MaterialConstants Package ver. 02 for Maple

by

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Abstract: This Maple worksheet describes a new preliminary Maple package called **MaterialConstants ver. 02 (July 15, 2014)**, whose main goal is to display in a material constants matrix **C** for materials with various types of symmetries. In particular, the main procedure of the package called **TransformedMaterialConstants** and aliased as **TCM**, applies desired material symmetries to a generic material constants matrix C which is a 6 x 6 symmetric real matrix. It then returns the material constants matrix **C** for the material with the specified symmetry(ies).

The package has been created and compiled under Maple 15 (Classic), but it also works in all subsequent versions of Maple through version 18. It uses some commands from two built-in Maple packages: LinearAlgebra and Groebner. Thus, all matrices are of type/Matrix.

The material presented in this wortksheet is divided into three sections followed by conclusions and references.

In **Section 1**, we describe mathematics behind procedures which implement certain mappings and new types. We provide simple examples of how these procedures work.

In **Section 2**, we describe in details how the main procedure **TransformedMaterialConstants** works. This procedure computes Groebner bases for certain ideals using a custom monomial order which is essentially an elimination order. In particular, this procedure can apply generators of the material symmetry group which are expressed as 3 x 3 orthogonal matrices. These matrices may be of type/orthogonal or of type/puresymbolic. For example, general rotation matrices in R^3 around coordinate axes x, y, and z by arbitrary (unspecified) angles theta[1], theta[2], and theta[3] are of type/puresymbolic (although they are also of type/orthogonal).

In **Section 3**, we give examples in which we compute and display the material constant matrix C for materials with various types of symmetries. This section is divided into two subsections:

--**Subsection 1: Standard materials:**
---monoclinic (see Example 8)
---orthotropic (see Example 9)
---transversely isotropic (see Example 10)
---isotropic (see Example 11)

--Subsection 2: Non-Standard Materials:
---cubic isotropic (see Example 12)
---tetragonal (see Example 13)
---trigonal (see Example 14)
---trigonal-hexagonal (see Example 15)

Cookeville, July 15, 2014

```
> restart:with(LinearAlgebra):with(MaterialConstants);
```

_known_types = [*orthogonal*, *puresymbolic*]

_known_aliases = [*RM* = *MaterialConstants*:-*ReflectionMatrix*,
TMC = *MaterialConstants*:-*TransformedMaterialConstants*]

_known_additional_protected_names = [*c*, ε, σ, θ]

[*C_constants*, *MCversion*, *ModuleLoad*, *ModuleUnload*, *ReflectionMatrix*, *SimilarityTransform*, *Teps*, *TepsMatrix*, *TransformedMaterialConstants*, *Tsigma*, *TsigmaMatrix*, *makeC*, *makeEpsilon*, *makeSigma*, *phi_eps*, *phi_eps_inv*, *phi_sigma*, *phi_sigma_inv*]

```
>
```

When the package is loaded, it displays **_known_types**, **_known_aliases**, and **_known_additional_protected_names**, and then, as usual, it displays a list of procedures in the package. Note that names 'c', 'epsilon', 'sigma' and 'theta' are protected.

Procedure **MCversion** displays information about the package. In particular, its version and the name of its source file are displayed.

```
> MCversion();
```

++

MaterialConstants - A Maple 15 Small Package for Computing Material Constants Tensor

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+++++This is MaterialConstants Package ver. 02 for Maple 15+++++

>

Section 1: Introduction

Procedure **makeSigma** defines a stress tensor **Sigma** as a 3 x 3 symmetric matrix with real symbolic entries. Since traditionally entries of **Sigma** are written as **sigma[i,j]**, the name 'sigma' is protected. This matrix is of type/puresymbolic.

```
> Sigma:=makeSigma(3,sigma);
  type(Sigma,puresymbolic);
```

$$\Sigma := \begin{bmatrix} \sigma_{1,1} & \sigma_{1,2} & \sigma_{1,3} \\ \sigma_{1,2} & \sigma_{2,2} & \sigma_{2,3} \\ \sigma_{1,3} & \sigma_{2,3} & \sigma_{3,3} \end{bmatrix}$$

true

>

Procedure **makeEpsilon** defines a strain tensor **Epsilon** as a 3 x 3 symmetric matrix with real symbolic entries. Since traditionally entries of **Epsilon** are written as **epsilon[i,j]**, the name 'epsilon' is protected. This matrix is of type/puresymbolic.

```
> Epsilon:=makeEpsilon(3,epsilon);
  type(Epsilon,puresymbolic);
```

$$E := \begin{bmatrix} \varepsilon_{1,1} & \varepsilon_{1,2} & \varepsilon_{1,3} \\ \varepsilon_{1,2} & \varepsilon_{2,2} & \varepsilon_{2,3} \\ \varepsilon_{1,3} & \varepsilon_{2,3} & \varepsilon_{3,3} \end{bmatrix}$$

true

>

Matrices **Sigma** and **Epsilon** belong to the space of real 3 x 3 symmetric matrices **Mat^S(3,R)** which is isomorphic to **R^6**. This isomorphism is realized via two procedures: **phi_sigma** and **phi_eps** which give maps **Mat^S(3,R) ---> R^6**. Their inverses are, respectively, **phi_sigma_inv** and **phi_eps_inv**. Thus, the image of the stress tensor **Sigma** under **phi_sigma** is a stress array written as a column vector in **R^6**. Likewise, the image of the strain tensor **Epsilon** under **phi_eps** is a strain array written as a column vector in **R^6**.

```
> sigma_array:=phi_sigma(Sigma);
  phi_sigma_inv(sigma_array);
```

$$sigma\_array := \begin{bmatrix} \sigma_{1,1} \\ \sigma_{2,2} \\ \sigma_{3,3} \\ \sigma_{1,2} \\ \sigma_{2,3} \\ \sigma_{1,3} \end{bmatrix}$$

$$\begin{bmatrix} \sigma_{1,1} & \sigma_{1,2} & \sigma_{1,3} \\ \sigma_{1,2} & \sigma_{2,2} & \sigma_{2,3} \\ \sigma_{1,3} & \sigma_{2,3} & \sigma_{3,3} \end{bmatrix}$$

```
> epsilon_array:=phi_eps(Epsilon);
  phi_eps_inv(epsilon_array);
```

$$epsilon\_array := \begin{bmatrix} \varepsilon_{1,1} \\ \varepsilon_{2,2} \\ \varepsilon_{3,3} \\ 2\,\varepsilon_{1,2} \\ 2\,\varepsilon_{2,3} \\ 2\,\varepsilon_{1,3} \end{bmatrix}$$

$$\begin{bmatrix} \varepsilon_{1,1} & \varepsilon_{1,2} & \varepsilon_{1,3} \\ \varepsilon_{1,2} & \varepsilon_{2,2} & \varepsilon_{2,3} \\ \varepsilon_{1,3} & \varepsilon_{2,3} & \varepsilon_{3,3} \end{bmatrix}$$

```
>
```

Procedure **SimilarityTransform** applies a similarity transformation **M--> T*M*T^(-1)** where **T** is an orthogonal matrix related to the material symmetry. Matrices **M** and **T** are either 3 x 3 or 6 x 6 matrices. **M** can be either the stress tensor matrix **Sigma** or the strain matrix **Epsilon**. Matrix **T** needs to be of type puresymbolic or orthogonal.

The 3 x 3 matrix **T** can be, for example, a reflection matrix with respect to some plane **P**, for example, a coordinate plane in **R^3**. Such matrix can be found via a procedure **ReflectionMatrix** (aliased as **RM**) which takes as an argument a list **[n_x, n_y, n_z]** of three components of a vector **n** normal to the reflection plane **P**.

For example, let **T** be the reflection with respect to the xy-plane for **monoclinic materials**:

```
> Tz:=ReflectionMatrix([0,0,1]);
  type(Tz,orthogonal);
```

$$Tz := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$true$$

Let's define a symbolic stress tensor **Sigma** and the corresponding to it stress array **sigma_1**:

```
> Sigma:=makeSigma(3,sigma); ##<<-- original stress tensor
  type(%,puresymbolic);
  sigma_1:=phi_sigma(Sigma); ##<<-- original stress array
```

$$\Sigma := \begin{bmatrix} \sigma_{1,1} & \sigma_{1,2} & \sigma_{1,3} \\ \sigma_{1,2} & \sigma_{2,2} & \sigma_{2,3} \\ \sigma_{1,3} & \sigma_{2,3} & \sigma_{3,3} \end{bmatrix}$$

$$true$$

$$sigma\_1 := \begin{bmatrix} \sigma_{1,1} \\ \sigma_{2,2} \\ \sigma_{3,3} \\ \sigma_{1,2} \\ \sigma_{2,3} \\ \sigma_{1,3} \end{bmatrix}$$

Let's find the new stress tensor **Sigmaprime** after the similarity transformation **Sigma ---> Tz*Sigma*Tz^(-1)** is applied where **Tz** is the reflection matrix with respect to the xy-plane. Then, let's find the corresponding new stress array **sigmaprime**:

```
> Sigmaprime:=SimilarityTransform(Sigma,Tz); ##<<-- new transformed
  stress tensor
  sigmaprime_1:=phi_sigma(Sigmaprime); ##<<-- new transformed stress
  array
```

$$Sigmaprime := \begin{bmatrix} \sigma_{1,1} & \sigma_{1,2} & -\sigma_{1,3} \\ \sigma_{1,2} & \sigma_{2,2} & -\sigma_{2,3} \\ -\sigma_{1,3} & -\sigma_{2,3} & \sigma_{3,3} \end{bmatrix}$$

$$sigmaprime\_1 := \begin{bmatrix} \sigma_{1,1} \\ \sigma_{2,2} \\ \sigma_{3,3} \\ \sigma_{1,2} \\ -\sigma_{2,3} \\ -\sigma_{1,3} \end{bmatrix}$$

We can repeat the above computation for the strain tensor **Epsilon** by mapping it via the similarity to **Epsilonprime**, and let's find the corresponding new strain array **epsilonprime**.

```
> Epsilon:=makeEpsilon(3,epsilon); ##<<-- original strain tensor
  epsilon_1:=phi_eps(Epsilon); ##<<-- original strain array
```

$$E := \begin{bmatrix} \varepsilon_{1,1} & \varepsilon_{1,2} & \varepsilon_{1,3} \\ \varepsilon_{1,2} & \varepsilon_{2,2} & \varepsilon_{2,3} \\ \varepsilon_{1,3} & \varepsilon_{2,3} & \varepsilon_{3,3} \end{bmatrix}$$

$$epsilon\_1 := \begin{bmatrix} \varepsilon_{1,1} \\ \varepsilon_{2,2} \\ \varepsilon_{3,3} \\ 2\,\varepsilon_{1,2} \\ 2\,\varepsilon_{2,3} \\ 2\,\varepsilon_{1,3} \end{bmatrix}$$

```
> Epsilonprime:=SimilarityTransform(Epsilon,Tz); ##<<-- new
  transformed strain tensor
  epsilonprime_1:=phi_eps(Epsilonprime); ##<<-- new transformed
  strain array
```

$$Epsilonprime := \begin{bmatrix} \varepsilon_{1,1} & \varepsilon_{1,2} & -\varepsilon_{1,3} \\ \varepsilon_{1,2} & \varepsilon_{2,2} & -\varepsilon_{2,3} \\ -\varepsilon_{1,3} & -\varepsilon_{2,3} & \varepsilon_{3,3} \end{bmatrix}$$

$$epsilonprime\_1 := \begin{bmatrix} \varepsilon_{1,1} \\ \varepsilon_{2,2} \\ \varepsilon_{3,3} \\ 2\,\varepsilon_{1,2} \\ -2\,\varepsilon_{2,3} \\ -2\,\varepsilon_{1,3} \end{bmatrix}$$

```
>
```

Procedures **TsigmaMatrix** and **TepsMatrix** are 6 x 6 matrices which map, for the given symmetry **T** entered as a 3 x 3 orthogonal matrix, matrices of the linear transformations **R^ 6---> R^6**, which, respectively, map the original stress array **sigma_1** to the new stress array **sigmaprime_1**, and, the original strain array **epsilon_1** to the new strain array **epsilonprime_1**. For the above symmetry **Tz**, we find:

```
> T_sigma:=TsigmaMatrix(Tz);
  'sigmaprime_1'=Multiply(T_sigma,sigma_1);
```

$$T\_sigma := \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}$$

$$sigmaprime\_1 = \begin{bmatrix} \sigma_{1,1} \\ \sigma_{2,2} \\ \sigma_{3,3} \\ \sigma_{1,2} \\ -\sigma_{2,3} \\ -\sigma_{1,3} \end{bmatrix}$$

```
> T_eps:=TepsMatrix(Tz);
  'epsilonprime_1'=Multiply(T_eps,epsilon_1);
```

$$T\_eps := \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}$$

$$epsilonprime\_1 = \begin{bmatrix} \varepsilon_{1,1} \\ \varepsilon_{2,2} \\ \varepsilon_{3,3} \\ 2\,\varepsilon_{1,2} \\ -2\,\varepsilon_{2,3} \\ -2\,\varepsilon_{1,3} \end{bmatrix}$$

```
>
```

Recall that it is always the case that **(Teps)^(-1) = (Tsigma)^t** where **t** denotes the transpose of the matrix.

```
> MatrixInverse(T_eps) = Transpose(T_sigma);
  Equal(lhs(%),rhs(%));
```

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}$$

$$true$$

```
>
```

Procedure **Tsigma** is a linear map **R^6 ---> R^6** which maps a 6 x 1 stress array **sigma_1** to a new stress array **sigmaprime_1** for the given symmetry **T**. See Diagram_1. Matrix **T** is a 3 x 3 matrix that represents the implied symmetry. It must be of type 'orthogonal' or 'puresymbolic'. Thus, **Tsigma** is the composition of the following maps:

Tsigma = phi_sigma o SimilarityTransform o phi_sigma_inv

Likewise, procedure **Teps** maps a 6 x 1 strain array **epsilon_1** to a new strain array **epsilonprime_1**. See Diagram_2. Matrix **T** is a 3 x 3 matrix that represents the implied symmetry. It must be of type 'orthogonal' or 'puresymbolic'. Thus, **Teps** is the composition of the following maps:

Teps = phi_eps o SimilarityTransform o phi_eps_inv

We continue with **T = Tz** defined above:

```
> 'sigma_1'=sigma_1; ##<<-- original stress array
  'sigmaprime_1'=Tsigma(sigma_1,Tz); ##<<-- new transformed stress
  array
```

$$sigma\_1 = \begin{bmatrix} \sigma_{1,1} \\ \sigma_{2,2} \\ \sigma_{3,3} \\ \sigma_{1,2} \\ \sigma_{2,3} \\ \sigma_{1,3} \end{bmatrix}$$

$$sigmaprime\_1 = \begin{bmatrix} \sigma_{1,1} \\ \sigma_{2,2} \\ \sigma_{3,3} \\ \sigma_{1,2} \\ -\sigma_{2,3} \\ -\sigma_{1,3} \end{bmatrix}$$

```
> 'epsilon_1'=epsilon_1; ##<<-- original strain array
  'epsilonprime_1'=Teps(epsilon_1,Tz); ##<<-- new transformed strain
  array
```

$$epsilon\_1 = \begin{bmatrix} \varepsilon_{1,1} \\ \varepsilon_{2,2} \\ \varepsilon_{3,3} \\ 2\,\varepsilon_{1,2} \\ 2\,\varepsilon_{2,3} \\ 2\,\varepsilon_{1,3} \end{bmatrix}$$

$$epsilonprime\_1 = \begin{bmatrix} \varepsilon_{1,1} \\ \varepsilon_{2,2} \\ \varepsilon_{3,3} \\ 2\,\varepsilon_{1,2} \\ -2\,\varepsilon_{2,3} \\ -2\,\varepsilon_{1,3} \end{bmatrix}$$

>

Procedure **makeC** defines a generic material constants matrix **C** as a 6 x 6 symmetric matrix with real symbolic entries. Since traditionally entries of **C** are written as **c[i,j]**, the name **'c'** is protected. This matrix is of type/puresymbolic.of size 6 x 6 using a symbol **'c'**.

```
> C:=makeC(6,c);
  type(C,puresymbolic);
```

$$C := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & c_{1,4} & c_{1,5} & c_{1,6} \\ c_{1,2} & c_{2,2} & c_{2,3} & c_{2,4} & c_{2,5} & c_{2,6} \\ c_{1,3} & c_{2,3} & c_{3,3} & c_{3,4} & c_{3,5} & c_{3,6} \\ c_{1,4} & c_{2,4} & c_{3,4} & c_{4,4} & c_{4,5} & c_{4,6} \\ c_{1,5} & c_{2,5} & c_{3,5} & c_{4,5} & c_{5,5} & c_{5,6} \\ c_{1,6} & c_{2,6} & c_{3,6} & c_{4,6} & c_{5,6} & c_{6,6} \end{bmatrix}$$

$$true$$

>

Procedure **C_constants** displays the number of independent and nonzero parameters in the material constants matrix **M**. The matrix **M** can either be the generic matrix **C** (no material symmetry of any kind) or the material constants matrix of a material with one or more symmetries. Matrix **M** is always compared to the default generic matrix **C** entered as a parameter. That is, this procedure is called as **C_constants[C](M)**.

```
> C_constants[C](C); ##<<-- M=C generic C
Number of nonzero parameters in the generic material constants matrix C is 36.
Number of independent parameters in the generic material constants matrix C is 21.
```

>

Recall now that the so-called **constitutive equation** relates components of the stress tensor **sigma[i,j]** with components of the strain tensor **epsilon[k,l]** this way:

sigma[i,j] = C[i,j,k,l]epsilon[k,l]

where **C[i,j,k,l]** are the compotents of the rank 4 tensor **C** that represents the material constants.

