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Relationships between some rotation descriptions for molecular replacement procedure

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The final purpose of the molecular replacement method (Rossmann & Blow, 1962; Crowther & Blow, 1967; Rossmann, 1990; Rossmann & Arnold, 1993; and references therein) is to find the position of a given search model in a given crystal. Another meaning of the term "molecular replacement", as a procedure to improve density distribution by averaging through non-crystallographic symmetry, is also widely used, however, to avoid any misleading, is not considered further in these notes. The search of the internal crystal symmetry (self-rotation analysis) as a tool to improve a molecular image is not considered here either.

A search atomic model is defined by a set of three-dimensional coordinates given in some *absolute* or *external* Cartesian coordinate system. The result of the molecular replacement search is a transformation which should be applied to these coordinates. The transformation can always be presented as a rotation plus a translation.

There is a number of different descriptions of rotations in three-dimensional space reflecting point of view of different authors. These variants differ by the definition of :

- a) the rotating object (body or coordinate system),
- b) direction of the rotation (clockwise or counter-clockwise, and how "clockwise" is defined),
- c) type of angles (Eulerian or polar),
- d) choice of parameters inside a given type of angles.

This variety is reasonable since different descriptions are convenient in different situations. Unfortunately, this very rich choice does not allow an easy understanding for users of different programs. Any of these definitions is easily used inside one program but their exact understanding is necessary when trying to compare the results of different programs. Actually, what the majority of crystallographers needs is simply to have *a rotation matrix, R, which should be applied to the coordinates of the model* to place it in the unit cell as the rotation function suggests. However, these matrices are not always derived explicitly while a large variety of options (a)-(d) are used in different programs and articles.

The program CONVROT is developed which calculates the rotation matrix for different types of rotation description and *vice versa*. Such approach solves two problems. First, it gives directly a rotation matrix which can be applied to the model coordinates in order to obtain a model orientation accordingly to the molecular replacement solution. Secondly, it allows to recalculate the rotational angles from any to any of these systems by use of 2N subroutines and not N*N, where N is the number of different rotation systems : N subroutines to go from rotation angles to the rotation matrix and N - for opposite operations. This also allows easy addition of any new rotation system.

The program can define all symmetry related rotation angles for a given one when the orthogonalisation agreement and the symmetry operations are known.

The program can work with the polar systems introduced by Rossmann & Blow (1962), Dodson et al. (1966), Crowther (1972, 1973) and the eulerian angles systems introduced by Rossmann & Blow (1962), Nordman (1966), Huber (1969), Crowther (1972, 1973), Lattman (1972), Navaza (1994). The system of direction cosines is also used (see, for example, Diamond, 1993). These system are used, in particular, in ALMN (Crowther, 1973; CCP4, 1994), in PROTEIN (Steigemann, 1974), in MERLOT (Fitzgerald, 1988), in X-PLOR (Brünger, 1992) and in AMoRe (Navaza, 1994).

Tables 1-2 give some basic formulae used by the program, the singular cases are not included. Table 1 uses the following notation:

$$\begin{array}{l}
 \text{RZ}(\xi) = \begin{array}{|c|c|c|c|} \hline \cos\xi & -\sin\xi & 0 & \\ \hline \sin\xi & \cos\xi & 0 & \\ \hline 0 & 0 & 1 & \\ \hline \end{array} \\
 \\
 \text{RY}(\xi) = \begin{array}{|c|c|c|c|} \hline \cos\xi & 0 & \sin\xi & \\ \hline 0 & 1 & 0 & \\ \hline -\sin\xi & 0 & \cos\xi & \\ \hline \end{array} \\
 \\
 \text{RX}(\xi) = \begin{array}{|c|c|c|c|} \hline 1 & 0 & 0 & \\ \hline 0 & \cos\xi & -\sin\xi & \\ \hline 0 & \sin\xi & \cos\xi & \\ \hline \end{array}
 \end{array}$$

Table 3 gives some simplest relationships between rotation angles.

The program is written on standard FORTRAN-77. The source is available by request from the author. Corresponding e-mail address is sacha@igbmc.u-strasbg.fr. Any reported comments, found mistakes and formulae improvements are appreciated. The full text of the notes will be published elsewhere. A new user-friendly version of the program is under development.

