethyl malonate; Propanedioic acid, diethyl ester; Carbethoxyacetic ester; Dicarbethoxymethane; ...

Compound CID: 7761

컴파운드 ID (PubChem ID)

MF: C₇H₁₂O₄ MW: 160.17g/mol

IUPAC Name: diethyl propanedioate

SMILES: CCOC(=O)CC(=O)OCC

InChIKey: IYXGSMUGOJNHAAZ-UHFFFAOYSA-N

InChI: InChI=1S/C7H12O4/c1-3-10-6(8)5-7(9)11-4-2/h3-5H2,1-2H3

Create Date: 2005-03-26

Summary

Similar Structures Search

Related Records

Index of /pubchem/Compounds			Index of /pubchem/Compounds		
Name	Last modified	Size	Name	Last modified	Size
Parent Directory		-	Parent Directory		-
DI_conf_per_cmpd/	2017-06-19 11:23	-	ASN/	2024-12-20 06:14	-
IO_conf_per_cmpd/	2016-04-11 11:22	-	SDF/	2024-12-20 06:14	-
FP/	2019-04-17 12:29	-	XML/	2024-12-20 06:14	-
ReferenceShapes/	2019-04-17 12:36	-	00000001_00025000.asn.gz	2017-06-19 11:23	21M
neighbors_3d/	2024-08-21 15:32	-	README	2016-04-11 11:22	3.5K
presentations/	2010-01-05 11:09	-			
README	2024-09-16 12:09	2.0K			
Release_notes.txt	2024-09-16 12:20	8.1K			
HHS Vulnerability Disclosure			HHS Vulnerability Disclosure		

malonic ester는 7761번

```

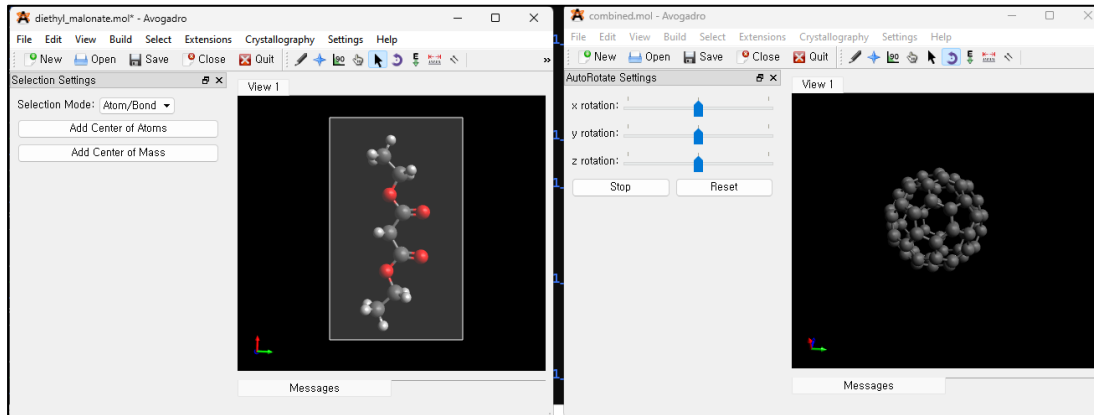
1661720      10
1661721
1661722      $$$$
1661723      7761
1661724      -OEChem-12192413473D
1661725
1661726      23  22  0      0      0      0      0      0  0999  V2000
1661727      -2.3374      -0.5665      -0.0040 O      0      0      0      0      0      0      0      0      0      0
1661728      -2.3373      -0.5664      -0.0022 O      0      0      0      0      0      0      0      0      0      0
1661729      -1.3628      1.5229      0.0003 O      0      0      0      0      0      0      0      0      0      0
1661730      -1.3629      1.5227      0.0033 O      0      0      0      0      0      0      0      0      0      0
1661731      0.0000      -0.4942      -0.0151 C      0      0      0      0      0      0      0      0      0      0
1661732      3.6346      0.0385      0.0069 C      0      0      0      0      0      0      0      0      0      0
1661733      -3.6346      0.0385      0.0062 C      0      0      0      0      0      0      0      0      0      0
1661734      1.2817      0.3027      -0.0061 C      0      0      0      0      0      0      0      0      0      0
1661735      -1.2818      0.3027      -0.0028 C      0      0      0      0      0      0      0      0      0      0
1661736      4.6864      -1.0504      0.0079 C      0      0      0      0      0      0      0      0      0      0
1661737      -4.6863      -1.0505      0.0057 C      0      0      0      0      0      0      0      0      0      0
1661738      -0.0011      -1.1888      -0.9222 H      0      0      0      0      0      0      0      0      0      0
1661739      0.0011      -1.1316      0.8762 H      0      0      0      0      0      0      0      0      0      0
1661740      3.7523      0.6660      -0.8836 H      0      0      0      0      0      0      0      0      0      0
1661741      3.7414      0.6572      0.9048 H      0      0      0      0      0      0      0      0      0      0
1661742      -3.7430      0.6575      0.9037 H      0      0      0      0      0      0      0      0      0      0
1661743      -3.7508      0.6656      -0.8848 H      0      0      0      0      0      0      0      0      0      0
1661744      5.6926      -0.6223      0.0162 H      0      0      0      0      0      0      0      0      0      0
1661745      4.5702      -1.6976      0.8836 H      0      0      0      0      0      0      0      0      0      0
1661746      4.5808      -1.6889      -0.8755 H      0      0      0      0      0      0      0      0      0      0
1661747      -5.6925      -0.6223      0.0121 H      0      0      0      0      0      0      0      0      0      0
1661748      -4.5792      -1.6892      -0.8771 H      0      0      0      0      0      0      0      0      0      0
1661749      -4.5716      -1.6973      0.8819 H      0      0      0      0      0      0      0      0      0      0
1661750      1  6  1  0  0  0  0
1661751      1  8  1  0  0  0  0
1661752      2  7  1  0  0  0  0
1661753      2  9  1  0  0  0  0
1661754      3  8  2  0  0  0  0
1661755      4  9  2  0  0  0  0
1661756      5  8  1  0  0  0  0
1661757      5  9  1  0  0  0  0
1661758      5  12  1  0  0  0  0
1661759      5  13  1  0  0  0  0
1661760      6  10  1  0  0  0  0
1661761      6  14  1  0  0  0  0
1661762      6  15  1  0  0  0  0

