Supporting Information for:

One-dimensional polymers containing strictly collinear metal ions: synthesis and XRPD characterization of homoleptic binary metal pyrazolates

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(10 Pages)

Compound: trispyrazolate iron (III)
Fe(pz)3

Space Group P 63/m

The lattice is centric primitive hexagonal Laue symmetry 6/m
Multiplicity of a general site is 12
The symmetry of the point 0,0,0 contains 1bar

Equivalent Positions

(1)	X	Y	Z	(2)	X-Y	X	1/2+Z	(3)	-Y	X-Y	Z
(4)	-X	-Y	1/2+Z	(5)	Y-X	-X	Z	(6)	Y	Y-X	1/2+Z

Lattice constants

a = 9.17454(33) b = A c = 7.2191(4)
Alpha = 90 Beta = 90 Gamma = 120
Cell volume = 526.24(4)

Fractional Atomic Coordinates

Name	X	Y	Z	Ui/Ue*100	Site sym	Mult	Type	Seq	Fractn
Fe	.000000	.000000	.000000	3.95(7)	-3	2	FE	1	1.0000
N	.1586(4)	.19284(33)	.15444(11)	5.95(7)	1	12	N	2	1.0000
C1	.2785(4)	.3510(4)	.09510(10)	5.95(7)	1	12	C	3	1.0000
C2	.3608(5)	.4449(4)	.250000	5.95(7)	M(001)	6	C	4	1.0000

Relevant Bond Distances and Angles

Vector	Length	Optr Cell	Neighbor atom coordinates		
Fe_Fe	3.60954(18)	2 0 0-1	.00000	.00000	-.50000
Fe_Fe	3.60954(18)	2 0 0 0	.00000	.00000	.50000
Fe_N	1.9788(23)	1 0 0 0	.15856	.19284	.15444

Fe_N	1.9788(23)	3 0 0 0	-.19284	-.03428	.15444
Fe_N	1.9788(23)	5 0 0 0	.03428	-.15856	.15444
Fe_N	1.9788(23)	-1 0 0 0	-.15856	-.19284	-.15444
Fe_N	1.9788(23)	-3 0 0 0	.19284	.03428	-.15444
Fe_N	1.9788(23)	-5 0 0 0	-.03428	.15856	-.15444
N_Fe	1.9788(23)	1 0 0 0	.00000	.00000	.00000
N_N	1.3797(15)	-4 0 0 1	.15856	.19284	.34556
N_C1	1.3794(13)	1 0 0 0	.27855	.35096	.09510
C1_N	1.3794(13)	1 0 0 0	.15856	.19284	.15444
C1_C1	2.2365(15)	-4 0 0 1	.27855	.35096	.40490
C1_C2	1.3828(12)	1 0 0 0	.36076	.44490	.25000
C2_C1	1.3828(12)	1 0 0 0	.27855	.35096	.09510
C2_C1	1.3828(12)	-4 0 0 1	.27855	.35096	.40490

Angle	Degrees	atom 1 loc	atom 3 loc
N_Fe_N	91.36(7)	1 0 0 0	3 0 0 0
N_Fe_N	91.36(7)	1 0 0 0	5 0 0 0
N_Fe_N	179.980(0)	1 0 0 0	-1 0 0 0
N_Fe_N	88.64(7)	1 0 0 0	-3 0 0 0
N_Fe_N	88.64(7)	1 0 0 0	-5 0 0 0
N_Fe_N	91.36(7)	3 0 0 0	5 0 0 0
N_Fe_N	88.64(7)	3 0 0 0	-1 0 0 0
N_Fe_N	180.000(0)	3 0 0 0	-3 0 0 0
N_Fe_N	88.64(7)	3 0 0 0	-5 0 0 0
N_Fe_N	88.64(7)	5 0 0 0	-1 0 0 0
N_Fe_N	88.64(7)	5 0 0 0	-3 0 0 0
N_Fe_N	179.980(0)	5 0 0 0	-5 0 0 0
N_Fe_N	91.36(7)	-1 0 0 0	-3 0 0 0
N_Fe_N	91.36(7)	-1 0 0 0	-5 0 0 0
N_Fe_N	91.36(7)	-3 0 0 0	-5 0 0 0
Fe_N_N	124.29(5)	1 0 0 0	-4 0 0 1
Fe_N_C1	127.49(8)	1 0 0 0	1 0 0 0
N_N_C1	108.09(5)	-4 0 0 1	1 0 0 0
C1_C1_C2	107.71(15)	1 0 0 0	1 0 0 0
C1_C2_C1	107.93(13)	1 0 0 0	-4 0 0 1

