MiCMoS
Milano Chemistry Molecular Simulation
Description and User Manual

Tutorials

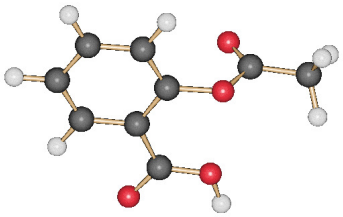
T2. Prepare a *.oeh* file compatible with the LJC parametrization and a charge density file for subsequent Pixel calculations

PURPOSE: In this tutorial, it is described how to prepare a *.oeh* structure file compatible with the LJC parametrization, that is, containing Electrostatic Potential (ESP) charges rather than the default Extended Hückel ones. At the same time, the production of a charge density file to be used in subsequent ***Pixelc*** calculations is also shown. The same test case used in Tutorial T1 is employed.

REFERENCE to main manual: Sections 2.1.2 (LJC potential); 3.1.2 (crypar.*par*) 3.2.5 (***Pixmt2***).

FILES: Click here to download the materials for this exercise:
https://sites.unimi.it/xtal_chem_group/images/MiCMoS_package/T2/sample.gjf
https://sites.unimi.it/xtal_chem_group/images/MiCMoS_package/T2/sample.oeh
https://sites.unimi.it/xtal_chem_group/images/MiCMoS_package/T2/sample.out
You also need the *runpixmt2* macro available in the batch directory of the package and a licence to run the Gaussian® quantum simulation package. File sample.*oeh* can be also obtained from Tutorial T1 and refers to ACSALA01, the $P2_1/c$ structure of acetylsalicylic acid. Place sample.*oeh* and pertinent (Windows/Unix) macros into your working directory.

You should have obtained the structure file sample.*oeh* in Tutorial T1 by use of the ***Retcif-Retcor-Retcha*** sequence. It refers to the solid-state structure of the acetylsalicylic acid shown in the picture below.



A printout of the sample.*oeh* file is given in the next page. Refer to the manual (Section 1.4.3) for a detailed description of all quantities and parameters. The Extended Hückel atomic point charges are suitable for the calculation of Coulomb-London-Pauli (CLP) energies. Recall that these will usually be damped by the 0.41 CLP factor (see manual, Section 3.1.2). This *.oeh* file is yet ready to enter ***Crysaa*** (Tutorial T4); however, you are going to learn here how to produce an *.oeh* file compatible with the Lennard-Jones-Coulomb (LJC) parametrization (see manual, Sections 2.1.2 and 4.1).

sample.oeh structure file

```
#SAMPLExx 'P 21/c'                          0.000     0.0      0.   0.00
   0          0.0
   11.4300    6.5910   11.3950    90.000    95.680    90.000
     0.0
   21
    1   0.15340   0.56400   0.06740   1  12   -0.0532
    2   0.24620   0.48770   0.00950   1  12    0.5755
    3   0.29830   0.30470   0.04160   1  12   -0.3439
    4   0.26040   0.19610   0.13380   1  12   -0.2316
    5   0.16960   0.26760   0.19310   1  12   -0.3232
    6   0.11650   0.44960   0.15980   1  12   -0.2388
    7   0.09030   0.75730   0.03760   1  10    1.3326
    8   0.36590   0.73840  -0.06370   1  10    1.3401
    9   0.39740   0.83780  -0.17280   1  13   -0.8859
   10   0.12030   0.86030  -0.05080   1  28   -0.9080
   11   0.01040   0.81180   0.09650   1  27   -1.2101
   12   0.28570   0.58780  -0.08800   1  23   -0.7525
   13   0.40360   0.78010   0.03450   1  27   -1.1311
   14   0.36868   0.24670  -0.00548   1   2    0.2969
   15   0.30217   0.05387   0.15979   1   2    0.2843
   16   0.14005   0.18175   0.26531   1   2    0.2872
   17   0.04492   0.50446   0.20628   1   2    0.2857
   18   0.31897   0.89723  -0.22149   1   3    0.3477
   19   0.45815   0.96037  -0.15004   1   3    0.3089
   20   0.43805   0.72830  -0.22643   1   3    0.3516
   21   0.07316   0.98776  -0.06274   1   6    0.6678
   0
   4
   1.0   0.0   0.0   0.0   1.0   0.0   0.0   0.0   1.0
  0.000000  0.000000  0.000000
  -1.0   0.0   0.0   0.0   1.0   0.0   0.0   0.0  -1.0
  0.000000  0.500000  0.500000
  -1.0   0.0   0.0   0.0  -1.0   0.0   0.0   0.0  -1.0
  0.000000  0.000000  0.000000
   1.0   0.0   0.0   0.0  -1.0   0.0   0.0   0.0   1.0
  0.000000 -0.500000 -0.500000
   3
   0
```

