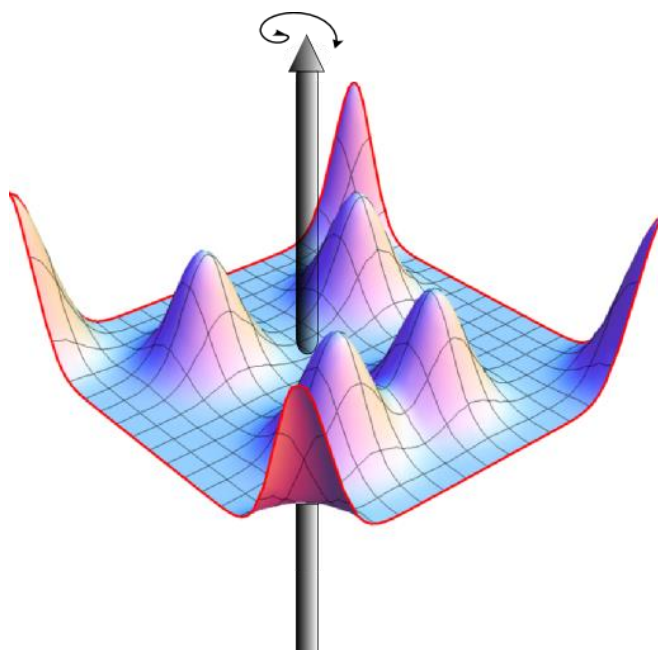Lobachevsky State University of Nizhni Novgorod

The computer program

PseudoSymmetry

(User Manual)

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Contents

1. The program PseudoSymmetry

PseudoSymmetry is the computer program for investigation of the pseudosymmetry in crystals. The functional of the electron density is used as the quantitative estimation of the degree of invariance of a crystal (see Section 2).

1.1. Features of the program PseudoSymmetry

1. The **PseudoSymmetry** program allows for calculation the degree of invariance of the electron density by different methods.

2. The electron density is calculated on the basis of structure factors which can be obtained through the following methods:

   2.1. The calculation of structure factors based on structural information about a crystal: lattice parameters, space group, atomic types, coordinates and scattering factors [1].

   2.2. The import of calculated structure factors from external sources.

2.3. The import of experimental structure factors from external sources.

3. Follow methods of calculation of the degree of invariance of the electron density are implemented:

3.1. The calculation of the degree of invariance of the electron density with respect to a transformation operator (**simple**, see Section 2.5.).

3.2. The refinement of the translation vector for the transformation operator. Search for the local maximum of the degree of invariance of the electron density (**refine**, see Section 2.7.).

3.3. The calculation of the map of the degree of invariance of the electron density for defined transformation matrix (**map**, see Section 2.6.).

3.4. Search for translation vectors of the transformation operator which correspond to local maxima of the degree of invariance of the electron density (**smart**, see Section 2.8.).

3.5. The calculation of atomic displacements (**displacement**, see Section 2.9.).

4. The program supports several formats of output data.

1.2.   System requirements

The **PseudoSymmetry** program is a console application. Windows (32/64, NT) 2000/XP/Vista/Windows 7 is required to launch the program. The program uses the libraries **FFTW** [2, 3] for **FFT** implementation. The required memory capacity depends on the size of the reciprocal space engaged in calculations (1 GB or higher is recommended). Most of the algorithms of the program involve **OpenMP** parallel computing (Open Multi-Processing), therefore, the program works best on multiprocessor and multicore systems.

The **PseudoSymmetry** program supports the high performance calculation on graphics processing units (**GPU**) with **CUDA** [4]. This feature requires **CUDA** compatible device installed on your computer. The **CUDA** calculation module uses **CUDA v.5** environment. Using **CUDA**-module allows substantially increase the speed of the calculation. The recommended memory size for **CUDA**-device is 512 MB or higher.

1.3.   Running PseudoSymmetry

The following command line instructions is recommended for the first run of the program

```
>ps temp "file name"
```

This command creates a template file for input parameters of the program **PseudoSymmetry**. The template file contains all the program options available in this version. Each option is provided with a brief description and is set to default. Detailed program options described in Section 3.

The following is the listing of the minimal input file of the program:

```
_pseudo_output   'path to the results of calculations'
_pseudo_input_type   cif

loop_
_pseudo_input_file
'the path to the CIF-file containing structural information about the crystal'

_pseudo_calc_threshold   0.08
_pseudo_calc_max_peaks   5

_pseudo_calc_method  smart

loop_
_pseudo_operator_name
_pseudo_operator_M11
_pseudo_operator_M12
_pseudo_operator_M13
_pseudo_operator_M21
_pseudo_operator_M22
_pseudo_operator_M23
_pseudo_operator_M31
_pseudo_operator_M32
_pseudo_operator_M33
_pseudo_operator_V1
_pseudo_operator_V2
_pseudo_operator_V3
'INV' -1 0 0 0 -1 0 0 0 -1 0 0 0
```

This file orders the computations of the degree of invariance of the electron density with respect to the inversion operator for 5 most strong values of the degree of invariance of the electron density (if available) for the crystal structure from the CIF-file. For details, see Sections 2 and 3.

The calculations are launched with the following command:

>ps "the name of the input file of program options"

For example, ps run "c:\ps\param1.txt".

2. The theoretical background

2.1. Transformation operators

A general transformation of the coordinate system consists of two parts, a linear part (matrix) and a shift of origin (translation vector) [5]. The linear part implies a change of orientation or length or both of the basis vectors. The shift of origin is defined by the shift vector, called a translation vector.

The transformation operator is denoted as

$$\hat{q} = \{q \,|\, \vec{t}\}, \tag{2.1.1}$$

where q is the linear part (next – the matrix), $\vec{t}$ is the translation vector. The action of the operator (2.1.1) on an arbitrary vector $\vec{r}$ has the form

$$\hat{q}\vec{r} = q\vec{r} + \vec{t}. \tag{2.1.2}$$

The translation vector of the transformation operator determines the type of the symmetry element. For example, the 2-fold axis along Z has the form

$$\left\{ \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \right\}, \tag{2.1.3}$$

the 2-fold screw axis along Z has the form

$$\left\{ \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0.5 \end{pmatrix} \right\}. \tag{2.1.4}$$

Also the translation vector of the transformation operator determines the position of the symmetry element. For example, the center of the inversion at (¼, ¼, ¼,) position has the form

$$\left\{ \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 0.5 \\ 0.5 \\ 0.5 \end{pmatrix} \right\}. \tag{2.1.5}$$

It should be noted that the vector $\vec{t}$ in the operator $\hat{q}$ is not equal to the vector determines the position of the corresponding element of the symmetry. For example, if the center of inversion is located at the point $\vec{p}$, then the corresponding the transformation operator takes the form $\{\bar{1} \,|\, 2\vec{p}\}$.

In the general case the position of the element of symmetry is convenient to find, using the following system of linear equations

$$\hat{q}\vec{p} = \vec{p}. \tag{2.1.6}$$

This system of equations is a system for finding the eigenvectors of the operator $\hat{q}$ corresponding to the eigenvalue +1.

