Magnetic and spectroscopic studies of iron and manganese complexes

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APPENDIX

1- IR and Raman spectra of the compounds described in chapter 2

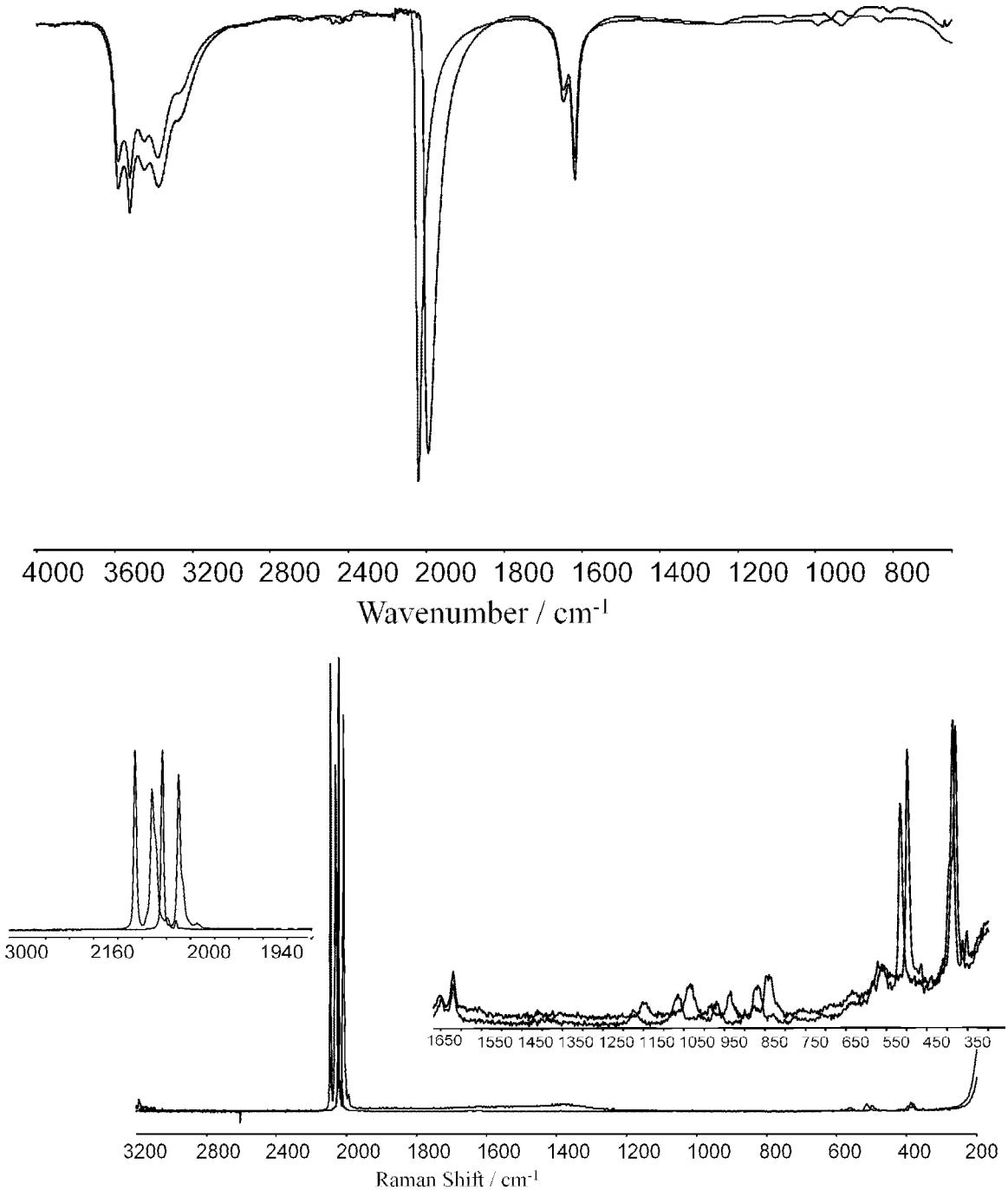

Figure A1: Solid state FTIR (upper) and Raman (lower) spectra of $K_4[Fe^{II}(^{12}CN)_6]$ and $K_4[Fe^{II}(^{13}CN)_6]$

