

Linear transformations of variance/covariance matrices

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Received 21 February 2011

Accepted 13 May 2011

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Many applications in crystallography require the use of linear transformations on parameters and their standard uncertainties. While the transformation of the parameters is textbook knowledge, the transformation of the standard uncertainties is more complicated and needs the full variance/covariance matrix. For the transformation of second-rank tensors it is suggested that the 3×3 matrix is re-written into a 9×1 vector. The transformation of the corresponding variance/covariance matrix is then straightforward and easily implemented into computer software. This method is applied in the transformation of anisotropic displacement parameters, the calculation of equivalent isotropic displacement parameters, the comparison of refinements in different space-group settings and the calculation of standard uncertainties of eigenvalues.

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1. Notation

* denotes the reciprocal space or dual space.

Bold capital letters define matrices.

$\vec{}$ define the *vec* operator or simply a vector which is represented as a column matrix.

$^{-1}$ denotes the inverse of a matrix, t the transpose of a matrix, and their combination $^{-t}$ denotes the transpose of the inverse of a matrix.

U^* is the dimensionless mean-square displacement tensor, U^{*ij} are its components. The corresponding temperature factor parameters are defined as¹

$$T = \exp(-2\pi^2[U^{*11}h^2 + U^{*22}k^2 + U^{*33}l^2 + 2U^{*12}hk + 2U^{*13}hl + 2U^{*23}kl]).$$

U is the displacement tensor defined with respect to the reciprocal-lattice basis (\mathbf{a}^* , \mathbf{a}^{*2} , \mathbf{a}^{*3}). U^{ij} are its components. The corresponding temperature-factor parameters are defined as²

$$T = \exp(-2\pi^2[U^{11}h^2(\mathbf{a}^*)^2 + U^{22}k^2(\mathbf{a}^{*2})^2 + U^{33}l^2(\mathbf{a}^{*3})^2 + 2U^{12}hka^* \mathbf{a}^{*2} + 2U^{13}hla^* \mathbf{a}^{*3} + 2U^{23}kla^* \mathbf{a}^{*3}]).$$

$\text{Var}(V)$ is the variance of V .

$\text{Cov}(V, W)$ is the covariance of V, W .

\otimes is the Kronecker product [see equation (29)].

¹ $U^* = \beta/(2\pi^2)$ (Grosse-Kunstleve & Adams, 2002; Giacovazzo, 2002). In the input for the *ORTEP-III* software these displacement parameters are called type 10.

² $U^{ij} = U^{*ij} a^{*i} a^{*j}$. In the input for the *ORTEP-III* software these displacement parameters are called type 8.

2. Introduction

Second-rank tensors are a very useful concept in crystallography (Sands, 1995; Lovett, 1999). Probably the most often employed application are the (harmonic) anisotropic displacement parameters in crystal structure refinement. Other important applications are in the description of physical properties, *e.g.* thermal expansion, electrical conductivity *etc.*

Linear transformations on second-rank tensors can easily be applied using matrix operations. Many crystallographic programs (*PLATON*, *ORTEP* *etc.*) have implemented routines to perform this. Less trivial is the application of linear operations to the standard uncertainties. To do this correctly the variance/covariance matrix is necessary, which is unfortunately not available in many output files (most prominent the CIF format). Additionally there is no generally applicable software available for this purpose. This prompted us to develop such a procedure. Nowadays, linear algebra is well available directly in programming languages or mathematical libraries (*LAPACK* *etc.*) via whole array assignments and operations. The matrix operations are then easily transferred into software.

Most calculations in crystal physics are performed in a Cartesian system (Haussühl, 2007). Also, rigid-body analysis based on a TLS model commonly uses Cartesian axes (Schomaker & Trueblood, 1998). After the structure refinement in the crystal system the parameters must first be transformed to the Cartesian system with a linear transformation.

In the least-squares refinement of a crystal structure a similar situation occurs: depending on the space-group setting, different lattice parameters must be used. These are related by

Table 1

A 3×3 variance/covariance matrix of the coordinates.

(x, y) is read as $\text{Cov}(x, y)$ and the following properties hold: $\text{Cov}(x, x) = \text{Var}(x)$, $\text{Cov}(x, y) = \text{Cov}(y, x)$. Values printed in bold are the six independent parameters of the matrix.

$$\begin{bmatrix} (\mathbf{x}, \mathbf{x}) & (\mathbf{x}, \mathbf{y}) & (\mathbf{y}, \mathbf{z}) \\ (\mathbf{y}, \mathbf{x}) & (\mathbf{y}, \mathbf{y}) & (\mathbf{y}, \mathbf{z}) \\ (\mathbf{z}, \mathbf{x}) & (\mathbf{z}, \mathbf{y}) & (\mathbf{z}, \mathbf{z}) \end{bmatrix}$$

linear transformations. Feast *et al.* (2009) argue that a setting with an oblique angle increases the correlation between parameters and difficulties can arise during the refinement. Taking the variance/covariance matrix into account in the linear transformation, the results of the refinement in the transformed setting can be compared with the transformed results.

3. Linear transformations of coordinates and their standard uncertainties

Let \mathbf{L} be a linear operation in the crystal coordinate system and \vec{v} the coordinate vector of an atom on a general position. Then, $\vec{v}' = \mathbf{L}\vec{v}$ is the new coordinate vector. If \mathbf{E} is the corresponding 3×3 variance/covariance matrix of the coordinate vector \vec{v} (Table 1), \mathbf{E}' is the variance/covariance matrix of \vec{v}' . \mathbf{E}' is calculated by the application of \mathbf{L} [see also equation (23) in §11.1],

$$\mathbf{E}' = \mathbf{L} \mathbf{E} \mathbf{L}' \quad (1)$$

3×3 3×3 3×3 3×3

4. Linear transformations of ADPs and their standard uncertainties

Let \mathbf{L} be a linear operation in the crystal coordinate system and \mathbf{U}^* be a symmetric tensor representing the anisotropic displacement parameters (ADPs) of an atom on a general position. From the nine components in \mathbf{U}^* the corresponding 9×9 variance/covariance matrix \mathbf{F}^* can be constructed (see §11.2). Only 21 elements (6 variances and 15 covariances) of this 9×9 matrix are independent (Table 2). $\mathbf{U}^{*'}$, the result of the application of the linear transformation \mathbf{L} on \mathbf{U}^* , is calculated by [see also equation (23) in §11.1]

$$\mathbf{U}^{*'} = \mathbf{L} \mathbf{U}^* \mathbf{L}' \quad (2)$$

3×3 3×3 3×3 3×3

Alternatively, the *vec* operator can be used [see also equation (30) in §11.2],

$$\vec{U}^{*'} = (\mathbf{L} \otimes \mathbf{L}) \vec{U}^* \quad (3)$$

9×1 9×9 9×1

From (2) and (3) the corresponding variance/covariance matrix is calculated as follows,

Table 2

A 9×9 variance/covariance matrix of U^{*ij} of an atom on a general position.