Let's consider a few examples of the analysis of systems of linear equations (2.1.6). Let the inversion operator has the form

$$\hat{q} = \{\overline{1} \mid \vec{t}\}. \tag{2.1.7}$$

Let's find from (2.1.6) the vector $\vec{p}$ which is the position of the center of inversion

$$\{\overline{1} \mid \vec{t}\}\vec{p} = \vec{p} \Rightarrow -\vec{p} + \vec{t} = \vec{p} \Rightarrow \vec{p} = \frac{1}{2}\vec{t}. \tag{2.1.8}$$

The center of inversion is located at half the translation $\vec{t}$. Consider another example. Let $\hat{q}$ is the 2-fold screw axis along Z

$$\hat{q} = \left\{ 2_z \mid \begin{pmatrix} t_x \\ t_y \\ 1/2 \end{pmatrix} \right\}, \tag{2.1.9}$$

This transformation operator has no stationary points ($\hat{q}\vec{r} \neq \vec{r}$ for all $\vec{r}$ in direct space). The system of the linear equation (2.1.6) has the next form

$$\begin{pmatrix} -p_x \\ -p_y \\ p_z \end{pmatrix} + \begin{pmatrix} t_x \\ t_y \\ 1/2 \end{pmatrix} = \begin{pmatrix} p_x \\ p_y \\ p_z \end{pmatrix}, \tag{2.1.10}$$

where $\begin{pmatrix} p_x \\ p_y \\ p_z \end{pmatrix} = \vec{p}$. After the transformation (2.1.10) obtain the expression

$$\begin{pmatrix} 2p_x \\ 2p_y \\ 0 \end{pmatrix} = \begin{pmatrix} t_x \\ t_y \\ 1/2 \end{pmatrix}. \tag{2.1.11}$$

The equation for p_z has no solution, this means that the coordinate p_z of the 2-fold screw axis along Z is not determined. In this case, p_z can have any value. Coordinates p_x and p_y are the corresponding coordinates of the axis of symmetry and are uniquely determined as

$$p_x = \frac{1}{2}t_x$$
$$p_y = \frac{1}{2}t_y$$

(2.1.12)

In such a way it is easy to find the position of any element of symmetry.

$$p_x = \frac{1}{2}t_x$$
$$p_y = \frac{1}{2}t_y$$

2.2. The functional of the degree of invariance of the electron density

The electron density of the crystal is limited, periodic, positive definite function and reflects the symmetry of the crystal. The symmetry of the electron density of the crystal is described by the same symmetry as the atomic structure. If the crystal is pseudosymmetric then some part of its electron density is invariant with respect to the group H, where H is the supergroup of the symmetry group G of the crystal ($H \supset G$).

The supergroup H can be decomposed into left cosets with respect to G as follows

$$H = G \cup h_1 G \cup h_2 G \cup ... \cup h_i G, \tag{2.2.1}$$

where h_i are operators of symmetry which belong to the supergroup H and do not belong to the group G ($h_i \in H \wedge h_i \notin G$).

In [6] proposed a method for estimates the symmetry of crystals with the functional of the degree of invariance of the electron density

$$\eta_{\hat{q}}[\rho(\vec{r})] = \frac{\int\limits_V \rho(\vec{r}) \rho(\hat{q}\vec{r}) dV}{\int\limits_V \rho^2(\vec{r}) dV}, \tag{2.2.2}$$

where $\rho(\vec{r})$ is an electron density, $\hat{q}$ is a transformation operator. The integration in (2.2.2) is over the unit cell volume V. Since the function of the electron density is non-negative range of possible values of the functional (2.2.2) is limited to the interval (0,1] (greater than 0 and less than or equal to 1). Quantity $\eta_{\hat{q}}[\rho(\vec{r})]$ characterizes the fraction of the electron density $\rho(\vec{r})$ of the crystal is invariant with respect to the transformation $\hat{q}$. If $\hat{q}$ is the symmetry operator and belongs to G, then $\eta_{\hat{q}}[\rho(\vec{r})]$ is identically equal to unity ($\eta_{g_i}[\rho(\vec{r})] \equiv 1, g_i \in G$). If $\hat{q} = h_i$ then $\eta_{h_i}[\rho(\vec{r})] \in (0,1)$.

The closer to the unit $\eta_{h_i}[\rho(\vec{r})]$, the greater the proportion of the electron density is invariant with respect to the transformation h_i and the higher the pseudosymmetry of the crystal.

Calculation of the functional (2.2.2) is conveniently carried out in reciprocal space. For this we use the expansion of the electron density in a Fourier series

$$\rho(\vec{r}) = \frac{1}{V} \sum_{\vec{H}} F(\vec{H}) \exp\left(-2\pi i (\vec{H}, \vec{r})\right), \tag{2.2.3}$$

where $\vec{H}$ is the vector of the reciprocal space, $F(\vec{H})$ is the structure factor, V is the unit cell volume. Summation in (2.2.3) is over all reciprocal space. Values of the structure factors $F(\vec{H})$ can be obtained in different ways, structural factors can be calculated analytically or measured experimentally. Analytical formula for the calculation of structure factors has the form

$$F(\vec{H}) = \sum_{j=1}^{N} f_j(\vec{H}) O_j T_j \exp\left(2\pi i\left(\vec{H}, \vec{r}_j\right)\right), \tag{2.2.4}$$

where $f_j(\vec{H})$ is the atomic scattering factor [1], O_j is the occupation of the j-th atom, T_j is the atomic Debye-Waller factor or the atomic temperature factor [7], $\vec{r}_j$ is coordinates of the j-th atoms. Summation in (2.2.4) is over all atoms (N) of the unit cell.

Rewrite (2.2.2) with (2.2.3) and (2.1.2)

$$\eta_q[\rho(\vec{r})] = \frac{\int_V \sum_{\vec{M}} F(\vec{M}) \exp\left(-2\pi i\left(\vec{M}, \vec{r}\right)\right) \sum_{\vec{H}} F(\vec{H}) \exp\left(-2\pi i\left(\vec{H}, q\vec{r} + \vec{t}\right)\right) dV}{\int_V \rho^2(\vec{r}) dV}. \tag{2.2.5}$$

Consider separately the numerator of (2.2.5) and carry out the regrouping of terms

$$\sum_{\vec{M}} \sum_{\vec{H}} F(\vec{H}) F(\vec{M}) \exp\left(-2\pi i\left(\vec{H}, \vec{t}\right)\right) \int_V \exp\left(-2\pi i\left\{\left(\vec{M}, \vec{r}\right) + \left(\vec{H}, q\vec{r}\right)\right\}\right) dV. \tag{2.2.6}$$

The integral in (2.2.6) is nonzero only at points, where argument of the exponential vanishes

$$\left(\vec{M}, \vec{r}\right) + \left(\vec{H}, q\vec{r}\right) = 0. \tag{2.2.7}$$

From (2.2.7) can obtain the relation for the vectors $\vec{H}$ and $\vec{M}$

$$\vec{M} = -q^T \vec{H}, \tag{2.2.8}$$

where q^T is the transposed matrix of $\hat{q}$. Upon condition (2.2.8) the integral in (2.2.6) is identically equal to unity. Rewrite (2.2.6) with (2.2.8)

$$\int_V \rho(\vec{r}) \rho(\hat{q}\vec{r}) dV = \sum_{\vec{H}} F(\vec{H}) F(-q^T \vec{H}) \exp\left(-2\pi i\left(\vec{H}, \vec{t}\right)\right). \tag{2.2.9}$$

