

Supporting Information

Two-Dimensional Metallic Chain Compounds $Y_5M_2Te_2$ ($M = Fe, Co, Ni$) That are Related to Gd_3MnI_3 . The Hydride Derivative $Y_5Ni_2Te_2D_{0.4}$

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Table S1. Single Crystal X-ray Data Collection and Refinement Parameters for $Y_3Fe_2Te_2$.

formula weight, g mol ⁻¹	811.42	PRIVILEGED DOCUMENT FOR REVIEW ONLY REC'D
space group, Z	$Cmcm$ (No. 63), 4	NOV 10 2003
lattice parameters, Å		INORG CHEM
<i>a</i>	3.9594(3)	
<i>b</i>	15.057(1)	
<i>c</i>	15.216(1)	
<i>V</i> , (Å ³)	907.1(2)	
<i>d</i> _{calc} , g/cm ³	5.976	
radiation; $2\theta_{max}$	Mo K_{α} ; 56°	
octants measured	$h, \pm k, \pm l$	
scan method	$\omega-2\theta$	
temperature, °C	23	
absorption method	2 ψ -scans, DIFABS	
relative transmission range	0.48 – 1.43	
μ , cm ⁻¹ (Mo K_{α})	41.421	
number of reflections:		
measured	3106	
unique observed ($I \geq 3\sigma(I)$)	305	
number of variables	31	
residuals R ; R_w , ^a %	4.6; 4.2	
goodness of fit	1.39	
secondary ext. coeff.	$2.8(2) \times 10^{-7}$	

^a $R = \sum ||F_o| - |F_c|| / \sum |F_o|$; $R_w = [\sum \omega (|F_o| - |F_c|)^2 / \sum \omega (F_o)^2]^{1/2}$, $\omega = 1/\sigma^2$.

Table S2. U_{ij} (\AA^2) values for $\text{Y}_5\text{Fe}_2\text{Te}_2$

Atom	U11	U22	U33	U12	U13	U23
Te1	0.0109(8)	0.011(1)	0.011(1)	0	0	0
Y1	0.013(1)	0.014(2)	0.009(1)	0	0	0
Y2	0.012(1)	0.011(2)	0.013(2)	0	0	0
Y3	0.012(2)	0.012(2)	0.015(2)	0	0	0
Fe1	0.017(3)	0.015(4)	0.007(3)	0	0	0
Fe2	0.008(3)	0.016(3)	0.012(3)	0	0	0

Table S3. Interatomic distances <math>< 4.0 \text{ \AA}</math> in

Atom	Atom	Mult.	Distance	Atom	Atom	Mult.	Distance
Te1	Te1	2x	3.9594(3)	Y3	Te1	2x	3.217(2)
	Te1		3.714(5)		Y1	4x	3.543(4)
	Y1	2x	3.281(3)		Y2	4x	3.551(3)
	Y1	2x	3.334(3)		Fe1		3.051(9)
	Y2		3.146(3)		Fe2		3.316(9)
	Y2	2x	3.162(3)				
	Y3		3.217(2)		Fe1	Y1	4x
			Y2	2x		2.928(6)	
			Y3			3.051(9)	
Y1	Te1	2x	3.281(3)	Fe2	Y2	4x	2.944(3)
	Te1	2x	3.334(3)		Y3		3.316(9)
	Y1		3.779(6)		Fe1	2x	2.296(4)
	Y2	2x	3.699(3)		Fe2	2x	2.296(4)
	Y3	2x	3.543(4)		Y1	2x	2.870(6)
	Fe1	2x	2.953(3)		Y2	4x	2.944(3)
	Fe2		2.870(6)		Y3		3.316(9)
Y2				Fe1	2x	2.296(4)	
	Te1		3.146(3)				
	Te1	2x	3.162(3)				
	Y1	4x	3.699(3)				
	Y2		3.8042(3)				
	Y3	2x	3.551(3)				
	Fe1		2.928(6)				
	Fe2	2x	2.944(3)				

Table S4. Single Crystal X-ray Data Collection and Refinement Parameters for $Y_5Ni_2Te_2(H)$.

formula weight, g mol ⁻¹	817.12
Space group, Z	<i>Pnma</i> (No. 62), 4
lattice parameters, Å	
<i>a</i>	14.384(4)
<i>b</i>	4.026(2)
<i>c</i>	15.895(7)
<i>V</i> , (Å ³)	920.5(6)
<i>d</i> _{calc} , g/cm ³	5.897
radiation; 2θ _{max}	Mo K _α ; 56°
octants measured	±h, ±k, ±l
scan method	ω-2θ
temperature, °C	23
absorption Method	SADABS
relative transmission range	0.73 – 1.69
μ, cm ⁻¹ (Mo K _α)	41.265
number of reflections:	
measured	7740
unique observed (<i>I</i> ≥ 3σ(<i>I</i>))	784
number of variables	56
residuals <i>R</i> ; <i>R</i> _ω , ^a %	3.4; 7.8
goodness of fit	0.58
secondary ext. coeff.	1.3(2) × 10 ⁻³

^a $R = \sum |F_o^2 - F_c^2| / \sum F_o^2$; $R_\omega = [\sum \omega ((F_o^2 - F_c^2)^2 / \sum \omega F_o^2)^2]^{1/2}$.