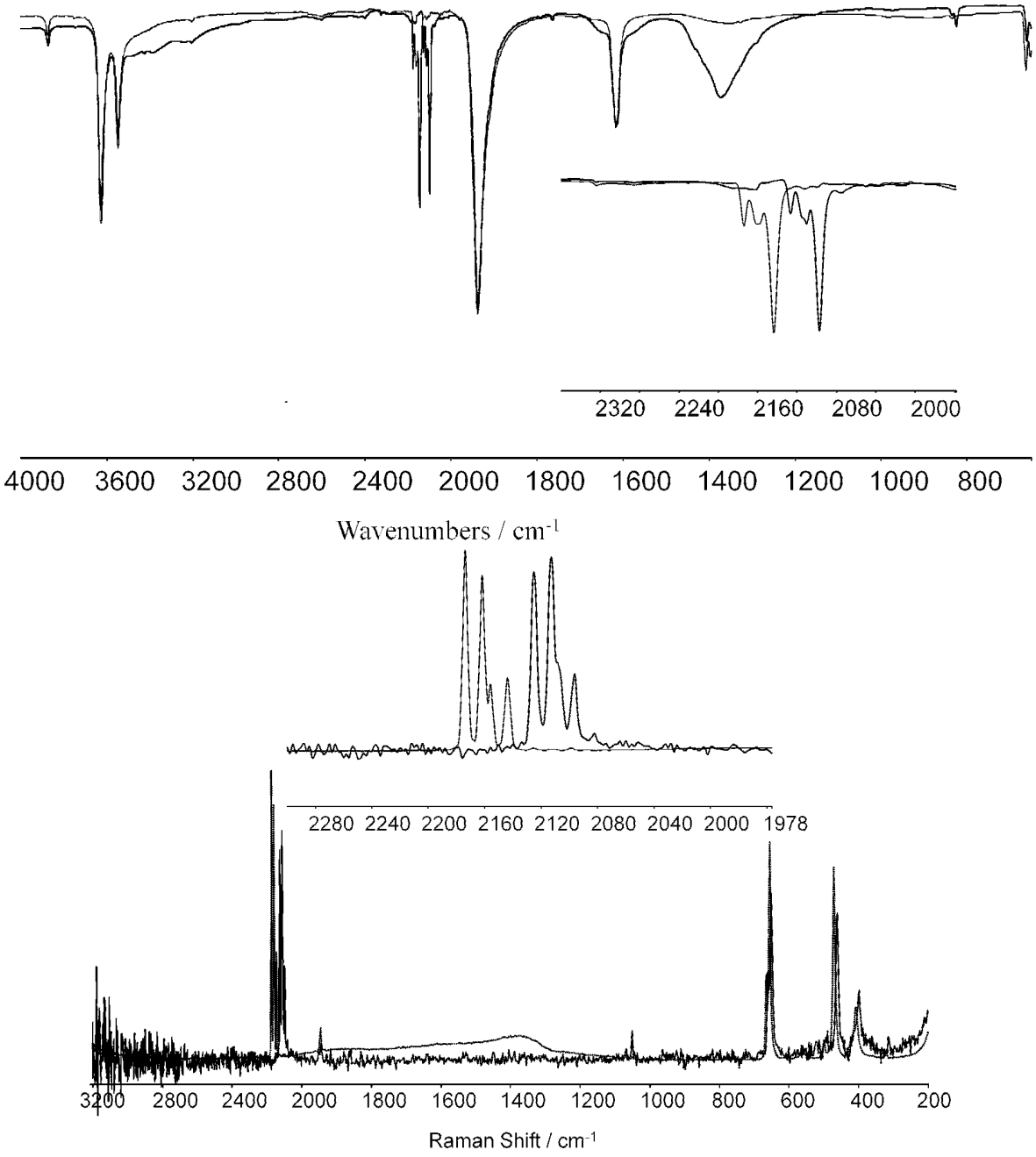

Figure A2: IR (upper) and Raman (bottom) spectra of $Na_2[Fe^{III}(^{13}CN)_5NO]$ (straight line) and $Na_2[Fe^{III}(CN)_5NO]$ (dotted lines)