Let's evaluate the integral in the denominator of (2.2.5). The integral can be computed by (2.2.9) by taking $\hat{q}$ equal to the identity transformation

$$\int_V \rho(\vec{r})\rho(\vec{r})dV = \sum_{\vec{H}} F(\vec{H})F(-\vec{H}) = \sum_{\vec{H}} \left| F(\vec{H}) \right|^2 . \tag{2.2.10}$$

Let's write the final expression for the calculation of (2.2.2)

$$\eta_{\hat{q}}[\rho(\vec{r})] = \frac{\sum_{\vec{H}} F(\vec{H})F(-q^T\vec{H})\exp\left(-2\pi i(\vec{H},\vec{t})\right)}{\sum_{\vec{H}} \left| F(\vec{H}) \right|^2}, \tag{2.2.11}$$

where $F(\vec{H})$ is the structure factor, q^T is the transposed matrix of the operator $\hat{q}$, $\vec{t}$ is the translation vector of the operator $\hat{q}$.

The range of summation indices (h, k and l) of the reciprocal vector $\vec{H}$ in (2.2.11) is limited. Calculation (2.2.11) for different ranges of (h, k and l) leads to obtaining different values of $\eta_{\hat{q}}[\rho(\vec{r})]$ for same electron density $\rho(\vec{r})$. Decrease the range of indices h, k and l leads to an electron density peak broadening and increasing of $\eta_{\hat{q}}[\rho(\vec{r})]$ value. Therefore, a comparison of the absolute values $\eta_{\hat{q}}[\rho(\vec{r})]$ for different crystals is possible only if the equivalence range h, k and l are used in (2.2.11).

For convenience and unification of the data ranges of the indices h, k and l describe the two characteristics. The first of them is $\dfrac{\sin\theta_{max}}{\lambda}$, where θ_{max} is the maximal diffraction angle, λ is the wave length. The value $\dfrac{\sin\theta_{max}}{\lambda}$ ranges from 0 to ∞, the dimension is the inverse angstroms (Å^{-1}).

The second characteristic of the range of indices h, k and l is *the resolution*, and is defined as the minimum interplanar spacing d_{min}, the dimension is angstroms (Å). Both characteristics are related by the equation Bragg.

$$d_{min} = \frac{1}{2}\left(\frac{\sin\theta_{max}}{\lambda}\right)^{-1}. \tag{2.2.12}$$

Interplanar spacing can be determined using the modulus of the reciprocal vector

$$d_{min} = \frac{1}{\left|\vec{H}_{max}\right|}. \tag{2.2.13}$$

Hence

$$\frac{\sin\theta_{max}}{\lambda} = \frac{1}{2}\left|\vec{H}_{max}\right|. \tag{2.2.14}$$

In calculations of (2.2.11) it is convenient to use the limitations of indices h, k and l are the following types of

$$|\vec{H}| < 2\frac{\sin\theta_{max}}{\lambda}, \qquad (2.2.15)$$

$$|\vec{H}| < \frac{1}{d_{min}}. \qquad (2.2.16)$$

By using formulas (2.2.15) and (2.2.16) the summation in equation (2.2.11) is over the indices inside the sphere with radius $|\vec{H}|$ in reciprocal space.

The **PseudoSymmetry** program using atomic scattering function with maximum domain of values $0 \leq \frac{\sin\theta}{\lambda} \leq 6$ Å^{-1}, $d_{min} = 0.083$ Å. See also Section 3.19.

For precise calculations of the electron density synthesis is recommended the resolution of 0.5 Å and less. Resolution value more than 0.5 Å could be used for broad-brush estimates. Time of calculation would decrease degree of invariance of the electron density peaks height would increase. Thereby, peak searching is more effective for resolution value more than 0.5 Å. Then, degree of invariance of the electron density maximums should be refined using resolution 0.5 Å or less.

2.3. The method of calculating the maps of the degree of invariance of the electron density for the crystal

Given the electron density of the crystal with the array of structure factors $F(\vec{H})$, and the symmetry operator with the matrix q. Then the functional (2.2.10) can be represented as the function of the translation $\vec{t} = \{t_x, t_y, t_z\}$

$$\eta(\vec{t}) = \frac{1}{K} \sum_{\vec{H}} G(\vec{H}) \exp\left(-2\pi i (\vec{H}, \vec{t})\right),$$ (2.3.1)

where $G(\vec{H}) = F(\vec{H})F(-q^T \vec{H})$ is the Fourier coefficient for the degree of invariance of the electron density with respect to the transformation matrix q, $K = \sum_{\vec{H}} |F(\vec{H})|^2$ is the normalization factor.

If q is the matrix of the inversion center, then the searching for the pseudoinversion center will be to find appropriate translation $\vec{t}^{\,max}$ of the maximum value of (2.3.1) ($\eta(\vec{t}^{\,max}) = \max \eta(\vec{t})$).

For high-speed computing (2.3.1) for grid points translations discrete fast Fourier transform (DFFT) is useful [2, 3]. This algorithm makes it possible to convert a set of Fourier coefficients $\{G(\vec{H})\}$ in an array of values $\{\eta(\vec{t})\}$ of the same dimension. For example, if the indices ranges of $\{G(\vec{H})\}$ are

$$\begin{aligned} h &\in [-N_1, N_1] \\ k &\in [-N_2, N_2], \\ l &\in [-N_3, N_3] \end{aligned}$$ (2.3.2)

then the array values $\{\eta(\vec{t})\}$ will be calculated at the points of the regular grid with the steps

$$\begin{aligned} \Delta t_x &= \frac{1}{2N_1 + 1} \\ \Delta t_y &= \frac{1}{2N_2 + 1}. \\ \Delta t_z &= \frac{1}{2N_3 + 1} \end{aligned}$$ (2.3.4)

To calculate FFT the **PseudoSymmetry** program uses the library **FFTW** [2]. FFT algorithms implemented in the library are working with indexes ranging from zero to some value. But in (2.3.1) index range includes negative values. Therefore, the formula (2.3.1) has been adapted. The array of values $G(\vec{H})$ represented in the form $\{G(\vec{M})\}$, where $\vec{M} = \{m, n, p\}$,

$$\begin{aligned} m &\in [0, 2N_1 + 1] \\ n &\in [0, 2N_2 + 1]. \\ p &\in [0, 2N_3 + 1] \end{aligned}$$ (2.3.5)

Define the vector with the minimal indices h, k and l

$$\vec{H}_0 = \{-N_1, -N_2 - N_3\}. \tag{2.3.6}$$

Then (2.3.1) can be written as

$$\eta(\vec{t}) = \frac{1}{K} \sum_{\vec{M}} G(\vec{M}) \exp\left(-2\pi i\left(\vec{M} + \vec{H}_0, \vec{t}\right)\right). \tag{2.3.7}$$

After transformation we obtain

$$\eta(\vec{t}) = \frac{\exp\left(-2\pi i\left(\vec{H}_0, \vec{t}\right)\right)}{K} \sum_{\vec{M}} G(\vec{M}) \exp\left(-2\pi i\left(\vec{M}, \vec{t}\right)\right). \tag{2.3.8}$$

The calculation of (2.3.8) is performed in two stages. First, the FFT is calculated from $\sum_{\vec{M}} G(\vec{M}) \exp\left(-2\pi i\left(\vec{M}, \vec{t}\right)\right)$, second, each result value is multiplied by $\dfrac{\exp\left(-2\pi i\left(\vec{H}_0, \vec{t}\right)\right)}{K}$.

