Supplementary Information for the paper entitled

"**Superconductivity of Pressure Stabilized Vanadium Hydrides"**

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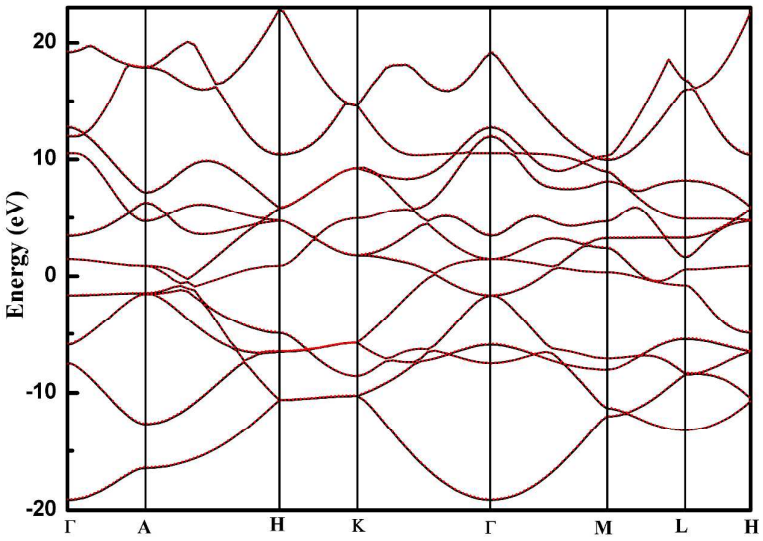

Figure S1 The band structure of $P6_3/mmc$-VH_5 at 200GPa. The black and red lines represented GGA and GGA+U, respectively.

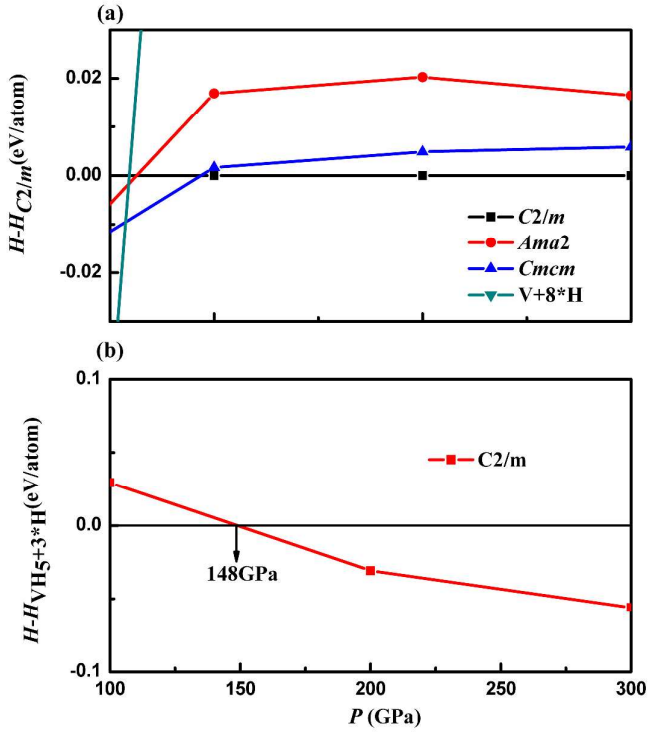

Figure S2 Calculated enthalpies per atom of various structures for VH_8 in the pressure range of 0–300 GPa with respect to $C2/m$ phase (a) and VH_5 and H_2 (b).

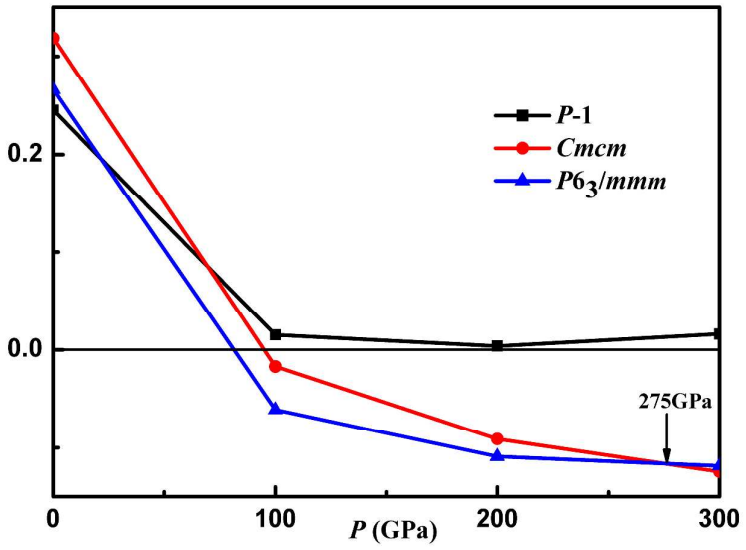

Figure S3 Calculated enthalpies per atom of various structures for VH_5 in the pressure range of 0–300 GPa with respect to VH_2 and H_2.