```

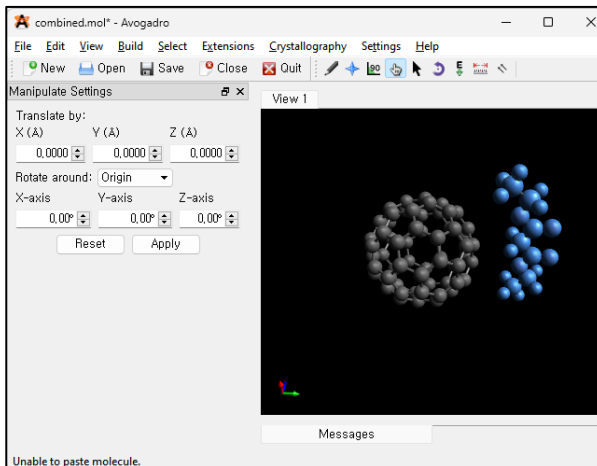
Step 2. 구조 러프하게 합치기:

풀러렌과 malonic ester 합치기

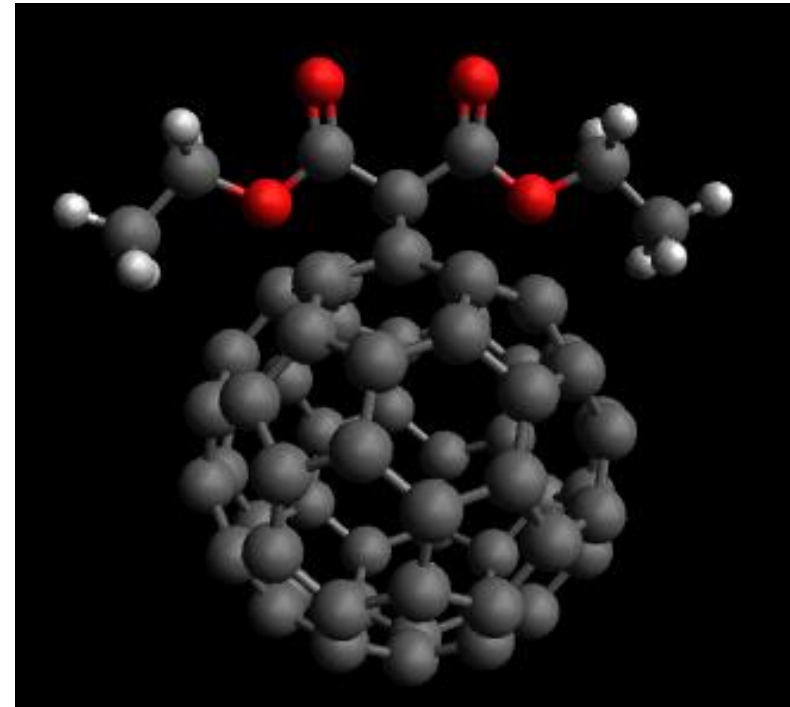
1) 두 구조를 동시에 볼 수 있게 두 창 띄우기




2) malonic ester를 복사 붙여넣기



3) 3D 에디터로 화합물들을 적절하게 돌려가며 원하는 구조로 러프하게 합체



4) 사라지지 않게 저장

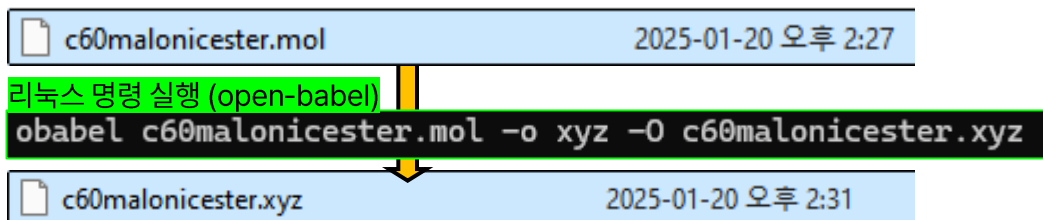
 c60malonicester.mol

2025-01-20 오후 2:27

Step 3. 파일 변환

.mol -> xyz -> .inp

1) openbabel로 .xyz로의 변환



2) .xyz 상의 내용을 선택해 복사

```

1 81
2
3 C ..... 3.27420 ..... -1.42970 ..... -0.06200
4 C ..... 3.57140 ..... -0.01920 ..... -0.08500
5 C ..... 3.31190 ..... 0.79090 ..... 1.07890
6 C ..... 2.71820 ..... -2.02920 ..... 1.12330
7 C ..... 2.77020 ..... -1.79900 ..... -1.36120
8 C ..... 3.25070 ..... 0.48310 ..... -1.39920
9 C ..... 2.73320 ..... 2.10420 ..... 0.93000
10 C ..... 2.75590 ..... 0.19130 ..... 2.26420
11 C ..... 1.65740 ..... -2.99890 ..... 1.01110
12 C ..... 2.45860 ..... -1.21920 ..... 2.28720
13 C ..... 1.70930 ..... -2.76870 ..... -1.47340

```

```

73 H ..... -1.69650 ..... 5.02610 ..... 4.36630
74 C ..... -0.88390 ..... 5.35280 ..... -0.67510
75 H ..... 0.21690 ..... 3.88990 ..... -4.17550
76 O ..... -0.76940 ..... 4.61040 ..... -1.81740
