# PLATON GUI: some hints

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## 1 Introduction

This small tutorial give some hints how to use the graphical user interface (GUI) of PLATON. The recommended reference for the use of PLATON is: Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7-13. The (L)UNIX version of PLATON can be downloaded at http://www.cryst.chem.uu.nl/platon/pl000000.html; a windows version of PLATON is available at http://www.chem.gla.ac.uk/∼louis/software/platon/. The main difference between the (L)INUX and Windows version is that the former gives access to the so-called 's' mode of PLATON. This is a mode in which PLATON is linked to different structure solving and refinement packages and the user is guided all along the solution and refinement process.

## 2 Main interface

Start Platon either via the command line by typing 'platon ecryst20.cif' or by starting PLATON via the WINGX toolbar.

If there is a corresponding .fcf file with the same name in the directory, PLATON will detect this automatically. All command that are in white can be clicked. The commands in blue are not accessible - in this case the CSD database is not found. If in the course of a PLATON session some tasks have been performed, the associated commands become blue and are no longer accessible. If for instance the .fcf file is not found then all tasks related to structure factors can not be performed, for instance structure factor validation (FCF-Valid in report).

# 3 Graphics

Either ORTEP or PLUTON can be used by clicking on the PLUTONauto or ORTEP command in the Graphics colum completely on the left. The functionality of both modes is pretty much the same, except that the ORTEP mode gives access to standard uncertainties for all kind of geometrical calculations. There is, ofcourse, only one style in 'ORTEP' mode, which is the typical thermal ellipsoid ORTEP style. In PLUTON there are 5 different styles available (Solid, Rod, CPK, Straw, and Stick).

## 3.1 ORTEP

Click on 'ORTEP' in the Graphics column of the main menu. The ORTEP windows the following window is displayed. There are three different ORTEP menus available by clicking on the three different parts of the OptionMenus box (see below figure):
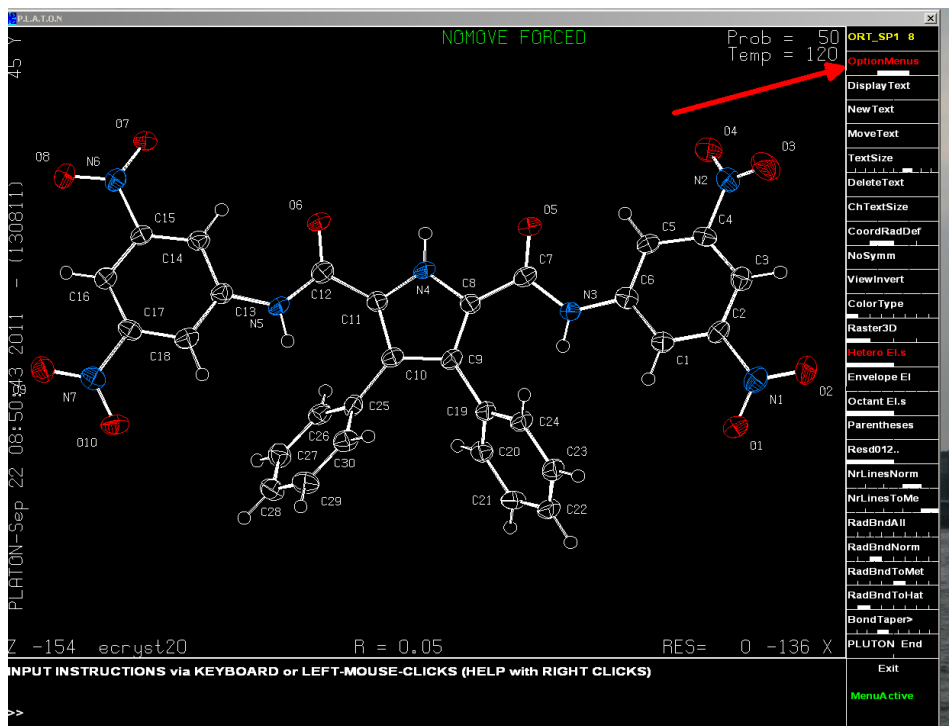
### 3.1.1 Changing the probability level of the ellipsoids