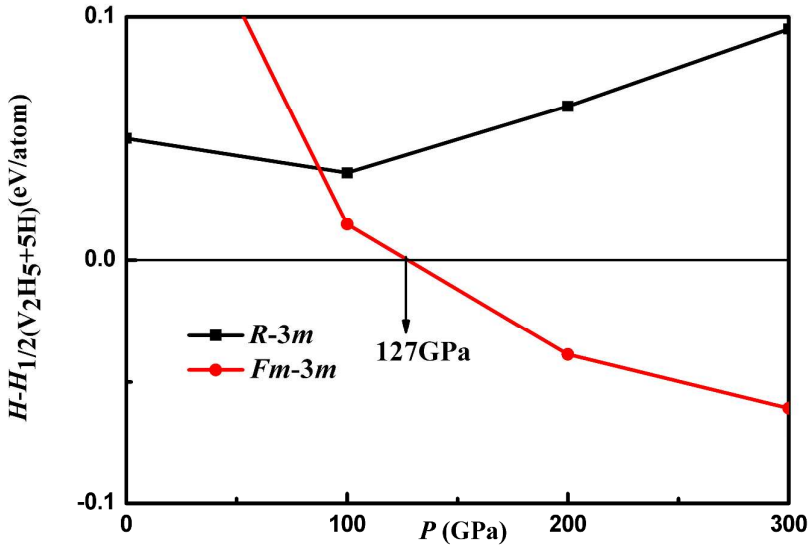

Figure S4 Calculated enthalpies per atom of various structures for VH_3 in the pressure range of 0–300 GPa with respect to V_2H_5 and H_2.

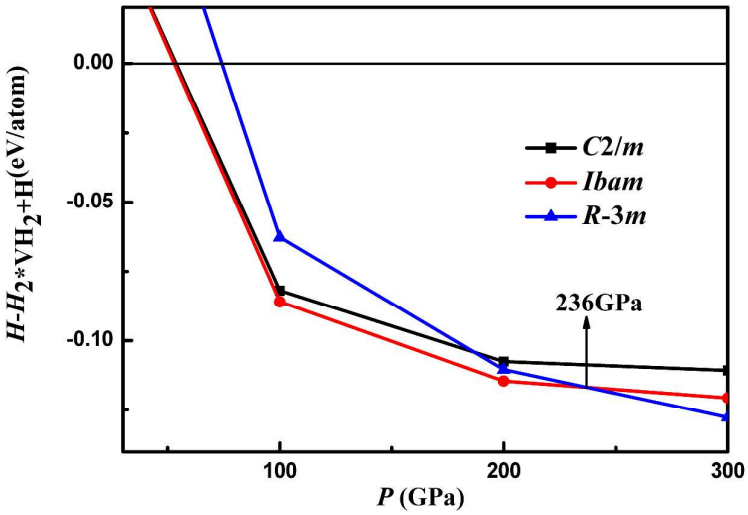

Figure S5 Calculated enthalpies per atom of various structures for V_2H_5 in the pressure range of 0–300 GPa with respect to VH_2 and H_2.

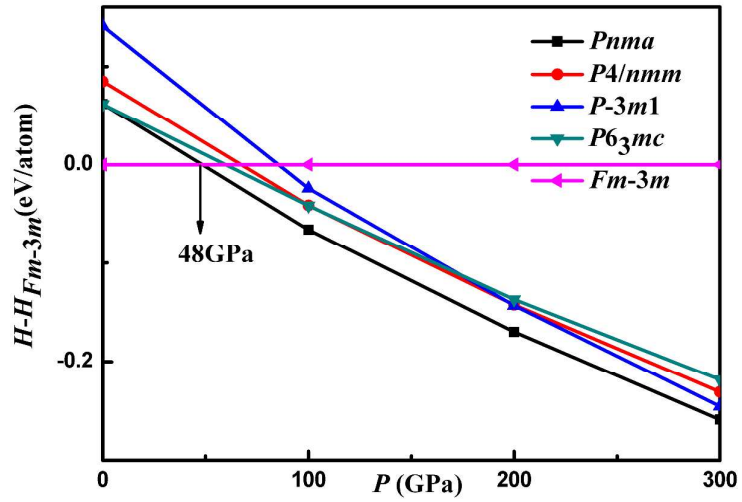

Figure S6 Calculated enthalpies per atom of various structures for VH_2 in the pressure range of 0–300 GPa with respect to *Fm*-3*m*-VH_2.

