

(Sr<sub>0.77</sub>Nd<sub>0.23</sub>)<sub>5</sub>Cu(Ce<sub>0.85</sub>Nd<sub>0.15</sub>)<sub>3</sub>O<sub>12.08</sub>

*hP28*

(189) *P-62m* – *k*<sup>2</sup>*gf*<sup>3</sup>*ec*

**Sr<sub>3.87</sub>Ce<sub>2.56</sub>Nd<sub>1.57</sub>CuO<sub>12.08</sub>** [1]

Structural features: Three infinite chains of edge-linked (Ce,Nd)O<sub>6</sub> octahedra are interconnected via common vertices with (Cu<sup>2+</sup>)O<sub>4</sub> tetrahedra (in part replaced by Cu<sup>+</sup>O<sub>2</sub> units).

Miyazaki Y. et al. (1999) [1]

Ce<sub>2.57</sub>CuNd<sub>1.57</sub>O<sub>12</sub>Sr<sub>3.86</sub>

*a* = 1.01849, *c* = 0.36289 nm, *c/a* = 0.356, *V* = 0.3260 nm<sup>3</sup>, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>k</i>	<i>m</i> ..	0.1108	0.1396	<sup>1</sup> / <sub>2</sub>	0.167	
O2	6 <i>k</i>	<i>m</i> ..	0.2497	0.4449	<sup>1</sup> / <sub>2</sub>		single atom Ce
M3	3 <i>g</i>	<i>m2m</i>	0.3325	0	<sup>1</sup> / <sub>2</sub>		octahedron O <sub>6</sub>
O4	3 <i>f</i>	<i>m2m</i>	0.1809	0	0	0.667	
O5	3 <i>f</i>	<i>m2m</i>	0.4597	0	0		coplanar triangle Ce <sub>2</sub> Sr
M6	3 <i>f</i>	<i>m2m</i>	0.6913	0	0		
Cu7	2 <i>e</i>	3. <i>m</i>	0	0	0.0952	0.5	
M8	2 <i>c</i>	-6..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0		tricapped trigonal prism O <sub>9</sub>

M3 = 0.857Ce + 0.143Nd; M6 = 0.660Sr + 0.340Nd; M8 = 0.942Sr + 0.058Nd

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: powder, diffractometer, neutrons, time-of-flight, *wR<sub>p</sub>* = 0.018

Remarks: Refinement on combined X-ray and neutron diffraction data. Short interatomic distances for partly occupied site(s).

References: [1] Miyazaki Y., Edwards P.P., Amamoto Y. (1999), Chem. Mater. 11, 564-568.