2.4. Searching for local maxima of the degree of invariance of the electron density

If given the transformation matrix q, then (2.3.1) will depend only on the translation vector $\vec{t} = \{t_x, t_y, t_z\}$. In this case, the extremum condition (2.3.1) is a system of equations

$$
\begin{cases}
\dfrac{\partial \eta}{\partial t_x} = 0 \\[2mm]
\dfrac{\partial \eta}{\partial t_y} = 0 \,. \\[2mm]
\dfrac{\partial \eta}{\partial t_z} = 0
\end{cases}
\tag{2.4.1}
$$

Therefore

$$
\begin{cases}
\displaystyle\sum_{\vec{H}} ihG(\vec{H})\exp\!\left(-2\pi i(ht_x + kt_y + lt_z)\right) = 0 \\[3mm]
\displaystyle\sum_{\vec{H}} ikG(\vec{H})\exp\!\left(-2\pi i(ht_x + kt_y + lt_z)\right) = 0 \,. \\[3mm]
\displaystyle\sum_{\vec{H}} ilG(\vec{H})\exp\!\left(-2\pi i(ht_x + kt_y + lt_z)\right) = 0
\end{cases}
\tag{2.4.2}
$$

The system of equations (2.4.2) is a nonlinear. A numerical method is used for solving of this system. We expand the exponential in power series up to quadratic term

$$
\begin{aligned}
\exp(ai\Delta x) &\approx \exp(aix_0) + ai\exp(aix_0)\Delta x - \frac{1}{2}a^2\exp(aix_0)\Delta x^2 = \\
&= \alpha + \beta\Delta x + \gamma\Delta x^2
\end{aligned}
\tag{2.4.3}
$$

where $\Delta x = x - x_0$, x_0 – the initial value; Δx – some small value; a – an arbitrary constant. Then the first equation in (2.4.2) with (2.4.3) can be written as

$$
\sum_{\vec{H}} G_h(\vec{H})\left(\alpha_h + \beta_h\Delta t_x + \gamma_h\Delta t_x^2\right) = 0,
\tag{2.4.4}
$$

where

$$
G_h(\vec{H}) = ihG(\vec{H})\exp\!\left(-2\pi i(kt_y + lt_z)\right),
\tag{2.4.5}
$$

$$
\begin{aligned}
\alpha_h &= \exp(-2\pi i h t_x) \\
\beta_h &= -2\pi i h \exp(-2\pi i h t_x) \quad . \\
\gamma_h &= -2\pi^2 h^2 \exp(-2\pi i h t_x)
\end{aligned}
\tag{2.4.6}
$$

After regrouping the terms in (2.4.4) we obtain the equation of the form

$$\sum_{\vec{H}} G_h(\vec{H})\alpha_h + \Delta t_x \sum_{\vec{H}} G_h(\vec{H})\beta_h + \Delta t_x^2 \sum_{\vec{H}} G_h(\vec{H})\gamma_h = 0. \qquad (2.4.7)$$

For convenience, introduce the notation

$$
\begin{aligned}
A_h &= \sum_{\vec{H}} G_h(\vec{H})\gamma_h \\
B_h &= \sum_{\vec{H}} G_h(\vec{H})\beta_h \\
C_h &= \sum_{\vec{H}} G_h(\vec{H})\alpha_h
\end{aligned} \qquad (2.4.8)
$$

Then (2.4.7) can be written in a more convenient form

$$A_h \Delta t_x^2 + B_h \Delta t_x + C_h = 0, \qquad (2.4.9)$$

The equation (2.4.9) is the quadratic equation in the general case with two roots

$$
\Delta t_{x1} = \frac{-B_h + \sqrt{D_h}}{2A_h}; \Delta t_{x2} = \frac{-B_h - \sqrt{D_h}}{2A_h}; \\
D_h = B^2 - 4A_h C_h \qquad (2.4.10)
$$

Because we are interested in the maximum of value (2.3.1), the shift of the coordinate x into point with a maximum value of the degree of invariance of the electron density is determined by the first root Δt_{x1}. Similarly, we can find other shifts of coordinates for the translation vector

$$
\begin{aligned}
\Delta t_x &= \frac{-B_h + \sqrt{D_h}}{2A_h} \\
\Delta t_y &= \frac{-B_k + \sqrt{D_k}}{2A_k} \\
\Delta t_z &= \frac{-B_l + \sqrt{D_l}}{2A_l}
\end{aligned} \qquad (2.4.11)
$$

The refinement of the vector components produced by the iterative scheme

$$\vec{t}_{i+1} = \vec{t}_i + \begin{pmatrix} \Delta t_{x,i} \\ \Delta t_{y,i} \\ \Delta t_{z,i} \end{pmatrix}, \qquad (2.4.12)$$

where i is the iteration number. The iteration with $i=0$ is the initial, $\vec{t}_0$ is the initial value close to the local maximum of (2.3.1).

The refinement of the scheme (2.4.12) to be made as long as values $\Delta t_{x,i}$, $\Delta t_{y,i}$ and $\Delta t_{z,i}$ does not become lower than a given accuracy of calculations

$$\left|\Delta t_x\right| + \left|\Delta t_y\right| + \left|\Delta t_z\right| < \delta \,, \qquad\qquad (2.4.13)$$

where δ is the precision. The value of δ appropriate to choose the lower accuracy of atomic coordinates determination, so if the atomic coordinates are defined up to $1 \cdot 10^{-4}$ then $\delta = 1 \cdot 10^{-6} \div 1 \cdot 10^{-7}$.

2.5.   The algorithm for calculating the degree of invariance of the electron density with respect to the transformation operator (simple)

The algorithm allows the calculation of the degree of invariance of the electron density with respect to the transformation operator

$$
\hat{q} = \left\{ \begin{pmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \end{pmatrix} \begin{pmatrix} t_x \\ t_y \\ t_z \end{pmatrix} \right\}.
\tag{2.5.1}
$$

For the calculations expression (2.2.11) is used. Limiting the range of indices of the reciprocal vector is carried out according to the formula (2.2.15) or (2.2.16) (see Section 3).

2.6.   The algorithm for calculation of three-dimensional maps of the degree of invariance of the electron density for a given transformation matrix (map)

The algorithm allows to calculate the degree of invariance of the three-dimensional map of the electron density for a given transformation matrix q (see Section 2.4.). Limiting the range of indices of the reciprocal vector is carried out according to the formula (2.2.15) or (2.2.16) (see Section 3).

