# Role of Iron(II) Dilution in the Magnetic and Photomagnetic Properties of the Series $[Fe_xZn_{1-x}(bpp)_2](NCSe)_2$

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## Electronic Supplementary Information

**Figure SI.1** Room temperature powder *X*-ray diffraction patterns of $[Fe_xZn_{1-x}(bpp)_2](NCSe)_2$ (x = 1, 0.6 and 0)

**Table SI.1 :** Elemental Analysis for the Mixed-Crystal complexes: $[Fe_xZn_{1-x}(bpp)_2](NCSe)_2$

- Details of the calculations for the kinetic studies.
- Structural Tables for the Mixed-Crystal complexe $[Fe_{0.6}Zn_{0.4}(bpp)_2](NCSe)_2$ at 120 K and 298 K.

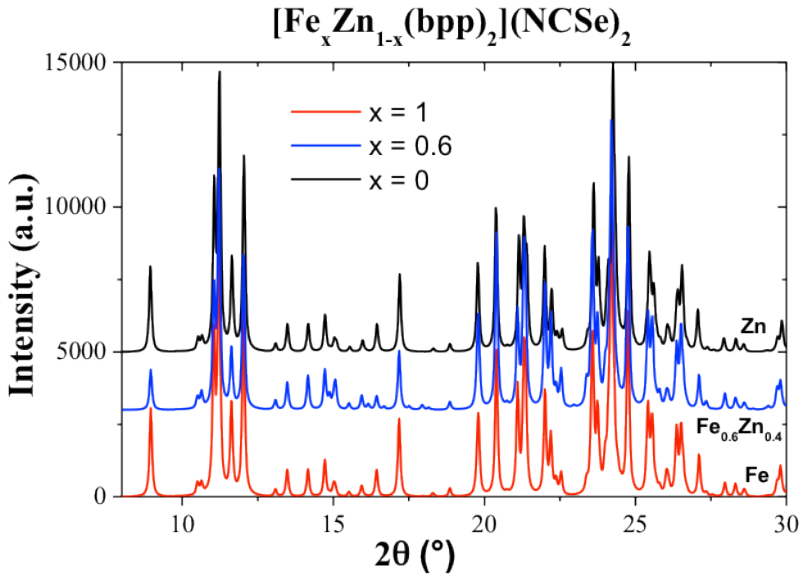


**Figure SI.1** Room temperature powder *X*-ray diffraction patterns of $[Fe_xZn_{1-x}(bpp)_2](NCSe)_2$ (x = 1, 0.6 and 0)

**Table SI.1 :** Elemental Analysis for the Mixed-Crystal complexes: $[Fe_xZn_{1-x}(bpp)_2](NCSe)_2$

| Compound | Calculate (% weight) | | | Experimental (% weight) | | |
|---|---|---|---|---|---|---|
| | C | H | N | C | H | N |
| **1** : $[Fe(bpp)_2](NCSe)_2$ | 41,88 | 2,63 | 24,42 | 41,53 | 2,62 | 24,50 |
| **2** :$[Fe_{0,8}Zn_{0,2}(bpp)_2](NCSe)_2$ | 41,76 | 2,62 | 24,35 | 41,40 | 2,59 | 24,31 |
| **3** :$[Fe_{0,6}Zn_{0,4}(bpp)_2](NCSe)_2$ | 41,65 | 2,62 | 24,28 | 41,52 | 2,61 | 24,48 |
| **4** : $[Fe_{0,45}Zn_{0,55}(bpp)_2](NCSe)_2$ | 41,56 | 2,61 | 24,23 | 41,13 | 2,59 | 24,25 |
| **5** : $[Fe_{0,22}Zn_{0,78}(bpp)_2](NCSe)_2$ | 41,43 | 2,60 | 24,16 | 41,00 | 2,58 | 24,23 |
| **6** : $[Fe_{0,11}Zn_{0,89}(bpp)_2](NCSe)_2$ | 41,37 | 2,60 | 24,12 | 40,82 | 2,50 | 23,83 |

**Details of the calculations for the kinetic study.**

The equations used in order to model the kinetic decay of the photoexcited HS state in the case of a cooperative system are recalled bellow:

$$\frac{\partial \gamma_{HS}}{\partial t} = -k^*_{HL}\gamma_{HS} \quad (1)$$

$$k^*_{HL}(T, \gamma_{HS}) = k_{HL}(T)\exp[\alpha(T)(1-\gamma_{HS})] \quad (2)$$

$$k_{HL}(T) = k_0 + k_\infty.\exp(-E_a / k_B T) \quad (3)$$

$$\frac{\partial \gamma_{HS}}{\partial t} = -\gamma_{HS}\left\{k_0 + k_\infty \exp\left(-E_a/k_B T\right)\right\}.\exp[\alpha(T)(1-\gamma_{HS})] \quad (4)$$

All the simulations have been realized using Origin 5.0 program. At each temperature, a simulation is done using 3 parameters, namely $\gamma_{HS}(t=0)$, $\alpha(T)$ and $k_{HL}(T)$. Integration of the first two equations is realized numerically by Origin 5.0 program.

More precisely, in the Origin 5.0 program, a column of equally spaced $\gamma_{HS}$ is created and the time at which a given $\gamma_{HS}$ is reached is calculated using the integration function of the Origin 5.0 program and an integrated version of equations 1 and 2:

$$t = \int_{\gamma_{HS}(t=0)}^{\gamma_{HS}(t)} \frac{d\gamma_{HS}}{-k_{HL}(T)\exp[\alpha(T)(1-\gamma_{HS})]\gamma_{HS}}$$

The Arrhenius plot of ln(kHL(T)) versus 1/T allows the determination of $E_a$ and $k_\infty$.

In order to get a reasonable fitting, it has also been necessary to take into account a Gaussian distribution of activation energy. Due to numerical difficulties, it has not been possible to use an exact distribution of activation energies. Instead, a standard deviation σ has been chosen, and a relaxation curve has been simulated for different activation energy values, namely $E_a$-3σ, $E_a$-2σ, $E_a$-σ, $E_a$, $E_a$+σ, $E_a$+2σ, $E_a$+3σ. The 7 different curves have thus been summed using the following Gaussian weighting: $E_a$ : 39.9 %, $E_a$±σ : 24.2 %, $E_a$±2σ : 5.4 %, $E_a$±3σ : 0.45 %.

The σ parameter has been determined through trial and error.

**bpp120K in P -1**

==========
S U P P L E M E N T A R Y  M A T E R I A L
==========

B E L O N G I N G  TO  T H E  P A P E R

b y

C o n t e n t s
==========

Table S1 - Crystal Data and Details of the Structure Determination for: bpp120 in P -1

Crystal Data

| | | | |
|---|---|---|---|
| Formula | | | ? |
| Formula Weight | | | 692.01 |
| Crystal System | | | Triclinic |
| Space group | | P-1 | (No. 2) |
| a, b, c [Angstrom] | 8.2142(16) | 8.353(2) | 19.855(4) |
| alpha, beta, gamma [deg] | 87.724(9) | 83.926(13) | 88.701(13) |
| V [Ang**3] | | | 1353.4(5) |
| Z | | | 2 |
| D(calc) [g/cm**3] | | | 1.698 |
| Mu(MoKa) [ /mm ] | | | 3.423 |
| F(000) | | | 683 |
| Crystal Size [mm] | | 0.00 x 0.00 x 0.00 | |

Data Collection

| | | | |
|---|---|---|---|
| Temperature (K) | | | ***** |
| Radiation [Angstrom] | | MoKa | 0.71073 |
| Theta Min-Max [Deg] | | | 0.0, 0.0 |
| Dataset | | 999:-99 ; 999:-99 ; 999:-99 | |
| Tot., Uniq. Data, R(int) | | 0, 0, 0.000 | |
| Observed data [I > 0.0 sigma(I)] | | | 0 |

Refinement

| | | | |
|---|---|---|---|
| Nref, Npar | | | 0, 0 |
| R, wR2, S | | 0.0000, 0.0000, 0.00 | |
| w = | | | |
| Max. and Av. Shift/Error | | | 0.00, 0.00 |
| Min. and Max. Resd. Dens. [e/Ang^3] | | | 0.00, 0.00 |

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: bpp120 in P -1

| Atom | x | y | z | U(eq) [Ang^2] |
|---|---|---|---|---|
| *Fe1 | 0.71931(7) | 0.23222(7) | 0.24807(3) | 0.0232(2) |
| *Zn1 | 0.71931(7) | 0.23222(7) | 0.24807(3) | 0.0232(2) |
| N1 | 0.5686(5) | 0.5897(5) | 0.2447(3) | 0.0435(17) |
| N2 | 0.6233(5) | 0.4510(5) | 0.2172(2) | 0.0297(12) |
| N3 | 0.7233(4) | 0.2137(5) | 0.14795(19) | 0.0252(12) |
| N4 | 0.8200(5) | 0.0064(5) | 0.2322(2) | 0.0319(14) |
| N5 | 0.8796(5) | -0.1154(6) | 0.2690(3) | 0.0477(17) |
| N6 | 0.3684(6) | 0.0704(5) | 0.2626(3) | 0.0442(17) |
| N7 | 0.4957(5) | 0.1408(5) | 0.2856(2) | 0.0319(14) |
| N8 | 0.7205(5) | 0.2514(5) | 0.3479(2) | 0.0284(12) |
| N9 | 0.9443(5) | 0.3288(5) | 0.2560(2) | 0.0306(12) |
| N10 | 1.0767(5) | 0.3725(5) | 0.2147(3) | 0.0450(17) |
| C1 | 0.5228(7) | 0.6935(7) | 0.1977(4) | 0.052(2) |
| C2 | 0.5467(6) | 0.6235(6) | 0.1354(3) | 0.0408(19) |
| C3 | 0.6098(6) | 0.4702(6) | 0.1505(3) | 0.0290(17) |
| C4 | 0.6651(6) | 0.3349(6) | 0.1097(3) | 0.0280(17) |
| C5 | 0.6621(6) | 0.3220(7) | 0.0406(3) | 0.0349(17) |
| C6 | 0.7205(7) | 0.1821(7) | 0.0107(3) | 0.0402(19) |
| C7 | 0.7830(6) | 0.0590(7) | 0.0494(3) | 0.0368(17) |
| C8 | 0.7829(6) | 0.0780(6) | 0.1186(2) | 0.0270(17) |
| C9 | 0.8424(6) | -0.0374(6) | 0.1678(3) | 0.0308(17) |
| C10 | 0.9167(7) | -0.1894(7) | 0.1639(4) | 0.047(2) |
| C11 | 0.9366(7) | -0.2350(7) | 0.2297(4) | 0.057(3) |
| C12 | 0.2606(7) | 0.0213(7) | 0.3144(4) | 0.055(3) |
| C13 | 0.3173(7) | 0.0597(7) | 0.3738(3) | 0.045(2) |
| C14 | 0.4661(6) | 0.1349(6) | 0.3540(3) | 0.0311(17) |

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued) for: bpp120 in P -1

| Atom | x | y | z | U(eq) [Ang^2] |
|---|---|---|---|---|
| C15 | 0.5910(6) | 0.2029(6) | 0.3902(3) | 0.0305(17) |
| C16 | 0.5854(7) | 0.2174(7) | 0.4599(3) | 0.0407(19) |
| C17 | 0.7179(7) | 0.2847(7) | 0.4851(3) | 0.046(2) |
| C18 | 0.8534(7) | 0.3320(7) | 0.4419(3) | 0.0412(17) |
| C19 | 0.8500(6) | 0.3154(6) | 0.3731(3) | 0.0309(17) |
| C20 | 0.9791(6) | 0.3583(6) | 0.3190(3) | 0.0303(17) |
| C21 | 1.1365(7) | 0.4204(7) | 0.3169(4) | 0.048(2) |
| C22 | 1.1943(7) | 0.4278(7) | 0.2497(4) | 0.056(3) |
| Se1 | 0.86428(8) | 0.80986(8) | 0.43577(3) | 0.0544(3) |
| N11 | 0.5915(7) | 0.6505(6) | 0.3802(3) | 0.0538(19) |
| C23 | 0.6990(8) | 0.7101(7) | 0.4028(3) | 0.044(2) |
| Se2 | 0.16967(8) | 0.32871(8) | 0.04954(3) | 0.0512(2) |
| N12 | 0.3294(6) | 0.0659(7) | 0.1246(3) | 0.0532(19) |
| C24 | 0.2703(7) | 0.1677(8) | 0.0947(3) | 0.043(2) |