By clicking in the different parts of the Probability box of the first menu the probability levels of the ellipsoids can be changed from 10% to 90%.
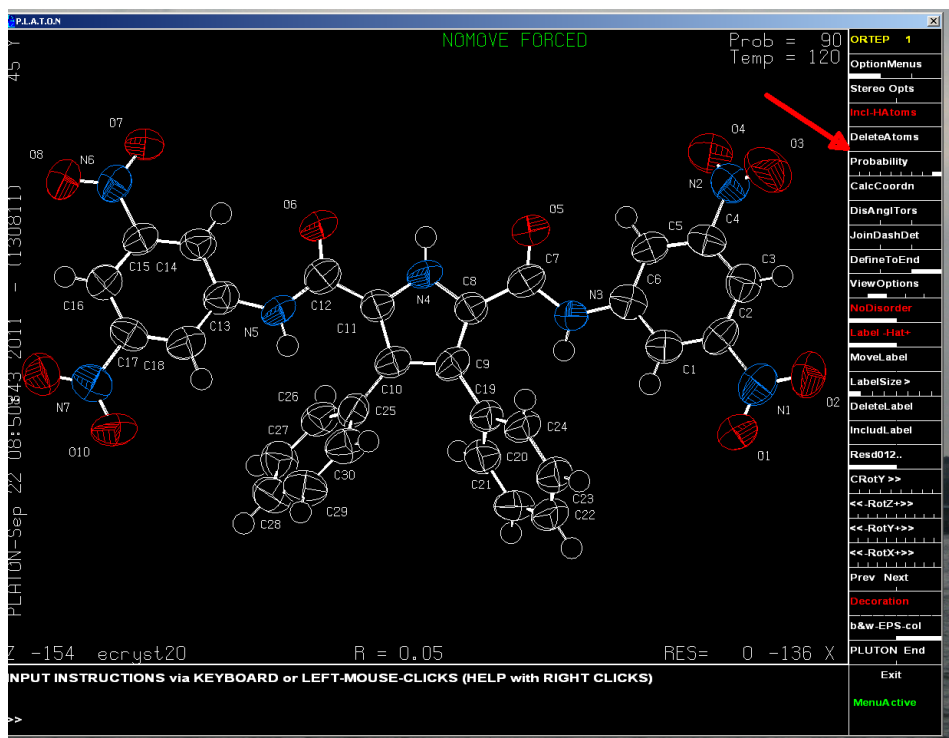


