

# jems preferences selection

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## Contents

<b>1</b>	<b>Atom tab</b>	<b>3</b>
<b>2</b>	<b>Color tab</b>	<b>3</b>
<b>3</b>	<b>Contour tab</b>	<b>4</b>
<b>4</b>	<b>Debug tab</b>	<b>4</b>
<b>5</b>	<b>Display tab</b>	<b>5</b>
<b>6</b>	<b>Font tab</b>	<b>6</b>
<b>7</b>	<b>Imaging tab</b>	<b>7</b>
<b>8</b>	<b>Indexing tab</b>	<b>8</b>
<b>9</b>	<b>Mail tab</b>	<b>9</b>
<b>10</b>	<b>Measuring tab</b>	<b>9</b>
<b>11</b>	<b>Microscope tab</b>	<b>10</b>
<b>12</b>	<b>Miscellany tab</b>	<b>10</b>

<b>13 Noise tab</b>	<b>11</b>
<b>14 OS tab</b>	<b>11</b>
<b>15 Save As tab</b>	<b>12</b>
<b>16 VM memory tab</b>	<b>12</b>
<b>17 Web help tab</b>	<b>13</b>

# 1 Atom tab

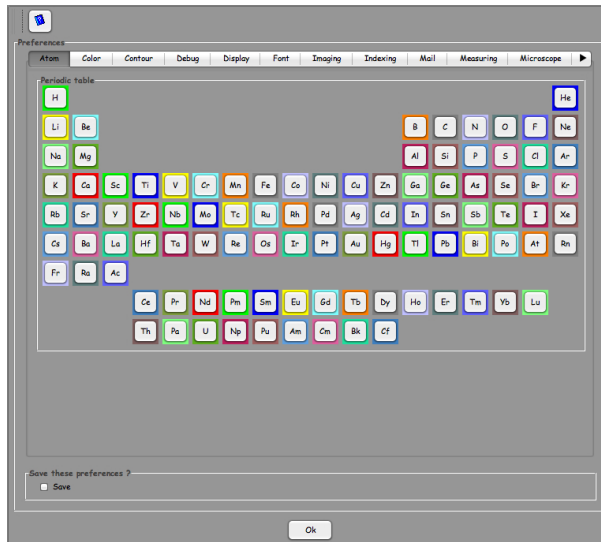


Figure 1: Atom tab: atom color selection. Figure 2: Color tab: text & panel background color selection.

The **Atom color** tab sets the atom colors<sup>1</sup>.

# 2 Color tab

The **Color** tab sets text, drawing and images background colors.

<sup>1</sup>Note that a tool tip text is attached to every control of the **Preferences dialog**.

### 3 Contour tab

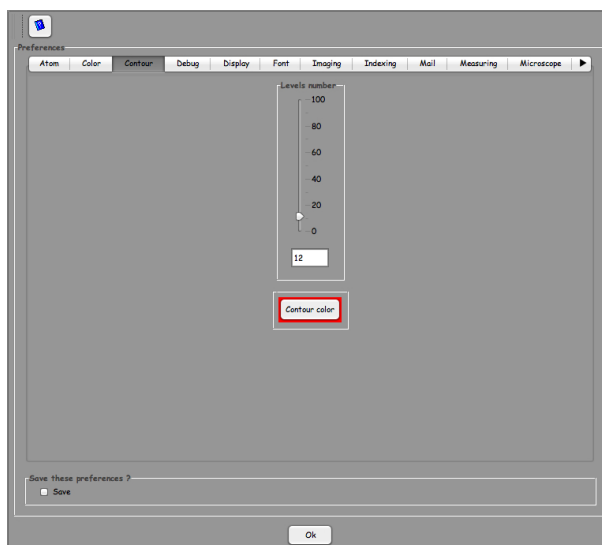


Figure 3: Contour tab: contour plot color and levels number selection.

