RESETTING A TRICLINIC UNIT-CELL IN THE CONVENTIONAL ORIENTATION

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Introduction

The rules for the conventional orientation of a triclinic crystal (Donnay and Mélon, 1933; Donnay, Tunell, and Barth, 1934; Donnay, 1943) are the following. The axes must be: (1) chosen along the shortest three translations; (2) named so as to satisfy the condition $c<a<b$; (3) oriented so that the axial cross is right-handed, with α and β both obtuse.

The first of these rules has been followed generally in the past, so that the problem of reorienting a triclinic crystal usually reduces to resetting the unit-cell, that is to say, renaming and reorienting the axes. Although this problem admits of a straightforward solution, it is encountered so often in crystallographic work that its treatment at this place should be of practical value.

Resetting a Triclinic Cell

The original axial elements are usually given in the form (right-handed axial cross):

$a_0=7.88$	$b_0=7.27$	$c_0=7.03$
$\alpha=89°59'$,	$\beta=95°16'$,	$\gamma=103°25'$,

Copy them, without the letters, as follows:

7.88,	7.27,	7.03
89°59′,	95°16′,	103°25′.

Relabel the axes c, a, b, in increasing order (so as to satisfy the condition $c<a<b$). The new labels of the interaxial angles are thereby determined (respectively: γ, α, β). Thus:

$b=7.88$	$a=7.27$,	$c=7.03$,
$\beta=89°59'$,	$\alpha=95°16'$,	$\gamma=103°25'$.

Two cases may occur: The arrangement of letters, read from left to right, either is or (as in the above example) is not a cyclic permutation of *a b c*.

I. If the arrangement is one of the three cyclic permutations (*a b c*, *b c a*, *c a b*), the axial cross has remained a right-handed one. If a reorientation of the axes is found to be necessary in order to comply with the convention "α and β both obtuse," two axes must change their signs in order that the axial cross remain right-handed.

Any one of four possibilities may arise: (1) α and β both obtuse; (2) α obtuse, but β acute; (3) β obtuse, but α acute; (4) α and β both acute.

(1) α and β both obtuse.—No further modification of the setting is needed.

(2) α obtuse, β acute.—A reorientation of axes is necessary to make the angle β obtuse. As two axes must be reversed, only one of the three interaxial angles can retain its character (obtuse or acute), namely, the angle comprised between the two axes that change their signs. Since α must remain obtuse, the axes to be reversed are b and c. After this transformation, β has changed from acute to obtuse (as desired), and γ has also changed its character (which is immaterial).

(3) β obtuse, α acute.—This case is similar to the one just considered. Reverse the signs of a and c; take the supplements of α and γ.

(4) α and β both acute.—The only angle that should retain its character (obtuse or acute) is γ. Reverse the signs of a and b; take the supplements of α and β.

II. If the arrangement of letters, obtained after renaming the axes, is not a cyclic permutation of $a\ b\ c$, but is one of the other three permutations ($a\ c\ b$, $c\ b\ a$, $b\ a\ c$), the axial cross has become left-handed. A reorientation of the axes is imperative in any case in order to restore the right-handed character of the axial cross; it may also be needed to bring the new setting into agreement with the rule "α and β both obtuse." The left-handed axial cross can be made right-handed in two ways only: either by changing the sign of a single axis, or by reversing all three axes.

The four possibilities to be examined are the same as before:

(1) α and β both obtuse.—Reverse all three axes. The axial cross again becomes right-handed. All interaxial angles keep the same values.

(2) α obtuse, β acute.—Reversing one axis only changes the character (obtuse or acute) of the two angles which this axis makes with the other two axes. The angle α cannot be changed; β must, and γ may, become obtuse. Reverse the sign of a; take the supplements of β and γ.

(3) β obtuse, α acute.—For the foregoing reasons, reverse the sign of b; take the supplements of α and γ.

(4) α and β both acute.—Change the sign of c; take the supplements of α and β.

