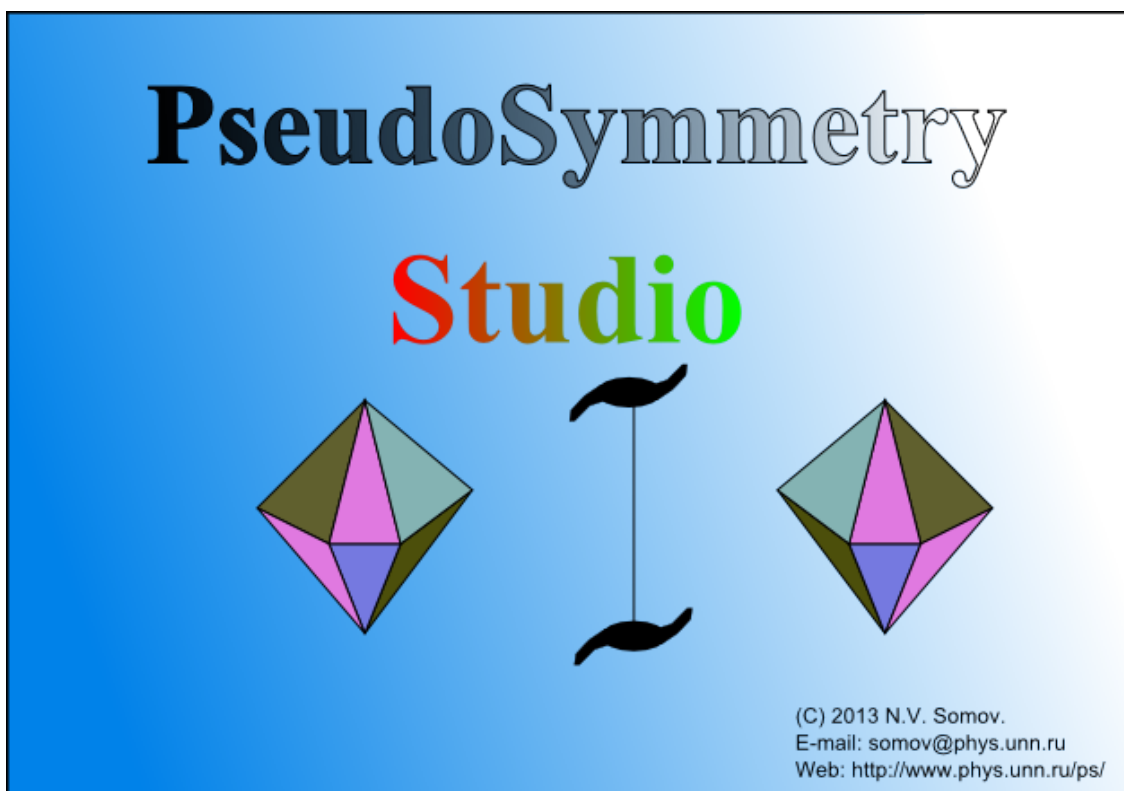


PseudoSymmetry Studio

Quick Start Guide



1. Install and launch **PseudoSymmetry Studio**.

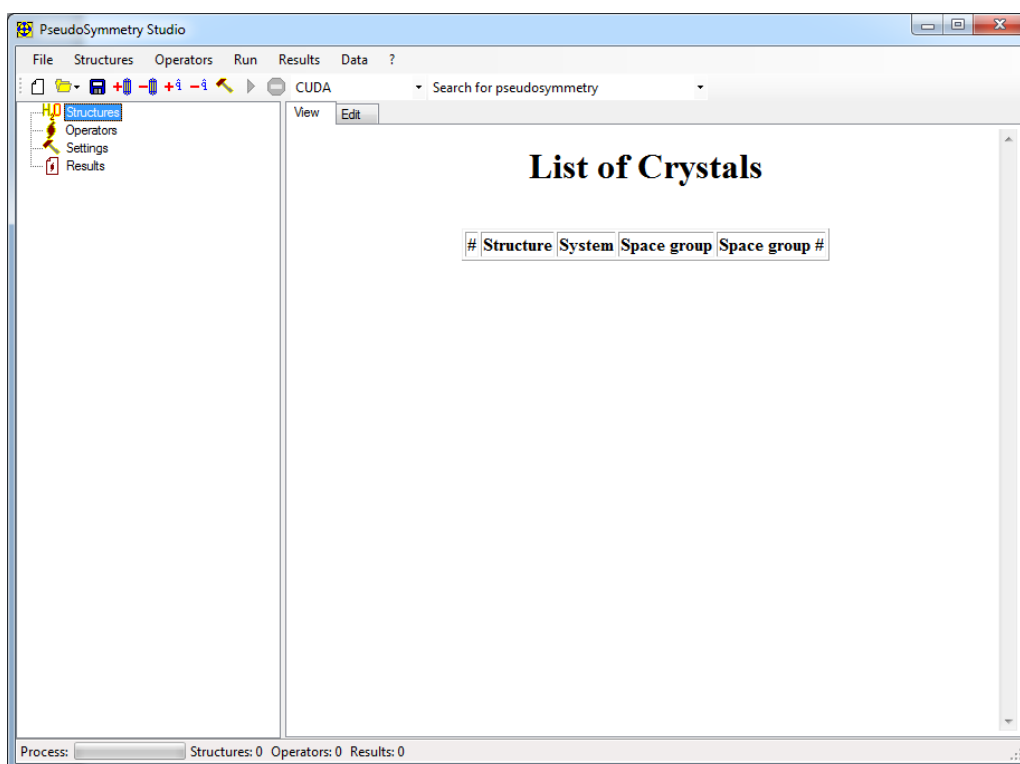


Fig. 1. Main window of **PseudoSymmetry Studio**

2. Click right mouse button on «Structure» in the navigator panel (left part of the PSS window) and import structure information from CIF-file or RES-file (see Fig. 2). Description of the CIF-file format you can