The matrix form of the above equation, which is much more convinient to use than the tensor form, relates the 6 x 1 stress array **sigma**, the 6 x 1 strain array **epsilon**, and the 6 x 6 material constants

matrix **C** through the matrix equation

sigma = C*epsilon.

This equation remains intact after **sigma**, **epsilon**, and **C** are transformed, namely,

sigma' = C'*epsilon'.

where **sigma' = TsigmaMatrix(sigma)**, **epsilon'=TepsMatrix(epsilon)**, and so **C'=Tsigma*C*(Teps)^(-1)**.

>

Procedure **TransformedMaterialConstants** (aliased as **TMC**) is the main procedure in the package. It displays the 6 x 6 material constants matrix for a material with multiple symmetries T_1, T_2, etc. **TCM** applies to a 6 x 6 symmetric generic material constants matrix **C** (entered as the first argument) symmetries represented by the orthogonal or puresymbolic matrices **T_1, T_2,....,** which are entered as the subsequent arguments. Then, the final matrix is compared to the generic matrix **C** entered also as a parameter.

That is, this procedure is called as

TransformedMaterialConstants[C](C,T_1,T_2,...) or **TMC[C](C,T_1,T_2,...).**

We summarize our example of the monoclinic material with the single plane symmetry **Tz** defined above and find its material constants matrix **C**.:

Example 1: Monoclinic material with a single plane of symmetry taken to be the xy-plane. It has 20 nonzero parameters among which 13 are independent.

```
> C:=makeC(6,c); ##<<-- original generic material constants matrix
  C
  Tz:=ReflectionMatrix([0,0,1]); ##<<-- reflection matrix w.r.t. the
  xy-plane
```

$$C := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & c_{1,4} & c_{1,5} & c_{1,6} \\ c_{1,2} & c_{2,2} & c_{2,3} & c_{2,4} & c_{2,5} & c_{2,6} \\ c_{1,3} & c_{2,3} & c_{3,3} & c_{3,4} & c_{3,5} & c_{3,6} \\ c_{1,4} & c_{2,4} & c_{3,4} & c_{4,4} & c_{4,5} & c_{4,6} \\ c_{1,5} & c_{2,5} & c_{3,5} & c_{4,5} & c_{5,5} & c_{5,6} \\ c_{1,6} & c_{2,6} & c_{3,6} & c_{4,6} & c_{5,6} & c_{6,6} \end{bmatrix}$$

$$Tz := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

```
> C1:=TMC[C](C,Tz); ##<<-- material constants matrix of monoclinic
  material with the xy-plane of symmertry
  C_constants[C](C1);
```

$$C1 := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & c_{1,4} & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & c_{2,4} & 0 & 0 \\ c_{1,3} & c_{2,3} & c_{3,3} & c_{3,4} & 0 & 0 \\ c_{1,4} & c_{2,4} & c_{3,4} & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & c_{5,6} \\ 0 & 0 & 0 & 0 & c_{5,6} & c_{6,6} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 20.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 13.
```

```
> Cprime:=Multiply(Multiply(T_sigma,C),MatrixInverse(T_eps));
```

$$Cprime := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & c_{1,4} & -c_{1,5} & -c_{1,6} \\ c_{1,2} & c_{2,2} & c_{2,3} & c_{2,4} & -c_{2,5} & -c_{2,6} \\ c_{1,3} & c_{2,3} & c_{3,3} & c_{3,4} & -c_{3,5} & -c_{3,6} \\ c_{1,4} & c_{2,4} & c_{3,4} & c_{4,4} & -c_{4,5} & -c_{4,6} \\ -c_{1,5} & -c_{2,5} & -c_{3,5} & -c_{4,5} & c_{5,5} & c_{5,6} \\ -c_{1,6} & -c_{2,6} & -c_{3,6} & -c_{4,6} & c_{5,6} & c_{6,6} \end{bmatrix}$$

Note that by equating **C** with **Cprime** we find the form of **C**:

```
> C=Cprime;
```

$$\begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & c_{1,4} & c_{1,5} & c_{1,6} \\ c_{1,2} & c_{2,2} & c_{2,3} & c_{2,4} & c_{2,5} & c_{2,6} \\ c_{1,3} & c_{2,3} & c_{3,3} & c_{3,4} & c_{3,5} & c_{3,6} \\ c_{1,4} & c_{2,4} & c_{3,4} & c_{4,4} & c_{4,5} & c_{4,6} \\ c_{1,5} & c_{2,5} & c_{3,5} & c_{4,5} & c_{5,5} & c_{5,6} \\ c_{1,6} & c_{2,6} & c_{3,6} & c_{4,6} & c_{5,6} & c_{6,6} \end{bmatrix} = \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & c_{1,4} & -c_{1,5} & -c_{1,6} \\ c_{1,2} & c_{2,2} & c_{2,3} & c_{2,4} & -c_{2,5} & -c_{2,6} \\ c_{1,3} & c_{2,3} & c_{3,3} & c_{3,4} & -c_{3,5} & -c_{3,6} \\ c_{1,4} & c_{2,4} & c_{3,4} & c_{4,4} & -c_{4,5} & -c_{4,6} \\ -c_{1,5} & -c_{2,5} & -c_{3,5} & -c_{4,5} & c_{5,5} & c_{5,6} \\ -c_{1,6} & -c_{2,6} & -c_{3,6} & -c_{4,6} & c_{5,6} & c_{6,6} \end{bmatrix}$$

From the above we see that:

c[1,5]=-c[1,5]=0, c[2,5]=-c[2,5]=0, c[3,5]=-c[3,5]=0, c[4,5]=-c[4,5]=0,
c[1,6]=-c[1,6]=0, c[2,6]=-c[2,6]=0, c[3,6]=-c[3,6]=0, c[4,6]=-c[4,6]=0,

hence **the material constants matrix C for a monoclinic material** is:

```
> 'C'=C1;
```

$$C = \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & c_{1,4} & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & c_{2,4} & 0 & 0 \\ c_{1,3} & c_{2,3} & c_{3,3} & c_{3,4} & 0 & 0 \\ c_{1,4} & c_{2,4} & c_{3,4} & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & c_{5,6} \\ 0 & 0 & 0 & 0 & c_{5,6} & c_{6,6} \end{bmatrix}$$

```
>
```

The above process of finding **C** for the given material symmetry (in the above example of monoclinic material it was the symmetry with respect to the xy-plane) is generalized to materials of any symmetry and it is formalized in the procedure **TransformedMaterialConstants** (or, **TMC**, for short) used as **TransformedMaterialConstants[C](C,T_1,T_2,...)** or **TMC[C](C,T_1,T_2,...),** where T_1, T_2, etc. are 3 x 3 orthogonal matrices that generate the symmetry group of the given material. See Section 2 where this procedure is analyzed step-by-step.

Thus, from the constitutive equation shown above we have:

```
> sigma_1=Multiply(C,epsilon_1); ##<<-- relation between original
  stress, strain and C
```

$$\begin{bmatrix} \sigma_{1,1} \\ \sigma_{2,2} \\ \sigma_{3,3} \\ \sigma_{1,2} \\ \sigma_{2,3} \\ \sigma_{1,3} \end{bmatrix} = \begin{bmatrix} c_{1,1}\,\varepsilon_{1,1} + c_{1,2}\,\varepsilon_{2,2} + c_{1,3}\,\varepsilon_{3,3} + 2\,c_{1,4}\,\varepsilon_{1,2} + 2\,c_{1,5}\,\varepsilon_{2,3} + 2\,c_{1,6}\,\varepsilon_{1,3} \\ c_{1,2}\,\varepsilon_{1,1} + c_{2,2}\,\varepsilon_{2,2} + c_{2,3}\,\varepsilon_{3,3} + 2\,c_{2,4}\,\varepsilon_{1,2} + 2\,c_{2,5}\,\varepsilon_{2,3} + 2\,c_{2,6}\,\varepsilon_{1,3} \\ c_{1,3}\,\varepsilon_{1,1} + c_{2,3}\,\varepsilon_{2,2} + c_{3,3}\,\varepsilon_{3,3} + 2\,c_{3,4}\,\varepsilon_{1,2} + 2\,c_{3,5}\,\varepsilon_{2,3} + 2\,c_{3,6}\,\varepsilon_{1,3} \\ c_{1,4}\,\varepsilon_{1,1} + c_{2,4}\,\varepsilon_{2,2} + c_{3,4}\,\varepsilon_{3,3} + 2\,c_{4,4}\,\varepsilon_{1,2} + 2\,c_{4,5}\,\varepsilon_{2,3} + 2\,c_{4,6}\,\varepsilon_{1,3} \\ c_{1,5}\,\varepsilon_{1,1} + c_{2,5}\,\varepsilon_{2,2} + c_{3,5}\,\varepsilon_{3,3} + 2\,c_{4,5}\,\varepsilon_{1,2} + 2\,c_{5,5}\,\varepsilon_{2,3} + 2\,c_{5,6}\,\varepsilon_{1,3} \\ c_{1,6}\,\varepsilon_{1,1} + c_{2,6}\,\varepsilon_{2,2} + c_{3,6}\,\varepsilon_{3,3} + 2\,c_{4,6}\,\varepsilon_{1,2} + 2\,c_{5,6}\,\varepsilon_{2,3} + 2\,c_{6,6}\,\varepsilon_{1,3} \end{bmatrix}$$

```
> sigmaprime_1=Multiply(Cprime,epsilonprime_1); ##<<-- relation
  between transformed stress, strain and C
```

$$\begin{bmatrix} \sigma_{1,1} \\ \sigma_{2,2} \\ \sigma_{3,3} \\ \sigma_{1,2} \\ -\sigma_{2,3} \\ -\sigma_{1,3} \end{bmatrix} = \begin{bmatrix} c_{1,1}\,\varepsilon_{1,1} + c_{1,2}\,\varepsilon_{2,2} + c_{1,3}\,\varepsilon_{3,3} + 2\,c_{1,4}\,\varepsilon_{1,2} + 2\,c_{1,5}\,\varepsilon_{2,3} + 2\,c_{1,6}\,\varepsilon_{1,3} \\ c_{1,2}\,\varepsilon_{1,1} + c_{2,2}\,\varepsilon_{2,2} + c_{2,3}\,\varepsilon_{3,3} + 2\,c_{2,4}\,\varepsilon_{1,2} + 2\,c_{2,5}\,\varepsilon_{2,3} + 2\,c_{2,6}\,\varepsilon_{1,3} \\ c_{1,3}\,\varepsilon_{1,1} + c_{2,3}\,\varepsilon_{2,2} + c_{3,3}\,\varepsilon_{3,3} + 2\,c_{3,4}\,\varepsilon_{1,2} + 2\,c_{3,5}\,\varepsilon_{2,3} + 2\,c_{3,6}\,\varepsilon_{1,3} \\ c_{1,4}\,\varepsilon_{1,1} + c_{2,4}\,\varepsilon_{2,2} + c_{3,4}\,\varepsilon_{3,3} + 2\,c_{4,4}\,\varepsilon_{1,2} + 2\,c_{4,5}\,\varepsilon_{2,3} + 2\,c_{4,6}\,\varepsilon_{1,3} \\ -c_{1,5}\,\varepsilon_{1,1} - c_{2,5}\,\varepsilon_{2,2} - c_{3,5}\,\varepsilon_{3,3} - 2\,c_{4,5}\,\varepsilon_{1,2} - 2\,c_{5,5}\,\varepsilon_{2,3} - 2\,c_{5,6}\,\varepsilon_{1,3} \\ -c_{1,6}\,\varepsilon_{1,1} - c_{2,6}\,\varepsilon_{2,2} - c_{3,6}\,\varepsilon_{3,3} - 2\,c_{4,6}\,\varepsilon_{1,2} - 2\,c_{5,6}\,\varepsilon_{2,3} - 2\,c_{6,6}\,\varepsilon_{1,3} \end{bmatrix}$$

```
>
```

Example 2: In this example we find the material constants matrix for an **orthotropic material** that has two planes of symmetry, say the xy- and the xz-plane. We will show that such material has 12 nonzero material constants and among them 9 independent.

```
> Tz:=ReflectionMatrix([0,0,1]); ##<<-- reflection matrix w.r.t. the
```

```
xy-plane
Ty:=ReflectionMatrix([0,1,0]); ##<<-- reflection matrix w.r.t. the
xz-plane
```

$$Tz := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$Ty := \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

We can successively apply the two symmetries. It is worth observing that the order in which these symmetries are applied does not matter.

```
> C1:=TMC[C](C,Tz); ##<<-- first reflective symmetry w.r.t. xy-plane
  is applied to C
  C_constants[C](C1);
```

$$C1 := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & c_{1,4} & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & c_{2,4} & 0 & 0 \\ c_{1,3} & c_{2,3} & c_{3,3} & c_{3,4} & 0 & 0 \\ c_{1,4} & c_{2,4} & c_{3,4} & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & c_{5,6} \\ 0 & 0 & 0 & 0 & c_{5,6} & c_{6,6} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 20.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 13.
```

```
> C2:=TMC[C](C1,Ty); ##<<-- second reflective symmetry w.r.t.
  xz-plane is applied to C1
  C_constants[C](C2);
```

$$C2 := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & 0 & 0 & 0 \\ c_{1,3} & c_{2,3} & c_{3,3} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{6,6} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 12.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 9.
```

A better way to compute the final matrix is with a single call to the procedure **TCM**. We also verify

directly that the order in which the symmetries are applied does not matter. That is, the material constants matrix is the same regardless of the order in which the symmetries are applied.

```
> TMC[C](C,Tz,Ty)=TMC[C](C,Ty,Tz); ##<<-- two reflective symmetries
  applied in two different orders
  Equal(lhs(%),rhs(%));
```

$$\begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & 0 & 0 & 0 \\ c_{1,3} & c_{2,3} & c_{3,3} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{6,6} \end{bmatrix} = \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & 0 & 0 & 0 \\ c_{1,3} & c_{2,3} & c_{3,3} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{6,6} \end{bmatrix}$$

true

```
>
```

Example 3: In this example we compute the material constants matrix for the material that has three planes of symmetry, say the xy-, the xz-, and the yz-plane. Again, this material like the orthotropuic material has 9 independent material constants. This is because, the reflective symmetries with respect to two coordinate planes imply the third reflective symmetry with respect to the third coordinate plane. **This means that the third reflective symmetry does not change the number of nonzero and independent constants in the material constants matrix of such material.**

In the following, we apply the third reflective symmetry **Tx** to the material constants matrix **C2** found in Example 2 and find that the resulting matrix **C3** actually equals **C2**..