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References

- Brünger, A.T. (1992) X-PLOR. Version 3.1. A System for X-ray Crystallography and NMR. Yale University, Connecticut, USA.
- Collaborative Computational Project, Number 4 (1994) *Acta Cryst.*, **D50**, 760-763
- Crowther, R.A. (1972) In : "*The Molecular Replacement Method*", M.G.Rossmann, ed., 173-178. New York: Gordon and Breach.
- Crowther, R.A. (1973) Manual "*The Fast Rotation Function*".
- Crowther, R.A. & Blow, D.M. (1967) *Acta Cryst.* **23**, 544-548.
- Diamond, R. (1993) In: "*International Tables for Crystallography*", U.Shmueli, ed., **B**, 345-373, Dordrecht, Boston, London: Kluwer Academic Publishers.
- Dodson, E., Harding, M.M., Hodgkin, D.C. & Rossmann, M.G. (1966) *J.Mol.Biol.*, **16**, 227-241.
- Fitzgerald., P. (1988) *J.Appl.Cryst.*, **21**, 273-278
- Goldstein, H. (1950) "*Classical Mechanics*", Cambridge, Massachusetts : Addison-Wesley Press.
- Huber, R. (1969) In : "*Crystallographic Computing Proc.*", F.R.Ahmed, ed., 96-102. Munksgaard: Copenhagen.
- Lattman, E.E. (1972) *Acta Cryst.*, **B28**, 1065-1068
- Navaza, J. (1994) *Acta Cryst.*, **A51**, 157-163
- Nordman, C.E. (1966) *Trans.Am.Crystallogr.Assoc.*, **2**, 29-38
- Rossmann, M.G., ed. (1972) "*The Molecular Replacement Method*. New York: Gordon and Breach.
- Rossmann, M.G. (1990) *Acta Cryst.* **A46**, 73-82.
- Rossmann, M.G. & Blow, D.M. (1962) *Acta Cryst.* **15**, 24-31.
- Rossmann, M.G. & Arnold, E. (1993) In : "*International Tables for Crystallography*", U.Shmueli, ed., **B**, 230-263, Dordrecht, Boston, London: Kluwer Academic Publishers.
- Steigemann, W. (1974) PhD thesis, Technische Univ., München, FRG

Table 1. Rotation angles and corresponding rotations. Matrices $R_X(\xi)$, $R_Y(\xi)$, $R_Z(\xi)$ for the primitive rotations are defined in the text. Most distributed molecular replacement program packages are indicated which use the corresponding rotation system.

