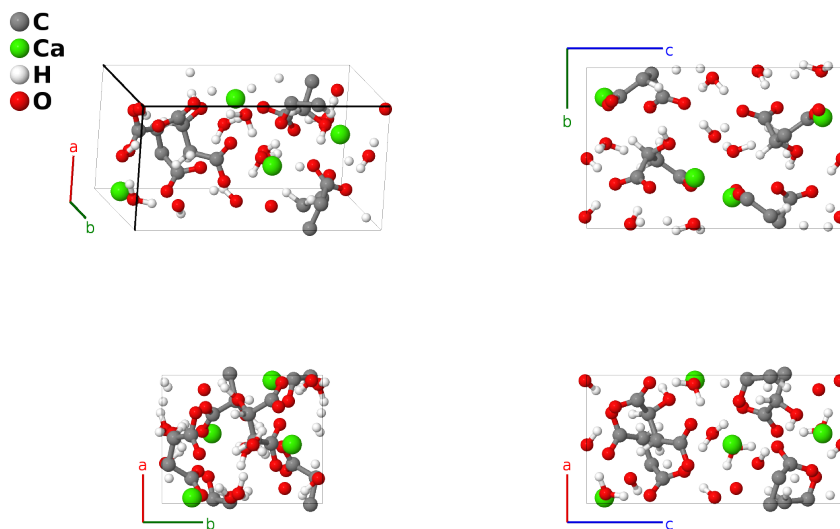


Ca-Malate-dihydrate ($\text{CaC}_4\text{H}_8\text{O}_7 \cdot 2\text{H}_2\text{O}$) Structure: A4BC8D7_oP80_19_4a_a_8a_7a-001

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<https://aflow.org/p/RRH1>

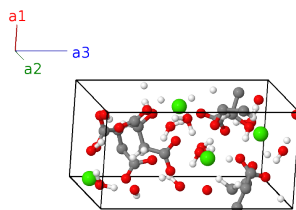
https://aflow.org/p/A4BC8D7_oP80_19_4a_a_8a_7a-001



Prototype	$\text{C}_4\text{CaH}_8\text{O}_7$
AFLOW prototype label	A4BC8D7_oP80_19_4a_a_8a_7a-001
ICSD	None
Pearson symbol	oP80
Space group number	19
Space group symbol	$P2_12_12_1$
AFLOW prototype command	<pre>aflow --proto=A4BC8D7_oP80_19_4a_a_8a_7a-001 --params=a, b/a, c/a, 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</pre>