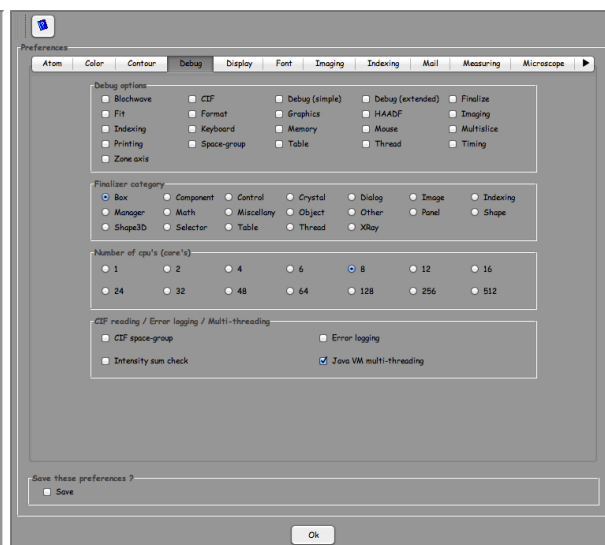


Figure 4: Debug tab: debug, finaliser and multithreading options.

The **Contour** tab sets the colour of the contour plots and the number of contour levels.

### 4 Debug tab

The **Debug** tag allows to debug jems operations (**Debug options**), to check that memory is released when dialogues and frames are close (**Finalizer category**), to set the number of available cores (**Number of cpu's**) and to set a few more options concerning .cif files reading (**CIF space-group**), error reporting (**Error loving**) and setting of java VM (**java VM multi-threading**).

When using a i7 processor set the core's number to 8 (i7 allows 2 threads per core).

## 5 Display tab

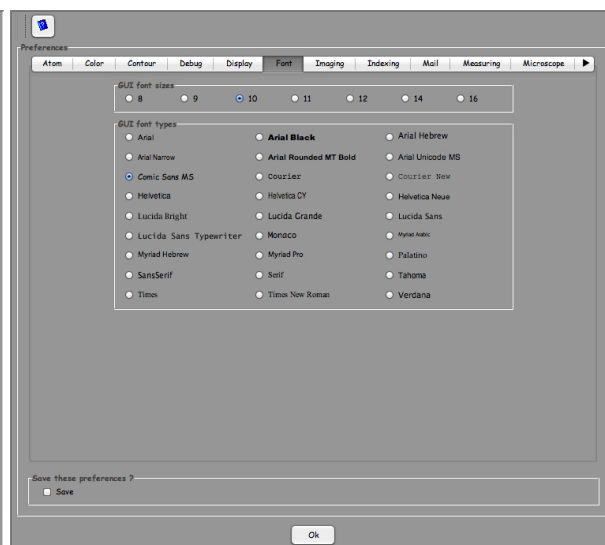
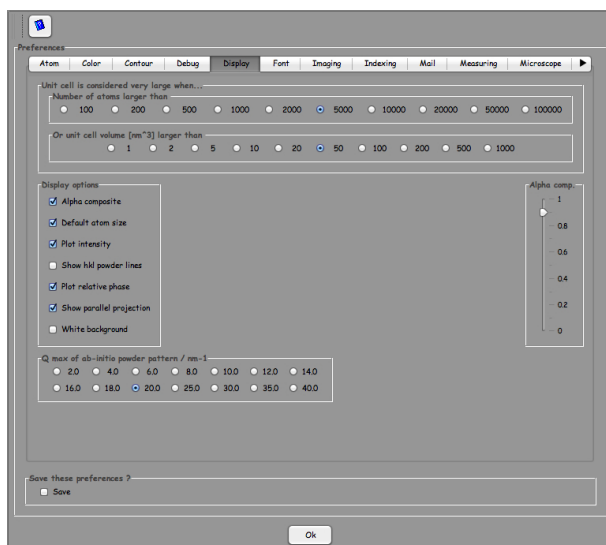


Figure 5: Display tab: sets several display options. Figure 6: Font tab: font type and size selection.