```
> Tx:=ReflectionMatrix([1,0,0]); ##<<-- reflection matrix w.r.t. the
  yz-plane
  C3:=TMC[C](C2,Tx);
  C_constants[C](C3);
```

$$Tx := \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$C3 := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & 0 & 0 & 0 \\ c_{1,3} & c_{2,3} & c_{3,3} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{6,6} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 12.
Number of independent parameters in the material constants matrix C of the given s
```

```
ymmetry is 9.
```

The above can also be shown as follows:

```
> TMC[C](C,Ty,Tz)=TMC[C](C,Ty,Tz,Tx);
  Equal(lhs(%),rhs(%));
```

$$\begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & 0 & 0 & 0 \\ c_{1,3} & c_{2,3} & c_{3,3} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{6,6} \end{bmatrix} = \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & 0 & 0 & 0 \\ c_{1,3} & c_{2,3} & c_{3,3} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{6,6} \end{bmatrix}$$

$$true$$

```
>
```

Section 2: Step-by-step Procedure TransformedMaterialConstants

In this section we show step-by step computations performed by the procedure **TransformedMaterialConstants**. As an example, we take a transversely isotropic material and verify that it has 5 independent material constants.

```
> restart:with(LinearAlgebra):with(MaterialConstants);
```

$$\_known\_types = [orthogonal, puresymbolic]$$

$$\_known\_aliases = [RM = MaterialConstants:\text{-}ReflectionMatrix,$$
$$TMC = MaterialConstants:\text{-}TransformedMaterialConstants]$$

$$\_known\_additional\_protected\_names = [c, \varepsilon, \sigma, \theta]$$

$$[C\_constants, MCversion, ModuleLoad, ModuleUnload, ReflectionMatrix, SimilarityTransform,$$
$$Teps, TepsMatrix, TransformedMaterialConstants, Tsigma, TsigmaMatrix, makeC, makeEpsilon,$$
$$makeSigma, phi\_eps, phi\_eps\_inv, phi\_sigma, phi\_sigma\_inv]$$

```
>
```

Example 4: In this example, we take a **transversely isotropic material**.

First, we define rotation matrices around the coordinate axes. Note that these general rotation matrices are both of type/orthogonal and type/puresymbolic, and that they are defined as functions of the rotation angle. Note also that the name **'theta'** is protected.

```
> T[xy]:=gamma->Matrix(3,3,[
  cos(gamma),sin(gamma),0,-sin(gamma),cos(gamma),0,0,0,1]);
  T[xy](theta[3]); ##<<-- rotation about the z-axis by angle
  theta[3]
  type(%,orthogonal);
  type(%%,puresymbolic);
```

$$T_{xy} := \gamma \to \mathrm{Matrix}(3, 3, [\cos(\gamma), \sin(\gamma), 0, -\sin(\gamma), \cos(\gamma), 0, 0, 0, 1])$$

$$\begin{bmatrix} \cos(\theta_3) & \sin(\theta_3) & 0 \\ -\sin(\theta_3) & \cos(\theta_3) & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$true$$

$$true$$

```
> T[xz]:=beta->Matrix(3,3,[cos(beta),0,sin(beta),0,1,0,-sin(beta),0,
  cos(beta)]);
  T[xz](theta[2]); ##<<-- rotation about the z-axis by angle
  theta[2]
```

$$T_{xz} := \beta \to \mathrm{Matrix}(3, 3, [\cos(\beta), 0, \sin(\beta), 0, 1, 0, -\sin(\beta), 0, \cos(\beta)])$$

$$\begin{bmatrix} \cos(\theta_2) & 0 & \sin(\theta_2) \\ 0 & 1 & 0 \\ -\sin(\theta_2) & 0 & \cos(\theta_2) \end{bmatrix}$$

```
> T[yz]:=alpha->Matrix(3,3,[1,0,0,0,cos(alpha),sin(alpha),0,-sin(alp
  ha),cos(alpha)]);
  T[yz](theta[1]); ##<<-- rotation about the z-axis by angle
  theta[1]
```

$$T_{yz} := \alpha \to \mathrm{Matrix}(3, 3, [1, 0, 0, 0, \cos(\alpha), \sin(\alpha), 0, -\sin(\alpha), \cos(\alpha)])$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta_1) & \sin(\theta_1) \\ 0 & -\sin(\theta_1) & \cos(\theta_1) \end{bmatrix}$$

We can also define a general rotation matrix which is the result of three consecutive rotations about the coordinate axes by the angles alpha, beta, and gamma.

```
> X1Y2Z3:=(alpha,beta,gamma)->Multiply(Multiply(T[yz](alpha),T[xz](b
  eta)),T[xy](gamma));
```

$$X1Y2Z3 := (\alpha, \beta, \gamma) \to LinearAlgebra{:}\text{-}Multiply(LinearAlgebra{:}\text{-}Multiply(T_{yz}(\alpha), T_{xz}(\beta)), T_{xy}(\gamma))$$

Then, the matrix of this general rotation parametrized by three arbitrary angle has the following form:

```
> X1Y2Z3(theta[1],theta[2],theta[3]);
```

$$[\cos(\theta_2)\cos(\theta_3), \cos(\theta_2)\sin(\theta_3), \sin(\theta_2)]$$

$$[-\sin(\theta_1)\sin(\theta_2)\cos(\theta_3) - \cos(\theta_1)\sin(\theta_3), -\sin(\theta_1)\sin(\theta_2)\sin(\theta_3) + \cos(\theta_1)\cos(\theta_3), \sin(\theta_1)\cos(\theta_2)]$$

$$[-\cos(\theta_1)\sin(\theta_2)\cos(\theta_3) + \sin(\theta_1)\sin(\theta_3), -\cos(\theta_1)\sin(\theta_2)\sin(\theta_3) - \sin(\theta_1)\cos(\theta_3),$$

$\cos(\theta_1)\cos(\theta_2)]$

Note that the above matrix is of type/puresymbolic:

```
> type(%,puresymbolic);
```

$$true$$

Of course, the individual rotation matrices around the coordinate axes can be easily recovered:

```
> X1Y2Z3(theta[1],0,0),X1Y2Z3(0,theta[2],0),X1Y2Z3(0,0,theta[3]);
```

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta_1) & \sin(\theta_1) \\ 0 & -\sin(\theta_1) & \cos(\theta_1) \end{bmatrix}, \begin{bmatrix} \cos(\theta_2) & 0 & \sin(\theta_2) \\ 0 & 1 & 0 \\ -\sin(\theta_2) & 0 & \cos(\theta_2) \end{bmatrix}, \begin{bmatrix} \cos(\theta_3) & \sin(\theta_3) & 0 \\ -\sin(\theta_3) & \cos(\theta_3) & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

```
> symmetry:=[xy,xz,yz]; ##<<-- collection of possible symmetries
```

$$symmetry := [xy, xz, yz]$$

```
> k:=1; ##<<-- picking a symmetry (don't use 'k' for anything
  else!)
```

$$k := 1$$

```
> TT:=T[symmetry[k]](theta[1]);##<<-- assigning the symmetry matrix
  to TT for further computation
```

$$TT := \begin{bmatrix} \cos(\theta_1) & \sin(\theta_1) & 0 \\ -\sin(\theta_1) & \cos(\theta_1) & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

```
> Sigma:=makeSigma(3,sigma);
```

$$\Sigma := \begin{bmatrix} \sigma_{1,1} & \sigma_{1,2} & \sigma_{1,3} \\ \sigma_{1,2} & \sigma_{2,2} & \sigma_{2,3} \\ \sigma_{1,3} & \sigma_{2,3} & \sigma_{3,3} \end{bmatrix}$$

```
>
```

The procedure **TransformedMaterialConstants** finds the material constants matrix **C** for a material with a symmetry group **G** whose generators **T_1, T_2,...,T_k**, are listed as arguments in

TransformedMaterialConstants[C](Cp,T_1,T_2,...,T_k)

This recursive procedure alaways takes the generic material constants matrix **C** as a parameter and it successively applies one symmetry at the time to the current material constants matrix **Cp** obtained from the previous step of the recursion. Thus, there are k steps where k is the number of generators in the sequence T_1,T_2,...,T_k.

First recursive step:
Cp := C

C1 := TransformedMaterialConstants[C](Cp,T_1)

Second recursive step:
Cp := C1
C2 := TransformedMaterialConstants[C](Cp,T_2)
.....

The final k-th recursive step:
Cp := C(k-1)
Ck := TransformedMaterialConstants[C](Cp,T_k)

At each resursive step i, the procedure applies computations shown in **Example 1** above for the given symmetry **T_i**, 1 <= i <= k.

Thus, we have as **INPUT** in **TransformedMaterialConstants[C](Cp,T1,T2,...,Tk)**:

INPUT:
Arguments: Cp, **T_1**, **T_2**, ..., **T_k** where **Cp** is a 6 x 6 symmetric matrix while **T_1**,..., **T_k** are orthogonal or purely symbolic 3 x 3 matrices that generate the material symmetry group
Parameter: C which is the generic material constants 6 x 6 symmetric matrix **C** with 36 symbolic entries **c[i,j]** of which 21 are independent

OUTPUT:
A material constants matrix **C** in block-diagonal form for a material with the symmetry group **G** generated by **T_1,..., T_k**.

In our example, there is only one generator **TT** and so the following steps refer to what happens in that single invocation of this procedure.

Knowns are : the stress tensor **Sigma** and the symmetry generator **TT**.

```
> 'Sigma'=Sigma;
  'TT'=TT;
```

$$\Sigma = \begin{bmatrix} \sigma_{1,1} & \sigma_{1,2} & \sigma_{1,3} \\ \sigma_{1,2} & \sigma_{2,2} & \sigma_{2,3} \\ \sigma_{1,3} & \sigma_{2,3} & \sigma_{3,3} \end{bmatrix}$$

$$TT = \begin{bmatrix} \cos(\theta_1) & \sin(\theta_1) & 0 \\ -\sin(\theta_1) & \cos(\theta_1) & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

```
>
```

Step 1: SimilarityTransformation is applied to the stress tensor **Sigma** with the rotational symmetry

given by **TT**, we find a new stress tensor **Sigmaprime** and a new stress array **sigmaprime_1**:

```
> Sigmaprime:=SimilarityTransform(Sigma,TT);
```

$$Sigmaprime :=$$

$$[\cos(\theta_1)\,(\sigma_{1,1}\cos(\theta_1)+\sigma_{1,2}\sin(\theta_1))+\sin(\theta_1)\,(\sigma_{1,2}\cos(\theta_1)+\sigma_{2,2}\sin(\theta_1)),$$
$$\cos(\theta_1)\,(-\sigma_{1,1}\sin(\theta_1)+\sigma_{1,2}\cos(\theta_1))+\sin(\theta_1)\,(-\sigma_{1,2}\sin(\theta_1)+\sigma_{2,2}\cos(\theta_1)),$$
$$\sigma_{1,3}\cos(\theta_1)+\sigma_{2,3}\sin(\theta_1)]$$
$$[-\sin(\theta_1)\,(\sigma_{1,1}\cos(\theta_1)+\sigma_{1,2}\sin(\theta_1))+\cos(\theta_1)\,(\sigma_{1,2}\cos(\theta_1)+\sigma_{2,2}\sin(\theta_1)),$$
$$-\sin(\theta_1)\,(-\sigma_{1,1}\sin(\theta_1)+\sigma_{1,2}\cos(\theta_1))+\cos(\theta_1)\,(-\sigma_{1,2}\sin(\theta_1)+\sigma_{2,2}\cos(\theta_1)),$$
$$-\sigma_{1,3}\sin(\theta_1)+\sigma_{2,3}\cos(\theta_1)]$$
$$[\sigma_{1,3}\cos(\theta_1)+\sigma_{2,3}\sin(\theta_1),\ -\sigma_{1,3}\sin(\theta_1)+\sigma_{2,3}\cos(\theta_1),\ \sigma_{3,3}]$$

```
> sigmaprime_1:=phi_sigma(Sigmaprime);
```

$$sigmaprime\_1 := \begin{bmatrix} \sigma_{1,1}\cos(\theta_1)^2+2\sin(\theta_1)\,\sigma_{1,2}\cos(\theta_1)+\sigma_{2,2}\sin(\theta_1)^2 \\ \sigma_{1,1}\sin(\theta_1)^2-2\sin(\theta_1)\,\sigma_{1,2}\cos(\theta_1)+\sigma_{2,2}\cos(\theta_1)^2 \\ \sigma_{3,3} \\ -\cos(\theta_1)\,\sigma_{1,1}\sin(\theta_1)+\sigma_{1,2}\cos(\theta_1)^2-\sigma_{1,2}\sin(\theta_1)^2+\sin(\theta_1)\,\sigma_{2,2}\cos(\theta_1) \\ -\sigma_{1,3}\sin(\theta_1)+\sigma_{2,3}\cos(\theta_1) \\ \sigma_{1,3}\cos(\theta_1)+\sigma_{2,3}\sin(\theta_1) \end{bmatrix}$$

```
>
```

Step 2: The generic 6 x 6 symmetric material constants matrix **C** is generated by the procedure **makeC** and a 6 x 6 matrix of the map **Tsigma** is computed by the procedure **TsigmaMatrix**:

```
> C:=makeC(6,c);
```

$$C := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & c_{1,4} & c_{1,5} & c_{1,6} \\ c_{1,2} & c_{2,2} & c_{2,3} & c_{2,4} & c_{2,5} & c_{2,6} \\ c_{1,3} & c_{2,3} & c_{3,3} & c_{3,4} & c_{3,5} & c_{3,6} \\ c_{1,4} & c_{2,4} & c_{3,4} & c_{4,4} & c_{4,5} & c_{4,6} \\ c_{1,5} & c_{2,5} & c_{3,5} & c_{4,5} & c_{5,5} & c_{5,6} \\ c_{1,6} & c_{2,6} & c_{3,6} & c_{4,6} & c_{5,6} & c_{6,6} \end{bmatrix}$$

```
> T_sigma:=TsigmaMatrix(TT);  ##<<-- finding matrix of Tsigma
```

$$T\_sigma := \begin{bmatrix} \cos(\theta_1)^2 & \sin(\theta_1)^2 & 0 & 2\cos(\theta_1)\sin(\theta_1) & 0 & 0 \\ \sin(\theta_1)^2 & \cos(\theta_1)^2 & 0 & -2\cos(\theta_1)\sin(\theta_1) & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ -\cos(\theta_1)\sin(\theta_1) & \cos(\theta_1)\sin(\theta_1) & 0 & \cos(\theta_1)^2 - \sin(\theta_1)^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cos(\theta_1) & -\sin(\theta_1) \\ 0 & 0 & 0 & 0 & \sin(\theta_1) & \cos(\theta_1) \end{bmatrix}$$

>

Step 3: The transformed material constants matrix **C'** is computed as a matrix product of the following three 6 x 6 matrices: **T_sigmaMatrix**, **C**, and **(T_sigmaMatrix)^t** . Recall from **Example 1** that

C' = Multiply(T_sigmaMatrix, C, (T_epsMatrix)^(-1))

but since **(T_epsMatrix)^(-1)= (T_sigmaMatrix)^t**, where **t** denotes the matrix tranpose, we compute

C' = Multiply(T_sigmaMatrix, C, (T_sigmaMatrix)^t)

because **it is easier to take the transpose of T_sigmaMatrix than compute the inverse of T_epsMatrix.** The entries of **C'** are simplified and the matrix is assigned to a (local) variable **C4**.

Note: We do not display matrix **C4** as it has complicated expressions.

```
> C4:=LinearAlgebra:-Map(simplify,LinearAlgebra:-Multiply(T_sigma,
  LinearAlgebra:-Multiply(C,LinearAlgebra:-Transpose(T_sigma)))):
```

>

Step 4: Once the transformed material constants matrix **C'** has been computed in **Step 3**, matrices **C** and **-C**' are added and assigned to a (local) variable **C5**. Requiring that **C5** is the zero matrix, this will result in a system **S** of **36** linear equations in **20** indetereminates **c[i,j]** whose coefficients are complicated expressions in the powers and products of sin(theta[1]), sin(theta[2]), sin(theta[3]), cos(theta[1]), cos(theta[2]), and cos(theta[3]) (in the most general case)..