(11, 12) is read as $\text{Cov}(U^{*11}, U^{*12})$ and the following properties hold: $\text{Cov}(U^{*ij}, U^{*ij}) = \text{Var}(U^{*ij})$, $\text{Cov}(U^{*ij}, U^{*kl}) = \text{Cov}(U^{*kl}, U^{*ij})$. Values printed in bold are the 21 independent parameters of the matrix.

$$\begin{bmatrix} (\mathbf{11}, \mathbf{11}) & (\mathbf{11}, \mathbf{12}) & (\mathbf{11}, \mathbf{13}) & (11, 12) & (\mathbf{11}, \mathbf{22}) & (\mathbf{11}, \mathbf{23}) & (11, 13) & (11, 23) & (\mathbf{11}, \mathbf{33}) \\ (12, 11) & (\mathbf{12}, \mathbf{12}) & (\mathbf{12}, \mathbf{13}) & (12, 12) & (\mathbf{12}, \mathbf{22}) & (\mathbf{12}, \mathbf{23}) & (12, 13) & (12, 23) & (\mathbf{12}, \mathbf{33}) \\ (13, 11) & (13, 12) & (\mathbf{13}, \mathbf{13}) & (13, 12) & (\mathbf{13}, \mathbf{22}) & (\mathbf{13}, \mathbf{23}) & (13, 13) & (13, 23) & (\mathbf{13}, \mathbf{33}) \\ (12, 11) & (12, 12) & (12, 13) & (12, 12) & (12, 22) & (12, 23) & (12, 13) & (12, 23) & (12, 33) \\ (22, 11) & (22, 12) & (22, 13) & (22, 12) & (\mathbf{22}, \mathbf{22}) & (\mathbf{22}, \mathbf{23}) & (22, 13) & (22, 23) & (\mathbf{22}, \mathbf{33}) \\ (23, 11) & (23, 12) & (23, 13) & (23, 12) & (23, 22) & (\mathbf{23}, \mathbf{23}) & (23, 13) & (23, 23) & (\mathbf{23}, \mathbf{33}) \\ (13, 11) & (13, 12) & (13, 13) & (13, 12) & (13, 22) & (13, 23) & (13, 13) & (13, 23) & (13, 33) \\ (23, 11) & (23, 12) & (23, 13) & (23, 12) & (23, 22) & (23, 23) & (23, 13) & (23, 23) & (23, 33) \\ (33, 11) & (33, 12) & (33, 13) & (33, 12) & (33, 22) & (33, 23) & (33, 13) & (33, 23) & (\mathbf{33}, \mathbf{33}) \end{bmatrix}$$

$$\mathbf{F}_{9 \times 9}^{* \vec{U}^{*'}} = (\mathbf{L} \otimes \mathbf{L}) \mathbf{F}_{9 \times 9}^{* \vec{U}^*} (\mathbf{L} \otimes \mathbf{L})^t \quad (4)$$

The standard uncertainty of each component of the \vec{U}^* vector can then easily be extracted from the square root of the diagonal elements of the variance/covariance matrix \mathbf{F}^* .

A symmetry operation is a linear operation without the change of the basis. In this case equations (2), (3) and (4) are also valid on the tensors \mathbf{U} and $\mathbf{F}_{\vec{U}}$.

5. Constrained refinement

When an atom is on a special position, the site symmetry implies constraints on some of the parameters (Prince *et al.*, 2004). In the most simple case the parameter is constrained to a certain value, *e.g.* some U^{ij} must be constrained to zero. In other cases two parameters are dependent on each other, *e.g.* U^{12} might be dependent on U^{11} . The latter case is difficult to detect in the CIF file because both parameters have standard uncertainties there. It is consequently not possible to recognize from the presence or absence of standard uncertainties whether a parameter was refined freely or constrained.

While an anisotropically refined atom on a general position has six ADPs and a 9×9 variance/covariance matrix \mathbf{F}^* (Table 2), constrained atoms have less than six independent ADPs and a smaller variance/covariance matrix (Table 3). It is not possible to apply a linear transformation on such a smaller variance/covariance matrix.

By definition, the correlation matrix only contains the refined parameters. An example is the .mat file written by the *SHELXL* software (Sheldrick, 2008). In the case of constrained atoms, the correlation matrix is incomplete concerning the coordinate vector and the ADP tensor: the constrained parameters are missing.³ The .mat file is thus different from the CIF file, which contains all parameters. Because our method only works with the 9×9 variance/covariance matrix of the ADPs, we have to construct the matrix from the CIF file. From the parameters in the CIF file the site symmetry can be derived and thus the dependency

³ It would indeed be helpful if the least-squares software would additionally store refinement restrictions into a file.

Table 3

Example of a 9×9 variance/covariance matrix of the ADPs of an atom on a mirror plane: $-y, -x, z$.

