Support Information

A New Series of Cyanide-Bridged Hetrobimetallic Fe^{III}-$Fe^{III}/Mn^{III}/Cu^{II}$ One-dimensional Complexes: Synthesis, Crystal Structures, and Magnetic Properties

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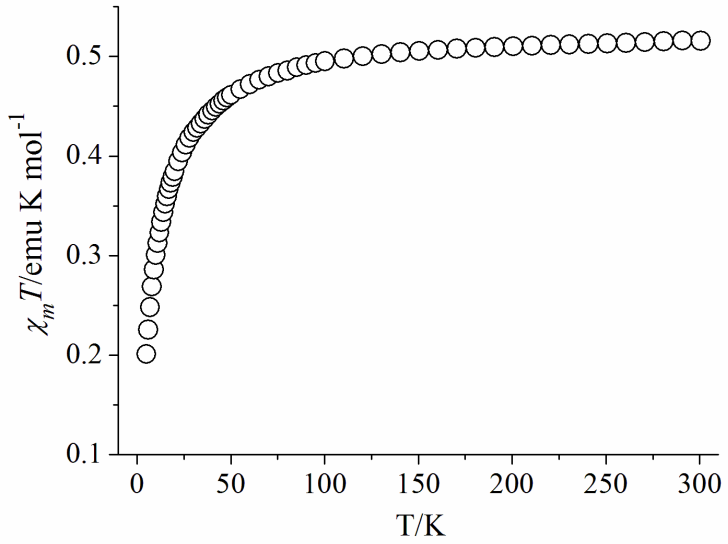
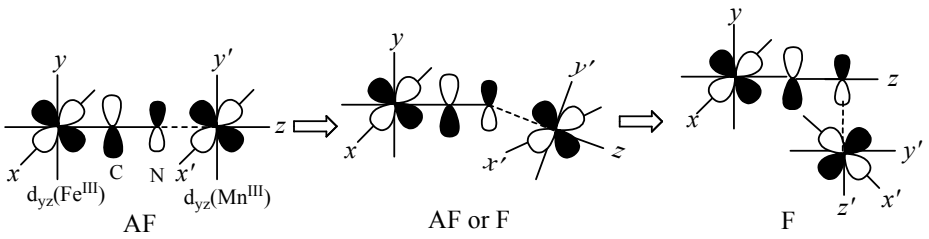
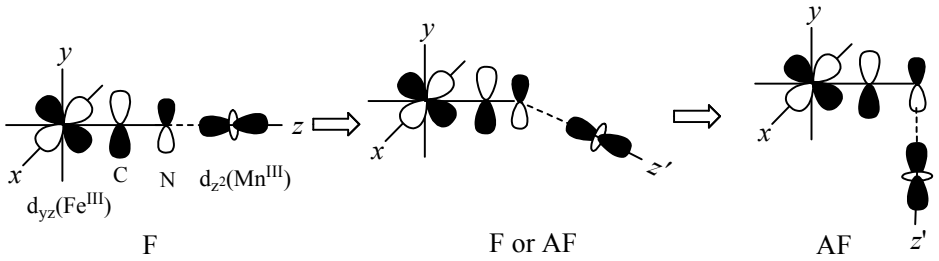


Figure. S1. Temperature dependence of $\chi_M T$ of compound **1**.



(a) d_{yz}-d_{yz} orbital overlap of two metal ions.



(b) d_{yz}-d_{z2} orbital overlap of two metal ions.

Figure S2. Different magnetic exchange situations with bent Fe-C≡N-Mn linkages.

Table S1. Comparison of the magnetic property of cyanide-bridged $Fe^{III}Mn^{III}$ complexes based on low-spin Fe(III) building blocks.