System	Limits for the triclinic group	Alternative solution	Rotation matrix as a product of matrices for elementary rotations	Program packages
<i>Polar</i> Rossmann,1962	$0 \leq \phi < 2\pi$ $0 \leq \psi \leq \pi$ $0 \leq \kappa < 2\pi$	$\phi = -\phi$ $\psi = -\psi + \pi$ $\kappa = -\kappa$	$R_Y(\phi) \cdot R_Z(-\psi) \cdot R_Y(-\kappa) \cdot R_Z(\psi) \cdot R_Y(-\phi)$	X-PLOR PROTEIN
<i>Polar</i> Dodson et al.,1966 Crowther,1972	$0 \leq \phi < 2\pi$ $0 \leq \psi \leq \pi$ or $0 \leq \omega \leq \pi$ $0 \leq \kappa < 2\pi$	$\phi = \phi + \pi$ $\psi = -\psi + \pi$ $\kappa = -\kappa$	$R_Z(\phi) \cdot R_Y(\psi) \cdot R_Z(-\kappa) \cdot R_Y(-\psi) \cdot R_Z(-\phi)$ $R_Z(\phi) \cdot R_Y(\omega) \cdot R_Z(-\kappa) \cdot R_Y(-\omega) \cdot R_Z(-\phi)$	ALMN AMoRe
<i>Direction cosines</i>	$0 \leq \kappa < 2\pi$ $-1 \leq \cos x \leq 1$ $-1 \leq \cos y \leq 1$ $-1 \leq \cos z \leq 1$ $\cos x^2 + \cos y^2 + \cos z^2 = 1$	$\kappa = -\kappa$ $\cos x = -\cos x$ $\cos y = -\cos y$ $\cos z = -\cos z$	can be written through recalculated angles	AMoRe
<i>Eulerian</i> Rossmann,1962	$0 \leq \theta_1 < 2\pi$ $0 \leq \theta_2 < 2\pi$ $0 \leq \theta_3 < 2\pi$	$\theta_1 = \theta_1 + \pi$ $\theta_2 = -\theta_2$ $\theta_3 = \theta_3 + \pi$	$R_Z(-\theta_3) \cdot R_X(-\theta_2) \cdot R_Z(-\theta_1)$	X-PLOR PROTEIN
<i>Eulerian</i> Lattman,1966	$0 \leq \theta_+ < 4\pi$ $0 \leq \theta_2 < 2\pi$ $-2\pi \leq \theta_- < 2\pi$	$\theta_1 = \theta_1 + 2\pi$ $\theta_2 = -\theta_2$ $\theta_3 = \theta_3$	$R_Z[-(\theta_+ - \theta_-)/2] \cdot R_X(-\theta_2) \cdot R_Z[-(\theta_+ + \theta_-)/2]$	X-PLOR
<i>Eulerian</i> Crowther,1972	$0 \leq \alpha < 2\pi$ $0 \leq \beta < 2\pi$ $0 \leq \gamma < 2\pi$	$\alpha = \alpha + \pi$ $\beta = -\beta$ $\gamma = \gamma + \pi$	$R_Z(-\gamma) \cdot R_Y(-\beta) \cdot R_Z(-\alpha)$	ALMN MERLOT
<i>Eulerian</i> Nordman,1966	$0 \leq \phi < 2\pi$ $0 \leq \theta < 2\pi$ $0 \leq \psi < 2\pi$	$\phi = \phi + \pi$ $\theta = -\theta$ $\psi = \psi + \pi$	$R_X(-\phi) \cdot R_Y(-\theta) \cdot R_X(-\psi)$	
<i>Eulerian</i> Huber,1969	$0 \leq \psi < 2\pi$ $0 \leq \theta < 2\pi$ $0 \leq \phi < 2\pi$	$\phi = \phi + \pi$ $\theta = -\theta$ $\psi = \psi + \pi$	$R_Z(\psi) \cdot R_X(\theta) \cdot R_Y(\phi)$	PROTEIN
<i>Eulerian</i> Navaza,1994	$0 \leq \alpha < 2\pi$ $0 \leq \beta < 2\pi$ $0 \leq \gamma < 2\pi$	$\alpha = \alpha + \pi$ $\beta = -\beta$ $\gamma = \gamma + \pi$	$R_Z(\alpha) \cdot R_Y(\beta) \cdot R_Z(\gamma)$	AMoRe

Table 2. Rotation matrices and angle recalculation for a general case. Following notations are used for brevity : $c\alpha=\cos\alpha$, $c\theta_1=\cos\theta_1$, $s\alpha=\sin\alpha$, $s\theta_1=\sin\theta_1$, etc; $c^2\alpha=\cos\alpha\cdot\cos\alpha$, $s^2\alpha=\sin\alpha\cdot\sin\alpha$, etc; $R_{jk}=R(j,k)$ is the k-th element of the j-th line of the rotation matrix; $\xi=\text{atan2}(q_1,q_2)$ stands for the angle ξ for with $\sin\xi=k\cdot q_1$ and $\cos\xi=k\cdot q_2$, where k and is a positive normalising factor (definition corresponds to the inserted FORTRAN function atan2)

