

NanoPDF64 Quick Start Guide

1. Make sure you are running 64 bit version of MS Windows. It seems to be a standard these days but who knows.

2. Download “nppackageXXXXX.zip” file by clicking on this link:

[Reasonably recent 64bit version](#) The packa
[Last 32bit ve](#)



Vista, W7

Unpack the “nppackage” folder to your Desktop

3. Download the file rastop.2.2.zip from RasTop's home page:

<http://www.geneinfinity.org/rastop/index.htm#download>

or directly from Sourceforge:

https://sourceforge.net/projects/rastop/files/latest/download?source=typ_redirect

Unpack “rastop” folder to your Desktop

4. Run NanoPDF64.exe from the “nppackage” folder on your Desktop.

5. Select Options → Settings

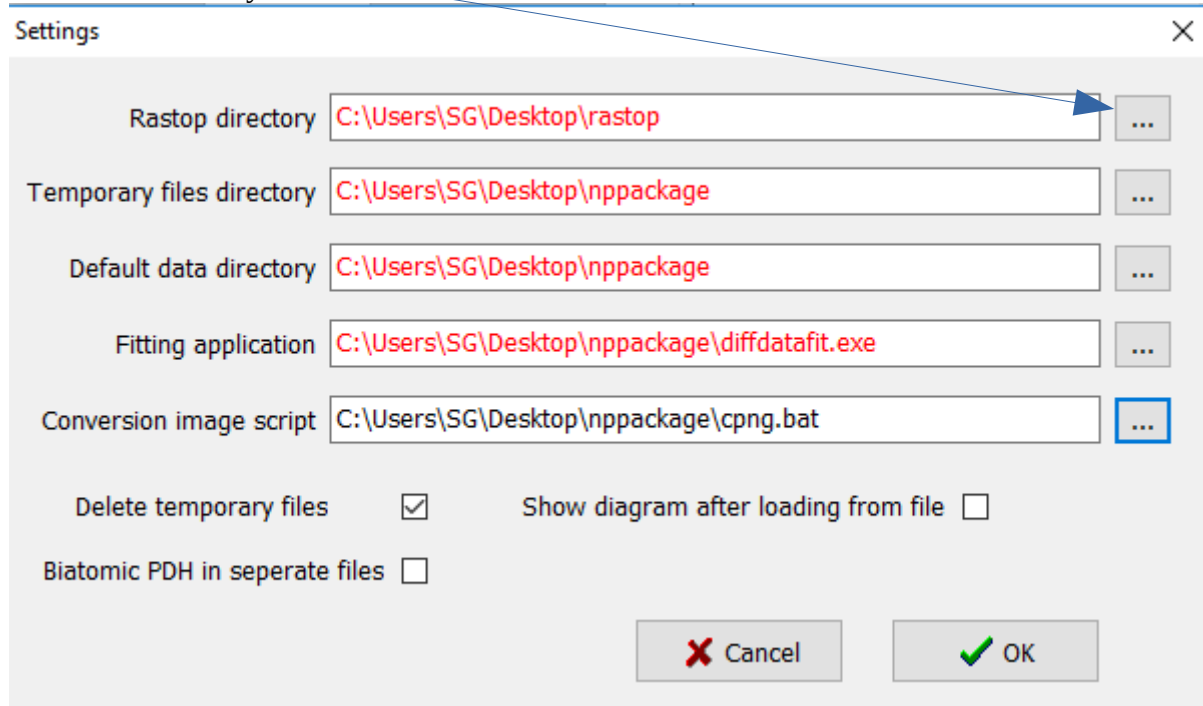
The screenshot displays the NanoPDF64 software interface. The 'Options' menu is open, with 'Settings' selected. The main window is divided into several sections:

- Element properties:** Includes a dropdown for 'F8', a 'biatomic lattice' section with two 'Ac' dropdowns, and a 'Build' button with a unit cell diagram.
- Crystal Structure:** Features radio buttons for 'diamond like', 'cubic I (bcc)', 'cubic F (fcc)', and 'hcp P', along with a 'cubic latt. prm. (Å)' input field set to '3'.
- Grain geometry:** Includes radio buttons for 'sphere' and 'cylinder', a 'cube' radio button, a 'size (Å)' input field set to '15', and a 'N' dropdown set to '5 l.p.'.
- Modify:** A button with a hammer icon.
- Calculations:** Contains tabs for 'PDH', 'RDH', and ' $\delta(r)$ '. It includes buttons for 'Diffraction pattern', 'G(r) PDF', and 'PDH', each with a 'Show' checkbox. A 'Show diagram' checkbox is also present.
- Parameters:** A sub-section with tabs for 'Parameters', 'Radiation', and 'TDS'. It features a table for 'Angle(2 θ)' and 'Q(1/Å)' with input fields for 'start', 'stop', and 'step' values.
- Range, step (in Angs):** A sub-section with tabs for 'Start, step, ...' and 'W.F.'. It includes input fields for 'start', 'stop', and 'step' values.
- Bin width:** An input field set to '0.0078125'.
- One Bin mode:** A checked checkbox.
- Visualizations:** Four small icons representing different data plots.

The right-hand pane displays a welcome message: '... WELCOME ... NanoPDF-64-ver.: Oct 10 2016'.

6. Set the required entries:

Use these buttons to search your disk



The screenshot shows a 'Settings' dialog box with the following fields and options:

- Rastop directory:** (A blue arrow points to this button from the text above.)
- Temporary files directory:**
- Default data directory:**
- Fitting application:**
- Conversion image script:**

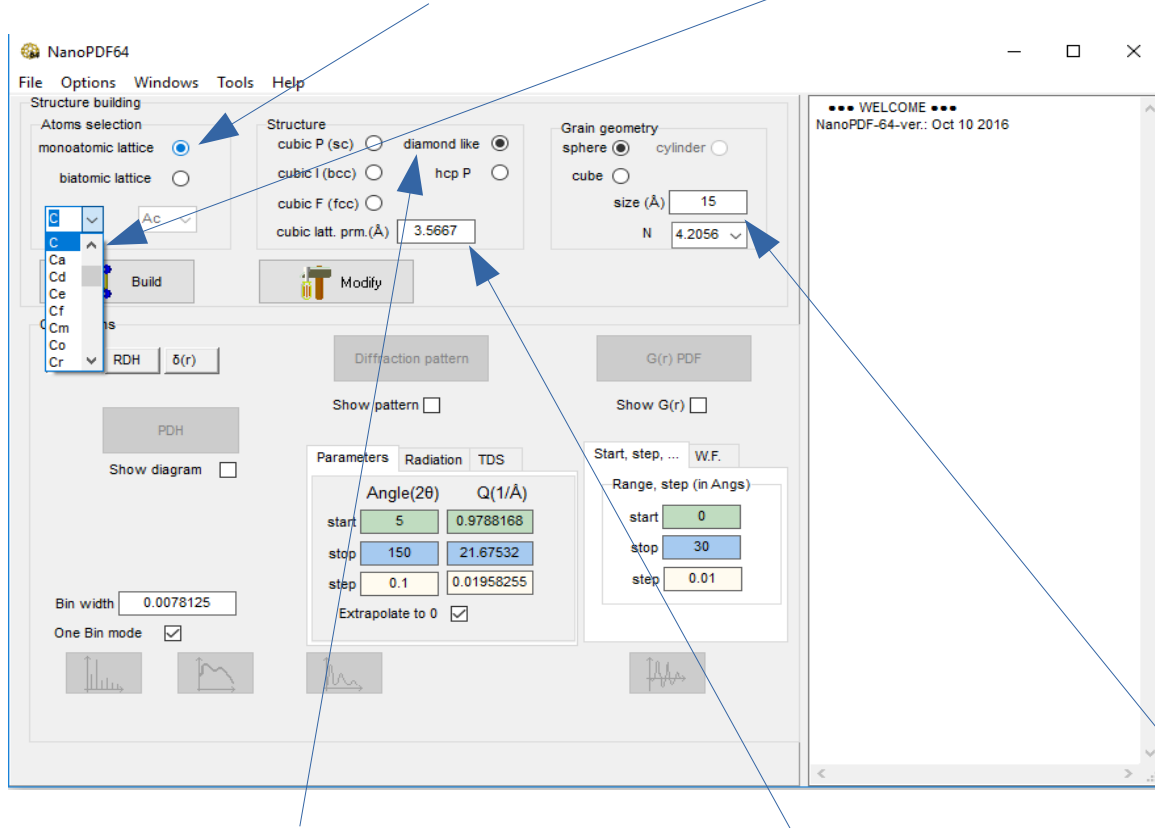
Below the fields are three checkboxes:

