Supplemental Material to the article "Phase Transitions in Tungsten Monoborides"

Crystal data

Table S1. Crystal structures of WB phases

Phase	Volume (Å^3/atom)	ρ (g/cm)^3	Lattice parameters	Coordinates			
				Atom	x	y	z
α-WB	10.44 10.3 [1]	15.48	$a = 3.139$ Å $c = 16.954$ Å $a = 3.115$ Å[1] $c = 16.930$ Å[1] $a = 3.116$ Å[2] $c = 16.930$ Å[2] $a = 3.126$ Å[3] $c = 16.901$ Å[3]	W B	0.000 0.000	0.000 0.000	0.803 0.656
β-WB	10.45	15.46	$a = 3.173$ Å $b = 8.501$ Å $c = 3.099$ Å	W B	0.000 0.000	−0.355 −0.061	0.250 0.250
$P\bar{4}2_1m$-WB	10.75	15.03	$a = b = 4.334$ Å $c = 6.861$ Å	W1 W2 B1 B2	0.000 0.754 0.753 0.500	0.000 0.254 0.747 0.000	0.500 0.131 0.239 0.383

Crystal structures of WB phases

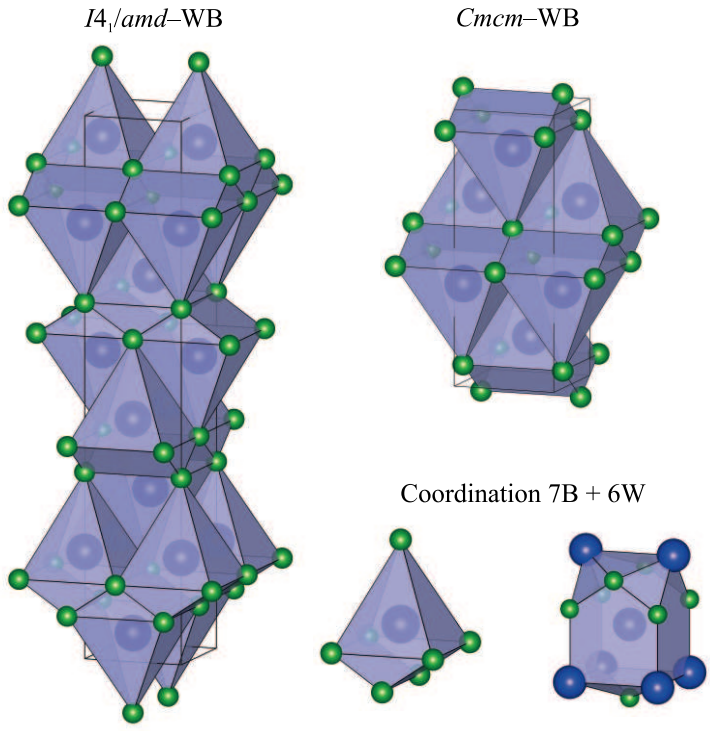

Fig. S1. Crystal structure of $I4_1/amd$ and $Cmcm$ phases

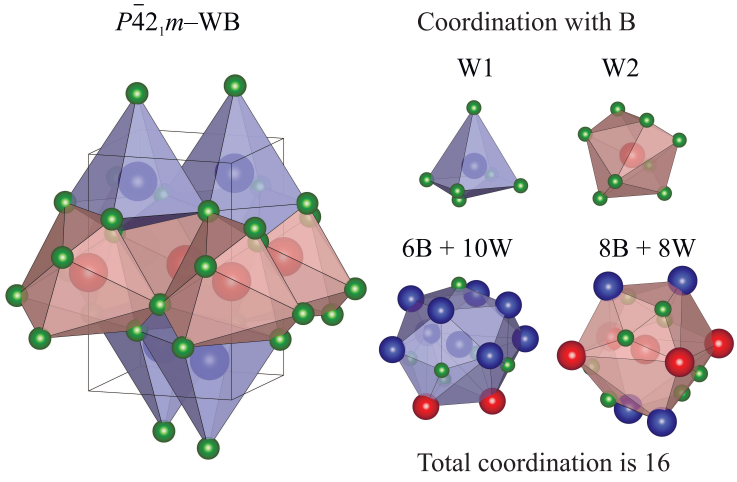

Fig. S2. Crystal structure of $P\bar{4}2_1m$-WB

Details of phase transition

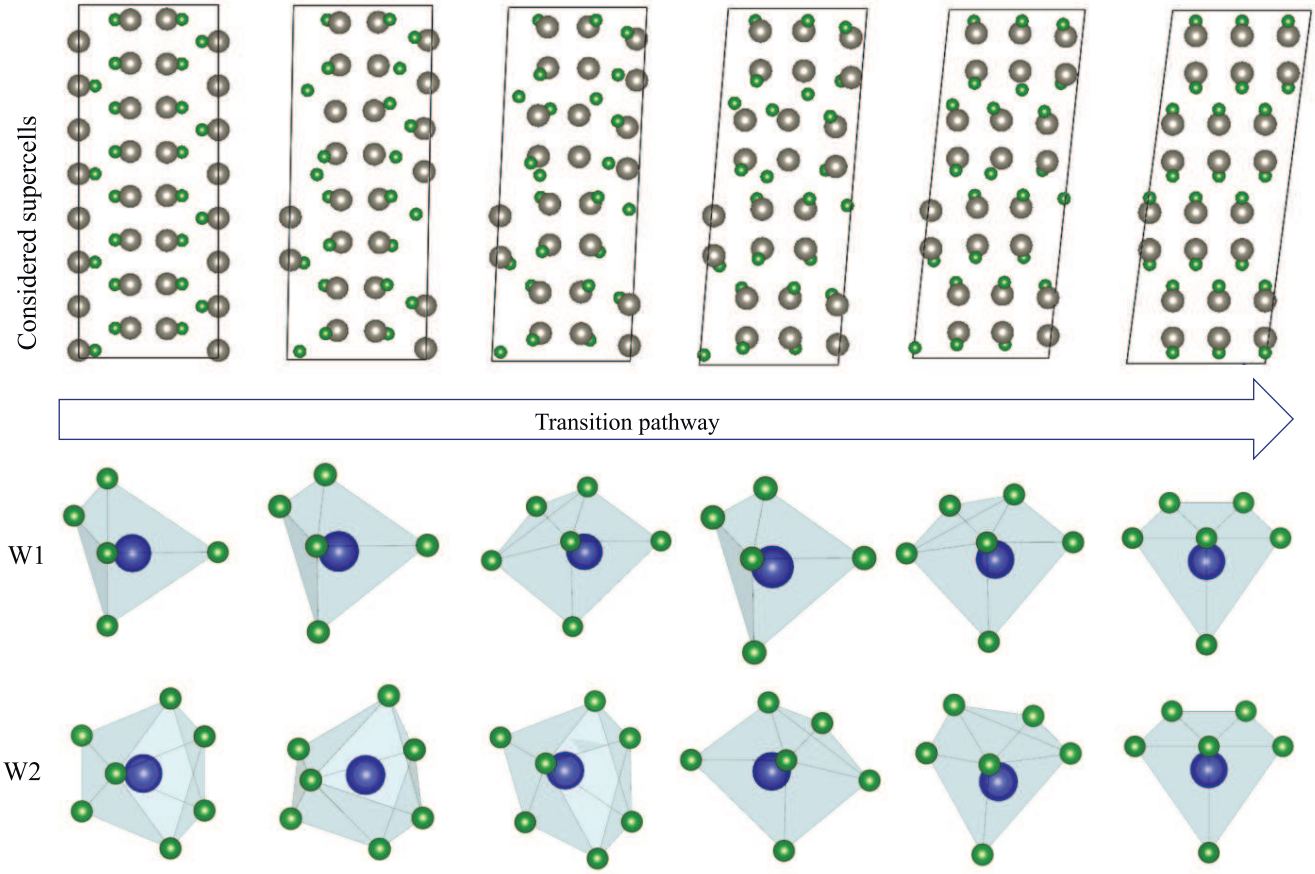

Fig. S3. (Top) Changes in crystal structure during the phase transition. (Bottom) Changes on boron coordination of symmetrically inequivalent atoms during the phase transition