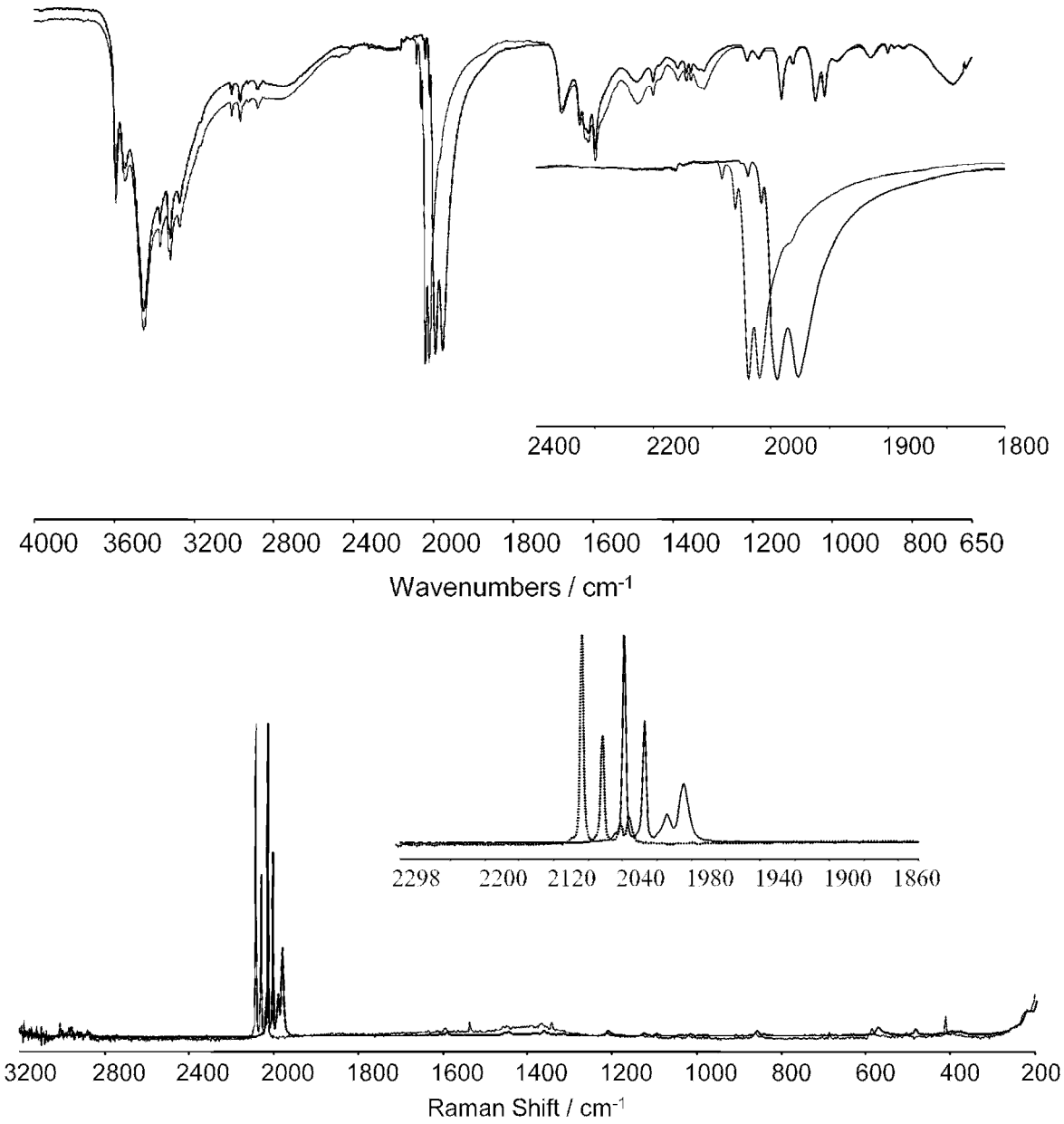

Figure A3: IR (upper) and Raman (bottom) spectra of $Na_3[Fe^{II}(^{13}CN)_5en]$ (straight lines) and $Na_3[Fe^{II}(CN)_5en]$ (dotted lines)