- Delete temporary files
- Show diagram after loading from file
- Biatomic PDH in seperate files

At the bottom are two buttons: and .

Accepted entries will show up in red. Don't worry about cpnb.bat. Confirm with "OK".

7. In main program window choose “monoatomic lattice” and select “C” from the drop-down list:



The program will suggest “diamond like” structure, the correct lattice parameter and spherical shape with 15Å radius.

8. Press “Build”. Check the number of atoms created. Choose Tools → Rastop → Ideal and look at the initial model of the nanocrystal in Rastop:

The screenshot shows the NanoPDF64 software interface. The 'Tools' menu is open, with 'Rastop' selected, and its sub-menu is also open, showing 'Ideal' as the selected option. The 'Build' button in the 'Atoms selection' panel is highlighted with a blue dashed border. The 'Ideal' model parameters are displayed in the 'Grain name' section: size (Å) is 15, and N (number of nodes) is 4,2056. The 'Parameters' section shows the following data:

Angle(2θ)	Q(1/Å)
start: 5	0.9788168
stop: 150	21.67532
step: 0.1	0.01958255

The 'Range, step (in Angs)' section shows: start: 0, stop: 32.8349557, step: 0.01. The 'Extrapolate to 0' checkbox is checked. The 'WELCOME' message in the terminal window reads: 'NanoPDF-64-ver.: Oct 1, 2016 ***** NEW STRUCTURE ***** diamond like, number of nodes=2506 ... center atoms ... index 0 C (x,y,z)=0,0,0'.

9. Press “PDH” to compute the pair distribution histogram.

The screenshot shows the NanoPDF64 software interface. The 'Calculations' section has the 'PDH' button highlighted with a blue dashed border. A blue arrow points from the text '9. Press “PDH” to compute the pair distribution histogram.' to this button. Below the 'PDH' button is a 'Show diagram' checkbox. In the 'Parameters' section, the 'Angle(2 θ)' and 'Q(1/Å)' fields are visible, with values 5, 150, 0.1, 0.9788168, 21.67532, and 0.01958255. The 'Range, step, ...' section shows 'start' at 0, 'stop' at 32.8349557, and 'step' at 0.01. At the bottom left, there are four icons representing different plots; the first icon, a histogram, is highlighted with a blue arrow pointing from the text 'Now the “graph” the button at the bottom becomes active. Press it to see the histogram.' The right-hand side of the window shows a terminal window with the following text:

```
*** WELCOME ***
NanoPDF-64-ver.: Oct 10 2016
***** NEW STRUCTURE *****
diamond like, number of nodes=2506
... center atoms ...
index 0
C
(x,y,z)=0,0,0
at num: 2506

... PDH CALCULATIONS ...
start time: 12:18:19
stop time: 12:18:20
```

Now the “graph” the button at the bottom becomes active. Press it to see the histogram.

10. Select radiation wavelength and the kind of diffraction data you want to calculate: $I(2\theta)$, $I(Q)$ or $S(Q)$. Press “Diffraction pattern”.

