

Table S1. Relative atomic coordinates of the calculated model of the priscillagrewite-(Y) structure with the  $a$  parameter = 12.50 Å.

Site	Atom	$x$	$y$	$z$
$X$	0.73Ca+0.27Y	0.125	0	0.25
$Y$	0.9Zr+0.07Ti+0.03Sb	0	0	0
$Z$	0.6Al+0.4Fe	0.375	0	0.25
O	O	0.032	0.054	0.653