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites have a S.O.F less than 1.0

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters
for: bpp120 in P -1

| Atom | x | y | z | U(iso) [Ang^2] |
|---|---|---|---|---|
| H1 | 0.48046 | 0.79867 | 0.20560 | 0.0619 |
| H1N | 0.56392 | 0.60878 | 0.28810 | 0.0521 |
| H2 | 0.52537 | 0.66845 | 0.09242 | 0.0489 |
| H5 | 0.62057 | 0.40762 | 0.01408 | 0.0419 |
| H5N | 0.88097 | -0.11639 | 0.31324 | 0.0567 |
| H6 | 0.71764 | 0.17076 | -0.03656 | 0.0482 |
| H6N | 0.35709 | 0.05818 | 0.21952 | 0.0533 |
| H7 | 0.82516 | -0.03652 | 0.02918 | 0.0441 |
| H10 | 0.94693 | -0.24816 | 0.12441 | 0.0560 |
| H10N | 1.08573 | 0.36597 | 0.17033 | 0.0538 |
| H11 | 0.98256 | -0.33376 | 0.24471 | 0.0689 |
| H12 | 0.16105 | -0.03160 | 0.31035 | 0.0663 |
| H13 | 0.26694 | 0.03980 | 0.41858 | 0.0543 |
| H16 | 0.49342 | 0.18216 | 0.48934 | 0.0487 |
| H17 | 0.71597 | 0.29854 | 0.53241 | 0.0541 |
| H18 | 0.94622 | 0.37465 | 0.45914 | 0.0491 |
| H21 | 1.19121 | 0.45092 | 0.35410 | 0.0573 |
| H22 | 1.29849 | 0.46507 | 0.23107 | 0.0673 |

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S4 - (An)isotropic Displacement Parameters
for: bpp120 in P -1

| Atom | U(1,1) or U | U(2,2) | U(3,3) | U(2,3) | U(1,3) | U(1,2) |
|---|---|---|---|---|---|---|
| Fe1 | 0.0204(4) | 0.0234(4) | 0.0258(3) | -0.0012(3) | -0.0027(3) | 0.0033(3) |
| Zn1 | 0.0204(4) | 0.0234(4) | 0.0258(3) | -0.0012(3) | -0.0027(3) | 0.0033(3) |
| N1 | 0.030(3) | 0.035(3) | 0.065(3) | -0.021(3) | 0.005(2) | -0.002(2) |
| N2 | 0.024(2) | 0.024(2) | 0.041(2) | -0.0108(19) | 0.0004(18) | -0.0021(18) |
| N3 | 0.019(2) | 0.020(2) | 0.036(2) | -0.0001(18) | -0.0005(17) | -0.0012(17) |
| N4 | 0.022(2) | 0.031(3) | 0.043(2) | 0.010(2) | -0.0086(19) | -0.0034(19) |
| N5 | 0.037(3) | 0.040(3) | 0.068(3) | 0.030(3) | -0.025(3) | -0.010(2) |
| N6 | 0.036(3) | 0.033(3) | 0.069(3) | -0.016(2) | -0.027(3) | 0.009(2) |
| N7 | 0.028(2) | 0.024(2) | 0.046(3) | -0.004(2) | -0.016(2) | 0.0081(19) |
| N8 | 0.027(2) | 0.020(2) | 0.038(2) | 0.0022(18) | -0.0050(19) | 0.0047(19) |
| N9 | 0.025(2) | 0.024(2) | 0.040(2) | 0.0054(19) | 0.0067(19) | 0.0048(19) |
| N10 | 0.035(3) | 0.034(3) | 0.060(3) | 0.005(2) | 0.019(2) | 0.005(2) |
| C1 | 0.032(3) | 0.026(4) | 0.096(5) | -0.010(3) | 0.002(3) | 0.008(3) |
| C2 | 0.029(3) | 0.026(3) | 0.068(4) | 0.003(3) | -0.009(3) | -0.003(2) |
| C3 | 0.025(3) | 0.022(3) | 0.041(3) | 0.001(2) | -0.010(2) | 0.002(2) |
| C4 | 0.022(3) | 0.023(3) | 0.039(3) | 0.001(2) | -0.004(2) | 0.000(2) |
| C5 | 0.037(3) | 0.036(3) | 0.032(3) | 0.003(2) | -0.007(2) | 0.000(3) |
| C6 | 0.039(3) | 0.050(4) | 0.032(3) | -0.008(3) | -0.003(2) | -0.002(3) |
| C7 | 0.038(3) | 0.032(3) | 0.041(3) | -0.008(2) | -0.005(2) | 0.004(3) |
| C8 | 0.022(3) | 0.023(3) | 0.036(3) | -0.003(2) | -0.002(2) | 0.000(2) |
| C9 | 0.024(3) | 0.021(3) | 0.048(3) | 0.001(2) | -0.007(2) | 0.000(2) |
| C10 | 0.034(3) | 0.025(3) | 0.082(5) | -0.006(3) | -0.013(3) | 0.003(3) |
| C11 | 0.035(4) | 0.020(4) | 0.120(6) | 0.015(4) | -0.028(4) | -0.003(3) |
| C12 | 0.029(3) | 0.025(4) | 0.113(6) | -0.009(4) | -0.013(4) | 0.002(3) |
| C13 | 0.032(3) | 0.033(4) | 0.069(4) | -0.003(3) | 0.001(3) | 0.001(3) |
| C14 | 0.025(3) | 0.022(3) | 0.046(3) | 0.001(2) | -0.005(2) | 0.005(2) |

Table S4 - (An)isotropic Displacement Parameters (continued)
for: bpp120 in P -1

| Atom | U(1,1) or U | U(2,2) | U(3,3) | U(2,3) | U(1,3) | U(1,2) |
|---|---|---|---|---|---|---|
| C15 | 0.030(3) | 0.022(3) | 0.038(3) | 0.003(2) | 0.001(2) | 0.001(2) |
| C16 | 0.042(3) | 0.041(4) | 0.037(3) | 0.002(3) | 0.002(3) | 0.007(3) |
| C17 | 0.054(4) | 0.049(4) | 0.035(3) | 0.003(3) | -0.015(3) | 0.005(3) |
| C18 | 0.042(3) | 0.036(3) | 0.048(3) | 0.001(3) | -0.018(3) | 0.002(3) |
| C19 | 0.029(3) | 0.025(3) | 0.040(3) | -0.003(2) | -0.011(2) | 0.009(2) |
| C20 | 0.026(3) | 0.022(3) | 0.043(3) | 0.000(2) | -0.007(2) | 0.008(2) |
| C21 | 0.025(3) | 0.028(3) | 0.093(5) | 0.005(3) | -0.018(3) | 0.004(3) |
| C22 | 0.025(3) | 0.036(4) | 0.106(6) | 0.004(4) | 0.001(3) | -0.003(3) |
| Se1 | 0.0558(4) | 0.0621(5) | 0.0469(4) | -0.0065(3) | -0.0137(3) | 0.0087(3) |
| N11 | 0.052(3) | 0.057(4) | 0.051(3) | -0.014(3) | 0.004(3) | 0.005(3) |
| C23 | 0.052(4) | 0.048(4) | 0.029(3) | -0.001(3) | 0.001(3) | 0.016(3) |
| Se2 | 0.0548(4) | 0.0481(4) | 0.0502(4) | -0.0031(3) | -0.0010(3) | -0.0067(3) |
| N12 | 0.053(3) | 0.050(4) | 0.059(3) | -0.018(3) | -0.011(3) | -0.001(3) |
| C24 | 0.042(4) | 0.043(4) | 0.044(3) | -0.015(3) | 0.004(3) | -0.009(3) |

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Table S5 - Bond Distances (Angstrom)
for: bpp120 in P -1

| | | | | | |
|---|---|---|---|---|---|
| Se1 | -C23 | 1.802(6) | N9 | -N10 | 1.339(6) |
| Se2 | -C24 | 1.818(6) | N10 | -C22 | 1.348(8) |
| Zn1 | -N4 | 2.065(4) | N1 | -H1N | 0.8800 |
| Zn1 | -N3 | 1.997(4) | N5 | -H5N | 0.8800 |
| Zn1 | -N9 | 2.057(4) | N6 | -H6N | 0.8800 |
| Zn1 | -N7 | 2.059(4) | N10 | -H10N | 0.8800 |
| Zn1 | -N2 | 2.070(4) | N11 | -C23 | 1.162(9) |
| Zn1 | -N8 | 1.996(4) | N12 | -C24 | 1.146(8) |
| Fe1 | -N3 | 1.997(4) | C1 | -C2 | 1.383(9) |
| Fe1 | -N4 | 2.065(4) | C2 | -C3 | 1.404(7) |
| Fe1 | -N2 | 2.070(4) | C3 | -C4 | 1.453(8) |
| Fe1 | -N8 | 1.996(4) | C4 | -C5 | 1.383(8) |
| Fe1 | -N9 | 2.057(4) | C5 | -C6 | 1.385(8) |
| Fe1 | -N7 | 2.059(4) | C6 | -C7 | 1.381(8) |
| N1 | -C1 | 1.326(9) | C7 | -C8 | 1.389(7) |
| N1 | -N2 | 1.348(6) | C8 | -C9 | 1.459(7) |
| N2 | -C3 | 1.344(7) | C9 | -C10 | 1.398(8) |
| N3 | -C8 | 1.353(6) | C10 | -C11 | 1.372(11) |
| N3 | -C4 | 1.351(7) | C12 | -C13 | 1.365(9) |
| N4 | -C9 | 1.337(7) | C13 | -C14 | 1.399(8) |
| N4 | -N5 | 1.343(7) | C14 | -C15 | 1.452(7) |
| N5 | -C11 | 1.338(8) | C15 | -C16 | 1.390(8) |
| N6 | -C12 | 1.342(9) | C16 | -C17 | 1.384(8) |
| N6 | -N7 | 1.341(6) | C17 | -C18 | 1.386(8) |
| N7 | -C14 | 1.353(7) | C18 | -C19 | 1.382(8) |
| N8 | -C19 | 1.352(7) | C19 | -C20 | 1.467(8) |
| N8 | -C15 | 1.343(7) | C20 | -C21 | 1.400(8) |
| N9 | -C20 | 1.346(7) | C21 | -C22 | 1.368(11) |

Table S5 - Bond Distances (Angstrom) (continued)
for: bpp120 in P -1

| | | | | | |
|---|---|---|---|---|---|
| C1 | -H1 | 0.9500 | C12 | -H12 | 0.9500 |
| C2 | -H2 | 0.9500 | C13 | -H13 | 0.9500 |
| C5 | -H5 | 0.9500 | C16 | -H16 | 0.9500 |
| C6 | -H6 | 0.9500 | C17 | -H17 | 0.9500 |
| C7 | -H7 | 0.9500 | C18 | -H18 | 0.9500 |
| C10 | -H10 | 0.9500 | C21 | -H21 | 0.9500 |
| C11 | -H11 | 0.9500 | C22 | -H22 | 0.9500 |

