Supplementary Material (ESI) for Chemical Communications

Multimode hydriding/dehydriding reactions of CaPd

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Table S1 Summary of crystallographic parameters of $CaPdD_{2.0}$ and $CaPdD_{2.4}$ (the space group $P3_2$ (no. 145) and $Z = 2$).

		$CaPdD_{2.0}$	$CaPdD_{2.4}$
Lattice	a (Å)	5.2112(6)	5.2029(9)
	c (Å)	6.2758(7)	6.3090(8)
Atoms			
Ca	g	1.0*	1.0*
	x	0.322(5)	0.334(13)
	y	0.330(5)	0.332(12)
	z	0.505(9)	0.495(3)
	B (Å^2)	0.3*	0.3*
Pd	g	1.0*	1.0*
	x	0.340(4)	0.324(7)
	y	0.346(3)	0.340(4)
	z	0	0
	B (Å^2)	0.68(17)	0.3(2)
D1	g	1.0*	1.0*
	x	0.668(6)	0.660(11)
	y	0.515(6)	0.504(10)
	z	0.199(6)	0.202(9)
	B (Å^2)	3.2(2)	1.51(15)
D2	g	1.0*	1.0*
	x	0.132(5)	0.157(7)
	y	0.451(4)	0.494(14)
	z	0.153(6)	0.165(11)
	B (Å^2)	3.2	1.51
D3	g	-	0.4*
	x	-	0.14(2)
	y	-	0.00(2)
	z	-	0.18(4)
	B (Å^2)	-	1.51
R_{wp}		0.0511	0.0972
R_F		0.0149	0.0278

Neutron scattering lengths of Ca, Pd and D are 4.70 fm, 5.91 fm and 6.671 fm,

respectively. Numbers in parentheses are estimated standard deviations of the last significant digit. R_{wp} and R_F are the weighted profile reliability factor on the observed and calculated intensities, and the structural reliability factor based on the integrated intensities, respectively. * Fixed in the Rietveld refinement.