The above discussion is summarized in a double-entry table (Table 1), which also gives the old-to-new transformation matrices for the 24 possible right-handed settings. This table should prove worthwhile as a labor-saving device, whenever a large number of triclinic cell reorientations are to be performed. The procedure is simple: rename the axes so that $c<a<b$; if, after renaming the axes, α and β are both acute, take

their supplements; if only one of them is acute, take its supplement and also that of γ; the old-to-new transformation matrix is then found in the table.

Examples

The triclinic species given in Wyckoff (1931, 1935) have been worked out as examples. In each case it has been assumed that the unit lengths were the shortest three translations. The examples are listed in groups, each under the appropriate transformation, indicated by its letter (cp. Table 1).

These examples probably constitute a representative sampling of the various types of setting used for triclinic crystals. They are instructive in providing a statistical survey and they also bring out certain special cases which require additional conventions.

If one of the two interaxial angles α and β is 90° (as in pectolite and wollastonite), two settings are found, as 90° is considered obtuse or acute in turn (transformations W and X, respectively). That setting which leads to γ obtuse is obviously the more desirable.

If both α and β are 90° (as in $3KPbCl_3 \cdot H_2O$), two sets of axial elements are likewise obtained, with supplementary values for γ (transformations O or R, and P or Q). Again the setting that makes γ obtuse should be preferred.

A case where $a=b$ has been encountered (H_3BO_3). Two settings are obtained (transformations A and W), which differ from each other by the interchange of α and β. To cope with such cases (which seldom occur), an additional convention may be devised (α smaller than β, for instance), although refinement of the measurements will usually reveal a difference between the unit lengths.

References

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TABLE 1. TRANSFORMATION MATRICES
(Old setting to new setting)

After renaming the axes:	In order to satisfy the condition $c<a<b$, the original $a_0b_0c_0$ become:					
	abc	*bca*	*cab*	*acb*	*cba*	*bac*
α and β both obtuse: Leave all angles un-unchanged	A $\begin{matrix}1&0&0\\0&1&0\\0&0&1\end{matrix}$	E $\begin{matrix}0&1&0\\0&0&1\\1&0&0\end{matrix}$	K $\begin{matrix}0&0&1\\1&0&0\\0&1&0\end{matrix}$	O $\begin{matrix}\bar{1}&0&0\\0&0&\bar{1}\\0&\bar{1}&0\end{matrix}$	S $\begin{matrix}0&0&\bar{1}\\0&\bar{1}&0\\\bar{1}&0&0\end{matrix}$	W $\begin{matrix}0&\bar{1}&0\\\bar{1}&0&0\\0&0&\bar{1}\end{matrix}$
α obtuse, β acute: Take supplements of β and γ	B $\begin{matrix}1&0&0\\0&\bar{1}&0\\0&0&\bar{1}\end{matrix}$	F $\begin{matrix}0&1&0\\0&0&\bar{1}\\\bar{1}&0&0\end{matrix}$	L $\begin{matrix}0&0&1\\\bar{1}&0&0\\0&\bar{1}&0\end{matrix}$	P $\begin{matrix}\bar{1}&0&0\\0&0&1\\0&1&0\end{matrix}$	T $\begin{matrix}0&0&\bar{1}\\0&1&0\\1&0&0\end{matrix}$	X $\begin{matrix}0&\bar{1}&0\\1&0&0\\0&0&1\end{matrix}$
β obtuse, α acute: Take supplements of α and γ	C $\begin{matrix}\bar{1}&0&0\\0&1&0\\0&0&\bar{1}\end{matrix}$	G $\begin{matrix}0&\bar{1}&0\\0&0&1\\\bar{1}&0&0\end{matrix}$	M $\begin{matrix}0&0&\bar{1}\\1&0&0\\0&\bar{1}&0\end{matrix}$	Q $\begin{matrix}1&0&0\\0&0&\bar{1}\\0&1&0\end{matrix}$	U $\begin{matrix}0&0&1\\0&\bar{1}&0\\1&0&0\end{matrix}$	Y $\begin{matrix}0&1&0\\\bar{1}&0&0\\0&0&1\end{matrix}$
α and β both acute: Take supplements of α and β	D $\begin{matrix}\bar{1}&0&0\\0&\bar{1}&0\\0&0&1\end{matrix}$	H $\begin{matrix}0&\bar{1}&0\\0&0&\bar{1}\\1&0&0\end{matrix}$	N $\begin{matrix}0&0&\bar{1}\\\bar{1}&0&0\\0&1&0\end{matrix}$	R $\begin{matrix}1&0&0\\0&0&1\\0&\bar{1}&0\end{matrix}$	V $\begin{matrix}0&0&1\\0&1&0\\\bar{1}&0&0\end{matrix}$	Z $\begin{matrix}0&1&0\\1&0&0\\0&0&\bar{1}\end{matrix}$

