Compound: Bis-imidazole, imidazolate, acetate nickel(II)

Crystal Data:

Space group P 21/a
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

The equivalent positions are:
(1) X Y Z (2) 1/2-X 1/2+Y -Z

Lattice constants are
a = 12.3467(7) b = 14.8671(8) c = 8.6676(6)
Alpha = 90 Beta = 112.788(5) Gamma = 90
Cell volume = 1466.81(16)

Fractional Atomic Coordinates:

Name	X	Y	Z	Ui/Ue*100	Site sym	Mult	Type	Seq	Fractn
Ni	.7334(7)	.2475(5)	.3578(9)	8.45(20)	1	4	NI	1	1.0000
N1	.5797(16)	.3058(23)	.3593(38)	10.45(20)	1	4	N	2	1.0000
N2	.3998(16)	.2877(23)	.3576(34)	10.45(20)	1	4	N	3	1.0000
C1	.4924(30)	.2435(8)	.3391(33)	10.45(20)	1	4	C	4	1.0000
C2	.5367(30)	.3897(13)	.3740(41)	10.45(20)	1	4	C	5	1.0000
C3	.4248(28)	.3787(18)	.3709(41)	10.45(20)	1	4	C	6	1.0000
N4	.6697(22)	.1173(9)	.3185(52)	10.45(20)	1	4	N	7	1.0000
N5	.6309(23)	-.0146(18)	.4091(42)	10.45(20)	1	4	N	8	1.0000
C4	.6693(27)	.0720(25)	.4572(25)	10.45(20)	1	4	C	9	1.0000
C5	.6137(23)	-.0242(16)	.2427(43)	10.45(20)	1	4	C	10	1.0000
C6	.6289(26)	.0592(27)	.1838(22)	10.45(20)	1	4	C	11	1.0000
N4	.8052(38)	.2402(18)	.6211(13)	10.45(20)	1	4	N	12	1.0000
N6	.9416(22)	.2269(15)	.8800(39)	10.45(20)	1	4	N	13	1.0000
C7	.9245(30)	.2331(19)	.7132(55)	10.45(20)	1	4	C	14	1.0000
C8	.7498(14)	.2469(23)	.7318(59)	10.45(20)	1	4	C	15	1.0000
C9	.8342(42)	.2390(23)	.8919(34)	10.45(20)	1	4	C	16	1.0000
O1	.6744(19)	.2978(9)	.0968(16)	10.45(20)	1	4	O	17	1.0000
O2	.7734(16)	.3882(9)	.3127(17)	10.45(20)	1	4	O	18	1.0000
C10	.7167(18)	.3790(8)	.1490(16)	10.45(20)	1	4	C	19	1.0000
C11	.7014(26)	.4569(11)	.0282(25)	10.45(20)	1	4	C	20	1.0000

Relevant Bond Distances and Angles:
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Vector	Length	Optr Cell	Neighbor atom coordinates		
Ni_N1	2.092(13)	1 0 0 0	.57973	.30584	.35935
Ni_N2	2.120(12)	-2 1 1 0	.89978	.21226	.35758
Ni_N4	2.068(11)	1 0 0 0	.66970	.11730	.31846
Ni_N4	2.107(10)	1 0 0 0	.80520	.24016	.62112
Ni_O1	2.220(12)	1 0 0 0	.67443	.29776	.09680
Ni_O2	2.218(13)	1 0 0 0	.77341	.38818	.31273

Angle	Degrees	atom 1 loc	atom 3 loc
N1_Ni_N2	169.8(19)	1 0 0 0	-2 1 1 0
N1_Ni_N4	95.8(13)	1 0 0 0	1 0 0 0
N1_Ni_O2	90.9(12)	1 0 0 0	1 0 0 0
N2_Ni_N4	94.3(12)	-2 1 1 0	1 0 0 0
N2_Ni_O2	89.3(11)	-2 1 1 0	1 0 0 0
N4_Ni_O2	95.9(13)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
N1_Ni	2.092(13)	1 0 0 0	.73345	.24751	.35776
N1_C1	1.3805(17)	1 0 0 0	.49235	.24354	.33908
N1_C2	1.3807(16)	1 0 0 0	.53666	.38973	.37400