find on: <http://www.iucr.org/resources/cif>, <http://it.iucr.org/G/>. Also you can use output file of the SHELX software (<http://shelx.uni-ac.gwdg.de/SHELX/>).

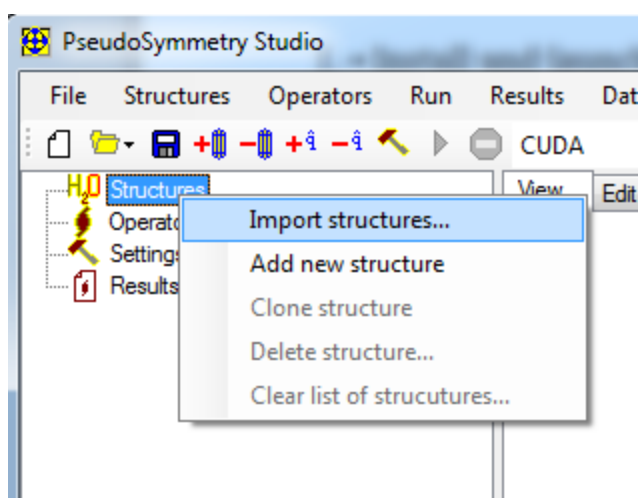


Fig. 2. Import structure information

It's also possible to input the crystal structure information manually («Add new structure», see Fig. 2). The editing of crystal structure information is carried out in special editor (see Fig. 3)