This data is used to call ***Pixmt2*** to produce a tentative template for the *.gjf* file input to GAUSSIAN. The command line is:

```
./run.pixmt2 sample
```

The program will print the following note:

```
#SAMPLExx 'P 21/c'
 structures read, good, wrong      1      1      0
 normal end of operation
```

At the same time, a file sample.*gjf* is produced, which can be given in input to Gaussian, as well as a file sample.*inp*, which contains the ***Pixelc*** instructions. Have now a look at the Gaussian input:

Gaussian input file for charge density:

```
#MP2/6-31G** guess=core nosym density=MP2 pop=esp cube=cards cube=frozencore

 #SAMPLExx 'P 21/c'   fragm   1

 0 1
 C   -0.085716    0.460623    0.896945
 C   -0.373875   -0.708472    0.188427
 C   -0.380093   -1.937870    0.811842
 C   -0.071578   -2.028279    2.149952
 C    0.224187   -0.896263    2.874995
 C    0.212509    0.336011    2.252839
 C   -0.081170    1.830335    0.318972
 C    0.270627   -0.650606   -2.071023
 C   -0.240159   -0.562203   -3.458201
 O   -0.409675    1.965100   -0.920154
 O    0.212968    2.794469    1.039243
 O   -0.745187   -0.674086   -1.165717
 O    1.414535   -0.695934   -1.743404
 H   -0.626403   -2.827820    0.251645
 H   -0.061470   -2.993600    2.634208
 H    0.464143   -0.971750    3.925251
 H    0.439028    1.221434    2.828283
 H   -0.854914    0.319937   -3.559910
 H    0.591336   -0.502641   -4.144841
 H   -0.829348   -1.439367   -3.681484
 H   -0.365771    2.921219   -1.209938

~/programs/MiCMoS/doc/static/SAMPLExxa.den
    0   -3.640000   -5.400000   -6.680000
  100    0.080000    0.000000    0.000000
  140    0.000000    0.080000    0.000000
  160    0.000000    0.000000    0.080000
```

The string `~/programs/MiCMoS/doc/static/SAMPLExxa.den` localizes the charge density cube file in the Unix/Linux environment default directory. You may change it at your convenience, for example to have the *.den* file written directly in your working directory. The Windows version of ***Pixmt2*** produces a `c:\MiCMoS\doc\static\SAMPLExxa.den` string instead.

CAUTION: The last blank line is mandatory for a proper Gaussian termination. If missing, the program might not print the density file!

You may edit the main commands in the first input line, for example to use modern Gaussian keywords; refer to the manual (Section 3.2.5) for step-by-step explanations.

CAUTION: It is recommended that you perform the calculation at least at the MP2/6-31G** level of theory and that you include the `nosym` keyword, unless you know exactly what you are doing.

