Magnetostructural Behavior in the Non-centrosymmetric Compound Nd_7Pd_3

Y. Mudryk, C. Ritter, D. Paudyal, A. Provino, S. K. Dhar, P. Manfrinetti, F. Fauth, V. K. Pecharsky

Supporting Information

Table S1. Interatomic distances, d_{ij}, in two Nd_7Pd_3 polymorphs.

*P*6$_3$*mc* polymorph at T = 35 K					*Cmc*2$_1$ polymorph at T = 10 K			
Atom 1	Atom 2	Count	$d_{1,2}$ [Å]		Atom 1	Atom 2	Count	$d_{1,2}$ [Å]
Nd1	Nd1	2x	3.4464		Nd11	Nd11	2x	3.4531
	Nd3	1x	3.5763			Nd3	1x	3.5963
	Nd2	2x	3.6881			Nd22	1x	3.6866
	Nd2	2x	3.8343			Nd21	1x	3.7057
	Nd3	1x	3.8763			Nd21	1x	3.8361
	Nd1	2x	3.8887			Nd22	1x	3.8444
	Nd3	1x	3.9074			Nd3	1x	3.8591
	Pd1	2x	2.9101			Nd11	1x	3.8670
	Pd1	2x	3.5317			Nd12	1x	3.8737
						Nd3	1x	3.9068
						Pd2	1x	2.8935
						Pd1	1x	2.9149
						Pd1	1x	3.5372
						Pd2	1x	3.5486
					Nd12	Nd12	2x	3.4531
						Nd3	1x	3.5925
						Nd21	2x	3.6977
						Nd21	2x	3.8418
						Nd3	1x	3.8564
						Nd11	2x	3.8737
						Nd3	1x	3.9056
						Pd1	2x	2.9034
						Pd1	2x	3.5331
Nd2	Nd1	2x	3.6881		Nd21	Nd11	1x	3.6977
	Nd2	2x	3.7883			Nd12	1x	3.7054
	Nd1	2x	3.8343			Nd22	1x	3.7917
	Nd3	1x	3.8548			Nd21	1x	3.7941
	Nd2	4x	3.8587			Nd11	1x	3.8362
	Pd	2x	2.9257			Nd12	1x	3.8419
	Pd	1x	3.0431			Nd21	2x	3.8495
	Pd	1x	3.6947			Nd22	1x	3.8551

						Nd3	1x	3.8575
						Nd22	1x	3.8640
						Pd1	1x	2.9291
						Pd2	1x	2.9450
						Pd1	1x	3.0282
						Pd1	1x	3.7119
					Nd22	Nd11	2x	3.6866
						Nd21	2x	3.7917
						Nd3	1x	3.8420
						Nd11	2x	3.8444
						Nd21	2x	3.8551
						Nd21	2x	3.8641
						Pd1	2x	2.9479
						Pd2	1x	3.0286
						Pd2	1x	3.7073
Nd3	Nd1	3x	3.5763		Nd3	Nd12	1x	3.5925
	Nd1	3x	3.8548			Nd11	2x	3.5963
	Nd2	3x	3.8763			Nd22	1x	3.8420
	Nd1	3x	3.9074			Nd12	1x	3.8562
	Pd	3x	2.9617			Nd21	2x	3.8575
						Nd11	2x	3.8591
						Nd12	1x	3.9056
						Nd11	2x	3.9068
						Pd2	1x	2.9554
						Pd1	2x	2.9581
Pd1	Nd1	2x	2.9101		Pd1	Nd12	1x	2.9034
	Nd2	2x	2.9257			Nd11	1x	2.9149
	Nd3	1x	2.9616			Nd21	1x	2.9291
	Nd2	1x	3.0431			Nd22	1x	2.9479
	Nd1	2x	3.5317			Nd3	1x	2.9581
	Nd2	1x	3.6947			Nd21	1x	3.0282
						Nd12	1x	3.5331
						Nd11	1x	3.5372
						Nd21	1x	3.7119
					Pd2	Nd11	2x	2.8935
						Nd21	2x	2.9450
						Nd3	1x	2.9554
						Nd22	1x	3.0286
						Nd11	2x	3.5486
						Nd22	1x	3.7073

Table S2. Calculated average Nd-Nd interatomic distances and variances.

*P*6$_3$*mc* polymorph at T = 35 K			*Cmc*2$_1$ polymorph at T = 10 K		
Atom 1	Average $d_{Nd\text{-}Nd}$ (Å)	Variance	Atom 1	Average $d_{Nd\text{-}Nd}$ (Å)	Variance
Nd1	3.7341	0.3127	Nd11	3.7347	0.285
			Nd12	3.7352	0.287
Nd2	3.810	0.0433	Nd21	3.8129	0.0356
			Nd22	3.8114	0.0444
Nd3	3.8037	0.2111	Nd3	3.803	0.1784