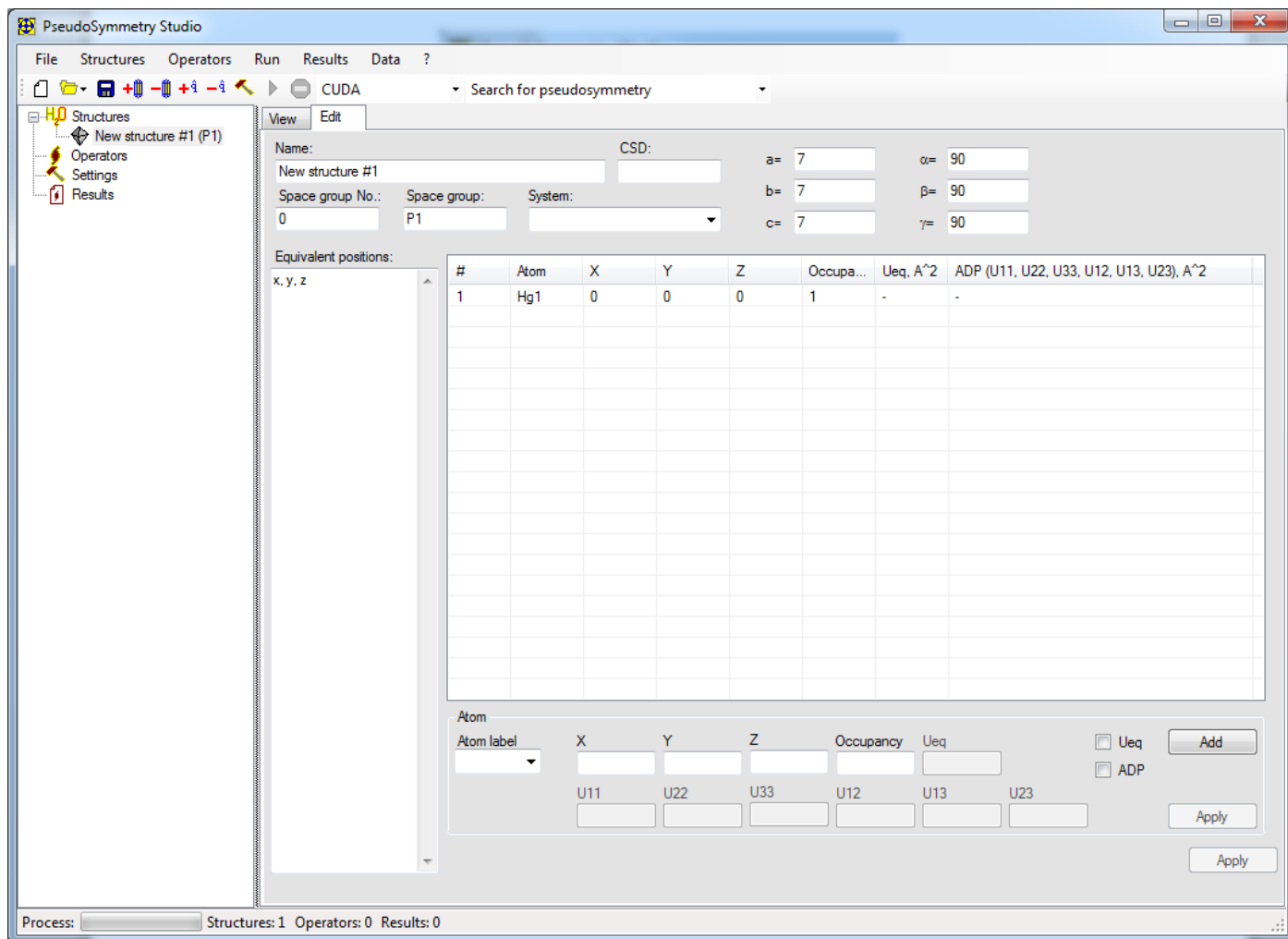


Fig. 3. Crystal structure information editor window

3. Add the operator of the transformation (see Fig. 4). For example, let we want calculate the degree of invariance of the electron density with respect to the inversion at $\mathbf{r}=(0.333, 0.666, 0.25)$ position. This transformation consists of the matrix \mathbf{m} and the translation vector \mathbf{t} :

$$\mathbf{m} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}; \mathbf{t} = 2 * \mathbf{r} = \begin{pmatrix} 0.666 \\ 1.332 \\ 0.5 \end{pmatrix}$$

The point of inversion is located at the half of the translation vector \mathbf{t} . Enter new components of translation vector as shows Fig. 5 and click «Apply».