Angle	Degrees	atom 1 loc	atom 3 loc
Ni_N1_C1	112.8(26)	1 0 0 0	1 0 0 0
Ni_N1_C2	139.3(26)	1 0 0 0	1 0 0 0
C1_N1_C2	107.93(15)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
N2_Ni	2.120(12)	-2 0 1 0	.23345	.25249	.35776
N2_C1	1.3805(17)	1 0 0 0	.49235	.24354	.33908
N2_C3	1.3814(16)	1 0 0 0	.42483	.37865	.37092

Angle	Degrees	atom 1 loc	atom 3 loc
Ni_N2_C1	136.7(27)	-2 0 1 0	1 0 0 0
Ni_N2_C3	115.3(27)	-2 0 1 0	1 0 0 0
C1_N2_C3	107.86(16)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C1_N1	1.3805(17)	1 0 0 0	.57973	.30584	.35935
C1_N2	1.3805(17)	1 0 0 0	.39978	.28774	.35758
C1_C2	2.2329(16)	1 0 0 0	.53666	.38973	.37400
C1_C3	2.2325(17)	1 0 0 0	.42483	.37865	.37092

Angle	Degrees	atom 1 loc	atom 3 loc

N1_C1_C3	107.9(28)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C2_N1	1.3807(16)	1 0 0 0	.57973	.30584	.35935
C2_C1	2.2329(16)	1 0 0 0	.49235	.24354	.33908
C2_C3	1.3804(16)	1 0 0 0	.42483	.37865	.37092

Angle	Degrees	atom 1 loc	atom 3 loc
C1_C2_C3	108.0(28)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C3_N2	1.3814(16)	1 0 0 0	.39978	.28774	.35758
C3_C1	2.2325(17)	1 0 0 0	.49235	.24354	.33908
C3_C2	1.3804(16)	1 0 0 0	.53666	.38973	.37400

Angle	Degrees	atom 1 loc	atom 3 loc
C1_C3_C2	107.9(28)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
N4_Ni	2.068(11)	1 0 0 0	.73345	.24751	.35776
N4_C4	1.3802(16)	1 0 0 0	.66926	.07201	.45723
N4_C6	1.3804(17)	1 0 0 0	.62890	.05923	.18382

Angle	Degrees	atom 1 loc	atom 3 loc
Ni_N4_C4	116.3(31)	1 0 0 0	1 0 0 0
Ni_N4_C6	135.7(31)	1 0 0 0	1 0 0 0
C4_N4_C6	107.96(13)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
N5_C4	1.3801(16)	1 0 0 0	.66926	.07201	.45723
N5_C5	1.3811(18)	1 0 0 0	.61366	-.02415	.24271

Angle	Degrees	atom 1 loc	atom 3 loc
C4_N5_C5	107.90(16)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C4_N4	1.3802(16)	1 0 0 0	.66970	.11730	.31846
C4_N5	1.3801(16)	1 0 0 0	.63088	-.01463	.40909
C4_C5	2.2324(16)	1 0 0 0	.61366	-.02415	.24271
C4_C6	2.2328(16)	1 0 0 0	.62890	.05923	.18382

Angle	Degrees	atom 1 loc	atom 3 loc
N4_C4_C6	108.0(32)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C5_N5	1.3811(18)	1 0 0 0	.63088	-.01463	.40909

C5_C4	2.2324(16)	1 0 0 0	.66926	.07201	.45723
C5_C6	1.3809(17)	1 0 0 0	.62890	.05923	.18382

Angle	Degrees	atom 1 loc	atom 3 loc
C4_C5_C6	107.8(32)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C6_N4	1.3804(17)	1 0 0 0	.66970	.11730	.31846
C6_C4	2.2328(16)	1 0 0 0	.66926	.07201	.45723
C6_C5	1.3809(17)	1 0 0 0	.61366	-.02415	.24271

Angle	Degrees	atom 1 loc	atom 3 loc
C4_C6_C5	107.8(32)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
N4_Ni	2.107(10)	1 0 0 0	.73345	.24751	.35776
N4_C7	1.3805(17)	1 0 0 0	.92445	.23309	.71321
N4_C8	1.3805(16)	1 0 0 0	.74982	.24688	.73180