### 3.1.2 Adding a nearby molecule and drawing non-covalent intermolecular interactions

By clicking on the CalcCoordn box of the first menu the user is asked to select an atom for which distances in a coordinating shell are calculated. Select the N4 atom and a new window opens which gives the coordination sphere around the N(4) atom (intra and inter). If a close contact is selected one can add the nearby ARU (Atomic Residue Unit) to the figure by clicking on the ARU number. Click on the number 10 close contact ARU number (2544.01) and the ARU is added to the plot.
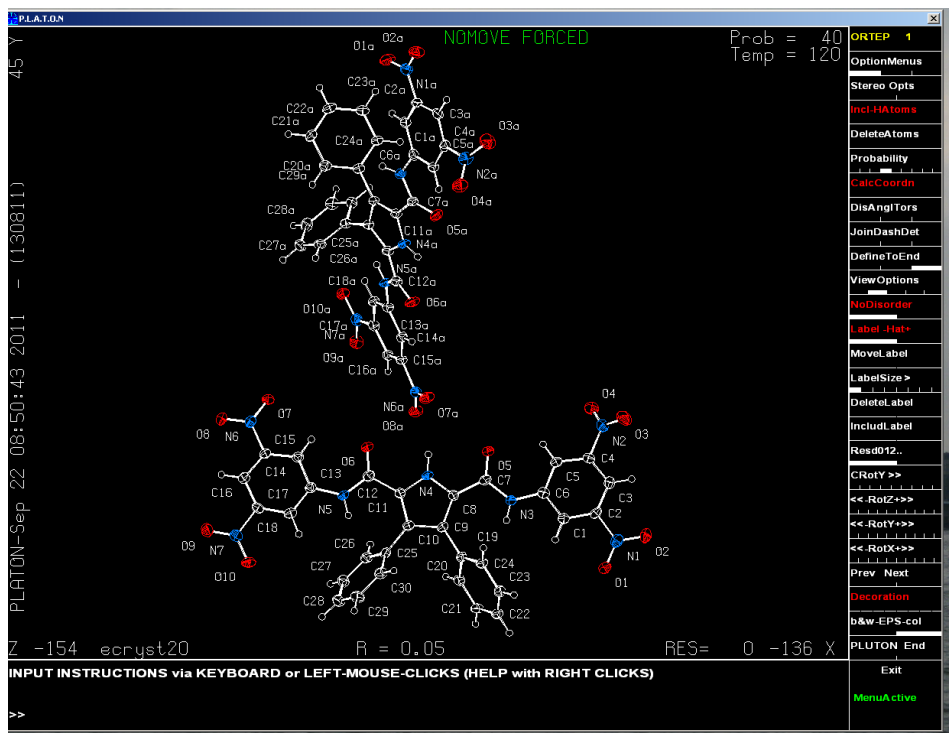
By clicking on the middle part of the JoinDashDet box and subsequently by clicking on the O7a and the N4 attached proton a dashed bond can be drawn in order to illustrate the short contact.
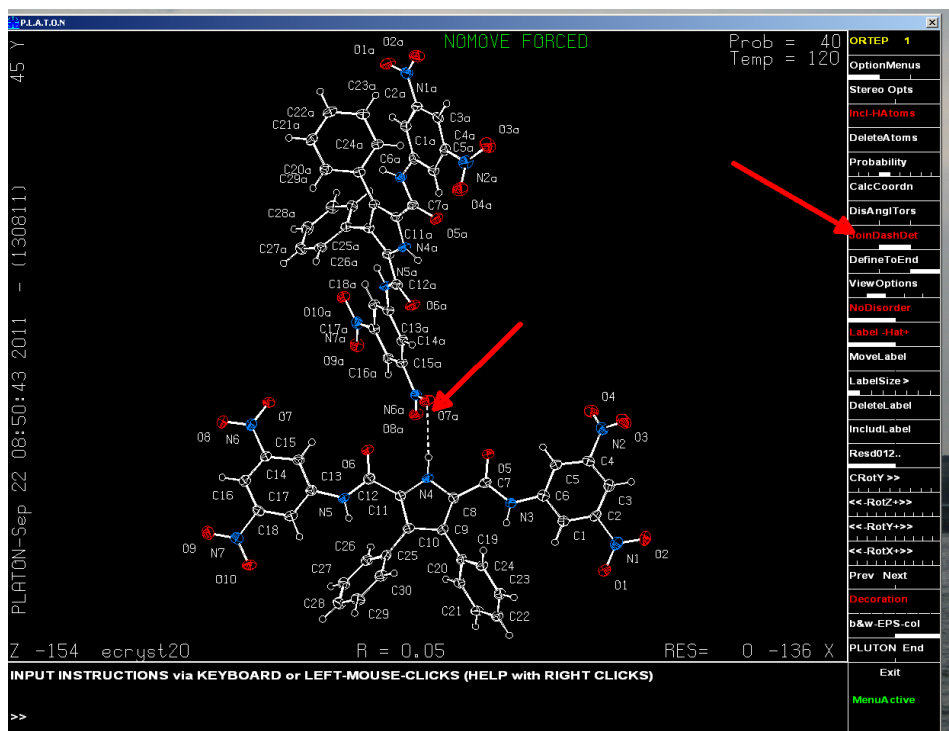


The word JoinDashDet is now in red meaning that the program is now in Drawing Bond mode. In order to quit this mode, click again on JoinDashDet and it becomes white again.