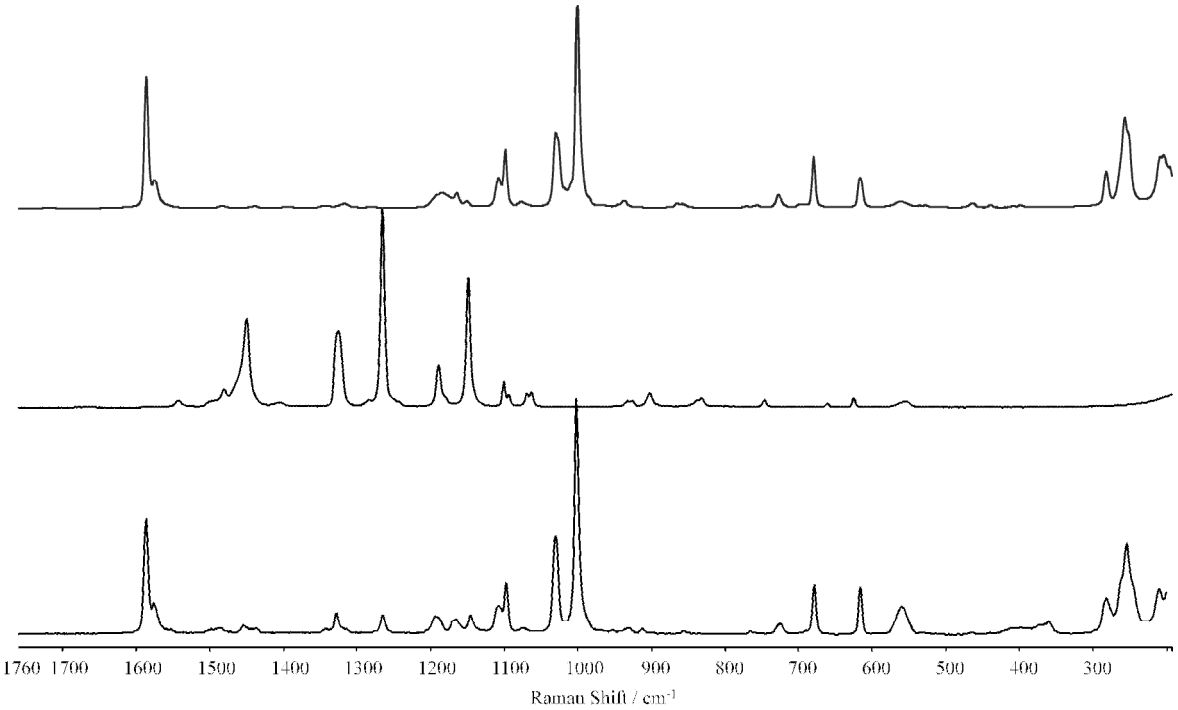

Figure A4: Raman spectra of Ph_4PCl (top), Imidazole (middle), and $(Ph_4P)_2[Fe^{III}(CN)_5im]$ $2H_2O$ (bottom)

2- Tables of the selected bonds lengths and angles for compounds 1, 2, 3 and 4 described in chapter 3

Table A1: Selected bond lengths (Å) and angles (deg)[a,b] for **1**

Co1-O1	2.119(3)	Fe1-C1_h	1.951(3)
Co1-N1	2.107(2)	N1-C1	1.145(4)
Co1-O1_b	2.119(3)	N2-C2	1.136(10)
Co1-N1_b	2.107(2)	N3-C3	1.380(7)
Co1-N1_d	2.107(2)	N3-C5	1.340(7)
Co1-N1_g	2.107(2)	N3-C3_a	1.380(7)
Fe1-N3	1.958(5)	N3-C5_a	1.340(7)
Fe1-C1	1.951(3)	N4-C4	1.360(12)
Fe1-C2	1.919(8)	N4-C5	1.341(13)
Fe1-C1_a	1.951(3)	C3-C4	1.359(9)
Fe1-C1_f	1.951(3)		
O1-Co1-N1	87.52(9)	C2-Fe1-C1_a	87.44(9)
O1-Co1-O1_b	180	C2-Fe1-C1_f	87.44(9)
O1-Co1-N1_b	92.48(9)	C2-Fe1-C1_h	87.44(9)
O1-Co1-N1_d	92.48(9)	C1_a-Fe1-C1_f	91.08(12)
O1-Co1-N1_g	87.52(9)	C1_a-Fe1-C1_h	88.69(12)
N1-Co1-O1_b	92.48(9)	C1_f-Fe1-C1_h	174.88(13)
N1-Co1-N1_b	88.70(9)	Co1-N1-C1	178.8(2)
N1-Co1-N1_d	180	Fe1-N3-C3	132.6(3)
N1-Co1-N1_g	91.30(9)	Fe1-N3-C5	121.4(4)
O1_b-Co1-N1_b	87.52(9)	Fe1-N3-C3_a	132.6(3)
O1_b-Co1-N1_d	87.52(9)	Fe1-N3-C5_a	121.4(4)
O1_b-Co1-N1_g	92.48(9)	C3-N3-C5	106.1(5)
N1_b-Co1-N1_d	91.30(9)	C3-N3-C3_a	94.9(5)
N1_b-Co1-N1_g	180	C3-N3-C5_a	11.2(5)
N1_d-Co1-N1_g	88.70(9)	C5-N3-C3_a	11.2(5)
N3-Fe1-C1	92.56(9)	C5-N3-C5_a	117.2(6)
N3-Fe1-C2	180	C3_a-N3-C5_a	106.1(5)
N3-Fe1-C1_a	92.56(9)	C4-N4-C5	103.5(7)
N3-Fe1-C1_f	92.56(9)	Fe1-C1-N1	177.7(3)
N3-Fe1-C1_h	92.56(9)	Fe1-C2-N2	180.00(3)
C1-Fe1-C2	87.44(9)	N3-C3-C4	105.8(5)
C1-Fe1-C1_a	174.88(13)	N4-C4-C3	111.6(6)
C1-Fe1-C1_f	88.69(12)	N3-C5-N4	113.0(6)
C1-Fe1-C1_h	91.08(12)		