Angle	Degrees	atom 1 loc	atom 3 loc
Ni_N4_C7	122.(4)	1 0 0 0	1 0 0 0
Ni_N4_C8	129.(4)	1 0 0 0	1 0 0 0
C7_N4_C8	107.95(16)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
N6_C7	1.3806(17)	1 0 0 0	.92445	.23309	.71321
N6_C9	1.3806(17)	1 0 0 0	.83420	.23901	.89191

Angle	Degrees	atom 1 loc	atom 3 loc
C7_N6_C9	107.93(16)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C7_N4	1.3805(17)	1 0 0 0	.80520	.24016	.62112
C7_N6	1.3806(17)	1 0 0 0	.94156	.22694	.87999
C7_C8	2.2329(16)	1 0 0 0	.74982	.24688	.73180
C7_C9	2.2328(16)	1 0 0 0	.83420	.23901	.89191

Angle	Degrees	atom 1 loc	atom 3 loc
N4_C7_C9	108.(4)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C8_N4	1.3805(16)	1 0 0 0	.80520	.24016	.62112
C8_C7	2.2329(16)	1 0 0 0	.92445	.23309	.71321
C8_C9	1.3802(16)	1 0 0 0	.83420	.23901	.89191

Angle	Degrees	atom 1 loc	atom 3 loc

C7_C8_C9	108.(4)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C9_N6	1.3806(17)	1 0 0 0	.94156	.22694	.87999
C9_C7	2.2328(16)	1 0 0 0	.92445	.23309	.71321
C9_C8	1.3802(16)	1 0 0 0	.74982	.24688	.73180

Angle	Degrees	atom 1 loc	atom 3 loc
C7_C9_C8	108.(4)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
O1_Ni	2.220(12)	1 0 0 0	.73345	.24751	.35776
O1_C10	1.3237(17)	1 0 0 0	.71668	.37898	.14899
O2_Ni	2.218(13)	1 0 0 0	.73345	.24751	.35776
O2_C10	1.3242(18)	1 0 0 0	.71668	.37898	.14899
C10_O1	1.3237(17)	1 0 0 0	.67443	.29776	.09680
C10_O2	1.3242(18)	1 0 0 0	.77341	.38818	.31273
C10_C11	1.5236(18)	1 0 0 0	.70142	.45693	.02821

Angle	Degrees	atom 1 loc	atom 3 loc
O1_C10_O2	115.81(17)	1 0 0 0	1 0 0 0
O1_C10_C11	122.11(17)	1 0 0 0	1 0 0 0
O2_C10_C11	122.08(17)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C11_C10	1.5236(18)	1 0 0 0	.71668	.37898	.14899

Compound: Bis-imidazole, bis-imidazolate palladium(II)

Crystal Data:

Space group P n c a
The lattice is centric primitive orthorhombic Laue symmetry mmm
Multiplicity of a general site is 8
The symmetry of the point 0,0,0 contains 1bar

The equivalent positions are:

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

Lattice constants are
a = 16.9300(10) b = 14.9344(9) c = 5.55825(28)
Alpha = 90 Beta = 90 Gamma = 90
Cell volume = 1405.35(14)

Fractional Atomic Coordinates:

Name	X	Y	Z	Ui/Ue*100	Site sym	Mult	Type	Seq	Fractn
Pd	.000000	.000000	.000000	2.47(8)	-1	4	PD	1	1.0000
N1	.0984(6)	.0797(12)	.0945(37)	4.47(8)	1	8	N	2	1.0000
N2	.2002(8)	.1312(14)	.3089(25)	4.47(8)	1	8	N	3	1.0000
C1	.1454(14)	.0631(9)	.2925(28)	4.47(8)	1	8	C	4	1.0000
C2	.1271(12)	.1552(14)	-.0190(22)	4.47(8)	1	8	C	5	1.0000
C3	.1926(11)	.1843(8)	.1068(38)	4.47(8)	1	8	C	6	1.0000
N3	.0724(12)	-.0762(11)	-.2373(27)	4.47(8)	1	8	N	7	1.0000
N4	.1580(8)	-.1522(9)	-.4647(36)	4.47(8)	1	8	N	8	1.0000
C4	.1508(9)	-.1006(14)	-.2597(30)	4.47(8)	1	8	C	9	1.0000
C5	.0305(4)	-.1182(13)	-.4180(35)	4.47(8)	1	8	C	10	1.0000
C6	.0830(13)	-.1680(11)	-.5529(24)	4.47(8)	1	8	C	11	1.0000