The screenshot shows the NanoPDF64 software interface. The 'Calculations' section is active, with the 'Diffraction pattern' button highlighted by a blue box. Below this, the 'Parameters' tab is selected, showing a wavelength λ of 0.56 Å and a 'Custom' dropdown. The 'Radiation' section has radio buttons for 'I' (selected), 'S', 'Angle(2 θ)', and 'Q(1/Å)'. The 'Range, step, ... W.F.' dialog box is open, showing a start value of 0, a stop value of 32.8349557, and a step of 0.01. At the bottom, a 'graph' button (represented by a small plot icon) is highlighted with a blue box. The right-hand pane displays a log window with the following text:

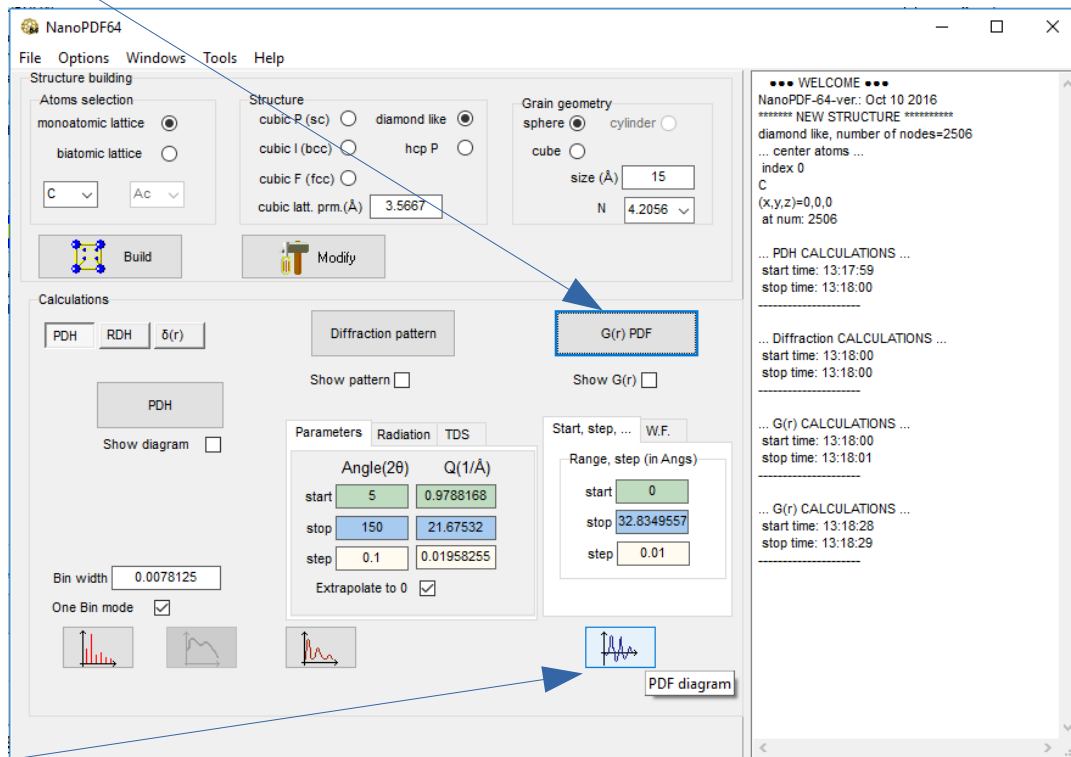
```
... WELCOME ...
NanoPDF-64-ver.: Oct 10 2016
***** NEW STRUCTURE *****
diamond like, number of nodes=2506
... center atoms ...
index 0
C
(x,y,z)=0,0,0
at num: 2506

... PDH CALCULATIONS ...
start time: 12:18:19
stop time: 12:18:20

... Diffraction CALCULATIONS ...
start time: 12:21:30
stop time: 12:21:30
```

The “graph” button at the bottom becomes active. Press it to see the pattern.

11. Press “G(r) PDF” button



The “graph” button at the bottom becomes active. Press it to see G(r).

12. Read manual to learn about all functionalities of NanoPDF64.