Table S5. U_{ij} (\AA^2) values for $\text{Y}_5\text{Ni}_2\text{Te}_2\text{H}$ (23 °C)

Atom	U11	U22	U33	U12	U13	U23
Te1	0.0109(5)	0.0127(5)	0.0089(5)	0	0.0001(4)	0
Te2	0.0131(5)	0.0102(4)	0.0122(5)	0	-0.0016(4)	0
Y1	0.0098(7)	0.0118(7)	0.0103(7)	0	-0.0005(5)	0
Y2	0.0110(7)	0.0119(7)	0.0099(7)	0	0.0002(5)	0
Y3	0.0140(8)	0.0130(7)	0.0087(7)	0	-0.0014(5)	0
Y4	0.0120(7)	0.0112(6)	0.0112(7)	0	-0.0003(6)	0
Y5	0.0136(8)	0.0118(7)	0.0100(7)	0	0.0007(5)	0
Ni1	0.0110(1)	0.012(1)	0.0138(9)	0	-0.0005(7)	0
Ni2	0.012(1)	0.013(1)	0.013(1)	0	-0.0001(8)	0

Table S6. Interatomic distances < 4.0 Å in $Y_5Ni_2Te_2(H)_x$ (23 °C)

Atom 1	Atom 2	Mult.	Distance	Atom 1	Atom 2	Mult.	Distance
Te1	Y1		3.199(2)	Y2	Y1		3.929(2)
	Y2		3.125(2)		Y1		3.514(2)
	Y3		3.114(2)		Y4	2x	3.804(2)
	Y3	2x	3.192(2)		Y5	2x	3.630(2)
	Y4	2x	3.212(2)		Ni1	2x	2.723(2)
				Ni2		2.814(2)	
Te2	Y1	2x	3.224(2)	Y3	Te1		3.114(2)
	Y2	2x	3.196(2)		Te1	2x	3.192(2)
	Y4		3.544(2)		Y1	2x	3.639(2)
	Y5		3.341(2)		Y4	2x	3.722(2)
	Y5	2x	3.184(2)		Y5		3.616(2)
Y1	Te1		3.199(2)	Y4	Ni1		2.847(2)
	Te2	2x	3.224(2)		Ni2	2x	2.748(2)
	Y2		3.929(2)		Te1	2x	3.212(2)
	Y2		3.514(2)		Te2		3.544(2)
	Y3	2x	3.639(2)		Y1	2x	3.564(2)
	Y4	2x	3.564(2)		Y2	2x	3.804(2)
	Ni1	2x	2.759(2)		Y3	2x	3.722(2)
	Ni2		3.140(3)		Y5	2x	3.614(2)
					Ni1		3.148(3)
	Te1		3.125(2)		Ni2		3.094(3)
Te2	2x	3.196(2)					

Table S6. (continued)

Y5	Te2		3.341(2)	Ni2	Y1		3.140(3)
	Te2	2x	3.184(2)		Y2		2.814(2)
	Y2	2x	3.630(2)		Y3	2x	2.748(2)
	Y3		3.616(2)		Y4		3.094(3)
	Y4	2x	3.614(2)		Y5	2x	2.802(2)
	Ni1		3.181(3)		Ni1	2x	2.701(2)
	Ni2	2x	2.802(2)				
Ni1	Y1	2x	2.759(2)				
	Y2	2x	2.723(2)				
	Y3		2.847(2)				
	Y4		3.148(3)				
	Y5		3.181(3)				
	Ni2	2x	2.701(2)				

Table S7. Interatomic distances <math>< 4.0 \text{ \AA}</math> in

Atom 1	Atom 2	Mult.	Distance	Atom 1	Atom 2	Mult.	Distance
Te1	Y1		3.196(6)	Y2	Y1		3.910(5)
	Y2		3.124(9)		Y1		3.502(5)
	Y3		3.102(9)		Y4	2x	3.772(6)
	Y3	2x	3.180(5)		Y5	2x	3.634(5)
	Y4	2x	3.189(4)		Ni1	2x	2.715(4)
				Ni2		2.808(5)	
Te2	Y1	2x	3.229(6)	Y3	Te1		3.102(9)
	Y2	2x	3.193(5)		Te1	2x	3.180(5)
	Y4		3.554(4)		Y1	2x	3.624(4)
	Y5		3.322(6)		Y4	2x	3.715(6)
	Y5	2x	3.155(7)		Y5		3.577(5)
Y1	Te1		3.196(6)	Y4	Ni1		2.814(5)
	Te2	2x	3.229(6)		Ni2	2x	2.725(3)
	Y2		3.910(5)		Te1	2x	3.189(4)
	Y2		3.502(5)		Te2		3.554(4)
	Y3	2x	3.624(4)		Y1	2x	3.552(5)
	Y4	2x	3.552(5)		Y2	2x	3.772(6)
	Ni1	2x	2.750(3)		Y3	2x	3.715(6)
	Ni2		3.142(5)		Y5	2x	3.590(5)
	D		2.31(2)		Ni1		3.131(7)
Y2	Te1		3.124(9)	D	Ni2		3.088(7)
	Te2	2x	3.193(5)		2x	2.259(4)	

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Table S7. (continued)

Y5	Te2		3.322(6)	Ni2	Y1		3.142(5)
	Te2	2x	3.155(7)		Y2		2.808(5)
	Y2	2x	3.634(5)		Y3	2x	2.725(3)
	Y3		3.577(5)		Y4		3.088(7)
	Y4	2x	3.590(5)		Y5	2x	2.788(3)
	Ni1		3.180(5)		Ni1	2x	2.694(2)
	Ni2	2x	2.788(3)				
	D		2.32(2)	D	Y1		2.31(2)
					Y4	2x	2.259(4)
Ni1	Y1	2x	2.750(3)		Y5		2.32(2)
	Y2	2x	2.715(4)				
	Y3		2.814(5)				
	Y4		3.131(7)				
	Y5		3.180(5)				
	Ni2	2x	2.694(2)				