Table S6 - Bond Angles (Degrees)
for: bpp120 in P -1

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N2 | -Zn1 | -N3 | 76.90(16) | N7 | -Fe1 | -N9 | 154.55(16) |
| N2 | -Zn1 | -N4 | 154.04(16) | N8 | -Fe1 | -N9 | 77.07(16) |
| N2 | -Zn1 | -N7 | 94.53(16) | N2 | -N1 | -C1 | 111.1(5) |
| N2 | -Zn1 | -N8 | 103.41(17) | Fe1 | -N2 | -N1 | 138.6(4) |
| N2 | -Zn1 | -N9 | 92.14(16) | Fe1 | -N2 | -C3 | 115.6(3) |
| N3 | -Zn1 | -N4 | 77.15(16) | Zn1 | -N2 | -N1 | 138.6(4) |
| N3 | -Zn1 | -N7 | 103.69(15) | Zn1 | -N2 | -C3 | 115.6(3) |
| N3 | -Zn1 | -N8 | 178.77(16) | N1 | -N2 | -C3 | 105.8(4) |
| N3 | -Zn1 | -N9 | 101.74(15) | Fe1 | -N3 | -C4 | 120.4(3) |
| N4 | -Zn1 | -N7 | 92.28(16) | Fe1 | -N3 | -C8 | 119.6(3) |
| N4 | -Zn1 | -N8 | 102.52(16) | Zn1 | -N3 | -C4 | 120.4(3) |
| N4 | -Zn1 | -N9 | 92.38(17) | Zn1 | -N3 | -C8 | 119.6(3) |
| N7 | -Zn1 | -N8 | 77.50(16) | C4 | -N3 | -C8 | 120.0(4) |
| N7 | -Zn1 | -N9 | 154.55(16) | Fe1 | -N4 | -N5 | 138.0(4) |
| N8 | -Zn1 | -N9 | 77.07(16) | Fe1 | -N4 | -C9 | 116.1(3) |
| N2 | -Fe1 | -N3 | 76.90(16) | Zn1 | -N4 | -N5 | 138.0(4) |
| N2 | -Fe1 | -N4 | 154.04(16) | Zn1 | -N4 | -C9 | 116.1(3) |
| N2 | -Fe1 | -N7 | 94.53(16) | N5 | -N4 | -C9 | 105.9(4) |
| N2 | -Fe1 | -N8 | 103.41(17) | N4 | -N5 | -C11 | 111.3(5) |
| N2 | -Fe1 | -N9 | 92.14(16) | N7 | -N6 | -C12 | 110.5(5) |
| N3 | -Fe1 | -N4 | 77.15(16) | Fe1 | -N7 | -N6 | 138.7(4) |
| N3 | -Fe1 | -N7 | 103.69(15) | Fe1 | -N7 | -C14 | 115.0(3) |
| N3 | -Fe1 | -N8 | 178.77(16) | Zn1 | -N7 | -N6 | 138.7(4) |
| N3 | -Fe1 | -N9 | 101.74(15) | Zn1 | -N7 | -C14 | 115.0(3) |
| N4 | -Fe1 | -N7 | 92.28(16) | N6 | -N7 | -C14 | 106.1(4) |
| N4 | -Fe1 | -N8 | 102.52(16) | Fe1 | -N8 | -C15 | 119.9(3) |
| N4 | -Fe1 | -N9 | 92.38(17) | Fe1 | -N8 | -C19 | 120.3(4) |
| N7 | -Fe1 | -N8 | 77.50(16) | Zn1 | -N8 | -C15 | 119.9(3) |

Table S6 - Bond Angles (Degrees) (continued)
for: bpp120 in P -1

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Zn1 | -N8 | -C19 | 120.3(4) | N3 | -C8 | -C7 | 121.2(4) |
| C15 | -N8 | -C19 | 119.8(4) | N3 | -C8 | -C9 | 112.0(4) |
| Fe1 | -N9 | -N10 | 137.9(3) | N4 | -C9 | -C10 | 110.3(5) |
| Fe1 | -N9 | -C20 | 116.4(3) | C8 | -C9 | -C10 | 134.6(6) |
| Zn1 | -N9 | -N10 | 137.9(3) | N4 | -C9 | -C8 | 115.1(4) |
| Zn1 | -N9 | -C20 | 116.4(3) | C9 | -C10 | -C11 | 104.8(6) |
| N10 | -N9 | -C20 | 105.7(4) | N5 | -C11 | -C10 | 107.7(5) |
| N9 | -N10 | -C22 | 111.4(5) | N6 | -C12 | -C13 | 108.9(5) |
| N2 | -N1 | -H1N | 124.00 | C12 | -C13 | -C14 | 104.6(5) |
| C1 | -N1 | -H1N | 124.00 | N7 | -C14 | -C13 | 110.0(5) |
| N4 | -N5 | -H5N | 124.00 | N7 | -C14 | -C15 | 115.7(5) |
| C11 | -N5 | -H5N | 124.00 | C13 | -C14 | -C15 | 134.3(5) |
| N7 | -N6 | -H6N | 125.00 | N8 | -C15 | -C14 | 111.8(5) |
| C12 | -N6 | -H6N | 125.00 | N8 | -C15 | -C16 | 121.7(5) |
| N9 | -N10 | -H10N | 124.00 | C14 | -C15 | -C16 | 126.5(5) |
| C22 | -N10 | -H10N | 124.00 | C15 | -C16 | -C17 | 118.0(5) |
| N1 | -C1 | -C2 | 108.8(5) | C16 | -C17 | -C18 | 120.6(5) |
| C1 | -C2 | -C3 | 103.8(5) | C17 | -C18 | -C19 | 118.3(5) |
| N2 | -C3 | -C2 | 110.5(5) | N8 | -C19 | -C20 | 111.4(5) |
| N2 | -C3 | -C4 | 115.7(5) | C18 | -C19 | -C20 | 127.0(5) |
| C2 | -C3 | -C4 | 133.8(5) | N8 | -C19 | -C18 | 121.6(5) |
| N3 | -C4 | -C3 | 111.4(5) | N9 | -C20 | -C19 | 114.8(4) |
| N3 | -C4 | -C5 | 121.1(5) | N9 | -C20 | -C21 | 110.2(5) |
| C3 | -C4 | -C5 | 127.5(5) | C19 | -C20 | -C21 | 134.9(6) |
| C4 | -C5 | -C6 | 118.9(5) | C20 | -C21 | -C22 | 105.0(6) |
| C5 | -C6 | -C7 | 120.2(5) | N10 | -C22 | -C21 | 107.6(5) |
| C6 | -C7 | -C8 | 118.6(5) | N1 | -C1 | -H1 | 126.00 |
| C7 | -C8 | -C9 | 126.9(5) | C2 | -C1 | -H1 | 126.00 |

Table S6 - Bond Angles (Degrees) (continued)
for: bpp120 in P -1

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C1 | -C2 | -H2 | 128.00 | C12 | -C13 | -H13 | 128.00 |
| C3 | -C2 | -H2 | 128.00 | C14 | -C13 | -H13 | 128.00 |
| C4 | -C5 | -H5 | 121.00 | C15 | -C16 | -H16 | 121.00 |
| C6 | -C5 | -H5 | 121.00 | C17 | -C16 | -H16 | 121.00 |
| C5 | -C6 | -H6 | 120.00 | C16 | -C17 | -H17 | 120.00 |
| C7 | -C6 | -H6 | 120.00 | C18 | -C17 | -H17 | 120.00 |
| C6 | -C7 | -H7 | 121.00 | C17 | -C18 | -H18 | 121.00 |
| C8 | -C7 | -H7 | 121.00 | C19 | -C18 | -H18 | 121.00 |
| C9 | -C10 | -H10 | 128.00 | C20 | -C21 | -H21 | 127.00 |
| C11 | -C10 | -H10 | 128.00 | C22 | -C21 | -H21 | 127.00 |
| N5 | -C11 | -H11 | 126.00 | N10 | -C22 | -H22 | 126.00 |
| C10 | -C11 | -H11 | 126.00 | C21 | -C22 | -H22 | 126.00 |
| N6 | -C12 | -H12 | 126.00 | Se1 | -C23 | -N11 | 177.7(6) |
| C13 | -C12 | -H12 | 126.00 | Se2 | -C24 | -N12 | 177.8(5) |

Table S7 - Torsion Angles (Degrees)
for: bpp120 in P -1

| | | | | |
|---|---|---|---|---|
| N9 | -Fe1 | -N3 | -C4 | -91.0(4) |
| N2 | -Fe1 | -N3 | -C8 | 179.3(4) |
| N3 | -Fe1 | -N2 | -N1 | -177.9(5) |
| N4 | -Fe1 | -N2 | -N1 | -176.2(4) |
| N7 | -Fe1 | -N2 | -N1 | 79.1(5) |
| N8 | -Fe1 | -N2 | -N1 | 0.9(5) |
| N9 | -Fe1 | -N2 | -N1 | -76.4(5) |
| N3 | -Fe1 | -N2 | -C3 | 0.9(3) |
| N4 | -Fe1 | -N2 | -C3 | 2.6(6) |
| N7 | -Fe1 | -N2 | -C3 | -102.1(4) |
| N8 | -Fe1 | -N2 | -C3 | 179.7(3) |
| N9 | -Fe1 | -N2 | -C3 | 102.5(4) |
| N2 | -Fe1 | -N3 | -C4 | -1.6(3) |
| N4 | -Fe1 | -N3 | -C4 | 179.2(4) |
| N7 | -Fe1 | -N3 | -C4 | 90.0(4) |
| N8 | -Fe1 | -N9 | -C20 | -1.1(4) |
| N7 | -Fe1 | -N8 | -C15 | -0.2(4) |
| N4 | -Fe1 | -N3 | -C8 | 0.0(3) |
| N7 | -Fe1 | -N3 | -C8 | -89.2(3) |
| N9 | -Fe1 | -N3 | -C8 | 89.8(4) |
| N2 | -Fe1 | -N4 | -N5 | 176.7(4) |
| N3 | -Fe1 | -N4 | -N5 | 178.4(5) |
| N7 | -Fe1 | -N4 | -N5 | -78.1(5) |
| N8 | -Fe1 | -N4 | -N5 | -0.4(5) |
| N9 | -Fe1 | -N4 | -N5 | 76.9(5) |
| N2 | -Fe1 | -N4 | -C9 | 0.3(6) |
| N3 | -Fe1 | -N4 | -C9 | 2.0(3) |
| N7 | -Fe1 | -N4 | -C9 | 105.5(4) |

Table S7 - Torsion Angles (Degrees) (continued)
for: bpp120 in P -1

| | | | | |
|---|---|---|---|---|
| N8 | -Fe1 | -N4 | -C9 | -176.8(4) |
| N9 | -Fe1 | -N4 | -C9 | -99.5(4) |
| N4 | -Fe1 | -N8 | -C15 | -89.8(4) |
| N9 | -Fe1 | -N7 | -N6 | -173.2(4) |
| N9 | -Fe1 | -N8 | -C15 | -179.4(4) |
| N2 | -Fe1 | -N8 | -C19 | -87.4(4) |
| N2 | -Fe1 | -N7 | -N6 | 82.2(5) |
| N3 | -Fe1 | -N7 | -N6 | 4.6(5) |
| N4 | -Fe1 | -N7 | -N6 | -72.8(5) |
| N8 | -Fe1 | -N7 | -N6 | -175.1(5) |
| N7 | -Fe1 | -N9 | -C20 | -3.0(6) |
| N2 | -Fe1 | -N7 | -C14 | -104.8(4) |
| N3 | -Fe1 | -N7 | -C14 | 177.7(3) |
| N4 | -Fe1 | -N7 | -C14 | 100.3(4) |
| N8 | -Fe1 | -N7 | -C14 | -2.0(3) |
| N9 | -Fe1 | -N7 | -C14 | -0.1(6) |
| N2 | -Fe1 | -N8 | -C15 | 91.5(4) |
| N2 | -Fe1 | -N9 | -N10 | -78.9(5) |
| N3 | -Fe1 | -N9 | -N10 | -1.9(5) |
| N4 | -Fe1 | -N9 | -N10 | 75.5(5) |
| N7 | -Fe1 | -N9 | -N10 | 175.9(4) |
| N4 | -Fe1 | -N8 | -C19 | 91.3(4) |
| N7 | -Fe1 | -N8 | -C19 | -179.2(4) |
| N9 | -Fe1 | -N8 | -C19 | 1.7(4) |
| N4 | -Fe1 | -N9 | -C20 | -103.4(4) |
| N8 | -Fe1 | -N9 | -N10 | 177.8(5) |
| N2 | -Fe1 | -N9 | -C20 | 102.2(4) |
| N3 | -Fe1 | -N9 | -C20 | 179.2(4) |

