

Supporting Information for:
Heavy Ligand Atom Induced Large Magnetic
Anisotropy in Mn(II) Complexes

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Table S1: Major coupling paramters between spin moments of different spin free states.

Complex	Spin free state in- dex	$ m_s\rangle$	Spin free state in- dex	$ m_s\rangle$	Coupling parameter(cm^{-1})
MnCl ₂	3	-2.5	2	-1.5	250.5
	3	-1.5	2	-2.5	250.5
	3	-1.5	2	-0.5	316.9
	3	-0.5	2	-1.5	316.9
	3	-0.5	2	0.5	336.1
	3	0.5	2	-0.5	336.1
	3	0.5	2	1.5	316.9
	3	1.5	2	0.5	316.9
	3	1.5	2	2.5	250.5
	3	2.5	2	1.5	250.5
MnBr ₂	3	-2.5	2	-2.5	2257.2
	3	-1.5	2	-1.5	1354.3
	3	-0.5	2	-0.5	451.4
	3	0.5	2	0.5	451.4
	3	1.5	2	1.5	1354.3
	3	2.5	2	2.5	2257.2
MnI ₂	3	-2.5	2	-2.5	4606.6
	3	-1.5	2	-1.5	2763.9
	3	-0.5	2	-0.5	921.3
	3	0.5	2	0.5	921.3
	3	1.5	2	1.5	2763.9

	3	2.5	2	2.5	4606.6
	3	-2.5	2	-1.5	137.0
	3	-1.5	2	-2.5	137.0
	3	-1.5	2	-0.5	173.3
Mn[N(SiH ₃) ₂] ₂	3	-0.5	2	-1.5	173.3
	3	-0.5	2	0.5	183.8
	3	0.5	2	-0.5	183.8
	3	0.5	2	1.5	173.3
	3	1.5	2	0.5	173.3
	3	1.5	2	2.5	137.0
	3	2.5	2	1.5	137.0
	4	-2.5	1	-2.5	164.0
	4	2.5	1	2.5	164.0
	2	-1.5	1	-0.5	1206.0
	2	-0.5	1	-1.5	1206.0
	2	-0.5	1	0.5	1279.2
(I)Mn[N(SiH ₃) ₂] ₂ ⁻	2	0.5	1	-0.5	1279.2
	2	0.5	1	1.5	1206.0
	2	1.5	1	0.5	1206.0
	7	-2.5	1	-2.5	1500.8
	7	2.5	1	2.5	1500.8
	7	-2.5	1	-2.5	1289.2
	8	2.5	1	2.5	1289.2