You can also draw dashed interaction bonds between centers of gravity or between a center of gravity and *e.g.* a proton (CH· · · $\pi$ interaction). *PLATON* can find automatically the centers of gravity of aromatic rings, just by clicking on the LabelCg button of the third Ortep menu. If the structure is already grown, you should use a different, more indirect way to find and visualize the center of gravity of a ring or another set of atoms. For this, just as an example, we create a 'short' contact between the O8a atom and the N4-C8-C9-C10-C11 ring.
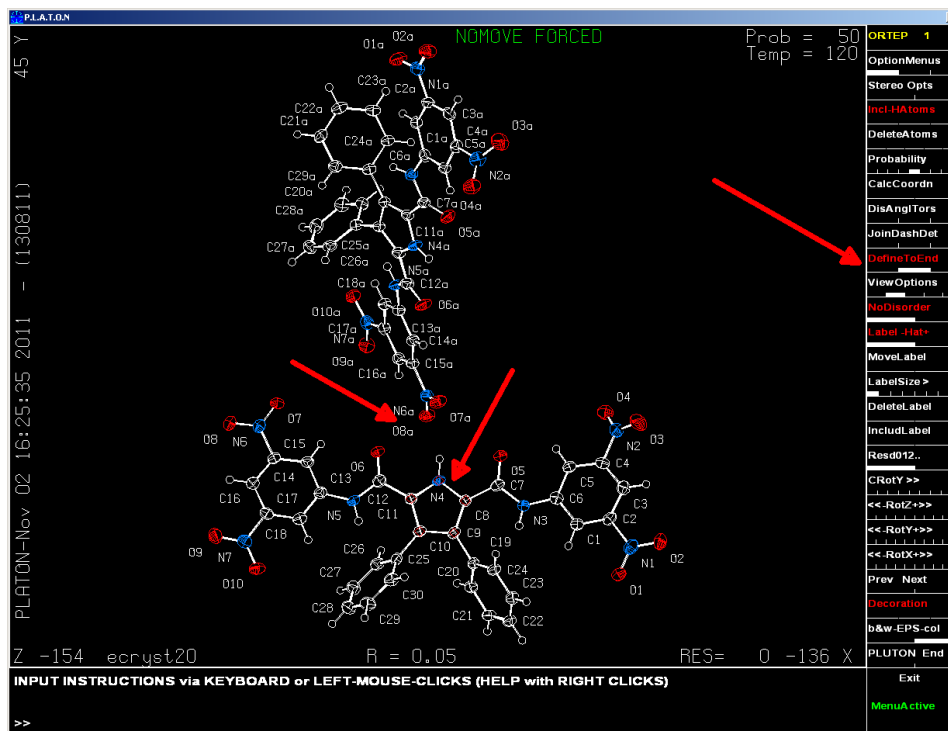
For this go to the first Ortep menu and click on DefineToEnd. Click on DefineToEnd which turns red and then click on the source atom O8a. When done the white rectangle in the DefineToEnd box goes to the middle and the next atoms will define the center of gravity Cg to be calculated. Click thus on N4-C8-C9-C10-C11 and then on the rightmost part of the DefineToEnd box.
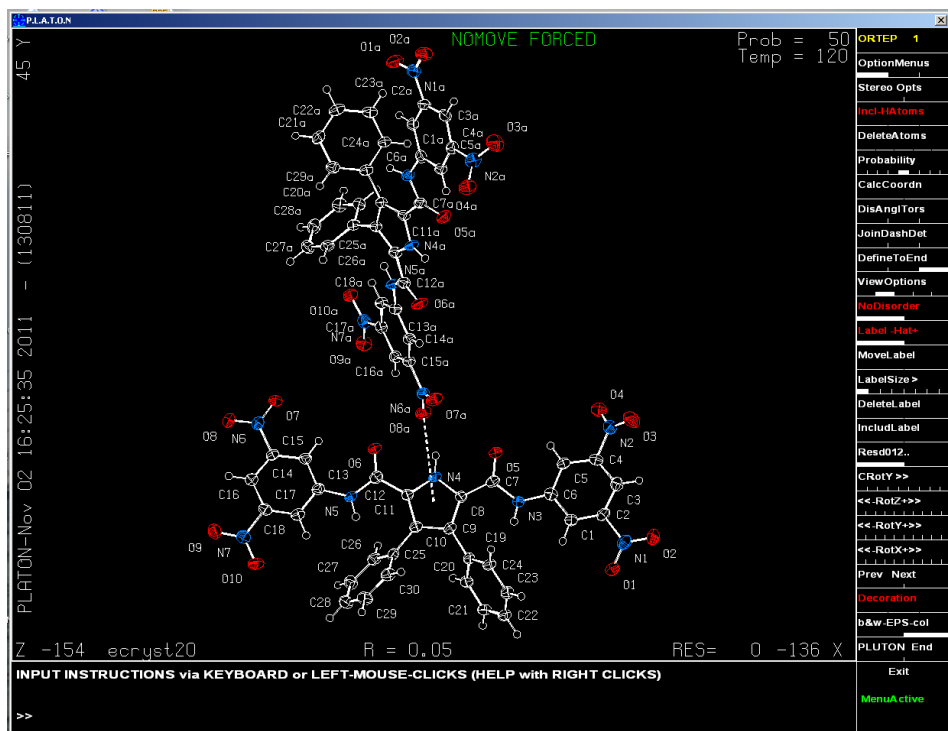