System	Matrix			Solution for a general case
<i>Polar</i> Rossmann,1962	$c\kappa+(1-c\kappa)\cdot s^2\psi\cdot c^2\phi$ $s\psi\cdot[(1-c\kappa)\cdot c\psi\cdot c\phi+s\kappa\cdot s\phi]$ $-(1-c\kappa)\cdot s^2\psi\cdot c\phi+s\kappa\cdot c\psi$	$s\psi\cdot[(1-c\kappa)\cdot c\psi\cdot c\phi+s\kappa\cdot s\phi]$ $c\kappa+(1-c\kappa)\cdot c^2\psi$ $-s\psi\cdot((1-c\kappa)\cdot c\psi\cdot s\phi+s\kappa\cdot c\phi)$	$-(1-c\kappa)\cdot s^2\psi\cdot c\phi\cdot s\phi-s\kappa\cdot c\psi$ $-s\psi\cdot[(1-c\kappa)\cdot c\psi\cdot s\phi-s\kappa\cdot c\phi]$ $c\kappa+(1-c\kappa)\cdot s^2\psi\cdot s^2\phi$	$\cos\kappa=(R_{11}+R_{22}+R_{33}-1)/2$ $\text{tg}\phi=-(R_{12}-R_{21})/(R_{23}-R_{32})$ $\text{tg}\psi\cdot\cos\phi=-(R_{23}-R_{32})/(R_{13}-R_{31})$
<i>Polar</i> Crowther,1972 Dodson, 1966 ($\psi=\omega$)	$c\kappa+(1-c\kappa)\cdot s^2\omega\cdot c^2\phi$ $(1-c\kappa)\cdot s^2\omega\cdot c\phi\cdot s\phi-s\kappa\cdot c\omega$ $s\omega\cdot[(1-c\kappa)\cdot c\omega\cdot c\phi+s\kappa\cdot s\phi]$	$(1-c\kappa)\cdot s^2\omega\cdot c\phi\cdot s\phi+s\kappa\cdot c\omega$ $c\kappa+(1-c\kappa)\cdot s^2\omega\cdot s^2\phi$ $s\omega\cdot[(1-c\kappa)\cdot c\omega\cdot s\phi-s\kappa\cdot c\phi]$	$s\omega\cdot[(1-c\kappa)\cdot c\omega\cdot c\phi-s\kappa\cdot s\phi]$ $s\omega\cdot[(1-c\kappa)\cdot c\omega\cdot s\phi+s\kappa\cdot c\phi]$ $c\kappa+(1-c\kappa)\cdot c^2\omega$	$\cos\kappa=(R_{11}+R_{22}+R_{33}-1)/2$ $\text{tg}\phi=-(R_{13}-R_{31})/(R_{23}-R_{32})$ $\text{tg}\omega\cdot\cos\phi=-(R_{23}-R_{32})/(R_{12}-R_{21})$
<i>Direction</i> <i>cosines</i>	$c\kappa+(1-c\kappa)\cdot c_x^2$ $(1-c\kappa)\cdot c_x\cdot c_y+s\kappa\cdot c_z$ $(1-c\kappa)\cdot c_z\cdot c_x-s\kappa\cdot c_y$	$(1-c\kappa)\cdot c_x\cdot c_y-s\kappa\cdot c_z$ $c\kappa+(1-c\kappa)\cdot c_y^2$ $(1-c\kappa)\cdot c_z\cdot c_y+s\kappa\cdot c_x$	$(1-c\kappa)\cdot c_z\cdot c_x+s\kappa\cdot c_y$ $(1-c\kappa)\cdot c_z\cdot c_y-s\kappa\cdot c_x$ $c\kappa+(1-c\kappa)\cdot c_z^2$	$\cos\kappa=(R_{11}+R_{22}+R_{33}-1)/2$ $\cos z/\cos x=(R_{12}-R_{21})/(R_{23}-R_{32})$ $\cos z/\cos x=-(R_{13}-R_{31})/(R_{23}-R_{32})$
<i>Eulerian</i> Rossmann,1962	$-s\theta_1\cdot c\theta_2\cdot s\theta_3+c\theta_1\cdot c\theta_3$ $-s\theta_1\cdot c\theta_2\cdot c\theta_3-c\theta_1\cdot s\theta_3$ $s\theta_1\cdot s\theta_2$	$c\theta_1\cdot c\theta_2\cdot s\theta_3+s\theta_1\cdot c\theta_3$ $c\theta_1\cdot c\theta_2\cdot c\theta_3-s\theta_1\cdot s\theta_3$ $-c\theta_1\cdot s\theta_2$	$s\theta_2\cdot s\theta_3$ $s\theta_2\cdot c\theta_3$ $c\theta_2$	$\theta_1=\text{atan2}(R_{31},-R_{32})$ $\cos\theta_2=R_{33}$ $\theta_1=\text{atan2}(R_{13}, R_{23})$