Table S7 - Torsion Angles (Degrees) (continued)
for: bpp120 in P -1

| | | | | |
|---|---|---|---|---|
| C1 | -N1 | -N2 | -Fe1 | 178.6(4) |
| N2 | -N1 | -C1 | -C2 | 0.1(6) |
| C1 | -N1 | -N2 | -C3 | -0.3(6) |
| Fe1 | -N2 | -C3 | -C2 | -178.8(3) |
| Fe1 | -N2 | -C3 | -C4 | -0.2(6) |
| N1 | -N2 | -C3 | -C4 | 179.0(4) |
| N1 | -N2 | -C3 | -C2 | 0.4(5) |
| Fe1 | -N3 | -C4 | -C3 | 1.8(5) |
| C8 | -N3 | -C4 | -C3 | -179.0(4) |
| C4 | -N3 | -C8 | -C7 | -1.2(7) |
| Fe1 | -N3 | -C8 | -C9 | -1.8(5) |
| C4 | -N3 | -C8 | -C9 | 179.0(4) |
| C8 | -N3 | -C4 | -C5 | 1.3(7) |
| Fe1 | -N3 | -C8 | -C7 | 178.0(4) |
| Fe1 | -N3 | -C4 | -C5 | -177.9(4) |
| C9 | -N4 | -N5 | -C11 | -0.8(6) |
| N5 | -N4 | -C9 | -C8 | 179.0(4) |
| N5 | -N4 | -C9 | -C10 | 0.2(6) |
| Fe1 | -N4 | -C9 | -C8 | -3.5(6) |
| Fe1 | -N4 | -N5 | -C11 | -177.5(4) |
| Fe1 | -N4 | -C9 | -C10 | 177.7(4) |
| N4 | -N5 | -C11 | -C10 | 1.1(6) |
| C12 | -N6 | -N7 | -C14 | 0.1(6) |
| C12 | -N6 | -N7 | -Fe1 | 173.6(4) |
| N7 | -N6 | -C12 | -C13 | -0.1(6) |
| N6 | -N7 | -C14 | -C13 | -0.2(6) |
| Fe1 | -N7 | -C14 | -C13 | -175.4(4) |
| N6 | -N7 | -C14 | -C15 | 179.0(4) |

Table S7 - Torsion Angles (Degrees) (continued)
for: bpp120 in P -1

| | | | | |
|---|---|---|---|---|
| Fe1 | -N7 | -C14 | -C15 | 3.8(6) |
| Fe1 | -N8 | -C15 | -C16 | -178.6(4) |
| C15 | -N8 | -C19 | -C20 | 179.2(4) |
| C19 | -N8 | -C15 | -C16 | 0.4(8) |
| Fe1 | -N8 | -C19 | -C20 | -1.9(6) |
| Fe1 | -N8 | -C15 | -C14 | 2.2(6) |
| C19 | -N8 | -C15 | -C14 | -178.9(4) |
| C15 | -N8 | -C19 | -C18 | 0.3(7) |
| Fe1 | -N8 | -C19 | -C18 | 179.2(4) |
| C20 | -N9 | -N10 | -C22 | 0.4(6) |
| N10 | -N9 | -C20 | -C19 | -178.8(4) |
| Fe1 | -N9 | -C20 | -C19 | 0.4(6) |
| Fe1 | -N9 | -C20 | -C21 | 178.8(4) |
| N10 | -N9 | -C20 | -C21 | -0.4(6) |
| Fe1 | -N9 | -N10 | -C22 | -178.6(4) |
| N9 | -N10 | -C22 | -C21 | -0.1(6) |
| N1 | -C1 | -C2 | -C3 | 0.2(6) |
| C1 | -C2 | -C3 | -N2 | -0.4(6) |
| C1 | -C2 | -C3 | -C4 | -178.6(6) |
| C2 | -C3 | -C4 | -C5 | -3.1(9) |
| N2 | -C3 | -C4 | -N3 | -1.0(6) |
| N2 | -C3 | -C4 | -C5 | 178.8(5) |
| C2 | -C3 | -C4 | -N3 | 177.2(5) |
| C3 | -C4 | -C5 | -C6 | -179.9(5) |
| N3 | -C4 | -C5 | -C6 | -0.2(8) |
| C4 | -C5 | -C6 | -C7 | -1.0(8) |
| C5 | -C6 | -C7 | -C8 | 1.2(8) |
| C6 | -C7 | -C8 | -C9 | 179.7(5) |

Table S7 - Torsion Angles (Degrees) (continued)
for: bpp120 in P -1

| | | | | |
|---|---|---|---|---|
| C6 | -C7 | -C8 | -N3 | -0.1(8) |
| C7 | -C8 | -C9 | -N4 | -176.4(5) |
| C7 | -C8 | -C9 | -C10 | 2.0(10) |
| N3 | -C8 | -C9 | -C10 | -178.2(6) |
| N3 | -C8 | -C9 | -N4 | 3.4(6) |
| N4 | -C9 | -C10 | -C11 | 0.4(6) |
| C8 | -C9 | -C10 | -C11 | -178.0(6) |
| C9 | -C10 | -C11 | -N5 | -0.9(6) |
| N6 | -C12 | -C13 | -C14 | 0.0(6) |
| C12 | -C13 | -C14 | -N7 | 0.1(6) |
| C12 | -C13 | -C14 | -C15 | -178.9(6) |
| C13 | -C14 | -C15 | -C16 | -4.1(10) |
| C13 | -C14 | -C15 | -N8 | 175.1(6) |
| N7 | -C14 | -C15 | -C16 | 177.0(5) |
| N7 | -C14 | -C15 | -N8 | -3.9(6) |
| C14 | -C15 | -C16 | -C17 | 179.5(5) |
| N8 | -C15 | -C16 | -C17 | 0.3(8) |
| C15 | -C16 | -C17 | -C18 | -1.7(9) |
| C16 | -C17 | -C18 | -C19 | 2.3(9) |
| C17 | -C18 | -C19 | -C20 | 179.8(5) |
| C17 | -C18 | -C19 | -N8 | -1.6(8) |
| N8 | -C19 | -C20 | -C21 | -176.9(6) |
| C18 | -C19 | -C20 | -C21 | 1.9(10) |
| N8 | -C19 | -C20 | -N9 | 0.9(6) |
| C18 | -C19 | -C20 | -N9 | 179.7(5) |
| C19 | -C20 | -C21 | -C22 | 178.3(6) |
| N9 | -C20 | -C21 | -C22 | 0.4(6) |
| C20 | -C21 | -C22 | -N10 | -0.2(6) |

Table S8 - Contact Distances(Angstrom)
for: bpp120 in P -1

| | | | | | |
|---|---|---|---|---|---|
| Se1 | .C18_l | 3.677(6) | N4 | .N8 | 3.168(6) |
| Se1 | .N5_a | 3.335(6) | N4 | .N9 | 2.974(6) |
| Se2 | .C5_k | 3.588(6) | N5 | .Se1_c | 3.335(6) |
| Se2 | .N10_b | 3.320(6) | N5 | .C23_c | 3.216(8) |
| Se1 | .H5N_a | 2.4800 | N6 | .N12 | 2.794(8) |
| Se1 | .H16_m | 3.1500 | N6 | .C22_b | 3.293(7) |
| Se1 | .H13_m | 3.2700 | N7 | .N8 | 2.539(6) |
| Se1 | .H18_l | 3.0800 | N7 | .N4 | 2.974(6) |
| Se2 | .H7_n | 2.9500 | N7 | .N3 | 3.190(5) |
| Se2 | .H10N_b | 2.4500 | N7 | .N2 | 3.033(6) |
| Se2 | .H5_k | 2.9800 | N7 | .C15 | 2.376(7) |
| N1 | .C11_a | 3.368(7) | N8 | .N7 | 2.539(6) |
| N1 | .C22_b | 3.377(7) | N8 | .N9 | 2.525(6) |
| N1 | .N11 | 2.784(8) | N8 | .N4 | 3.168(6) |
| N2 | .N7 | 3.033(6) | N8 | .C20 | 2.329(7) |
| N2 | .N3 | 2.529(6) | N8 | .N2 | 3.192(6) |
| N2 | .N8 | 3.192(6) | N8 | .C14 | 2.315(6) |
| N2 | .N9 | 2.972(6) | N9 | .N2 | 2.972(6) |
| N2 | .C4 | 2.368(7) | N9 | .N4 | 2.974(6) |
| N3 | .N7 | 3.190(5) | N9 | .N8 | 2.525(6) |
| N3 | .C9 | 2.331(6) | N9 | .N3 | 3.145(5) |
| N3 | .N2 | 2.529(6) | N9 | .C19 | 2.371(7) |
| N3 | .N4 | 2.533(6) | N10 | .Se2_f | 3.320(6) |
| N3 | .N9 | 3.145(5) | N10 | .C24_f | 3.245(8) |
| N3 | .C3 | 2.317(6) | N11 | .N1 | 2.784(8) |
| N4 | .N3 | 2.533(6) | N12 | .N6 | 2.794(8) |
| N4 | .C8 | 2.360(6) | N1 | .H22_b | 2.5200 |
| N4 | .N7 | 2.974(6) | N2 | .H22_b | 2.6500 |

Table S8 - Contact Distances(Angstrom) (continued)
for: bpp120 in P -1

| | | | | | |
|---|---|---|---|---|---|
| N5 | .H12_d | 2.6500 | C19 | .C23 | 3.545(8) |
| N6 | .H1_e | 2.6800 | C20 | .C12_d | 3.600(8) |
| N9 | .H11_a | 2.8400 | C21 | .C12_d | 3.465(8) |
| N10 | .H11_a | 2.6300 | C21 | .C13_d | 3.527(8) |
| N11 | .H1N | 1.9100 | C22 | .C1_d | 3.574(9) |
| N11 | .H17_m | 2.9400 | C22 | .N1_d | 3.377(7) |
| N12 | .H6_n | 2.7500 | C22 | .N6_d | 3.293(7) |
| N12 | .H6N | 1.9200 | C22 | .C11_a | 3.520(8) |
| C1 | .C9_a | 3.483(8) | C23 | .C16_m | 3.461(9) |
| C1 | .C10_a | 3.392(8) | C23 | .C19 | 3.545(8) |
| C1 | .C11_a | 3.591(8) | C23 | .N5_a | 3.216(8) |
| C1 | .C22_b | 3.574(9) | C23 | .C18 | 3.467(8) |
| C2 | .C10_a | 3.557(8) | C24 | .N10_b | 3.245(8) |
| C5 | .C24 | 3.538(8) | C24 | .C7_n | 3.563(9) |
| C5 | .Se2_g | 3.588(6) | C24 | .C5 | 3.538(8) |
| C7 | .C24_h | 3.563(9) | C1 | .H22_b | 2.7000 |
| C9 | .C1_e | 3.483(8) | C2 | .H22_b | 2.9400 |
| C10 | .C1_e | 3.392(8) | C2 | .H5 | 3.0700 |
| C10 | .C2_e | 3.557(8) | C3 | .H22_b | 2.8700 |
| C11 | .C22_e | 3.520(8) | C10 | .H7 | 3.0800 |
| C11 | .N1_e | 3.368(7) | C13 | .H16 | 3.0600 |
| C11 | .C1_e | 3.591(8) | C20 | .H11_a | 2.9100 |
| C12 | .C20_b | 3.600(8) | C21 | .H11_a | 2.8100 |
| C12 | .C21_b | 3.465(8) | C21 | .H18 | 3.0900 |
| C13 | .C21_b | 3.527(8) | C22 | .H11_a | 2.6200 |
| C16 | .C23_i | 3.461(9) | C23 | .H5N_a | 2.6100 |
| C18 | .Se1_j | 3.677(6) | C23 | .H1N | 2.8000 |
| C18 | .C23 | 3.467(8) | C23 | .H16_m | 2.7000 |