The short contact shows up as a dashed line between O8a and the center of gravity of the aromatic ring. Note that the defined center of gravity can be used for other dashed lines or calculations. You can draw a dashed line to O7a (with the Dash part of JoinDashDet) by clicking on the center and then on O7a. Or you can determine the distance from the center to another atom (with the Dis part of DisAnglTors box), *e.g.* from the center to O7a. Note that clicked atoms (or centers) are generally represented by a small red rhombus. This rhombus will not be printed.
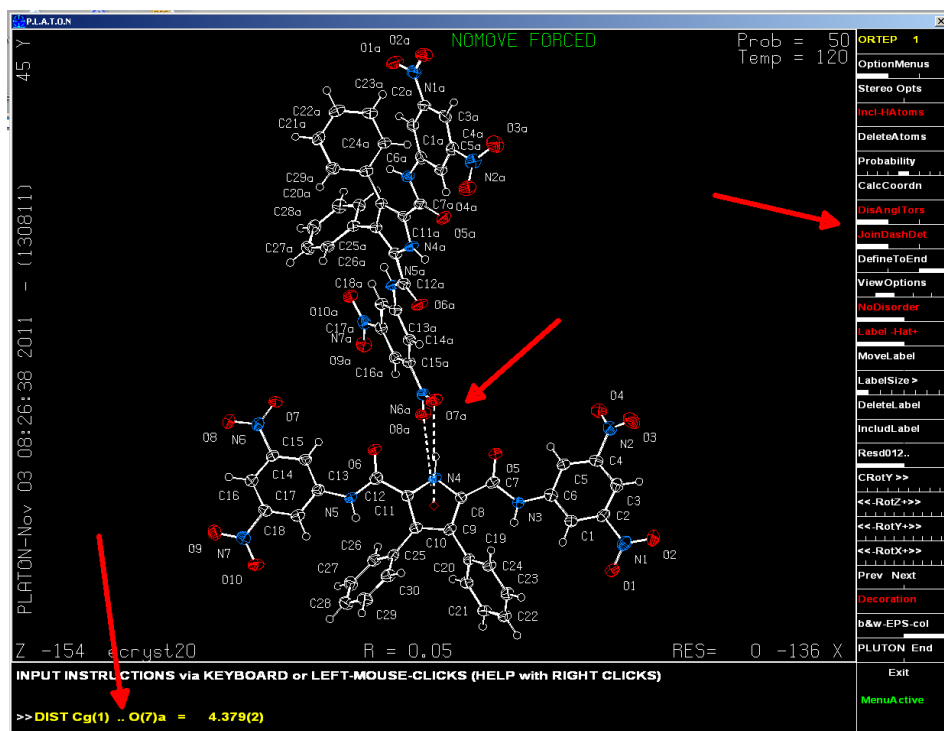
### 3.1.3 Calculating bond distances, angles, torsion angles, and least-squares planes with standard uncertainties.