(11, 12) is read as $\text{Cov}(U^{11}, U^{12})$ and the following properties hold: $\text{Cov}(U^{ij}, U^{ij}) = \text{Var}(U^{ij})$, $\text{Cov}(U^{ij}, U^{kl}) = \text{Cov}(U^{kl}, U^{ij})$. Dashed elements are constrained covariances not present in the .mat file.

$$\begin{bmatrix} \text{(11, 11)} & \text{(11, 12)} & - & - & - & \text{(11, 23)} & - & - & \text{(11, 33)} \\ - & \text{(12, 12)} & - & - & - & \text{(12, 23)} & - & - & \text{(12, 33)} \\ - & - & - & - & - & - & - & - & - \\ - & - & - & - & - & - & - & - & - \\ - & - & - & - & - & - & - & - & - \\ - & - & - & - & - & \text{(23, 23)} & - & - & \text{(23, 33)} \\ - & - & - & - & - & - & - & - & - \\ - & - & - & - & - & - & - & - & - \\ - & - & - & - & - & - & - & - & \text{(33, 33)} \end{bmatrix}$$

between parameters. From the .mat file we can then extract the variances and covariances.

The effect of the site symmetry on the coordinates can be found by solving the equation

$$\mathbf{S}\vec{x} = \vec{x}, \quad (5)$$

where \mathbf{S} is the symmetry operation (*i.e.* a linear transformation) which leaves the coordinates unchanged and \vec{x} the vector coordinate. A similar equation is used for the ADPs (it is not necessary to operate on \mathbf{U}^* as there is no change of basis during a symmetry operation),

$$\mathbf{S}\mathbf{U}\mathbf{S}^t = \mathbf{U}. \quad (6)$$

For the variance/covariance matrix, equations (5) and (6) are not sufficient to derive the missing elements (Table 3). But from the equalities found for the coordinates and ADPs we are able to complete these missing elements.

In the simple case when the parameter is constrained to a certain value, its standard uncertainty and its variance are zero and its covariance with any parameter is also zero.

The situation is more complicated if two parameters are dependent on each other. For example, if an atom is located on a mirror plane in space group $R3m$, the following constraints are imposed by symmetry: $x = -y$ on the coordinates and $U^{22} = U^{11}$, $U^{13} = -U^{23}$ on the ADPs [e.g. atom Cl2 in $3\text{C}_7\text{H}_9\text{ClO}_3 \cdot \text{CHCl}_3$ (Tafeenko *et al.*, 2009)]. From the .mat file written by *SHELXL* (Sheldrick, 2008) the four variances of the ADPs U^{11} , U^{33} , U^{23} , U^{12} and the corresponding six covariances can be derived. Consequently, we have to complete the 11 missing elements in the variances/covariances matrix of the ADPs (see Table 3) in order to obtain the complete \mathbf{F} (Table 2). These 11 missing elements are not independent and can be found using variable substitutions and the properties of covariances,⁴

⁴ $\text{Cov}(V, V) = \text{Var}(V)$, $\text{Var}(aV + bW) = a^2\text{Var}(V) + b^2\text{Var}(W) + 2ab\text{Cov}(V, W)$, $\text{Cov}(aV + bW, cX + dY) = ac\text{Cov}(V, X) + ad\text{Cov}(V, Y) + bc\text{Cov}(W, X) + bd\text{Cov}(W, Y)$.

$$\begin{aligned} \text{Cov}(U^{11}, U^{22}) &= \text{Cov}(U^{11}, U^{11}) = \text{Var}(U^{11}), \\ \text{Cov}(U^{12}, U^{13}) &= \text{Cov}(U^{12}, -U^{23}) = -\text{Cov}(U^{12}, U^{23}), \\ \text{Cov}(U^{12}, U^{22}) &= \text{Cov}(U^{12}, U^{11}), \\ \text{Var}(U^{13}) &= \text{Var}(-U^{23}) = \text{Var}(U^{23}), \\ \text{Cov}(U^{13}, U^{11}) &= \text{Cov}(-U^{23}, U^{11}) = -\text{Cov}(U^{23}, U^{11}), \\ \text{Cov}(U^{13}, U^{22}) &= \text{Cov}(-U^{23}, U^{11}) = -\text{Cov}(U^{23}, U^{11}), \\ \text{Cov}(U^{13}, U^{23}) &= \text{Cov}(U^{13}, -U^{13}) = -\text{Var}(U^{13}), \\ \text{Cov}(U^{13}, U^{33}) &= \text{Cov}(-U^{23}, U^{33}) = -\text{Cov}(U^{23}, U^{33}), \\ \text{Var}(U^{22}) &= \text{Var}(U^{11}), \\ \text{Cov}(U^{22}, U^{33}) &= \text{Cov}(U^{11}, U^{33}), \\ \text{Cov}(U^{23}, U^{22}) &= \text{Cov}(U^{23}, U^{11}). \end{aligned} \quad (7)$$

The implementation is usually based on the matrix of constraints \mathbf{M} (Watkin, 2008). \mathbf{M} is a $p \times q$ matrix mapping p parameters to a reduced set of q independent parameters. The construction of \mathbf{M} is made by finding the relationship between the parameters. This procedure is necessary because there is no straightforward way to recover \mathbf{M} purely from the correlation matrix or the CIF file. For example, the constraints $U^{22} = U^{11}$ and $U^{13} = -U^{23}$ give the following constraint matrix,

$$\begin{bmatrix} U^{11} \\ U^{21} \\ U^{31} \\ U^{12} \\ U^{22} \\ U^{32} \\ U^{13} \\ U^{23} \\ U^{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} U^{11} \\ U^{33} \\ U^{23} \\ U^{12} \end{bmatrix}. \quad (8)$$

\mathbf{M}

The full 9×9 variance/covariance matrix \mathbf{F} and the variance/covariance matrix with missing elements \mathbf{F}_m (derived from the .mat file) are related by the following equation (Watkin, 2008),

$$\mathbf{F} = \mathbf{M}\mathbf{F}_m\mathbf{M}^t. \quad (9)$$

6. Isotropic displacement parameters

Isotropic displacement parameters are a special case of ADPs where the magnitudes of displacement are equal in all directions. In an orthonormal (Cartesian) coordinate system the tensor representative of the isotropic displacement parameter is diagonal with all diagonal elements equal. This tensor has the dimension of length² as in the CIF file and needs to be converted to a dimensionless tensor before applying any linear operations (see §11).

