Supporting Information

Ferromagnetic nitrides with the β -Mn structure; $\text{Fe}_{2-x}\text{M}_x\text{Mo}_3\text{N}$ ($\text{M} = \text{Ni, Pd, Pt}$)

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Table S1: Crystal data for $\text{Fe}_{2-x}\text{M}_x\text{Mo}_3\text{N}$ ($\text{M} = \text{Ni, Pd, Pt}$) derived from neutron diffraction data

Composition* (Instrument)	T / K	$a_c / \text{\AA}$	8c site			12d site			4a site (N)	$R_{wp} (\chi^2)$
			Atom type (Occ.)	x	$U_{iso} / \text{\AA}^2$	Atom type	$y(12d)$	$U_{iso} / \text{\AA}^2$	$U_{iso} / \text{\AA}^2$	
Fe_{0.75}Ni_{1.25}Mo₃N (D1B)	200	6.621(1)	Fe (0.375) Ni (0.625)	0.0679(3)	0.000(2)	Mo	0.2028(5)	0.006(2)	0.002(3)	0.0259 (30.19)
	5	6.607(1)	Fe (0.375) Ni (0.625)	0.0678(2)	0.000(2)	Mo	0.2025(5)	0.007(2)	0.002(2)	0.0260 (30.41)
Fe_{0.5}Pd_{1.5}Mo₃N (D2B)	200	6.7906(2)	Fe (0.25) Pd (0.75)	0.0646(3)	0.0087(9)	Mo	0.2045(3)	0.007(1)	0.011(1)	0.0487 (1.946)
	5	6.7855(2)	Fe (0.25) Pd (0.75)	0.6445(2)	0.0088(7)	Mo	0.2039(2)	0.0062(9)	0.0118(9)	0.0394 (2.276)
Fe_{1.5}Pd_{0.5}Mo₃N (D2B)	200	6.7036(8)	Fe (0.75) Pd (0.25)	0.0687(3)	0.000(2)	Mo	0.2045(4)	0.013(2)	0.006(2)	0.0215 (20.06)
	5	6.6837(5)	Fe (0.75) Pd (0.25)	0.0686(3)	0.001(2)	Mo	0.2042(4)	0.013(2)	0.005(2)	0.0217 (19.96)
Fe_{0.75}Pt_{1.25}Mo₃N (D2B)	300	6.7894(1)	Fe (0.411) Pt (0.589)	0.06522(8)	0.0074(2)	Mo (0.936) Pt (0.064)	0.20422(9)	0.0078(2)	0.0069(3)	0.0429 (3.884)
	5	6.7803(1)	Fe (0.411) Pt (0.589)	0.06499(8)	0.0045(2)	Mo (0.936) Pt (0.064)	0.20417(9)	0.0050(2)	0.0051(2)	0.0464 (6.446)
FePtMo₃N (D2B)	300	6.77144(3)	Fe (0.5) Pt (0.5)	0.06637(7)	0.0082(2)	Mo	0.20433(7)	0.0064(2)	0.0075(2)	0.0377 (3.172)
	10	6.7632(1)	Fe (0.5) Pt (0.5)	0.06616(6)	0.0045(1)	Mo	0.20416(7)	0.0039(1)	0.0058(2)	0.0393 (3.903)

* β -Mn structure M_2T_3X : Space group $P4_132$; M (8c) x,x,x ; T (12d) $1/8, y, 0.25+y$; X (4a) $3/8, 3/8, 3/8$

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