Click on the the most-right Tors part of the DisAngTors box (the word becomes red). Then click on four atoms (here O2, N1, C2, C3 in the lower molecule) in order to calculate the torsion angle with standard uncertainty. The torsion angle is displayed at the bottom line in yellow. If there are no standard uncertainties available for the coordinates, then no standard uncertainty is given. The same can ofcourse be done for any distance or angle.
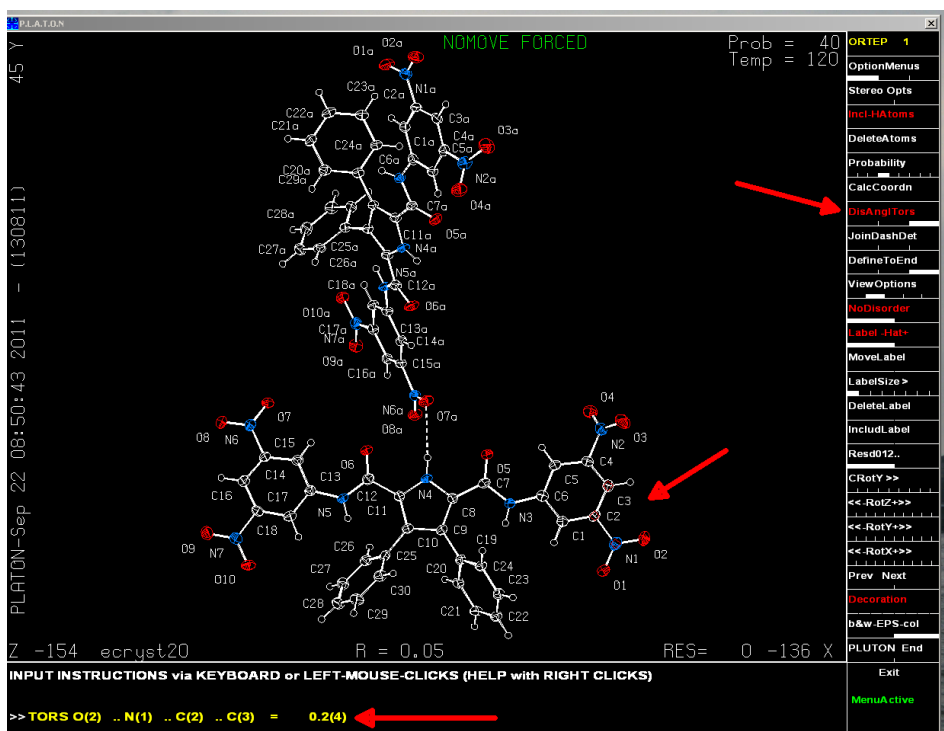


