

University of Groningen

Magnetic and spectroscopic studies of iron and manganese complexes

Tchouka, Héloïse

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version

Publisher's PDF, also known as Version of record

Publication date:

2011

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Tchouka, H. (2011). *Magnetic and spectroscopic studies of iron and manganese complexes: from molecular materials to catalysis*. s.n.

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

APPENDIX

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

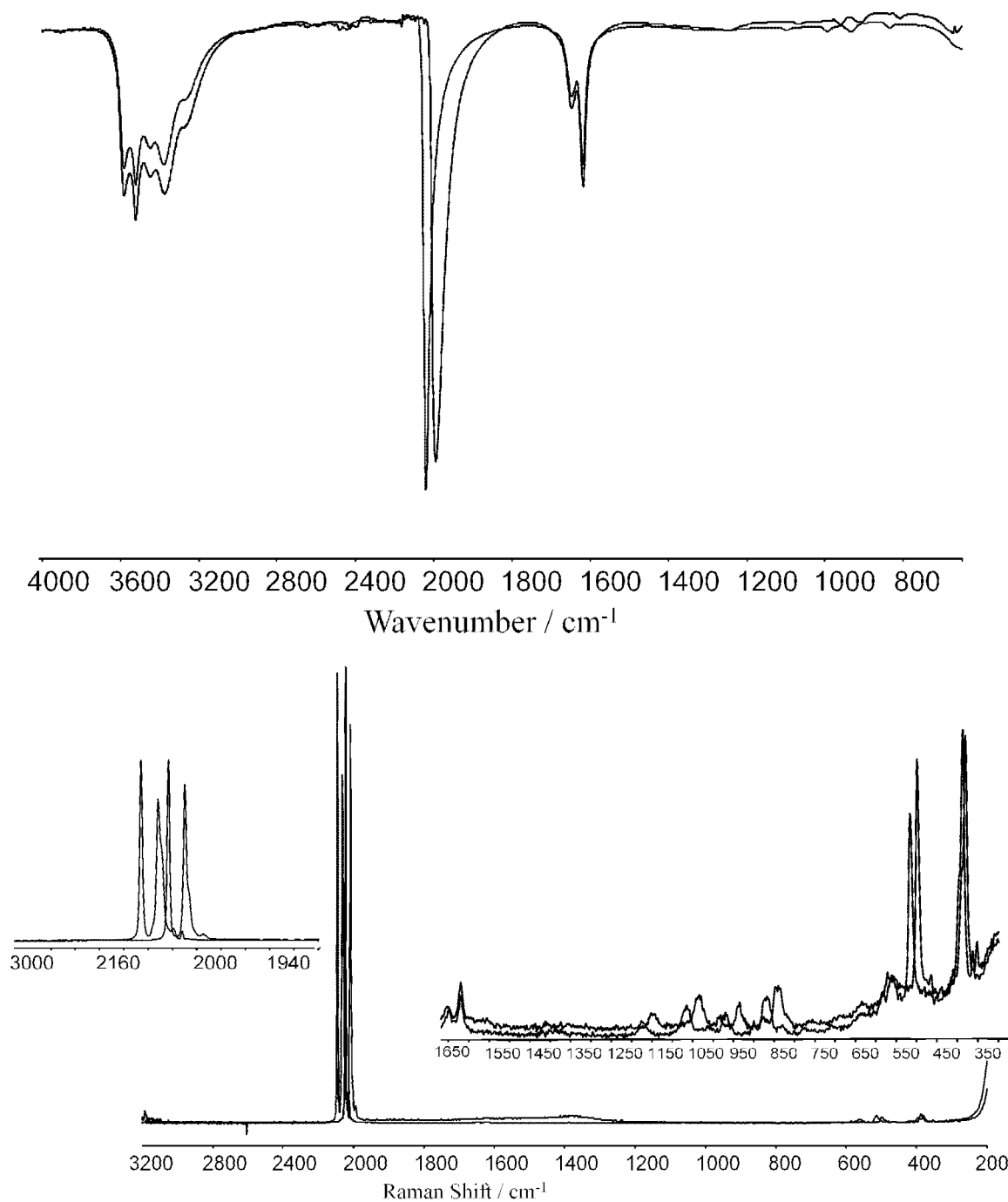


Figure A1: Solid state FTIR (upper) and Raman (lower) spectra of $K_4[Fe^{II}(^{12}CN)_6]$ and $K_4[Fe^{II}(^{13}CN)_6]$

