# NIELINIOWA OPTYKA MOLEKULARNA

## chapter 1

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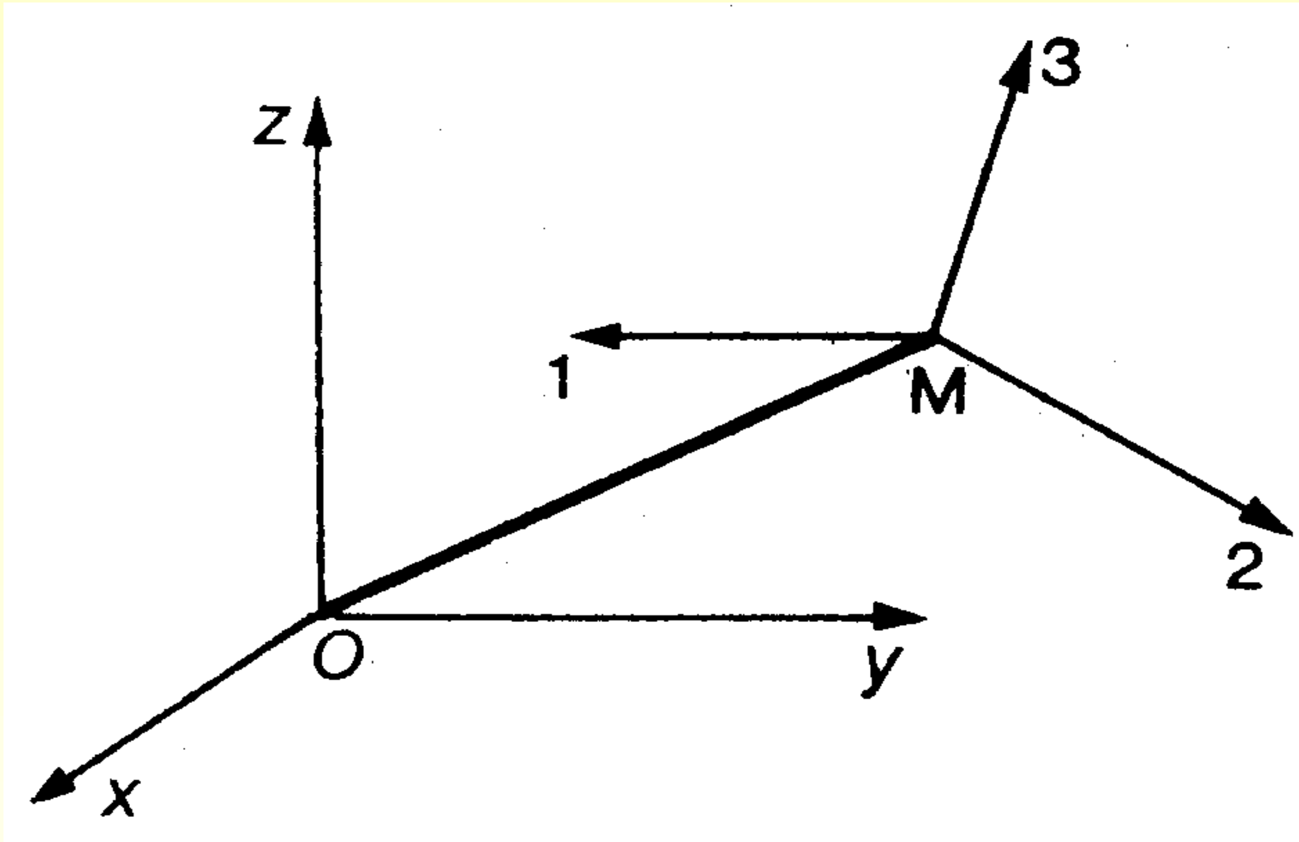
# ELEMENTS OF THE VECTOR AND TENSOR ANALYSIS

## Reference frames

The spatial properties of material systems usually are described three-fold Euclidean space. In order to describe the physical phenomena going in space the appropriate reference frame must be chosen. In principle this choice is arbitrary and we select it in such a way that the physical process is described univocally and the most conveniently. Generally it is convenient, in Euclidean space, to deal with the rectangular Cartesian reference frame. The Cartesian reference frame Oxyz connected with the quiescent material system we call the nieruchomy? reference frame and/or the laboratory frame whereas the frame M123 connected to the microsystem (atom or molecule) of this material system we call the moving system and/or the molecular system. We will use only the right angle reference systems (the direction of $Oz$ in connection to directions $Ox$ and $Oy$ defines regula sruby prawoskretnej.) The components of a point in the quiescent frame $Oxyz$ we denote by $x_i$ where latin index $i$ called the free index runs through $x, y, z$. Similarly in the molecular frame M123 the components of a point read $x_1, x_2, x_3$ or briefly $x_\alpha$, where the greek symbol $\alpha$ runs over the values 1,2,3.

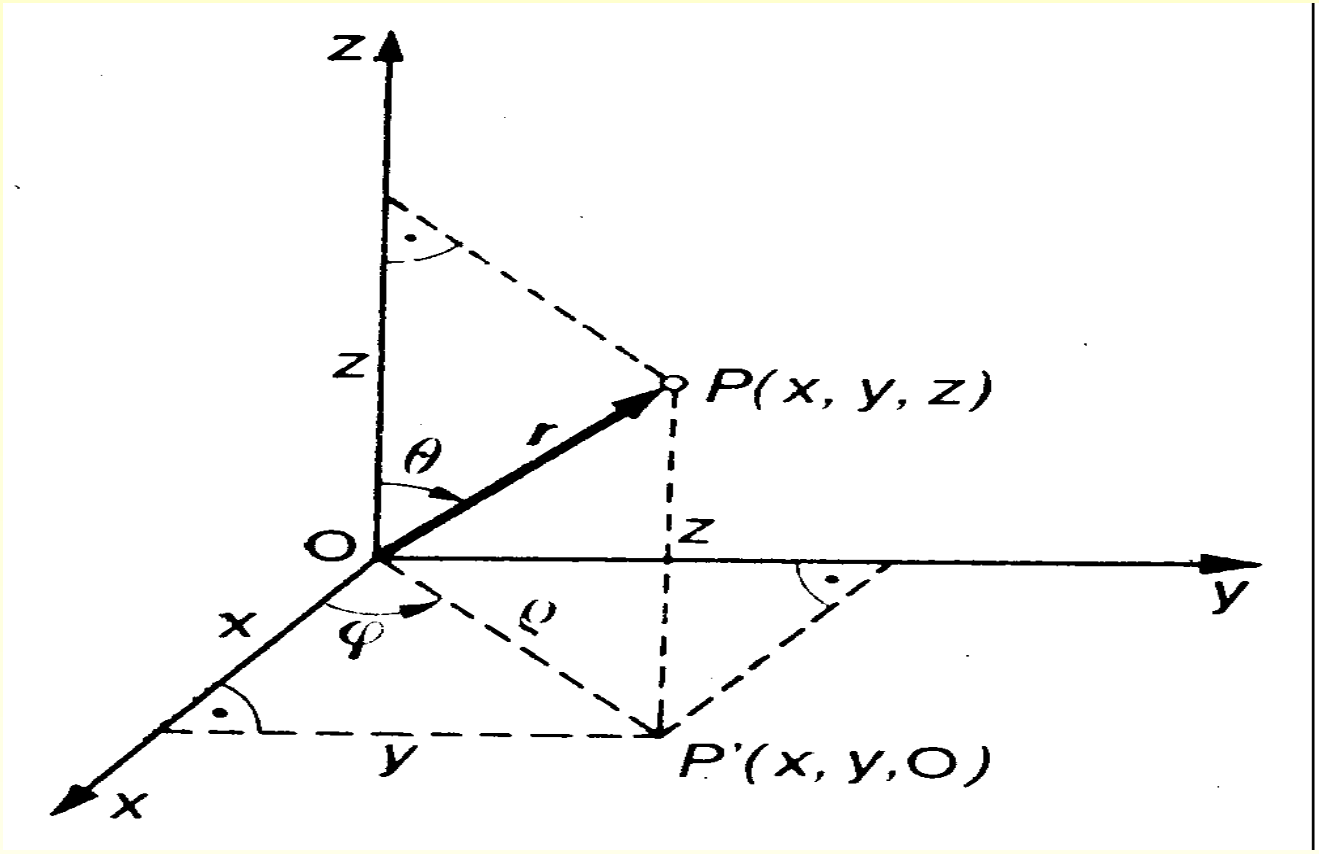



Rysunek 1: The laboratory reference frame XYZ versus the molecular reference frame 123

