

Supplementary Table Standardized atomic positions of Ca₂PO₄Cl

Site	Atom	Wyckoff position	<i>x</i>	<i>y</i>	<i>z</i>	sof
Ca1	Ca ²⁺	4 <i>c</i>	0.6336(1)	0.25	0	1
Ca2	Ca ²⁺	4 <i>d</i>	0.1286(2)	0.0280(1)	0.25	1
P1	P ⁵⁺	4 <i>c</i>	0.1381(2)	0.25	0	1
O1	O ²⁻	8 <i>e</i>	0.0105(4)	0.7723(3)	0.1145(1)	1
O2	O ²⁻	8 <i>e</i>	0.2840(4)	0.0764(3)	0.0233(2)	1
Cl1	Cl ¹⁻	4 <i>d</i>	0.5185(2)	0.2827(3)	0.25	1

Original data taken from literature (Greenblatt *et al.*, 1967)