

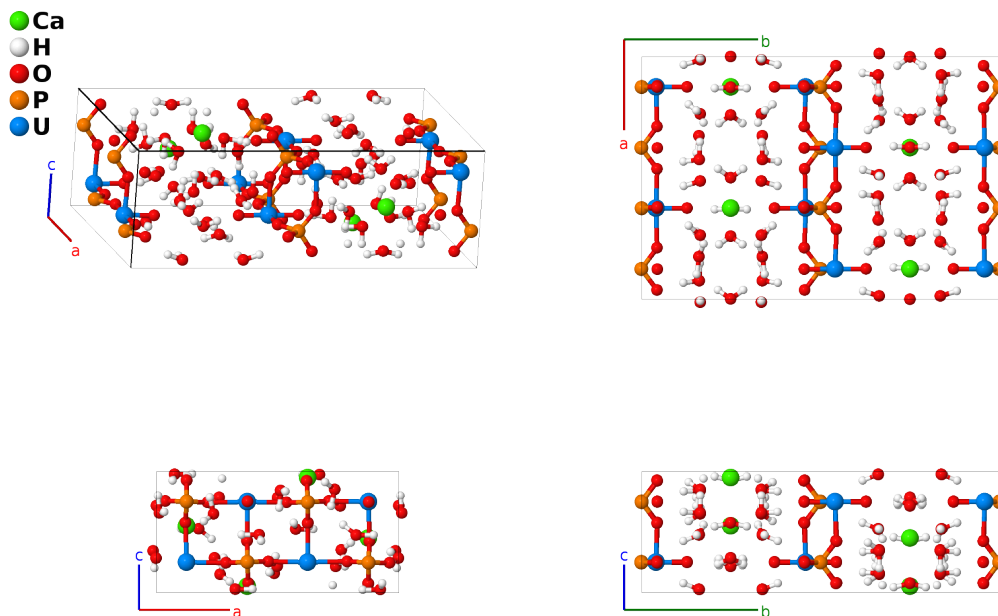
# Autunite $\text{Ca}[(\text{UO}_2)(\text{PO}_4)]_2(\text{H}_2\text{O})_{11}$ Structure: AB22C23D2E2\_oP200\_62\_c\_11d\_3c10d\_d\_d-001

This structure originally had the label AB22C23D2E2\_oP200\_62\_c\_11d\_3c10d\_d\_d. Calls to that address will be redirected here.

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

[https://aflow.org/p/AB22C23D2E2\\_oP200\\_62\\_c\\_11d\\_3c10d\\_d\\_d-001](https://aflow.org/p/AB22C23D2E2_oP200_62_c_11d_3c10d_d_d-001)



|                         |  |
|-------------------------|--|
| Prototype               | $\text{CaH}_{22}\text{O}_{23}\text{P}_2\text{U}_2$   |
| AFLOW prototype label   | AB22C23D2E2_oP200_62_c_11d_3c10d_d_d-001   |
| Mineral name            | autunite   |
| ICSD                    | 96812  |
| Pearson symbol          | oP200  |
| Space group number      | 62   |
| Space group symbol      | $Pnma$   |
| AFLOW prototype command | <pre>aflow --proto=AB22C23D2E2_oP200_62_c_11d_3c10d_d_d-001       --params=a, b/a, c/a, x1, z1, x2, z2, x3, z3, x4, 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</pre> |

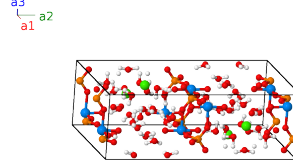
- Autunite,  $\text{Ca}(\text{UO}_2)_2(\text{PO}_4)_2 \cdot n\text{H}_2\text{O}$ , is found in three varieties:

- Naturally occurring autunite, with  $n > 10$ , and
- partially dehydrated meta-autunite (I) ( $6 \leq n \leq 10$ ).
- Further dehydration in the laboratory produces meta-autunite (II).
- The original determination of the autunite structure designated  $H5_9$  by (Herrmann, 1941) was a tetragonal structure, none of the positions of the oxygen atom or water molecules was determined. (Locock, 2003) find a pseudo-tetragonal ( $a \approx 2c$ ) unit cell which doubles the size of the original cell. They were able to locate all of the atoms in the structure.
- (Locock, 2003) found the (4c) calcium site to be occupied only 86% of the time.

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### Simple Orthorhombic primitive vectors

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




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### Basis vectors

|                   | Lattice coordinates   |     | Cartesian coordinates  | Wyckoff position | Atom type |
|-------------------|---|-----|--|------------------|-----------|
| $\mathbf{B}_1$    | $= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$                                  | $=$ | $ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$                                  | (4c)             | Ca I      |
| $\mathbf{B}_2$    | $= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$ | (4c)             | Ca I      |
| $\mathbf{B}_3$    | $= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$                                 | $=$ | $-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$                                 | (4c)             | Ca I      |
| $\mathbf{B}_4$    | $= (x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$  | (4c)             | Ca I      |
| $\mathbf{B}_5$    | $= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$                                  | $=$ | $ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$                                  | (4c)             | O I       |
| $\mathbf{B}_6$    | $= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$ | (4c)             | O I       |
| $\mathbf{B}_7$    | $= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$                                 | $=$ | $-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$                                 | (4c)             | O I       |
| $\mathbf{B}_8$    | $= (x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$  | (4c)             | O I       |
| $\mathbf{B}_9$    | $= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$                                  | $=$ | $ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$                                  | (4c)             | O II      |
| $\mathbf{B}_{10}$ | $= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$ | (4c)             | O II      |
| $\mathbf{B}_{11}$ | $= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$                                 | $=$ | $-ax_3 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$                                 | (4c)             | O II      |
| $\mathbf{B}_{12}$ | $= (x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$  | (4c)             | O II      |
| $\mathbf{B}_{13}$ | $= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$                                  | $=$ | $ax_4 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$                                  | (4c)             | O III     |
| $\mathbf{B}_{14}$ | $= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$ | (4c)             | O III     |
| $\mathbf{B}_{15}$ | $= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$                                 | $=$ | $-ax_4 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$                                 | (4c)             | O III     |
| $\mathbf{B}_{16}$ | $= (x_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$  | (4c)             | O III     |
| $\mathbf{B}_{17}$ | $= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$  | $=$ | $ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$  | (8d)             | H I       |
| $\mathbf{B}_{18}$ | $= -(x_5 - \frac{1}{2}) \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$         | $=$ | $-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$         | (8d)             | H I       |
| $\mathbf{B}_{19}$ | $= -x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$                         | $=$ | $-ax_5 \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$                         | (8d)             | H I       |















## References

- [1] A. J. Locock and P. C. Burns, *The crystal structure of synthetic autunite,  $Ca[(UO_2)(PO_4)]_2(H_2O)_{11}$* , Am. Mineral. **88**, 240–244 (2003), doi:10.2138/am-2003-0128.
- [2] K. Herrmann, ed., *Strukturbericht Band VI 1938* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1941).

## Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).