The **Display** tab deals with the display of jems drawings. The **Unit cell ...** box defines conditions to display crystal structures with minimum resolution. The **Display options** set:

1. **Alpha composite**: transparency of drawings and images. Alpha composite is set using using the slider **Alpha comp.**.
2. **Default atom size**: set the atom radius to a 50 pm default.
3. **Plot intensity**: plot the intensity of the reflections instead of the amplitude as a function of crystal thickness.
4. **Show hkl powder lines**: when set displays the hkl powder lines on transfer function plots.
5. **Show parallel projection**: show a parallel projection of the structure in jems main window.
6. **White background**: plots drawing on a white background.

The **Q max ...** set of controls places a limit on the powder lines displays.

## 6 Font tab

The **Font** tab allows to select a given font and size. The number of available fonts depends on the operating system (OS).

## 7 Imaging tab

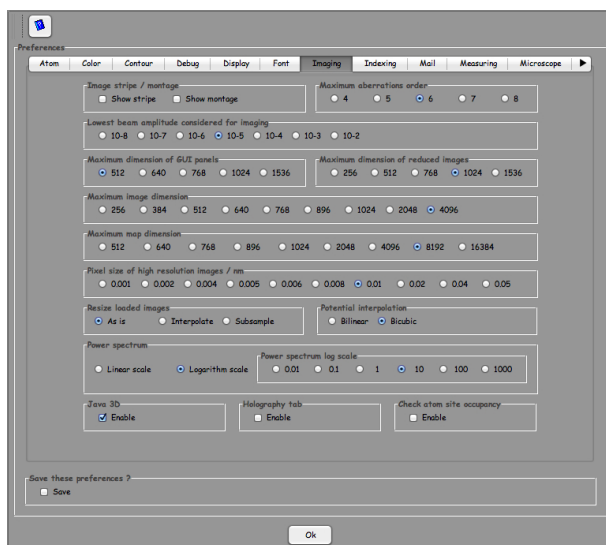


Figure 7: Imaging tab: image simulation op-

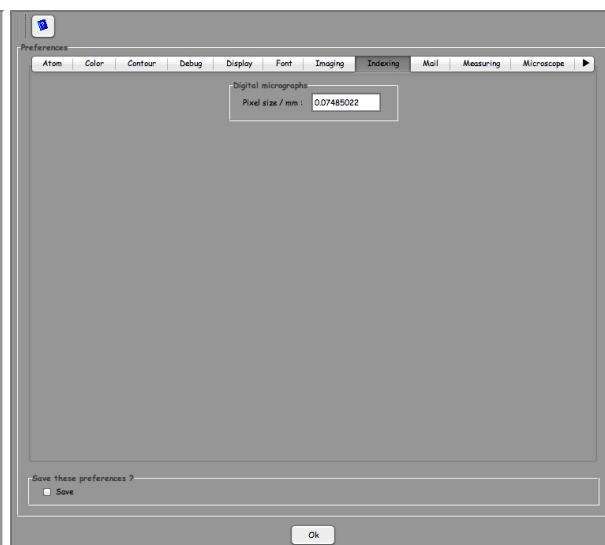


Figure 8: Indexing tab: experimental pixel size.

The **Imaging** tab groups controls and settings related to image simulation and graphical user interface (GUI). Typical settings are show in Figure 7. When using a large screen, the **Maximum dimension of GUI panels** can be increased to 1024 or more, allowing to calculate, for example, large CBED and LACBED patterns. The **Maximum image dimension** defines the maximum size of calculated images. The **Maximum map dimension** defines the maximum size of images map.

The **Pixel size of high resolution images / nm** sets the sampling used by the multislice calculation. A typical value is 0.001 nm.

The **Resize loaded images** set how experimental images are resized before being displayed. **Potential interpolation** sets the method employed to interpolate projected potential.

The **Java 3D**, **Holography tab** and **Check atom site occupancy** check boxes allow to display crystal structures using OpenGL, to simulate holograms and to check the occupancy of every atom site in a structure.

## 8 Indexing tab

The **Indexing** tab sets the experimental pixel size.