2.7.   The algorithm for finding a local maximum degree of invariance of the electron density for a given transformation operator (refine)

The algorithm implements the method of finding a local maximum degree of invariance of the electron density with respect to the specified transformation operator described in Section 2.5. For successful work of this algorithm it is necessary to give translation vector is in close to a local maximum degree of invariance of the electron density, otherwise the algorithm may be non-convergent. If the algorithm is non-convergent, then output values of the components of the translation vector and the degree of invariance of the electron density will be equal **–4**. Limiting the range of indices of the reciprocal vector is carried out according to the formula (2.2.15) or (2.2.16) (see Section 3).

2.8. The algorithm of the investigation of pseudosymmetric features of the electron density of the crystal (smart)

Input data to this algorithm are an array of structural factors calculated by the **PseudoSymmetry** program structural data, or derived from external sources, and the matrix that specifies the type of investigation pseudosymmetry (translational, inversion, rotational, etc.). Limiting the range of indices of the reciprocal vector is carried out according to the formula (2.2.15) or (2.2.16) (see Section 3).

Initially, the map of the degree of invariance of the electron density is calculated. The size of the map depends on (2.2.15) or (2.2.16) (see Sections 2.3 and 3). Following conditions are necessary for point $\eta_{i,j,k}$ to be a peak

$$
\begin{cases}
\eta_{i,j,k} > \eta^{\min} \\
\eta_{i,j,k} > \eta_{i-1,j,k} \\
\eta_{i,j,k} > \eta_{i+1,j,k} \\
\eta_{i,j,k} > \eta_{i,j-1,k} \\
\eta_{i,j,k} > \eta_{i,j+1,k} \\
\eta_{i,j,k} > \eta_{i,j,k-1} \\
\eta_{i,j,k} > \eta_{i,j,k+1}
\end{cases}
, \tag{2.8.1}
$$

where $\eta^{\min}$ is a specified minimum value of the degree of invariance of the electron density.

The resulting array of peaks is sorted, and for a specified number of the strongest peaks is performed refinement of degree of invariance of the electron density (see Section 2.5.). If the local maximum of the degree of invariance of the electron density is not found, such the peak is rejected as a false. The final calculations of degree of invariance of the electron density are made only for peaks with well refined positions of the maxima.

2.9. The algorithm of the calculation of atomic displacements

Often, in the process of the study pseudosymmetric features of crystals need to find out the location of the atoms which creates the pseudosymmetry of the atomic structure. The calculation of the distances between atoms of the original structure and transformed atoms with respect to the operator of the pseudosymmetry is convenient for the solution of such problem.

Let the structure given as the set of vectors of centers of mass of atoms

$$S = \{\vec{r}_i\}. \tag{2.9.1}$$

Let also the set S contains the full set of atoms in the unit cell (the atoms are multiplied by symmetry operators of G), and given some pseudosymmetry operator $\hat{h}$. Let the operator $\hat{h}$ acts on the structure S, and then we get the transformed structure

$$S' = \hat{h}S = \{\hat{h}\vec{r}_i\} = \{\vec{r}_i'\}. \tag{2.9.2}$$

Obviously, if $\hat{h} \in G$ then

$$S' = S. \tag{2.9.3}$$

If the operator $\hat{h}$ describes some pseudosymmetrical transformation of S ($\hat{h} \notin G$ and $\hat{h} \in H$) then the equality in (2.9.3) becomes the approximate equality. In this case, only the part of elements for S and S' are equals or approximately equals ($\vec{r}_i' \approx \vec{r}_j$).

For every atom $\vec{r}_k$ of the original structure S determines the shortest distance between $\vec{r}_k$ and some atom $\vec{r}_i'$ of S'

$$\Delta r_k = \min\left(\left|\vec{r}_k - \vec{r}_i'\right|\right). \tag{2.9.4}$$

The value Δr_k is called the atomic displacement. The small value of Δr_k denotes the approximate equality $\vec{r}_k$ and $\vec{r}_i'$, it means peaks of electron densities of atoms $\vec{r}_k$ and $\vec{r}_i$ overlap. Only atoms with the small value Δr_k influence on the degree of invariance of the electron density.

Therefore, only small atomic displacements limited by some threshold $\Delta r^{\max}$ are considered efficiently.

$$\Delta r_k < \Delta r^{\max}. \tag{2.9.5}$$

For this convenient to form tables which consist of atoms of the original structure, transformed atoms with respect to $\hat{h}$ and values of atomic displacements (Tab. 2.9.1).

Tab. 2.9.1. Atomic displacements for MoO_2 crystal (sp. gr. $P2_1$). The pseudosymmetry operator is $\{T|(0.0, 0.5, 0.0)\}$. In atom labels after the sign "_" indicates the number of symmetrically equivalent positions: 0 – {-x, y+1/2, -z}, 1 – {x, y, z}.

Исходный атом ($\vec{r}_k$)	Преобразованный атом ($\vec{r}_i' = \hat{h}\vec{r}_i$)	Атомное смещение, Å (Δr_k)
Mo1_1	Mo1_0	0.0001
Mo2_1	Mo2_0	0.0001
Mo2_1	Mo2_0	0.0001
Mo2_0	Mo2_1	0.0001
O2_0	O2_0	1.3256
O2_1	O2_1	1.3256

Molybdenum atoms are well superposed by the operator pseudosymmetry $(T|\{0.0, 0.5, 0.0\})$, atomic displacements are less than standard deviation for atoms of structure (Tab. 2.9.1.). The atomic displacement for oxygen atoms is 1.3256 Å, this means that oxygen atoms do not significantly affect the increase of the crystal symmetry. The degree of invariance of the electron density with respect to $\{T|(0.0, 0.5, 0.0)\}$ is $\eta=0.976$, and this value almost completely determined by the pseudosymmetric location of molybdenum atoms.

3. The input file format

The input file is a text file and is organized on the basis of CIF-file [8]. Data items start with «_», after follow values. Values of data items can have several formats. The **Simple value** can have the numerical or string type (for example, «0.56», «simple»). The **String** is the specified string value with the maximum length up to 80 symbols. Strings written in apostrophes (for example, 'C:\pseudo symmetry\data'). The **Text** is the multiline text block contained between two markers «;». For example:

;
Some text…
;

Lines beginning with «#» character are considered a comment. The following is the description of **PseudoSymmetry** program options, and examples of their use.

3.1.   _pseudo_use_U и _pseudo_use_Ueq_only

Values: **yes**, **no**

These options are used to control the calculation of the Debye-Waller factor with atomic displacement parameters (ADP).

Examples:

The Debye-Waller factor is not calculated. It is the model of fixed spherically symmetric atoms:

_pseudo_use_U   **no**

The Debye-Waller factor is calculated for all atoms. If the atom is given at the same time equivalent and anisotropic displacement parameters are the anisotropic Debye-Waller factor is calculated:

_pseudo_use_U   **yes**

_pseudo_use_Ueq_only   **no**

If you want to force the calculation of the Debye-Waller factor in the isotropic form it should be used:

_pseudo_use_U   **yes**

_pseudo_use_Ueq_only   **yes**

3.2.   _pseudo_trim_data_type

Values: **none**, **mind**, **sintl**

Set as limit the range of indices of the reciprocal vector. The numerical value is specified by the option **_pseudo_trim_value**.

none – used for the external structure amplitudes (use a specially defined cases). Calculations are made for the range $[-\max(|h|), \max(|h|)]$, $[-\max(|k|), \max(|k|)]$ и $[-\max(|l|), \max(|l|)]$.

mind – limitation of the formula (2.2.16). The parameter **_pseudo_trim_value** should contain the minimum value of the interplanar spacing in angstroms.

sintl – limitation of the formula (2.2.15). The parameter **_pseudo_trim_value** should contain the maximum value of $\sin\theta/\lambda$ in inverse angstroms.