Relevant Bond Distances and Angles:

Vector	Length	Optr	Cell	Neighbor atom coordinates		
Pd_N1	2.115(7)	1	0 0 0	.09844	.07973	.09449
Pd_N1	2.115(7)	-1	0 0 0	-.09844	-.07973	-.09449
Pd_N3	2.130(8)	1	0 0 0	.07243	-.07621	-.23730
Pd_N3	2.130(8)	-1	0 0 0	-.07243	.07621	.23730

Angle	Degrees	atom 1 loc	atom 3 loc

N1_Pd_N1	179.980(0)	1 0 0 0	-1 0 0 0
N1_Pd_N3	90.1(6)	1 0 0 0	1 0 0 0
N1_Pd_N3	89.9(6)	1 0 0 0	-1 0 0 0
N1_Pd_N3	89.9(6)	-1 0 0 0	1 0 0 0
N1_Pd_N3	90.1(6)	-1 0 0 0	-1 0 0 0
N3_Pd_N3	180.000(0)	1 0 0 0	-1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
N1_Pd	2.115(7)	1 0 0 0	.00000	.00000	.00000
N1_C1	1.3805(11)	1 0 0 0	.14543	.06306	.29248
N1_C2	1.3800(10)	1 0 0 0	.12712	.15521	-.01900

Angle	Degrees	atom 1 loc	atom 3 loc
Pd_N1_C1	123.4(18)	1 0 0 0	1 0 0 0
Pd_N1_C2	128.6(18)	1 0 0 0	1 0 0 0
C1_N1_C2	108.00(7)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
N2_C1	1.3805(11)	1 0 0 0	.14543	.06306	.29248
N2_C3	1.3810(11)	1 0 0 0	.19260	.18431	.10677

Angle	Degrees	atom 1 loc	atom 3 loc
C1_N2_C3	107.86(11)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C1_N1	1.3805(11)	1 0 0 0	.09844	.07973	.09449
C1_N2	1.3805(11)	1 0 0 0	.20022	.13125	.30892
C1_C2	2.2332(10)	1 0 0 0	.12712	.15521	-.01900
C1_C3	2.2321(11)	1 0 0 0	.19260	.18431	.10677

Angle	Degrees	atom 1 loc	atom 3 loc
N1_C1_C3	107.9(18)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C2_N1	1.3800(10)	1 0 0 0	.09844	.07973	.09449
C2_C1	2.2332(10)	1 0 0 0	.14543	.06306	.29248
C2_C3	1.3808(11)	1 0 0 0	.19260	.18431	.10677

Angle	Degrees	atom 1 loc	atom 3 loc
C1_C2_C3	107.9(18)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C3_N2	1.3810(11)	1 0 0 0	.20022	.13125	.30892
C3_C1	2.2321(11)	1 0 0 0	.14543	.06306	.29248
C3_C2	1.3808(11)	1 0 0 0	.12712	.15521	-.01900

Angle	Degrees	atom 1 loc	atom 3 loc
C1_C3_C2	107.8(18)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
N3_Pd	2.130(8)	1 0 0 0	.00000	.00000	.00000
N3_C4	1.3809(11)	1 0 0 0	.15076	-.10061	-.25974
N3_C5	1.3808(11)	1 0 0 0	.03048	-.11821	-.41799

Angle	Degrees	atom 1 loc	atom 3 loc
Pd_N3_C4	138.6(16)	1 0 0 0	1 0 0 0
Pd_N3_C5	113.4(16)	1 0 0 0	1 0 0 0
C4_N3_C5	107.96(8)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
N4_C4	1.3808(11)	1 0 0 0	.15076	-.10061	-.25974
N4_C6	1.3816(11)	1 0 0 0	.08298	-.16802	-.55293