Table S8 - Contact Distances(Angstrom) (continued)
for: bpp120 in P -1

| | | | | | |
|---|---|---|---|---|---|
| C24 | .H10N_b | 2.6300 | H10N | .Se2_f | 2.4500 |
| C24 | .H7_n | 2.9200 | H10N | .C24_f | 2.6300 |
| C24 | .H6_n | 3.0900 | H11 | .N9_e | 2.8400 |
| C24 | .H6N | 2.7700 | H11 | .N10_e | 2.6300 |
| H1 | .N6_a | 2.6800 | H11 | .C20_e | 2.9100 |
| H1 | .H6N_a | 2.3900 | H11 | .C21_e | 2.8100 |
| H1N | .C23 | 2.8000 | H11 | .C22_e | 2.6200 |
| H1N | .N11 | 1.9100 | H12 | .N5_b | 2.6500 |
| H5 | .H5_k | 2.5800 | H12 | .H5N_b | 2.4200 |
| H5 | .C2 | 3.0700 | H13 | .Se1_i | 3.2700 |
| H5 | .Se2_g | 2.9800 | H16 | .C13 | 3.0600 |
| H5N | .Se1_c | 2.4800 | H16 | .Se1_i | 3.1500 |
| H5N | .C23_c | 2.6100 | H16 | .C23_i | 2.7000 |
| H5N | .H12_d | 2.4200 | H17 | .N11_i | 2.9400 |
| H6 | .N12_h | 2.7500 | H18 | .C21 | 3.0900 |
| H6 | .C24_h | 3.0900 | H18 | .Se1_j | 3.0800 |
| H6N | .N12 | 1.9200 | H22 | .N1_d | 2.5200 |
| H6N | .C24 | 2.7700 | H22 | .N2_d | 2.6500 |
| H6N | .H1_e | 2.3900 | H22 | .C1_d | 2.7000 |
| H7 | .C10 | 3.0800 | H22 | .C2_d | 2.9400 |
| H7 | .Se2_h | 2.9500 | H22 | .C3_d | 2.8700 |
| H7 | .C24_h | 2.9200 | | | |

Table S9 - Hydrogen Bonds (Angstrom, Deg)
for: bpp120 in P -1

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N1 | -- H1N | .. N11 | 0.8800 | 1.9100 | 2.784(8) | 171.00 | . |
| N5 | -- H5N | .. Se1 | 0.8800 | 2.4800 | 3.335(6) | 166.00 | 1_545 |
| N6 | -- H6N | .. N12 | 0.8800 | 1.9200 | 2.794(8) | 171.00 | . |
| N10 | -- H10N | .. Se2 | 0.8800 | 2.4500 | 3.320(6) | 168.00 | 1_655 |
| C7 | -- H7 | .. Se2 | 0.9500 | 2.9500 | 3.845(6) | 158.00 | 2_655 |
| C22 | -- H22 | .. N1 | 0.9500 | 2.5200 | 3.377(7) | 151.00 | 1_655 |

Translation of Symmetry Code to Equiv.Pos

a =[ 1565.00 ] = x,1+y,z
b =[ 1455.00 ] = -1+x,y,z
c =[ 1545.00 ] = x,-1+y,z
d =[ 1655.00 ] = 1+x,y,z
g =[ 2665.00 ] = 1-x,1-y,-z
h =[ 2655.00 ] = 1-x,-y,-z
i =[ 2666.00 ] = 1-x,1-y,1-z
j =[ 2766.00 ] = 2-x,1-y,1-z
k =[ 2665.00 ] = 1-x,1-y,-z
l =[ 2766.00 ] = 2-x,1-y,1-z
m =[ 2666.00 ] = 1-x,1-y,1-z

**bpp 298K in P -1**

==========
S U P P L E M E N T A R Y  M A T E R I A L
==========

B E L O N G I N G  TO  T H E  P A P E R

b y

C o n t e n t s
==========

Table S1 - Crystal Data and Details of the Structure Determination for: bpp in P -1

| Crystal Data | | | |
|---|---|---|---|
| Formula | | | ? |
| Formula Weight | | | 692.48 |
| Crystal System | | | Triclinic |
| Space group | | P-1 | (No. 2) |
| a, b, c [Angstrom] | 8.368(1) | 8.426(2) | 19.889(5) |
| alpha, beta, gamma [deg] | 87.024(8) | 83.163(6) | 88.898(9) |
| V [Ang**3] | | | 1390.4(5) |
| Z | | | 2 |
| D(calc) [g/cm**3] | | | 1.654 |
| Mu(MoKa) [ /mm ] | | | 3.348 |
| F(000) | | | 684 |
| Crystal Size [mm] | | 0.00 x 0.00 x 0.00 | |

| Data Collection | | | |
|---|---|---|---|
| Temperature (K) | | | ***** |
| Radiation [Angstrom] | | MoKa | 0.71073 |
| Theta Min-Max [Deg] | | | 0.0, 0.0 |
| Dataset | | 999:-99 ; 999:-99 ; 999:-99 | |
| Tot., Uniq. Data, R(int) | | 0, 0, | 0.000 |
| Observed data [I > 0.0 sigma(I)] | | | 0 |

| Refinement | | | |
|---|---|---|---|
| Nref, Npar | | | 0, 0 |
| R, wR2, S | | 0.0000, 0.0000, 0.00 | |
| w = | | | |
| Max. and Av. Shift/Error | | | 0.00, 0.00 |
| Min. and Max. Resd. Dens. [e/Ang^3] | | | 0.00, 0.00 |

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: bpp in P -1

| Atom | x | y | z | U(eq) [Ang^2] |
|---|---|---|---|---|
| *Fe1 | 0.73503(8) | 0.22740(8) | 0.24897(3) | 0.0450(3) |
| *Zn1 | 0.73503(8) | 0.22740(8) | 0.24897(3) | 0.0450(3) |
| N1 | 0.5834(5) | 0.5967(5) | 0.2367(2) | 0.0541(17) |
| N2 | 0.6377(5) | 0.4564(5) | 0.2125(2) | 0.0433(16) |
| N3 | 0.7365(5) | 0.2126(5) | 0.14346(19) | 0.0432(16) |
| N4 | 0.8402(5) | -0.0061(5) | 0.2248(2) | 0.0504(17) |
| N5 | 0.9067(6) | -0.1310(6) | 0.2563(3) | 0.0650(17) |
| N6 | 0.3756(6) | 0.0602(5) | 0.2736(2) | 0.0608(17) |
| N7 | 0.5027(5) | 0.1325(5) | 0.2933(2) | 0.0483(17) |
| N8 | 0.7273(5) | 0.2512(5) | 0.35451(19) | 0.0446(16) |
| N9 | 0.9661(5) | 0.3264(5) | 0.2647(2) | 0.0504(17) |
| N10 | 1.1054(6) | 0.3690(5) | 0.2278(3) | 0.0586(17) |
| C1 | 0.5376(7) | 0.6935(7) | 0.1865(3) | 0.068(3) |
| C2 | 0.5614(7) | 0.6168(7) | 0.1279(3) | 0.063(2) |
| C3 | 0.6239(6) | 0.4696(6) | 0.1458(3) | 0.0458(17) |
| C4 | 0.6776(6) | 0.3319(6) | 0.1067(3) | 0.0473(19) |
| C5 | 0.6695(7) | 0.3233(7) | 0.0377(3) | 0.061(2) |
| C6 | 0.7232(8) | 0.1857(8) | 0.0074(3) | 0.072(3) |
| C7 | 0.7850(7) | 0.0635(7) | 0.0445(3) | 0.063(2) |
| C8 | 0.7915(6) | 0.0795(6) | 0.1130(3) | 0.0498(19) |
| C9 | 0.8540(6) | -0.0383(6) | 0.1590(3) | 0.0482(19) |
| C10 | 0.9299(7) | -0.1858(7) | 0.1491(3) | 0.069(3) |
| C11 | 0.9588(8) | -0.2403(8) | 0.2121(4) | 0.081(3) |
| C12 | 0.2704(8) | 0.0178(7) | 0.3269(3) | 0.074(3) |
| C13 | 0.3268(7) | 0.0623(7) | 0.3839(3) | 0.069(3) |
| C14 | 0.4733(7) | 0.1327(7) | 0.3607(3) | 0.054(2) |

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued) for: bpp in P -1

| Atom | x | y | z | U(eq) [Ang^2] |
|---|---|---|---|---|
| C15 | 0.5948(7) | 0.2056(6) | 0.3952(3) | 0.053(2) |
| C16 | 0.5840(8) | 0.2247(8) | 0.4650(3) | 0.075(3) |
| C17 | 0.7100(10) | 0.2934(8) | 0.4906(3) | 0.086(3) |
| C18 | 0.8453(8) | 0.3373(8) | 0.4486(3) | 0.072(3) |
| C19 | 0.8501(7) | 0.3156(6) | 0.3796(3) | 0.052(2) |
| C20 | 0.9837(7) | 0.3569(6) | 0.3287(3) | 0.051(2) |
| C21 | 1.1361(7) | 0.4183(7) | 0.3321(4) | 0.071(3) |
| C22 | 1.2079(7) | 0.4251(7) | 0.2670(4) | 0.076(3) |
| Se1 | 0.86985(10) | 0.81452(10) | 0.42767(4) | 0.0928(3) |
| N11 | 0.6039(8) | 0.6627(8) | 0.3715(3) | 0.097(3) |
| C23 | 0.7079(9) | 0.7194(9) | 0.3947(3) | 0.076(3) |
| Se2 | 0.18568(9) | 0.31273(9) | 0.06115(3) | 0.0846(3) |
| N12 | 0.3426(7) | 0.0514(7) | 0.1346(3) | 0.089(3) |
| C24 | 0.2831(8) | 0.1519(8) | 0.1051(3) | 0.066(3) |

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites have a S.O.F less than 1.0

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters
for: bpp in P -1

| Atom | x | y | z | U(iso) [Ang^2] |
|---|---|---|---|---|
| H1 | 0.49641 | 0.79615 | 0.19124 | 0.0816 |
| H1N | 0.57879 | 0.62068 | 0.27835 | 0.0648 |
| H2 | 0.54039 | 0.65473 | 0.08509 | 0.0749 |
| H5 | 0.62899 | 0.40792 | 0.01265 | 0.0734 |
| H5N | 0.91462 | -0.13948 | 0.29908 | 0.0777 |
| H6 | 0.71732 | 0.17594 | -0.03856 | 0.0869 |
| H6N | 0.36378 | 0.04340 | 0.23216 | 0.0727 |
| H7 | 0.82212 | -0.02912 | 0.02398 | 0.0756 |
| H10 | 0.95513 | -0.23559 | 0.10851 | 0.0827 |
| H10N | 1.12570 | 0.36110 | 0.18467 | 0.0705 |
| H11 | 1.00670 | -0.33742 | 0.22270 | 0.0972 |
| H12 | 0.17388 | -0.03387 | 0.32512 | 0.0892 |
| H13 | 0.27869 | 0.04893 | 0.42843 | 0.0828 |
| H16 | 0.49336 | 0.19158 | 0.49351 | 0.0900 |
| H17 | 0.70330 | 0.31020 | 0.53672 | 0.1030 |
| H18 | 0.93220 | 0.38075 | 0.46586 | 0.0865 |
| H21 | 1.17913 | 0.44811 | 0.37054 | 0.0849 |
| H22 | 1.31067 | 0.46234 | 0.25229 | 0.0906 |