7. Practical application 1: refinement in different space-group settings

In the triclinic and monoclinic crystal systems the choice of the unit cell is not unique. Different space-group settings in the monoclinic system normally lead to different cell parameters; famous examples are the settings $P2_1/n$ versus $P2_1/c$ and $C2/c$

Table 4
Parameters of O14 and C13 of methylene aziridine.

Parameter	Refined in $P2_1/n$	$P2_1/c$ setting transformed from the $P2_1/n$ refinement	Refined in $P2_1/c$
O14			
x	0.35897 (11)	0.72706 (16)	0.72703 (16)
y	0.74314 (12)	0.25686 (12)	0.25684 (12)
z	0.63191 (11)	0.36809 (11)	0.36807 (11)
U^{11}	0.04682 (85)	0.06219 (99)	0.06227 (99)
U^{22}	0.02399 (70)	0.02399 (70)	0.02368 (69)
U^{33}	0.05938 (101)	0.05938 (101)	0.05922 (101)
U^{23}	0.00258 (63)	-0.00306 (65)	-0.00306 (65)
U^{13}	-0.00735 (72)	0.04677 (90)	0.04679 (91)
U^{12}	-0.00165 (63)	-0.00165 (63)	-0.00185 (63)
Eigenvalues	0.02369 (70)	0.02369 (70)	0.02341 (69)
	0.04239 (61)	0.04239 (61)	0.04214 (61)
	0.06476 (64)	0.06476 (64)	0.06479 (65)
C13			
x	0.48537 (15)	0.85708 (21)	0.85711 (21)
y	0.13692 (23)	0.86308 (23)	0.86308 (23)
z	0.62829 (16)	0.37171 (16)	0.37174 (16)
U^{11}	0.03135 (101)	0.04285 (116)	0.04269 (117)
U^{22}	0.04763 (123)	0.04763 (123)	0.04765 (122)
U^{33}	0.05264 (134)	0.05264 (134)	0.05267 (135)
U^{23}	0.00808 (95)	-0.00436 (99)	-0.00457 (99)
U^{13}	-0.00006 (91)	0.03666 (113)	0.03674 (113)
U^{12}	0.00237 (103)	0.00237 (103)	0.00234 (103)
Eigenvalues	0.02788 (102)	0.02788 (102)	0.02731 (101)
	0.05015 (89)	0.05015 (89)	0.05031 (90)
	0.05370 (91)	0.05370 (91)	0.05370 (91)

versus $I2/a$. In some of these settings the cell angles can become very oblique. It has been reported that refinement in oblique cells has increased correlation between selected parameters, potentially making the refinement unstable (Dunitz, 1995).

The molecule methylene aziridine (Feast *et al.*, 2009) can be described in space group $P2_1/n$ with cell parameters $a = 13.8593$ (3), $b = 10.5242$ (2), $c = 14.8044$ (4) Å, $\beta = 92.0014$ (7)° or space group $P2_1/c$ with cell parameters $a = 13.8594$ (2), $b = 10.5243$ (2), $c = 19.9230$ (3) Å, $\beta = 132.0439$ (7)°. In the oblique cell setting, Feast *et al.* (2009) highlight an increase of the correlation between refined parameters. For our study we re-refined the structure based on the deposited reflection data. The asymmetric unit contains 28 non-H atoms, which have been refined freely with ADPs. As an example we consider here atoms C13, O14, C111 and O102. On these atoms we demonstrate how to transform the refined coordinates, ADPs and their covariances into different unit-cell settings.

The unit-cell transformation from $P2_1/n$ to $P2_1/c$ has the transformation matrix \mathbf{A} applied to the column vector of cell parameters,

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ -1 & 0 & -1 \end{bmatrix}. \quad (10)$$

Consequently, for the column vector of coordinates and ADPs, \mathbf{A}^{-t} is used,

$$\mathbf{A}^{-t} = \begin{bmatrix} 1 & 0 & -1 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}. \quad (11)$$

The original refinement (Feast *et al.*, 2009) had been performed with the *CRYSTALS* package (Betteridge *et al.*, 2003). Our re-refinement was performed with *SHELXL* (Sheldrick, 2008). The refined parameters obtained from *SHELXL* and from Feast *et al.* (2009) were identical within standard uncertainties. The result of the $P2_1/n$ refinement is given in the left-hand column of Table 4 and of the $P2_1/c$ refinement in the right-hand column. The middle column of Table 4 shows the $P2_1/n$ results transformed to the $P2_1/c$ setting using our own *Python* routine (see supplementary material⁵). The transformation has been applied on the coordinates, ADPs, eigenvalues of the ADPs, and all standard uncertainties. The full variance/covariance matrix has been used, as obtained from the .mat file generated by *SHELXL* (Sheldrick, 2008) with the 'MORE -1' instruction.

Fig. 1 displays the correlation matrix of four atoms from the $P2_1/c$ refinement (left) and the $P2_1/n$ refinement (right). It is evident from the graphs that these two correlation matrices are very different. These graphs support thus the conclusions about correlations by Feast *et al.* (2009). However, from the previous it follows that the correlation matrices can be compared only if the relevant linear transformation is used. The difference between the correlation matrix from the $P2_1/c$ refinement and the transformed matrix from the $P2_1/n$ refinement is shown in Fig. 2. For the four atoms shown the maximum deviation is only 0.015. It can thus be concluded that the refinement is independent of the unit-cell setting.

In applying the transformations and in the preparation of Figs. 1 and 2 the correlation between different atoms has been ignored. We also ignored the correlation between the coordinates and the ADPs of the same atom. This corresponds to a block diagonal least-squares refinement.⁶

8. Practical application 2: eigenvalues and eigenvectors of ADPs

Calculation of eigenvalues and eigenvectors of second-rank tensors is not trivial but readily available in programming languages or mathematic software (see §11.3). To calculate the eigenvalues of the ADPs in a non-orthogonal coordinate system, it is necessary to use the reciprocal metric tensor $\mathbf{G}^* = \mathbf{G}^{-1}$.

