

Supporting Information

Cyanide-Bridged Fe(III)-Mn(III) Bimetallic Systems Assembled from the
fac-Fe Tricyanide and Mn Schiff bases: Structures, Magnetic Properties,
and DFT Calculations

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Table S1. Computed data of DFT calculations for **3**.

		HS	BS
Spin density	Fe	1.04835	-1.03864
	Mn	3.84395	3.84461
$\langle S^2 \rangle$		8.8026	4.8019
E(a.u.)		-4774.57712542	-4774.57705180

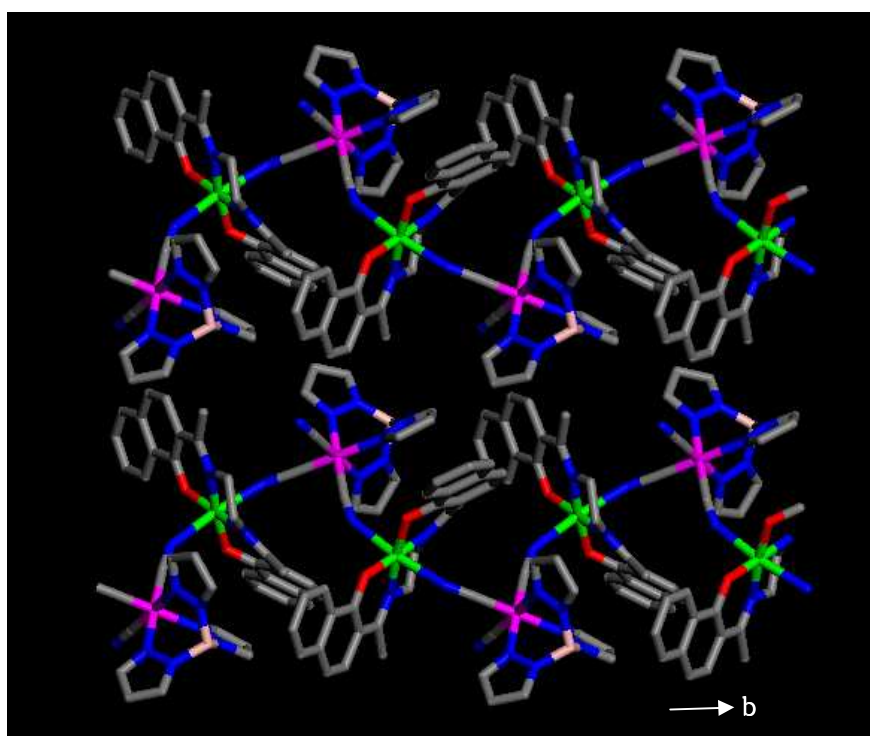


Figure S1. 1D structure of **5** displaying zigzag patterns along the *b*-axis

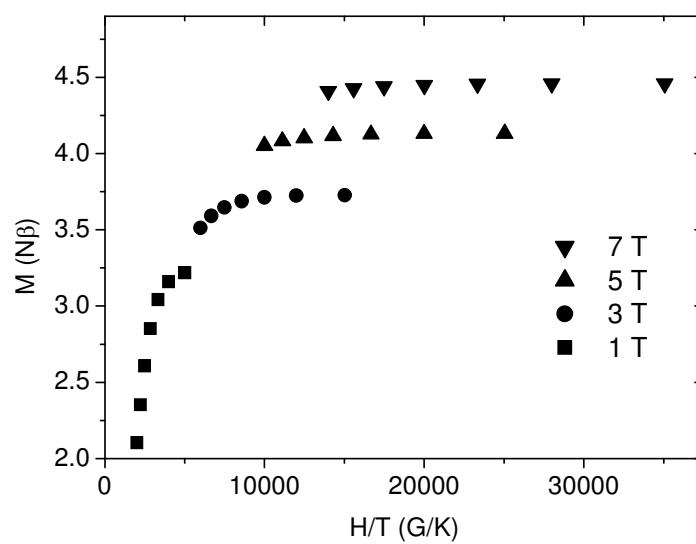


Figure S2. Plots of reduce magnetization versus H/T for **5**.