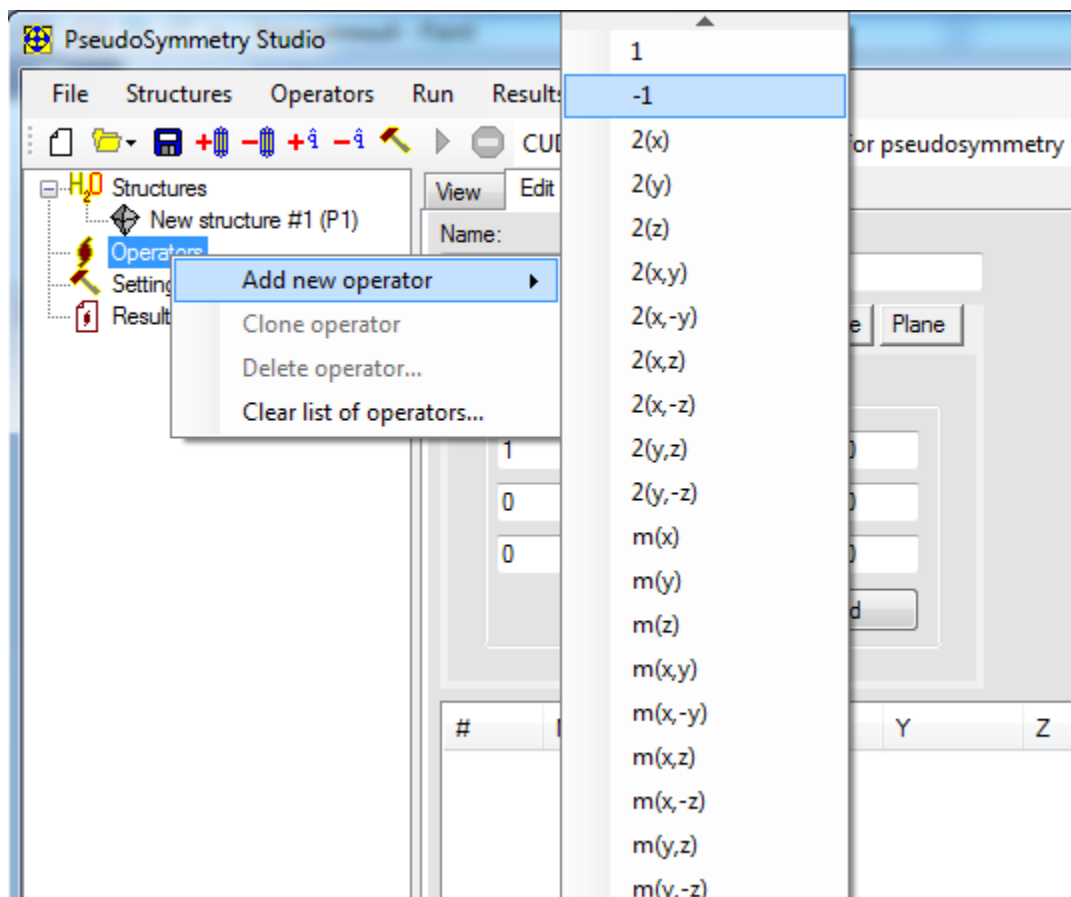


Fig. 4. Adding of the transformation operator

On Fig. 5 shows the editor for transformation operator.