77 H ..... -0.14430 ..... 6.11340 ..... -3.09990
78 O ..... -1.09530 ..... 6.55610 ..... -0.62510
79 C ..... -0.91480 ..... 5.33650 ..... -3.04240
80 C ..... -0.76260 ..... 4.37830 ..... -4.20450
81 H ..... -0.86840 ..... 4.90130 ..... -5.15900
82 H ..... -1.51530 ..... 3.58470 ..... -4.15080
83 H ..... -1.90550 ..... 5.80330 ..... -3.07470
84

```

3) c60malonicester.inp라는 파일을 만들어 다음과 같이 입력후 그 아래에 아까 복사한 내용도 이어 붙이기

```

1  ! B3LYP def2-SVP Opt TightSCF ALLPOP KEEPDENS
2
3  %pal
4  num_procs 8
5  end
6
7  * xyz 0 1
8  C ..... 3.27420 ..... -1.42970 ..... -0.06200
9  C ..... 3.57140 ..... -0.01920 ..... -0.08500
10 C ..... 3.31190 ..... 0.79090 ..... 1.07890
11 C ..... 2.71820 ..... -2.02920 ..... 1.12330
12 C ..... 2.77020 ..... -1.79900 ..... -1.36120
13 C ..... 3.25070 ..... 0.48310 ..... -1.39920

```

병렬CPU 사용 구분
(open mpi 설정 하지 않았다면 사용 못함. 이 경우 이 줄들은 제거하고 실행)

- 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.

c60malonicester.inp 2025-01-20 오후 2:32

Step 4. Orca로 구조 최적화

Orca 명령어 실행

1) Orca 명령어 실행

```
(base) [yongsang@ga04 inp]$ orca c60malonicester.inp > c60malonicester.out
```

2) 계산 완료될 때까지 기다리기..