## 9 Mail tab

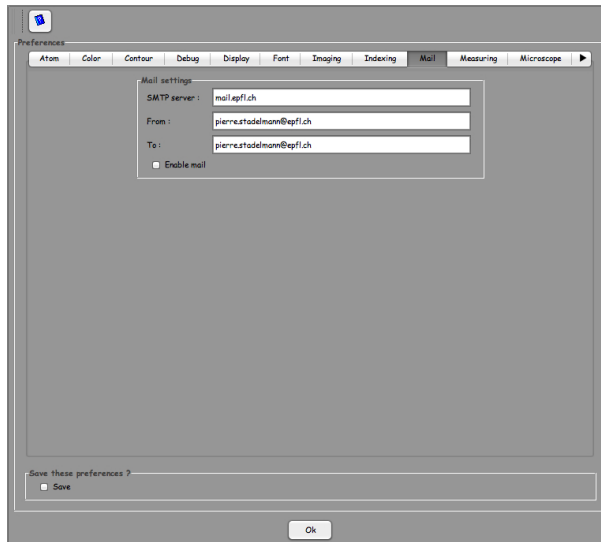


Figure 9: Mail tab: e-mail settings.

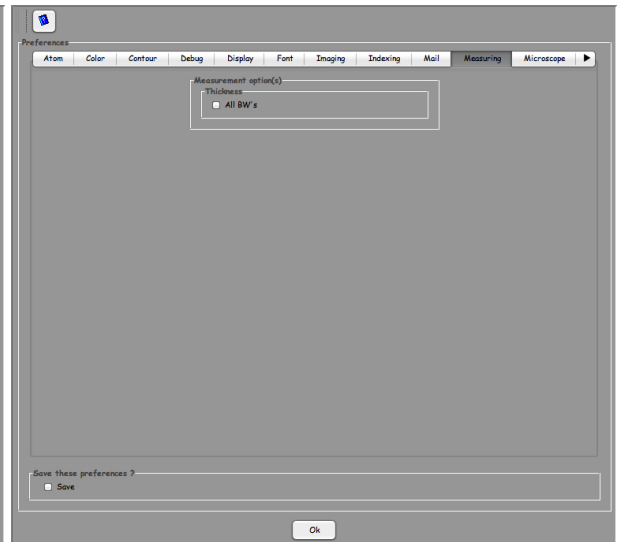


Figure 10: Measuring tab: QCBED profile option.

The **Mail** tab defines the out going mail server, your e-mail address and the e-mail address of the recipient. The **Enable mail** check box is used to mail newly created crystal files.

## 10 Measuring tab

The **Measuring** tab defines how QCBED thickness profiles are calculated. QCBED uses the Bloch wave method and a limited number of reflections can be included in the calculations.

## 11 Microscope tab

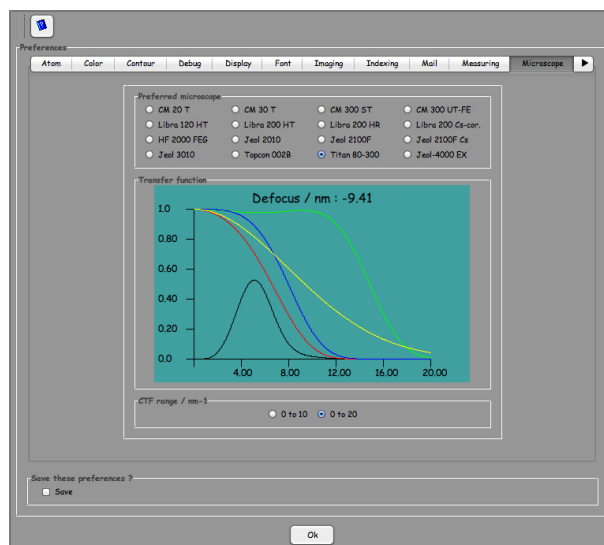


Figure 11: Microscope tab: defines the default microscope.