compounds	structure	Mn-$N_{cyanide}$ (Å)	C≡N-Mn (°)	magnetism	ref.
$[Mn(salen)(EtOH)]_3[Fe(CN)_6]$	tetranuclear	2.249(2)-2.307(2)	170.7(2), 161.9(2), 148.9	AF AF F	S1
$(NEt_4)[\{Mn(salen)\}_2Fe(CN)_6]$	2D	2.266(3) 2.337(3)	167.8(3) 146.2(2)	AF AF	S2
rac-$(NEt_4)[Mn(salmen)(MeOH)]_2[Fe(CN)_6]$	trinuclear	2.219(9)	164.7(9)	F	S3
$[NEt_4]_2[Mn(saldmen)(H_2O)][Fe(CN)_6]$	dinuclear	2.198(9)	162.4(8)	F	S4
$K[Mn(3\text{-}MeOsalen)]_2Fe(CN)_6$	2D	2.290(5) 2.415(5)	169.5(5) 137.2(4)	F F	S5
$[Mn(salpn)(CH_3OH)]_4[Fe(CN)_6]ClO_4$	pentanuclear	2.261(3) 2.259(5)	160.2(3) 151.3(3)	F	S6
$[Mn_4(saltmen)_4Fe(CN)_6]ClO_4$	2D	2.19(1)	156.1(10)	F	S5
$[NEt_4]_2[Mn(acacen)][Fe(CN)_6]$	1D	2.316(4)	156.2(3)	F	S7
$Mn_3((R,R)\text{-}Salcy)_3(H_2O)_2Fe(CN)_6$	1D	2.398(4)-2.251(4)	143.0(3), 152.9(3)	AF	S8
$K(18C6)(2\text{-}PrOH)_2\{Mn(acacen)\}_2\{Fe(CN)_6\}$	2D	2.331(3) 2.439(3)	152.0(3) 154.8(3)	F	S9
$\{[Mn(salen)]_6[Fe(CN)_6]\}[Fe(CN)_6]$	heptanuclear	2.334(2)	150.74(14)	F	S10
$\{Fe(CN)_4[CNMn(salen)(MeOH)]_2\}\{[Mn(salen)(H_2O)]_2\}[Mn(salen)(H_2O)(MeOH)]_2[Fe(CN)_6]$	trinuclear	2.30(1)	149(1)	F	S11
$(NEt_4)[Mn_2(salmen)_2(MeOH)_2Fe(CN)_6]$	1D	2.179(3)	146.7(4)	F	S12
$K[(5\text{-}Brsalen)_2(H_2O)_2Mn_2Fe(CN)_6]$	trinuclear	2.331(5)	142.6(5)	F	S13
$Mn_3((R,R)\text{-}Salcy)_3(H_2O)_2Fe(CN)_6$	1D	2.398(4)-2.251(4)	143.0(3)–152.9(3)	AF	S14
$\{[Mn(3\text{-}EtOSalen)]_6[Fe(CN)_6]\}[Fe(CN)_6]$	hetpanuclear	2.299(4)	152.0(3)	F	S15
$[Mn(3\text{-}MeOSalen)]_3[Fe(CN)_5(1\text{-}CH3im)]ClO_4$	tetranulcear	2.244(6)-2.268(6)	142.5(5)-147.5(5)	F	S15
$[Mn(3\text{-}EtOSalen)]_3[Fe(CN)_5(1\text{-}CH3im)]ClO_4$	tetranulcear	2.245(6)-2.253(6)	146.1(5)-157.2(5)	F	S15
$[Mn_2(5\text{-}Brsalen)_2Fe(CN)_5(1\text{-}CH_3im)]$	trinuclear	2.236(6), 2.222(6)	160.0(5) 154.3(5)	F	S16
$[Mn_2(5\text{-}Clsalen)_2(H_2O)_2Fe(CN)_5(1\text{-}CH_3im)]$	trinuclear	2.243(5)	149.8(5)	F	S16
$[Mn_2(5\text{-}Clsaltmen)_2(H_2O)_2Fe(CN)_5(1\text{-}CH_3im)]$	trinuclear	2.311(3), 2.258(3)	159.7(3), 157.8(3)	F	S16
$[Mn_2(5\text{-}Brsaltmen)_2(H_2O)_2Fe(CN)_5(1\text{-}CH_3im)]$	trinuclear	2.323(3), 2.266(3)	159.4(2), 157.2(3)	F	S16