다루는 화합물에 원자 수가 많고 복잡하며, ALLPOP, KEEPDENS 키워드까지 이용했으므로 계산시간이 다소 걸림,,,

~~개인적으로 CPU 8개를 병렬 처리해 9시간이 걸렸다.~~

https://drive.google.com/drive/folders/1YW7PAblm_rfhhtjExgnEx-pJsSxePLoR

파일들은 여기에 저장해두었다.

3) 완료 후 아웃풋들 확인

```
(base) [yongsang@ga04 inp]$ ls
c60malonicester.bibtex      c60malonicester.engrad  c60malonicester.out
c60malonicester.densities   c60malonicester.gbw     c60malonicester.property.txt
c60malonicester.densitiesinfo c60malonicester.inp     c60malonicester_trj.xyz
c60malonicester.eldens.cube c60malonicester.opt     c60malonicester.xyz
```

.inp 확장자를 제외하면 11개의 파일이 새로 생겼다

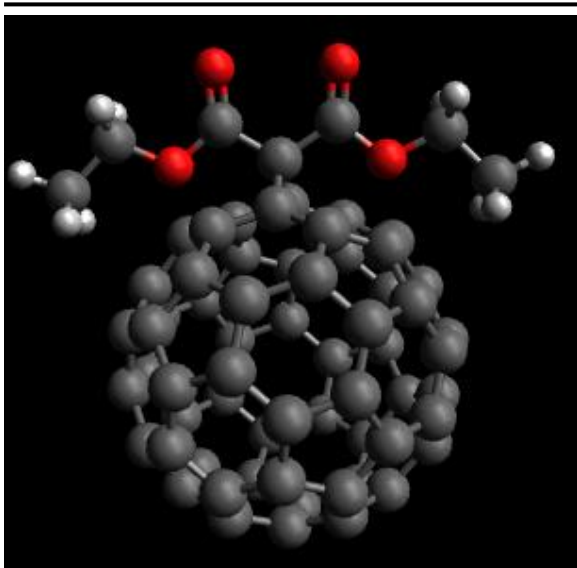
Step 4. Orca로 구조 최적화

계산 결과 시각화 및 올바르게 최적화 되었는지 체크

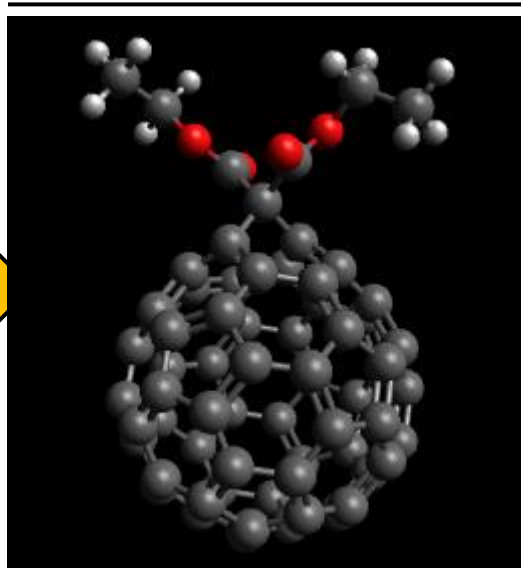
1) Avogadro로 새로 생긴 .xyz파일 열기

2) 최적화 전 / 레퍼런스 와 비교

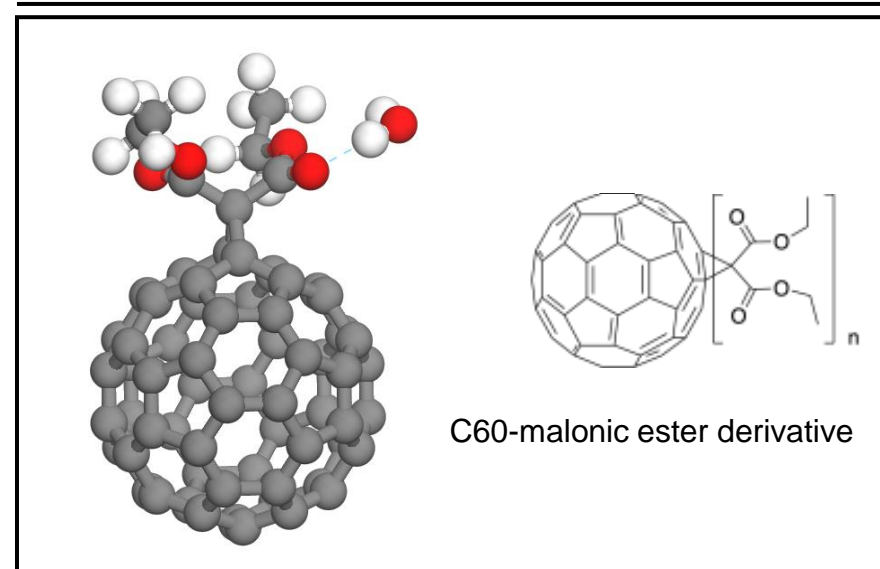
*최적화 전 .xyz파일



*최적화 후 .xyz파일



*레퍼런스



*최적화 전과 비교했을 때, 확실히 구조가 바뀐 것을 확인할 수 있으며

* 레퍼런스와 비교했을때 구조가 일치하는 것을 알 수 있다.

1) orca_plot 명령을 이용한 .cube 파일 생성

```
orca_plot [redacted] -i
```

c60malonicester.qbw

2025-01-20 오후 11:34

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
MD/Operator   ... 0 0
Output file   ... (null)
Format        ... Grid3d/Cube
Resolution    ... 40 40 40
Boundaries    ... -12.509708 12.493060 (x direction)
              ... -11.085077 11.085070 (y direction)
              ... -7.005949 7.004752 (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 configuration 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 1

```

```
Plot-Type is presently: 1
-----
Searching for Ground State Electron or Spin Densities: ...
1 - molecular orbitals
2 - (scf) electron density ..... (scf) ) => AVAILABLE
3 - (scf) spin density ..... (scf) ) - NOT AVAILABLE
4 - natural orbitals
5 - corresponding orbitals
6 - atomic orbitals
7 - mdc1 electron density ..... (mdc1p) ) - NOT AVAILABLE
8 - mdc1 spin density ..... (mdc1s) ) - NOT AVAILABLE
9 - 00-RI-MP2 density ..... (pmp2re) ) - NOT AVAILABLE
10 - 00-RI-MP2 spin density ..... (pmp2ur) ) - NOT AVAILABLE