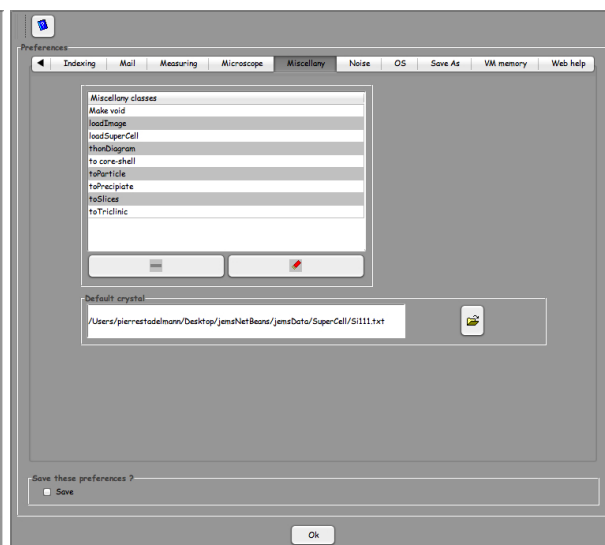


Figure 12: Miscellany tab: defines the default crystal.

The **Microscope** tab sets the microscope characteristics<sup>2</sup> and the range of the contrast transfer function (CTF) plots. Note that  $20 \text{ nm}^{-1}$  corresponds to  $0.5 \text{ \AA}$ .

## 12 Miscellany tab

The **Miscellany** tab sets primarily the default crystal, i.e. the crystal that is loaded at start time.

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<sup>2</sup>Microscopes not defined here can be created using the *Microscope dialogue*.

## 13 Noise tab

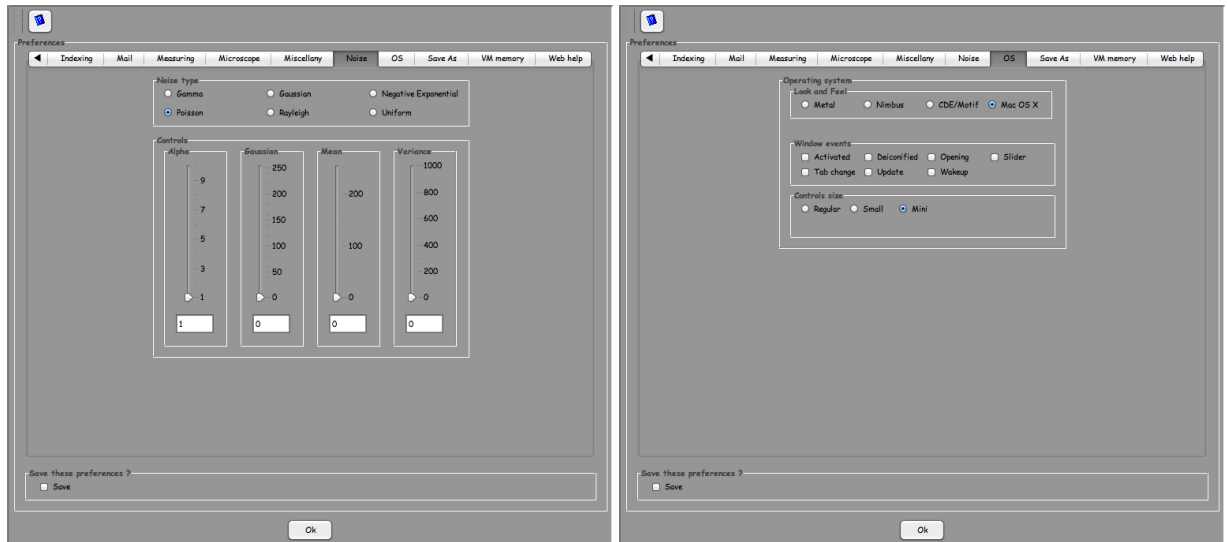


Figure 13: Noise tab: characteristics of the graphical noise that can be added to simulated images. Figure 14: OS tab: look and feel of graphical user interface.

The **Noise** tab defines the type and amplitude of the noise that can be added to simulated images.