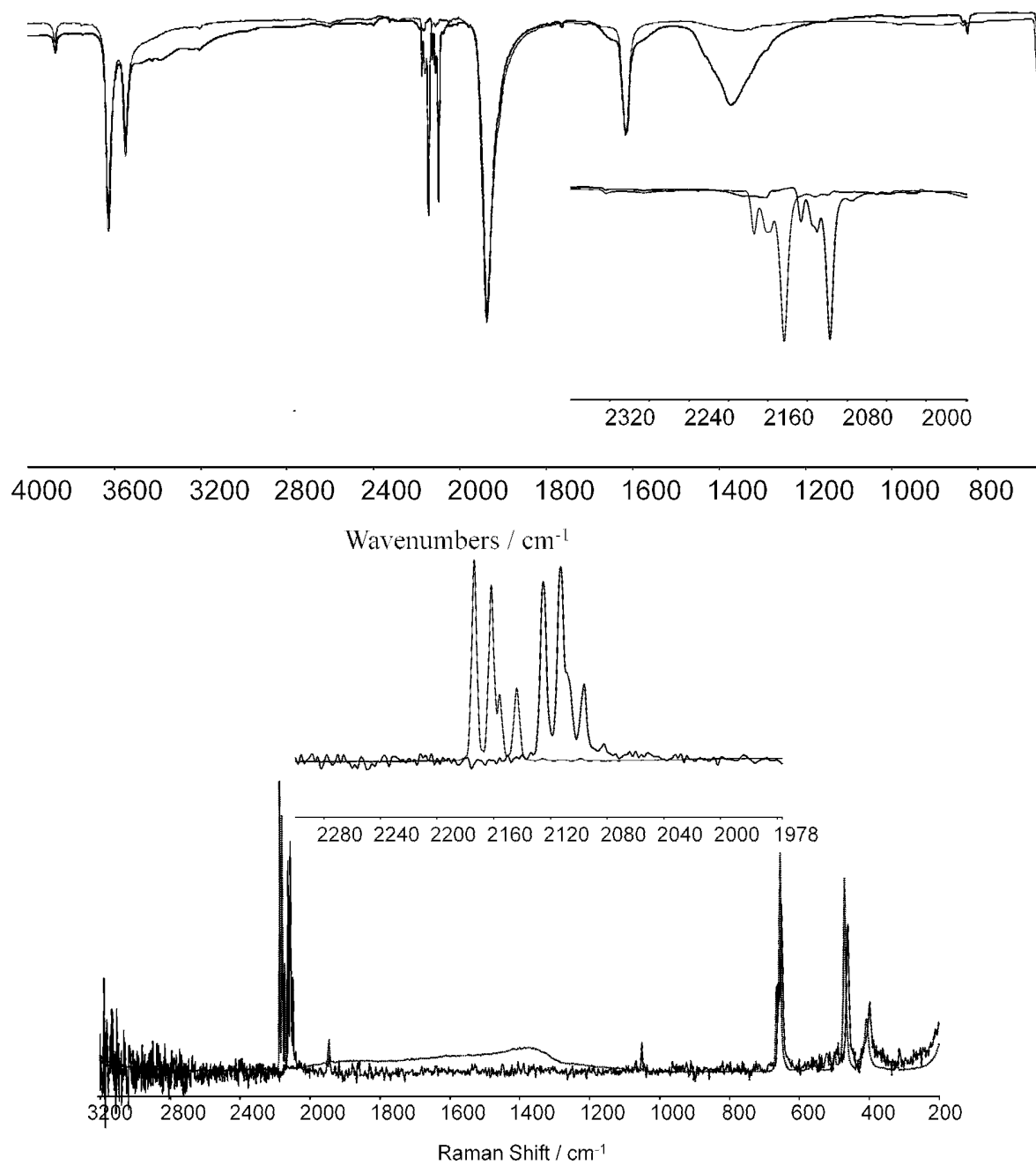


Figure A2: IR (upper) and Raman (bottom) spectra of $\text{Na}_2[\text{Fe}^{\text{III}}(^{13}\text{CN})_5\text{NO}]$ (straight line) and $\text{Na}_2[\text{Fe}^{\text{III}}(\text{CN})_5\text{NO}]$ (dotted lines)