11 - MP2 relaxed density ..... (pmp2ur) ) - NOT AVAILABLE
12 - MP2 unrelaxed density ..... (pmp2re) ) - NOT AVAILABLE
13 - MP2 relaxed spin density ..... (pmp2ur) ) - 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 ..... (autoc1pre) ) - NOT AVAILABLE
20 - AutoCI unrelaxed density ..... (autoc1pre) ) - NOT AVAILABLE
21 - AutoCI relaxed spin density ..... (autoc1ur) ) - 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-ROCIIS) - NOT AVAILABLE
25 - CAS unrelaxed transition AO density ..... (Tdens-CAS ) - NOT AVAILABLE
26 - ICE unrelaxed transition AO density ..... (Tdens-ICE ) - NOT AVAILABLE
27 - MRCI unrelaxed transition AO density ..... (Tdens-MRCI ) - 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 - ROCS unrelaxed transition MO density ..... (Tdens-ROCSMO) ) - NOT AVAILABLE
31 - CAS unrelaxed transition MO density ..... (Tdens-CASMO) ) - NOT AVAILABLE
32 - ICE unrelaxed transition MO density ..... (Tdens-ICEMO) ) - NOT AVAILABLE
33 - MRCI unrelaxed transition MO density ..... (Tdens-MRCIMO) ) - 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-CASQDPSOC) ) - NOT AVAILABLE
36 - DCCAS QDPT unrelaxed transition AO density ..... (Tdens-CASQDPSOC) ) - NOT AVAILABLE
37 - CAS CUSTOM E QDPT unrelaxed transition AO density ..... (Tdens-CASCUSTOMEQDPSOC) ) - NOT AVAILABLE
38 - QDPT QDPT unrelaxed transition AO density ..... (Tdens-CASPTQDPSOC) ) - NOT AVAILABLE
39 - GEOMET2 QDPT unrelaxed transition AO density ..... (Tdens-CASQDPTQDPSOC) ) - NOT AVAILABLE
40 - RCIS QDPT unrelaxed transition AO density ..... (Tdens-RCISQDPSOC) ) - NOT AVAILABLE
41 - RCIS QDPT unrelaxed transition AO density ..... (Tdens-RCISQDPSOC) ) - NOT AVAILABLE
42 - ..... relaxed transition AO density ..... (Tdens-LFTQDPSOC) ) - NOT AVAILABLE

```

Enter Type:

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 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:

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
```