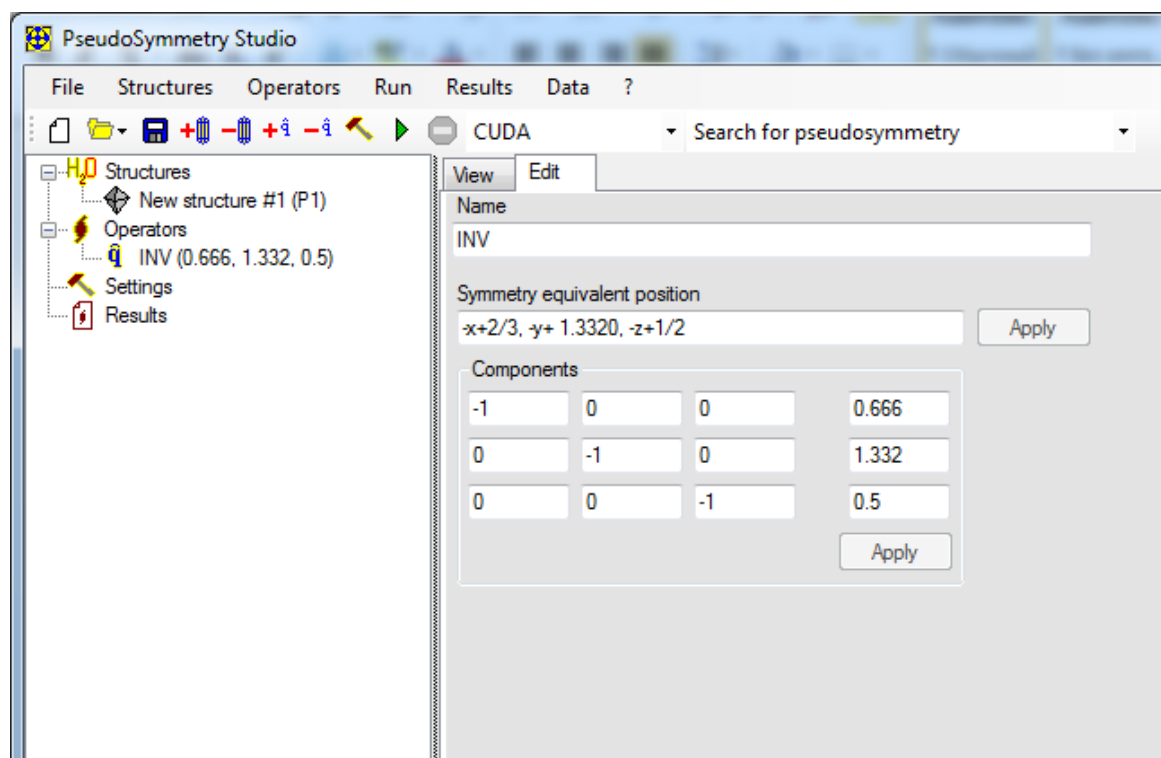


Fig. 5. Input the transformation operator (inversion)

Note: The translation vector is not required if you use «Search for pseudosymmetry» method. In this case the translation vector determined automatically by the maximum of the degree of invariance of the electron density.

4. You can choose additional option in the settings editor window (Fig. 6). In this window you can set the type of the target calculation device (CPU – central processor, CUDA – High performance calculation on NVidia GPU (if you have CUDA-device, <https://developer.nvidia.com/cuda-zone>)).

The calculation method:

- **Search for pseudosymmetry** – search for peak of the degree of invariance of the electron density for the specific rotation matrix.
- **Refine for pseudosymmetry** – refine the translation vector for transformation operator.
- **Calculate for pseudosymmetry** – Calculate the degree of invariance of the electron density with respect to the specific transformation operator.