\mathbf{G} is defined as (Dunitz, 1995, p. 227)

$$\mathbf{G} = \begin{bmatrix} a^2 & ab \cos(\gamma) & ac \cos(\beta) \\ ab \cos(\gamma) & b^2 & bc \cos(\alpha) \\ ac \cos(\beta) & bc \cos(\alpha) & c^2 \end{bmatrix}. \quad (12)$$

⁵ Results of the $P2_1/n$ refinement which are discussed in this paper are available from the IUCr electronic archives (Reference: PC5002). Services for accessing these data are described at the back of the journal.

⁶ The situation might be different in the case of a full matrix refinement. Still, there is strong evidence for the same behavior. Additionally, weighting schemes might introduce numerical problems.

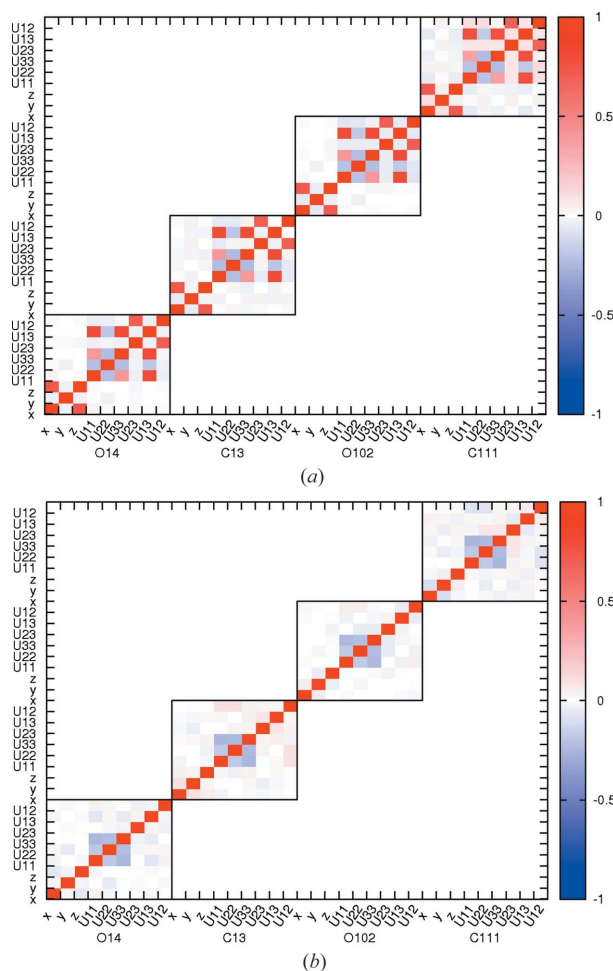


Figure 1

Correlation matrix from *SHELXL* using color coding. Correlation between parameters of different atoms are not reported. (a) Methylene aziridine refined in space group $P2_1/c$. (b) Methylene aziridine refined in space group $P2_1/n$.

The variance/covariance matrix \mathbf{F}_λ of the eigenvalues of a second-rank tensor can be calculated as

$$\mathbf{F}_\lambda = [\mathbf{Q}^t \otimes (\mathbf{G}^* \mathbf{Q})^{-1}] \mathbf{F}_{\vec{u}^*} [\mathbf{Q}^t \otimes (\mathbf{G}^* \mathbf{Q})^{-1}]^t, \quad (13)$$

where \mathbf{Q} is the matrix of the eigenvectors (see also §11.3).

Because $\mathbf{G}^* = \mathbf{G}^{-1}$, this can be simplified to

$$\mathbf{F}_\lambda = [\mathbf{Q}^t \otimes (\mathbf{Q}^{-1} \mathbf{G})] \mathbf{F}_{\vec{u}^*} [\mathbf{Q} \otimes (\mathbf{Q}^{-1} \mathbf{G})]. \quad (14)$$

The standard uncertainties of the eigenvalues λ can be obtained from the square root of the diagonal terms of the \mathbf{F}_λ matrix. As an example, the eigenvalues and their standard uncertainties of the ADPs of atoms O14 and C13 from Feast *et al.* (2009) are shown in Table 4.

9. Practical application 3: normal coordinate analysis

Normal coordinate analysis of crystal structures measured at multiple temperatures can be performed with the *NKA* software (Bürgi & Capelli, 2000; Capelli *et al.*, 2000). The input for this software must be in 1 (C_1) symmetry. If a molecule is on a special position, the coordinates, the ADPs and their standard

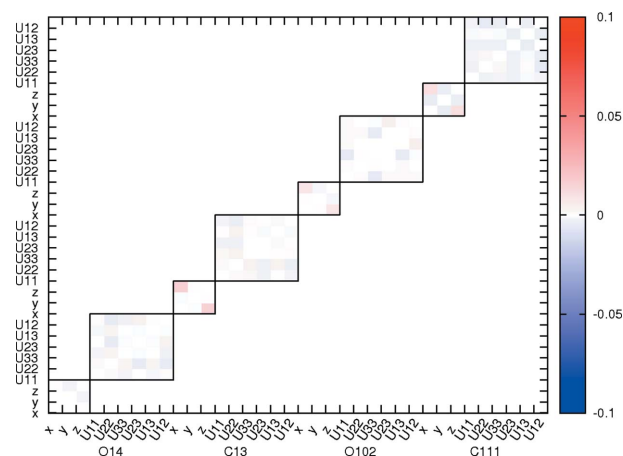


Figure 2

Difference between the correlations of parameters in the $P2_1/n$ and the $P2_1/c$ refinement. The correlations of the $P2_1/n$ refinement have been transformed to the $P2_1/c$ setting. The maximum deviation is 0.015.

uncertainties have to be expanded to 1 (C_1) symmetry (Smeets *et al.*, 2011). The correct symmetry is then introduced later by the choice of appropriate local coordinate systems for the atoms.

The *Python* program (see supplementary material) will perform this expansion to 1 (C_1) symmetry using the site symmetry and the CIF and .mat files from *SHELXL* as input.