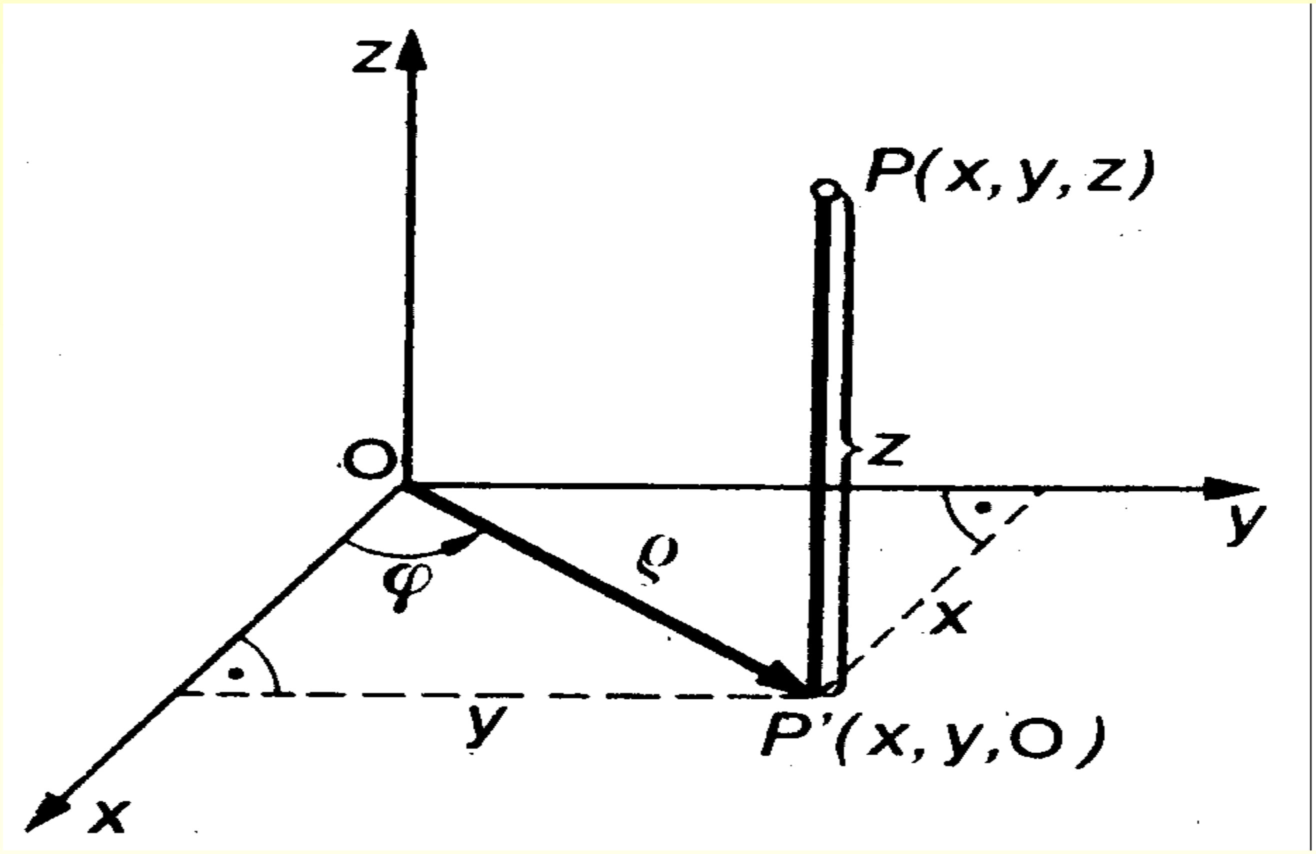
## Vector calculus

Physical properties which magnitude is given completely by the real number we named the scalar quantities or shortly scalars. The examples of scalar values are: mass, temperature, volume, potential, energy.

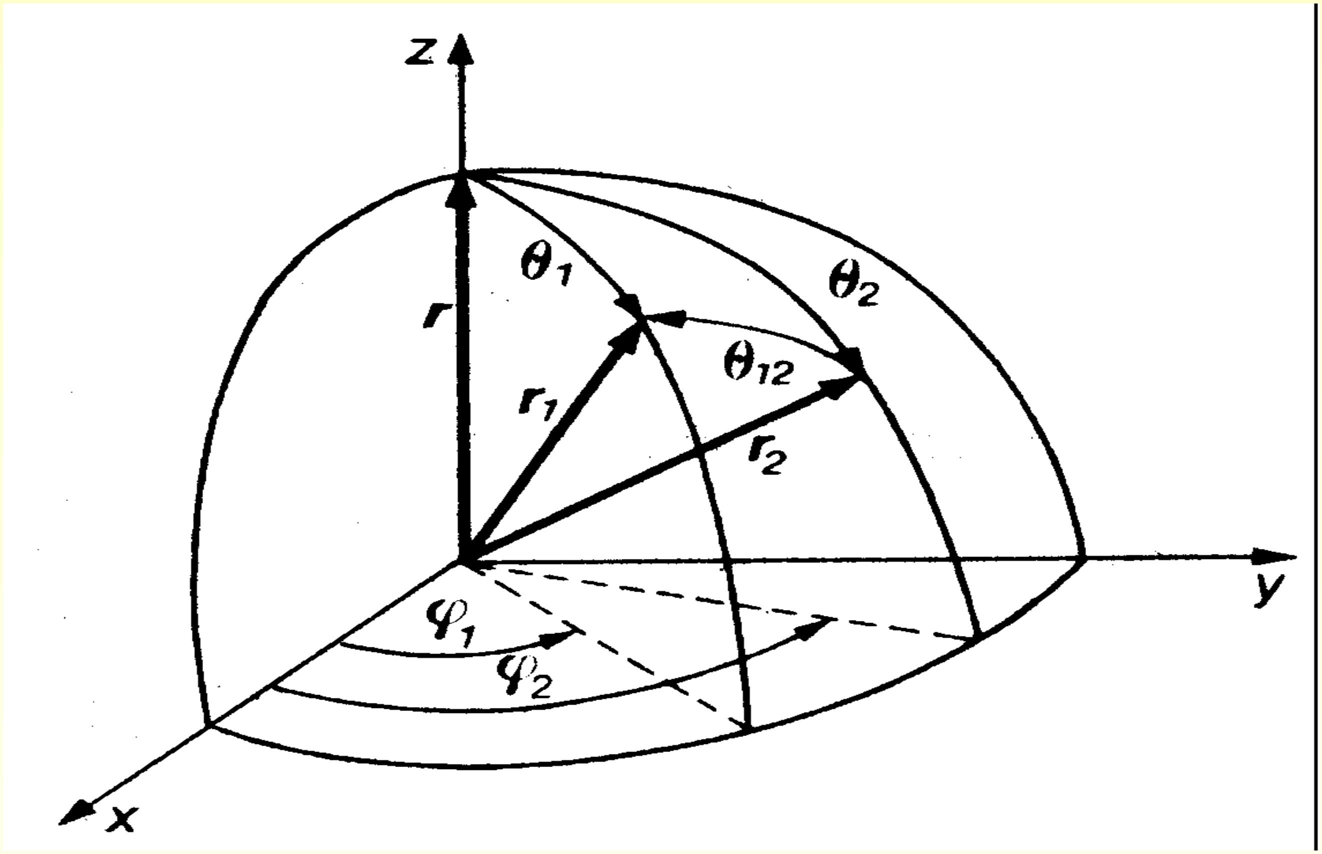
In physics occur also the vector values.