Note: We do not display matrix **C5** as it has complicated expressions.

```
> C5:=LinearAlgebra:-Map(factor,LinearAlgebra:-MatrixAdd(C4,-C)):
  ##<<-- subtracting C from transformed C' stored in C4
```

>

Step 5: The system **S** from **Step 6** will be eventually solved using the Groebner basis method. In this step, one collects all the entries of the matrix **C5** into a set while replacing, for short, sin(theta[1]), sin(theta[2]), and sin(theta[3]) with, respectively, new indetereminates ss[1], ss[2], ss[3]. Likewise, cos(theta[1]), cos(theta[2]), and cos(theta[3]) are replaced with, respectively, new indetereminates

cc[1], cc[2], cc[3]. All zeros, i.e., trivial equations of the form 0=0 are removed from the system. Then, all remaining equations are collected with respect to the six new indeterminates ss[1], ss[2], ss[3], cc[1], cc[2], cc[3]. The resulting equations are assigned to a (local) variable eqs. We show these equations below.

```
> eqs:=LinearAlgebra:-Map(collect,convert(remove(member,

  subs({cos(theta[1])=cc[1],sin(theta[1])=ss[1],cos(theta[2])=cc[2],
  sin(theta[2])=ss[2],cos(theta[3])=cc[3],sin(theta[3])=ss[3]},

  {seq(seq(C5[i,j],i=1..6),j=1..6)}),{0}),list),[cc[1],ss[1],cc[2],s
  s[2],cc[2],ss[2]]);
```

$$
\begin{aligned}
eqs := [&(-c_{1,1}+2\,c_{1,2}+4\,c_{4,4}-c_{2,2})\,cc_1^{\,4}+(-4\,c_{1,4}+4\,c_{2,4})\,ss_1\,cc_1^{\,3}\\
&+(c_{1,1}-2\,c_{1,2}-4\,c_{4,4}+c_{2,2})\,cc_1^{\,2}+(-2\,c_{2,4}+2\,c_{1,4})\,ss_1\,cc_1, c_{3,5}\,cc_1-c_{3,6}\,ss_1-c_{3,5},\\
&c_{3,5}\,ss_1+c_{3,6}\,cc_1-c_{3,6}, 2\,c_{3,4}\,cc_1^{\,2}+(-c_{1,3}+c_{2,3})\,ss_1\,cc_1-2\,c_{3,4},\\
&2\,c_{5,6}\,cc_1^{\,2}+(c_{5,5}-c_{6,6})\,ss_1\,cc_1-2\,c_{5,6}, (c_{1,3}-c_{2,3})\,cc_1^{\,2}+2\,c_{3,4}\,cc_1\,ss_1-c_{1,3}+c_{2,3},\\
&(-c_{1,3}+c_{2,3})\,cc_1^{\,2}-2\,c_{3,4}\,cc_1\,ss_1+c_{1,3}-c_{2,3}, (c_{5,5}-c_{6,6})\,cc_1^{\,2}-2\,cc_1\,c_{5,6}\,ss_1-c_{5,5}+c_{6,6},\\
&(-c_{5,5}+c_{6,6})\,cc_1^{\,2}+2\,cc_1\,c_{5,6}\,ss_1+c_{5,5}-c_{6,6},\\
&(c_{1,6}-c_{2,6}-2\,c_{4,5})\,cc_1^{\,3}+(c_{1,5}-c_{2,5}+2\,c_{4,6})\,ss_1\,cc_1^{\,2}+(c_{2,6}+2\,c_{4,5})\,cc_1-c_{1,6}+c_{2,5}\,ss_1,\\
&(c_{1,5}-c_{2,5}+2\,c_{4,6})\,cc_1^{\,3}+(-c_{1,6}+2\,c_{4,5}+c_{2,6})\,ss_1\,cc_1^{\,2}+(c_{2,5}-2\,c_{4,6})\,cc_1-c_{1,5}-c_{2,6}\,ss_1,\\
&(-c_{1,6}+2\,c_{4,5}+c_{2,6})\,cc_1^{\,3}+(-c_{1,5}+c_{2,5}-2\,c_{4,6})\,ss_1\,cc_1^{\,2}+(c_{1,6}-2\,c_{4,5})\,cc_1-c_{2,6}+c_{1,5}\,ss_1,\\
&(-c_{1,5}+c_{2,5}-2\,c_{4,6})\,cc_1^{\,3}+(c_{1,6}-c_{2,6}-2\,c_{4,5})\,ss_1\,cc_1^{\,2}+(c_{1,5}+2\,c_{4,6})\,cc_1-c_{2,5}-c_{1,6}\,ss_1,\\
&(-c_{1,6}+2\,c_{4,5}+c_{2,6})\,cc_1^{\,3}+(-c_{1,5}+c_{2,5}-2\,c_{4,6})\,ss_1\,cc_1^{\,2}+(-c_{2,6}+c_{1,6}-c_{4,5})\,cc_1+c_{4,6}\,ss_1\\
&-c_{4,5}, (c_{1,5}-c_{2,5}+2\,c_{4,6})\,cc_1^{\,3}+(-c_{1,6}+2\,c_{4,5}+c_{2,6})\,ss_1\,cc_1^{\,2}+(-c_{4,6}+c_{2,5}-c_{1,5})\,cc_1\\
&-c_{4,5}\,ss_1-c_{4,6}, (c_{1,1}-2\,c_{1,2}-4\,c_{4,4}+c_{2,2})\,cc_1^{\,4}+(4\,c_{1,4}-4\,c_{2,4})\,ss_1\,cc_1^{\,3}\\
&+(4\,c_{4,4}+2\,c_{1,2}-2\,c_{1,1})\,cc_1^{\,2}-4\,c_{1,4}\,cc_1\,ss_1-c_{2,2}+c_{1,1}, (c_{1,1}-2\,c_{1,2}-4\,c_{4,4}+c_{2,2})\,cc_1^{\,4}\\
&+(4\,c_{1,4}-4\,c_{2,4})\,ss_1\,cc_1^{\,3}+(4\,c_{4,4}+2\,c_{1,2}-2\,c_{2,2})\,cc_1^{\,2}+4\,c_{2,4}\,cc_1\,ss_1+c_{2,2}-c_{1,1},\\
&(4\,c_{1,4}-4\,c_{2,4})\,cc_1^{\,4}+(-c_{1,1}+2\,c_{1,2}+4\,c_{4,4}-c_{2,2})\,ss_1\,cc_1^{\,3}+(-3\,c_{1,4}+5\,c_{2,4})\,cc_1^{\,2}\\
&+(c_{2,2}-c_{1,2}-2\,c_{4,4})\,ss_1\,cc_1-c_{1,4}-c_{2,4}, (-4\,c_{1,4}+4\,c_{2,4})\,cc_1^{\,4}\\
&+(c_{1,1}-2\,c_{1,2}-4\,c_{4,4}+c_{2,2})\,ss_1\,cc_1^{\,3}+(-3\,c_{2,4}+5\,c_{1,4})\,cc_1^{\,2}+(-c_{1,1}+c_{1,2}+2\,c_{4,4})\,ss_1\,cc_1\\
&-c_{1,4}-c_{2,4}]
\end{aligned}
$$

>

Step 6: In preparation for using the Groebner basis method, we must tell Maple that the six new indeterminates ss[1], ss[2], ss[3], cc[1], cc[2], cc[3] are not independent but satisfy the Pythagorean identity. Thus, we add three such identities to the system eqs.

```
> eqs:=[op(eqs),cc[1]^2+ss[1]^2-1,cc[2]^2+ss[2]^2-1,cc[3]^2+ss[3]^2-
  1]; ##<<-- adding extra conditions
```

$$
\begin{aligned}
eqs := [&(-c_{1,1} + 2\,c_{1,2} + 4\,c_{4,4} - c_{2,2})\,cc_1^{\,4} + (-4\,c_{1,4} + 4\,c_{2,4})\,ss_1\,cc_1^{\,3} \\
&+ (c_{1,1} - 2\,c_{1,2} - 4\,c_{4,4} + c_{2,2})\,cc_1^{\,2} + (-2\,c_{2,4} + 2\,c_{1,4})\,ss_1\,cc_1, c_{3,5}\,cc_1 - c_{3,6}\,ss_1 - c_{3,5}, \\
&c_{3,5}\,ss_1 + c_{3,6}\,cc_1 - c_{3,6}, 2\,c_{3,4}\,cc_1^{\,2} + (-c_{1,3} + c_{2,3})\,ss_1\,cc_1 - 2\,c_{3,4}, \\
&2\,c_{5,6}\,cc_1^{\,2} + (c_{5,5} - c_{6,6})\,ss_1\,cc_1 - 2\,c_{5,6}, (c_{1,3} - c_{2,3})\,cc_1^{\,2} + 2\,c_{3,4}\,cc_1\,ss_1 - c_{1,3} + c_{2,3}, \\
&(-c_{1,3} + c_{2,3})\,cc_1^{\,2} - 2\,c_{3,4}\,cc_1\,ss_1 + c_{1,3} - c_{2,3}, (c_{5,5} - c_{6,6})\,cc_1^{\,2} - 2\,cc_1\,c_{5,6}\,ss_1 - c_{5,5} + c_{6,6}, \\
&(-c_{5,5} + c_{6,6})\,cc_1^{\,2} + 2\,cc_1\,c_{5,6}\,ss_1 + c_{5,5} - c_{6,6}, \\
&(c_{1,6} - c_{2,6} - 2\,c_{4,5})\,cc_1^{\,3} + (c_{1,5} - c_{2,5} + 2\,c_{4,6})\,ss_1\,cc_1^{\,2} + (c_{2,6} + 2\,c_{4,5})\,cc_1 - c_{1,6} + c_{2,5}\,ss_1, \\
&(c_{1,5} - c_{2,5} + 2\,c_{4,6})\,cc_1^{\,3} + (-c_{1,6} + 2\,c_{4,5} + c_{2,6})\,ss_1\,cc_1^{\,2} + (c_{2,5} - 2\,c_{4,6})\,cc_1 - c_{1,5} - c_{2,6}\,ss_1, \\
&(-c_{1,6} + 2\,c_{4,5} + c_{2,6})\,cc_1^{\,3} + (-c_{1,5} + c_{2,5} - 2\,c_{4,6})\,ss_1\,cc_1^{\,2} + (c_{1,6} - 2\,c_{4,5})\,cc_1 - c_{2,6} + c_{1,5}\,ss_1, \\
&(-c_{1,5} + c_{2,5} - 2\,c_{4,6})\,cc_1^{\,3} + (c_{1,6} - c_{2,6} - 2\,c_{4,5})\,ss_1\,cc_1^{\,2} + (c_{1,5} + 2\,c_{4,6})\,cc_1 - c_{2,5} - c_{1,6}\,ss_1, \\
&(-c_{1,6} + 2\,c_{4,5} + c_{2,6})\,cc_1^{\,3} + (-c_{1,5} + c_{2,5} - 2\,c_{4,6})\,ss_1\,cc_1^{\,2} + (-c_{2,6} + c_{1,6} - c_{4,5})\,cc_1 + c_{4,6}\,ss_1 \\
&- c_{4,5}, (c_{1,5} - c_{2,5} + 2\,c_{4,6})\,cc_1^{\,3} + (-c_{1,6} + 2\,c_{4,5} + c_{2,6})\,ss_1\,cc_1^{\,2} + (-c_{4,6} + c_{2,5} - c_{1,5})\,cc_1 \\
&- c_{4,5}\,ss_1 - c_{4,6}, (c_{1,1} - 2\,c_{1,2} - 4\,c_{4,4} + c_{2,2})\,cc_1^{\,4} + (4\,c_{1,4} - 4\,c_{2,4})\,ss_1\,cc_1^{\,3} \\
&+ (4\,c_{4,4} + 2\,c_{1,2} - 2\,c_{1,1})\,cc_1^{\,2} - 4\,c_{1,4}\,cc_1\,ss_1 - c_{2,2} + c_{1,1}, (c_{1,1} - 2\,c_{1,2} - 4\,c_{4,4} + c_{2,2})\,cc_1^{\,4} \\
&+ (4\,c_{1,4} - 4\,c_{2,4})\,ss_1\,cc_1^{\,3} + (4\,c_{4,4} + 2\,c_{1,2} - 2\,c_{2,2})\,cc_1^{\,2} + 4\,c_{2,4}\,cc_1\,ss_1 + c_{2,2} - c_{1,1}, \\
&(4\,c_{1,4} - 4\,c_{2,4})\,cc_1^{\,4} + (-c_{1,1} + 2\,c_{1,2} + 4\,c_{4,4} - c_{2,2})\,ss_1\,cc_1^{\,3} + (-3\,c_{1,4} + 5\,c_{2,4})\,cc_1^{\,2} \\
&+ (c_{2,2} - c_{1,2} - 2\,c_{4,4})\,ss_1\,cc_1 - c_{1,4} - c_{2,4}, (-4\,c_{1,4} + 4\,c_{2,4})\,cc_1^{\,4} \\
&+ (c_{1,1} - 2\,c_{1,2} - 4\,c_{4,4} + c_{2,2})\,ss_1\,cc_1^{\,3} + (-3\,c_{2,4} + 5\,c_{1,4})\,cc_1^{\,2} + (-c_{1,1} + c_{1,2} + 2\,c_{4,4})\,ss_1\,cc_1 \\
&- c_{1,4} - c_{2,4}, cc_1^{\,2} + ss_1^{\,2} - 1, cc_2^{\,2} + ss_2^{\,2} - 1, cc_3^{\,2} + ss_3^{\,2} - 1\,]
\end{aligned}
$$

>

Step 7: We collect all indetermines **c[i,j]** from the generic material constants matrix **C** in a new (local) list **Cindets** which we reverse, and the reversed list is assigned to **Cindetsrev**. The reason this list is reversed is because in the end we want to reduce the free coefficients in C in such a way as to express

the indeterminates **c[i,j]** with higher-valued indices in terms of those with lower-valued indices. That is, we want to eliminate indeterminates **c[i,j]** with higher-valued indices.

Since we will be solving the system **S** stored in eqs using the Groebner basis method, we will need a monomial order. Since we want to eliminate the indeterminates ss[1], ss[2], ss[3], cc[1], cc[2], cc[3], we will use the elimination order **'lexdeg'** from the Maple's Groebner package. This monomial order is stored in a variable **Tmonord**. Thus, we assign

Tmonord := lexdeg([ss[1], ss[2], ss[3], cc[1], cc[2], cc[3]], Cindetsrev).

Finally, we collect all 22 polynomial equations in the system **eqs** to a list **F**. .

```
> Cindets:=[seq(seq(C[i,j],j=i..6),i=1..6)]; ##<<-- all
  indeterminates in C
```

$$Cindets := [c_{1,1}, c_{1,2}, c_{1,3}, c_{1,4}, c_{1,5}, c_{1,6}, c_{2,2}, c_{2,3}, c_{2,4}, c_{2,5}, c_{2,6}, c_{3,3}, c_{3,4}, c_{3,5}, c_{3,6}, c_{4,4}, c_{4,5}, c_{4,6}, c_{5,5}, c_{5,6}, c_{6,6}]$$

```
> Cindetsrev:=[seq(Cindets[nops(Cindets)-i+1],i=1..nops(Cindets))];
  ##<<-- reversed indeterminates in C
```

$$Cindetsrev := [c_{6,6}, c_{5,6}, c_{5,5}, c_{4,6}, c_{4,5}, c_{4,4}, c_{3,6}, c_{3,5}, c_{3,4}, c_{3,3}, c_{2,6}, c_{2,5}, c_{2,4}, c_{2,3}, c_{2,2}, c_{1,6}, c_{1,5}, c_{1,4}, c_{1,3}, c_{1,2}, c_{1,1}]$$

```
> Tmondord:=lexdeg([cc[1],ss[1],cc[2],ss[2],cc[3],ss[3]],Cindetsrev)
  ; ##<<-- defining elimination order
```

$$Tmondord := \mathrm{lexdeg}([cc_1, ss_1, cc_2, ss_2, cc_3, ss_3], [c_{6,6}, c_{5,6}, c_{5,5}, c_{4,6}, c_{4,5}, c_{4,4}, c_{3,6}, c_{3,5}, c_{3,4}, c_{3,3}, c_{2,6}, c_{2,5}, c_{2,4}, c_{2,3}, c_{2,2}, c_{1,6}, c_{1,5}, c_{1,4}, c_{1,3}, c_{1,2}, c_{1,1}])$$

```
> F:=[seq(expand(p),p=eqs)]; ##<<-- assigning all equations to a
  list F
  nops(F);
```