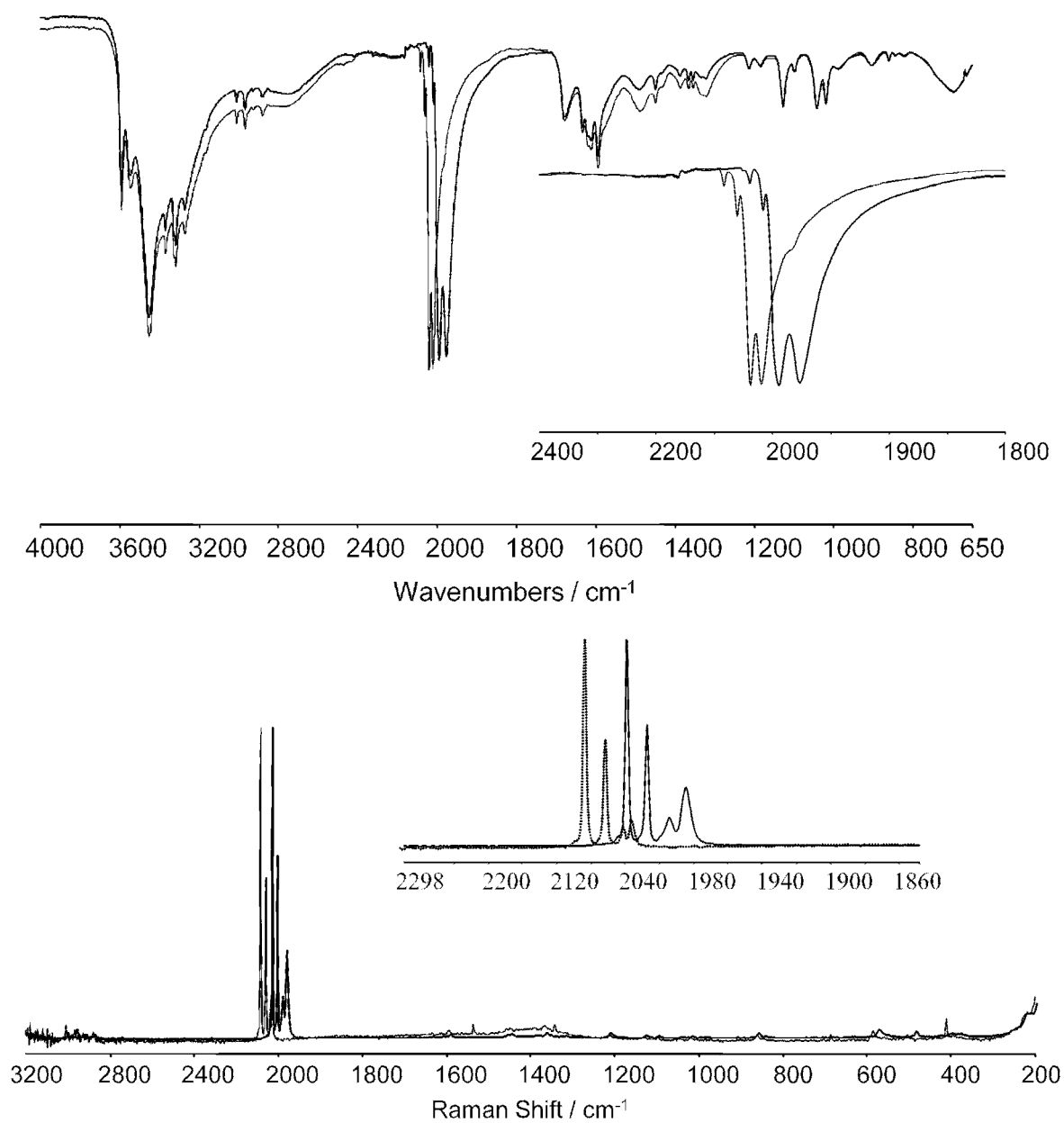


Figure A3: IR (upper) and Raman (bottom) spectra of Na₃[Fe^{II}(¹³CN)₅en] (straight lines) and Na₃[Fe^{II}(CN)₅en] (dotted lines)

