

Lu₃Co_{7.77}Sn₄***hP30*****(186) *P6₃mc* – c⁴b²a****Lu₃Co_{7.77}Sn₄** [2]; Ca₃Ni₈In₄ [3]

Structural features: Lu₃(Co₃) layers (the Lu atoms and the centers of Co₃ triangles form a triangle mesh) and puckered Co₅Sn₄ layers (a CoSn hexagon mesh with every fourth hexagon centered by an additional Co) alternate along [001]. Lu₃ trigonal clusters perpendicular to [001] are interconnected via Lu-Lu distances of similar length to form a 3D-framework. Substitution derivative of BaLi₄.

Canepa F. et al. (2000) [1]

Co_{7.93}Lu₃Sn₄*a* = 0.8757, *c* = 0.7446 nm, *c/a* = 0.850, *V* = 0.4945 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Co1	6 <i>c</i>	. <i>m</i> .	0.163	0.837	0.0598		pseudo Frank-Kasper Co ₅ Sn ₄ Lu ₄
Sn2	6 <i>c</i>	. <i>m</i> .	0.1724	0.8276	0.4282		icosahedron Co ₈ Lu ₄
Lu3	6 <i>c</i>	. <i>m</i> .	0.5255	0.4745	0.2153		pseudo Frank-Kasper Co ₈ Sn ₆ Lu ₄
Co4	6 <i>c</i>	. <i>m</i> .	0.8983	0.1017	0.2464		icosahedron Co ₇ Sn ₃ Lu ₂
Sn5	2 <i>b</i>	3. <i>m</i> .	¹ / ₃	² / ₃	0.0165		bicapped square prism Co ₄ Lu ₆
Co6	2 <i>b</i>	3. <i>m</i> .	¹ / ₃	² / ₃	0.3693	0.93	pseudo Frank-Kasper Sn ₄ Lu ₆ Co ₃
Co7	2 <i>a</i>	3. <i>m</i> .	0	0	0.0		icosahedron Co ₉ Sn ₃

Transformation from published data: origin shift 0 0 0.2847

Experimental: single crystal, diffractometer, X-rays, R = 0.035

Remarks: Identical to the phases called RCo₃Sn in the literature. Vacancies were observed only for the Lu-compound.

References: [1] Canepa F., Cirafici S., Fornasini M.L., Manfrinetti P., Merlo F., Palenzona A., Pani M. (2000), J. Alloys Compd. 297, 109-113. [2] Skolozdra R., Garcia Landa B., Fruchart D., Gignoux D., Soubeyroux J.L., Aksel'rud L. (1996), J. Alloys Compd. 235, 210-215. [3] Zaremba V.I., Muts I.R., Kalychak Y.M., Hoffmann R.D., Pöttgen R. (2001), J. Solid State Chem. 160, 415-420.