[a]Estimated standard deviations in the last significant digits are given in parentheses. [b]Symmetry code: [_a] -1-x, 1/2-y, z; [_b] x, -y, -z; [_c] -x, 1/2+y, -z; [_d] -x, -y, -z; [_e] x, 1/2+y, -z; [_f] -1-x, y, z; [_g] -x, y, z; [_h] x, 1/2-y, z; [_i] -1/2-x, y, -1/2-z.

Table A2: selected bond lengths (Å) and angles (deg)[a,b] for **2**

Fe-N6	1.958(8)	O1-C9	1.415(12)
Fe-C1	1.956(14)	O2-C10	1.465(11)
Fe-C4	1.935(12)	N1-C1	1.144(18)
Fe-C5_b	1.928(15)	N2-C2	1.18(2)
Fe-C2_c	1.926(16)	N3-C3	1.15(2)
Fe-C3_e	1.937(16)	N4-C4	1.156(16)
Mn-O1	2.188(8)	N5-C5	1.178(19)
Mn-O2	2.278(9)	N6-C6	1.332(13)
Mn-N1	2.214(11)	C6-C8	1.374(11)
Mn-N2	2.159(13)	N7-C6	1.328(14)
Mn-N3	2.214(13)	N7-C7	1.392(15)
Mn-N5	2.217(12)	C7-C8	1.360(14)
N6-Fe-C1	91.45)	N1-Mn-N2	178.1(5)
N6-Fe-C4	174.4(6)	N1-Mn-N3	91.1(4)
N6-Fe-C5_b	94.1(6)	N1-Mn-N5	88.5(4)
N6-Fe-C2_c	90.1(6)	N2-Mn-N3	90.8(5)
N6-Fe-C3_e	91.2(6)	N2-Mn-N5	89.6(5)
C1-Fe-C4	85.5(6)	N3-Mn-N5	172.3(5)
C1-Fe-C5_b	87.9(6)	Mn-O1-C9	124.4(6)
C1-Fe-C2_c	94.8(6)	Mn-O2-C10	127.9(6)
C1-Fe-C3_e	176.1(6)	Mn-N1-C1	142.4(11)
C4-Fe-C5_b	89.1(6)	Mn-N2-C2	179.2(13)
C4-Fe-C2_c	86.7(6)	Mn-N3-C3	174.0(12)
C4-Fe-C3_e	92.1(6)	Mn-N5-C5	163.4(12)
C5_b-Fe-C2_c	174.7(6)	Fe-N6-C6	124.9(7)
C5_b-Fe-C3_e	89.0(6)	Fe-N6-C8	128.8(6)
C2_c-Fe-C3_e	88.0(7)	C6-N6-C8	106.2(7)
O1-Mn-O2	174.2(4)	C6-N7-C7	108.5(9)
O1-Mn-N1	87.4(4)	Fe-C1-N1	176.8(13)
O1-Mn-N2	92.9(4)	N2-C2-Fe_d	179.7(17)
O1-Mn-N3	94.2(4)	N3-C3-Fe_f	176.9(14)
O1-Mn-N5	93.5(4)	Fe-C4-N4	177.0(11)
O2-Mn-N1	87.1(4)	N5-C5-Fe_a	174.6(13)
O2-Mn-N2	92.6(4)	N6-C6-N7	110.5(9)
O2-Mn-N3	84.0(4)	N7-C7-C8	104.9(9)
O2-Mn-N5	88.3(4)	N6-C8-C7	109.8(8)