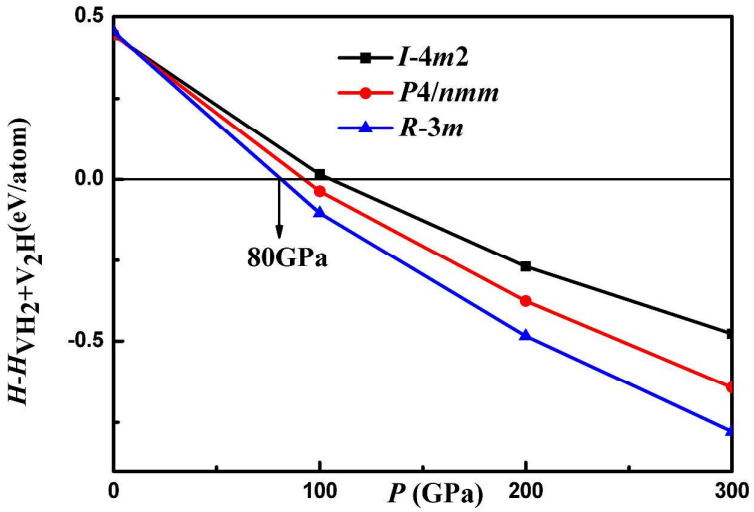

Figure S7 Calculated enthalpies per atom of various structures for VH in the pressure range of 0–300 GPa with respect to VH_2 and V_2H.

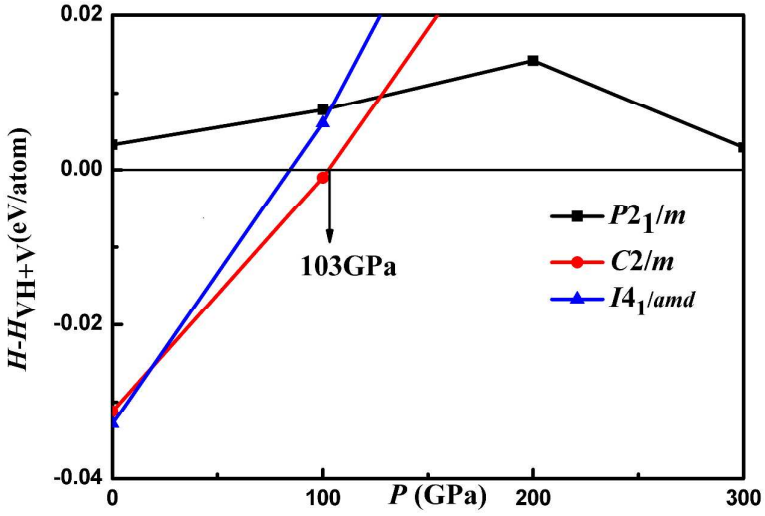

Figure S8 Calculated enthalpies per atom of various structures for V_2H in the pressure range of 0–300 GPa

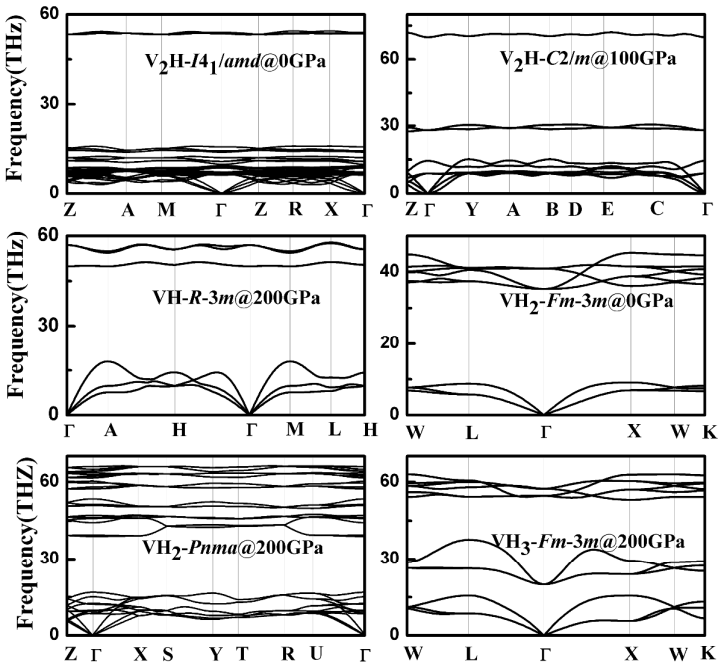

Figure S9 Phonon dispersion of the V_2H, VH, VH_2 and VH_3 at different pressures.