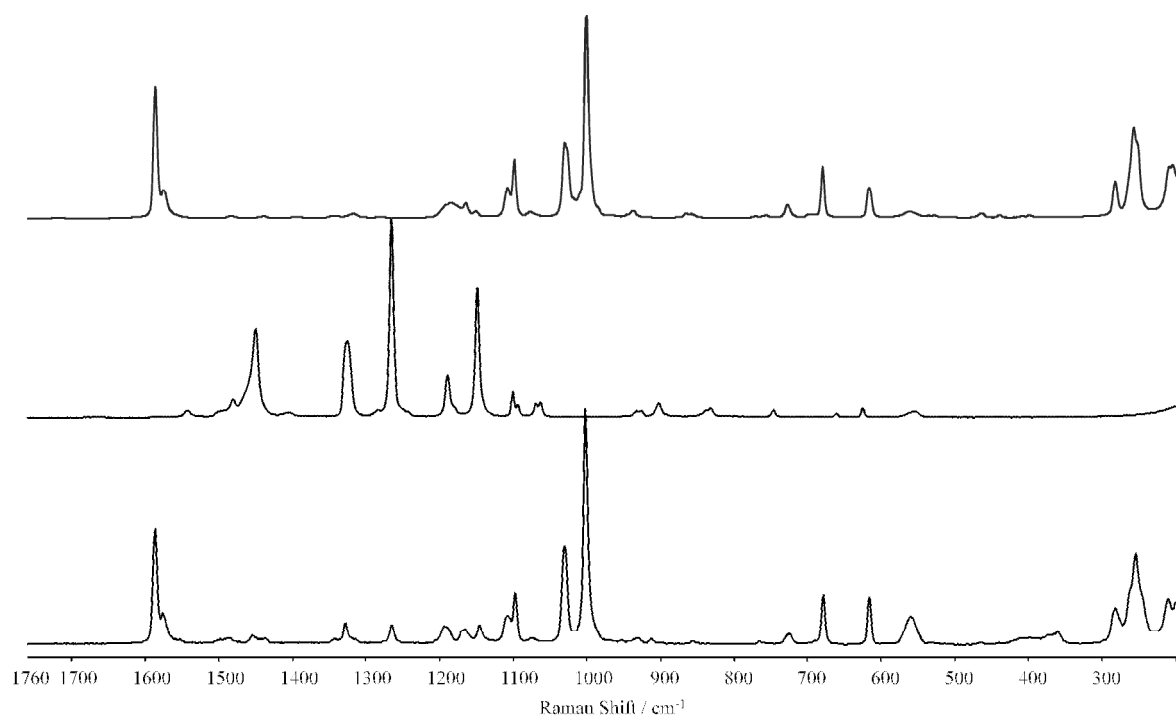


Figure A4: Raman spectra of Ph₄PCl (top), Imidazole (middle), and (Ph₄P)₂[Fe^{III}(CN)₅im] 2H₂O (bottom)

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)		

^aEstimated standard deviations in the last significant digits are given in parentheses.

^bSymmetry 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)

^aEstimated standard deviations in the last significant digits are given in parentheses.

^bSymmetry code: [_a] -1+x, y, z; [_b] 1+x, y, z; [_c] 2-x, -1/2+y, 1/2-z; [_d] 2-x, 1/2+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)

^aEstimated standard deviations in the last significant digits are given in parentheses.

^bSymmetry 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)

^aEstimated standard deviations in the last significant digits are given in parentheses.

^bSymmetry 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;