

Co <sub>3</sub> H	<i>hP</i> 12	(186) <i>P</i> 6 <sub>3</sub> <i>mc</i> – b <sup>3</sup> a <sup>3</sup>
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**CoH<sub>0.34</sub>** [1]

Structural features: Close-packed Co layers in h stacking; H in octahedral voids, with a strong preference for voids in every third interlayer.

Fedotov V.K. et al. (1999) [1]

Co<sub>3</sub>H<sub>1.01</sub>

$a = 0.2555$ ,  $c = 1.2406$  nm,  $c/a = 4.856$ ,  $V = 0.0701$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Co1	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.08767		trigonal prism H <sub>6</sub>
Co2	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.41167		trigonal prism H <sub>6</sub>
Co3	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.75		trigonal prism H <sub>6</sub>
H4	2 <i>a</i>	3 <i>m.</i>	0	0	0.0	0.97	octahedron Co <sub>6</sub>
H5	2 <i>a</i>	3 <i>m.</i>	0	0	0.16667	0.02	octahedron Co <sub>6</sub>
H6	2 <i>a</i>	3 <i>m.</i>	0	0	0.33333	0.02	octahedron Co <sub>6</sub>

Transformation from published data (*P*6<sub>3</sub>): origin shift 0 0 0.33333

Experimental: powder, diffractometer, neutrons,  $R_p = 0.090$ ,  $T = 120$  K

Remarks: Phase stable at  $T < 230$ -260 K; homogeneity range CoH<sub>x</sub>,  $0.34 < x < 0.5$ . The description in space group (173) *P*6<sub>3</sub> in [1] does not take into consideration all symmetry elements of the proposed structure.

References: [1] Fedotov V.K., Antonov V.E., Antonova T.E., Bokhenkov E.L., Dorner B., Grosse G., Wagner F.E. (1999), J. Alloys Compd. 291, 1-7.