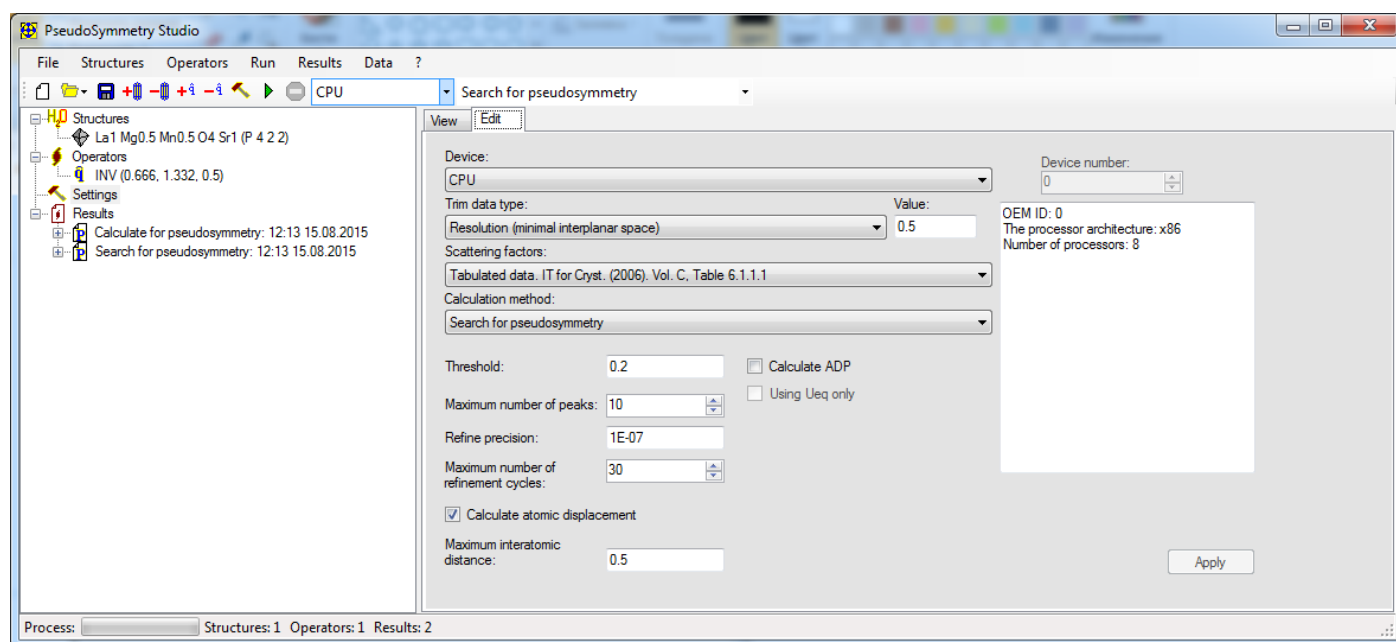


Fig. 6. The settings editor window.

Calculate atomic displacements – enables the calculations of atomic displacements which determines the difference between real and ideal symmetric positions.

5. Launch the calculation (see Fig. 7). Also you can use main menu «Run» or shortcut key F9.

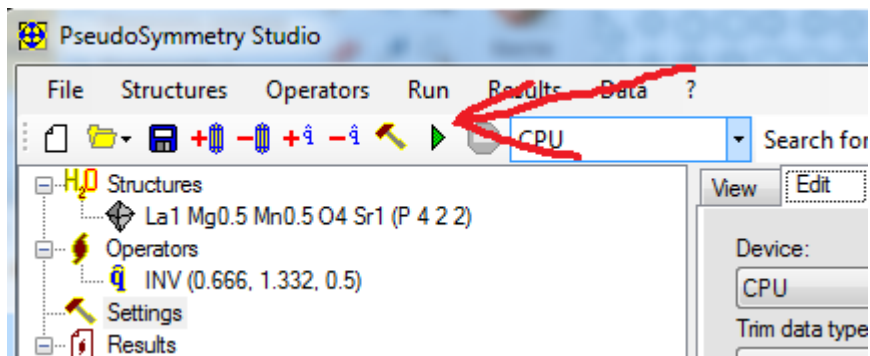


Fig. 7. Launch the calculation.