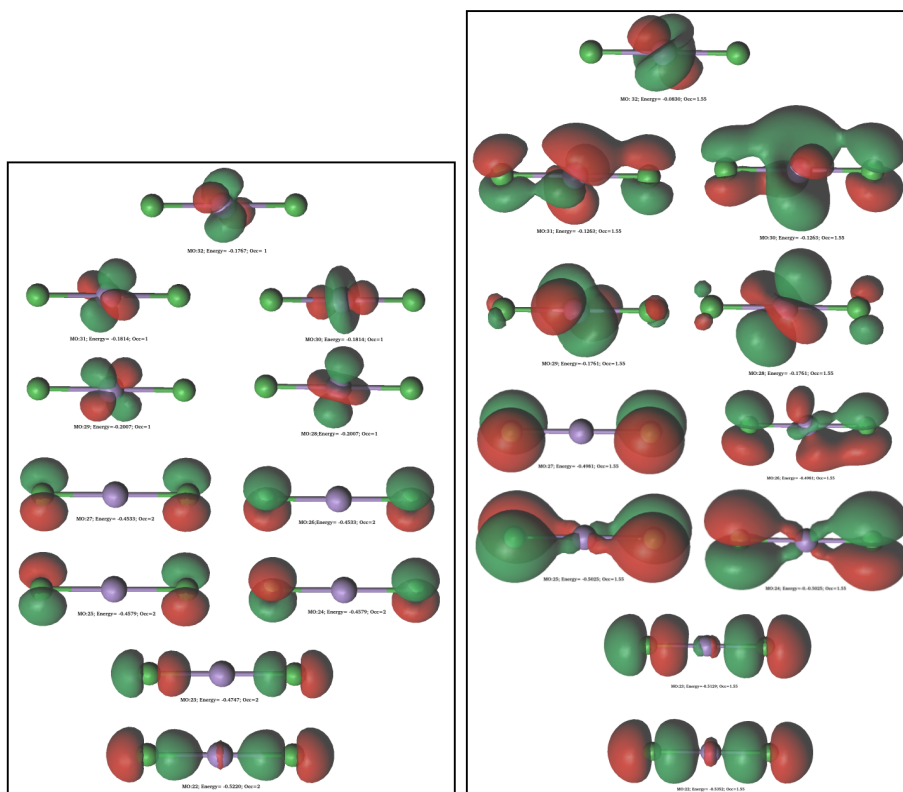


Figure S1: Orbitals of expanded active space (17,11) of MnCl_2 (a) before and (b) after state average CASSCF calculation.

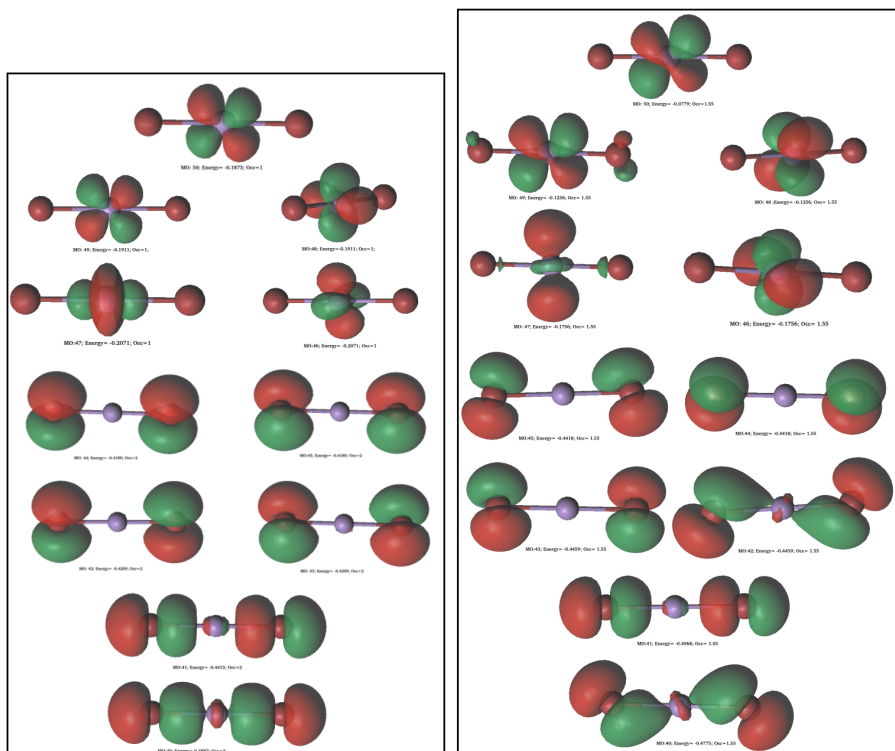


Figure S2: Orbitals of expanded active space (17,11) of MnBr₂ (a) before and (b) after state average CASSCF calculation.