Simple Orthorhombic primitive vectors

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



$$\begin{aligned}
\mathbf{B}_{28} &= (x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3 = a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (4a) & \text{H II} \\
\mathbf{B}_{29} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (4a) & \text{H III} \\
\mathbf{B}_{30} &= -(x_8 - \frac{1}{2}) \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 = -a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{H III} \\
\mathbf{B}_{31} &= -x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3 = -ax_8 \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{H III} \\
\mathbf{B}_{32} &= (x_8 + \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3 = a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (4a) & \text{H III} \\
\mathbf{B}_{33} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (4a) & \text{H IV} \\
\mathbf{B}_{34} &= -(x_9 - \frac{1}{2}) \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 = -a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{H IV} \\
\mathbf{B}_{35} &= -x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3 = -ax_9 \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{H IV} \\
\mathbf{B}_{36} &= (x_9 + \frac{1}{2}) \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3 = a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (4a) & \text{H IV} \\
\mathbf{B}_{37} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (4a) & \text{H V} \\
\mathbf{B}_{38} &= -(x_{10} - \frac{1}{2}) \mathbf{a}_1 - y_{10} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3 = -a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{H V} \\
\mathbf{B}_{39} &= -x_{10} \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3 = -ax_{10} \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{H V} \\
\mathbf{B}_{40} &= (x_{10} + \frac{1}{2}) \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 - z_{10} \mathbf{a}_3 = a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (4a) & \text{H V} \\
\mathbf{B}_{41} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 = ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (4a) & \text{H VI} \\
\mathbf{B}_{42} &= -(x_{11} - \frac{1}{2}) \mathbf{a}_1 - y_{11} \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3 = -a(x_{11} - \frac{1}{2}) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{H VI} \\
\mathbf{B}_{43} &= -x_{11} \mathbf{a}_1 + (y_{11} + \frac{1}{2}) \mathbf{a}_2 - (z_{11} - \frac{1}{2}) \mathbf{a}_3 = -ax_{11} \hat{\mathbf{x}} + b(y_{11} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{11} - \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{H VI} \\
\mathbf{B}_{44} &= (x_{11} + \frac{1}{2}) \mathbf{a}_1 - (y_{11} - \frac{1}{2}) \mathbf{a}_2 - z_{11} \mathbf{a}_3 = a(x_{11} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{11} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (4a) & \text{H VI} \\
\mathbf{B}_{45} &= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 = ax_{12} \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (4a) & \text{H VII} \\
\mathbf{B}_{46} &= -(x_{12} - \frac{1}{2}) \mathbf{a}_1 - y_{12} \mathbf{a}_2 + (z_{12} + \frac{1}{2}) \mathbf{a}_3 = -a(x_{12} - \frac{1}{2}) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + c(z_{12} + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{H VII} \\
\mathbf{B}_{47} &= -x_{12} \mathbf{a}_1 + (y_{12} + \frac{1}{2}) \mathbf{a}_2 - (z_{12} - \frac{1}{2}) \mathbf{a}_3 = -ax_{12} \hat{\mathbf{x}} + b(y_{12} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{12} - \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{H VII} \\
\mathbf{B}_{48} &= (x_{12} + \frac{1}{2}) \mathbf{a}_1 - (y_{12} - \frac{1}{2}) \mathbf{a}_2 - z_{12} \mathbf{a}_3 = a(x_{12} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{12} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}} & (4a) & \text{H VII} \\
\mathbf{B}_{49} &= x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3 = ax_{13} \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (4a) & \text{H VIII} \\
\mathbf{B}_{50} &= -(x_{13} - \frac{1}{2}) \mathbf{a}_1 - y_{13} \mathbf{a}_2 + (z_{13} + \frac{1}{2}) \mathbf{a}_3 = -a(x_{13} - \frac{1}{2}) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + c(z_{13} + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{H VIII} \\
\mathbf{B}_{51} &= -x_{13} \mathbf{a}_1 + (y_{13} + \frac{1}{2}) \mathbf{a}_2 - (z_{13} - \frac{1}{2}) \mathbf{a}_3 = -ax_{13} \hat{\mathbf{x}} + b(y_{13} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{13} - \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{H VIII} \\
\mathbf{B}_{52} &= (x_{13} + \frac{1}{2}) \mathbf{a}_1 - (y_{13} - \frac{1}{2}) \mathbf{a}_2 - z_{13} \mathbf{a}_3 = a(x_{13} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{13} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{13} \hat{\mathbf{z}} & (4a) & \text{H VIII} \\
\mathbf{B}_{53} &= x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3 = ax_{14} \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (4a) & \text{O I} \\
\mathbf{B}_{54} &= -(x_{14} - \frac{1}{2}) \mathbf{a}_1 - y_{14} \mathbf{a}_2 + (z_{14} + \frac{1}{2}) \mathbf{a}_3 = -a(x_{14} - \frac{1}{2}) \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + c(z_{14} + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O I}
\end{aligned}$$

References

- [1] C.-I. Brädín and B.-O. Söderberg, *The Crystal Structure of Ca-Malate-dihydrate, $CaC_4H_4O_5 \cdot 2H_2O$* , Acta Chem. Scand. **20**, 730–738 (1966), doi:10.3891/acta.chem.scand.20-0730.