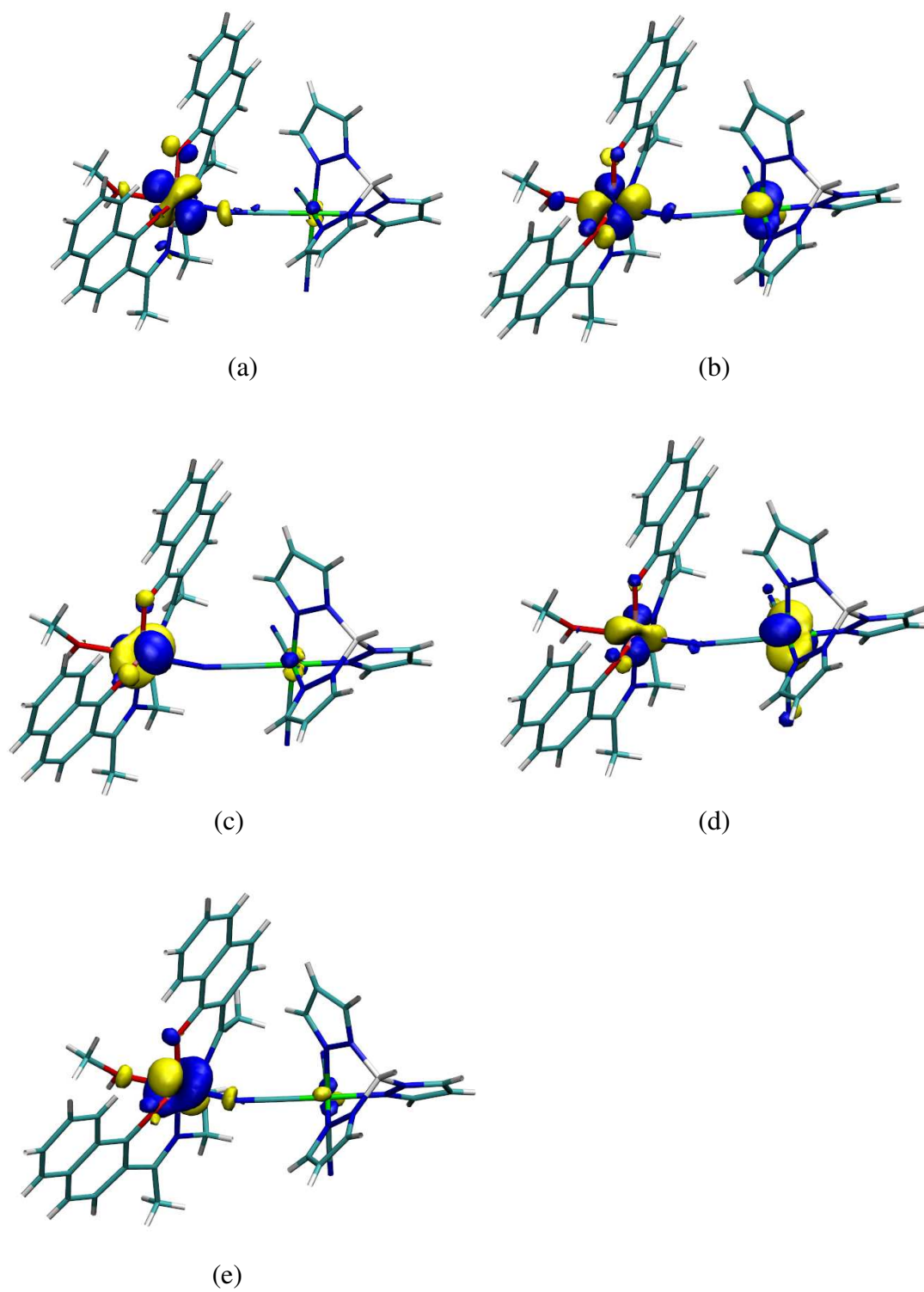


Figure S3. Magnetic natural orbitals for the high-spin configuration of **3**.