Example:

_pseudo_trim_data_type   mind

_pseudo_trim_value   0.5

3.3.   _pseudo_trim_value

Value: **Numerical**

Contains a numeric value of the range of indices reciprocal vector (see also **_pseudo_trim_data_type**).

3.4.   _pseudo_use_log

Value: **yes**, **no**

This option allows the using of the log file. The log file contains information on the calculation.

3.5.   _pseudo_log_name

Value: **File name (string)**

This option sets the name of the log file. For display the log file on the console use the value **'CON'**.

3.6.   _pseudo_work_dir

Value: **Directory (string)**

This option sets the working directory. The working directory is appended to a file name (the file name **'file.ext'** does change to '**working directory\file.ext**'). Full path to the file does not change (full file name

'**C:\pseudo\file.ext**' does not change). The exception is the log file name. It is not uses the working directory (only direct path). For example, **_pseudo_work_dir 'C:\pseudo\data'**.

3.7.   _pseudo_output_type

Value: **cif1**, **cif2**

This option sets the format of the output file.

cif1 − defines following format of the output data:

q_{11} q_{12} q_{13} v_1

q_{21} q_{22} q_{23} v_2

q_{31} q_{32} q_{33} v_3 η

Where q_{11}- q_{33} are components of the transformation matrix, v_1–v_3 are components of the translation vector, η is the value of the degree of invariance of the electron density. This format is recommended for visual analysis of the results.

cif2 − defines following format of the output data:

q_{11} q_{12} q_{13} q_{21} q_{22} q_{23} q_{31} q_{32} q_{33} v_1 v_2 v_3 η

The data for one operator is represented as the single line. For more information, see also Section 4.

3.8.   _pseudo_output

Value: **file name (string)**

This option sets the output file name with results (See also Section **_pseudo_output_type**). For example,

_pseudo_output_type   **cif1**

_pseudo_output   **'out.pscif'**

3.9.   _pseudo_input_type

Value: **cif**, **fcf_fo**, **fcf_fc**

This option sets the format of the input file with structural information or with the array of structure factors.

cif – the input file has the **CIF** format [8], and contains structural information (symmetry, cell, atoms). In this case structure factors will be calculated by the formula (2.2.4) (see also Section 3.1.). Files can contain one or more structures.

fcf_fo or **fcf_fc** – defines the file with calculated (**fcf_fc**) or with observed (**fcf_fo**) structure factors. The format of the file should be similar to the format of the FCF-file for **SHELX'97** [9]. The file should contain unit cell, space group, the independent part of structure factors. If in the file indicated the resolution of the data (option **_reflns_d_resolution_high**) then this resolution will be used for limiting of the reciprocal vector (see Sections 3.2. and 3.3.). Suitable for the calculations are files containing fields of **_refln_F_meas**, **_refln_A_calc**, **_refln_B_calc** (**SHELX** instruction **LIST 3**) and files containing fields of **_refln_F_squared_meas**, **_refln_F_calc**, **_refln_phase_calc** (**SHELX** instruction **LIST 6**).

The transformation of structure factors with respect to symmetry operators carried out as follows. Let the structure factor for some $\vec{H}$ has the simple form

$$F(\vec{H}) = \sum_{j=1}^{N} f_j e^{2\pi i(\vec{H},\vec{r}_j)} \ . \tag{3.9.1}$$

Obviously, if we transform all atoms of the structure with coordinates $\vec{r}_j$ with respect to the operator $\hat{g} = \{g \mid \vec{p}\}$ which belongs to the space group of the crystal, then the value of the structure factor for same $\vec{H}$ does not change.

$$F(\vec{H}) = \sum_{j=1}^{N} f_j e^{2\pi i(\vec{H},\hat{g}\vec{r}_j)} \ . \tag{3.9.2}$$

After the transformation (3.9.2) we obtain

$$F(\vec{H}) = e^{2\pi i(\vec{H},\vec{p})} \sum_{j=1}^{N} f_j e^{2\pi i(g^T \vec{H},\vec{r}_j)} \ , \tag{3.9.3}$$

where g^T is the transpose transformation matrix. From (3.9.3) we obtain the expression for the structure factors transformation with respect to $\hat{g}$

$$F(g^T \vec{H}) = e^{-2\pi i(\vec{H},\vec{p})} F(\vec{H}) \ . \tag{3.9.4}$$

Using the formula (3.9.4) transform all of independent structural factors from the file. So, is filled all the reciprocal space. If the symmetry group of the crystal does not contain the inversion center then in the reciprocal space are added Friedel opposites

$$F(-\vec{H}) = F^*(\vec{H}) \ . \tag{3.9.5}$$

3.10. _pseudo_input_file

Value: **file path (string)**

This option defines the input file path (see Section 3.9.). The option **_pseudo_input_file** can only be used as part of the loop item. The value of this option can contains some file path or some directory with a filter. For example, the calculation for two CIF files carried out as follows

```
_pseudo_input_type cif
loop_
_pseudo_input_file
'c:\pseudo\data\cif\1.cif'
'c:\pseudo\data\cif\2.cif'
```

You can also use directory with the extension filter

```
loop_
_pseudo_input_file
'c:\pseudo\data\cif\*.cif'
```

In this case, the program will process all files with extension **cif** in the directory "**c:\pseudo\data\cif**". Subdirectories will not be processed.

3.11. _pseudo_calc_method

Value: **simple**, **map**, **refine**, **smart**

This option sets the calculation method.

simple − the calculation of the degree of invariance of the electron density with respect to the specified transformation operator (see Section 2.5).

map − the calculation of the map of the degree of invariance of the electron density for the specified transformation matrix (see Section 2.6.).

refine − the refinement of the translation vector for the specified transformation operator. This method searches for the local maximum of the degree of invariance of the electron density for the specified transformation operator (initial approximation) (see Section 2.7.).

smart − the method of investigation of pseudosymmetric features of the crystal (see Section 2.8.).

3.12. _pseudo_calc_threshold

Value: **Number**

This option uses in the method **smart** (see Sections 3.11. and 2.8.), and sets $\eta^{\min}$ in the condition (2.8.1).

3.13. _pseudo_calc_max_peaks

Value: **Number (integer)**

This option uses in the method **smart** (see Sections 3.11. and 2.8.), and sets the number of strongest peaks which will be used to refine.

3.14. _pseudo_refine_precision

Value: **Number**

This option uses in methods **smart** and **refine** (see Sections 3.11., 2.7., 2.8.), and sets δ the precision of the refinement in (2.4.13).

3.15. _pseudo_refine_maxcycles

Value: **Number (integer)**

This option uses in methods **smart** and **refine** (see Sections 3.11., 2.7., 2.8.), and sets the maximum number of refinement cycles (see Section 2.4.). If the specified number of refinement cycles is not enough to obtain the specified precision, the refinement will stop without some messages.