$$F := [-cc_1^4 c_{1,1} + 2\,cc_1^4 c_{1,2} + 4\,cc_1^4 c_{4,4} - cc_1^4 c_{2,2} - 4\,cc_1^3 c_{1,4}\,ss_1 + 4\,ss_1 c_{2,4} cc_1^3 + c_{1,1} cc_1^2 - 2\,c_{1,2} cc_1^2 - 4\,cc_1^2 c_{4,4} + c_{2,2} cc_1^2 - 2\,c_{2,4} cc_1\,ss_1 + 2\,c_{1,4} cc_1\,ss_1, c_{3,5} cc_1 - c_{3,6} ss_1 - c_{3,5}, c_{3,5} ss_1 + c_{3,6} cc_1 - c_{3,6}, -c_{1,3} cc_1\,ss_1 + c_{2,3} cc_1\,ss_1 + 2\,c_{3,4} cc_1^2 - 2\,c_{3,4}, cc_1 c_{5,5}\,ss_1 - ss_1 c_{6,6} cc_1 + 2\,c_{5,6} cc_1^2 - 2\,c_{5,6}, c_{1,3} cc_1^2 + 2\,c_{3,4} cc_1\,ss_1 + c_{2,3} - c_{2,3} cc_1^2 - c_{1,3}, c_{2,3} cc_1^2 - 2\,c_{3,4} cc_1\,ss_1 + c_{1,3} - c_{1,3} cc_1^2 - c_{2,3}, c_{5,5} cc_1^2 - 2\,cc_1 c_{5,6}\,ss_1 + c_{6,6} - c_{6,6} cc_1^2 - c_{5,5}, 2\,cc_1 c_{5,6}\,ss_1 + c_{6,6} cc_1^2 + c_{5,5} - c_{5,5} cc_1^2 - c_{6,6}, cc_1^2 c_{1,5}\,ss_1 + 2\,cc_1^2 ss_1 c_{4,6} + c_{2,5}\,ss_1 - ss_1 c_{2,5} cc_1^2 - 2\,cc_1^3 c_{4,5} + c_{2,6} cc_1 + cc_1^3 c_{1,6} - cc_1^3 c_{2,6} + 2\,c_{4,5} cc_1 - c_{1,6}, -cc_1^2 c_{1,6}\,ss_1 + 2\,cc_1^2 ss_1 c_{4,5} - c_{2,6}\,ss_1 + ss_1 c_{2,6} cc_1^2 + 2\,cc_1^3 c_{4,6} + c_{2,5} cc_1 + cc_1^3 c_{1,5} - cc_1^3 c_{2,5} - 2\,c_{4,6} cc_1$$

$$-c_{1,5},\ ss_1\,c_{2,5}\,cc_1^{\,2}-2\,cc_1^{\,2}\,ss_1\,c_{4,6}+c_{1,5}\,ss_1-cc_1^{\,2}\,c_{1,5}\,ss_1+2\,cc_1^{\,3}\,c_{4,5}+c_{1,6}\,cc_1+cc_1^{\,3}\,c_{2,6}$$
$$-cc_1^{\,3}\,c_{1,6}-2\,c_{4,5}\,cc_1-c_{2,6},\ -ss_1\,c_{2,6}\,cc_1^{\,2}-2\,cc_1^{\,2}\,ss_1\,c_{4,5}-c_{1,6}\,ss_1+cc_1^{\,2}\,c_{1,6}\,ss_1-2\,cc_1^{\,3}\,c_{4,6}$$
$$+c_{1,5}\,cc_1+cc_1^{\,3}\,c_{2,5}-cc_1^{\,3}\,c_{1,5}+2\,c_{4,6}\,cc_1-c_{2,5},\ -2\,cc_1^{\,2}\,ss_1\,c_{4,6}-cc_1^{\,2}\,c_{1,5}\,ss_1+c_{4,6}\,ss_1$$
$$+ss_1\,c_{2,5}\,cc_1^{\,2}+cc_1^{\,3}\,c_{2,6}-c_{2,6}\,cc_1+c_{1,6}\,cc_1+2\,cc_1^{\,3}\,c_{4,5}-cc_1^{\,3}\,c_{1,6}-c_{4,5}\,cc_1-c_{4,5},\ ss_1\,c_{2,6}\,cc_1^{\,2}$$
$$+2\,cc_1^{\,2}\,ss_1\,c_{4,5}-c_{4,5}\,ss_1-cc_1^{\,2}\,c_{1,6}\,ss_1-cc_1^{\,3}\,c_{2,5}-c_{4,6}\,cc_1+c_{2,5}\,cc_1+2\,cc_1^{\,3}\,c_{4,6}+cc_1^{\,3}\,c_{1,5}$$
$$-c_{1,5}\,cc_1-c_{4,6},\ 4\,cc_1^{\,3}\,c_{1,4}\,ss_1-4\,ss_1\,c_{2,4}\,cc_1^{\,3}-4\,c_{1,4}\,cc_1\,ss_1+2\,c_{1,2}\,cc_1^{\,2}+cc_1^{\,4}\,c_{2,2}+c_{1,1}$$
$$-2\,c_{1,1}\,cc_1^{\,2}-2\,cc_1^{\,4}\,c_{1,2}+4\,cc_1^{\,2}\,c_{4,4}+cc_1^{\,4}\,c_{1,1}-4\,cc_1^{\,4}\,c_{4,4}-c_{2,2},\ -4\,ss_1\,c_{2,4}\,cc_1^{\,3}$$
$$+4\,cc_1^{\,3}\,c_{1,4}\,ss_1+4\,c_{2,4}\,cc_1\,ss_1+2\,c_{1,2}\,cc_1^{\,2}+cc_1^{\,4}\,c_{1,1}+c_{2,2}-2\,c_{2,2}\,cc_1^{\,2}-2\,cc_1^{\,4}\,c_{1,2}$$
$$+4\,cc_1^{\,2}\,c_{4,4}+cc_1^{\,4}\,c_{2,2}-4\,cc_1^{\,4}\,c_{4,4}-c_{1,1},\ -cc_1^{\,3}\,c_{1,1}\,ss_1+2\,cc_1^{\,3}\,c_{1,2}\,ss_1+4\,cc_1^{\,3}\,ss_1\,c_{4,4}$$
$$+c_{2,2}\,cc_1\,ss_1-c_{1,2}\,cc_1\,ss_1-2\,c_{4,4}\,cc_1\,ss_1-ss_1\,cc_1^{\,3}\,c_{2,2}-3\,c_{1,4}\,cc_1^{\,2}+5\,c_{2,4}\,cc_1^{\,2}-c_{2,4}$$
$$+4\,cc_1^{\,4}\,c_{1,4}-4\,cc_1^{\,4}\,c_{2,4}-c_{1,4},\ ss_1\,cc_1^{\,3}\,c_{2,2}-2\,cc_1^{\,3}\,c_{1,2}\,ss_1-4\,cc_1^{\,3}\,ss_1\,c_{4,4}-c_{1,1}\,cc_1\,ss_1$$
$$+c_{1,2}\,cc_1\,ss_1+2\,c_{4,4}\,cc_1\,ss_1+cc_1^{\,3}\,c_{1,1}\,ss_1-3\,c_{2,4}\,cc_1^{\,2}+5\,c_{1,4}\,cc_1^{\,2}-c_{1,4}+4\,cc_1^{\,4}\,c_{2,4}$$
$$-4\,cc_1^{\,4}\,c_{1,4}-c_{2,4},\ cc_1^{\,2}+ss_1^{\,2}-1,\ cc_2^{\,2}+ss_2^{\,2}-1,\ cc_3^{\,2}+ss_3^{\,2}-1\,]$$

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>

Step 8: Using **Groebner:-Basis** command, we compute the Groebner basis **GB** for the ideal **<F>** with respect to the elimination order **Tmonord**. The Groebner basis **GB** for **<F>** has 55 polynomials.

```
> GB:=Groebner:-Basis(F,Tmonord); ##<<-- compute Groebner basis for
  ideal <F>
  nops(GB);
```

$$GB := [\,c_{1,6}\,cc_1+c_{4,5}\,cc_1-c_{1,6}-c_{4,5},\ c_{1,5}\,cc_1-c_{4,6}\,cc_1-c_{1,5}+c_{4,6},$$
$$c_{2,6}\,cc_1-c_{4,5}\,cc_1-c_{2,6}+c_{4,5},\ c_{2,5}\,cc_1+c_{4,6}\,cc_1-c_{2,5}-c_{4,6},\ c_{3,6}\,cc_1-c_{3,6},\ c_{3,5}\,cc_1-c_{3,5},$$
$$cc_1^{\,2}+ss_1^{\,2}-1,\ c_{1,6}\,ss_1+c_{4,5}\,ss_1,\ c_{1,5}\,ss_1-c_{4,6}\,ss_1,\ c_{2,6}\,ss_1-c_{4,5}\,ss_1,\ c_{2,5}\,ss_1+c_{4,6}\,ss_1,$$
$$c_{2,4}\,ss_1+c_{1,4}\,ss_1,\ c_{2,2}\,ss_1-c_{1,1}\,ss_1,\ c_{3,4}\,ss_1,\ c_{5,6}\,ss_1,\ -c_{1,3}\,ss_1+c_{2,3}\,ss_1,\ c_{5,5}\,ss_1-ss_1\,c_{6,6},\ c_{3,6}\,ss_1,$$
$$c_{3,5}\,ss_1,\ cc_2^{\,2}+ss_2^{\,2}-1,\ cc_3^{\,2}+ss_3^{\,2}-1,\ 2\,cc_1^{\,2}\,c_{4,5}-c_{4,5}\,cc_1-c_{4,5},\ 2\,cc_1^{\,2}\,c_{4,6}-c_{4,6}\,cc_1-c_{4,6},$$
$$c_{2,4}\,cc_1^{\,2}+c_{1,4}\,cc_1^{\,2}-c_{2,4}-c_{1,4},\ c_{2,2}\,cc_1^{\,2}-c_{1,1}\,cc_1^{\,2}-c_{2,2}+c_{1,1},\ c_{3,4}\,cc_1^{\,2}-c_{3,4},\ c_{5,6}\,cc_1^{\,2}-c_{5,6},$$
$$c_{2,3}\,cc_1^{\,2}-c_{1,3}\,cc_1^{\,2}-c_{2,3}+c_{1,3},\ c_{5,5}\,cc_1^{\,2}-c_{6,6}\,cc_1^{\,2}-c_{5,5}+c_{6,6},\ 2\,c_{4,5}\,ss_1\,cc_1+c_{4,5}\,ss_1,$$
$$2\,c_{4,6}\,ss_1\,cc_1+c_{4,6}\,ss_1,\ c_{1,4}\,cc_1\,ss_1,\ c_{1,1}\,cc_1\,ss_1-2\,c_{4,4}\,cc_1\,ss_1-c_{1,2}\,cc_1\,ss_1,\ c_{1,4}\,c_{4,5}\,cc_1-c_{1,4}\,c_{4,5},$$

$$c_{2,4}\,c_{4,5}\,cc_1 - c_{2,4}\,c_{4,5},$$
$$c_{1,1}\,c_{4,5}\,cc_1 - 2\,c_{4,4}\,c_{4,5}\,cc_1 - c_{1,2}\,c_{4,5}\,cc_1 - c_{1,1}\,c_{4,5} + 2\,c_{4,4}\,c_{4,5} + c_{1,2}\,c_{4,5},$$
$$c_{2,2}\,c_{4,5}\,cc_1 - 2\,c_{4,4}\,c_{4,5}\,cc_1 - c_{1,2}\,c_{4,5}\,cc_1 - c_{2,2}\,c_{4,5} + 2\,c_{4,4}\,c_{4,5} + c_{1,2}\,c_{4,5},$$
$$c_{3,4}\,c_{4,5}\,cc_1 - c_{3,4}\,c_{4,5},\ c_{5,6}\,c_{4,5}\,cc_1 - c_{5,6}\,c_{4,5},\ c_{2,3}\,c_{4,5}\,cc_1 - c_{1,3}\,c_{4,5}\,cc_1 - c_{2,3}\,c_{4,5} + c_{1,3}\,c_{4,5},$$
$$c_{5,5}\,c_{4,5}\,cc_1 - c_{6,6}\,c_{4,5}\,cc_1 - c_{5,5}\,c_{4,5} + c_{6,6}\,c_{4,5},\ c_{1,4}\,c_{4,6}\,cc_1 - c_{1,4}\,c_{4,6},\ c_{2,4}\,c_{4,6}\,cc_1 - c_{2,4}\,c_{4,6},$$
$$c_{1,1}\,c_{4,6}\,cc_1 - 2\,c_{4,4}\,c_{4,6}\,cc_1 - c_{1,2}\,c_{4,6}\,cc_1 - c_{1,1}\,c_{4,6} + 2\,c_{4,4}\,c_{4,6} + c_{1,2}\,c_{4,6},$$
$$c_{2,2}\,c_{4,6}\,cc_1 - 2\,c_{4,4}\,c_{4,6}\,cc_1 - c_{1,2}\,c_{4,6}\,cc_1 - c_{2,2}\,c_{4,6} + 2\,c_{4,4}\,c_{4,6} + c_{1,2}\,c_{4,6},$$
$$c_{3,4}\,c_{4,6}\,cc_1 - c_{3,4}\,c_{4,6},\ c_{5,6}\,c_{4,6}\,cc_1 - c_{5,6}\,c_{4,6},\ c_{2,3}\,c_{4,6}\,cc_1 - c_{1,3}\,c_{4,6}\,cc_1 - c_{2,3}\,c_{4,6} + c_{1,3}\,c_{4,6},$$
$$c_{5,5}\,c_{4,6}\,cc_1 - c_{6,6}\,c_{4,6}\,cc_1 - c_{5,5}\,c_{4,6} + c_{6,6}\,c_{4,6},\ c_{1,4}\,c_{4,5}\,ss_1,$$
$$c_{1,1}\,c_{4,5}\,ss_1 - 2\,c_{4,4}\,c_{4,5}\,ss_1 - c_{1,2}\,c_{4,5}\,ss_1,\ c_{1,4}\,c_{4,6}\,ss_1,\ c_{1,1}\,c_{4,6}\,ss_1 - 2\,c_{4,4}\,c_{4,6}\,ss_1 - c_{1,2}\,c_{4,6}\,ss_1,$$
$$cc_1^{\,3}\,c_{1,4} - c_{1,4}\,cc_1,\ cc_1^{\,3}\,c_{1,1} - 2\,cc_1^{\,3}\,c_{4,4} - cc_1^{\,3}\,c_{1,2} - c_{1,1}\,cc_1 + 2\,cc_1\,c_{4,4} + c_{1,2}\,cc_1\,]$$

