

Supplementary materials

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

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**Table S1.** The Wyckoff positions of the centered atoms inside the Macky or pseudo-Mackay 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
Mackay (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-Mackay 1 @ 12 @ 38	Cr11(0.25000, 0.75000, 0.50000) (4c; -1)
	$\mu$ -Al <sub>4</sub> Cr pseudo-Mackay 1 @ 12 @ 41	Cr2(0.00000, 0.00000, 0.25000) (2b; -6m2)
	$\theta$ -Al <sub>45</sub> Cr <sub>7</sub> pseudo-Mackay 1 @ 12 @ 38	Cr3(0.50000, 0.50000, 0.50000) (2c; 2/m)
		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)
1 @ 12 @ 46	$\epsilon$ -Al <sub>4</sub> Cr	
	$\eta$ -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)