One result of the normal coordinate analysis is the ε tensor, which is a temperature-independent term. ε is a symmetric second-rank tensor and thus analogous to an ADP tensor. The standard uncertainties of the eigenvalues of the ε tensor can again be calculated using equation (13). As in the case of ADPs, the ε tensor must be positive definite to be physically meaningful. The calculation of the eigenvalues and their standard uncertainties is thus very useful for assessing the quality of the analysis. As the ε tensor is symmetric and expressed in a Cartesian coordinate system, the matrix of the eigenvectors \mathbf{Q} is orthogonal ($\mathbf{Q}^{-1} = \mathbf{Q}^t$) and the metric tensor is the identity matrix. From equation (13) we find

$$\begin{aligned} \mathbf{F}_\lambda &= [\mathbf{Q}^t \otimes (\mathbf{G}^* \mathbf{Q})^{-1}] \mathbf{F}_\varepsilon [\mathbf{Q}^t \otimes (\mathbf{G}^* \mathbf{Q})^{-1}]^t, \\ \mathbf{F}_\lambda &= (\mathbf{Q}^t \otimes \mathbf{Q}^t) \mathbf{F}_\varepsilon (\mathbf{Q} \otimes \mathbf{Q}). \end{aligned} \quad (15)$$

Table 5 shows the ε tensors of atoms Cu, N and C in tris-(ethylenediamine)copper(II) sulfate (Smeets *et al.*, 2011).

10. Practical application 4: equivalent isotropic ADPs

Equivalent isotropic ADPs U_{equiv} should be reported with their standard uncertainties (Trueblood *et al.*, 1996). The calculation of these standard uncertainties is not straightforward, because it can involve the transformation to an orthogonal coordinate system (Fischer & Tillmanns, 1988). Therefore, in many instances approximations are used for the calculation (Schomaker & Marsh, 1983; Watkin, 2000).

U_{equiv} is the arithmetic average of the ADPs in the Cartesian coordinate system,

Table 5

ε tensor components and eigenvalues (\AA^2) in tris(ethylenediamine)copper(II) sulfate (Smeets *et al.*, 2011).

	Components						Eigenvalues		
	ε_{11}	ε_{22}	ε_{33}	ε_{12}	ε_{13}	ε_{23}	λ_1	λ_2	λ_3
$\varepsilon(\text{Cu})$	0.0041 (2)	0.0041 (2)	0.0016 (3)	0	0	0	0.00408 (19)	0.00407 (19)	0.0016 (3)
$\varepsilon(\text{N})$	0.0302 (2)	0.0058 (3)	0.0117 (3)	-0.0009 (2)	-0.0012 (2)	0.0037 (2)	0.03038 (18)	0.0133 (3)	0.0040 (3)
$\varepsilon(\text{C})$	0.0101 (3)	0.0033 (4)	0.0135 (5)	0.0001 (3)	-0.0038 (3)	0.0013 (4)	0.0160 (6)	0.0077 (3)	0.0030 (5)

$$U_{\text{equiv}} = \frac{1}{3} \left(U_{\text{cart}}^{11} + U_{\text{cart}}^{22} + U_{\text{cart}}^{33} \right). \quad (16)$$

The ADPs expressed in the Cartesian coordinate system are calculated from the \mathbf{U}^* tensor using an orthogonalization matrix (Dunitz, 1995, p. 237),

$$\begin{bmatrix} a & b \cos \gamma & c \cos \beta \\ 0 & b \sin \gamma & [c(\cos \alpha - \cos \beta \cos \gamma)]/\sin \gamma \\ 0 & 0 & cv/\sin \gamma \end{bmatrix}, \quad (17)$$

with $v = abc(1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma)^{1/2}$.

The orthogonalization matrix represents a linear transformation. This means that the orthogonalization matrix can also be applied on the variance/covariance matrix of the ADPs using equation (3). The variance of U_{equiv} is then derived from the components of the variance/covariance matrix on a Cartesian basis,

$$\begin{aligned} \text{Var}(U_{\text{equiv}}) &= \text{Var} \left[\frac{1}{3} (U_{\text{cart}}^{11} + U_{\text{cart}}^{22} + U_{\text{cart}}^{33}) \right] \\ &= \frac{1}{9} [\text{Var}(U_{\text{cart}}^{11}) + \text{Var}(U_{\text{cart}}^{22}) + \text{Var}(U_{\text{cart}}^{33}) \\ &\quad + 2\text{Cov}(U_{\text{cart}}^{11}, U_{\text{cart}}^{22}) + 2\text{Cov}(U_{\text{cart}}^{11}, U_{\text{cart}}^{33}) \\ &\quad + 2\text{Cov}(U_{\text{cart}}^{22}, U_{\text{cart}}^{33})]. \end{aligned} \quad (18)$$

11. Mathematical background

A linear map or linear application or linear transformation is a transformation in the Euclidean physical space that preserves the operations of vector addition and scalar multiplication (Zeidler, 2004, ch. 2.3). Typically, a symmetry operation and a change of coordinate system are linear maps.

Let V, W be two vector spaces, and $\mathbf{L} : V \mapsto W$ be a linear map between \mathbf{V} and \mathbf{W} . Letting W^*, V^* be the corresponding dual vector spaces, we define the dual homomorphism $\mathbf{L}^* : W^* \mapsto V^*$. A vector in this article is always noted as a column matrix. Mathematicians define a vector in the dual space as a row matrix which implies $\mathbf{L} = \mathbf{L}^*$ and \mathbf{L} is pre-multiplied or post-multiplied by a vector depending on the vector space (Shmueli, 2001). Let (a_i, \dots, a_n) be a direct basis of a vector space; the reciprocal basis (a^{*i}, \dots, a^{*n}) of the dual space is defined as $a^{*i} a_j = 1$ if $i = j$ or 0 otherwise.

The components of a vector denoted by an asterisk (*) are covariant and defined with respect to the reciprocal basis. Also, a second-rank tensor denoted by an asterisk (*) is defined with respect to the reciprocal basis.

Interesting dual homomorphism properties in the present context are:

$$\begin{aligned} \text{If } \mathbf{L} : V \mapsto W \text{ then } \mathbf{L}^{-1} : W \mapsto V. \\ \text{If } \mathbf{L} : V \mapsto W \text{ then } \mathbf{L}^t : W^* \mapsto V^*. \\ \text{If } \mathbf{L} : V \mapsto W \text{ then } \mathbf{L}^{-t} : V^* \mapsto W^*. \end{aligned} \quad (19)$$

The vector space V is the direct crystallographic space; the reciprocal crystallographic space is the vector space V^* . As a result a linear map \mathbf{L} in the direct space is the linear map \mathbf{L}^{-t} in the reciprocal space. Additionally, the components of a vector are named contravariant in the direct space and covariant in the reciprocal space.