## 14 OS tab

The **OS** tab sets the *Look and Feel* of the user interface and allows to activate a few type of windows events (when not taking into account by the OS).

## 15 Save As tab

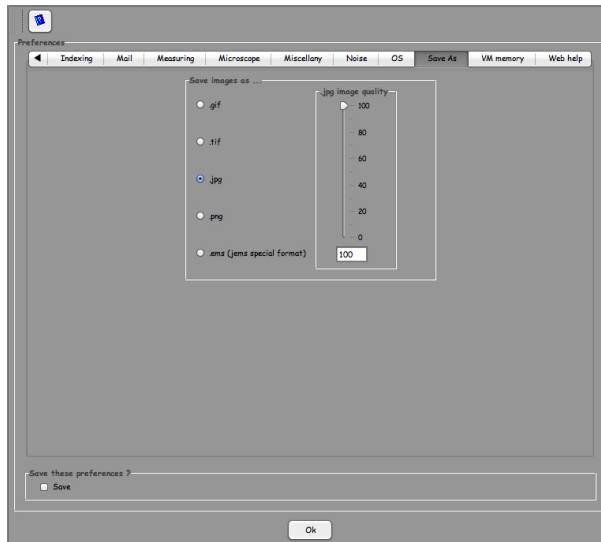


Figure 15: Save As tab: format of saved images.

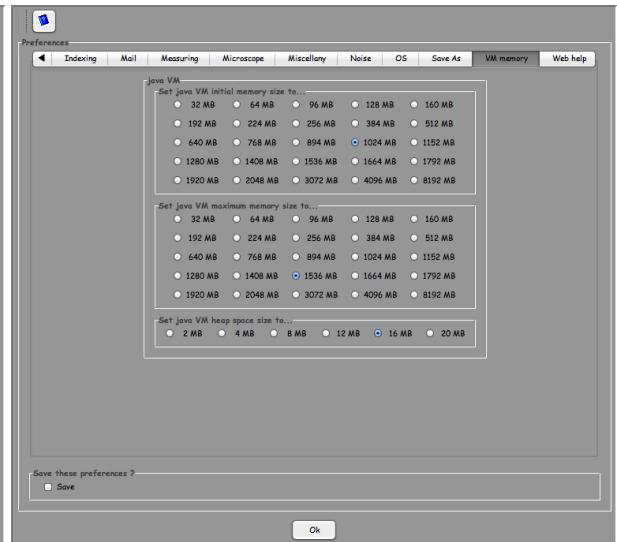


Figure 16: VM memory tab: java VM memory settings.

The **Save As** tab defines in which format images or drawings must be saved<sup>3</sup>.

## 16 VM memory tab

The **VM memory** tab defines the size of java VM memory allocated at start time, the maximum size of java VM memory and the stack size.

<sup>3</sup>The jems format is not always available.

## 17 Web help tab

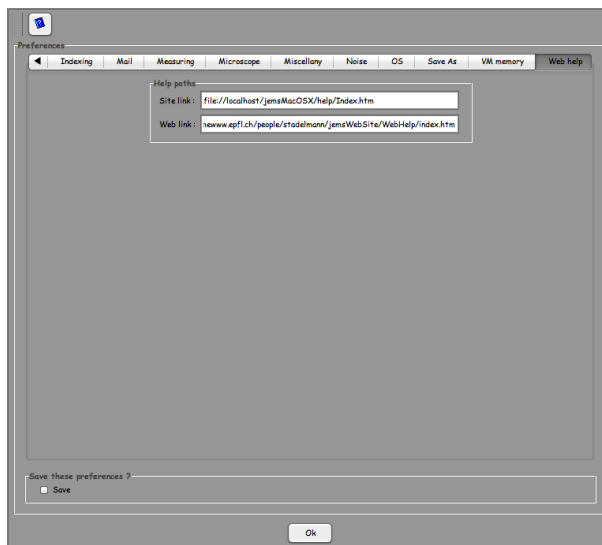


Figure 17: Web help tab: url of help files.

The **Web help** tab defines the url of jems help files and the url web site where more info is available.