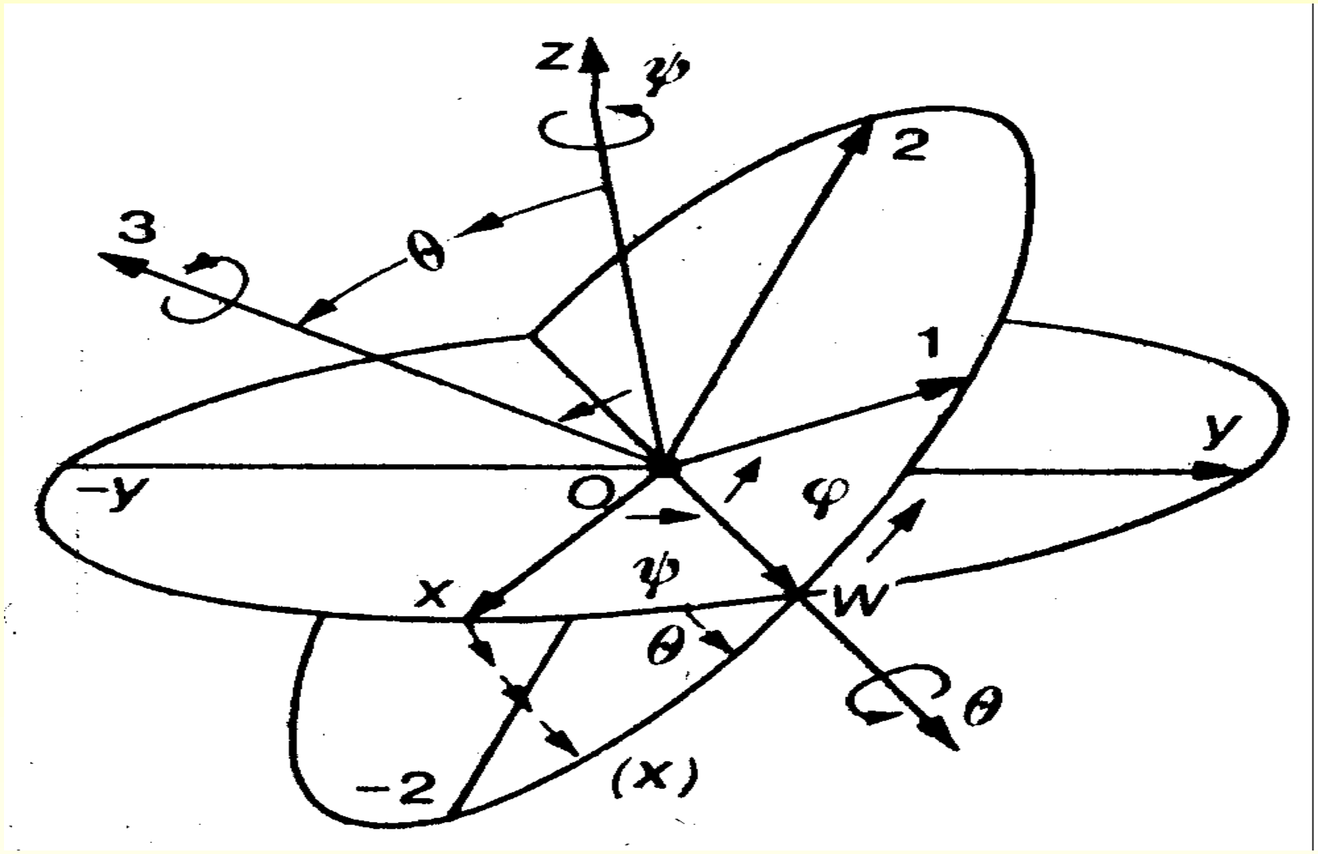

Rysunek 2: A spherical reference frame




Rysunek 3: A cylindrical reference frame




Rysunek 4: The angle between vectors $\mathbf{r}_1$ and $\mathbf{r}_2$




Rysunek 5: The Eulers's angles

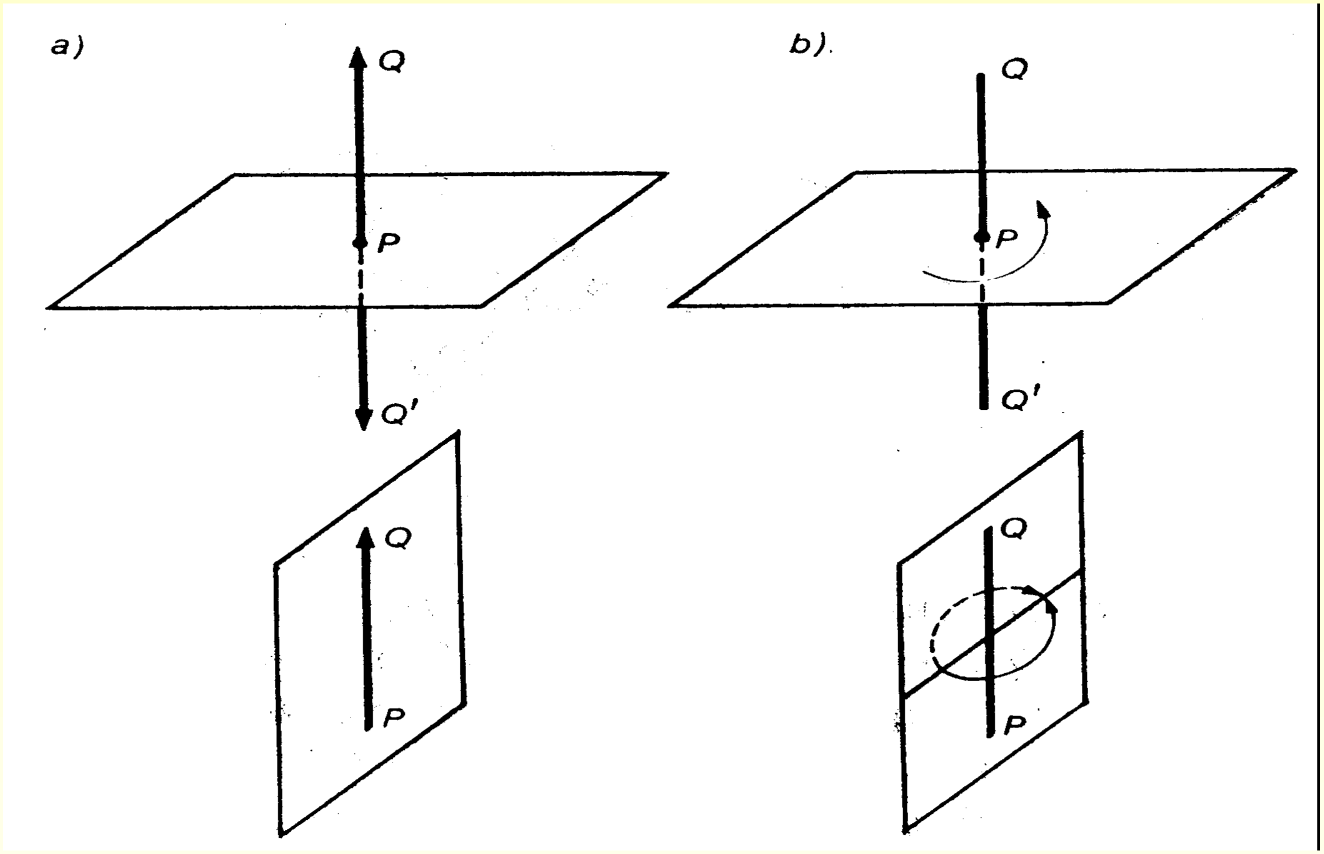
## Cartesian tensors

In physics beside scalars and vectors we use tensor quantities. The scalar is the zero order (rank) [a] tensor. We denote it by $T^{(0)}$. Previously described vector quantities we name the first rank tensors $T^{(1)}$ and as we have shown they are fully described by their components $T_x, T_y, T_z$ along axes $Ox, Oy, Oz$ of a selected Cartesian reference frame. In index (or tensor) notation the first rank tensor we denote by $T_i$, where the free index runs over $x, y, z$. In the matrix notation the first rank tensor we write in the form of