[a]Estimated standard deviations in the last significant digits are given in parentheses. [b]Symmetry code: [_a] -1+x, y, z; [_b] 1+x, y, z; [_c] 2-x, -1/2+y, 1/2-z; [_d] 2-x, ½+y, 1/2-z; [_e] 3-x, -1/2+y, 1/2-z; [_f] 3-x, 1/2 +y, 1/2 -z

Table A3: Selected bond lengths (Å) and angles (deg)[a,b] for **3**

Zn-N1	2.059(2)	Fe-C1_k	1.940(2)
Zn-N2	2.097(2)	N1-C1	1.147(3)
Zn-N3	2.024(3)	N2-C2	1.147(3)
Zn-N1_i	2.059(2)	N3-C3	1.167(4)
Zn-N2_i	2.097(2)	N4-C4	1.341(5)
Fe-N4	1.966(3)	N4-C6	1.377(5)
Fe-C1	1.940(2)	N5-C4	1.341(5)
Fe-C2_c	1.942(2)	N5-C5	1.353(6)
Fe-C3_e	1.919(4)	C5-C6	1.374(6)
Fe-C2_h	1.942(2)		
N1-Zn-N2	87.28(8)	C2_c-Fe-C3_e	89.76(10)
N1-Zn-N3	103.69(8)	C2_c-Fe-C2_h	88.17(9)
N1-Zn-N1_i	88.56(8)	C2_c-Fe-C1_k	91.99(9)
N1-Zn-N2_i	155.03(9)	C3_e-Fe-C2_h	89.76(10)
N2-Zn-N3	101.22(8)	C3_e-Fe-C1_k	87.96(10)
N2-Zn-N1_i	155.03(9)	C2_h-Fe-C1_k	177.72(11)
N2-Zn-N2_i	86.19(8)	Zn-N1-C1	174.4(2)
N3-Zn-N1_i	103.69(8)	Zn-N2-C2	175.7(2)
N3-Zn-N2_i	101.22(8)	Zn-N3-C3	155.7(3)
N1_j-Zn-N2_i	87.28(8)	Fe-N4-C4	124.8(2)
N4-Fe-C1	90.61(9)	Fe-N4-C6	128.0(2)
N4-Fe-C2_c	91.67(9)	C4-N4-C6	107.2(3)
N4-Fe-C3_e	178.01(12)	C4-N5-C5	109.1(4)
N4-Fe-C2_h	91.67(9)	Fe-C1-N1	177.2(2)
N4-Fe-C1_k	90.61(9)	N2-C2-Fe_b	178.6(2)
C1-Fe-C2_c	177.72(11)	N3-C3-Fe_d	176.0(3)
C1-Fe-C3_e	87.96(10)	N4-C4-N5	109.2(3)
C1-Fe-C2_h	91.99(9)	N5-C5-C6	106.7(3)
C1-Fe-C1_k	87.77(9)	N4-C6-C5	107.8(3)

[a]Estimated standard deviations in the last significant digits are given in parentheses. [b]Symmetry code: [_a] 3/2-x, 1-y, -1/2+z; [_b] -1/2+x, 3/2-y, 1/2-z; [_c] 1/2+x, 3/2-y, 1/2-z; [_d] 1-x, -1/2+y, 1-z; [_e] 1-x, 1/2+y, 1-z; [_f] 1-x, 1-y, 1-z; [_g] -1/2+x, y, 1/2-z; [_h] 1/2+x, y, 1/2-z; [_i] 3/2-x, 1/2+y, -1/2+z; [_j] x, 1/2-y, z; [_k] x, 3/2-y, z.

