

Supplementary materials

# Pressure Induced Disorder-Order Phase Transitions in the Al<sub>4</sub>Cr Phases

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**Citation:** Fan, C.; Geng, X.; Wen, B. Pressure Induced Disorder-Order Phase Transitions in the Al<sub>4</sub>Cr Phases. *Crystals* **2022**, *12*, 1008. <https://doi.org/10.3390/cryst12071008>

Academic Editor: Daniel Errandonea

Received: 23 June 2022

Accepted: 19 July 2022

Published: 21 July 2022

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**Table S1.** The Wyckoff positions of the centered atoms inside the Macky or pseudo-Macky cluster for the  $\epsilon$ - and  $\mu$ -Al<sub>4</sub>Cr phase along with the  $\eta$ -Al<sub>11</sub>Cr<sub>2</sub> phase.

Nanocluster Type	Phase	Center Atom Coordinates of Nanocluster
Macky (1 @ 12@42)	$\epsilon$ -Al <sub>4</sub> Cr 1 @ 12@42	Cr10(0.50000,-0.06080,0.25000) (4c; m2m)
	$\eta$ -Al <sub>11</sub> Cr <sub>2</sub> pseudo-Macky 1 @ 12@38	Cr11(0.25000,0.75000,0.50000) (4c; -1)
	$\mu$ - Al <sub>4</sub> Cr pseudo-Macky 1 @ 12@ 41	Cr2(0.00000,0.00000,0.25000) (2b;-6m2)
	$\theta$ - Al <sub>45</sub> Cr <sub>7</sub> pseudo-Macky 1 @ 12@ 38	Cr3(0.50000,0.50000,0.50000) (2c; 2/m)
1 @ 12@46	$\epsilon$ -Al <sub>4</sub> Cr	Al13(0.50000, 0.18285, 0.25000) (4c; m2m)
		Al14(0.50000,0.07444, 0.25000) (4c; m2m)
		Al17(0.50000,0.25398,0.17920) (8f; m..)
		Al23(0.00000,0.19190,0.51390) (8f; m..)
		Al27(0.81860,0.14117,0.13300) (16h 1)
	$\eta$ -Al <sub>11</sub> Cr <sub>2</sub>	Al36(0.44124, 0.64688, 0.49235) (8f; 1)
		Al28(0.75770, 0.85334, 0.80867) (8f; 1)
$\mu$ - Al <sub>4</sub> Cr	Al3(0.25590,0.36707,0.49559) (24l; 1)	
	Al10(0.03077,-0.41351,0.15948) (24l; 1)	
	Al22(0.50978,0.49022,0.25000) (6h; mm2)	
		Al23(-0.23891,0.38054,0.25000 6h mm2)