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Compound: bispyrazolate cobalt (II)
Co(pz)2

Space Group I b a m

The lattice is centric I-centered orthorhombic Laue symmetry mmm
Multiplicity of a general site is 16
The symmetry of the point 0,0,0 contains 1bar

Equivalent Positions

(1)	X	Y	Z	(2)	1/2-X	1/2+Y	Z
(3)	1/2+X	1/2-Y	Z	(4)	-X	-Y	Z

Lattice Constants

a = 7.5239(5) b = 14.3461(9) c = 7.4331(5)
Alpha = 90 Beta = 90 Gamma = 90
Cell volume = 802.31(9)

Fractional Atomic Coordinates

Name	X	Y	Z	Ui/Ue*100	Site sym	Mult	Type	Seq	Fractn
Co	.500000	.000000	.250000	3.32(12)	222	4	Co	1	1.0000
N	.3395(8)	.0764(5)	.09286(12)	5.32(12)	1	16	N	2	1.0000
C1	.2023(9)	.1334(5)	.15012(12)	5.32(12)	1	16	C	3	1.0000
C2	.1343(13)	.1779(7)	.000000	5.32(12)	M(001)	8	C	4	1.0000

Relevant Bond Distances and Angles

Vector	Length	Optr Cell	Neighbor atom coordinates		
Co_Co	3.71653(25)	-1 1 0 0	.50000	.00000	-.25000
Co_Co	3.71653(25)	-1 1 0 1	.50000	.00000	.75000

Co_N	2.0062(29)	1	0	0	0	.33950	.07643	.09286
Co_N	2.0062(29)	4	1	0	0	.66050	-.07643	.09286
Co_N	2.0062(29)	-102	0	0	0	.33950	-.07643	.40714
Co_N	2.0062(29)	-103	1	0	0	.66050	.07643	.40714
N_Co	2.0062(29)	1	0	0	0	.50000	.00000	.25000
N_N	1.3805(18)	-4	0	0	0	.33950	.07643	-.09286
N_C1	1.3836(16)	1	0	0	0	.20233	.13340	.15012
C1_N	1.3836(16)	1	0	0	0	.33950	.07643	.09286
C1_C1	2.2317(18)	-4	0	0	0	.20233	.13340	-.15012
C1_C2	1.3833(16)	1	0	0	0	.13433	.17786	.00000
C2_C1	1.3833(16)	1	0	0	0	.20233	.13340	.15012
C2_C1	1.3833(16)	-4	0	0	0	.20233	.13340	-.15012

Angle	Degrees	atom 1	loc			atom 3	loc		
N_Co_N	108.79(13)	1	0	0	0	4	1	0	0
N_Co_N	106.0(4)	1	0	0	0	-102	0	0	0
N_Co_N	113.7(5)	1	0	0	0	-103	1	0	0
N_Co_N	113.7(5)	4	1	0	0	-102	0	0	0
N_Co_N	106.0(4)	4	1	0	0	-103	1	0	0
N_Co_N	108.79(13)	-102	0	0	0	-103	1	0	0
Co_N_N	125.61(6)	1	0	0	0	-4	0	0	0
Co_N_C1	126.35(10)	1	0	0	0	1	0	0	0
N_N_C1	107.92(6)	-4	0	0	0	1	0	0	0
C1_C1_C2	107.46(19)	1	0	0	0	1	0	0	0
C1_C2_C1	107.54(20)	1	0	0	0	-4	0	0	0

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Compound: trispyrazolate cobalt (III)
Co(pz)3

