

$(\text{Ca}_{0.05}\text{Y}_{0.95})_3\text{Cu}_3\text{O}_{7.62}$  $hP40$  $(176) P6_3/m - ih^2\Gamma^2eca$  $(\text{Y}_{0.95}\text{Ca}_{0.05})\text{CuO}_{2.54}$  [1]

Structural features: Puckered triangle-mesh  $(\text{Y,Ca})_3\text{O}_6$  layers alternate with planar  $\text{Cu}_3\text{O}_2$  layers (Cu triangle mesh with part of the triangles centered by O) (disordered vacancies and site splitting).  $(\text{Y,Ca})\text{O}_8$  cubes,  $(\text{Y,Ca})\text{O}_7$  deficient cubes (one vertex missing) and distorted  $\text{CuO}_4$  squares share atoms to form a 3D-framework.

Natali Sora I. et al. (1997) [1]

 $\text{Ca}_{0.15}\text{Cu}_3\text{O}_{7.62}\text{Y}_{2.85}$  $a = 0.61991$  nm,  $c = 1.12059$  nm,  $c/a = 1.808$ ,  $V = 0.3729$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12i	1	0.345	0.0182	0.0879		
Cu2	6h	$m..$	0.023	0.338	$\frac{1}{4}$	0.81	
Cu3	6h	$m..$	0.399	0.04	$\frac{1}{4}$	0.19	
M4	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.028	0.5	
M5	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.5053	0.5	
M6	4e	3..	0	0	0.028	0.5	
O7	2c	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.81	
O8	2a	$-6..$	0	0	$\frac{1}{4}$	0.81	coplanar triangle $\text{Cu}_3$

 $\text{M4} = 0.95\text{Y} + 0.05\text{Ca}$ ;  $\text{M5} = 0.95\text{Y} + 0.05\text{Ca}$ ;  $\text{M6} = 0.95\text{Y} + 0.05\text{Ca}$ Experimental: powder, diffractometer, neutrons,  $R_p = 0.071$ ,  $T = 293$  K

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Natali Sora I., Huang Q., Santoro A., Cava R.J., Krajewski J.J., Peck W.F. Jr. (1997), Nuovo Cimento Soc. Ital. Fis. D 19, 1093-1101.