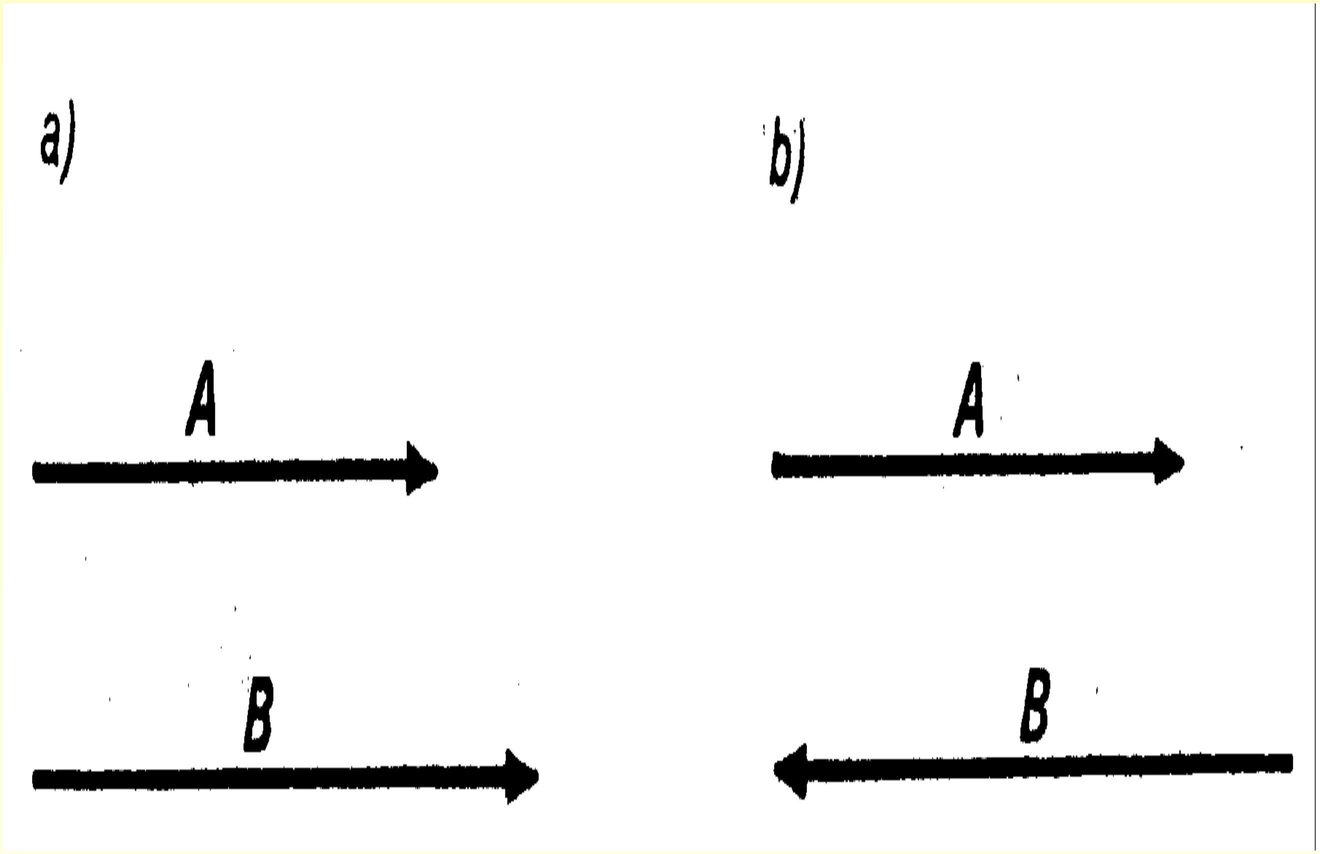
[a] We use expression tensor's rank instead of order since the word order we will use to subsequent terms of the perturbation calculus

one column (or one row) symbol

$$(T_i) = \begin{pmatrix} T_x \\ T_y \\ T_z \end{pmatrix} = (T_x \, T_y \, T_z) \tag{1}$$



