

NAME _____
HW 6

Characterization of Materials
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Space Group **62** is **Pnma** (orthorhombic) has crystals such as **Perovskites** (**CaTiO₃** **LaMnO₃**)

Pnma (No. 62) Wyckoff Positions

Multiplicity Wyckoff Letter Coordinates (fractional, conventional setting)

4	a	(0, 0, 0)
4	b	(0, $\frac{1}{2}$, 0)
4	c	($\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$)
4	d	(x, $\frac{1}{4}$, z)
8	e	(x, y, z)
4	f	(x, 0, z)
4	g	(x, $\frac{1}{2}$, z)

CaTiO₃ in Pnma has the 4 Ca atoms start at **(0.487, 0.25, 0.991)** and the 4 Ti start at **(0,0,0)**

Similar to others, like F has the start position and the face centering translations, or I that adds (1/2, 1/2, 1/2,) to the starting position, Pnma has the following added translations to the starting position: (1/2, 1/2, 1/2), (0, 1/2, 0), (1/2, 0, 1/2).

AI SAYS: Ca occupies **4c** positions; Ti occupies **4a** positions.

Question: did AI give the correct Wyckoff letter for the Ca atoms and if not, what is the correct Wyckoff letter (a, b, c, d, e, f, g) and why?. ANS letter _____
Why?