Aufgabe 2 (i):

Für Au-P1:

$\Delta_1 = 9.9933(0.33863-0.24277) = 0.957958$

$\Delta_1^2 = 0.917683$

$\Delta_2 = 23.917(0.30980-0.28317) = 0.636910$

$\Delta_2^2 = 0.405654$

$\Delta_3 = 15.180(0.58099-0.71103) = -1.974007$

$\Delta_3^2 = 3.896704$

und $2\ \Delta_1\ \Delta_3 \cos\beta = 0.366434$

$d^2 = \Delta_1^2 + \Delta_2^2 + \Delta_3^2 + 2\ \Delta_1\ \Delta_3 \cos\beta = 5.586475$

d = **2.364 Å**

Analog: Au-P2 = **2.388 Å**, P1···P2 = **3.446 Å**

Nach der Cosinus-Regel:

cos (P1-Au-P2) = $(2.364^2 + 2.388^2 - 3.446^2) / (2 \times 2.364 \times 2.388)$

(P1-Au-P2) = **92.96°**

Aufgabe 2 (ii):

E = **MA** (**E** orthonormale Achsen, **A** Kristallachsen, **M** Transformationsmatrix **E**→**A**)

Bei Koordinaten gilt **X** = $(\mathbf{M}^{-1})^T\mathbf{x}$ (**X** orthonormale Koordinaten, **x** Kristallkoordinaten)

$$(\mathbf{M}^{-1})^T = \begin{pmatrix} a & 0 & c\cos\beta \\ 0 & b & 0 \\ 0 & 0 & c\sin\beta \end{pmatrix} = \begin{pmatrix} 9.9933 & 0 & -1.47076 \\ 0 & 23.917 & 0 \\ 0 & 0 & 15.1086 \end{pmatrix}$$

Für Au: $\mathbf{X}_{Au} = (\mathbf{M}^{-1})^T \begin{pmatrix} 0.33863 \\ 0.30980 \\ 0.58099 \end{pmatrix}$

$X_{Au} = (9.9933 \times 0.33863) - (1.47076 \times 0.58099) = 2.5295$

$Y_{Au} = 23.917 \times 0.30980 = 7.4095$

$Z_{Au} = 15.1086 \times 0.58099 = 8.7780$

Analog: P1 auf 1.3803, 6.7726, 10.7427, P2 auf 1.3141, 9.4600, 8.5821

$d^2(\text{Au-P1}) = (2.5295 - 1.3803)^2 + (7.4095 - 6.7726)^2 + (10.7427 - 8.7780)^2 = 5.5863$

d(Au-P1) = **2.364 Å**

usw.

Aufgabe 3 (Teil (ii)(b))**:**

$$\mathbf{G'} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ -1 & 0 & -1 \end{pmatrix} \begin{pmatrix} \mathbf{a.a} & \mathbf{a.b} & \mathbf{a.c} \\ \mathbf{a.b} & \mathbf{b.b} & \mathbf{b.c} \\ \mathbf{a.c} & \mathbf{b.c} & \mathbf{c.c} \end{pmatrix} \begin{pmatrix} 1 & 0 & -1 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$= \begin{pmatrix} \mathbf{a.a} & \mathbf{a.b} & \mathbf{a.c} \\ -\mathbf{a.b} & -\mathbf{b.b} & -\mathbf{b.c} \\ -\mathbf{a.a}-\mathbf{a.c} & -\mathbf{a.b}-\mathbf{b.c} & -\mathbf{a.c}-\mathbf{c.c} \end{pmatrix} \begin{pmatrix} 1 & 0 & -1 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$= \begin{pmatrix} \mathbf{a.a} & -\mathbf{a.b} & -\mathbf{a.a}-\mathbf{a.c} \\ -\mathbf{a.b} & \mathbf{b.b} & \mathbf{a.b}+\mathbf{b.c} \\ -\mathbf{a.a}-\mathbf{a.c} & \mathbf{a.b}+\mathbf{b.c} & \mathbf{a.a}+2\mathbf{a.c}+\mathbf{c.c} \end{pmatrix}$$

[bei a = 4.902, b = 12.345, c = 7.213, β = 104.56, cos β = -0.251]

$$= \begin{pmatrix} 24.03 & 0 & -24.03+8.89 \\ 0 & 152.40 & 0 \\ -24.03+8.89 & 0 & 24.03-2(8.89)+52.03 \end{pmatrix}$$

ergibt: $a' = a$, $b' = b$, $c' = \sqrt{58.28}$ = **7.634**

a' c' cos β' = -15.14, cos β' = -15.14/(4.902×7.634) = -0.405, β' = **113.86°**.