Angle	Degrees	atom 1 loc	atom 3 loc
C4_N4_C6	107.86(11)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C4_N3	1.3809(11)	1 0 0 0	.07243	-.07621	-.23730
C4_N4	1.3808(11)	1 0 0 0	.15799	-.15224	-.46466
C4_C5	2.2338(11)	1 0 0 0	.03048	-.11821	-.41799
C4_C6	2.2329(12)	1 0 0 0	.08298	-.16802	-.55293

Angle	Degrees	atom 1 loc	atom 3 loc
N3_C4_C6	107.9(17)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C5_N3	1.3808(11)	1 0 0 0	.07243	-.07621	-.23730
C5_C4	2.2338(11)	1 0 0 0	.15076	-.10061	-.25974
C5_C6	1.3806(11)	1 0 0 0	.08298	-.16802	-.55293

Angle	Degrees	atom 1 loc	atom 3 loc
C4_C5_C6	108.0(17)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C6_N4	1.3816(11)	1 0 0 0	.15799	-.15224	-.46466
C6_C4	2.2329(12)	1 0 0 0	.15076	-.10061	-.25974
C6_C5	1.3806(11)	1 0 0 0	.03048	-.11821	-.41799

Angle	Degrees	atom 1 loc	atom 3 loc
C4_C6_C5	107.9(17)	1 0 0 0	1 0 0 0

Compound: Bis-imidazole, bis-imidazolate platinum(II)

Crystal Data:

Space group P 21/c
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

The equivalent positions are:
(1) X Y Z (2) -X 1/2+Y 1/2-Z

Lattice constants are
a = 5.34033(29) b = 15.6798(9) c = 8.6555(5)
Alpha = 90 Beta = 103.354(4) Gamma = 90
Cell volume = 705.17(7)

Fractional Atomic Coordinates:

Name	X	Y	Z	Ui/Ue*100	Site sym	Mult	Type	Seq	Fractn
Pt	.000000	.000000	.000000	2.77(9)	-1	2	PT	1	1.0000
N1	.2964(35)	.0636(12)	.1597(26)	4.77(9)	1	4	N	2	1.0000
N2	.6282(37)	.1468(11)	.2714(35)	4.77(9)	1	4	N	3	1.0000
C1	.481(6)	.1181(18)	.1282(18)	4.77(9)	1	4	C	4	1.0000
C2	.348(4)	.0512(12)	.3222(31)	4.77(9)	1	4	C	5	1.0000
C3	.535(5)	.1093(16)	.3913(12)	4.77(9)	1	4	C	6	1.0000
N3	.0191(55)	-.1048(13)	.1754(26)	4.77(9)	1	4	N	7	1.0000
N4	-.0760(53)	.2685(7)	.2042(28)	4.77(9)	1	4	N	8	1.0000
C4	-.139(4)	.3170(19)	.3232(27)	4.77(9)	1	4	C	9	1.0000
C5	.130(4)	.3927(14)	.2138(33)	4.77(9)	1	4	C	10	1.0000
C6	.120(5)	.3105(19)	.1548(21)	4.77(9)	1	4	C	11	1.0000

Relevant Bond Distances and Angles:

Vector	Length	Optr Cell	Neighbor atom coordinates		
Pt_N1	2.098(11)	1 0 0 0	.29635	.06360	.15972
Pt_N1	2.098(11)	-1 0 0 0	-.29635	-.06360	-.15972
Pt_N3	2.223(11)	1 0 0 0	.01915	-.10479	.17536
Pt_N3	2.223(11)	-1 0 0 0	-.01915	.10479	-.17536

Angle	Degrees	atom 1 loc	atom 3 loc
N1_Pt_N1	179.960(0)	1 0 0 0	-1 0 0 0
N1_Pt_N3	89.6(8)	1 0 0 0	1 0 0 0
N1_Pt_N3	90.4(8)	1 0 0 0	-1 0 0 0
N1_Pt_N3	90.4(8)	-1 0 0 0	1 0 0 0
N1_Pt_N3	89.6(8)	-1 0 0 0	-1 0 0 0
N3_Pt_N3	180.000(0)	1 0 0 0	-1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
N1_Pt	2.098(11)	1 0 0 0	.00000	.00000	.00000
N1_C1	1.3808(20)	1 0 0 0	.48139	.11812	.12816
N1_C2	1.3826(21)	1 0 0 0	.34797	.05123	.32217