.cube 파일 생성!!

c60malonicester.eldens.cube

2025-01-20 오후 11:42

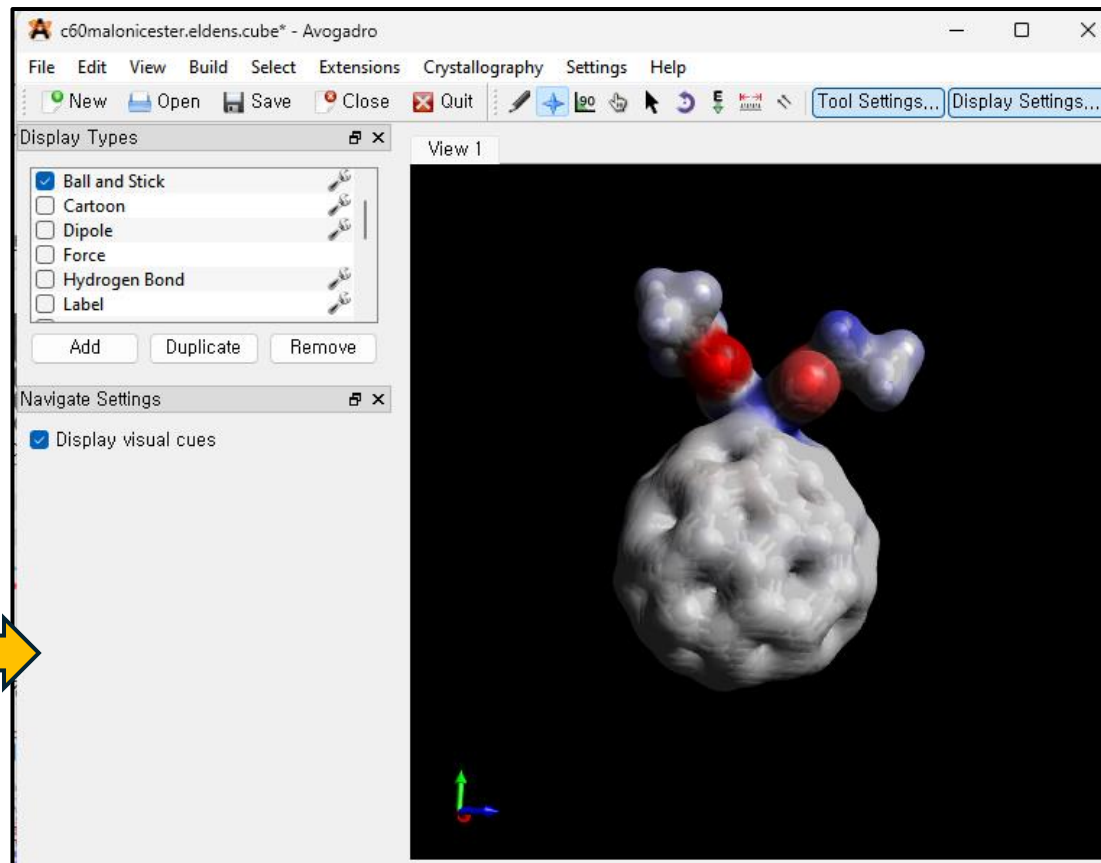
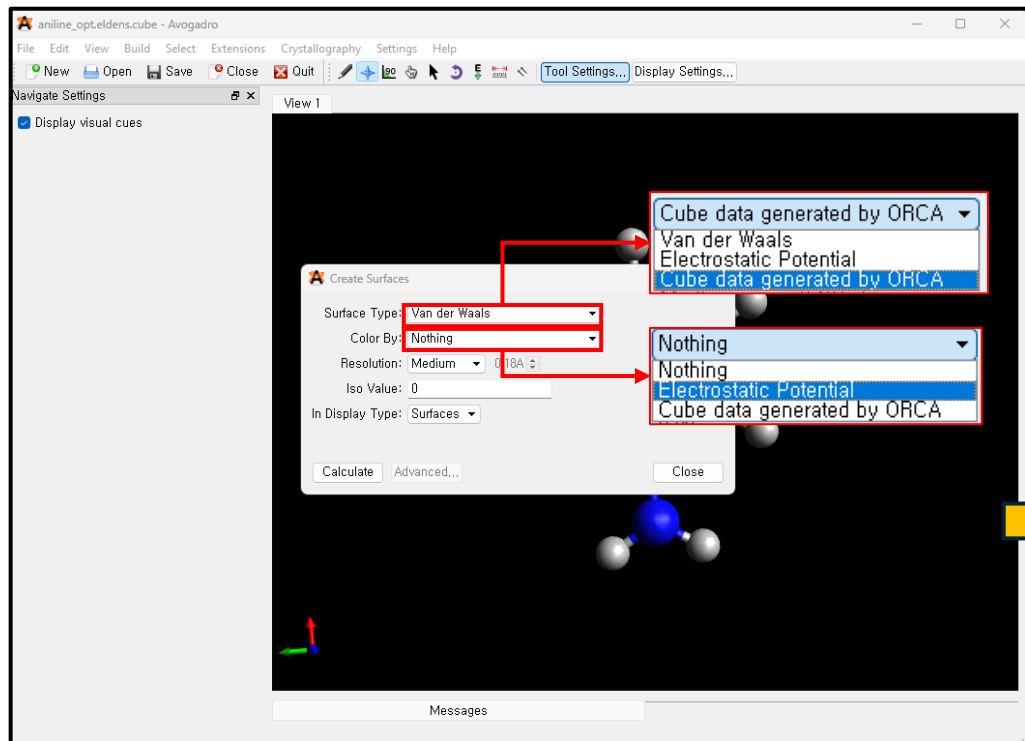
```
Calling PlotGrid3d with ATOM-A,B=0,0
Entering PlotGrid3d with Plotttype =2
*** PLOTTING FINISHED ***
Output file: aniline_opt.eldens.cube
-----
Current-settings:
PlotType      ... DENSITY-PLOT