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S4 - (An)isotropic Displacement Parameters
for: bpp in P -1

| Atom | U(1,1) or U | U(2,2) | U(3,3) | U(2,3) | U(1,3) | U(1,2) |
|---|---|---|---|---|---|---|
| Fe1 | 0.0461(5) | 0.0477(5) | 0.0417(4) | -0.0045(3) | -0.0069(3) | 0.0023(3) |
| Zn1 | 0.0461(5) | 0.0477(5) | 0.0417(4) | -0.0045(3) | -0.0069(3) | 0.0023(3) |
| N1 | 0.046(3) | 0.053(3) | 0.065(3) | -0.013(2) | -0.009(2) | -0.002(2) |
| N2 | 0.043(3) | 0.038(3) | 0.050(2) | -0.0067(19) | -0.0083(19) | 0.002(2) |
| N3 | 0.046(3) | 0.037(3) | 0.047(2) | -0.004(2) | -0.0074(19) | 0.003(2) |
| N4 | 0.052(3) | 0.043(3) | 0.056(3) | 0.002(2) | -0.008(2) | 0.001(2) |
| N5 | 0.062(3) | 0.053(3) | 0.081(3) | 0.011(3) | -0.019(3) | -0.003(3) |
| N6 | 0.059(3) | 0.053(3) | 0.072(3) | -0.008(3) | -0.012(3) | -0.002(3) |
| N7 | 0.039(3) | 0.049(3) | 0.059(3) | -0.007(2) | -0.012(2) | -0.002(2) |
| N8 | 0.042(3) | 0.050(3) | 0.043(2) | -0.004(2) | -0.010(2) | 0.001(2) |
| N9 | 0.041(3) | 0.043(3) | 0.066(3) | -0.006(2) | -0.001(2) | 0.003(2) |
| N10 | 0.049(3) | 0.046(3) | 0.078(3) | -0.003(2) | 0.003(3) | 0.006(2) |
| C1 | 0.064(4) | 0.043(4) | 0.098(5) | 0.003(4) | -0.019(4) | 0.010(3) |
| C2 | 0.068(4) | 0.054(4) | 0.068(4) | 0.002(3) | -0.022(3) | 0.005(3) |
| C3 | 0.045(3) | 0.038(3) | 0.056(3) | 0.001(2) | -0.014(2) | 0.002(3) |
| C4 | 0.047(3) | 0.046(4) | 0.050(3) | -0.003(3) | -0.010(2) | -0.003(3) |
| C5 | 0.074(4) | 0.060(4) | 0.051(3) | 0.001(3) | -0.018(3) | 0.002(3) |
| C6 | 0.088(5) | 0.087(5) | 0.043(3) | -0.011(3) | -0.009(3) | 0.000(4) |
| C7 | 0.071(4) | 0.063(4) | 0.057(3) | -0.020(3) | -0.008(3) | 0.008(3) |
| C8 | 0.048(3) | 0.050(4) | 0.051(3) | -0.007(3) | -0.002(2) | -0.003(3) |
| C9 | 0.042(3) | 0.042(4) | 0.061(3) | -0.007(3) | -0.006(2) | 0.000(3) |
| C10 | 0.067(4) | 0.049(4) | 0.090(5) | -0.016(3) | -0.003(4) | 0.014(3) |
| C11 | 0.081(5) | 0.043(4) | 0.118(6) | 0.001(4) | -0.012(4) | 0.013(4) |
| C12 | 0.059(4) | 0.072(5) | 0.091(5) | 0.003(4) | -0.007(4) | -0.018(4) |
| C13 | 0.054(4) | 0.079(5) | 0.070(4) | 0.009(3) | 0.007(3) | -0.015(3) |
| C14 | 0.053(4) | 0.052(4) | 0.056(3) | -0.002(3) | -0.005(3) | 0.006(3) |

Table S4 - (An)isotropic Displacement Parameters (continued)
for: bpp in P -1

| Atom | U(1,1) or U | U(2,2) | U(3,3) | U(2,3) | U(1,3) | U(1,2) |
|---|---|---|---|---|---|---|
| C15 | 0.058(4) | 0.055(4) | 0.045(3) | -0.004(3) | -0.002(3) | 0.005(3) |
| C16 | 0.091(5) | 0.084(5) | 0.046(3) | -0.001(3) | 0.007(3) | -0.002(4) |
| C17 | 0.125(7) | 0.091(6) | 0.044(3) | -0.008(3) | -0.018(4) | -0.013(5) |
| C18 | 0.084(5) | 0.079(5) | 0.057(4) | -0.009(3) | -0.022(4) | -0.006(4) |
| C19 | 0.056(4) | 0.051(4) | 0.050(3) | -0.004(3) | -0.013(3) | 0.007(3) |
| C20 | 0.047(4) | 0.038(3) | 0.070(4) | -0.010(3) | -0.020(3) | 0.007(3) |
| C21 | 0.053(4) | 0.067(5) | 0.098(5) | -0.015(4) | -0.028(4) | -0.003(3) |
| C22 | 0.035(4) | 0.062(5) | 0.131(6) | -0.006(4) | -0.012(4) | 0.000(3) |
| Se1 | 0.0965(6) | 0.1102(7) | 0.0742(5) | -0.0107(4) | -0.0187(4) | 0.0002(5) |
| N11 | 0.100(5) | 0.125(6) | 0.069(4) | -0.023(4) | -0.012(3) | 0.003(4) |
| C23 | 0.090(6) | 0.087(5) | 0.049(4) | -0.007(3) | -0.002(3) | 0.024(4) |
| Se2 | 0.0999(6) | 0.0811(5) | 0.0724(4) | -0.0012(4) | -0.0096(4) | -0.0030(4) |
| N12 | 0.109(5) | 0.080(4) | 0.080(4) | -0.013(3) | -0.021(3) | 0.010(4) |
| C24 | 0.077(5) | 0.066(5) | 0.056(4) | -0.015(3) | -0.008(3) | -0.009(4) |

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S5 - Bond Distances (Angstrom)
for: bpp in P -1

| | | | | | |
|---|---|---|---|---|---|
| Se1 | -C23 | 1.794(7) | N9 | -N10 | 1.346(7) |
| Se2 | -C24 | 1.808(7) | N10 | -C22 | 1.334(8) |
| Zn1 | -N4 | 2.193(4) | N1 | -H1N | 0.8600 |
| Zn1 | -N3 | 2.107(4) | N5 | -H5N | 0.8600 |
| Zn1 | -N9 | 2.183(4) | N6 | -H6N | 0.8600 |
| Zn1 | -N7 | 2.185(4) | N10 | -H10N | 0.8600 |
| Zn1 | -N2 | 2.202(4) | N11 | -C23 | 1.155(10) |
| Zn1 | -N8 | 2.112(4) | N12 | -C24 | 1.145(9) |
| Fe1 | -N3 | 2.107(4) | C1 | -C2 | 1.354(8) |
| Fe1 | -N4 | 2.193(4) | C2 | -C3 | 1.383(8) |
| Fe1 | -N2 | 2.202(4) | C3 | -C4 | 1.464(8) |
| Fe1 | -N8 | 2.112(4) | C4 | -C5 | 1.388(8) |
| Fe1 | -N9 | 2.183(4) | C5 | -C6 | 1.378(9) |
| Fe1 | -N7 | 2.185(4) | C6 | -C7 | 1.365(9) |
| N1 | -C1 | 1.343(7) | C7 | -C8 | 1.384(8) |
| N1 | -N2 | 1.350(6) | C8 | -C9 | 1.448(8) |
| N2 | -C3 | 1.344(7) | C9 | -C10 | 1.397(8) |
| N3 | -C8 | 1.349(7) | C10 | -C11 | 1.359(10) |
| N3 | -C4 | 1.334(7) | C12 | -C13 | 1.352(8) |
| N4 | -C9 | 1.341(7) | C13 | -C14 | 1.390(8) |
| N4 | -N5 | 1.342(7) | C14 | -C15 | 1.455(8) |
| N5 | -C11 | 1.337(9) | C15 | -C16 | 1.398(8) |
| N6 | -C12 | 1.333(8) | C16 | -C17 | 1.374(10) |
| N6 | -N7 | 1.343(6) | C17 | -C18 | 1.369(10) |
| N7 | -C14 | 1.334(7) | C18 | -C19 | 1.390(8) |
| N8 | -C19 | 1.331(7) | C19 | -C20 | 1.451(8) |
| N8 | -C15 | 1.343(7) | C20 | -C21 | 1.396(8) |
| N9 | -C20 | 1.337(7) | C21 | -C22 | 1.360(11) |

Table S5 - Bond Distances (Angstrom) (continued)
for: bpp in P -1

| | | | | | |
|---|---|---|---|---|---|
| C1 | -H1 | 0.9300 | C12 | -H12 | 0.9300 |
| C2 | -H2 | 0.9300 | C13 | -H13 | 0.9300 |
| C5 | -H5 | 0.9300 | C16 | -H16 | 0.9300 |
| C6 | -H6 | 0.9300 | C17 | -H17 | 0.9300 |
| C7 | -H7 | 0.9300 | C18 | -H18 | 0.9300 |
| C10 | -H10 | 0.9300 | C21 | -H21 | 0.9300 |
| C11 | -H11 | 0.9300 | C22 | -H22 | 0.9300 |

Table S6 - Bond Angles (Degrees)
for: bpp in P -1

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N2 | -Zn1 | -N3 | 74.10(16) | N7 | -Fe1 | -N9 | 148.23(15) |
| N2 | -Zn1 | -N4 | 148.24(15) | N8 | -Fe1 | -N9 | 73.88(16) |
| N2 | -Zn1 | -N7 | 95.46(16) | N2 | -N1 | -C1 | 110.4(4) |
| N2 | -Zn1 | -N8 | 103.48(16) | Fe1 | -N2 | -N1 | 139.6(3) |
| N2 | -Zn1 | -N9 | 93.95(16) | Fe1 | -N2 | -C3 | 115.3(3) |
| N3 | -Zn1 | -N4 | 74.18(16) | Zn1 | -N2 | -N1 | 139.6(3) |
| N3 | -Zn1 | -N7 | 105.13(16) | Zn1 | -N2 | -C3 | 115.3(3) |
| N3 | -Zn1 | -N8 | 177.52(17) | N1 | -N2 | -C3 | 105.1(4) |
| N3 | -Zn1 | -N9 | 106.63(16) | Fe1 | -N3 | -C4 | 120.4(3) |
| N4 | -Zn1 | -N7 | 94.41(16) | Fe1 | -N3 | -C8 | 120.1(3) |
| N4 | -Zn1 | -N8 | 108.25(16) | Zn1 | -N3 | -C4 | 120.4(3) |
| N4 | -Zn1 | -N9 | 93.35(16) | Zn1 | -N3 | -C8 | 120.1(3) |
| N7 | -Zn1 | -N8 | 74.43(16) | C4 | -N3 | -C8 | 119.5(4) |
| N7 | -Zn1 | -N9 | 148.23(15) | Fe1 | -N4 | -N5 | 138.9(4) |
| N8 | -Zn1 | -N9 | 73.88(16) | Fe1 | -N4 | -C9 | 115.2(3) |
| N2 | -Fe1 | -N3 | 74.10(16) | Zn1 | -N4 | -N5 | 138.9(4) |
| N2 | -Fe1 | -N4 | 148.24(15) | Zn1 | -N4 | -C9 | 115.2(3) |
| N2 | -Fe1 | -N7 | 95.46(16) | N5 | -N4 | -C9 | 105.8(4) |
| N2 | -Fe1 | -N8 | 103.48(16) | N4 | -N5 | -C11 | 110.7(5) |
| N2 | -Fe1 | -N9 | 93.95(16) | N7 | -N6 | -C12 | 110.8(4) |
| N3 | -Fe1 | -N4 | 74.18(16) | Fe1 | -N7 | -N6 | 139.0(3) |
| N3 | -Fe1 | -N7 | 105.13(16) | Fe1 | -N7 | -C14 | 115.9(4) |
| N3 | -Fe1 | -N8 | 177.52(17) | Zn1 | -N7 | -N6 | 139.0(3) |
| N3 | -Fe1 | -N9 | 106.63(16) | Zn1 | -N7 | -C14 | 115.9(4) |
| N4 | -Fe1 | -N7 | 94.41(16) | N6 | -N7 | -C14 | 105.0(4) |
| N4 | -Fe1 | -N8 | 108.25(16) | Fe1 | -N8 | -C15 | 119.0(4) |
| N4 | -Fe1 | -N9 | 93.35(16) | Fe1 | -N8 | -C19 | 120.1(4) |
| N7 | -Fe1 | -N8 | 74.43(16) | Zn1 | -N8 | -C15 | 119.0(4) |