{[Et_4N][Mn(acacen)Fe$(CN)_5$(1-CH_3im)]}	1D	2.331(4)	144.4(4)	AF	S16
{[Mn_4(saltmen)$_4$Fe$(CN)_5$(1-CH_3im)]}$_n$[ClO_4]	2D	2.197(8)	157.3(7)	F	S16
[Mn(salen)][Fe(pzcq)$(CN)_3$]	1D	2.288(3), 2.263(3)	152.2(3), 158.3(3)	AF	S17
[Mn(salcy)][Fe(mpzcq)$(CN)_3$]	1D	2.287(5) 2.298(5)	169.1(4) 154.3(5)	AF	S18
[Mn(salen)][Fe(mpzcq)$(CN)_3$]	dinuclear	2.275(3)	164.1(2)	AF	S18
[Mn((*R,R*)-Salcy)][Fe(pcq)$(CN)_3$]	1D	2.279(7) 2.275(7)	153.0(7) 166.4(7)	F	S19
[Mn((R,R)-Salcy)Fe(Tp)$(CN)_3$]	1D	2.281(5) 2.308(5)	162.8(4) 149.5(4)	F	S20
[Mn((R,R)Salcy)Fe(bpca)$(CN)_3$]	1D	2.3132(16) 2.3440(15)	147.69(15) 147.78(14)	AF	S20
[(Tp)Fe$(CN)_3]_2$[Mn(acphen)]$_2$	dinuclear	2.185(5)	149.5(4)	F	S21
[(Tp)Fe$(CN)_3]_2$[Mn(5-Bracphen)]$_2$	dinuclear	2.175(7)	151.5(6)	F	S21
[(Tp)Fe$(CN)_3]_2$[Mn(salen)]$_2$	dinuclear	2.218(3)	154.4(3)	AF	S21
[(Tp)Fe$(CN)_3$][Mn(1-napen)(H_2O)]	dinuclear	2.334(2)	156.31(19)	F	S22
[(Tp)Fe$(CN)_3$][Mn(5-Clsalen)(H_2O)]	dinuclear	2.307(4)	157.7(4)	F	S22
[(Tp)Fe$(CN)_3$][Mn(2-acnapen)(MeOH)]	dinuclear	2.247(3)	159.0(3)	F	S22
[(Tp)Fe$(CN)_3$][Mn(3-MeOsalen)(H_2O)]	dinuclear	2.298(4)	163.8(4)	AF	S22
[(Tp)Fe$(CN)_3$][Mn(2-acnapen)]	1D	2.372(3) 2.322(3)	149.3(3) 148.7(3)	F	S22
[Fe(iqc)$(CN)_3$][Mn(salen)]	1D	2.315(3) 2.273(3)	174.1(3) 167.1(3)	F	S23
[Fe(iqc)$(CN)_3$][Mn(5-Fsalen)]	1D	2.313(4) 2.281(4)	141.6(3) 151.4(3)	AF	S23
[Fe(iqc)$(CN)_3$][Mn(5-Clsalen)]	1D	2.260(7) 2.278(7)	155.2(8) 154.2(7)	AF	S23
[Fe(iqc)$(CN)_3$][Mn(5-Brsalen)]	1D	2.269(4) 2.265(4)	156.4(4) 147.6(3)	AF	S23
[Fe(pcq)$(CN)_3$Mn(saltmen)(CH_3OH)]	dinuclear	2.258(3)	153.2(2)	AF	S24
[Fe(bpca)$(CN)_3$Mn(3-MeO- salen)(H_2O)]	dinuclear	2.298(2)	146.09(18)	AF	S24
[Fe(bpca)$(CN)_3$Mn(salpen)]	1D	2.360(2) 2.324(2)	144.24(18) 151.70(18)	AF	S24
[Fe(bpca)-$(CN)_3$Mn(saltmen)]	1D	2.302(7) 2.337(6)	152.8(6) 153.8(7)	AF	S24
[Fe(bpca)$(CN)_3$Mn(5-Me-saltmen)]	1D	2.371(4) 2.314(4)	162.7(3) 169.7(3)	F	S24
[Fe(pcq)$(CN)_3$Mn(5-Me-saltmen)]	1D	2.366(4) 2.305(4)	160.9(4) 169.4(4)	F	S24
[Fe(bpb)$(CN)_2$Mn(saltmen)]	1D	2.243(6)-	148.9(6)-	F	S24