ElDens File   ... aniline_opt.scfp
Output file    ... aniline_opt.eldens.cube
Format        ... Grid3d/Cube
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 6. Generate Surface

Avogadro 상에서 Generate Surface 실행하기



.mol2 파일로 저장!

c60malonicester.eldens.cube.mol2

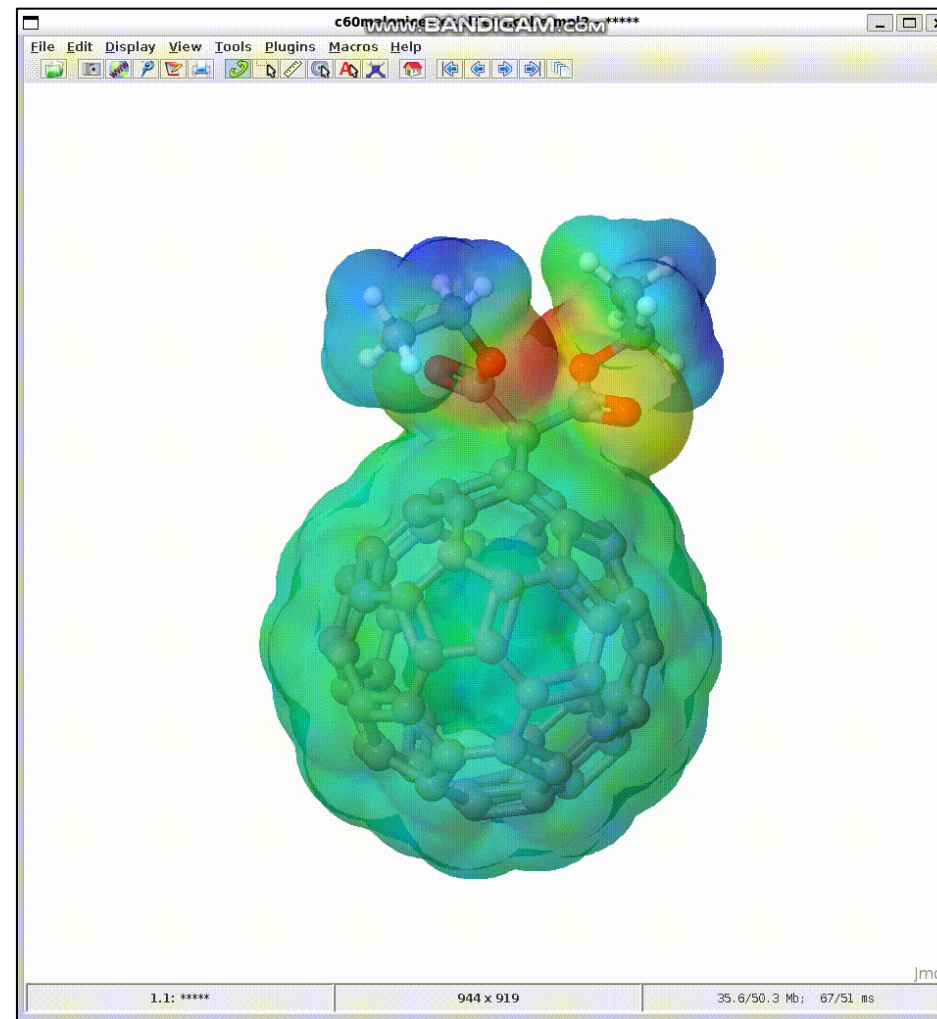
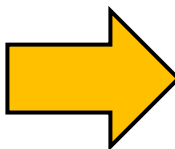