Table S6 - Bond Angles (Degrees) (continued)
for: bpp in P -1

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Zn1 | -N8 | -C19 | 120.1(4) | N3 | -C8 | -C7 | 121.1(5) |
| C15 | -N8 | -C19 | 120.9(5) | N3 | -C8 | -C9 | 113.2(5) |
| Fe1 | -N9 | -N10 | 138.6(4) | N4 | -C9 | -C10 | 110.2(5) |
| Fe1 | -N9 | -C20 | 115.7(3) | C8 | -C9 | -C10 | 132.6(5) |
| Zn1 | -N9 | -N10 | 138.6(4) | N4 | -C9 | -C8 | 117.2(5) |
| Zn1 | -N9 | -C20 | 115.7(3) | C9 | -C10 | -C11 | 104.6(5) |
| N10 | -N9 | -C20 | 105.7(4) | N5 | -C11 | -C10 | 108.6(6) |
| N9 | -N10 | -C22 | 111.0(5) | N6 | -C12 | -C13 | 108.9(6) |
| N2 | -N1 | -H1N | 125.00 | C12 | -C13 | -C14 | 104.1(5) |
| C1 | -N1 | -H1N | 125.00 | N7 | -C14 | -C13 | 111.2(5) |
| N4 | -N5 | -H5N | 125.00 | N7 | -C14 | -C15 | 116.1(5) |
| C11 | -N5 | -H5N | 125.00 | C13 | -C14 | -C15 | 132.7(6) |
| N7 | -N6 | -H6N | 125.00 | N8 | -C15 | -C14 | 114.5(5) |
| C12 | -N6 | -H6N | 125.00 | N8 | -C15 | -C16 | 120.3(5) |
| N9 | -N10 | -H10N | 125.00 | C14 | -C15 | -C16 | 125.2(6) |
| C22 | -N10 | -H10N | 124.00 | C15 | -C16 | -C17 | 118.7(6) |
| N1 | -C1 | -C2 | 108.7(5) | C16 | -C17 | -C18 | 120.4(6) |
| C1 | -C2 | -C3 | 104.8(5) | C17 | -C18 | -C19 | 118.7(6) |
| N2 | -C3 | -C2 | 111.0(5) | N8 | -C19 | -C20 | 113.6(5) |
| N2 | -C3 | -C4 | 116.2(5) | C18 | -C19 | -C20 | 125.3(5) |
| C2 | -C3 | -C4 | 132.8(5) | N8 | -C19 | -C18 | 121.1(5) |
| N3 | -C4 | -C3 | 113.9(5) | N9 | -C20 | -C19 | 116.5(5) |
| N3 | -C4 | -C5 | 122.0(5) | N9 | -C20 | -C21 | 110.2(5) |
| C3 | -C4 | -C5 | 124.1(5) | C19 | -C20 | -C21 | 133.2(6) |
| C4 | -C5 | -C6 | 118.0(5) | C20 | -C21 | -C22 | 104.9(6) |
| C5 | -C6 | -C7 | 120.4(6) | N10 | -C22 | -C21 | 108.2(6) |
| C6 | -C7 | -C8 | 119.0(5) | N1 | -C1 | -H1 | 126.00 |
| C7 | -C8 | -C9 | 125.7(5) | C2 | -C1 | -H1 | 126.00 |

Table S6 - Bond Angles (Degrees) (continued)
for: bpp in P -1

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C1 | -C2 | -H2 | 128.00 | C12 | -C13 | -H13 | 128.00 |
| C3 | -C2 | -H2 | 128.00 | C14 | -C13 | -H13 | 128.00 |
| C4 | -C5 | -H5 | 121.00 | C15 | -C16 | -H16 | 121.00 |
| C6 | -C5 | -H5 | 121.00 | C17 | -C16 | -H16 | 121.00 |
| C5 | -C6 | -H6 | 120.00 | C16 | -C17 | -H17 | 120.00 |
| C7 | -C6 | -H6 | 120.00 | C18 | -C17 | -H17 | 120.00 |
| C6 | -C7 | -H7 | 120.00 | C17 | -C18 | -H18 | 121.00 |
| C8 | -C7 | -H7 | 121.00 | C19 | -C18 | -H18 | 121.00 |
| C9 | -C10 | -H10 | 128.00 | C20 | -C21 | -H21 | 128.00 |
| C11 | -C10 | -H10 | 128.00 | C22 | -C21 | -H21 | 128.00 |
| N5 | -C11 | -H11 | 126.00 | N10 | -C22 | -H22 | 126.00 |
| C10 | -C11 | -H11 | 126.00 | C21 | -C22 | -H22 | 126.00 |
| N6 | -C12 | -H12 | 126.00 | Se1 | -C23 | -N11 | 177.4(6) |
| C13 | -C12 | -H12 | 126.00 | Se2 | -C24 | -N12 | 178.1(6) |

Table S7 - Torsion Angles (Degrees)
for: bpp in P -1

| | | | | |
|---|---|---|---|---|
| N3 | -Fe1 | -N2 | -N1 | -178.4(5) |
| N3 | -Fe1 | -N2 | -C3 | 1.9(3) |
| N4 | -Fe1 | -N2 | -N1 | -175.1(4) |
| N4 | -Fe1 | -N2 | -C3 | 5.2(5) |
| N7 | -Fe1 | -N2 | -N1 | 77.4(5) |
| N7 | -Fe1 | -N2 | -C3 | -102.3(4) |
| N8 | -Fe1 | -N2 | -N1 | 2.2(5) |
| N8 | -Fe1 | -N2 | -C3 | -177.5(3) |
| N9 | -Fe1 | -N2 | -N1 | -72.2(5) |
| N9 | -Fe1 | -N2 | -C3 | 108.1(4) |
| N2 | -Fe1 | -N3 | -C4 | -2.8(4) |
| N2 | -Fe1 | -N3 | -C8 | 179.7(4) |
| N4 | -Fe1 | -N3 | -C4 | 179.0(4) |
| N4 | -Fe1 | -N3 | -C8 | 1.5(4) |
| N7 | -Fe1 | -N3 | -C4 | 88.6(4) |
| N7 | -Fe1 | -N3 | -C8 | -88.8(4) |
| N9 | -Fe1 | -N3 | -C4 | -92.2(4) |
| N9 | -Fe1 | -N3 | -C8 | 90.3(4) |
| N2 | -Fe1 | -N4 | -N5 | 172.7(5) |
| N2 | -Fe1 | -N4 | -C9 | -2.5(5) |
| N3 | -Fe1 | -N4 | -N5 | 176.0(6) |
| N3 | -Fe1 | -N4 | -C9 | 0.9(3) |
| N7 | -Fe1 | -N4 | -N5 | -79.5(5) |
| N7 | -Fe1 | -N4 | -C9 | 105.4(4) |
| N8 | -Fe1 | -N4 | -N5 | -4.4(6) |
| N8 | -Fe1 | -N4 | -C9 | -179.6(3) |
| N9 | -Fe1 | -N4 | -N5 | 69.7(5) |
| N9 | -Fe1 | -N4 | -C9 | -105.5(4) |

Table S7 - Torsion Angles (Degrees) (continued)
for: bpp in P -1

| | | | | |
|---|---|---|---|---|
| N2 | -Fe1 | -N7 | -N6 | 81.9(5) |
| N2 | -Fe1 | -N7 | -C14 | -103.9(4) |
| N3 | -Fe1 | -N7 | -N6 | 7.0(5) |
| N3 | -Fe1 | -N7 | -C14 | -178.8(4) |
| N4 | -Fe1 | -N7 | -N6 | -67.8(5) |
| N4 | -Fe1 | -N7 | -C14 | 106.4(4) |
| N8 | -Fe1 | -N7 | -N6 | -175.6(5) |
| N8 | -Fe1 | -N7 | -C14 | -1.4(4) |
| N9 | -Fe1 | -N7 | -N6 | -171.5(4) |
| N9 | -Fe1 | -N7 | -C14 | 2.7(6) |
| N2 | -Fe1 | -N8 | -C15 | 90.3(4) |
| N2 | -Fe1 | -N8 | -C19 | -87.4(4) |
| N4 | -Fe1 | -N8 | -C15 | -91.2(4) |
| N4 | -Fe1 | -N8 | -C19 | 91.1(4) |
| N7 | -Fe1 | -N8 | -C15 | -1.7(4) |
| N7 | -Fe1 | -N8 | -C19 | -179.4(4) |
| N9 | -Fe1 | -N8 | -C15 | -179.4(4) |
| N9 | -Fe1 | -N8 | -C19 | 2.9(4) |
| N2 | -Fe1 | -N9 | -N10 | -79.7(5) |
| N2 | -Fe1 | -N9 | -C20 | 100.4(4) |
| N3 | -Fe1 | -N9 | -N10 | -5.1(5) |
| N3 | -Fe1 | -N9 | -C20 | 175.0(4) |
| N4 | -Fe1 | -N9 | -N10 | 69.4(5) |
| N4 | -Fe1 | -N9 | -C20 | -110.6(4) |
| N7 | -Fe1 | -N9 | -N10 | 173.3(4) |
| N7 | -Fe1 | -N9 | -C20 | -6.6(5) |
| N8 | -Fe1 | -N9 | -N10 | 177.4(5) |
| N8 | -Fe1 | -N9 | -C20 | -2.5(4) |

Table S7 - Torsion Angles (Degrees) (continued)
for: bpp in P -1

| | | | | |
|---|---|---|---|---|
| C1 | -N1 | -N2 | -Fe1 | -179.8(4) |
| C1 | -N1 | -N2 | -C3 | 0.0(6) |
| N2 | -N1 | -C1 | -C2 | 0.1(6) |
| Fe1 | -N2 | -C3 | -C2 | 179.8(4) |
| Fe1 | -N2 | -C3 | -C4 | -1.0(6) |
| N1 | -N2 | -C3 | -C2 | 0.0(6) |
| N1 | -N2 | -C3 | -C4 | 179.2(4) |
| Fe1 | -N3 | -C4 | -C3 | 3.2(6) |
| Fe1 | -N3 | -C4 | -C5 | -176.9(4) |
| C8 | -N3 | -C4 | -C3 | -179.3(4) |
| C8 | -N3 | -C4 | -C5 | 0.6(8) |
| Fe1 | -N3 | -C8 | -C7 | 176.2(4) |
| Fe1 | -N3 | -C8 | -C9 | -3.5(6) |
| C4 | -N3 | -C8 | -C7 | -1.2(8) |
| C4 | -N3 | -C8 | -C9 | 179.1(4) |
| Fe1 | -N4 | -N5 | -C11 | -176.4(4) |
| C9 | -N4 | -N5 | -C11 | -1.0(6) |
| Fe1 | -N4 | -C9 | -C8 | -3.0(6) |
| Fe1 | -N4 | -C9 | -C10 | 176.9(4) |
| N5 | -N4 | -C9 | -C8 | -179.7(4) |
| N5 | -N4 | -C9 | -C10 | 0.2(6) |
| N4 | -N5 | -C11 | -C10 | 1.4(7) |
| C12 | -N6 | -N7 | -Fe1 | 175.0(4) |
| C12 | -N6 | -N7 | -C14 | 0.4(6) |
| N7 | -N6 | -C12 | -C13 | 0.1(7) |
| Fe1 | -N7 | -C14 | -C13 | -176.8(4) |
| Fe1 | -N7 | -C14 | -C15 | 4.0(6) |
| N6 | -N7 | -C14 | -C13 | -0.7(6) |