Leave the DisAngTors mode by clicking on the word (it becomes white). Least-squares planes, angles between planes, and closest distances between atoms and planes can be calculated with LsplWithEnd and LsplDistEnd in the lower part of the third OptionMenus.
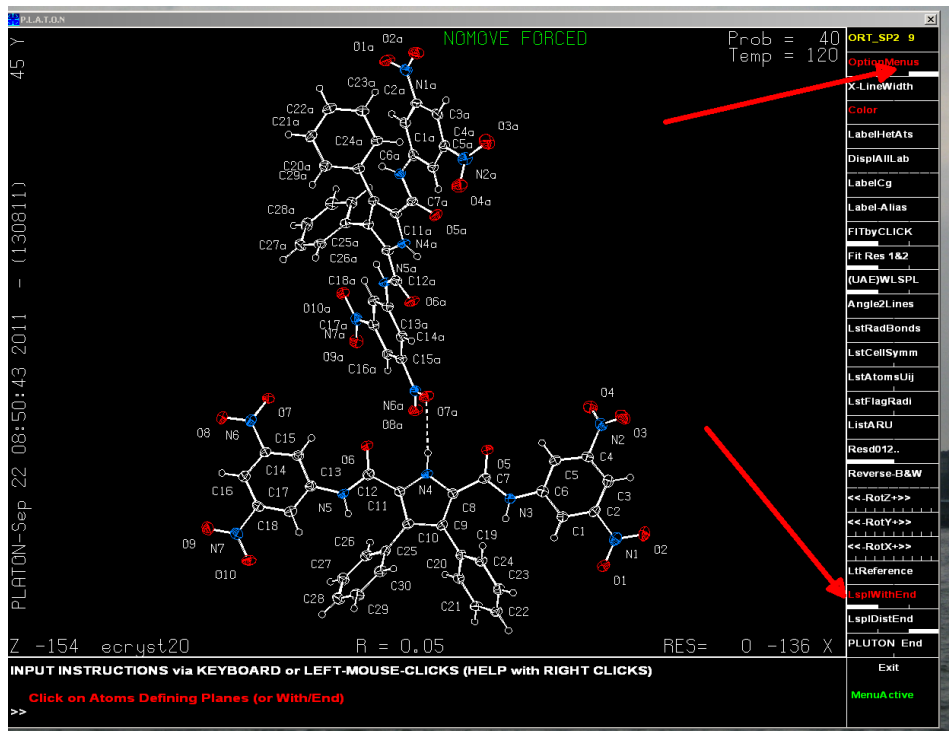
Click on the 6 atoms C1-C6 of the phenyl ring of the lower molecule. If you click now on the right-most part of LsplWithEnd the results of the least-squares plane calculation of this ring wll be given. If you click on the other hand on the middle part (With) then you can click new atoms inorder to define a new least-squares plane, for instance C19-C24. The program, when clicked on End of LsplWithEnd will give the results of the least-squares calculations of the two planes and the dihedral angle with standard uncertainty between the two planes.
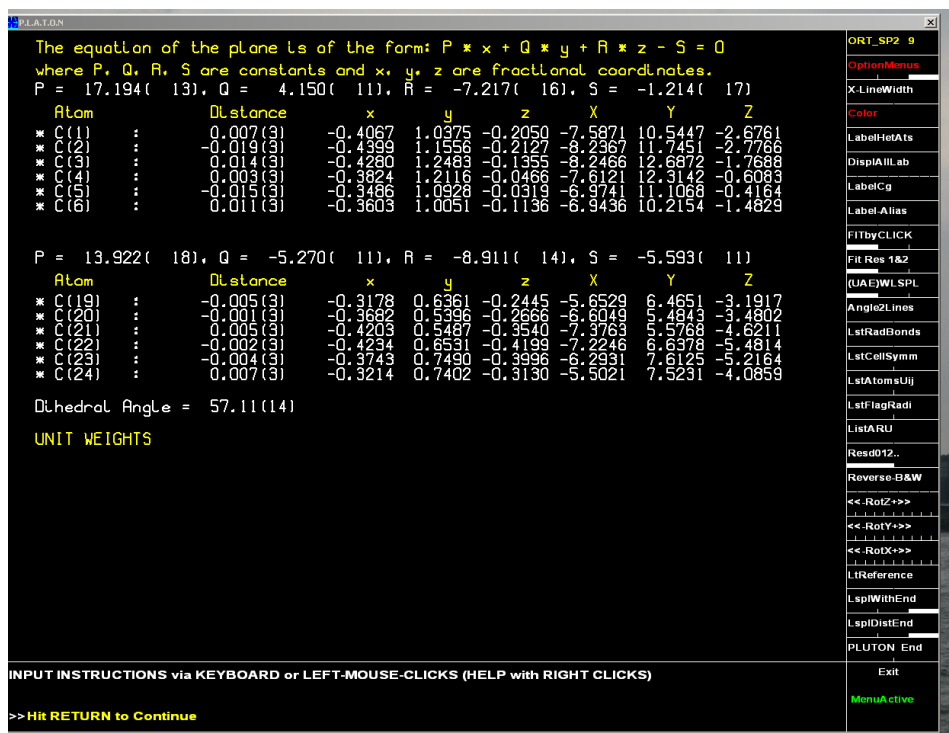


Press return to go back to the main ORTEP window. You can calculate the closest distance of one or more atoms to a least-squares plane by clicking on LsplDistEnd. Define the least-squares plane, click on the middle part Dist of LsplDistEnd. Click on one or more atoms. Once finished click on End, and the results will be displayed in a a new window. The first 6 atoms define the least-squares-plane whereas the closest distance to this plane is given for the following three non-starred atoms. Hit return to go back to the main Ortep window.

### 3.1.4 Making high-quality figures

The standard way to make high-quality figures is by pressing the black and white or color button in the first menu. Normally you would like to suppress the text in the margins before sending the picture to the file. this can simply be done by clicking on the the Decoration box which is by default activated (in red). Each time you click on the b&w-EPS-col box a new page is added to the output file in encapsulated postscript (EPS) format. Tools exist to convert this file to other formats, such as pdf or png.



Another possibility is to create files in POVRAY format, but this is only possible in PLUTON mode (sixth menu - PovrayResol). If the POVRAY engine is defined, then it starts up the created file. If not, it creates a file with extension .pov in the working directory.