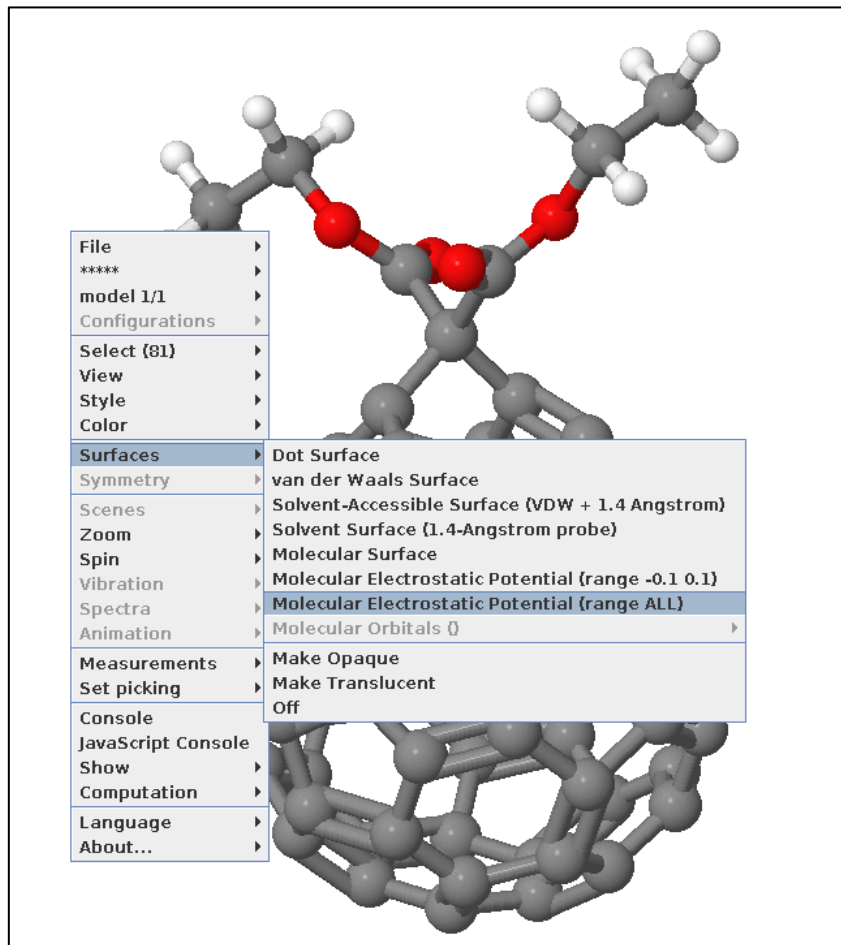
2025-01-20 오후 11:43

Step 7. Jmol로 ESP 확인

https://drive.google.com/drive/folders/1YW7PAbLm_rfhhtjExgnEx-pJsSxePLoR

jmol프로그램으로 ESP 확인

c60malonicester.eldens.cube.mol2 2025-01-20 오후 11:43



|| 구조 최적화와 전자밀도 계산 과정에서 나온 Output파일들 공유 링크

https://drive.google.com/drive/folders/1YW7PAbLm_rfhhtjExgnEx-pJsSxePLoR