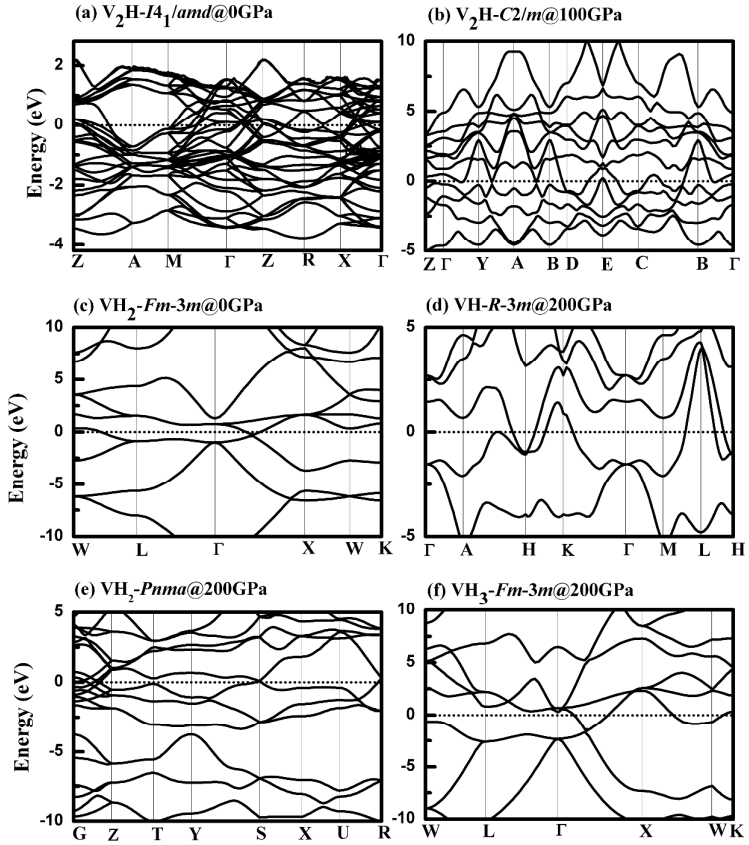

Figure S10 Band structure of the V_2H, VH, VH_2 and VH_3 at different pressures.

Table S1 Detailed structural information of the predicted stable H-V compounds at selected pressures.

Phases	*P*	Lattice constants	Atomic coordinates			
V_2H-$I4_1$/amd	0	*a*=*b*=5.856 (6.001[a])	V(16h)	0.751	0.500	0.604
		c=6.665 (6.619 [b])	H (8b)	0.250	0.500	0.875
		α=*β*=*γ*=90				
V_2H-C2/m	100	*a*= 4.003	V(4i)	0.044	0.000	0.769
		b= 2.674	H (2b)	0.500	0.000	0.500
		c= 5.251				
		α=*γ*=90				
		β=130				
VH-R-3m	150	*a*=*b*=2.534	V(3a)	0.000	0.000	0.000
		c=5.349	H (3b)	0.000	0.000	0.500
		α=*β*=90				
		γ=120				
VH_2-*Fm*-3*m*	30	*a*=*b*=*c*=4.029	V (4a)	0.000	0.000	0.000
		α=*β*=*γ*=90	H (4c)	0.250	0.750	0.250
VH_2-*Pnma*	200	*a*= 4.059	V (4c)	0.735	0.750	0.089
		b= 2.516	H (4c)	0.626	0.750	0.422
		c= 4.489	H (4c)	0.022	0.750	0.726
		α=*β*=*γ*=90				
VH_3-*Fm*-3*m*	200	*a*=*b*= *c*=3.714	V (2c)	0.500	0.500	0.500
		8.540	H (2c)	0.000	0.000	0.000
		α=*β*=*γ*=90	H (4f)	0.250	0.750	0.750
VH_3-*Pnma*	150	*a*= 4.854	V (4c)	0.317	0.250	0.854
		b= 3.402	H (4c)	0.116	0.250	0.431
		c= 3.884	H (4c)	0.662	0.750	0.739
		α=*β*=*γ*=90	H (4a)	0.000	0.500	0.000
VH_5-$P6_3$/*mmm*	100	*a*=*b*=2.589	V (1a)	0.000	0.000	0.000
		c=3.322	H (4h)	0.333	0.667	0.729
		α=*β*=90	H (1b)	0.000	0.000	0.500
		γ=120				
VH_5-*Cmcm*	300	*a*= 4.294	V (4c)	0.000	0.808	0.750
		b= 5.703	H (8g)	0.659	0.645	0.250
		c= 2.355	H (8g)	0.789	0.949	0.250
		α=*β*=*γ*=90	H (4c)	0.500	0.047	0.750
VH_8-C2/m	200	*a*= 4.294	V (2a)	0.000	0.000	0.000
		b= 5.703	H (4i)	0.277	0.000	0.799

		c= 2.355 *α*=*β*=*γ*=90	H (4i) H (4i) H (4i)	0.916 0.709 0.545	0.000 0.000 0.000	0.572 0.586 0.752