Space Group P 63/m
The lattice is centric primitive hexagonal Laue symmetry 6/m
Multiplicity of a general site is 12
The symmetry of the point 0,0,0 contains 1bar

Equivalent Positions

(1)	X	Y	Z	(2)	X-Y	X	1/2+Z	(3)	-Y	X-Y	Z
(4)	-X	-Y	1/2+Z	(5)	Y-X	-X	Z	(6)	Y	Y-X	1/2+Z

Lattice Constants

a = 9.19657(31) b = A c = 7.10514(30)
Alpha = 90 Beta = 90 Gamma = 120
Cell volume = 520.422(33)

Fractional Atomic Coordinates

Name	X	Y	Z	Ui/Ue*100	Site sym	Mult	Type	Seq	Fractn
Co	.000000	.000000	.000000	2.42(6)	-3	2	CO	1	1.0000
N	.1553(4)	.1918(4)	.15295(11)	4.42(6)	1	12	N	2	1.0000
C1	.2758(4)	.3490(4)	.09258(11)	4.42(6)	1	12	C	3	1.0000
C2	.3551(6)	.4451(5)	.250000	4.42(6)	M(001)	6	C	4	1.0000

Relevant Bond Distances and Angles

Vector	Length	Optr Cell	Neighbor atom coordinates		
Co_Co	3.55257(15)	2 0 0-1	.00000	.00000	-.50000
Co_Co	3.55257(15)	2 0 0 0	.00000	.00000	.50000
Co_N	1.9524(25)	1 0 0 0	.15527	.19176	.15295

Co_N	1.9524(25)	3 0 0 0	-.19176	-.03649	.15295
Co_N	1.9524(25)	5 0 0 0	.03649	-.15527	.15295
Co_N	1.9524(25)	-1 0 0 0	-.15527	-.19176	-.15295
Co_N	1.9524(25)	-3 0 0 0	.19176	.03649	-.15295
Co_N	1.9524(25)	-5 0 0 0	-.03649	.15527	-.15295
N_Co	1.9524(25)	1 0 0 0	.00000	.00000	.00000
N_N	1.3792(15)	-4 0 0 1	.15527	.19176	.34705
N_C1	1.3784(13)	1 0 0 0	.27576	.34896	.09258
C1_N	1.3784(13)	1 0 0 0	.15527	.19176	.15295
C1_C1	2.2370(15)	-4 0 0 1	.27576	.34896	.40742
C1_C2	1.3856(12)	1 0 0 0	.35505	.44512	.25000
C2_C1	1.3856(12)	1 0 0 0	.27576	.34896	.09258
C2_C1	1.3856(12)	-4 0 0 1	.27576	.34896	.40742

Angle	Degrees	atom 1 loc	atom 3 loc
N_Co_N	92.02(8)	1 0 0 0	3 0 0 0
N_Co_N	92.02(8)	1 0 0 0	5 0 0 0
N_Co_N	179.966(0)	1 0 0 0	-1 0 0 0
N_Co_N	87.98(8)	1 0 0 0	-3 0 0 0
N_Co_N	87.98(8)	1 0 0 0	-5 0 0 0
N_Co_N	92.02(8)	3 0 0 0	5 0 0 0
N_Co_N	87.98(8)	3 0 0 0	-1 0 0 0
N_Co_N	180.000(0)	3 0 0 0	-3 0 0 0
N_Co_N	87.98(8)	3 0 0 0	-5 0 0 0
N_Co_N	87.98(8)	5 0 0 0	-1 0 0 0
N_Co_N	87.98(8)	5 0 0 0	-3 0 0 0
N_Co_N	180.000(0)	5 0 0 0	-5 0 0 0
N_Co_N	92.02(8)	-1 0 0 0	-3 0 0 0
N_Co_N	92.02(8)	-1 0 0 0	-5 0 0 0
N_Co_N	92.02(8)	-3 0 0 0	-5 0 0 0
Co_N_N	123.82(5)	1 0 0 0	-4 0 0 1
Co_N_C1	127.99(8)	1 0 0 0	1 0 0 0
N_N_C1	108.13(5)	-4 0 0 1	1 0 0 0
C1_C1_C2	107.98(15)	1 0 0 0	1 0 0 0
C1_C2_C1	107.65(13)	1 0 0 0	-4 0 0 1