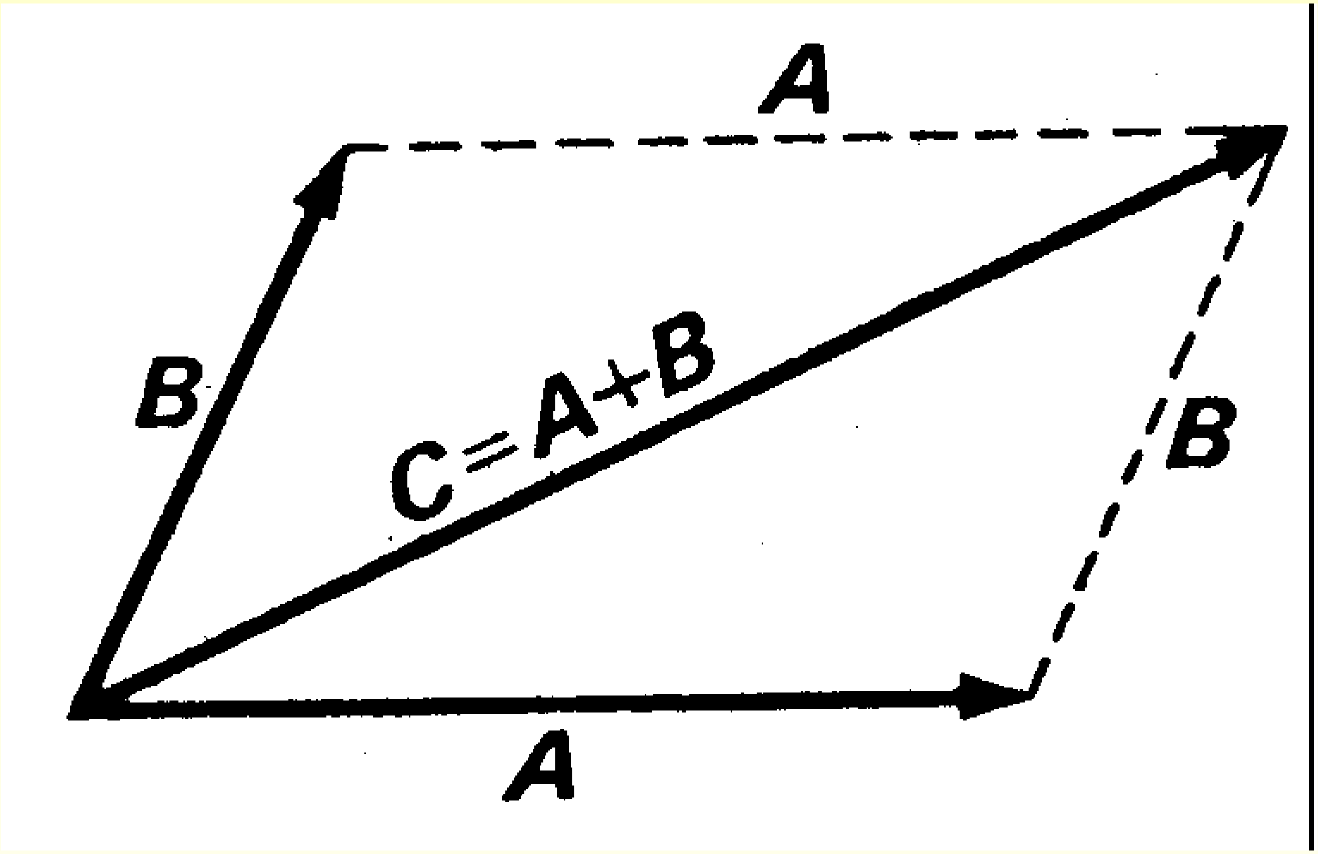

Rysunek 6: Polar and axial vectors



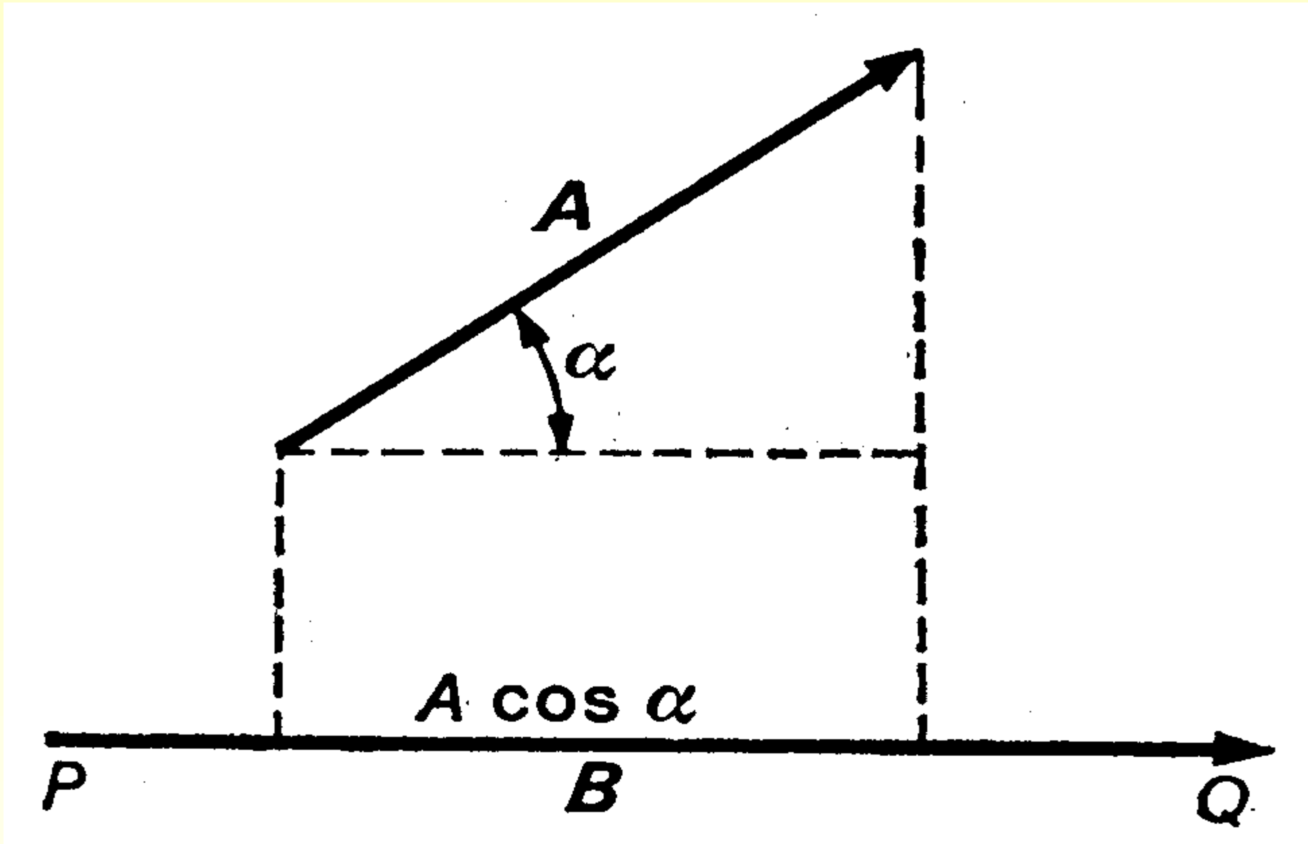

Rysunek 7: Colinear and anticolinear vectors

The second rank tensor $T^{(2)}$ we denote by the symbol $T_{ij}$ with two lower subscripts $i, j$. In the matrix form it reads

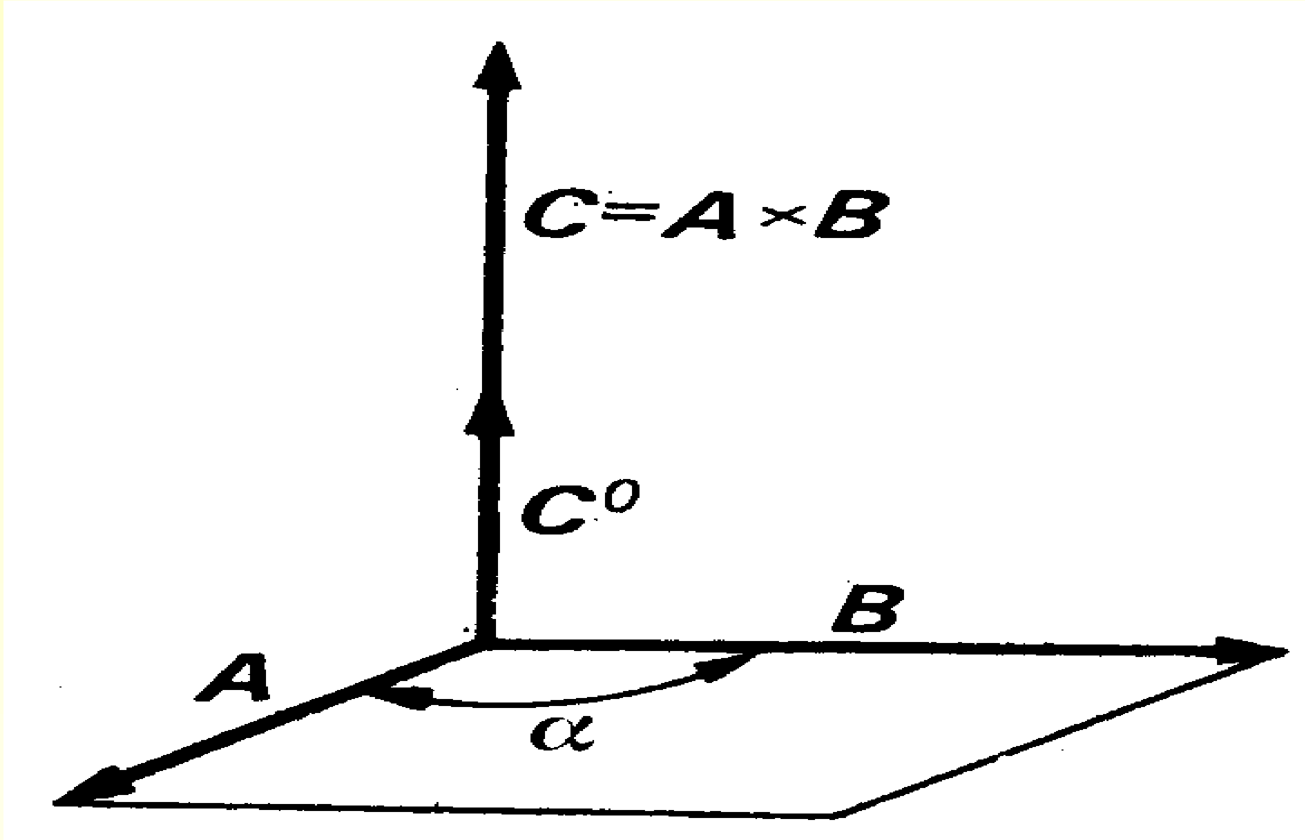
$$(T_{ij}) = \begin{pmatrix} T_{xx} & T_{xy} & T_{xz} \\ T_{yx} & T_{yy} & T_{yz} \\ T_{zx} & T_{zy} & T_{zz} \end{pmatrix} \tag{2}$$



