

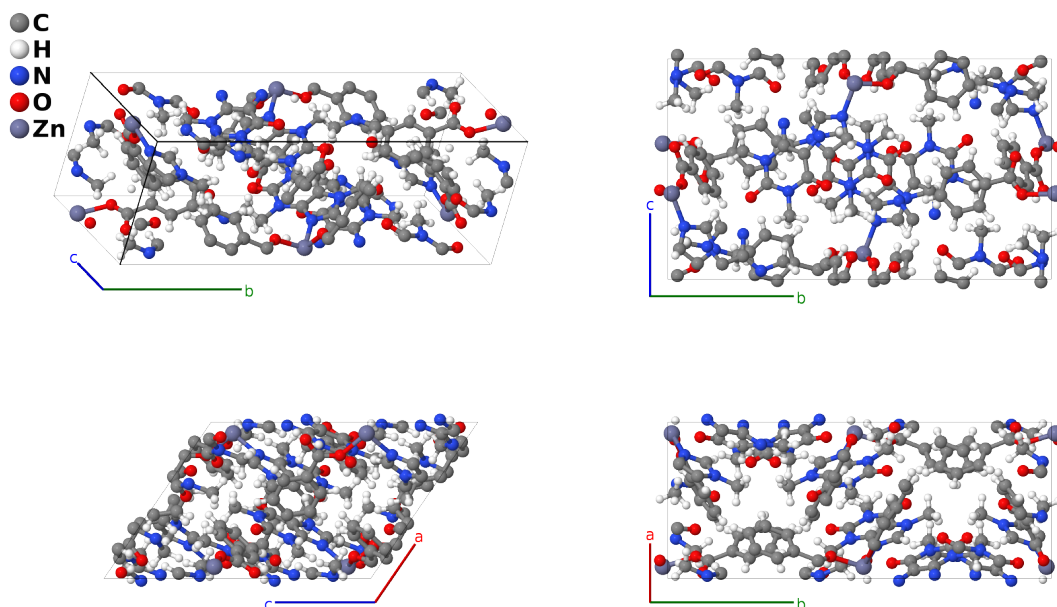
# [Zn<sub>2</sub>(Benzoato)<sub>4</sub>(Caffeine)<sub>2</sub>]<sub>2</sub> – Caffeine (C<sub>30</sub>H<sub>30</sub>N<sub>8</sub>O<sub>8</sub>Zn) Structure:

## A30B30C8D8E\_mP308\_14\_30e\_30e\_8e\_8e\_e-001

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<https://afLOW.org/p/6QN7>

[https://afLOW.org/p/A30B30C8D8E\\_mP308\\_14\\_30e\\_30e\\_8e\\_8e\\_e-001](https://afLOW.org/p/A30B30C8D8E_mP308_14_30e_30e_8e_8e_e-001)

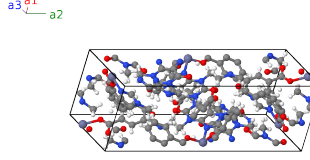


Prototype	C <sub>30</sub> H <sub>30</sub> N <sub>8</sub> O <sub>8</sub> Zn
AFLOW prototype label	A30B30C8D8E_mP308_14_30e_30e_8e_8e_e-001
CCDC	687128
Pearson symbol	mP308
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	<pre>afLOW --proto=A30B30C8D8E_mP308_14_30e_30e_8e_8e_e-001 --params=a,b/a,c/a,β,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,y5,z5,x6,y6,z6,x7, y7,z7,x8,y8,z8,x9,y9,z9,x10,y10,z10,x11,y11,z11,x12,y12,z12,x13,y13,z13,x14,y14,z14,x15, y15,z15,x16,y16,z16,x17,y17,z17,x18,y18,z18,x19,y19,z19,x20,y20,z20,x21,y21,z21,x22,y22, z22,x23,y23,z23,x24,y24,z24,x25,y25,z25,x26,y26,z26,x27,y27,z27,x28,y28,z28,x29,y29,z29, x30,y30,z30,x31,y31,z31,x32,y32,z32,x33,y33,z33,x34,y34,z34,x35,y35,z35,x36,y36,z36,x37, y37,z37,x38,y38,z38,x39,y39,z39,x40,y40,z40,x41,y41,z41,x42,y42,z42,x43,y43,z43,x44,y44, z44,x45,y45,z45,x46,y46,z46,x47,y47,z47,x48,y48,z48,x49,y49,z49,x50,y50,z50,x51,y51,z51, x52,y52,z52,x53,y53,z53,x54,y54,z54,x55,y55,z55,x56,y56,z56,x57,y57,z57,x58,y58,z58,x59, y59,z59,x60,y60,z60,x61,y61,z61,x62,y62,z62,x63,y63,z63,x64,y64,z64,x65,y65,z65,x66,y66, z66,x67,y67,z67,x68,y68,z68,x69,y69,z69,x70,y70,z70,x71,y71,z71,x72,y72,z72,x73,y73,z73, x74,y74,z74,x75,y75,z75,x76,y76,z76,x77,y77,z77</pre>

- (Fındoráková, 2010) present this structure in the  $P2_1/n$  setting of space group #14. We used FINDSYM to change this to the standard  $P2_1/c$  setting.