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Compound: bispyrazolate nickel (II) - alpha form
alpha-Ni(pz)2

Space Group C m c m

The lattice is centric C-centered orthorhombic Laue symmetry mmm
Multiplicity of a general site is 16
The symmetry of the point 0,0,0 contains 1bar

Equivalent Positions

(1)	X	Y	Z	(2)	-X	Y	Z
(3)	X	-Y	1/2+Z	(4)	-X	-Y	1/2+Z

Lattice Constants

a = 16.6758(11) b = 6.4872(4) c = 6.9423(6)
Alpha = 90 Beta = 90 Gamma = 90
Cell volume = 751.01(9)

Fractional Atomic Coordinates

Name	X	Y	Z	Ui/Ue*100	Site sym	Mult	Type	Seq	Fractn
Ni	.000000	.000000	.000000	6.87(8)	2/M(100)	4	NI	1	1.0000
N	.08011(20)	.1209(6)	.15062(8)	8.87(8)	1	16	N	2	1.0000
C1	.14581(25)	.2327(6)	.08947(8)	8.87(8)	1	16	C	3	1.0000
C2	.18046(36)	.3213(8)	.250000	8.87(8)	M(001)	8	C	4	1.0000

Relevant Bond Distances and Angles

Vector	Length	Optr Cell	Neighbor atom coordinates		
Ni_N	1.8690(33)	1 0 0 0	.08011	.12091	.15062
Ni_N	1.8690(33)	2 0 0 0	-.08011	.12091	.15062

Ni_N	1.8690(33)	-1 0 0 0	-.08011	-.12091	-.15062
Ni_N	1.8690(33)	-2 0 0 0	.08011	-.12091	-.15062
N_Ni	1.8690(33)	1 0 0 0	.00000	.00000	.00000
N_N	1.3798(11)	-4 0 0 1	.08011	.12091	.34938
N_C1	1.3809(9)	1 0 0 0	.14581	.23274	.08947
C1_N	1.3809(9)	1 0 0 0	.08011	.12091	.15062
C1_C1	2.2288(11)	-4 0 0 1	.14581	.23274	.41053
C1_C2	1.3805(9)	1 0 0 0	.18046	.32127	.25000
C2_C1	1.3805(9)	1 0 0 0	.14581	.23274	.08947
C2_C1	1.3805(9)	-4 0 0 1	.14581	.23274	.41053

Angle	Degrees	atom 1 loc	atom 3 loc
N_Ni_N	91.25(15)	1 0 0 0	2 0 0 0
N_Ni_N	179.980(0)	1 0 0 0	-1 0 0 0
N_Ni_N	88.75(15)	1 0 0 0	-2 0 0 0
N_Ni_N	88.75(15)	2 0 0 0	-1 0 0 0
N_Ni_N	180.000(0)	2 0 0 0	-2 0 0 0
N_Ni_N	91.25(15)	-1 0 0 0	-2 0 0 0
Ni_N_N	124.02(7)	1 0 0 0	-4 0 0 1
Ni_N_C1	127.99(9)	1 0 0 0	1 0 0 0
N_N_C1	107.904(34)	-4 0 0 1	1 0 0 0
C1_C1_C2	107.61(11)	1 0 0 0	1 0 0 0
C1_C2_C1	107.66(11)	1 0 0 0	-4 0 0 1

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Compound: bispyrazolate nickel (II) - beta form
beta-Ni(pz)2

Space Group P 21/m
The lattice is centric primitive monoclinic Laue symmetry 2/m
Multiplicity of a general site is 4
The unique axis is b
The symmetry of the point 0,0,0 contains 1bar

Equivalent Positions
(1) X Y Z (2) -X 1/2+Y -Z

Lattice Constants
a = 8.9673(18) b = 6.9752(13) c = 6.0158(14)
Alpha = 90 Beta = 98.502(12) Gamma = 90
Cell volume = 372.15(13)