Second-rank tensors may be written as square matrices. Most second-rank tensors of physical properties are symmetric and can be represented by a quadric surface. They are constructed following the relation (with C a constant) (Sands, 1995, p. 70)

$$\vec{x}'^t \mathbf{T} \vec{x} = C. \quad (20)$$

The anisotropic displacement tensor \mathbf{U}^* is defined with respect to a reciprocal-lattice basis (Trueblood *et al.*, 1996). Thus, the vector \vec{x}^* is covariant and the tensor \mathbf{U}^* defined by this vector is doubly contravariant,

$$\vec{x}^{*t} \mathbf{U}^* \vec{x}^* = C. \quad (21)$$

Variance/covariance matrices can also be described by a quadric surface and their representing tensors are doubly contravariant.

11.1. Linear maps on doubly contravariant symmetric tensors

Let \vec{x} be a vector of vector space V with respect to a direct basis. \vec{x}' is the result of the application of a linear map \mathbf{L} on \vec{x} . Using matrices, the equation is

$$\vec{x}' = \mathbf{L} \vec{x}. \quad (22)$$

The application of the same linear map \mathbf{L} on a doubly contravariant tensor \mathbf{T}^* is

$$\mathbf{T}^{*'} = \mathbf{L} \mathbf{T}^* \mathbf{L}^t. \quad (23)$$

Proof. Let \mathbf{T}^* be a doubly contravariant tensor representing a quadratic equation defined with respect to a reciprocal basis. The basis is not necessarily orthogonal:

$$\vec{x}^{*t} \mathbf{T}^* \vec{x}^* = C. \quad (24)$$

Let \vec{x}^* and $\vec{x}^{*'}$ be two vectors defined with respect to a reciprocal basis (a^{1*}, \dots, a^{n*}) . $\vec{x}^{*'}$ is the result of the application of a linear map \mathbf{L}^* on \vec{x}^* . Let \vec{x} and \vec{x}' be two vectors defined with

respect to the corresponding direct basis (a_1, \dots, a_n) . $a^{*i}a_j = 1$ if $i = j$ or 0 otherwise. \vec{x}' is the result of the application of a linear map \mathbf{L} on \vec{x} . Using the definition and properties of dual space [equation (19)] we obtain

$$\begin{aligned} \vec{x}^{*'} &= \mathbf{L}^* \vec{x}^* \\ \vec{x}^{*'} &= \mathbf{L}^{-t} \vec{x}^* \quad \text{dual-space property} \\ \vec{x}^* &= \mathbf{L}^t \vec{x}^{*'} \end{aligned} \quad (25)$$

Finally, by injecting (25) into (24) we obtain

$$\begin{aligned} \vec{x}^{*t} \mathbf{T}^* \vec{x}^* &= C, \\ (\mathbf{L}^t \vec{x}^{*'})^t \mathbf{T}^* (\mathbf{L}^t \vec{x}^*) &= C, \\ \vec{x}^{*t} (\mathbf{L} \mathbf{T}^* \mathbf{L}^t) \vec{x}^* &= C. \end{aligned} \quad (26)$$

11.2. Vectorization of the product of square matrices

Let a square $n \times n$ matrix \mathbf{B} be pre-multiplied by a matrix \mathbf{A} and post-multiplied by a matrix \mathbf{C} . It is a very common operation in linear applications such as symmetry operations on tensors,

$$\mathbf{P} = \begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{1n} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} b_{11} & \cdots & b_{1n} \\ \vdots & \ddots & \vdots \\ b_{1n} & \cdots & b_{nn} \end{bmatrix} \begin{bmatrix} c_{11} & \cdots & c_{1n} \\ \vdots & \ddots & \vdots \\ c_{1n} & \cdots & c_{nn} \end{bmatrix} \quad (27)$$

A B C

We define $\vec{\cdot}$ as the *vec* operator (Henderson & Searle, 1981). \mathbf{P} and \mathbf{B} are re-written as a vector by stacking all the columns on top of each other (Soler & van Gelder, 1991). The first column is on top of the second one and so on until all the columns are stacked. The resulting vector has size n^2 ,

$$\vec{\mathbf{B}} = \begin{bmatrix} b_{11} \\ \vdots \\ b_{n1} \\ - \\ b_{1i} \\ \vdots \\ b_{ni} \\ - \\ b_{1n} \\ \vdots \\ b_{nn} \end{bmatrix}.$$

The equivalent vector operation of equation (27) is written

$$\vec{\mathbf{P}} = \mathbf{D} \vec{\mathbf{B}} \quad (28)$$

$n^2 \times n^2$ $n^2 \times 1$

The \mathbf{D} matrix is constructed from matrices \mathbf{A} and \mathbf{C} using the Kronecker product. The Kronecker product, denoted by \otimes , is an operation on two matrices of arbitrary size resulting in a block matrix.

If \mathbf{A} is an $m \times n$ matrix and \mathbf{C} is a $p \times q$ matrix, then the Kronecker product $\mathbf{D} = \mathbf{A} \otimes \mathbf{C}$ is an $mp \times nq$ block matrix and is constructed as follows (Horn & Johnson, 1991; Roth, 1934),