At this point the Molecular Orbital MP2/6-31G** calculation must be carried out to obtain the density grid. The output of the Gaussian run, sample.*out* or sample.*log* depending on program version and settings, also carries atomic charges fitted against the molecular Electrostatic Potential (ESP charges); many of them are not too different from the CLP ones (Extended Hückel) scaled by the 0.41 fudge factor (see Sections 2.1.1 and 3.1.2), but those over the hydrogen bonding atoms are much larger:

Gaussian output file (excerpt)

```
Charges from ESP fit, RMS=   0.00107 RRMS=   0.06707:
ESP charges:
               1
     1  C   -0.138519
     2  C    0.399191
     3  C   -0.243598
     4  C   -0.081407
     5  C   -0.139335
     6  C   -0.127001
     7  C    0.668790
     8  C    0.808153
     9  C   -0.530410
    10  O   -0.542022
    11  O   -0.524557
    12  O   -0.481345
    13  O   -0.513135
    14  H    0.159469
    15  H    0.121766
    16  H    0.132037
    17  H    0.148517
    18  H    0.161244
    19  H    0.140612
    20  H    0.155416
    21  H    0.426136
Sum of ESP charges =   0.00000
```

Together with the Gaussian output, a charge density file in the "cube" format (`SAMPLExxa.den`; see manual, Section A5 in the Appendix) should now be available in the directory you have indicated in the last input block of .*gjf* file.

Now, make a copy of your sample.*oeh* file:

```
cp sample.oeh samplesp.oeh
```

The ESP charges must be somehow substituted for the CLP charges in the samplesp.*oeh* file. You can do this by hand, or using any smart text editor, as you prefer.

Note that the order of atoms in the Gaussian input .*gjf* file produced by ***Pixmt2*** strictly follows that in the .*oeh* file. This means that you do not have to concern with chemical identities of the various atoms. You should only replace the last column of the block of atom coordinates/identities in the .*oeh* file with the one sketched in the excerpt of the Gaussian output above.

In the end, the new structure file should look like the printout in the next page. This file is ready to enter the ***Crysaa*** routine for the evaluation of lattice energies with atomic charges compatible with LJC potentials (Tutorial T4).

samplesp.oeh file, with updated ESP charges

```
#SAMPLExx 'P 21/c'  esp charges
    0
    11.430     6.591    11.395     90.00     95.68     90.00
       0.0
   21
    1    0.1534    0.5640    0.0674  1 12 -0.1385
    2    0.2462    0.4877    0.0095  1 12  0.3992
    3    0.2983    0.3047    0.0416  1 12 -0.2436
    4    0.2604    0.1961    0.1338  1 12 -0.0814
    5    0.1696    0.2676    0.1931  1 12 -0.1393
    6    0.1165    0.4496    0.1598  1 12 -0.1270
    7    0.0903    0.7573    0.0376  1 10  0.6688
    8    0.3659    0.7384   -0.0637  1 10  0.8082
    9    0.3974    0.8378   -0.1728  1 13 -0.5304
   10    0.1203    0.8603   -0.0508  1 28 -0.5420
   11    0.0104    0.8118    0.0965  1 27 -0.5246
   12    0.2857    0.5878   -0.0880  1 23 -0.4813
   13    0.4036    0.7801    0.0345  1 27 -0.5131
   14    0.3687    0.2467   -0.0055  1  2  0.1595
   15    0.3022    0.0539    0.1598  1  2  0.1218
   16    0.1400    0.1817    0.2653  1  2  0.1320
   17    0.0449    0.5045    0.2063  1  2  0.1485
   18    0.3190    0.8972   -0.2215  1  3  0.1612
   19    0.4581    0.9604   -0.1500  1  3  0.1406
   20    0.4381    0.7283   -0.2264  1  3  0.1554
   21    0.0732    0.9878   -0.0627  1  6  0.4261
    0
    4
   1.0   0.0   0.0   0.0   1.0   0.0   0.0   0.0   1.0
  0.000000  0.000000  0.000000
  -1.0   0.0   0.0   0.0   1.0   0.0   0.0   0.0  -1.0
  0.000000  0.500000  0.500000
  -1.0   0.0   0.0   0.0  -1.0   0.0   0.0   0.0  -1.0
  0.000000  0.000000  0.000000
   1.0   0.0   0.0   0.0  -1.0   0.0   0.0   0.0   1.0
  0.000000 -0.500000 -0.500000
    3
    0
```