

$\text{Cd}_{0.57}\text{Mn}_{0.43}\text{S}$	$hP6$	$(186) P6_3mc - b^3$
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# $\text{Cd}_{0.57}\text{Mn}_{0.43}\text{S}$ [1]

Structural features: Close-packed S layers in h stacking; (Cd,Mn) in tetrahedral voids (stacking sequence BbCc, distinct positions for Cd and Mn). (Cd,Mn) $\text{S}_4$  tetrahedra share vertices to form a 3D-framework. Variant of ZnO with site splitting.

Rodic D. et al. (1996) [1]

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$a = 0.40683$ ,  $c = 0.66007$  nm,  $c/a = 1.622$ ,  $V = 0.0946$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Mn1	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.0	0.43	
Cd2	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.018	0.57	
S3	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.393		

Transformation from published data:  $-x, -y, -z$ ; origin shift 0 0 0.107

Experimental: powder, diffractometer, X-rays,  $R_B = 0.043$

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

References: [1] Rodic D., Spasojevic V., Bajorek A., Onnerud P. (1996), J. Magn. Magn. Mater. 152, 159-164.