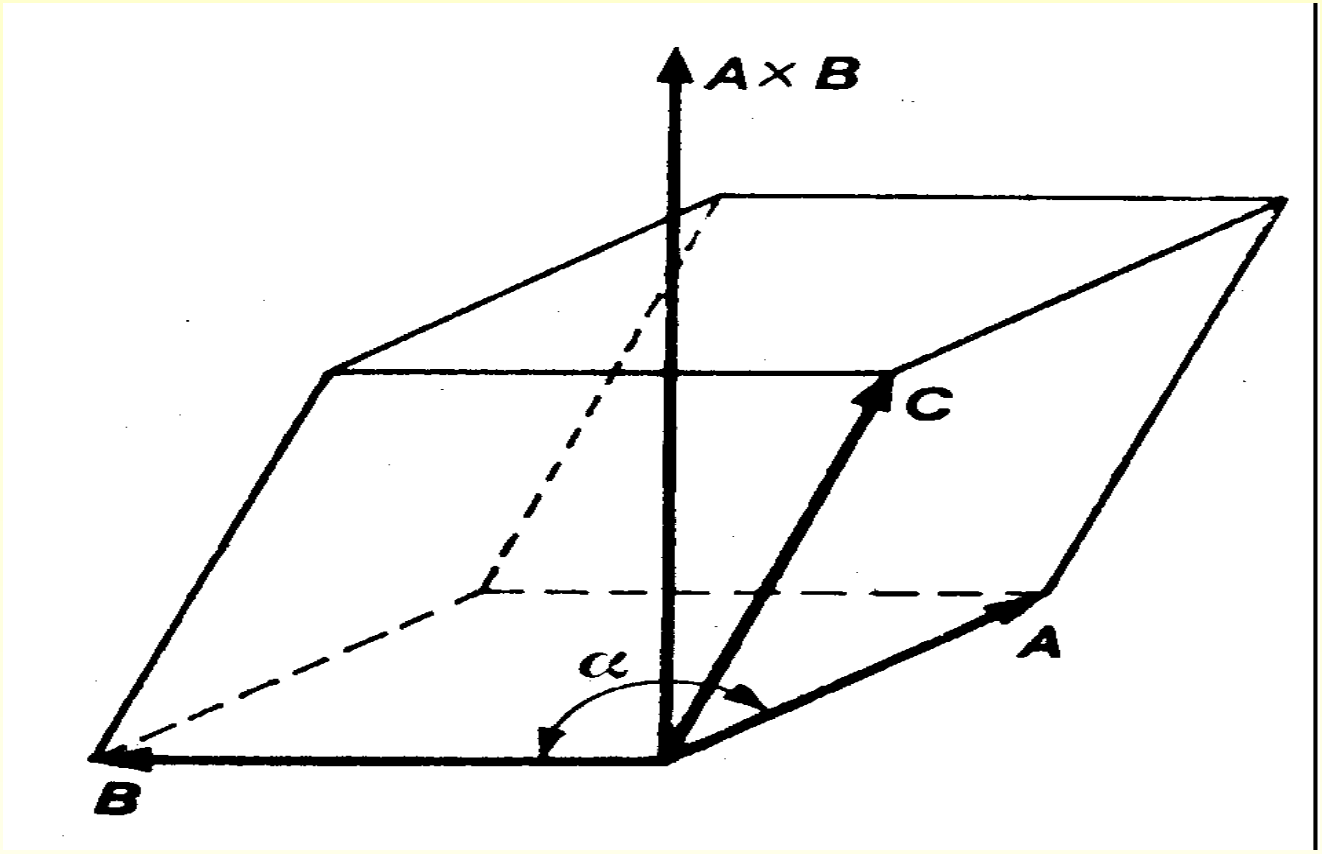

Rysunek 8: The sum of vectors



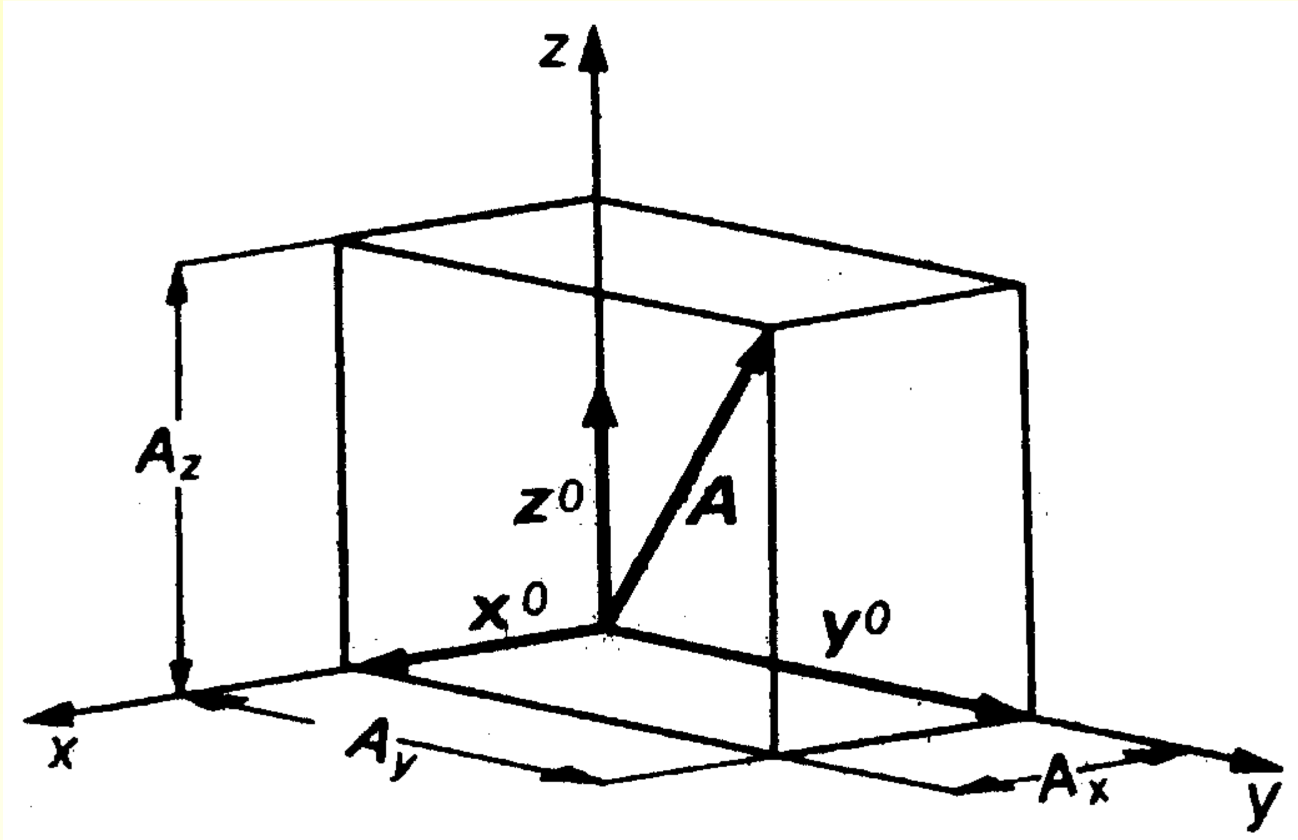

Rysunek 9: The projection of vector **A** on vector **B**




Rysunek 10: Multiplication of vectors **A** and **B**




Rysunek 11: The mixed multiplication of vectors bf A, **B** and **C**



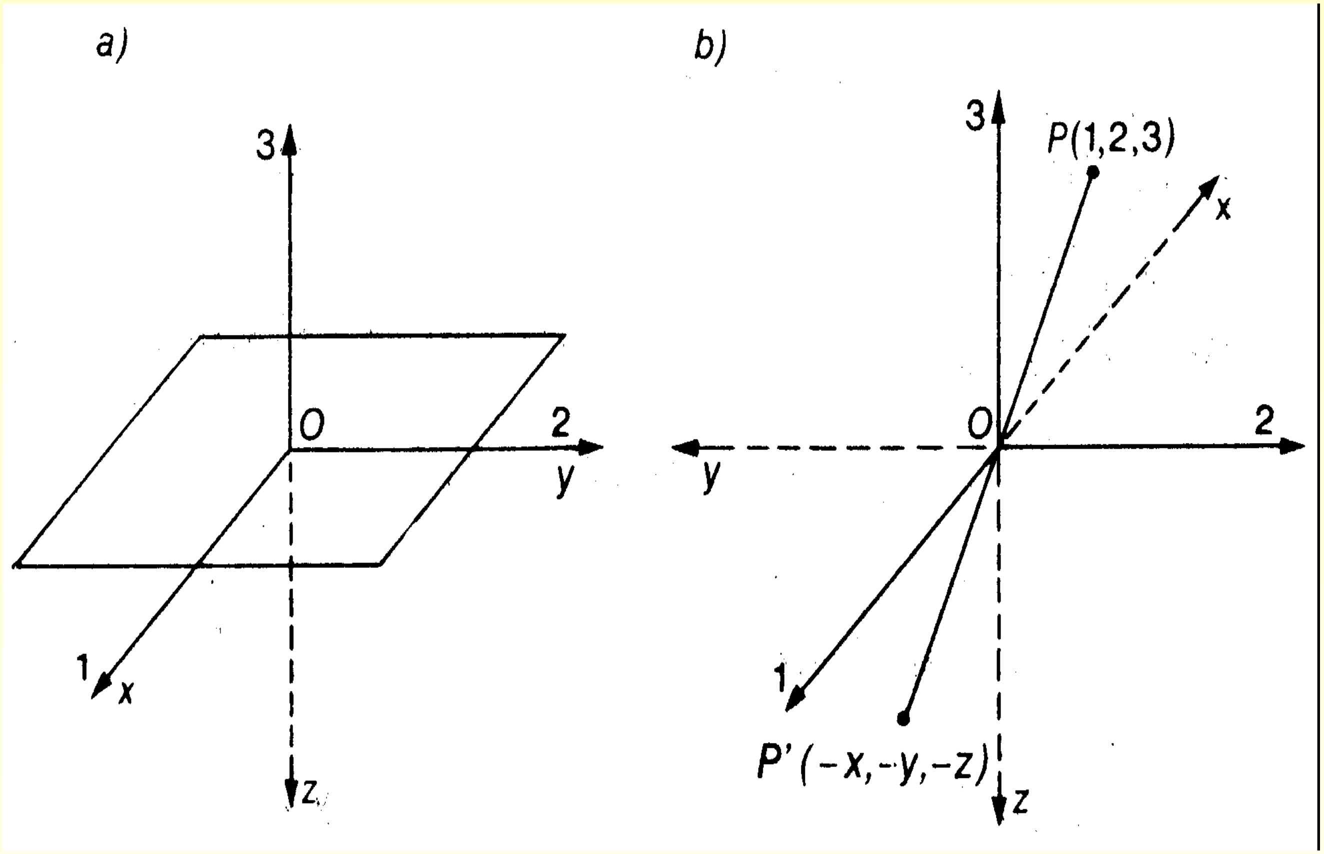

Rysunek 12: The vector **A** in Cartesian reference frame

The examples of the second rank tensors are: respectively the electric and magnetic primitivity tensors $\epsilon_{ij}$ and $\mu_{ij}$, the linear electric polarizability tensor $a_{ij}$. Among the third rank tensors we have: piezoelectric tensor $t_{ijk}$, the nonlinear polarizability (hyperpolarizability) tensor $B_{ijk}$ etc.

## Properties of second rank tensors

We discuss the transformation properties of tensor components between two different reference frames. We define the first rank tensor (the polar vector) as the quantity having, in respect to the frame $Ox_i$ three components $T_i$, Eq.(1), transforming between laboratory and molecular reference frames according to

$$T_i = c_{i\alpha} T_\alpha \tag{3}$$




Rysunek 13: Transformation of vectors

In a similar way we define the second rank tensor as the quantity having, in respect to the reference frame $x_i$, 9 components, Eq.(2), transforming in the following way

$$T_{ij} = c_{i\alpha}\, c_{j\beta}\, T_{\alpha\beta} \tag{4}$$

Let us remind that the indices $i$ and $j$ are free ones whereas the indices $\alpha$ and $\beta$ are the connected ones and we perform, according to the Einstein convention, summation over the connected indices. Then we transform Eq.(4) into its expanded form

$$\begin{aligned} T_{ij} &= c_{i1}\, c_{j1}\, T_{11} + c_{i1}\, c_{j2}\, T_{12} + c_{i1}\, c_{j3}\, T_{13} + c_{i2}\, c_{j1}\, T_{21} \\ &+ c_{i2}\, c_{j2}\, T_{22} + c_{i2}\, c_{j3}\, T_{23} + c_{i3}\, c_{j1}\, T_{31} + c_{i3}\, c_{j2}\, T_{32} + c_{i3}\, c_j \end{aligned}$$

Having in mind that for each pair of indices $i, j$ both running over $x, y, z$ we obtain one equation, then finally we have 9 equations with 9 components each. With this example we can see the advantages of the tensor techniques being simultaneously simple, compact and clear.

The inverse transformation of the second rank tensor from molecular to laboratory reference system reads

$$T_{\alpha\beta} = c_{\alpha i}\, c_{\beta j}\, T_{ij} \tag{6}$$

## Tensor addition

We can add or substrate only tensors of the same rank and of the same indices and defined in at the same point and the same reference frame. By the sum two tensors $A_{ij}$ and $B_{ij}$ we mean the third tensor $C_{ij}$ which components are the sums of the respective adding tensors

$$C_{ij} = A_{ij} + B_{ij} \tag{7}$$

The tensor is symmetric when

$$S_{ij} = S_{ji} \tag{8}$$

and is antisymmetic if

$$A_{ij} = -A_{ji} \tag{9}$$