55

```
>
```

Step 9: From the Groebner basis **GB**, we eliminate all polynomials which do not contain at least one parameter c[i,j] from the material constants matrix C. That is, we eliminate all trigonometric identities among the indeterminates **ss[1], ss[2], ss[3], cc[1], cc[2], cc[3]**. The resulting list is assigned to a variable **L1**. It contains 52 polynomials since the three Pythagorean identities added earlier got now removed.

```
> L1:=[]: ##<<-- this list will contain only those polynomials in GB
  which contain at least one parameter c[i,j]
  for p in GB do
      if not evalb(`intersect`(indets(p),convert(Cindets,set))={})
  then L1:=[p,op(L1)] end if;
  end do;
> 'L1'=L1;
  nops(L1);
```

$$L1 = [\,cc_1^{\,3}\,c_{1,1} - 2\,cc_1^{\,3}\,c_{4,4} - cc_1^{\,3}\,c_{1,2} - c_{1,1}\,cc_1 + 2\,cc_1\,c_{4,4} + c_{1,2}\,cc_1,\ cc_1^{\,3}\,c_{1,4} - c_{1,4}\,cc_1,$$
$$c_{1,1}\,c_{4,6}\,ss_1 - 2\,c_{4,4}\,c_{4,6}\,ss_1 - c_{1,2}\,c_{4,6}\,ss_1,\ c_{1,4}\,c_{4,6}\,ss_1,\ c_{1,1}\,c_{4,5}\,ss_1 - 2\,c_{4,4}\,c_{4,5}\,ss_1 - c_{1,2}\,c_{4,5}\,ss_1,$$
$$c_{1,4}\,c_{4,5}\,ss_1,\ c_{5,5}\,c_{4,6}\,cc_1 - c_{6,6}\,c_{4,6}\,cc_1 - c_{5,5}\,c_{4,6} + c_{6,6}\,c_{4,6},$$
$$c_{2,3}\,c_{4,6}\,cc_1 - c_{1,3}\,c_{4,6}\,cc_1 - c_{2,3}\,c_{4,6} + c_{1,3}\,c_{4,6},\ c_{5,6}\,c_{4,6}\,cc_1 - c_{5,6}\,c_{4,6},\ c_{3,4}\,c_{4,6}\,cc_1 - c_{3,4}\,c_{4,6},$$
$$c_{2,2}\,c_{4,6}\,cc_1 - 2\,c_{4,4}\,c_{4,6}\,cc_1 - c_{1,2}\,c_{4,6}\,cc_1 - c_{2,2}\,c_{4,6} + 2\,c_{4,4}\,c_{4,6} + c_{1,2}\,c_{4,6},$$
$$c_{1,1}\,c_{4,6}\,cc_1 - 2\,c_{4,4}\,c_{4,6}\,cc_1 - c_{1,2}\,c_{4,6}\,cc_1 - c_{1,1}\,c_{4,6} + 2\,c_{4,4}\,c_{4,6} + c_{1,2}\,c_{4,6},$$
$$c_{2,4}\,c_{4,6}\,cc_1 - c_{2,4}\,c_{4,6},\ c_{1,4}\,c_{4,6}\,cc_1 - c_{1,4}\,c_{4,6},\ c_{5,5}\,c_{4,5}\,cc_1 - c_{6,6}\,c_{4,5}\,cc_1 - c_{5,5}\,c_{4,5} + c_{6,6}\,c_{4,5},$$
$$c_{2,3}\,c_{4,5}\,cc_1 - c_{1,3}\,c_{4,5}\,cc_1 - c_{2,3}\,c_{4,5} + c_{1,3}\,c_{4,5},\ c_{5,6}\,c_{4,5}\,cc_1 - c_{5,6}\,c_{4,5},\ c_{3,4}\,c_{4,5}\,cc_1 - c_{3,4}\,c_{4,5},$$

$$c_{2,2}\,c_{4,5}\,cc_1 - 2\,c_{4,4}\,c_{4,5}\,cc_1 - c_{1,2}\,c_{4,5}\,cc_1 - c_{2,2}\,c_{4,5} + 2\,c_{4,4}\,c_{4,5} + c_{1,2}\,c_{4,5},$$
$$c_{1,1}\,c_{4,5}\,cc_1 - 2\,c_{4,4}\,c_{4,5}\,cc_1 - c_{1,2}\,c_{4,5}\,cc_1 - c_{1,1}\,c_{4,5} + 2\,c_{4,4}\,c_{4,5} + c_{1,2}\,c_{4,5},$$
$$c_{2,4}\,c_{4,5}\,cc_1 - c_{2,4}\,c_{4,5},\ c_{1,4}\,c_{4,5}\,cc_1 - c_{1,4}\,c_{4,5},\ c_{1,1}\,cc_1\,ss_1 - 2\,c_{4,4}\,cc_1\,ss_1 - c_{1,2}\,cc_1\,ss_1,\ c_{1,4}\,cc_1\,ss_1,$$
$$2\,c_{4,6}\,ss_1\,cc_1 + c_{4,6}\,ss_1,\ 2\,c_{4,5}\,ss_1\,cc_1 + c_{4,5}\,ss_1,\ c_{5,5}\,cc_1^{\,2} - c_{6,6}\,cc_1^{\,2} - c_{5,5} + c_{6,6},$$
$$c_{2,3}\,cc_1^{\,2} - c_{1,3}\,cc_1^{\,2} - c_{2,3} + c_{1,3},\ c_{5,6}\,cc_1^{\,2} - c_{5,6},\ c_{3,4}\,cc_1^{\,2} - c_{3,4},\ c_{2,2}\,cc_1^{\,2} - c_{1,1}\,cc_1^{\,2} - c_{2,2} + c_{1,1},$$
$$c_{2,4}\,cc_1^{\,2} + c_{1,4}\,cc_1^{\,2} - c_{2,4} - c_{1,4},\ 2\,cc_1^{\,2}\,c_{4,6} - c_{4,6}\,cc_1 - c_{4,6},\ 2\,cc_1^{\,2}\,c_{4,5} - c_{4,5}\,cc_1 - c_{4,5},\ c_{3,5}\,ss_1,$$
$$c_{3,6}\,ss_1,\ c_{5,5}\,ss_1 - ss_1\,c_{6,6},\ -c_{1,3}\,ss_1 + c_{2,3}\,ss_1,\ c_{5,6}\,ss_1,\ c_{3,4}\,ss_1,\ c_{2,2}\,ss_1 - c_{1,1}\,ss_1,\ c_{2,4}\,ss_1 + c_{1,4}\,ss_1,$$
$$c_{2,5}\,ss_1 + c_{4,6}\,ss_1,\ c_{2,6}\,ss_1 - c_{4,5}\,ss_1,\ c_{1,5}\,ss_1 - c_{4,6}\,ss_1,\ c_{1,6}\,ss_1 + c_{4,5}\,ss_1,\ c_{3,5}\,cc_1 - c_{3,5},$$
$$c_{3,6}\,cc_1 - c_{3,6},\ c_{2,5}\,cc_1 + c_{4,6}\,cc_1 - c_{2,5} - c_{4,6},\ c_{2,6}\,cc_1 - c_{4,5}\,cc_1 - c_{2,6} + c_{4,5},$$
$$c_{1,5}\,cc_1 - c_{4,6}\,cc_1 - c_{1,5} + c_{4,6},\ c_{1,6}\,cc_1 + c_{4,5}\,cc_1 - c_{1,6} - c_{4,5}\,]$$

52

>

Step 10: Remember we need to solve the polynomial equations in the list **L1** above for the indeterminates **c[i,j]** while treating the six additional indeterminates **ss[1], ss[2], ss[3], cc[1], cc[2], cc[3]** as arbitrary. Thus, we must find all coefficients from the polynomials in **L1** which have been collected with respect to these six indeterminates . To remove redundancies, we collect these coefficients into a set **L2**: This set contains **66** polynomials exclusively in the indeterminates **c[i,j]**. However, these polynomials may be algebraically dependent.

```
> L2:={seq(coeffs(p,[cc[1],ss[1],cc[2],ss[2],cc[3],ss[3]]),p=L1)};
  ##<<-- this list will contain all coefficients of cc and ss in
  polynomials p in L1
  nops(L2);
```

$$L2 := \{\, c_{1,4},\ c_{3,4},\ c_{3,5},\ c_{3,6},\ c_{4,5},\ c_{4,6},\ c_{5,6},\ c_{1,4}\,c_{4,5},\ c_{1,4}\,c_{4,6},\ c_{2,4}\,c_{4,5},\ c_{2,4}\,c_{4,6},\ c_{3,4}\,c_{4,5},\ c_{3,4}\,c_{4,6},$$
$$c_{5,6}\,c_{4,5},\ c_{5,6}\,c_{4,6},\ -c_{1,4},\ -c_{3,4},\ -c_{3,5},\ -c_{3,6},\ -c_{4,5},\ 2\,c_{4,5},\ -c_{4,6},\ 2\,c_{4,6},\ -c_{5,6},\ -c_{1,4}\,c_{4,5},\ -c_{1,4}\,c_{4,6},$$
$$-c_{2,4}\,c_{4,5},\ -c_{2,4}\,c_{4,6},\ -c_{3,4}\,c_{4,5},\ -c_{3,4}\,c_{4,6},\ -c_{5,6}\,c_{4,5},\ -c_{5,6}\,c_{4,6},\ -c_{1,3} + c_{2,3},\ c_{1,3} - c_{2,3},\ -c_{1,4} - c_{2,4},$$
$$c_{1,4} + c_{2,4},\ -c_{1,5} + c_{4,6},\ c_{1,5} - c_{4,6},\ -c_{1,6} - c_{4,5},\ c_{1,6} + c_{4,5},\ -c_{2,2} + c_{1,1},\ c_{2,2} - c_{1,1},\ -c_{2,5} - c_{4,6},$$
$$c_{2,5} + c_{4,6},\ -c_{2,6} + c_{4,5},\ c_{2,6} - c_{4,5},\ -c_{5,5} + c_{6,6},\ c_{5,5} - c_{6,6},\ -c_{2,3}\,c_{4,5} + c_{1,3}\,c_{4,5},\ c_{2,3}\,c_{4,5} - c_{1,3}\,c_{4,5},$$
$$-c_{2,3}\,c_{4,6} + c_{1,3}\,c_{4,6},\ c_{2,3}\,c_{4,6} - c_{1,3}\,c_{4,6},\ -c_{5,5}\,c_{4,5} + c_{6,6}\,c_{4,5},\ c_{5,5}\,c_{4,5} - c_{6,6}\,c_{4,5},$$
$$-c_{5,5}\,c_{4,6} + c_{6,6}\,c_{4,6},\ c_{5,5}\,c_{4,6} - c_{6,6}\,c_{4,6},\ -c_{1,1} + c_{1,2} + 2\,c_{4,4},\ c_{1,1} - 2\,c_{4,4} - c_{1,2},$$
$$c_{1,1}\,c_{4,5} - 2\,c_{4,4}\,c_{4,5} - c_{1,2}\,c_{4,5},\ c_{1,1}\,c_{4,6} - 2\,c_{4,4}\,c_{4,6} - c_{1,2}\,c_{4,6},\ -c_{1,2}\,c_{4,5} + c_{2,2}\,c_{4,5} - 2\,c_{4,4}\,c_{4,5},$$
$$-c_{1,2}\,c_{4,6} + c_{2,2}\,c_{4,6} - 2\,c_{4,4}\,c_{4,6},\ 2\,c_{4,4}\,c_{4,5} + c_{1,2}\,c_{4,5} - c_{1,1}\,c_{4,5},\ 2\,c_{4,4}\,c_{4,5} + c_{1,2}\,c_{4,5} - c_{2,2}\,c_{4,5},$$
$$2\,c_{4,4}\,c_{4,6} + c_{1,2}\,c_{4,6} - c_{1,1}\,c_{4,6},\ 2\,c_{4,4}\,c_{4,6} + c_{1,2}\,c_{4,6} - c_{2,2}\,c_{4,6}\,\}$$

66

>

Step 11: To remove all possible algebraic dependencies among the polynomials in the set **L2**, we will compute a Groebner basis **L3** for the ideal **<L2>** generated by the polynomials in **L2**. This Groebner basis will be computed with respect to a lexicographic order **'plex'(c[6,6],..., c[1,1])**. This is because we want to eliminate those indeterminates **c[i,j]** which have higher-valued indices and express them in terms of the indeterminates **c[i,j]** with lower-valued indices. This monomial order is stored in a variable **Trevplexmonord**.

```
> Trevplexmonord:=plex(op(Cindetsrev));
```

$$Trevplexmonord := \mathrm{plex}(c_{6,6}, c_{5,6}, c_{5,5}, c_{4,6}, c_{4,5}, c_{4,4}, c_{3,6}, c_{3,5}, c_{3,4}, c_{3,3}, c_{2,6}, c_{2,5}, c_{2,4}, c_{2,3}, c_{2,2}, c_{1,6}, c_{1,5}, c_{1,4}, c_{1,3}, c_{1,2}, c_{1,1})$$

>

Step 12: Now we compute Groebner basis **L3** for **<L2>**. **L3** has **16** polynomials, each of which must be 0.

```
> L3:=Groebner:-Basis(L2,Trevplexmonord); ##<<-- we reduce list L2
  to just generators by computing Groebner basis for <L2> w.r.t.
  plex(op(Cindetsrev)) order
  nops(L3);
```

$$L3 := [c_{1,4}, c_{1,5}, c_{1,6}, c_{2,2} - c_{1,1}, -c_{1,3} + c_{2,3}, c_{2,4}, c_{2,5}, c_{2,6}, c_{3,4}, c_{3,5}, c_{3,6}, -c_{1,1} + c_{1,2} + 2\,c_{4,4}, c_{4,5}, c_{4,6}, c_{5,6}, -c_{5,5} + c_{6,6}]$$

16

>

Step 13: In order to properly solve the nontrivial equations of the form **p = 0** for every polynomial **p** in **L3**, that is, solve for those indeterminates **c[i,j]** which are "greater" with respect to the monomial order **Trevplexmonord** defined above, we solve each polynomial equation **p = 0** for the **LeadingMonomial(p)** taken with respect to the monomial order **Trevplexmonord**. Then, for each equation **p = 0**, we set up a sequence of equations of the form

LeadingMonomial(p,Trevplexmonord) = solve(p,LeadingMonomial(p,Trevoplexmonord)) for each p in **L3**.

We will need these equations as we will need to substitute them into the generic material coefficients matrix **C**.

```
> L4:=[seq(Groebner:-LeadingMonomial(p,Trevplexmonord)=solve(p,Groeb
  ner:-LeadingMonomial(p,Trevplexmonord)),p=L3)];
```

$$L4 := \left[c_{1,4} = 0, c_{1,5} = 0, c_{1,6} = 0, c_{2,2} = c_{1,1}, c_{2,3} = c_{1,3}, c_{2,4} = 0, c_{2,5} = 0, c_{2,6} = 0, c_{3,4} = 0, \right.$$

$$c_{3,5}=0,\ c_{3,6}=0,\ c_{4,4}=\frac{1}{2}c_{1,1}-\frac{1}{2}c_{1,2},\ c_{4,5}=0,\ c_{4,6}=0,\ c_{5,6}=0,\ c_{6,6}=c_{5,5}\Big]$$

>

Step 14: We finally use the list **L4** to make substitutions into the generic material constants matrix **C** and return the result.

```
> Cnew[symmetry[k]]:=subs(L4,C);
```

$$Cnew_{xy}:=\begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & 0 & 0 \\ c_{1,2} & c_{1,1} & c_{1,3} & 0 & 0 & 0 \\ c_{1,3} & c_{1,3} & c_{3,3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}c_{1,1}-\frac{1}{2}c_{1,2} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{5,5} \end{bmatrix}$$

>

Thus, all of the above steps can be done with the single call to the procedure **TransformedMaterialConstants** (aliased as **TMC**), as follows:

```
> TMC[C](C,TT);
  C_constants[C](%);
```

$$\begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & 0 & 0 \\ c_{1,2} & c_{1,1} & c_{1,3} & 0 & 0 & 0 \\ c_{1,3} & c_{1,3} & c_{3,3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}c_{1,1}-\frac{1}{2}c_{1,2} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{5,5} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 12.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 5.
```

>

Thus, any **transversely isotropic** material with one rotational symmetry has **12 nonzero parameters in C among which 5 are independent.** We summarize these findings in the next example.

Example 6 (transversely istropic): Displaying three standard rotation matrices:

```
> T[xy](theta[3]),T[xz](theta[2]),T[yz](theta[1]);
```

$$\begin{bmatrix} \cos(\theta_3) & \sin(\theta_3) & 0 \\ -\sin(\theta_3) & \cos(\theta_3) & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} \cos(\theta_2) & 0 & \sin(\theta_2) \\ 0 & 1 & 0 \\ -\sin(\theta_2) & 0 & \cos(\theta_2) \end{bmatrix}, \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta_1) & \sin(\theta_1) \\ 0 & -\sin(\theta_1) & \cos(\theta_1) \end{bmatrix}$$

>

Computing material constants matrix for transversily isotropic materials by applying one rotational symmetry to **C**. Each has 5 free parameters, and 12 independent parameters:

```
> SymCxy:=TMC[C](C,T[xy](theta[3]));  ##<<-- applying xy symmetry to
  C
  C_constants[C](SymCxy);
```

$$SymCxy := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & 0 & 0 \\ c_{1,2} & c_{1,1} & c_{1,3} & 0 & 0 & 0 \\ c_{1,3} & c_{1,3} & c_{3,3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,2} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{5,5} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 12.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 5.
```

```
> SymCxz:=TMC[C](C,T[xz](theta[2]));  ##<<-- applying xz symmetry to
  C
  C_constants[C](SymCxz);
```

$$SymCxz := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{1,2} & 0 & 0 & 0 \\ c_{1,3} & c_{1,2} & c_{1,1} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{4,4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,3} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 12.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 5.
```

```
> SymCyz:=TMC[C](C,T[yz](theta[1]));  ##<<-- applying yz symmetry to
  C
  C_constants[C](SymCyz);
```

$$SymCyz := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,2} & 0 & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & 0 & 0 & 0 \\ c_{1,2} & c_{2,3} & c_{2,2} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2}c_{2,3} + \frac{1}{2}c_{2,2} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{4,4} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 12.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 5.
```

```
>
```

Example 7 (isotropic material). Thus, we apply to the material constants matrices of three transversily isotropic materials displayed above additional symmetries.

