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DFT and MM Description of the Structure and Magnetic Properties of Manganese Complexes with X-phenylcyanamido Bridging Ligand

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Supplementary Material

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Tables 1S –CFF parameters for all investigated complexes

Table 1S/1 - Bond stretching parameters

	k_r (kJ/mol Å ²)	r_0 (Å)		k_r (kJ/mol Å ²)	r_0 (Å)
Mn-N	1256.03	2.150	C _p -C _p	921.09	1.40
Mn-O	418.68	2.240	C _p -H	962.95	1.00
Mn-N _{ph}	628.01	2.300	C _p -Cl	628.01	1.76
O-C _{sp3}	628.01	1.390	C _p -F	628.01	1.34
O-H	628.01	0.870	N _{ph} -C _p	1046.69	1.38
C _{sp3} -C _{sp3}	2653.23	1.340	N _{ph} -C _{sp}	1046.69	1.29
C _{sp3} -H	628.01	0.960	N- C _{sp}	1046.69	1.17

Table 1S/2 – Angle bending parameters

	k_{θ} (kJ/mol rad ²)	θ (rad)		k_{θ} (kJ/mol rad ²)	θ (rad)
Mn-N _{ph} -C _p	125.60	2.18	C _p -C _p -N _{ph}	209.34	2.18
Mn-N-C _{sp}	1256.03	2.69	C _p -C _p -C _p	209.34	2.18
C _{sp} -N _{ph} -C _p	3349.40	2.09	H-C _p -C _p	209.34	2.18
N-Mn-N	209.34	1.58	Cl-C _p -C _p	209.34	2.18
N _{ph} -Mn-N _{ph}	20.93	2.82	F-C _p -C _p	209.34	2.18
O-Mn-N	209.34	1.49	H-O-C _{sp3}	2052.34	1.96
O-Mn- N _{ph} cis	209.34	3.01	H-C _{sp3} -O	259.24	2.18
O-Mn-N _{trans}	1046.69	3.04	H-C _{sp3} -H	192.93	1.86
N-Mn-N _{ph} cis	20.93	1.84	H-C _p -N _{ph}	293.07	2.18
N-Mn-N _{trans}	209.34	2.75	C _{sp3} -C _{sp3} -O	259.24	1.96
Mn-O-C _{sp3}	753.66	2.15	C _{sp3} -C _{sp3} -H	259.24	1.91
Mn-O-H	293.11	1.99			
N _{ph} -C _{sp} -N	2093.38	3.06			
C _p -N _{ph} -C _p	209.34	1.83			

Table 1S /3 – Torsion angle parameters

	k_{Φ} (kJ/mol)	n		k_{Φ} (kJ/mol)	n
N-Mn-N _{ph} -C _{sp}	0.004	12	C _p -C _p -C _p -C _p	29.307	-2
O-Mn-N-C _{sp}	4.187	12	H-C _p -C _p -H	523.344	-2
Mn-N-C _{sp} -N _{ph}	41.868	-2	H-C _p -C _p -X	314.006	-2
C _{sp} -N-C _p -N	0.029	-2	Mn-N _{ph} -C _p -H	4.187	-2
N _{ph} -Mn-O-C _{sp3}	0.029	3	H-C _p -C _p -C _p	14.654	-2
N _{ph} -Mn-N _{ph} -C _p	20.934	3	N _{ph} -C _p -C _p -N _{ph}	29.307	-2
O-Mn-A -C _p	29.307	3	C _p -A -C _p -H	29.307	-2
C _p -N _{ph} -C _p -C _p	29.307	-2	H-C _{sp3} -O-Mn	13.942	3
Mn-N _{ph} -C _p -C _p	523.344	-2	H-C _{sp3} -C _{sp3} -H	0.084	3
N _{ph} -C _p -C _p -C _p	29.307	-2	O-C _{sp3} -C _{sp3} -H	0.167	3
N-Mn-N-C _{sp}	4.187	3	O-Mn-N _{ph} -C _{sp}	4.187	3
N _{ph} -Mn-N-C _{sp}	0.004	3	Mn-N _{ph} -C _{sp} -N	41.868	-2

X=Cl, F

Table 1S /4– Electrostatic parameters

	esu		esu
Mn	0.882	N	-0.048
Cl	-0.130	C _{sp3}	0.401
F	-0.216	C _p , C _{sp}	0.131
O	-0.310	H	-0.116

Table 1S /5 – Van der Waals parameters

	ε (kJ/mol)	r^* (Å)		ε (kJ/mol)	r^* (Å)
Mn-C _p	0.54	3.24	F-N	0.25	3.42
Mn-C _{sp} ³	0.54	3.10	Cl-H	0.46	3.53
N-C _p	0.21	3.76	F-H	0.21	3.10
N- C _{sp} ³	0.21	3.76	Mn- C _{sp}	0.59	3.24
N-Mn	0.21	3.72	Mn-O	2.26	3.94
N- C _{sp}	0.21	3.76	Mn-Mn	0.63	2.60
C _p - C _p	0.17	3.88	C _{sp} ³ - C _{sp}	0.17	3.88
C _{sp} ³ - C _{sp} ³	0.17	3.88	C _{sp} - C _{sp}	0.17	3.88
C _{sp} ³ - C _p	0.17	3.88	H- C _{sp}	0.21	3.34
H-H	0.21	3.00	Cl- C _{sp}	0.42	3.97
H- C _{sp} ³	0.21	3.34	F- C _{sp}	0.21	3.54
H- C _p	0.21	3.34	O- C _{sp}	0.21	3.64
H-Mn	0.54	2.70	C _p - C _{sp}	0.17	3.88
N-H	0.21	3.32	Cl-N	0.50	3.85
N-N	0.21	3.60	H-O	0.25	3.24
Cl-Cl	1.00	4.00	Cl-O	0.50	3.85
F-F	0.25	3.20	F-O	0.21	3.34
Cl- C _p	0.42	3.97	O- C _p	0.21	3.64
F- C _p	0.21	3.54	O-N	0.21	3.56
Cl- C _{sp} ³	0.42	3.97	O-Mn	0.59	3.08
F- C _{sp} ³	0.21	3.54	O- C _{sp} ³	1.97	3.64
Cl-Mn	0.50	3.28	O-O	0.21	3.48
F-Mn	0.38	2.90	H-H	0.21	3.00