3.16. _pseudo_operator_name, _pseudo_operator_M11, _pseudo_operator_M12, _pseudo_operator_M13, _pseudo_operator_M21, _pseudo_operator_M22, _pseudo_operator_M23, _pseudo_operator_M31, _pseudo_operator_M32, _pseudo_operator_M33, _pseudo_operator_V1, _pseudo_operator_V2, _pseudo_operator_V3

Values: **string** (for _pseudo_operator_name), **number** (for _pseudo_operator_[])

These options set transformation operators, and are used only in the loop item. Specified operators are used for the calculation of the degree of invariance of the electron density. Below is an example of the list of transformation operators. This list contains inversion at the origin and the translation {0.5, 0.5, 0.5}

```
loop_
_pseudo_operator_name
_pseudo_operator_M11
_pseudo_operator_M12
_pseudo_operator_M13
_pseudo_operator_M21
_pseudo_operator_M22
_pseudo_operator_M23
_pseudo_operator_M31
_pseudo_operator_M32
_pseudo_operator_M33
_pseudo_operator_V1
_pseudo_operator_V2
_pseudo_operator_V3
'IN'   -1   0   0   0   -1   0   0   0   -1   0     0     0
'TR'    1   0   0   0    1   0   0   0    1   0.5   0.5   0.5
```

_pseudo_operator_name – this option sets the name of the transformation operator. The names of the operators are defined by the user.

_pseudo_operator_M11-33 – these options are nine components of the transformation matrix.

_pseudo_operator_V1-3 – these options are three components of the translation vector.

3.17. _pseudo_displacement

Value: **yes, no**

This option enables the calculation of atomic displacements (see Section 2.9.). For this calculation need atomic coordinates, therefore the format of input files should be **cif** (see Section 3.9.). Atomic displacements are calculated for same operators which are used for the calculation of the degree of invariance of the electron density. The maximum value of atomic displacements Δr^{max} is determined the option **_pseudo_displacement_maxdistance** (see Sections 2.9. and 3.18.). The format of results is described in Section 4.11.

3.18. _pseudo_displacement_maxdistance

Value: **number (default 1.5 Å)**

This option is determined the maximum value of output atomic displacements Δr^{max} in angstroms (see Section 2.9.).

3.19. _pseudo_atom_type_scat_source

Values: **it6111**, **it6114** (default **it6111**)

This option allows choose the way of the calculation atomic scattering functions. Default value is **it6111**, this value corresponded to mean atomic scattering factors in electrons for free atoms (See tab. 6.1.1.1 [1]). Intermediate values are determined by linear fit of the two closest points. The domain of values of the atomic scattering functions of this method is $0 \leq \dfrac{\sin \theta}{\lambda} \leq 6$ Å^{-1}.

If value of this option is **it6114**, atomic scattering function is defined by formula (6.1.1.15 [1]), values of coefficients is obtained form (tab. 6.1.1.4 [1]). The domain of values of the atomic scattering functions of this method is $0 \leq \dfrac{\sin \theta}{\lambda} \leq 2$ Å^{-1}.

3.20. _pseudo_calc_device

Values: **cpu**, **cuda** (default **cpu**)

This option determines the calculation module:

cpu – the calculation on the central processing unit (**CPU**). Acceleration of calculations is performed by **OpenMP** technology.

cuda – the calculation on the **CUDA**-device [4]. Using this option requires the **CUDA**-device installed in your computer (see Section 1.2.). The calculation on the **CUDA**-device (on **CUDA**-module) may take a shorter time.

Note:

1. The **CUDA**-module do not supports **displacement** method (see Section 3.11.), therefore if the option **_pseudo_displacement** is **yes**, the calculation of atomic displacements carried out on **CPU**.

2. The **CUDA**-module do not supports the calculation with structure factors obtained from other sources. The **CUDA**-module supports structure factors calculated by structure information and atomic scattering functions **it6114** (exponential approximation up to 2 Å^{-1}, see Section 3.19.).

3.21. _pseudo_calc_device_cuda_num

Value: **Integer** (default 0)

This option determines the number of the CUDA-device that will be used to calculate [4].

4. The file format of the results

The results file is the text file with the CIF format [8] (see also Section 3.).

4.1. _pseudo_date

This option contains the current date.

4.2. _pseudo_version

This option contains the current version of the program **PseudoSymmetry**.

4.3. _pseudo_structure_name

This option contains the name the structure.

4.4. _pseudo_code_CSD

This option contains the reference code of the structure in the database (if exist).

4.5. _cell_length_a, _cell_length_b, _cell_length_c, _cell_angle_alpha, _cell_angle_beta, _cell_angle_gamma

These options contain information about the unit cell.

4.6. _pseudo_use_U, _pseudo_use_Ueq_only, _pseudo_trim_data_type, _pseudo_trim_value, _pseudo_input_type, _pseudo_calc_method,

_pseudo_calc_threshold, _pseudo_calc_max_peaks, _pseudo_refine_maxcycles,
_pseudo_refine_precision

These options are repeated values similar options given in the input file (see Section 3.).

4.7.   _pseudo_limit_h_min, _pseudo_limit_h_max, _pseudo_limit_k_min, _pseudo_limit_k_max, _pseudo_limit_l_min, _pseudo_limit_l_max

These options contain limiting values of indices of the reciprocal vector.

4.8.   _atom_type_symbol, _atom_type_scat_source

These options contain information about the source of atomic scattering factors.

4.9.   _pseudo_operator_name, _pseudo_operator_M11, _pseudo_operator_M12, _pseudo_operator_M13, _pseudo_operator_V1, _pseudo_operator_M21, _pseudo_operator_M22, _pseudo_operator_M23, _pseudo_operator_V2, _pseudo_operator_M31, _pseudo_operator_M32, _pseudo_operator_M33, _pseudo_operator_V3, _pseudo_pseudo_ed

These options contain the results of the calculation of the degree of invariance of the electron density. The option **_pseudo_operator_name** contains the name of the transformation operator (from the input file). Options **_pseudo_operator_M11-33** and **_pseudo_operator_V1-3** contain components of the transformation operator (see also Section 3.16.). The option **_pseudo_pseudo_ed** contains the value of the degree of invariance of the electron density.

For example, the output in the format **cif1**:

loop_
_pseudo_operator_name
_pseudo_operator_M11
_pseudo_operator_M12
_pseudo_operator_M13
_pseudo_operator_V1
_pseudo_operator_M21
_pseudo_operator_M22

_pseudo_operator_M23
_pseudo_operator_V2
_pseudo_operator_M31
_pseudo_operator_M32
_pseudo_operator_M33
_pseudo_operator_V3
_pseudo_pseudo_ed
'INV'
 -1.000 0.000 0.000   0.3333
  0.000 -1.000 0.000   0.3333
  0.000 0.000 -1.000   0.0000   0.98272

For example, the output in the format **cif2**:

loop_
_pseudo_operator_name
_pseudo_operator_M11
_pseudo_operator_M12
_pseudo_operator_M13
_pseudo_operator_M21
_pseudo_operator_M22
_pseudo_operator_M23
_pseudo_operator_M31
_pseudo_operator_M32
_pseudo_operator_M33
_pseudo_operator_V1
_pseudo_operator_V2
_pseudo_operator_V3
_pseudo_pseudo_ed
'INV' -1.000 0.000 0.000 0.000 -1.000 0.000 0.000 0.000 -1.000 0.3333 0.3333 0.0000 0.98272

4.10. _pseudo_displacement

This option indicates usage of the calculation of atomic displacements (see Section 2.9.).

