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Supporting Information

From antiferromagnetic to ferromagnetic exchange in a family of oxime-based Mn^{III} dimers: a magneto-structural study

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Table S1 Computed overlap integral values of complexes **1**-**4**.

Complex 1	**Alpha/Beta**	dxy	dxz	dyz	dz2	dx2-y2
	dxy	-0.19711	0.10603	0.18111	-0.10483	-0.31314
	dyz	0.07562	-0.08634	0.28211	-0.02702	-0.09679
	dxz	-0.01044	-0.11199	-0.08549	-0.03386	-0.1447
	dz2	0.03345	0.12915	-0.05576	0.08449	0.01766
	dx2-y2	-0.11877	0.03753	-0.01067	-0.02269	-0.08876

Complex 2	**Alpha/Beta**	dxy	dxz	dyz	dz2	dx2-y2
	dyz	-0.09916	-0.0755	0.004883	0.10056	0.03267
	dxy	-0.15079	-0.07006	0.07971	-0.10796	0.36422
	dxz	-0.18503	-0.19975	-0.05443	-0.004	0.01488
	dz2	0.04433	-0.00737	-0.0909	0.05744	0.01282
	dx2-y2	-0.12504	0.09851	0.00872	-0.02178	-0.14188

Complex 3	**Alpha/Beta**	dxz	dyz	dxy	dz2	dx2-y2
	dyz	-0.08662	-0.03976	0.07319	0.09004	0.00668
	dxy	-0.00449	-0.04178	-0.39522	-0.08964	0.19424
	dxz	-0.21098	-0.04084	-0.06893	0.03117	0.12133
	dz2	0.00591	0.02899	-0.16681	-0.04892	-0.0237
	dx2-y2	-0.04866	0.08886	-0.2856	0.01456	0.15764

Complex 4	**Alpha/Beta**	dxy	dyz	dxz	dz2	dx2-y2
	dyz	0.10174	0.26288	-0.16419	0.00479	0.01221
	dxy	0.12153	0.00912	0.06013	-0.1738	-0.11855
	dxz	-0.02341	0.08591	0.34739	0.02209	-0.03955
	dz2	0.04309	0.01903	-0.00284	-0.00092	-0.02566
	dx2-y2	-0.26465	-0.02646	0.22811	-0.01456	-0.06878

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Table S2 Computed spin density values for Mn^{III} ions, oxygen atoms (oxo, oxime) and nitrogen atoms (oxime) of complexes **1**-**4**.

	1	**2**	**3**	**4**
Mn 1	3.817	3.815	3.846	3.834
Mn2	3.842	3.847	3.817	3.806
O3 (oxo)	0.077	0.076	0.076	0.080
O4 (oxime)	0.030	0.034	0.032	0.033
N5 (oxime)	-0.039	-0.028	-0.031	-0.031

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Figure S1 Computed spin density plots (A-C) for complexes **2**-**4** respectively.