LIST OF EXAMPLES

Transformation and Substance	Old Setting			New Setting
(A) Albite, $NaAlSi_3O_8$	8.14	12.86	7.17	
	94° 3′	116°29′	88° 9′	
Calcium sulfate urea, $CaSO_4\cdot CO(NH_2)_2$	14.74	14.95	6.47	
	91°26′	90°22′	86°42′	
4 Nitro-2-Methylaminotoluene, (red form)	7.6	8.5	7.5	
	113°	98°	109°	
Aenigmatite	18.3	18.3	10.6	
	96°30′	96°30′	113°30′	
Kyanite, Al_2SiO_5	7.09	7.72	5.56	
	90° 5′	101° 2′	105°44′	
Ammonium hydrogen fumarate, $C_4H_7NO_4$	7.00	7.44	6.56	
	107° 1′	117°58′	69°16′	
Fumaric acid	7.60	15.11	6.61	
	90°40′	111° 5′	89°48′	
Boric acid, H_3BO_3	7.04	7.04	6.56	
	92°30′	101°10′	120°	
Celsian[1]	8.63	13.10	7.29	
	ca. 90°	116°	ca. 90°	
Andesine	8.14	12.86	7.17	
	93°23′	116°28′	89°59′	
Tungstic trioxide[2] WO_3	7.28	7.48	3.82	
	ca. 90°	ca. 90°	ca. 90°	