$$\begin{aligned} \mathbf{D} &= \mathbf{A} \otimes \mathbf{C} \\ &= \begin{bmatrix} a_{11}c_{11} & \cdots & a_{11}c_{1q} & \cdots & a_{1n}c_{11} & \cdots & a_{1n}c_{1q} \\ a_{11}c_{21} & \cdots & a_{11}c_{2q} & \cdots & a_{1n}c_{21} & \cdots & a_{1n}c_{2q} \\ \vdots & \ddots & \vdots & & \vdots & \ddots & \vdots \\ a_{11}c_{p1} & \cdots & a_{11}c_{pq} & \cdots & a_{1n}c_{p1} & \cdots & a_{1n}c_{pq} \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ a_{m1}c_{11} & \cdots & a_{m1}c_{1q} & \cdots & a_{mn}c_{11} & \cdots & a_{mn}c_{1q} \\ a_{m1}c_{21} & \cdots & a_{m1}c_{2q} & \cdots & a_{mn}c_{21} & \cdots & a_{mn}c_{2q} \\ \vdots & \ddots & \vdots & & \vdots & \ddots & \vdots \\ a_{m1}c_{p1} & \cdots & a_{m1}c_{pq} & \cdots & a_{mn}c_{p1} & \cdots & a_{mn}c_{pq} \end{bmatrix} \\ &= \begin{bmatrix} a_{11} \mathbf{C} & \cdots & a_{1n} \mathbf{C} \\ \vdots & & \vdots \\ a_{m1} \mathbf{C} & \cdots & a_{mn} \mathbf{C} \end{bmatrix}. \end{aligned} \quad (29)$$

Finally, the equivalent vector operation of equation (27) is written (Petersen & Pedersen, 2008; Horn & Johnson, 1991)

$$\vec{\mathbf{P}} = (\mathbf{C}^t \otimes \mathbf{A}) \vec{\mathbf{B}} \quad (30)$$

$n^2 \times n^2$ $n^2 \times 1$

The variance/covariance matrix of a vector is usually represented by ‘extending’ the vector into a second-rank tensor. The construction of a variance/covariance matrix of a two-dimensional matrix is not trivial. The difficulty is in which order the indices of the resulting variance/covariance matrix are sorted. If the indices are ordered randomly, the linear map \mathbf{L} [equation (26)] is no longer valid for the variance/covariance matrix.

This difficulty in the construction of the variance/covariance matrix can be circumvented by re-writing the initial two-dimensional matrix into a vector (Soler & van Gelder, 1991). Any linear application on the vector is valid on the corresponding variance/covariance matrix \mathbf{F} using equation (26).

11.3. Eigenvalues of second-rank tensors and their standard uncertainties

In a non-orthogonal coordinate system eigenvalue decomposition cannot be performed without a metric tensor (Sands, 1995, p. 72). In this case the generalized eigenvalue problem is to find a vector \vec{v} that obeys $\mathbf{T}\vec{v} = \lambda\mathbf{G}\vec{v}$, where \mathbf{T} is the tensor of the initial ADPs. Depending in which space \mathbf{T} is represented, \mathbf{G} is the metric tensor or reciprocal metric tensor.⁷ λ is a diagonal matrix containing the eigenvalues. The eigenvalues are then obtained by solving the equation $\det(\mathbf{T} - \lambda\mathbf{G}) = 0$ (in an orthonormal coordinate system the metric tensor \mathbf{G} is substituted by the identity matrix).

Using matrix notation, the following equality holds,

⁷ In the *Python* programming language only the *scipy* extension provides the `scipy.linalg.eig` function which accepts the use of a metric tensor. From the *numpy* extension, `numpy.linalg.eig` is not suitable (see supplementary material).

$$\mathbf{T} = \mathbf{GQ}\boldsymbol{\lambda}\mathbf{Q}^{-1}. \quad (31)$$

By expressing $\boldsymbol{\lambda}$ as a function of \mathbf{T} and then applying the *vec* operator [see equation (30)], we obtain

$$\begin{aligned} \boldsymbol{\lambda} &= (\mathbf{GQ})^{-1}\mathbf{TQ}, \\ \vec{\boldsymbol{\lambda}} &= [\mathbf{Q}' \otimes (\mathbf{GQ})^{-1}]\vec{\mathbf{T}}. \end{aligned} \quad (32)$$

\mathbf{Q} and \mathbf{G} are linear maps, as are \mathbf{Q}' , \mathbf{Q}^{-1} and \mathbf{G}^{-1} . Also, the Kronecker product defines a linear map (Rowland, 2011). Consequently, $\mathbf{Q}' \otimes (\mathbf{GQ})^{-1}$ is a linear map. Application of a linear map on a doubly contravariant tensor [see equation (23)] gives us the expression of the variance/covariance matrix of $\boldsymbol{\lambda}$ and thus the standard uncertainties of the eigenvalues,

$$\mathbf{F}_{\vec{\boldsymbol{\lambda}}} = [\mathbf{Q}' \otimes (\mathbf{GQ})^{-1}]\mathbf{F}_{\vec{\mathbf{T}}}[\mathbf{Q}' \otimes (\mathbf{GQ})^{-1}]'. \quad (33)$$

11.4. The .mat file from SHELXL

The .mat file can be written by the *SHELXL* software (Sheldrick, 2008) using the 'MORE -1' instruction. The first section of this file provides the refined parameters, their values and their standard uncertainties. The second part consists of the correlations between the parameters given as an upper triangular matrix. The correlation elements are written sequentially in fixed format, ten elements per row. Thereby, the diagonal elements equal 1 (correlation of a parameter with itself). The variances can be derived from the standard uncertainties σ in the first part of the .mat file. The covariances can be derived from the correlations in the second part of the .mat file, e.g.

$$\text{Cov}(1, 2) = \sigma_1\sigma_2\text{Corr}(1, 2). \quad (34)$$

12. Conclusions

We describe a method to apply a linear transformation to the standard uncertainties using the *vec* operator and the variance/covariance matrix. This method has been used to explain the relationship between two correlation matrices expressed in different unit-cell settings.

13. Supplementary material

The supplementary material contains a small example as a *Python* script. A more complex *Python* script is available from the author or on the Debroglie website (<http://www.debroglie.net/>). This script reads in a CIF file and a .mat file from *SHELXL*. The software flow is controlled by command-line parameters. It is possible to expand all the structure parameters to *P1*, apply a transformation matrix or a symmetry operation, and convert all parameters into Cartesian space. The output is written on the terminal or into an SPF file for the *PLATON* software (Spek, 2009).

We thank Roelof W. Bruggeman (Mathematisch Instituut, Universiteit Utrecht) for his helpful advice on dual homomorphism, and David J. Watkin (University of Oxford) for fruitful discussions about least-squares refinements and about the nomenclature of ADPs.

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