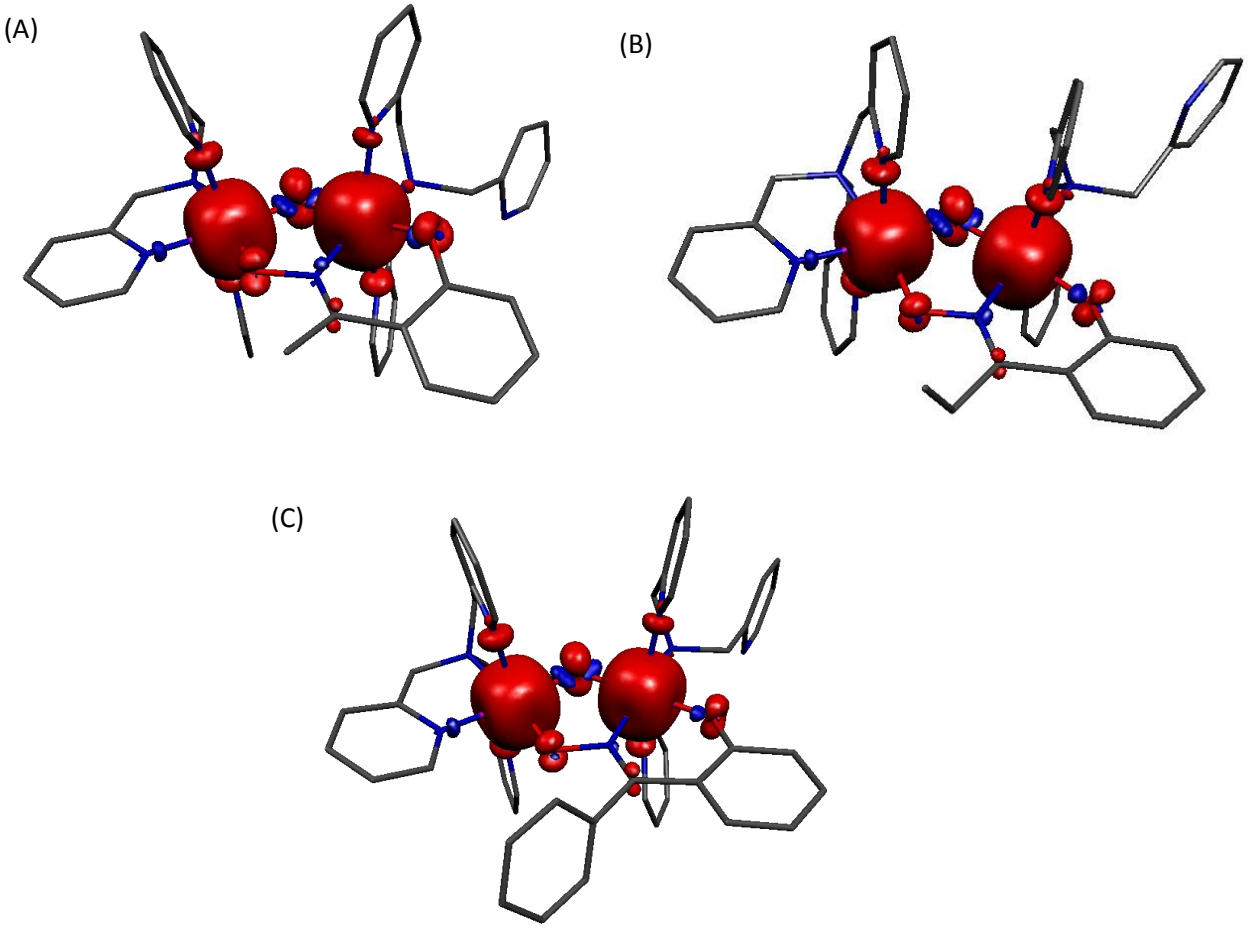

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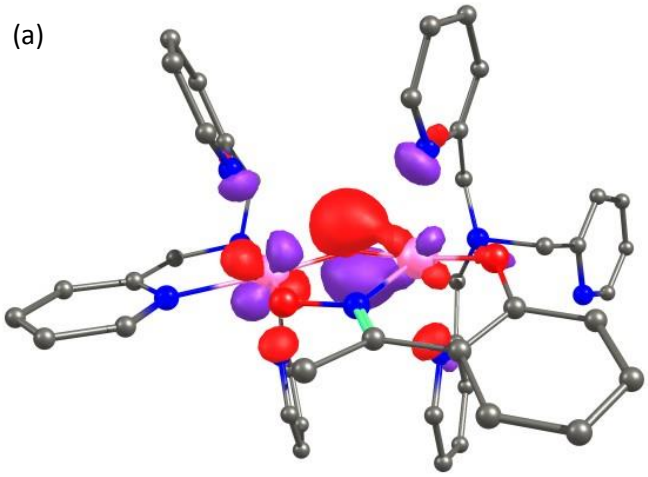
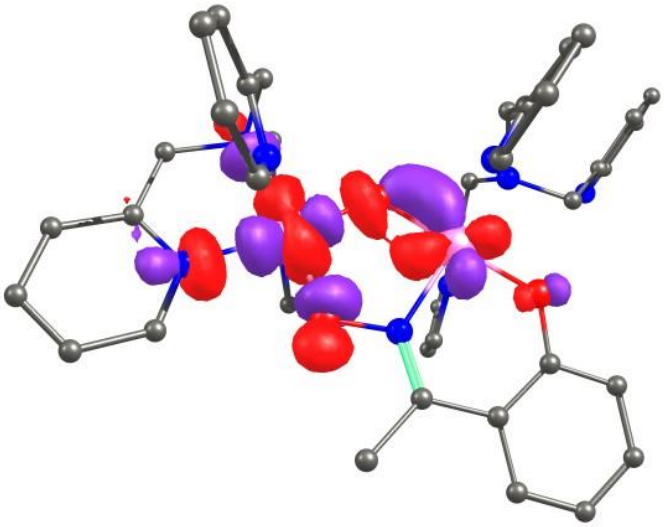
Figure S2: Qualitative MO diagram computed for complex 2: (a) d_{xz} orbital; (b) $d_x2_{-y}2$ orbital (alpha); (c) $d_{x^2-y^2}$ orbital (beta)