LIST OF EXAMPLES—*Continued*

Transformation and Substance	Old Setting			New Setting		
(B) Stilbene+2 mol. 1,3,5 Trinitrobenzene,	12.7	15.4	7.7	12.7	15.4	7.7
$C_6H_5CH{=}CHC_6H_5 \cdot 2[C_6H_3(NO_2)_3]$	102°16′	85°30′	87°35′	102°16′	94°30′	92°25′
(C) Copper sulfate pentahydrate,	6.07	10.78	5.89	6.07	10.78	5.89
$CuSO_4 \cdot 5H_2O$	82° 5′	107° 8′	102°41′	97°55′	107° 8′	77°19′
Rhodonite, $Mn_4Ca(SiO_3)_5$	7.77	12.45	6.74	7.77	12.45	6.74
	85°10′	94° 4′	111°29′	94°50′	94° 4′	68°31′
Racemic acid (anhydrous),	7.18	9.71	4.98	7.18	9.71	4.98
$COOH(CHOH)_2COOH$	82°20′	118° 0′	72°58′	97°40′	118° 0′	107° 2′
Racemic acid monohydrate, $C_4H_4O_6 \cdot H_2O$	8.09	10.03	4.81	8.09	10.03	4.81
	76° 2′	96°57′	120° 8′	103°58′	96°57′	59°52′
(D) Thallium mesotartrate, $Tl_2C_4H_4O_6$	13.26	16.12	7.63	13.26	16.12	7.63
	75°54′	86°37′	82°14′	104° 6′	93°23′	82°14′
Cholesteryl salicylate, $C_{34}H_{50}O_3$	9.68	12.52	6.31	9.68	12.52	6.31
	85°53′	77°41′	84° 1′	94° 7′	102°19′	84° 1′
(E) No example found						
(F) Hexamethyl benzene, $C_6(CH_3)_6$	9.01	8.92_6	5.34_4	8.92_6	9.01	5.34_4
	44°27′	116°43′	119°34′	116°43′	135°33′	60°26′
(G) Bisethylene diamino platinous chloride,	8.37	4.95	6.86	6.86	8.37	4.95
Pt $(C_2H_8N_2)_2Cl_2$	100°46′	111°40′	81°56′	98° 4′	100°46′	68°20′
Racemic methyl ephedrine hydroiodide,	11.2	7.67	7.68	7.68	11.2	7.67
$C_{11}H_{17}ON \cdot HI$	108°55′	95°36′	84°15′	95°45′	108°45′	84°24′
(H) Cyclododecane, $C_{12}H_{24}$	7.84	5.44	7.82	7.82	7.84	5.44
	98°18′	64°	81°	99°	98°18′	64°
(K) Anorthite, $CaAl_2Si_2O_8$	8.21	12.95	14.16	12.95	14.16	8.21
	93°13′	115°56′	91°12′	115°56′	91°12′	93°13′
(L) Labradorite	8.21	12.95	14.16	12.95	14.16	8.21
	93°21′	116° 3′	89°55′	116° 3′	90° 5′	86°29′
Babingtonite	6.73	7.54	12.43	7.54	12.43	6.73
	112°22′	93°48′	86° 9′	93°48′	93°51′	67°37′
(M) (N) No example found.						
(O) Potassium lead chloride hydrate,[3]	14.35	9.05	14.50	14.35	14.50	9.05
$3KPbCl_3 \cdot H_2O$	ca. 90°	113°	ca. 90°	ca. 90°	ca. 90°	113°
(P) Sodium iodide dihydrate, $NaI \cdot 2H_2O$	6.85	5.76	7.16	6.85	7.16	5.76
	98°	119°	68½°	98°	111½°	61°
p-Cyano-o-Nitro-p′-Methoxystilbene,	8.50	7.45	13.35	8.50	13.35	7.45
$C_6H_3(CN)(NO_2)CH{=}CHC_6H_4(OCH_3)$	98° 6′	106°20′	75°40′	98° 6′	104°20′	73°40′
Potassium mesotartrate dihydrate,	7.02	6.90	11.02	7.02	11.02	6.90
$K_2C_4H_4O_6 \cdot 2H_2O$	95°44′	102°52′	61°46′	95°44′	118°14′	77° 8′
(Q) α-Potassium dichromate, $K_2Cr_2O_7$	7.50	7.38	13.40	7.50	13.40	7.38
	82° 0′	96°13′	90°51′	98° 0′	90°51′	83°47′
(R) 2,7 dinitroanthraquinone fluorene,	8.2	7.4	19.0	8.2	19.0	7.4
$C_{14}H_6(NO_2)_2O_2$, $(C_6H_4)_2CH_2$	78°	82°	ca. 80°	102°	ca. 100°	82°
(S) Potassium persulfate, $K_2S_2O_8$	5.11	6.51	5.48	5.48	6.51	5.11
	96°45′	90°10′	95°15′	95°15′	90°10′	96°45′
Copper sulfate pentahydrate[4]	5.12	10.7	5.97	5.97	10.7	5.12
$CuSO_4 \cdot 5H_2O$	82°16′	107°26′	102°40′	102°40′	107°26′	82°16′
(T) (U) (V) No example found						
(W) Pectolite, $NaHCa_2(SiO_3)_3$	7.91	7.08	7.05	7.08	7.91	7.05
	90°	95°10′	103° 0′	95°10′	90°	103° 0′
Wollastonite, $CaSiO_3$	7.88	7.27	7.03	7.27	7.88	7.03
	90°	95°16′	103°25′	95°16′	90°	103°25′
Malonic acid, $CH_2(COOH)_2$	8.36	5.33	5.14	5.33	8.36	5.14
	94°56′	103°56′	71°30′	103°56′	94°56′	71°30′
(Y) (Z) No example found						

[1] Transformation C leads to the same axial elements as transformation A.
[2] Transformations A, B, C, and D lead to the same results.
[3] Transformation R would lead to the same results.
[4] Example of a redetermination that changes the setting.—Compare transformation C.