<i>Eulerian</i> Lattmann,1966	$[(1-c\theta_2)\cdot c\theta_-+(1+c\theta_2)\cdot c\theta_+]/2$ $[(1-c\theta_2)\cdot s\theta_--(1+c\theta_2)\cdot s\theta_+]/2$ $\sin[(\theta_++\theta_-)/2]\cdot s\theta_2$	$[(1-c\theta_2)\cdot s\theta_-+(1+c\theta_2)\cdot s\theta_+]/2$ $[(1+c\theta_2)\cdot c\theta_+-(1-c\theta_2)\cdot c\theta_-]/2$ $-\cos[(\theta_++\theta_-)/2]\cdot s\theta_2$	$s[(\theta_+-\theta_-)/2] s\theta_2$ $c[(\theta_+-\theta_-)/2] s\theta_2$ $c\theta_2$	$\theta_+=\text{atan2}(R_{31},-R_{32})+\text{atan2}(R_{13}, R_{23})$ $\cos\theta_2=R_{33}$ $\theta_-=\text{atan2}(R_{31},-R_{32})-\text{atan2}(R_{13}, R_{23})$
<i>Eulerian</i> Crowther,1972	$c\alpha\cdot c\beta\cdot c\gamma-s\alpha\cdot s\gamma$ $-c\alpha\cdot c\beta\cdot s\gamma-s\alpha\cdot c\gamma$ $c\alpha\cdot s\beta$	$s\alpha\cdot c\beta\cdot c\gamma+c\alpha\cdot s\gamma$ $-s\alpha\cdot c\beta\cdot s\gamma+c\alpha\cdot c\gamma$ $s\alpha\cdot s\beta$	$-s\beta\cdot c\gamma$ $s\beta\cdot s\gamma$ $c\beta$	$\alpha=\text{atan2}(R_{32}, R_{31})$ $\cos\beta=R_{33}$ $\gamma=\text{atan2}(R_{23},-R_{13})$
<i>Eulerian</i> Nordman,1966	$c\theta$ $s\phi\cdot s\theta$ $c\phi\cdot s\theta$	$s\theta\cdot s\psi$ $-s\phi\cdot c\theta\cdot s\psi+c\phi\cdot c\psi$ $-c\phi\cdot c\theta\cdot s\psi-s\phi\cdot c\psi$	$-s\theta\cdot c\psi$ $s\phi\cdot c\theta\cdot c\psi+c\phi\cdot s\psi$ $c\phi\cdot c\theta\cdot c\psi-s\phi\cdot s\psi$	$\phi=\text{atan2}(R_{21},R_{31})$ $\cos\theta=R_{11}$ $\psi=\text{atan2}(R_{12}, -R_{13})$
<i>Eulerian</i> Huber,1969	$c\psi\cdot c\phi\cdot s\psi\cdot s\theta\cdot s\phi$ $s\psi\cdot c\phi+c\psi\cdot s\theta\cdot s\phi$ $-c\theta\cdot s\phi$	$-s\psi\cdot c\theta$ $c\psi\cdot c\theta$ $s\theta$	$c\psi\cdot s\phi+s\psi\cdot s\theta\cdot c\phi$ $s\psi\cdot s\phi\cdot c\psi\cdot s\theta\cdot c\phi$ $c\theta\cdot c\phi$	$\phi=\text{atan2}(-R_{31},R_{33})$ $\sin\theta=R_{32}$ $\psi=\text{atan2}(-R_{12}, R_{22})$
<i>Eulerian</i> Navaza, 1994	$c\alpha\cdot c\beta\cdot c\gamma-s\alpha\cdot s\gamma$ $s\alpha\cdot c\beta\cdot c\gamma+c\alpha\cdot s\gamma$ $-s\beta\cdot c\gamma$	$-c\alpha\cdot c\beta\cdot s\gamma-s\alpha\cdot c\gamma$ $-s\alpha\cdot c\beta\cdot s\gamma+c\alpha\cdot c\gamma$ $s\beta\cdot s\gamma$	$c\alpha\cdot s\beta$ $s\alpha\cdot s\beta$ $c\beta$	$\alpha=\text{atan2}(R_{23},-R_{13})$ $\cos\beta=R_{33}$ $\gamma=\text{atan2}(R_{32}, R_{31})$