6. See results. For showing results click on **Results** in navigator (see Fig. 7-8).

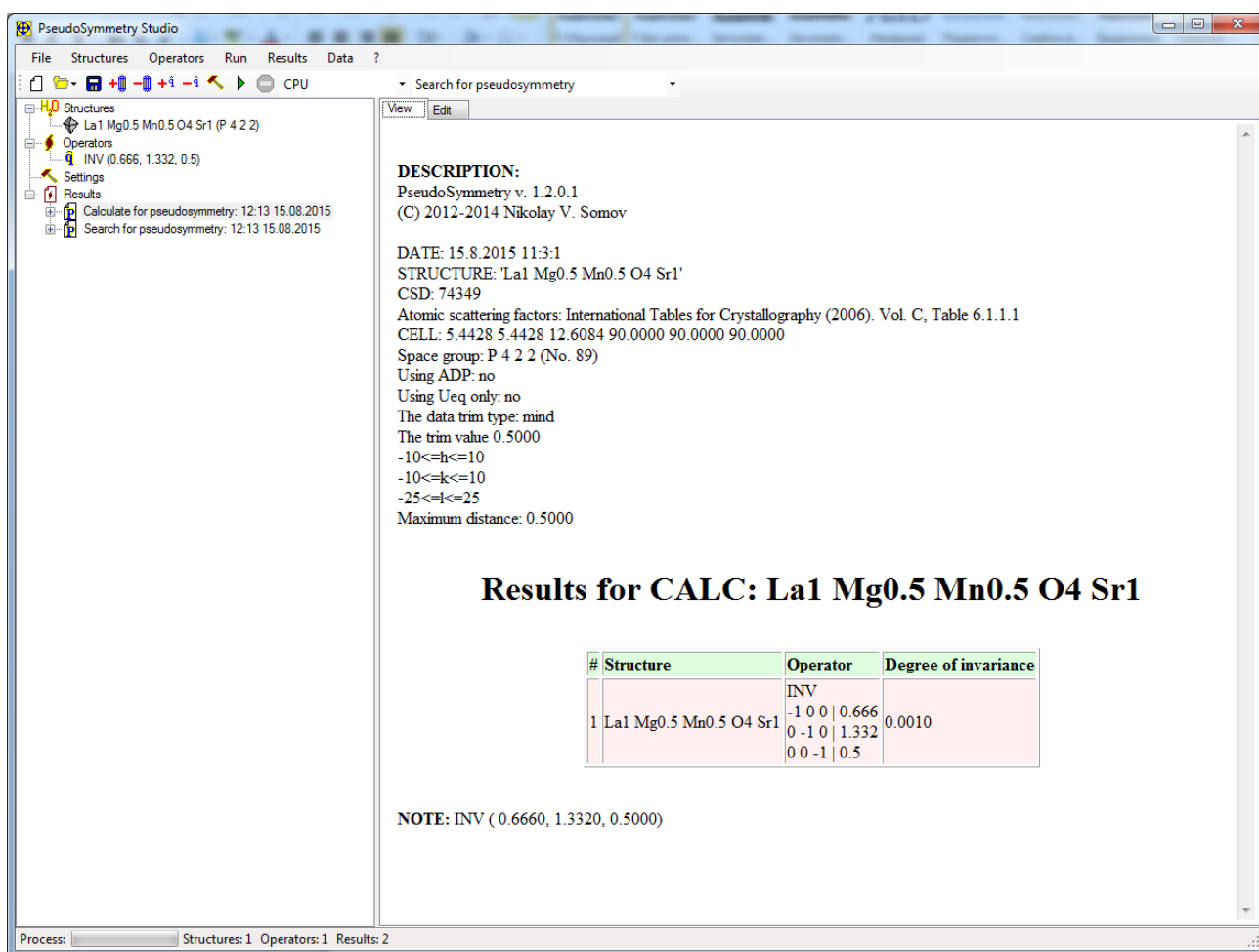


Fig. 7. Result for the inversion at (0.333, 0.666, 0.25) position. Uses *Calculate for pseudosymmetry* method