Angle	Degrees	atom 1 loc	atom 3 loc
Pt_N1_C1	129.0(22)	1 0 0 0	1 0 0 0
Pt_N1_C2	123.1(21)	1 0 0 0	1 0 0 0
C1_N1_C2	107.72(19)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
N2_C1	1.3806(19)	1 0 0 0	.48139	.11812	.12816
N2_C3	1.3808(20)	1 0 0 0	.53525	.10929	.39129

Angle	Degrees	atom 1 loc	atom 3 loc
C1_N2_C3	107.94(14)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C1_N1	1.3808(20)	1 0 0 0	.29635	.06360	.15972
C1_N2	1.3806(19)	1 0 0 0	.62816	.14683	.27145
C1_C2	2.2317(20)	1 0 0 0	.34797	.05123	.32217
C1_C3	2.2331(19)	1 0 0 0	.53525	.10929	.39129

Angle	Degrees	atom 1 loc	atom 3 loc
N1_C1_C3	107.9(22)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C2_N1	1.3826(21)	1 0 0 0	.29635	.06360	.15972
C2_C1	2.2317(20)	1 0 0 0	.48139	.11812	.12816
C2_C3	1.3822(21)	1 0 0 0	.53525	.10929	.39129

Angle	Degrees	atom 1 loc	atom 3 loc
C1_C2_C3	107.6(22)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C3_N2	1.3808(20)	1 0 0 0	.62816	.14683	.27145
C3_C1	2.2331(19)	1 0 0 0	.48139	.11812	.12816
C3_C2	1.3822(21)	1 0 0 0	.34797	.05123	.32217

Angle	Degrees	atom 1 loc	atom 3 loc
C1_C3_C2	107.8(22)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
N3_Pt	2.223(11)	1 0 0 0	.00000	.00000	.00000
N3_C4	1.3810(20)	2 0-1 0	.13870	-.18297	.17678
N3_C5	1.3813(20)	2 0-1 0	-.12992	-.10730	.28618

Angle	Degrees	atom 1 loc	atom 3 loc
Pt_N3_C4	127.6(23)	1 0 0 0	2 0-1 0
Pt_N3_C5	123.5(23)	1 0 0 0	2 0-1 0
C4_N3_C5	107.93(13)	2 0-1 0	2 0-1 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
N4_C4	1.3825(21)	1 0 0 0	-.13870	.31703	.32322
N4_C6	1.3836(22)	1 0 0 0	.11971	.31047	.15482

Angle	Degrees	atom 1 loc	atom 3 loc
C4_N4_C6	107.38(21)	1 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C4_N3	1.3810(20)	2 0 0 0	-.01915	.39521	.32464
C4_N4	1.3825(21)	1 0 0 0	-.07597	.26850	.20421
C4_C5	2.2337(18)	1 0 0 0	.12992	.39270	.21382
C4_C6	2.2290(21)	1 0 0 0	.11971	.31047	.15482

Angle	Degrees	atom 1 loc	atom 3 loc
N3_C4_C6	107.7(24)	2 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C5_N3	1.3813(20)	2 0 0 0	-.01915	.39521	.32464
C5_C4	2.2337(18)	1 0 0 0	-.13870	.31703	.32322
C5_C6	1.3831(21)	1 0 0 0	.11971	.31047	.15482

Angle	Degrees	atom 1 loc	atom 3 loc
C4_C5_C6	107.6(24)	2 0 0 0	1 0 0 0

Vector	Length	Optr Cell	Neighbor atom coordinates		
C6_N4	1.3836(22)	1 0 0 0	-.07597	.26850	.20421
C6_C4	2.2290(21)	1 0 0 0	-.13870	.31703	.32322
C6_C5	1.3831(21)	1 0 0 0	.12992	.39270	.21382

Angle	Degrees	atom 1 loc	atom 3 loc
C4_C6_C5	107.3(24)	1 0 0 0	1 0 0 0