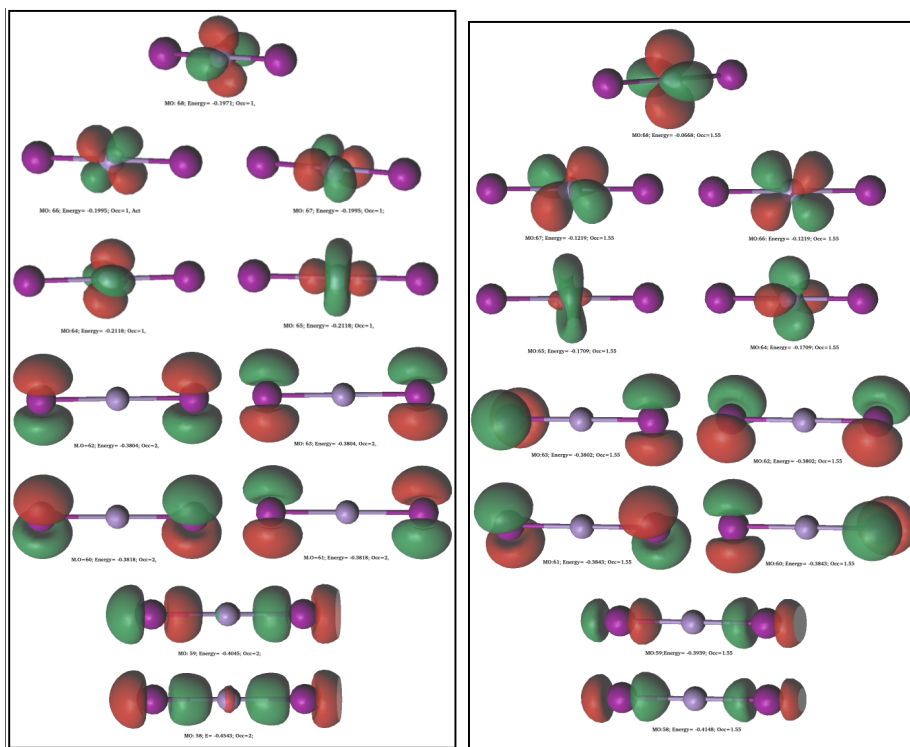


Figure S3: Orbitals of expanded active space (17,11) of MnI_2 (a) before and (b) after state average CASSCF calculation..

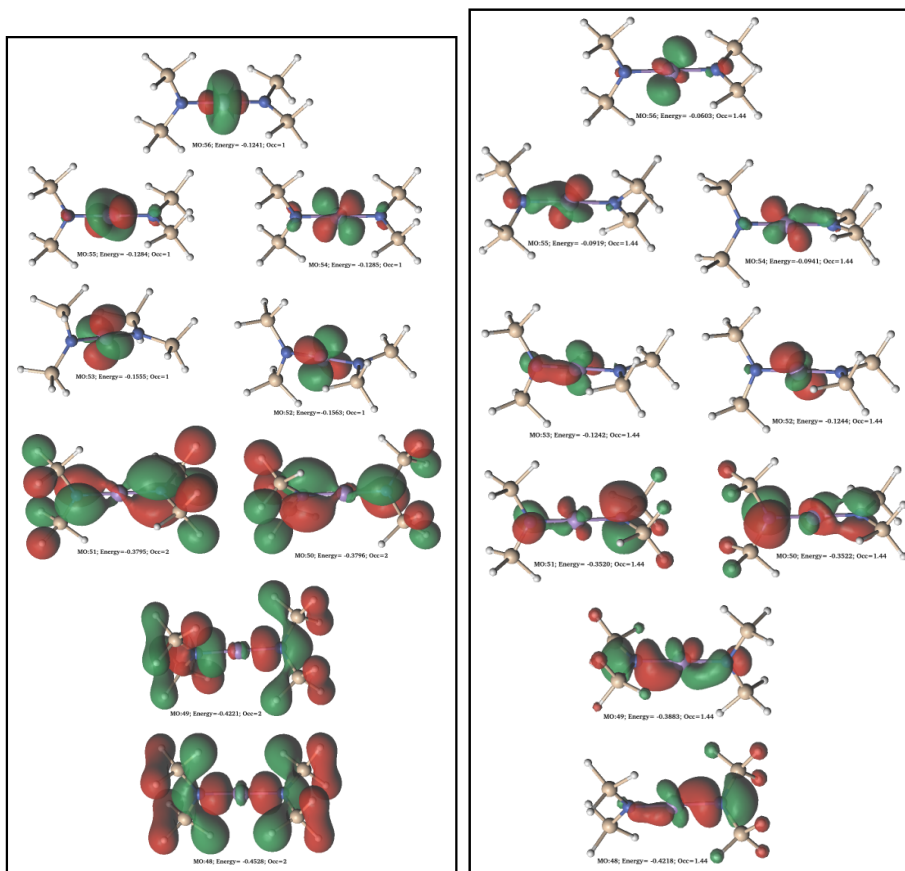


Figure S4: Orbitals of expanded active space (13,9) of $\text{Mn}[\text{N}(\text{SiH}_3)_2]_2$ (a) before and (b) after state average CASSCF calculation.