The symmetry and antisymmetry properties of the tensor are the reference frame independent. Each tensor of the second rank $T_{ij}$ we be univocally divided as a sum of the symmetric $S_{ij}$ and antisymmetric $A_{ij}$ tensors

$$T_{ij} = S_{ij} + A_{ij} \tag{10}$$

where

$$S_{ij} = \frac{1}{2}\left(T_{ij} + T_{ij}\right) \tag{11}$$

is the symmetric tensor, and

$$A_{ij} = \frac{1}{2}\left(T_{ij} - T_{ij}\right) \tag{12}$$

stands for the antisymmetric tensor.

According to Eqs (11) and (12) the symmetric tensor in three dimensional space posses 6 independent components: 3 diagonal components $S_{xx}, S_{yy}, S_{zz}$ and three off diagonal components $S_{xy} = S_{yx}, S_{yz} = S_{zy}, S_{zx} = S_{xz}$. The $S_{ij}$ tensor can be written in the form of the diagonally symmetric matrix

$$(S_{ij}) = \begin{pmatrix} S_{xx} & S_{xy} & S_{xz} \\ S_{xy} & S_{yy} & S_{yz} \\ S_{xz} & S_{yz} & S_{zz} \end{pmatrix} \tag{13}$$

The Kronecker delta, $\delta_{ij}$, tensor serves as an example of the symmetric tensor which we write in the form of the unit matrix form

$$(\delta_{ij}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{14}$$

The antisymmetric tensor, in the Cartesian space, posses only 3 off diagonal components: $A_{xy} = -A_{yx}, A_{yz} = -A_{zy}, A_{zx} = -A_{xz}$ since according to Eq(12) the diagonal components vanish. In the matix form we write the antisymmetric tensor in the following form

$$(A_{ij}) = \begin{pmatrix} 0 & A_{xy} & A_{xz} \\ -A_{xy} & 0 & A_{yz} \\ -A_{xz} & -A_{yz} & 0 \end{pmatrix} \tag{15}$$

## Contraction of tensors

In tensor calculus we often use the operation of contraction of a tensor. In this way we obtain a new tensor with its rank lowered by two to the origin tensor rank. This operation is of a specific tensorial character and has no equivalence in other arithmetic operations. The contraction consists in the summation over the pair of selected tensor indices. E.g. when within in the third rank tensor $T_{ijk}$ we sum over the indices $j$ and $k$ the new first rank tensor $T_{ijj}$ will result. In a similar way by contraction of its indices from the second rank tensor $T_{ij}$ we obtain the zero rank tensor–in other words scalar. In the case of the higher rank tensors contraction can be done several times (manifolds?). When in the $n-th$ rank tensor the contraction is performed p–times as a result we obtain the tensor of the rank lowered by $2p$

$$T^{(n)} \stackrel{n-fold\, contraction}{\longrightarrow} T^{(n-2)} \tag{16}$$

Now we are in a position to give the definition of the n-th rank tensor in the d-fold space. By this tensor we understand the set of $d^n$ components $T_{\alpha_1,...,\alpha_n}, (\alpha_n = 1.2, 3, ..., d)$ connected to the Cartesian reference sets in the way that by changing the set they transform by the rule given by Eq(**??**).

