

Supporting Information

**The effects of ordered carbon vacancies on stability and
thermo-mechanical properties of V_8C_7 compared with VC**

XiaoYu Chong, YeHua Jiang, Rong Zhou and Jing Feng^{*}

Faculty of Material Science and Engineering, Kunming University of Science and Technology, Kunming 650093,

People's Republic of China

Table S1 Structural information for ordered VC and V_8C_7

Phase	VC	V_8C_7
Space group	Fm-3m	P4 ₃ 32
Z	4	4
Volume (Å ³)	72.25	582.18
Density (g/cm ³)	5.79	5.61
a (Å)	4.165	8.350
V Wyckoff site	4a (0, 0, 0)	8c (0.375, 0.375, 0.375)
		24e (0.125, 0.375, 0.125)
C Wyckoff site	4b (0.5, 0.5, 0.5)	4a (0.125, 0.125, 0.125)
		12d (0.125, 0.625, 0.625)
		12d (0.125, 0.375, 0.875)

Corresponding author: Tel:+1 6174964295, Fax:+1 857-259-2445
E-mails address: jingfeng@kmust.edu.cn