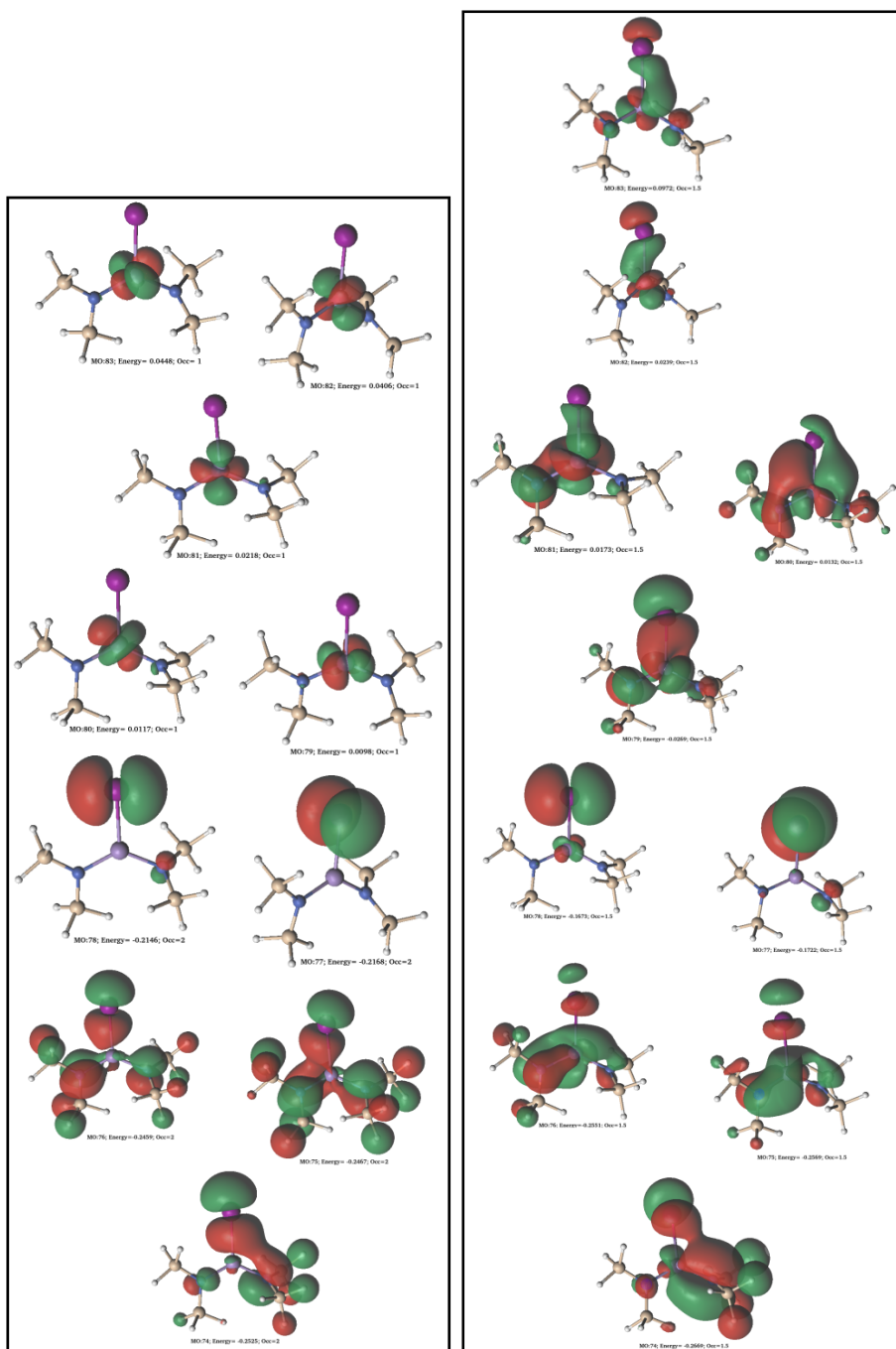


Figure S5: Orbitals of expanded active space (15,10) of $(I)Mn[N(SiH_3)_2]_2^-$ (a) before and (b) after state average CASSCF calculation.