Table S7 - Torsion Angles (Degrees) (continued)
for: bpp in P -1

| | | | | |
|---|---|---|---|---|
| N6 | -N7 | -C14 | -C15 | -180.0(5) |
| Fe1 | -N8 | -C15 | -C14 | 4.2(6) |
| Fe1 | -N8 | -C15 | -C16 | -177.9(4) |
| C19 | -N8 | -C15 | -C14 | -178.1(5) |
| C19 | -N8 | -C15 | -C16 | -0.2(8) |
| Fe1 | -N8 | -C19 | -C18 | 177.8(4) |
| Fe1 | -N8 | -C19 | -C20 | -2.7(6) |
| C15 | -N8 | -C19 | -C18 | 0.2(8) |
| C15 | -N8 | -C19 | -C20 | 179.6(5) |
| Fe1 | -N9 | -N10 | -C22 | 179.9(4) |
| C20 | -N9 | -N10 | -C22 | -0.2(6) |
| Fe1 | -N9 | -C20 | -C19 | 2.0(6) |
| Fe1 | -N9 | -C20 | -C21 | 179.6(4) |
| N10 | -N9 | -C20 | -C19 | -177.9(4) |
| N10 | -N9 | -C20 | -C21 | -0.4(6) |
| N9 | -N10 | -C22 | -C21 | 0.7(6) |
| N1 | -C1 | -C2 | -C3 | -0.1(6) |
| C1 | -C2 | -C3 | -N2 | 0.1(6) |
| C1 | -C2 | -C3 | -C4 | -179.0(6) |
| N2 | -C3 | -C4 | -N3 | -1.3(7) |
| N2 | -C3 | -C4 | -C5 | 178.8(5) |
| C2 | -C3 | -C4 | -N3 | 177.7(6) |
| C2 | -C3 | -C4 | -C5 | -2.2(9) |
| N3 | -C4 | -C5 | -C6 | 0.6(8) |
| C3 | -C4 | -C5 | -C6 | -179.5(5) |
| C4 | -C5 | -C6 | -C7 | -1.2(9) |
| C5 | -C6 | -C7 | -C8 | 0.6(9) |
| C6 | -C7 | -C8 | -N3 | 0.7(8) |

Table S7 - Torsion Angles (Degrees) (continued)
for: bpp in P -1

| | | | | |
|---|---|---|---|---|
| C6 | -C7 | -C8 | -C9 | -179.7(6) |
| N3 | -C8 | -C9 | -N4 | 4.2(7) |
| N3 | -C8 | -C9 | -C10 | -175.6(6) |
| C7 | -C8 | -C9 | -N4 | -175.5(5) |
| C7 | -C8 | -C9 | -C10 | 4.7(10) |
| N4 | -C9 | -C10 | -C11 | 0.7(7) |
| C8 | -C9 | -C10 | -C11 | -179.5(6) |
| C9 | -C10 | -C11 | -N5 | -1.2(7) |
| N6 | -C12 | -C13 | -C14 | -0.5(7) |
| C12 | -C13 | -C14 | -N7 | 0.8(7) |
| C12 | -C13 | -C14 | -C15 | 179.9(6) |
| N7 | -C14 | -C15 | -N8 | -5.3(7) |
| N7 | -C14 | -C15 | -C16 | 176.9(6) |
| C13 | -C14 | -C15 | -N8 | 175.6(6) |
| C13 | -C14 | -C15 | -C16 | -2.2(10) |
| N8 | -C15 | -C16 | -C17 | 1.2(9) |
| C14 | -C15 | -C16 | -C17 | 178.8(6) |
| C15 | -C16 | -C17 | -C18 | -2.1(10) |
| C16 | -C17 | -C18 | -C19 | 2.0(10) |
| C17 | -C18 | -C19 | -N8 | -1.1(9) |
| C17 | -C18 | -C19 | -C20 | 179.6(6) |
| N8 | -C19 | -C20 | -N9 | 0.3(7) |
| N8 | -C19 | -C20 | -C21 | -176.5(6) |
| C18 | -C19 | -C20 | -N9 | 179.8(5) |
| C18 | -C19 | -C20 | -C21 | 3.0(10) |
| N9 | -C20 | -C21 | -C22 | 0.8(6) |
| C19 | -C20 | -C21 | -C22 | 177.8(6) |
| C20 | -C21 | -C22 | -N10 | -0.9(7) |

Table S8 - Contact Distances(Angstrom)
for: bpp in P -1

| | | | | | |
|---|---|---|---|---|---|
| Se1 | .N5_a | 3.394(6) | N6 | .N12 | 2.816(7) |
| Se1 | .C18_n | 3.785(7) | N6 | .C22_b | 3.358(7) |
| Se2 | .N10_b | 3.359(6) | N7 | .N2 | 3.246(6) |
| Se2 | .C5_p | 3.700(6) | N7 | .N8 | 2.600(6) |
| Se1 | .H16_o | 3.2500 | N7 | .N4 | 3.212(6) |
| Se1 | .H18_n | 3.2100 | N7 | .C15 | 2.367(7) |
| Se1 | .H5N_a | 2.5500 | N8 | .C20 | 2.329(7) |
| Se1 | .H13_o | 3.2400 | N8 | .N9 | 2.582(6) |
| Se1 | .H12_m | 3.3000 | N8 | .C14 | 2.353(7) |
| Se2 | .H7_q | 3.0100 | N8 | .N7 | 2.600(6) |
| Se2 | .H10N_b | 2.5000 | N9 | .N8 | 2.582(6) |
| Se2 | .H5_p | 3.0600 | N9 | .N4 | 3.183(6) |
| N1 | .C11_a | 3.424(8) | N9 | .C19 | 2.372(7) |
| N1 | .N11 | 2.792(7) | N9 | .N2 | 3.206(6) |
| N2 | .N9 | 3.206(6) | N10 | .Se2_f | 3.359(6) |
| N2 | .C4 | 2.385(7) | N10 | .C24_f | 3.318(8) |
| N2 | .N7 | 3.246(6) | N11 | .N1 | 2.792(7) |
| N2 | .N3 | 2.597(6) | N12 | .N6 | 2.816(7) |
| N3 | .N2 | 2.597(6) | N1 | .H22_b | 2.5500 |
| N3 | .C9 | 2.336(7) | N2 | .H22_b | 2.7600 |
| N3 | .N4 | 2.594(6) | N5 | .H12_d | 2.9100 |
| N3 | .C3 | 2.345(7) | N6 | .H1_e | 2.9200 |
| N4 | .N3 | 2.594(6) | N9 | .H11_a | 2.9300 |
| N4 | .N9 | 3.183(6) | N10 | .H11_a | 2.5900 |
| N4 | .N7 | 3.212(6) | N11 | .H1N | 1.9400 |
| N4 | .C8 | 2.381(7) | N12 | .H6_q | 2.8700 |
| N5 | .Se1_c | 3.394(6) | N12 | .H6N | 1.9700 |
| N5 | .C23_c | 3.250(9) | N12 | .H1_e | 2.7500 |

Table S8 - Contact Distances(Angstrom) (continued)
for: bpp in P -1

| | | | | | |
|---|---|---|---|---|---|
| C1 | .C10_a | 3.440(8) | C23 | .H1N | 2.8400 |
| C1 | .C9_a | 3.489(8) | C24 | .H10N_b | 2.6600 |
| C5 | .Se2_g | 3.700(6) | C24 | .H7_q | 3.0500 |
| C9 | .C1_e | 3.489(8) | C24 | .H6N | 2.8000 |
| C10 | .C1_e | 3.440(8) | H1 | .H6N_a | 2.4700 |
| C11 | .N1_e | 3.424(8) | H1 | .N12_j | 2.7500 |
| C12 | .C21_b | 3.539(8) | H1 | .N6_a | 2.9200 |
| C13 | .C21_b | 3.534(9) | H1N | .C23 | 2.8400 |
| C16 | .C23_h | 3.528(9) | H1N | .N11 | 1.9400 |
| C18 | .Se1_i | 3.785(7) | H5 | .C2 | 2.9600 |
| C18 | .C23 | 3.554(10) | H5 | .Se2_g | 3.0600 |
| C19 | .C23 | 3.598(9) | H5N | .C23_c | 2.6600 |
| C21 | .C13_d | 3.534(9) | H5N | .H12_d | 2.4800 |
| C21 | .C12_d | 3.539(8) | H5N | .Se1_c | 2.5500 |
| C22 | .N6_d | 3.358(7) | H6 | .N12_k | 2.8700 |
| C23 | .C16_o | 3.528(9) | H6N | .N12 | 1.9700 |
| C23 | .N5_a | 3.250(9) | H6N | .C24 | 2.8000 |
| C23 | .C18 | 3.554(10) | H6N | .H1_e | 2.4700 |
| C23 | .C19 | 3.598(9) | H7 | .C24_k | 3.0500 |
| C24 | .N10_b | 3.318(8) | H7 | .Se2_k | 3.0100 |
| C1 | .H22_b | 2.9000 | H7 | .C10 | 2.9800 |
| C2 | .H5 | 2.9600 | H10N | .Se2_f | 2.5000 |
| C10 | .H7 | 2.9800 | H10N | .C24_f | 2.6600 |
| C13 | .H16 | 2.9800 | H11 | .N9_e | 2.9300 |
| C21 | .H18 | 2.9900 | H11 | .N10_e | 2.5900 |
| C22 | .H11_a | 2.7700 | H11 | .C22_e | 2.7700 |
| C23 | .H16_o | 2.7500 | H12 | .N5_b | 2.9100 |
| C23 | .H5N_a | 2.6600 | H12 | .H5N_b | 2.4800 |

Table S8 - Contact Distances(Angstrom) (continued)
for: bpp in P -1

| | | | | | |
|---|---|---|---|---|---|
| H12 | .Se1_l | 3.3000 | H18 | .Se1_i | 3.2100 |
| H13 | .Se1_h | 3.2400 | H18 | .C21 | 2.9900 |
| H16 | .C13 | 2.9800 | H22 | .C1_d | 2.9000 |
| H16 | .Se1_h | 3.2500 | H22 | .N2_d | 2.7600 |
| H16 | .C23_h | 2.7500 | H22 | .N1_d | 2.5500 |

Table S9 - Hydrogen Bonds (Angstrom, Deg)
for: bpp in P -1

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| N1 | -- H1N | .. N11 | 0.8600 | 1.9400 | 2.792(7) | 171.00 | . |
| N5 | -- H5N | .. Se1 | 0.8600 | 2.5500 | 3.394(6) | 167.00 | 1_545 |
| N6 | -- H6N | .. N12 | 0.8600 | 1.9700 | 2.816(7) | 168.00 | . |
| N10 | -- H10N | .. Se2 | 0.8600 | 2.5000 | 3.359(6) | 175.00 | 1_655 |
| C11 | -- H11 | .. N10 | 0.9300 | 2.5900 | 3.503(8) | 166.00 | 1_545 |
| C22 | -- H22 | .. N1 | 0.9300 | 2.5500 | 3.458(7) | 167.00 | 1_655 |

Translation of Symmetry Code to Equiv.Pos

a =[ 1565.00 ] = x,1+y,z
b =[ 1455.00 ] = -1+x,y,z
c =[ 1545.00 ] = x,-1+y,z
d =[ 1655.00 ] = 1+x,y,z
g =[ 2665.00 ] = 1-x,1-y,-z
h =[ 2666.00 ] = 1-x,1-y,1-z
i =[ 2766.00 ] = 2-x,1-y,1-z
j =[ 1565.00 ] = x,1+y,z
k =[ 2655.00 ] = 1-x,-y,-z
l =[ 1445.00 ] = -1+x,-1+y,z
m =[ 1665.00 ] = 1+x,1+y,z
n =[ 2766.00 ] = 2-x,1-y,1-z
o =[ 2666.00 ] = 1-x,1-y,1-z
p =[ 2665.00 ] = 1-x,1-y,-z
q =[ 2655.00 ] = 1-x,-y,-z