-- First, to **SymCxy** matrix with the xy-symmetry we apply additional xz-symmetry, and obtain matrix **SymCxyxz**.
-- Second, to **SymCxz** matrix with the xz-symmetry we apply additional xy-symmetry, and obtain matrix **SymCxzxy**
-- Third, we compare these matrices and find that they are identical with two free parameters **c[1,1]** and **c[1,2]**.
-- Fourth, we apply additional yz-symmetry to the matrix **SymCxyxz**.
-- Fifth, we find out that applying third symmetry does not reduce the number of free parameters **c[1,1]** and **c[1,2]**.

```
> SymCxyxz:=TMC[C](SymCxy,T[xz](theta[2]));      ##<<-- applying xz
  symmetry to SymCxy
  SymCxzxy:=TMC[C](SymCxz,T[xy](theta[3]));      ##<<-- applying xy
  symmetry to SymCxz
  Equal(SymCxyxz,SymCxzxy);                      ##<<-- comparing the
  above two matrices
  SymCxyxzyz:=TMC[C](SymCxyxz,T[yz](theta[1])); ##<<-- applying
  third symmetry
  Equal(SymCxyxz,SymCxyxzyz);                    ##<<-- comparing the
  above two matrices
```

$$SymCxyxz := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,2} & 0 & 0 & 0 \\ c_{1,2} & c_{1,1} & c_{1,2} & 0 & 0 & 0 \\ c_{1,2} & c_{1,2} & c_{1,1} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,2} \end{bmatrix}$$

$$SymCxzxy := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,2} & 0 & 0 & 0 \\ c_{1,2} & c_{1,1} & c_{1,2} & 0 & 0 & 0 \\ c_{1,2} & c_{1,2} & c_{1,1} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,2} \end{bmatrix}$$

true

$$SymCxyxzyz := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,2} & 0 & 0 & 0 \\ c_{1,2} & c_{1,1} & c_{1,2} & 0 & 0 & 0 \\ c_{1,2} & c_{1,2} & c_{1,1} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,2} \end{bmatrix}$$

true

```
> C_constants[C](SymCxyxzyz);
Number of nonzero parameters in the material constants matrix C of the given symme
try is 12.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 2.
```

```
>
```

Section 3: Examples of Materials with Various Symmetries

In this section we systematically find material constants matrices for materials with various

symmetries. We divide these materials into standard and non-standard.

```
> restart:with(MaterialConstants);
```

$$\_known\_types = [orthogonal, puresymbolic]$$

$$\_known\_aliases = [RM = MaterialConstants:\text{-}ReflectionMatrix, TMC = MaterialConstants:\text{-}TransformedMaterialConstants]$$

$$\_known\_additional\_protected\_names = [c, \varepsilon, \sigma, \theta]$$

$$[C\_constants, MCversion, ModuleLoad, ModuleUnload, ReflectionMatrix, SimilarityTransform, Teps, TepsMatrix, TransformedMaterialConstants, Tsigma, TsigmaMatrix, makeC, makeEpsilon, makeSigma, phi\_eps, phi\_eps\_inv, phi\_sigma, phi\_sigma\_inv]$$

```
>
```

Subsection 1: Standard Materials

Example 8: Monoclinic materials have **one plane of (reflective) symmetry**, which can always be chosen to be one of the coordinate planes. Their material constants matrix **C** has **20 nonzero constants among which 13 are indepednent**.

```
> C:=makeC(6,c); ##<<-- defining generic C
  C_constants[C](C);
```

$$C := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & c_{1,4} & c_{1,5} & c_{1,6} \\ c_{1,2} & c_{2,2} & c_{2,3} & c_{2,4} & c_{2,5} & c_{2,6} \\ c_{1,3} & c_{2,3} & c_{3,3} & c_{3,4} & c_{3,5} & c_{3,6} \\ c_{1,4} & c_{2,4} & c_{3,4} & c_{4,4} & c_{4,5} & c_{4,6} \\ c_{1,5} & c_{2,5} & c_{3,5} & c_{4,5} & c_{5,5} & c_{5,6} \\ c_{1,6} & c_{2,6} & c_{3,6} & c_{4,6} & c_{5,6} & c_{6,6} \end{bmatrix}$$

```
Number of nonzero parameters in the generic material constants matrix C is 36.
Number of independent parameters in the generic material constants matrix C is 21.
```

```
> T[rxy]:=ReflectionMatrix([0,0,1]); ##<<-- reflection w.r.t. the
  xy-plane
  MCrxy:=TMC[C](C,T[rxy]);
  C_constants[C](MCrxy);
```

$$T_{rxy} := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$MCrxy := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & c_{1,4} & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & c_{2,4} & 0 & 0 \\ c_{1,3} & c_{2,3} & c_{3,3} & c_{3,4} & 0 & 0 \\ c_{1,4} & c_{2,4} & c_{3,4} & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & c_{5,6} \\ 0 & 0 & 0 & 0 & c_{5,6} & c_{6,6} \end{bmatrix}$$

Number of nonzero parameters in the material constants matrix C of the given symmetry is 20.
Number of independent parameters in the material constants matrix C of the given symmetry is 13.

```
>
```

```
> T[rxz]:=ReflectionMatrix([0,1,0]); ##<<-- reflection w.r.t. the
  xz-plane
  MCrxz:=TMC[C](C,T[rxz]);
  C_constants[C](MCrxz);
```

$$T_{rxz} := \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$MCrxz := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & 0 & c_{1,6} \\ c_{1,2} & c_{2,2} & c_{2,3} & 0 & 0 & c_{2,6} \\ c_{1,3} & c_{2,3} & c_{3,3} & 0 & 0 & c_{3,6} \\ 0 & 0 & 0 & c_{4,4} & c_{4,5} & 0 \\ 0 & 0 & 0 & c_{4,5} & c_{5,5} & 0 \\ c_{1,6} & c_{2,6} & c_{3,6} & 0 & 0 & c_{6,6} \end{bmatrix}$$

Number of nonzero parameters in the material constants matrix C of the given symmetry is 20.
Number of independent parameters in the material constants matrix C of the given symmetry is 13.

```
>
```

```
> T[ryz]:=ReflectionMatrix([1,0,0]); ##<<-- reflection w.r.t. the
  yz-plane
  MCryz:=TMC[C](C,T[ryz]);
  C_constants[C](MCryz);
```

$$T_{ryz} := \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$MCryz := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & c_{1,5} & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & 0 & c_{2,5} & 0 \\ c_{1,3} & c_{2,3} & c_{3,3} & 0 & c_{3,5} & 0 \\ 0 & 0 & 0 & c_{4,4} & 0 & c_{4,6} \\ c_{1,5} & c_{2,5} & c_{3,5} & 0 & c_{5,5} & 0 \\ 0 & 0 & 0 & c_{4,6} & 0 & c_{6,6} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 20.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 13.
```

```
>
```

Example 9: Orthotropic materials have **three planes of (reflective) symmetry**. As such their material constants matrix **C** has **12 nonzero constants of which 9 are indepedent.**

```
> PlaneSym3:=TMC[C](C,T[rxy],T[rxz],T[ryz]);
  C_constants[C](PlaneSym3);
```

$$PlaneSym3 := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & 0 & 0 & 0 \\ c_{1,3} & c_{2,3} & c_{3,3} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{6,6} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 12.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 9.
```

```
>
```

Example 10: Transversely isotropic materials have **one plane of isotropic (rotational) symmetry**. As such their material constants matrix C has **12 nonzero constants of which 5 are independent.**

Let's define three rotation matrices:

```
> T[xy]:=gamma->Matrix(3,3,[cos(gamma),sin(gamma),0,-sin(gamma),cos(
  gamma),0,0,0,1]);
  T[xz]:=beta->Matrix(3,3,[cos(beta),0,sin(beta),0,1,0,-sin(beta),0,
  cos(beta)]);
  T[yz]:=alpha->Matrix(3,3,[1,0,0,0,cos(alpha),sin(alpha),0,-sin(alp
  ha),cos(alpha)]);
```

$$T_{xy} := \gamma \rightarrow \mathrm{Matrix}(3, 3, [\cos(\gamma), \sin(\gamma), 0, -\sin(\gamma), \cos(\gamma), 0, 0, 0, 1])$$

$$T_{xz} := \beta \rightarrow \mathrm{Matrix}(3, 3, [\cos(\beta), 0, \sin(\beta), 0, 1, 0, -\sin(\beta), 0, \cos(\beta)])$$

$$T_{yz} := \alpha \to \text{Matrix}(3, 3, [1, 0, 0, 0, \cos(\alpha), \sin(\alpha), 0, -\sin(\alpha), \cos(\alpha)])$$

>

Let's calculate now material constants matrices **C** for transversely isotropic materials with one rotational plane of symmetry, which can always be chosen to be one of the coordinate planes.

```
> TransIso[xy]:=TMC[C](C,T[xy](theta[3])); ##<<-- rotational
  symmetry in the xy-plane
  C_constants[C](TransIso[xy]);
```

$$TransIso_{xy} := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & 0 & 0 \\ c_{1,2} & c_{1,1} & c_{1,3} & 0 & 0 & 0 \\ c_{1,3} & c_{1,3} & c_{3,3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,2} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{5,5} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 12.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 5.
```

```
> TransIso[xz]:=TMC[C](C,T[xz](theta[2])); ##<<-- rotational
  symmetry in the xz-plane
  C_constants[C](TransIso[xz]);
```

$$TransIso_{xz} := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{1,2} & 0 & 0 & 0 \\ c_{1,3} & c_{1,2} & c_{1,1} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{4,4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,3} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 12.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 5.
```

```
> TransIso[yz]:=TMC[C](C,T[yz](theta[1])); ##<<-- rotational
  symmetry in the yz-plane
  C_constants[C](TransIso[yz]);
```

$$TransIso_{yz} := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,2} & 0 & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & 0 & 0 & 0 \\ c_{1,2} & c_{2,3} & c_{2,2} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2}c_{2,2} - \frac{1}{2}c_{2,3} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{4,4} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 12.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 5.
```

```
>
```

Example 11: Isotropic materials have a **complete rotational symmetry.** As such their material constant matrices have **12 nonzero constants of which 2 are independent.**

```
> Isotropic:=TMC[C](C,T[xy](theta[3]),T[xz](theta[2]));
  C_constants[C](Isotropic);
```

$$Isotropic := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,2} & 0 & 0 & 0 \\ c_{1,2} & c_{1,1} & c_{1,2} & 0 & 0 & 0 \\ c_{1,2} & c_{1,2} & c_{1,1} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,2} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 12.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 2.
```

```
>
```

Subsection 2: Nonstandard Materials

In this subsection, we discuss only four nonstandard materials and compute for each their material constants matrix **C**.

1. Cubic Isotropic Crystals -- 12 nonzero constants, 3 independent (3 planes of reflective symmetry with respect to any three planes at any angles)

2. Tetragonal Crystals -- 12 nonzero constants, 6 independent (2 planes of symmetry) with planes of symmetry not orthogonal but rotated at quarter angles: Pi/4, 2*Pi/4, 3*Pi/4

Note: When the rotation is at 2*Pi/4 = Pi/2, then there are 12 nonzero constants and 9 independent constants.

3. Trigonal Crystals -- 18 nonzero constants, 6 independent (3 planes of symmetry) [close to orthotropic] planes of symmetry are not orthogonal but are rotated at "third angles": Pi/3, 2*Pi/3

4. Trigonal-Hexagonal Crystals -- 24 nonzero constants, 7 independent (3 planes of symmetry) [mixture of trigonal, orthotropic, and monoclinic]
planes of symmetry are not orthogonal but are rotated at "third angles": Pi/3, 2*Pi/3

>

Example 12: Cubic isotropic crystals -- 12 nonzero constants, 3 independent (3 planes of reflective symmetry with respect to any three planes at any angles)

```
> Theta[1],Theta[2]:=Pi/4,3*Pi/4; ##<<-- picking some angles
```

$$\Theta_1, \Theta_2 := \frac{\pi}{4}, \frac{3\,\pi}{4}$$

```
> nv1:=[0,cos(Theta[1]),sin(Theta[1])]; ##<<-- normal vector to
  plane P1
  nv2:=[0,cos(Theta[2]),sin(Theta[2])]; ##<<-- normal vector to
  plane P2
  nv3:=[cos(Theta[1]),sin(Theta[1]),0]; ##<<-- normal vector to
  plane P3
```

$$nv1 := \left[0, \frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right]$$

$$nv2 := \left[0, -\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right]$$

$$nv3 := \left[\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}, 0\right]$$

```
> Rv1:=RM(nv1); ##<<-- reflection matrix w.r.t. plane P1
  Rv2:=RM(nv2); ##<<-- reflection matrix w.r.t. plane P2
  Rv3:=RM(nv3); ##<<-- reflection matrix w.r.t. plane P3
```

$$Rv1 := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix}$$

$$Rv2 := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

$$Rv3 := \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

```
> CubicIsotropic:=TMC[C](C,Rv1,Rv2,Rv3);##<<-- all three reflections
  are needed
```

$$CubicIsotropic := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,2} & 0 & 0 & 0 \\ c_{1,2} & c_{1,1} & c_{1,2} & 0 & 0 & 0 \\ c_{1,2} & c_{1,2} & c_{1,1} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{4,4} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{4,4} \end{bmatrix}$$

```
> C_constants[C](CubicIsotropic);
Number of nonzero parameters in the material constants matrix C of the given symme
try is 12.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 3.
```

```
>
```

Comments: Cubic isotropic crystal has six plane symmetry: three reflections w.r.t. the coordinate planes and three reflections w.r.t. three planes at 45 degree angles to the coordinate planes. This is because of the atoms located at the centers of the faces.

```
>
```

Example 13: Tetragonal Crystals -- 12 nonzero constants, 6 independent (2 planes of symmetry) Planes of symmetry are not orthogonal but are rotated at quarter angles: Pi/4, 2*Pi/4, 3*Pi/4

Note: When the angle is 2*Pi/4 = Pi/2, then there are 12 nonzero constants among which 9 independent.

```
> nv1:=[0,0,1]:
> Tnv1:=ReflectionMatrix(nv1);     ##<<-- reflection with respect to
  the xy plane
```

$$Tnv1 := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

```
> MC1:=TMC[C](C,Tnv1);  ##<<-- first reflection is with respect to
  the xy plane
  C_constants[C](MC1);
```

$$MC1 := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & c_{1,4} & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & c_{2,4} & 0 & 0 \\ c_{1,3} & c_{2,3} & c_{3,3} & c_{3,4} & 0 & 0 \\ c_{1,4} & c_{2,4} & c_{3,4} & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & c_{5,6} \\ 0 & 0 & 0 & 0 & c_{5,6} & c_{6,6} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 20.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 13.
```

```
> nv2:=[0,sqrt(2)/2,sqrt(2)/2]; ##<<-- second reflection is with
  respect to a plane that makes Pi/4 angle with the xy plane
  Tnv2:=ReflectionMatrix(nv2);
  MC2:=TMC[C](MC1,Tnv2);
  C_constants[C](MC2);
```

$$nv2 := \left[0, \frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right]$$

$$Tnv2 := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix}$$

$$MC2 := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,2} & 0 & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & 0 & 0 & 0 \\ c_{1,2} & c_{2,3} & c_{2,2} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{4,4} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 12.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 6.
```

```
>
```

The above transformations can be accomplished with one invocation of the procedure **TMC**:

```
> Tetragonal:=TMC[C](C,Tnv2,Tnv1);
```

$$Tetragonal := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,2} & 0 & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & 0 & 0 & 0 \\ c_{1,2} & c_{2,3} & c_{2,2} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{4,4} \end{bmatrix}$$

```
> C_constants[C](Tetragonal);
```
```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 12.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 6.
```
```
>
```

As we see, there are 12 nonzero constants and 6 are independent in C.