4.11. _pseudo_displacement_maxdistance

This option contains the maximum output atomic displacement Δr^{max} in angstroms (п. 2.9.).

4.12. _pseudo_displacement_table

This option contains output tables of atomic displacements for different transformation operators (see Section 2.9.), and it has the multiline format.

The table of atomic displacements has the following format. At first, outputs the transformation operator $\hat{h}$

The operator name

$q_{11}\ q_{12}\ q_{13}\ |\ v_1$

$q_{21}\ q_{22}\ q_{23}\ |\ v_2$

$q_{31}\ q_{32}\ q_{33}\ |\ v_3$

The following is a table of atomic displacements (see Tab. 4.11.1).

Tab. 4.11.1. The sample table of atomic displacements.

Atom 1	Atom 2	Distance, A	X1	Y1	Z1	X2	Y2	Z2
U3_0	U2_0	0.08076	0.333	0.497	0.668	0.327	0.4936	0.671
U3_1	U2_1	0.08076	0.667	0.997	0.332	0.673	0.9936	0.329
U4_1	U4_0	0.08093	0.169	0.229	0.806	0.169	0.2346	0.806

Atom labels in (Tab. 4.11.1) have the following format:

The atom label in cif-file _ the number of a symmetry equivalent position.

The first number of a symmetry equivalent position is zero, and the order corresponds to the order in the cif-file. The column *Atom 1* contains atoms $\vec{r}_k$ of the original structure (see Section 2.9.), and the column *Atom 2* contains atoms $\vec{r}_i'$ which satisfy conditions (2.9.4) and (2.9.5). Because $\hat{h}\vec{r}_i = \vec{r}_i'$, in the column *Atom 2* contains atom labels for the original structure $\vec{r}_i$. The column *Distance* contains atomic displacements Δr_k (2.9.4.) in angstroms. The following columns X1, Y1 and Z1 contain coordinates of atoms $\vec{r}_k$ for the original structure, and columns X2, Y2 и Z2 contain the coordinates of transformed atoms $\vec{r}_i' = \hat{h}\vec{r}_i$.

Data in the table of atomic displacements is sorted ascending atomic displacements and limited to the maximum atomic displacement, given by the option **_pseudo_displacement_maxdistance** (see Section 3.18.).

If the calculation carries out for several operators, results are output sequentially in the previously described format. The orders of results for atomic displacements and the degree of invariance the electron density are same (see following example).

The example of the results file:

```
. . . . . . . . . . . . . . . . . . . . .
_pseudo_displacement  yes
_pseudo_displacement_maxdistance   1.5000

_pseudo_displacement_table
;
INV
 -1.000    0.000    0.000  |   0.50000
  0.000   -1.000    0.000  |  -0.00044
  0.000    0.000   -1.000  |  -0.00000

 Atom 1  Atom 2    Distance, A     X1      Y1      Z1      X2      Y2      Z2
  Mo2_1   Mo1_0       0.002142  0.4650  0.0000  0.2320  0.4650  0.9996  0.2320
  Mo2_0   Mo1_1       0.002142  0.5350  0.5000  0.7680  0.5350  0.4996  0.7680
  Mo1_1   Mo2_0       0.002142  0.9650  0.5000  0.2320  0.9650  0.4996  0.2320
  Mo1_0   Mo2_1       0.002142  0.0350  0.0000  0.7680  0.0350  0.9996  0.7680
   O2_1    O4_0       0.094718  0.1200  0.7800  0.1100  0.1200  0.7996  0.1100
   O2_0    O4_1       0.094718  0.8800  0.2800  0.8900  0.8800  0.2996  0.8900
. . . . . . . . . . . . . . . . . . . . .
   O1_0    O3_1       0.191578  0.1600  0.6800  0.6100  0.1600  0.7196  0.6100
INV
 -1.000    0.000    0.000  |   0.00000
  0.000   -1.000    0.000  |   0.50003
  0.000    0.000   -1.000  |   0.00000

 Atom 1  Atom 2    Distance, A     X1      Y1      Z1      X2      Y2      Z2
  Mo1_1   Mo1_0       0.000141  0.9650  0.5000  0.2320  0.9650  0.5000  0.2320
  Mo1_0   Mo1_1       0.000141  0.0350  0.0000  0.7680  0.0350  0.0000  0.7680
  Mo2_1   Mo2_0       0.000141  0.4650  0.0000  0.2320  0.4650  0.0000  0.2320
  Mo2_0   Mo2_1       0.000141  0.5350  0.5000  0.7680  0.5350  0.5000  0.7680
   O2_0    O2_0       1.325563  0.8800  0.2800  0.8900  0.1200  0.2200  0.1100
. . . . . . . . . . . . . . . . . . .
   O3_0    O2_1       1.453962  0.6600  0.7800  0.6100  0.8800  0.7200  0.8900
INV
 -1.000    0.000    0.000  |   0.07128
  0.000   -1.000    0.000  |  -0.00029
  0.000    0.000   -1.000  |   0.53639

 Atom 1  Atom 2    Distance, A     X1      Y1      Z1      X2      Y2      Z2
  Mo1_0   Mo1_0       0.006563  0.0350  0.0000  0.7680  0.0363  0.9997  0.7684
  Mo2_0   Mo2_0       0.006563  0.5350  0.5000  0.7680  0.5363  0.4997  0.7684
   O3_0    O4_0       0.213235  0.6600  0.7800  0.6100  0.6913  0.7997  0.6464
    . . . . . . . . . . . . . . . . . . . . .
  Mo2_1    O1_1       1.446421  0.4650  0.0000  0.2320  0.2313  0.8197  0.1464
. . . . . . . . . . . . . . . . . . . . .
;

loop_
_pseudo_operator_name
_pseudo_operator_M11
_pseudo_operator_M12
_pseudo_operator_M13
_pseudo_operator_V1
_pseudo_operator_M21
_pseudo_operator_M22
_pseudo_operator_M23
_pseudo_operator_V2
_pseudo_operator_M31
_pseudo_operator_M32
_pseudo_operator_M33
_pseudo_operator_V3
_pseudo_pseudo_ed
'INV'
 -1.000    0.000    0.000     0.5000
  0.000   -1.000    0.000    -0.0004
  0.000    0.000   -1.000    -0.0000      0.99474
'INV'
 -1.000    0.000    0.000     0.0000
  0.000   -1.000    0.000     0.5000
  0.000    0.000   -1.000     0.0000      0.97599
'INV'
 -1.000    0.000    0.000     0.0713
```

```
   0.000  -1.000   0.000   -0.0003
   0.000   0.000  -1.000    0.5364     0.50604
. . . . . . . . . . . . . . . . . . . . . . . .
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