		2.326(6)	165.9(7)		
[Mn(5-Cl-salen)Fe(bpClb)$(CN)_2$]	1D	2.258(4)-2.277(4)	149.5(4)-154.3(3)	F	S25
[Mn(5-Cl-salen)Fe(bpb)$(CN)_2$]	1D	2.270(7)-2.339(7)	149.1(7)-160.8(7)	F	S25
[Mn(5-Br-salen)Fe(bpb)$(CN)_2$]	1D	2.304(3)-2.372(3)	149.0(3)-161.3(2)	F	S25
[Mn(5-Me-salen)Fe(bpb)$(CN)_2$]	1D	2.308(3)-2.376(3)	147.5(2)-160.9(3)	F	S25
[Mn(saltn)(MeOH)][Fe(bpb)$(CN)_2$]	dinuclear	2.256(3)	167.4(3)	F	S26
[Mn(saltn)(H_2O)Fe(bpmb)$(CN)_2$]	dinuclear	2.272(3)	166.7(3)	F	S26
[Mn(saltn)(MeOH)Fe(bpClb)$(CN)_2$]	dinuclear	2.268(4)	166.8(4)	F	S26
[Mn_2(5-Br-saltn)$_2$$(H_2O)$(EtOH)Fe(bpb)$(CN)_2$][Fe(bpb)$(CN)_2$]	trinuclear	2.251(16) 2.154(14)	166.6(13) 162.7(12)	AF AF	S26
[Mn_2(5-Cl-saltn)$_2$$(CH_3OH)$(EtOH)Fe(bpb)$(CN)_2$][Fe(bpb)$(CN)_2$]	trinuclear	2.251(7) 2.207(7)	166.7(6) 158.3(7)	F F	S26
{[Fe(bpb)$(CN)_2$][Mn(TMeOPP)(CH_3CH_2OH)]}	dinuclear	2.245(3)	160.3(2)	F	S27
{[Fe(bpb)$(CN)_2$][Mn(TClPP)(CH_3OH)]}	dinuclear	2.258(4)	159.9(3)	F	S27
{[Fe(bpmb)$(CN)_2$)]$_2$[Mn(TPP)]}[Mn(TPP)$(CH_3OH)_2$]	trinuclear	2.321(2)	159.9(2)	F	S27
{[Fe(bpb)$(CN)_2$)]$_2$[Mn(TPP)]}[Mn(TPP)$(CH_3OH)_2$]	trinuclear	2.275(2)	159.4(2)	F	S27
{[Fe(bpb)$(CN)_2$][Mn(TNPP)(H_2O)]}	dinuclear	2.330(4)	158.4(4)	F	S27
[Mn(salen)]$_6$[Fe(bpmb)$(CN)_2$]$_6$	wheel	2.258(5) 2.354(4)	140.8(4) 163.3(5)	F	S28
[Mn(salen)]$_6$[Fe(bpClb)$(CN)_2$]$_6$	wheel	2.250(4)-2.320(4)	138.4(4) 161.4(6)	F	S29
[Mn(salen)]$_6$[Fe(bpdmb)$(CN)_2$]$_6$	wheel	2.234(7)-2.256(6)	141.6(5) 170.2(6)	F	S29
[Mn(salen)][Fe(bpb)$(CN)_2$]	1D	2.301(3), 2.439(3)	158.6(3) 151.8(3)	AF	S28
[Mn(5-Brsalpn)]$_6$[Fe(bpmb)$(CN)_2$]$_6$	wheel	2.234(7), 2.256(6)	147.7(7) 158.2(6)	F	S29
[Mn(5-Clsalpn)]$_6$[Fe(bpmb)$(CN)_2$]$_6$	wheel	2.236(4), 2.259(4)	145.8(4) 158.4(3)	F	S29
[Mn(5-Clsalpn)]$_2$[Fe(bpmb)$(CN)_2$]$_2$	tetranuclear	2.280(4)-2.349(3)	147.2(3)-155.4(3)	F	S29
[Mn(3-MeOSalen)][Fe(bpb)$(CN)_2$]$_2$	dinuclear	2.257(3)	164.1(3)	AF	S30

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