However, when the angle between the planes is Pi/2 then we have **12 nonzero parameters among which 9 are independent:**

```
> nv2:=[0,1,0]; ##<<-- second reflection is with respect to a plane
  that makes Pi/2 angle with the xy plane
  Tnv2:=ReflectionMatrix(nv2);
  MC2:=TMC[C](MC1,Tnv2);
  C_constants[C](MC2);
```

$$nv2 := [0, 1, 0]$$

$$Tnv2 := \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$MC2 := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & 0 & 0 & 0 \\ c_{1,3} & c_{2,3} & c_{3,3} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{6,6} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 12.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 9.
```

```
> nv2:=[0,sqrt(2)/2,-sqrt(2)/2]; ##<<-- second reflection is with
  respect to a plane that makes 3*Pi/4 angle with the xy plane
  Tnv2:=ReflectionMatrix(nv2);
  MC2:=TMC[C](MC1,Tnv2);
  C_constants[C](MC2);
```

$$nv2 := \left[0, \frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}\right]$$

$$Tnv2 := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

$$MC2 := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,2} & 0 & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & 0 & 0 & 0 \\ c_{1,2} & c_{2,3} & c_{2,2} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{4,4} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 12.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 6.
```

>

As we see, there are 12 nonzero constants and 6 are independent in C.

>

Example 14: Trigonal Crystals -- 18 nonzero constants, 6 independent (3 planes of symmetry)

-- Planes of reflective symmetry are not orthogonal but are rotated at "third angles": Pi/3, 2*Pi/3.
-- The first plane can always be picked up to be one of the coordinate planes with the other two planes tilted to the first by Pi/3 and 2*Pi/3 angles, respectively.

There are six cases to consider:

A. First plane of reflective symmetry is the xz-plane while the other two planes are tilted.
(a) the x-axis is the common axis to all three planes:

```
> nv1:=[0,1,0];                          ##<<-- normal vector to plane
  P1
  nv2:=[0,cos(Pi/3),sin(Pi/3)];          ##<<-- normal vector to plane
  P2
  nv3:=[0,cos(2*Pi/3),sin(2*Pi/3)];      ##<<-- normal vector to plane
  P3
```

$$nv1 := [0, 1, 0]$$

$$nv2 := \left[0, \frac{1}{2}, \frac{\sqrt{3}}{2}\right]$$

$$nv3 := \left[0, \frac{-1}{2}, \frac{\sqrt{3}}{2}\right]$$

```
> Tnv1:=RM(nv1); ##<<-- reflection matrix w.r.t. plane P1
  Tnv2:=RM(nv2); ##<<-- reflection matrix w.r.t. plane P2
  Tnv3:=RM(nv3); ##<<-- reflection matrix w.r.t. plane P3
```

$$Tnv1 := \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$Tnv2 := \begin{bmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ 0 & -\frac{\sqrt{3}}{2} & \frac{-1}{2} \end{bmatrix}$$

$$Tnv3 := \begin{bmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} \\ 0 & \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{bmatrix}$$

```
> out6:=TMC[C](C,Tnv1);
  C_constants[C](out6);
```

$$out6 := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & 0 & c_{1,6} \\ c_{1,2} & c_{2,2} & c_{2,3} & 0 & 0 & c_{2,6} \\ c_{1,3} & c_{2,3} & c_{3,3} & 0 & 0 & c_{3,6} \\ 0 & 0 & 0 & c_{4,4} & c_{4,5} & 0 \\ 0 & 0 & 0 & c_{4,5} & c_{5,5} & 0 \\ c_{1,6} & c_{2,6} & c_{3,6} & 0 & 0 & c_{6,6} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 20.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 13.
```

```
> out7:=TMC[C](out6,Tnv2);
  C_constants[C](out7);
```

$$out7 := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,2} & 0 & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & 0 & 0 & c_{2,6} \\ c_{1,2} & c_{2,3} & c_{2,2} & 0 & 0 & -c_{2,6} \\ 0 & 0 & 0 & c_{4,4} & c_{2,6} & 0 \\ 0 & 0 & 0 & c_{2,6} & \frac{1}{2}c_{2,2} - \frac{1}{2}c_{2,3} & 0 \\ 0 & c_{2,6} & -c_{2,6} & 0 & 0 & c_{4,4} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 18.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 6.
```

```
> out8:=TMC[C](out7,Tnv3);
```

```
C_constants[C](out8);
```

$$out8 := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,2} & 0 & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & 0 & 0 & c_{2,6} \\ c_{1,2} & c_{2,3} & c_{2,2} & 0 & 0 & -c_{2,6} \\ 0 & 0 & 0 & c_{4,4} & c_{2,6} & 0 \\ 0 & 0 & 0 & c_{2,6} & \frac{1}{2}c_{2,2} - \frac{1}{2}c_{2,3} & 0 \\ 0 & c_{2,6} & -c_{2,6} & 0 & 0 & c_{4,4} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 18.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 6.
```

Note that **symmetries w.r.t. two of the planes P1 and P2 imply symmetry with respect to the third plane P3**. Thus, the material constants matrix **C** can be found by invoking the procedure **TMC** ones:

```
> TMC[C](C,Tnv1,Tnv2);
  C_constants[C](%);
```

$$\begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,2} & 0 & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & 0 & 0 & c_{2,6} \\ c_{1,2} & c_{2,3} & c_{2,2} & 0 & 0 & -c_{2,6} \\ 0 & 0 & 0 & c_{4,4} & c_{2,6} & 0 \\ 0 & 0 & 0 & c_{2,6} & \frac{1}{2}c_{2,2} - \frac{1}{2}c_{2,3} & 0 \\ 0 & c_{2,6} & -c_{2,6} & 0 & 0 & c_{4,4} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 18.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 6.
```

```
>
```

As we see, there are 18 nonzero constants and 6 are independent in C.

```
>
```

(b) the z-axis is the common axis to all three planes:

```
> nv1:=[0,1,0];                          ##<<-- normal vector to plane
  P1
  nv2:=[sin(Pi/3),cos(Pi/3),0];          ##<<-- normal vector to plane
  P2
  nv3:=[sin(2*Pi/3),cos(2*Pi/3),0];      ##<<-- normal vector to plane
  P3
```

$$nv1 := [0, 1, 0]$$

$$nv2 := \left[\frac{\sqrt{3}}{2}, \frac{1}{2}, 0\right]$$

$$nv3 := \left[\frac{\sqrt{3}}{2}, \frac{-1}{2}, 0\right]$$

```
> Tnv1:=RM(nv1); ##<<-- reflection matrix w.r.t. plane P1
  Tnv2:=RM(nv2); ##<<-- reflection matrix w.r.t. plane P2
  Tnv3:=RM(nv3); ##<<-- reflection matrix w.r.t. plane P3
```

$$Tnv1 := \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$Tnv2 := \begin{bmatrix} \frac{-1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$Tnv3 := \begin{bmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

```
> TMC[C](C,Tnv1,Tnv2);
  C_constants[C](%);
```

$$\begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & 0 & c_{1,6} \\ c_{1,2} & c_{1,1} & c_{1,3} & 0 & 0 & -c_{1,6} \\ c_{1,3} & c_{1,3} & c_{3,3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,2} & -c_{1,6} & 0 \\ 0 & 0 & 0 & -c_{1,6} & c_{5,5} & 0 \\ c_{1,6} & -c_{1,6} & 0 & 0 & 0 & c_{5,5} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 18.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 6.
```

```
>
```

As we see, there are 18 nonzero constants and 6 are independent in C.

```
>
```

B. First plane of reflective symmetry is the yz-plane, while the other two planes are tilted.

(a) the z-axis is the common axis to all three planes:

```
> nv1:=[1,0,0];                          ##<<-- normal vector to plane
  P1
  nv2:=[cos(Pi/3),sin(Pi/3),0];          ##<<-- normal vector to plane
  P2
  nv3:=[cos(2*Pi/3),sin(2*Pi/3),0];      ##<<-- normal vector to plane P3
```

$$nv1 := [1, 0, 0]$$

$$nv2 := \left[\frac{1}{2}, \frac{\sqrt{3}}{2}, 0\right]$$

$$nv3 := \left[\frac{-1}{2}, \frac{\sqrt{3}}{2}, 0\right]$$

```
> Tnv1:=RM(nv1);  ##<<-- reflection matrix w.r.t. plane P1
  Tnv2:=RM(nv2);  ##<<-- reflection matrix w.r.t. plane P2
  Tnv3:=RM(nv3);  ##<<-- reflection matrix w.r.t. plane P3
```

$$Tnv1 := \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$Tnv2 := \begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{-1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$Tnv3 := \begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

```
> TMC[C](C,Tnv1,Tnv2);
  C_constants[C](%);
```

$$\begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & c_{1,5} & 0 \\ c_{1,2} & c_{1,1} & c_{1,3} & 0 & -c_{1,5} & 0 \\ c_{1,3} & c_{1,3} & c_{3,3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,2} & 0 & c_{1,5} \\ c_{1,5} & -c_{1,5} & 0 & 0 & c_{5,5} & 0 \\ 0 & 0 & 0 & c_{1,5} & 0 & c_{5,5} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 18.
```

```
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 6.
```

```
>
```

(b) the y-axis is the common axis to all three planes:

```
> nv1:=[1,0,0];                          ##<<-- normal vector to plane
  P1
  nv2:=[cos(Pi/3),0,sin(Pi/3)];          ##<<-- normal vector to plane
  P2
  nv3:=[cos(2*Pi/3),0,sin(2*Pi/3)];      ##<<-- normal vector to plane P3
```

$$nv1 := [1, 0, 0]$$

$$nv2 := \left[\frac{1}{2}, 0, \frac{\sqrt{3}}{2}\right]$$

$$nv3 := \left[\frac{-1}{2}, 0, \frac{\sqrt{3}}{2}\right]$$

```
> Tnv1:=RM(nv1);  ##<<-- reflection matrix w.r.t. plane P1
  Tnv2:=RM(nv2);  ##<<-- reflection matrix w.r.t. plane P2
  Tnv3:=RM(nv3);  ##<<-- reflection matrix w.r.t. plane P3
```

$$Tnv1 := \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$Tnv2 := \begin{bmatrix} \frac{1}{2} & 0 & -\frac{\sqrt{3}}{2} \\ 0 & 1 & 0 \\ -\frac{\sqrt{3}}{2} & 0 & \frac{-1}{2} \end{bmatrix}$$

$$Tnv3 := \begin{bmatrix} \frac{1}{2} & 0 & \frac{\sqrt{3}}{2} \\ 0 & 1 & 0 \\ \frac{\sqrt{3}}{2} & 0 & \frac{-1}{2} \end{bmatrix}$$

```
> TMC[C](C,Tnv1,Tnv2);
  C_constants[C](%);
```

$$\begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & c_{1,5} & 0 \\ c_{1,2} & c_{2,2} & c_{1,2} & 0 & 0 & 0 \\ c_{1,3} & c_{1,2} & c_{1,1} & 0 & -c_{1,5} & 0 \\ 0 & 0 & 0 & c_{4,4} & 0 & c_{1,5} \\ c_{1,5} & 0 & -c_{1,5} & 0 & c_{4,4} & 0 \\ 0 & 0 & 0 & c_{1,5} & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,3} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 18.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 6.
```

```
>
```

C. First plane of reflective symmetry is the xy-plane, while the other two planes are tilted.

(a) the y-axis is the common axis to all three planes:

```
> nv1:=[0,0,1];                          ##<<-- normal vector to plane
  P1
  nv2:=[sin(Pi/3),0,cos(Pi/3)];          ##<<-- normal vector to plane
  P2
  nv3:=[sin(2*Pi/3),0,cos(2*Pi/3)];      ##<<-- normal vector to plane
  P3
```

$$nv1 := [0, 0, 1]$$

$$nv2 := \left[\frac{\sqrt{3}}{2}, 0, \frac{1}{2}\right]$$

$$nv3 := \left[\frac{\sqrt{3}}{2}, 0, \frac{-1}{2}\right]$$

```
> Tnv1:=RM(nv1); ##<<-- reflection matrix w.r.t. plane P1
  Tnv2:=RM(nv2); ##<<-- reflection matrix w.r.t. plane P2
  Tnv3:=RM(nv3); ##<<-- reflection matrix w.r.t. plane P3
```

$$Tnv1 := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$Tnv2 := \begin{bmatrix} \frac{-1}{2} & 0 & -\frac{\sqrt{3}}{2} \\ 0 & 1 & 0 \\ -\frac{\sqrt{3}}{2} & 0 & \frac{1}{2} \end{bmatrix}$$

$$Tnv3 := \begin{bmatrix} \frac{-1}{2} & 0 & \frac{\sqrt{3}}{2} \\ 0 & 1 & 0 \\ \frac{\sqrt{3}}{2} & 0 & \frac{1}{2} \end{bmatrix}$$

```
> TMC[C](C,Tnv1,Tnv2);
  C_constants[C](%);
```

$$\begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & c_{1,4} & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{1,2} & 0 & 0 & 0 \\ c_{1,3} & c_{1,2} & c_{1,1} & -c_{1,4} & 0 & 0 \\ c_{1,4} & 0 & -c_{1,4} & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{4,4} & -c_{1,4} \\ 0 & 0 & 0 & 0 & -c_{1,4} & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,3} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 18.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 6.
```

```
>
```

(b) the x-axis is the common axis to all three planes:

```
> nv1:=[0,0,1];                          ##<<-- normal vector to plane
  P1
  nv2:=[0,sin(Pi/3),cos(Pi/3)];          ##<<-- normal vector to plane
  P2
  nv3:=[0,sin(2*Pi/3),cos(2*Pi/3)];      ##<<-- normal vector to plane P3
```

$$nv1 := [0, 0, 1]$$

$$nv2 := \left[0, \frac{\sqrt{3}}{2}, \frac{1}{2}\right]$$

$$nv3 := \left[0, \frac{\sqrt{3}}{2}, \frac{-1}{2}\right]$$

```
> Tnv1:=RM(nv1);  ##<<-- reflection matrix w.r.t. plane P1
  Tnv2:=RM(nv2);  ##<<-- reflection matrix w.r.t. plane P2
  Tnv3:=RM(nv3);  ##<<-- reflection matrix w.r.t. plane P3
```

$$Tnv1 := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$Tnv2 := \begin{bmatrix} 1 & 0 & 0 \\ 0 & \frac{-1}{2} & -\frac{\sqrt{3}}{2} \\ 0 & -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix}$$

$$Tnv3 := \begin{bmatrix} 1 & 0 & 0 \\ 0 & \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ 0 & \frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix}$$

```
> TMC[C](C,Tnv1,Tnv2);
  C_constants[C](%);
```

$$\begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,2} & 0 & 0 & 0 \\ c_{1,2} & c_{2,2} & c_{2,3} & c_{2,4} & 0 & 0 \\ c_{1,2} & c_{2,3} & c_{2,2} & -c_{2,4} & 0 & 0 \\ 0 & c_{2,4} & -c_{2,4} & c_{4,4} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2}c_{2,2} - \frac{1}{2}c_{2,3} & -c_{2,4} \\ 0 & 0 & 0 & 0 & -c_{2,4} & c_{4,4} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 18.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 6.
```

```
>
```

Example 15: Trigonal-Hexagonal Crystals -- 12 nonzero constants, 5 independent (3 planes of symmetry) [mixture of trigonal, orthotropic, and monoclinic] planes of symmetry are not orthogonal but are rotated at "third angles": Pi/3, 2*Pi/3

```
> sixfoldrot:=T[xy](Pi/3);
```

$$sixfoldrot := \begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

```
> refl:=T[rxy];
```

$$refl := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

```
> out1:=TMC[C](C,sixfoldrot,refl);
```

```
C_constants[C](out1);
```

$$out1 := \begin{bmatrix} c_{1,1} & c_{1,2} & c_{1,3} & 0 & 0 & 0 \\ c_{1,2} & c_{1,1} & c_{1,3} & 0 & 0 & 0 \\ c_{1,3} & c_{1,3} & c_{3,3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}c_{1,1} - \frac{1}{2}c_{1,2} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{5,5} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{5,5} \end{bmatrix}$$

```
Number of nonzero parameters in the material constants matrix C of the given symme
try is 12.
Number of independent parameters in the material constants matrix C of the given s
ymmetry is 5.
```

>

Conclusions

--It would be interesting to connect the block-diagonal structure to irreducible inequivalent representations of the groups of symmetry of each material.
--It would be interesting to systematically apply theory of crystallographic groups in teaching about material properties.
--It would be interesting to extend this package to piezoelectric materials for which the strain-electric displacement constitutive equation in matrix form involves a 9 x 9 matrix.

References

[1] T. Janssen, "Crystallographic Groups", North-Holland/American Elsevier, New York, 1973
[2] A. Erturk and D. J. Inman, "Piezoelectric Energy Harvesting", Appendix A, 1st ed., John Wiley and Sons, Ltd. 2011

>

>

Cookeville, January 19, 2015