## Contraction of the product of tensors

With the use of the unit Kronecker tensor $\delta_{ij}$ in its matrix form, Eq.(**??**), we easily note that the one-fold contraction is equivalent to multiplying of the tensor by the unit tensor $\delta_{ij}$

$$\begin{aligned} T_{ij}\,\delta_{ij} &= T_{ii} \quad (\text{scalar}) \\ T_{ijk}\,\delta_{jk} &= T_{ijj} \quad (\text{vector}) \\ T_{ijkl}\,\delta_{kl} &= T_{ijkk} \quad (\text{second rank tensor}) \\ T_{ijkl}\,\delta_{ij}\,\delta_{kl} &= T_{iijj} \quad (\text{scalar}) \end{aligned} \tag{17}$$

We carry on contraction not only on tensors but also on products of tensors. E.g. let us take into account the second rank tensor $T_{ij}$ and the third rank tensor $T_{ijk}$; the product $T_{ij}\,Tklm$ is the fifth rank tensor. When now we carry on the contraction over pair of indices, let's say $j$ and $m$ we obtain the third rank tensor

$$T_{ij}\,T_{klm}\,\delta_{jm} = T_{ij}\,T_{klj} = ?T_{ikl} \tag{18}$$

The above process we call the contraction of the product of tensors $T_{ij}$ and $T_{klm}$ over the indices $j$ and $m$.
In the general case when we have the product of the tensors of ranks $r$ and $s$ $T^{(r)}\,T^{(s)} = T_{i_1,\dots,i_r}\,T_{k_1,\dots,k_s}$ than by one–fold contraction over arbitrary pair of indices we obtain the new tensor of the rank $r+s-2$. Generally a tensor of the rank $r+s$ over the p–fold contraction gives the new tensor of the rank $r+s-2\,p$

$$T^{(r)}\,T^{(s)} \ \overset{p-fold\, contraction}{\longrightarrow}\ T^{(r+s-2\,p)} \tag{19}$$

The product of the type of Eq.(18) based on the combination of the external tensor product and contraction we sometimes call the internal tensor product.

## The trace of tensor

Using ono–fold, two–fold etc. contraction of the tensor of a given rank leads to tensor invariants or tensor traces, e.g.

$$\begin{aligned} \mathrm{Tr}(T_{ij}) &= T_{ij}\,\delta_{ij} = T_{ii} \\ \mathrm{Tr}(T_{ijkl}) &= T_{iijj} \quad etc \end{aligned} \tag{20}$$

In particular the trace of the unit Kronecker tensor is 3.

$$\mathrm{Tr}(\delta_{ij}) = \delta_{ij}\,\delta_{ij} = \delta_{11} + \delta_{22} + \delta_{33} \tag{21}$$

Let's focus of our attention on another property of the unit Kronecker tensor $\delta_{ij}$, which we call the property of replacement (substitution) of indices

$$
\begin{aligned}
T_i\,\delta_{ij} &= T_j, \quad T_{ij}\,\delta_{jk} = T_{ik} \\
T_{ijk}\,\delta_{kl} &= T_{ijl} \\
\delta_{ij}\,\delta_{jk} &= \delta_{ik}, \quad etc.
\end{aligned} \tag{22}
$$

where in the process of calculating the product of $T_i$ and $\delta_{ij}$ the index $i$ has been substituted by the index $j$.

The symmetric second rank tensor, Eq.(11), can be written in the form of a sum

$$
S_{ij} = K_{ij} + D_{ij} \tag{23}
$$

where

$$
K_{ij} = \frac{1}{3}\,S_{kk}\,\delta_{ij} \tag{24}
$$

is the spherical tensor or the isotropic tensor given by the trace of the symmetric tensor $S_{kk} = rmTr(S_{kl})$ and the unit tensor $\delta_{ij}$, whereas the tensor

$$D_{ij}\, S_{ij} - \frac{1}{3}\, S_{kk}\, \delta_{ij} \tag{25}$$

we call the deviator or anisotropic tensor. We can easily prove that the trace of the anisotropic tensor vanishes

$$\mathrm{Tr}\, D_{ij} = D_{ii} = 0 \tag{26}$$

since the trace $\mathrm{Tr}\, \delta_{ij} = \delta_{ii} = 3$.

## Symmetrization of tensors

Previously we have shown that the symmetric part of the second rank tensor can be written in the form of Eq.(11). We note that it is the arithmetic mean value of the tensors $T_{ij}$ and $T_{ji}$ resultintg from two possible interchange of the indices $i$ and $j$. This symmetrization operation we can extend to the tensor of an arbitrary rank and in respect to all its indices as well as to some selected group of indices. When we intend to symmetrize the tensor in respect to $s$ its indices then we perform $s!$ their permutations and next we take the arthmetic average of all the tensors obtained in this way. When the indices under symmetrization form a compact group then the result of the symmetrization we write in the round parenthesis, e.g. $(ijk)$. In the other case we can use the symbol $(ij|kl|m)$, where the indices between the vertical lines are exempted from the symmetrization. In the case of the second rank tensor, $s = 2$, the symmetrization is given by Eq.(11), whereas in the case of the third rank tensor the symmetrization process in respect to the indices $j$ and $k$ reads

$$T_{i(jk)} = \frac{1}{2}\left(T_{ijk} + T_{ikj}\right) \tag{27}$$

When we intend to symmetrize the third rank tensor over its all three indices, $s = 3$, then we have $3! = 6$ permutations and then instead of Eq.(27) we obtian

$$T_{(ijk)} = \frac{1}{6}\left(T_{ijk} + T_{jki} + T_{kij} + T_{jik} + T_{ikj} + T_{kji}\right) \tag{28}$$

In a similar way we perform the symmetrization over arbitrary number of indices in result obtaining the symmetric tensor over the indices active in a process of symmetrization.

We call the tensor the totally symmetric or just symmetric according to some number of its indices when it does not change within these indices interchange.

## Antisymmetrization (alternation) of tensors

In the case of the second rank tensor the result of its antisymmetrization is given by Eq.(12). The process of antisymmetrization of a tensor in respect to its $s$ indices goes in the following way: we perform $s!$ permutations on these indices and in the case of even (cyclic) permutations we leave the sign of the tensor unchanged whereas in the case of odd permutations we change its sign. Finally we calculate the mean arthmetic value over all $s!$ terms. Usually the indices involed in the antisymmetrization process we write in the square parenthesis [...]. For $s = 3$ the antisymmetrization of the third rank tensor $T_{ijk}$ gives

$$T_{[ijk]} = \frac{1}{6}\left(T_{ijk} + T_{jki} + T_{kij} - T_{jik} - T_{kji} - T_{ikj}\right) \quad (29)$$

We call the tensor antisymmetric in respect to some indices when it changes the sign after the interchange of an arbitrary pair of these indices (then it changes the sign with respect to the odd number of their permutations and leaves the sign unchanged to even number of permutations). According to these properties for the antisymmetric second rank tensor we have

$$A_{ij} = -A_{ji} \tag{30}$$

whereas for the third rand tensor we obtain

$$A_{ijk} = -A_{jik} = A_{jki} = -A_{kij} = A_{kij} = -A_{ikj} \tag{31}$$

It is easy to note the the trace of the second rank tensor vanishs

$$\mathrm{Tr}\,(A_{ij}) = A_{ij}\,\delta_{ij} = A_{ii} = 0 \tag{32}$$

We can separate the tensor on its symmetric and antisymmetric part, e.g. for the second rank tensor we have

$$T_{ij} = S_{ij} + A_{ij} = T_{(ij)} + T_{[ij]} \tag{33}$$

In a similar way we separate the third rank tensor

$$T_{ijk} = T_{(ijk)} + T_{[ijk]} + \frac{2}{3}\left(T_{[ij]k} + T_{[kj]i}\right) + \frac{2}{3}\left(T_{(ij)k} - T_{k(ji)}\right) \tag{34}$$