

Superconductivity with high hardness in Mo_3C_2

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Supporting information

Table S1 Experiment data and the crystal details obtained from the Rietveld refinement

Identification code		Mo_3C_2	
Formula weight		311.84	
Radiation		Cu $K\alpha$	
Wavelength (Å)		1.5418	
Crystal system		Hexagonal	
Space group		$P6/mmm$	
Unit cell dimensions (Å)		$a = b = 3.016$	
		$c = 14.6444(3)$	
		$\alpha = \beta = 90^\circ$	
		$\gamma = 120^\circ$	
Volume (Å ³)		115.36(0)	
Θ range/degree		20 - 80	
Residuals		$R_p = 0.0807$	
		$R_{wp} = 0.1152$	
		$\chi^2 = 5.407$	
Atomic position	Wyckoff	(x, y, z)	Occupation
Mo1	2b	(0,0,0.2500)	1
Mo2	4f	(0.33333,0.66667,0.08467)	1
C1	2a	(0,0,0)	0.7981
C2	4f	(0.33333,0.66667,0.66981)	0.5037