Aufgabe 4. Orthorhombische Zelle, a = 36.837, b = 10.5429, c = 11.5357 Å.

C1	0.18430	0.3496	0.5751
C2	0.14452	0.3199	0.5552
C3	0.13395	0.3534	0.4309
C4	0.13756	0.4958	0.4085

Orthogonalkoordinaten = Kristallkoordinaten × Achsenlänge (orthorhombisch!):

C1	6.7891	3.6858	6.6342
C2	5.3237	3.3727	6.4046
C3	4.9343	3.7259	4.9707
C4	5.0673	5.2272	4.7123

C1 auf den Ursprung verschieben:

C1	0	0	0
C2	-1.4654	-0.3131	-0.2296
C3	-1.8546	0.0401	-1.6635
C4	-1.7218	1.5414	-1.9219

C3 von *C* auf *C'* verschieben (Vektor -*AB*):

C3'	x :	-1.8546 - (-1.4654) =	-0.3892
	y :	0.0401 - (-0.3131) =	0.3532
	z :	-1.6635 - (-0.2296) =	-1.4339

C4 von *D* auf *D'* verschieben (Vektor -*AB*-*AC*):

C4'	x :	-1.7218 - (-1.4654) - (-0.3892)=	0.1328
	y :	1.5414 - (-0.3131) - (0.3532) =	1.5013
	z :	-1.9219 - (-0.2296) - (-1.4339)=	-0.2584

Neue Lagen:

C1	0	0	0
C2	-1.4654	-0.3131	-0.2296
C3'	-0.3892	0.3532	-1.4339
C4'	0.1328	1.5013	-0.2584

$d_{AB} = \sqrt{(1.4654^2 + 0.3131^2 + 0.2296^2)} = 1.5160$ Å

$d_{AC'} = \sqrt{(0.3892^2 + 0.3532^2 + 1.4339^2)} = 1.5272$ Å

$d_{AD'} = \sqrt{(0.1328^2 + 1.5013^2 + 0.2584^2)} = 1.5292$ Å

$d_{BC'} = \sqrt{\{(1.4654 - 0.3892)^2 + (0.3131 + 0.3532)^2 + (1.4339 - 0.2296)^2\}} = 1.7471$ Å

$d_{BD'} = \sqrt{\{(1.4654 + 0.1328)^2 + (0.3131 + 1.5013)^2 + (0.2584 - 0.2296)^2\}} = 2.4181$ Å

$d_{C'D'} = \sqrt{\{(0.3892 + 0.1328)^2 + (1.5013 - 0.3532)^2 + (1.4339 - 0.2584)^2\}} = 1.7241$ Å

$\cos \gamma = \{(AB)^2 + (AC')^2 - (BC')^2\} / 2 (AB)(AC')$

$= (1.5160^2 + 1.5272^2 - 1.7471^2\}/2 (1.5160)(1.5272)$

$\gamma = 70.072°$

$\cos \beta = \{(AB)^2 + (AD')^2 - (BD')^2\} / 2 (AB)(AD')$

$= (1.5160^2 + 1.5292^2 - 2.4181^2\}/2 (1.5160)(1.5292)$

$\beta = 105.134°$

$\cos \alpha = \{(AC')^2 + (AD')^2 - (C'D')^2\} / 2 (AC')(AD')$

$= (1.5272^2 + 1.5292^2 - 1.7241^2\}/2 (1.5272)(1.5292)$

$\alpha = 68.679°$

$\cos\omega = (\cos\alpha \cos\gamma - \cos\beta) / \sin\alpha \sin\gamma$

$= \quad (0.36359 \times 0.34034 + 0.26108) / (0.93156 \times 0.94012)$

$\omega = \pm 63.9°$

Das Vorzeichen von ω ergibt sich aus dem Tripelprodukt $(A \rightarrow B) \cdot (A \rightarrow C' \times A \rightarrow D')$

$$= \det \begin{pmatrix} -1.4654 & -0.3131 & -0.2296 \\ -0.3892 & 0.3532 & -1.4339 \\ 0.1328 & 1.5013 & -0.2584 \end{pmatrix} = -3.05$$

(Pseudo-Zelle hat linkshändiges Achsensystem)

Ergebnis: **ω = -63.9°**