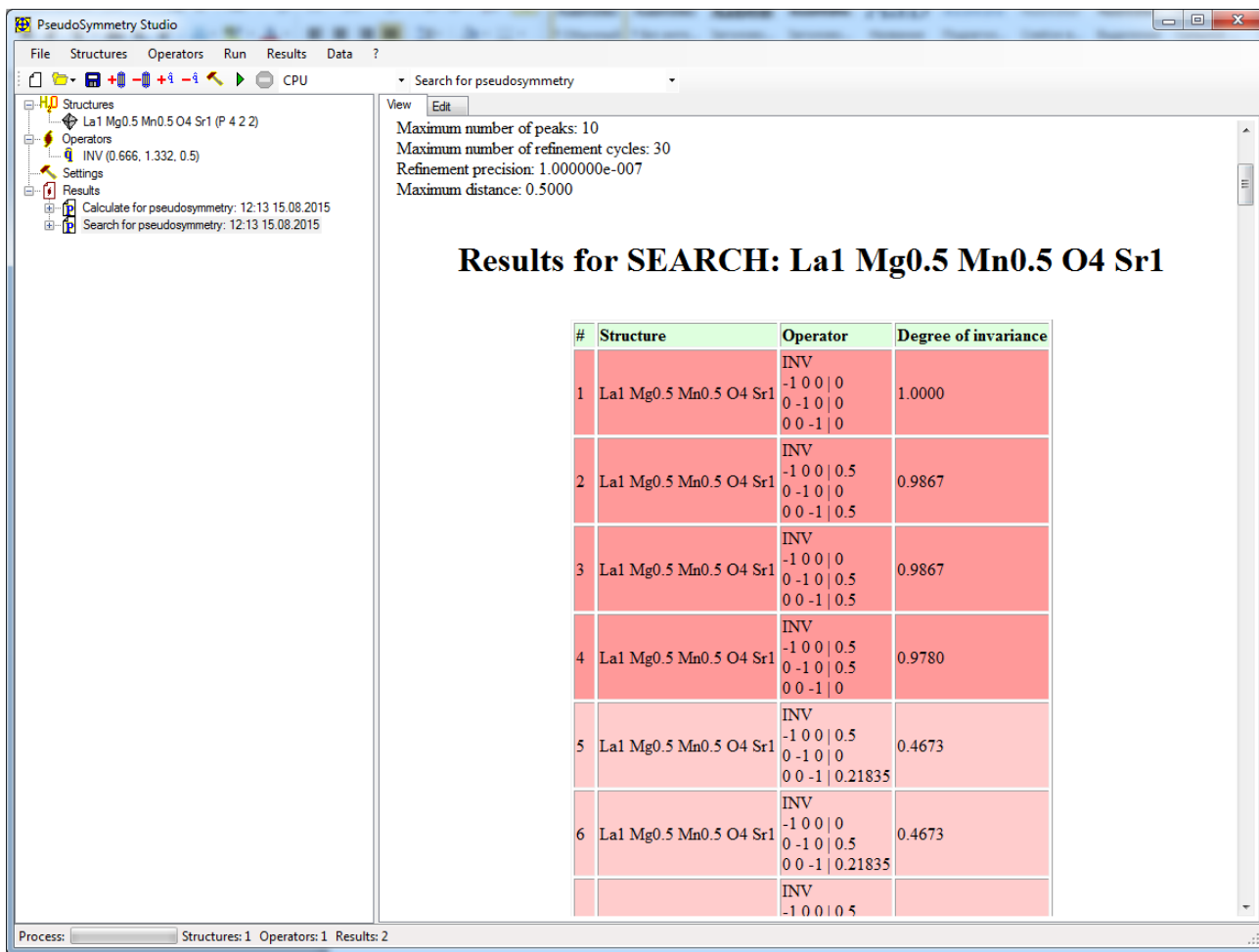


Fig. 8. Results for the inversion (*Search for pseudosymmetry* method)

The short conclusion for the La1 Mg0.5 Mn0.5 O4 Sr1 crystal: possible error in the space group for this crystal. Because the degree of invariance of the electron density with respect to the inversion at (0, 0, 0) position is **1.0** (maximal value). Possible that the La1 Mg0.5 Mn0.5 O4 Sr1 crystal structure is centrosymmetrical.