Table 3a. Basic relationships between polar rotation angles. The polar angles used by Dodson et al.(1966) are the same as the ones defined by Crowther with a small change in notation (ψ instead of ω). AMoRe (Navaza, 1994) uses the polar angles similar to the ones by Crowther only for the self-rotation, therefore the sign of κ is not defined.

	Rossmann, 1962; κ^r, ϕ^r, ψ^r	Crowther, 1972; $\kappa^c, \phi^c, \omega^c$	Direction cosines
Rossmann 1962 κ^r, ϕ^r, ψ^r		$\kappa^r = \kappa^c$ $\cos \psi^r = \sin \omega^c \cdot \sin \phi^c$ $\text{tg} \phi^r = -\cos \omega^c / (\sin \omega^c \cdot \cos \phi^c)$	$\kappa^r = -\kappa^d$ $\cos \psi^r = \cos y$ $\text{tg} \phi^r = (-\cos z, \cos x)$
Crowther 1972 $\kappa^c, \phi^c, \omega^c$	$\kappa^c = \kappa^r$ $\cos \omega^c = -\sin \psi^r \sin \phi^r$ $\text{tg} \phi^c = \cos \psi^r / (\sin \psi^r \cdot \cos \phi^r)$		$\kappa^c = -\kappa^d$ $\cos \omega^c = \cos z$ $\text{tg} \phi^c = (\cos y, \cos x)$
direction cosines	$\kappa^d = -\kappa^r$ $\cos x = \sin \psi^r \cdot \cos \phi^r$ $\cos y = \cos \psi^r$ $\cos z = -\sin \psi^r \cdot \sin \phi^r$	$\kappa^d = -\kappa^c$, $\cos x = \sin \omega^c \cdot \cos \phi^c$ $\cos y = \sin \omega^c \cdot \sin \phi^c$ $\cos z = \cos \omega^c$	

Table 3b. Basic relationships between some Eulerian rotation angles. Angles defined by Nordman (1966) and Huber (1969) are not included in the table because their recalculation through corresponding rotation matrix elements (Table 2) seems to be more rational.

	Rossmann, 1962 $\theta_1, \theta_2, \theta_3$	Lattman, 1966 $\theta_+, \theta_2', \theta_-$	Crowther, 1972 $\alpha^c, \beta^c, \gamma^c$	Navaza, 1994 $\alpha^a, \beta^a, \gamma^a$
Rossmann 1962 $\theta_1, \theta_2, \theta_3$		$\theta_1 = (\theta_+ + \theta_-) / 2$ $\theta_2 = \theta_2'$ $\theta_3 = (\theta_+ - \theta_-) / 2$	$\theta_1 = \alpha^c + \pi / 2$ $\theta_2 = \beta^c$ $\theta_3 = \gamma^c - \pi / 2$	$\theta_1 = -\gamma^a + \pi / 2$ $\theta_2 = -\beta$ $\theta_3 = -\alpha - \pi / 2$
Lattman 1966 $\theta_+, \theta_2', \theta_-$	$\theta_+ = \theta_1 + \theta_3$ $\theta_2' = \theta_2$ $\theta_- = \theta_1 - \theta_3$		$\theta_+ = \alpha^c + \gamma$ $\theta_2' = \beta^c$ $\theta_- = \gamma^c - \alpha^c + \pi$	$\theta_+ = -\alpha - \gamma$ $\theta_2' = -\beta$ $\theta_- = \alpha - \gamma + \pi$
Crowther 1972 $\alpha^c, \beta^c, \gamma^c$	$\alpha = \theta_1 + \pi$ $\beta = \theta_2$ $\gamma = \theta_3 + \pi$	$\alpha = (\theta_+ - \theta_-) / 2 + \pi$ $\beta = \theta_2'$ $\gamma = (\theta_+ + \theta_-) / 2 + \pi$		$\alpha^c = -\gamma^a$ $\beta^c = -\beta^a$ $\gamma^c = -\alpha^a$
Navaza 1994 $\alpha^a, \beta^a, \gamma^a$	$\alpha^a = -\theta_3 + \pi$ $\beta^a = -\theta_2$ $\gamma^a = -\theta_1 + \pi$	$\alpha^a = -(\theta_+ - \theta_-) / 2 + \pi$ $\beta^a = -\theta_2'$ $\gamma^a = -(\theta_+ + \theta_-) / 2 + \pi$	$\alpha^a = -\gamma^c$ $\beta^a = -\beta^c$ $\gamma^a = -\alpha^c$	