Fractional Atomic Coordinates

Name	X	Y	Z	Ui/Ue*100	Site sym	Mult	Type	Seq	Fractn
Ni	.000000	.000000	.000000	8.49(32)	-1	2	NI	1	1.0000
N1	.17668(27)	.15060(14)	.0495(30)	10.49(32)	1	4	N	2	1.0000
C1	.32651(28)	.09041(13)	.1022(33)	10.49(32)	1	4	C	3	1.0000
C2	.41520(40)	.250000	.1433(31)	10.49(32)	M(010)	2	C	4	1.0000
N2	-.09292(157)	.15055(14)	.2009(17)	10.49(32)	1	4	N	5	1.0000
C3	-.16948(134)	.09069(14)	.3755(15)	10.49(32)	1	4	C	6	1.0000
C4	-.19239(183)	.250000	.5018(15)	10.49(32)	M(010)	2	C	7	1.0000

Relevant Bond Distances and Angles

Vector	Length	Optr Cell	Neighbor atom coordinates		
Ni_N1	1.8875(17)	1 0 0 0	.17668	.15060	.04947
Ni_N1	1.8875(17)	-1 0 0 0	-.17668	-.15060	-.04947
Ni_N2	1.8856(16)	1 0 0 0	-.09292	.15055	.20090
Ni_N2	1.8856(16)	-1 0 0 0	.09292	-.15055	-.20090

N1_Ni	1.8875(17)	1 0 0 0	.00000	.00000	.00000
N1_N1	1.3866(19)	-2 0 1 0	.17668	.34940	.04947
N1_C1	1.3986(16)	1 0 0 0	.32651	.09041	.10218
C1_N1	1.3986(16)	1 0 0 0	.17668	.15060	.04947
C1_C1	2.2264(19)	-2 0 1 0	.32651	.40959	.10218
C1_C2	1.3692(17)	1 0 0 0	.41520	.25000	.14329
C2_C1	1.3692(17)	1 0 0 0	.32651	.09041	.10218
C2_C1	1.3692(17)	-2 0 1 0	.32651	.40959	.10218
N2_Ni	1.8856(16)	1 0 0 0	.00000	.00000	.00000
N2_N2	1.3873(19)	-2 0 1 0	-.09292	.34944	.20090
N2_C3	1.4010(16)	1 0 0 0	-.16948	.09069	.37555
C3_N2	1.4010(16)	1 0 0 0	-.09292	.15055	.20090
C3_C3	2.2224(20)	-2 0 1 0	-.16948	.40931	.37555
C3_C4	1.3784(20)	1 0 0 0	-.19239	.25000	.50180
C4_C3	1.3784(20)	1 0 0 0	-.16948	.09069	.37555
C4_C3	1.3784(20)	-2 0 1 0	-.16948	.40931	.37555

Angle	Degrees	atom 1 loc	atom 3 loc
N1_Ni_N1	179.972(0)	1 0 0 0	-1 0 0 0
N1_Ni_N2	91.7(4)	1 0 0 0	1 0 0 0
N1_Ni_N2	88.3(4)	1 0 0 0	-1 0 0 0
N1_Ni_N2	88.3(4)	-1 0 0 0	1 0 0 0
N1_Ni_N2	91.7(4)	-1 0 0 0	-1 0 0 0
N2_Ni_N2	179.980(0)	1 0 0 0	-1 0 0 0
Ni_N1_N1	123.82(5)	1 0 0 0	-2 0 1 0
Ni_N1_C1	128.64(12)	1 0 0 0	1 0 0 0
N1_N1_C1	107.47(6)	-2 0 1 0	1 0 0 0
C1_C1_C2	108.05(20)	1 0 0 0	1 0 0 0
C1_C2_C1	108.78(20)	1 0 0 0	-2 0 1 0
Ni_N2_N2	123.84(5)	1 0 0 0	-2 0 1 0
Ni_N2_C3	128.80(9)	1 0 0 0	1 0 0 0
N2_N2_C3	107.34(6)	-2 0 1 0	1 0 0 0
C3_C3_C4	107.60(23)	1 0 0 0	1 0 0 0
C3_C4_C3	107.44(26)	1 0 0 0	-2 0 1 0

References