(a)



(b)



(c)

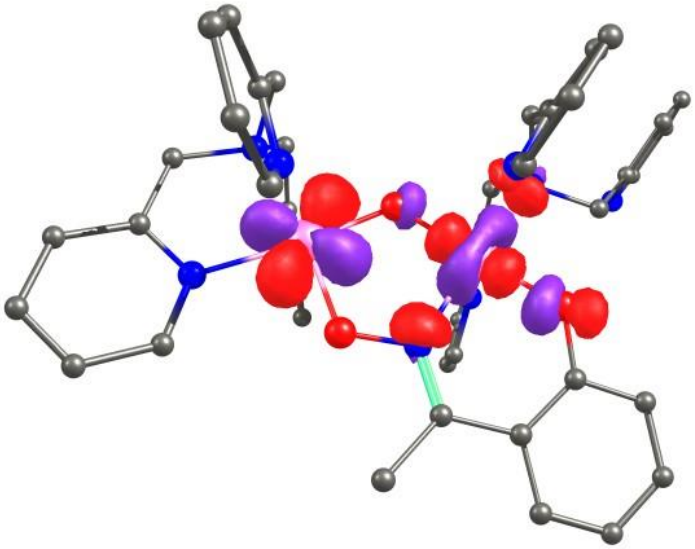


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Table S3 Computed overlap integral values for different torsion angles of complex **1**.

1.1	**Alpha/Beta**	dxy	dxz	dyz	dz2	dx2-y2
	dxy	0.19671	0.09327	0.03479	-0.10372	0.34177
	dyz	-0.05111	0.1001	-0.26054	0.04301	-0.03398
	dxz	0.02931	-0.11036	0.00591	-0.01125	-0.11751
	dz2	0.0428	0.0537	0.0215	0.00891	-0.01547
	dx2-y2	-0.10946	0.01086	0.02237	-0.02139	-0.08541

8.4	**Alpha/Beta**	dxy	dxz	dyz	dz2	dx2-y2
	dxy	-0.19711	0.10603	0.18111	-0.10483	-0.31314
	dyz	0.07562	-0.08634	0.28211	-0.02702	-0.09679
	dxz	-0.01044	-0.11199	-0.08549	-0.03386	-0.1447
	dz2	0.03345	0.12915	-0.05576	0.08449	0.01766
	dx2-y2	-0.11877	0.03753	-0.01067	-0.02269	-0.08876

16.7	**Alpha/Beta**	dxy	dyz	dxz	dz2	dx2-y2
	dyz	0.00835	-0.10062	-0.01275	-0.06813	0.028577
	dxy	-0.14768	-0.09747	0.06486	-0.10474	-0.22166
	dxz	0.05886	-0.16031	0.06721	0.04815	-0.15633
	dz2	0.02032	0.00071	0.1717	0.12695	-0.04891
	dx2-y2	-0.11762	-0.08657	0.05407	-0.02026	0.11033

25.1	**Alpha/Beta**	dxy	dxz	dyz	dz2	dx2-y2
	dxy	-0.14424	0.10423	0.05497	-0.05096	-0.20567
	dyz	0.03084	-0.08954	0.014846	0.02429	-0.0574
	dxz	0.05886	-0.22317	0.06721	0.04815	-0.15633
	dz2	0.02032	-0.00221	0.1717	0.12695	-0.04981
	dx2-y2	-0.11762	0.01569	0.05407	-0.02026	0.11033