

Table S1. The hexagonal symmetry-P63/m space group. Retrieved from Journal of Applied Crystallography, 43,320-327,2010.

a	b	c	α	β	γ	
9.421	9.421	6.88	90	90	120	
Atom	Site	Occ	x	y	z	U
Ca	4f	0.33333	0.33333	0.6667	0.00092	0.019
Ca	6h	1	0.24525	0.99333	0.25	0.019
P	6h	1	0.39811	0.36952	0.25	0.019
O	6h	1	0.32711	0.48474	0.25	0.019
O	6h	1	0.58616	0.465	0.25	0.019
O	12i	1	0.43152	0.25583	0.07261	0.019
O	4e	0.5	0	0	0.18819	0.019