Table A4: Selected bond lengths (Å) and angles (deg)[a,b] for **4**

Fe-N4	1.969(4)	N5-C4	1.342(6)
Fe-C1	1.927(6)	N5-C6	1.373(7)
Fe-C2	1.942(4)	N6-C7	1.335(6)
Fe-C3	1.947(4)	N6-C11	1.351(6)
Fe -C4	1.942(4)	N7-C12	1.342(6)
Fe-C5	1.947(4)	N7-C16	1.339(7)
Mn-N2	2.215(3)	C5-C6	1.352(9)
Mn-N6	2.267(4)	C7-C8	1.391(6)
Mn-N7	2.341(4)	C8-C9	1.377(7)

Mn-N3_b	2.227(3)	C9-C10	1.373(8)
Mn-N3_d	2.227(3)	C10-C11	1.387(8)
Mn-N2_g	2.215(3)	C11-C12	1.486(7)
N1-C1	1.153(8)	C12-C13	1.402(8)
N2-C2	1.155(5)	C13-C14	1.372(8)
N3-C3	1.156(5)	C14-C15	1.376(9)
N4-C4	1.331(7)	C15-C16	1.387(8)
N4-C5	1.387(8)		

N4-Fe-C1	178.2(2)	C3-N3-Mn_c	163.2(3)
N4-Fe-C2	90.36(14)	Fe-N4-C4	126.3(3)
N4-Fe-C3	90.62(13)	Fe-N4-C5	128.0(3)
N4-Fe-C2_f	90.36(14)	C4-N4-C5	105.7(4)
N4-Fe-C3_f	90.62(13)	C4-N5-C6	108.0(4)
C1-Fe-C2	88.35(16)	Mn-N6-C7	120.6(3)
C1-Fe-C3	90.68(16)	Mn-N6-C11	120.6(3)
C1-Fe-C2_f	88.35(16)	C7-N6-C11	118.8(4)
C1-Fe-C3_f	90.68(16)	Mn-N7-C12	117.9(3)
C2-Fe-C3	92.92(16)	Mn-N7-C16	123.1(4)
C2-Fe-C2_f	87.14(16)	C12-N7-C16	119.0(5)
C2-Fe-C3_f	179.02(15)	Fe-C1-CN1	176.2(5)
C3-Fe-C2_f	179.02(15)	Fe-C2-N2	176.2(3)
C3-Fe-C3_f	87.00(16)	Fe-C3-N3	176.5(3)
C2_f -Fe-C3_f	92.92(16)	N4-C4-N5	110.6(4)
N2-Mn-N6	130.05(9)	N4-C5-C6	109.4(5)
N2-Mn-N7	82.95(11)	N5-C6-C5	106.3(5)
N2-Mn-N3_b	138.52(11)	N6-C7-C8	122.2(5)
N2-Mn-N3_d	81.19(10)	C7-C8-C9	119.4(5)
N2-Mn-N2_g	84.85(11)	C8-C9-C10	118.2(5)
N6-Mn-N7	70.23(14)	C9-C10-C11	120.5(5)
N6-Mn-N3_b	87.36(11)	N6-C11-C10	121.0(5)
N6-Mn-N3_d	87.36(11)	N6-C11-C12	115.2(4)
N6-Mn-N2_g	130.05(9)	C10-C11-C12	123.9(5)
N7-Mn-N3_b	133.05(8)	N7-C12-C11	116.1(4)
N7-Mn-N3_d	133.05(8)	N7-C12-C13	121.1(5)
N7-Mn-N2_g	82.95(11)	C11-C12-C13	122.8(4)
N3_b-Mn-N3_d	83.95(10)	C12-C13-C14	119.1(6)
N3_b-Mn-N2_g	81.19(10)	C13-C14-C15	119.9(5)
N3_d-Mn-N2_g	138.52(11)	C14-C15-C16	118.2(5)
Mn-N2-C2	157.6(3)	N7-C16-C15	122.7(6)

[a]Estimated standard deviations in the last significant digits are given in parentheses. [b]Symmetry code: [_a] x, -1/2-y, z; [_b] -1/2+x, 1/2-y, 1/2-z; [_c] 1/2+x, 1/2-y, 1/2-z; [_d] -1/2+x, y, 1/2-z; [_e] 1/2+x, y, 1/2-z; [_f] x, -1/2-y, z; [_g] x, 1/2-y, z;