### Simple Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4e)	C I
$\mathbf{B}_2$	$-x_1 \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_1 + c(z_1 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C I
$\mathbf{B}_3$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(4e)	C I
$\mathbf{B}_4$	$x_1 \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_1 + c(z_1 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C I
$\mathbf{B}_5$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4e)	C II
$\mathbf{B}_6$	$-x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_2 + c(z_2 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C II
$\mathbf{B}_7$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4e)	C II
$\mathbf{B}_8$	$x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C II
$\mathbf{B}_9$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4e)	C III
$\mathbf{B}_{10}$	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C III
$\mathbf{B}_{11}$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4e)	C III
$\mathbf{B}_{12}$	$x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C III
$\mathbf{B}_{13}$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4e)	C IV
$\mathbf{B}_{14}$	$-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C IV
$\mathbf{B}_{15}$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4e)	C IV
$\mathbf{B}_{16}$	$x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C IV
$\mathbf{B}_{17}$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4e)	C V
$\mathbf{B}_{18}$	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_5 + c(z_5 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C V
$\mathbf{B}_{19}$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4e)	C V
$\mathbf{B}_{20}$	$x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C V

$$\begin{aligned}
\mathbf{B}_{21} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= (ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}} &(4e) & \text{C VI} \\
\mathbf{B}_{22} &= -x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - &= -(ax_6 + c(z_6 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + &(4e) & \text{C VI} \\
&\quad (z_6 - \frac{1}{2}) \mathbf{a}_3 & \quad b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{23} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}} &(4e) & \text{C VI} \\
\mathbf{B}_{24} &= x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 &= (ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - &(4e) & \text{C VI} \\
& & \quad b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{25} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= (ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}} &(4e) & \text{C VII} \\
\mathbf{B}_{26} &= -x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - &= -(ax_7 + c(z_7 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + &(4e) & \text{C VII} \\
&\quad (z_7 - \frac{1}{2}) \mathbf{a}_3 & \quad b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{27} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}} &(4e) & \text{C VII} \\
\mathbf{B}_{28} &= x_7 \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 &= (ax_7 + c(z_7 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - &(4e) & \text{C VII} \\
& & \quad b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{29} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= (ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}} &(4e) & \text{C VIII} \\
\mathbf{B}_{30} &= -x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - &= -(ax_8 + c(z_8 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + &(4e) & \text{C VIII} \\
&\quad (z_8 - \frac{1}{2}) \mathbf{a}_3 & \quad b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{31} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 &= -(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}} &(4e) & \text{C VIII} \\
\mathbf{B}_{32} &= x_8 \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 &= (ax_8 + c(z_8 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - &(4e) & \text{C VIII} \\
& & \quad b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{33} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 &= (ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}} &(4e) & \text{C IX} \\
\mathbf{B}_{34} &= -x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - &= -(ax_9 + c(z_9 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + &(4e) & \text{C IX} \\
&\quad (z_9 - \frac{1}{2}) \mathbf{a}_3 & \quad b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{35} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 &= -(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}} &(4e) & \text{C IX} \\
\mathbf{B}_{36} &= x_9 \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 &= (ax_9 + c(z_9 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - &(4e) & \text{C IX} \\
& & \quad b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{37} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= (ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}} &(4e) & \text{C X} \\
\mathbf{B}_{38} &= -x_{10} \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 - &= -(ax_{10} + c(z_{10} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + &(4e) & \text{C X} \\
&\quad (z_{10} - \frac{1}{2}) \mathbf{a}_3 & \quad b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{39} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= -(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} - &(4e) & \text{C X} \\
& & \quad cz_{10} \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{40} &= x_{10} \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 + &= (ax_{10} + c(z_{10} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - &(4e) & \text{C X} \\
&\quad (z_{10} + \frac{1}{2}) \mathbf{a}_3 & \quad b(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{41} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 &= (ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}} &(4e) & \text{C XI} \\
\mathbf{B}_{42} &= -x_{11} \mathbf{a}_1 + (y_{11} + \frac{1}{2}) \mathbf{a}_2 - &= -(ax_{11} + c(z_{11} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + &(4e) & \text{C XI} \\
&\quad (z_{11} - \frac{1}{2}) \mathbf{a}_3 & \quad b(y_{11} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{11} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{43} &= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 &= -(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} - &(4e) & \text{C XI} \\
& & \quad cz_{11} \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{44} &= x_{11} \mathbf{a}_1 - (y_{11} - \frac{1}{2}) \mathbf{a}_2 + &= (ax_{11} + c(z_{11} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - &(4e) & \text{C XI} \\
&\quad (z_{11} + \frac{1}{2}) \mathbf{a}_3 & \quad b(y_{11} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{45} &= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 &= (ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}} &(4e) & \text{C XII} \\
\mathbf{B}_{46} &= -x_{12} \mathbf{a}_1 + (y_{12} + \frac{1}{2}) \mathbf{a}_2 - &= -(ax_{12} + c(z_{12} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + &(4e) & \text{C XII} \\
&\quad (z_{12} - \frac{1}{2}) \mathbf{a}_3 & \quad b(y_{12} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{12} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{47} &= -x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3 &= -(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} - &(4e) & \text{C XII} \\
& & \quad cz_{12} \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{48} &= x_{12} \mathbf{a}_1 - (y_{12} - \frac{1}{2}) \mathbf{a}_2 + &= (ax_{12} + c(z_{12} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - &(4e) & \text{C XII} \\
&\quad (z_{12} + \frac{1}{2}) \mathbf{a}_3 & \quad b(y_{12} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{12} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}
\end{aligned}$$























## References

- [1] L. Findorá'ková, K. Györyová, M. K. J. Moncol, and M. Melník, *Crystal Structure and Physical Characterisation of  $[Zn_2(Benzoato)_4(Caffeine)_2] \cdot 2 Caffeine$* , *J. Chem. Crystallogr.* **40**, 145–150 (2010), doi:10.1007/s10870-009-9619-8.