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Synthesis, Structure and Hirshfeld Surface Analysis of a New Iron Complex [Fe(N4Py)(tenspr)] (tenspr)

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Abstract

We report the synthesis, crystal structure and Hirshfeld surface analysis of Fe(II) complex based on a pentadentate N4Py (N4Py = N,N-bis(2-pyridylmethyl)-N-(bis-2-pyridylmethyl)amine) and polynitrile tenspr (1,1,3,3-tetracyano-2-thioethylpropenide) ligands, [Fe(N4Py)(tenspr)](tenspr) (**I**). The X-ray result, indicates that (**I**) is low-spin Fe(II) complex. The tenspr molecule in the complex exhibits disorder over two sets of atomic sites having occupancies of 0.681 (6) and 0.319 (6). The crystal packing of (**I**) is established by weak intermolecular C-H...N/S hydrogen bond, C-N... π and stacking interactions. Hirshfeld surface analysis employing three-dimensional molecular surface contours and enrichment ratio calculations have been used to understand the intermolecular interactions present in the structure.

Keywords

Crystal structure, Polynitrile anion, Disorder, Hydrogen bonding, π -stacking interactions, Supramolecular assembly, Hirshfeld surface analysis.

Introduction

As a consequence of their ability to link metal ions in a variety of different ways, organic polynitrile anions, either functioning alone or in combination with neutral co-ligands, provide opportunities for the generation of molecular architectures with varying dimensions and topologies [1-7]. The presence of other potential donor groups such as those derived from –OH, –SH or –NH₂, together with their rigidity and electronic delocalization, mean that polynitrile anions can also lead to new magnetic and luminescent coordination polymers based on transition-metal ions [8-12]. Furthermore, the use of polynitrile anions for the synthesis of interesting discrete and polymeric bistable materials has been described [13-16]. It was during the course of attempts to prepare such complexes with N,N-bis(2-pyridylmethyl)-N-bis(2-pyridyl)methylamine (N4Py) as a co-ligand that the title complex, **(I)**, was unexpectedly obtained. Herein, the crystal and molecular structure of **I** are described. A study complemented by an analysis of the molecular packing by calculating the Hirshfeld surfaces study.

EXPERIMENTAL

Synthesis

All chemical reagents and solvents are commercially available and were used without further purification. Compound **(I)** was prepared using a mixture of iron(II) sulfate heptahydrate (28 mg, 0.1 mmol), N4Py (37 mg, 0.1 mmol) and Ktenspr (48 mg, 0.2 mmol) in mixed solvents of water/methanol (3:1 v/v, 20 ml). The mixture was sealed in a Teflon-lined autoclave and held at 403 K for 3d, and then cooled to room temperature at a rate of 10 K per hour (yield 27%). Red prismatic crystals of **(I)** suitable for single-crystal X-ray diffraction analysis were selected.

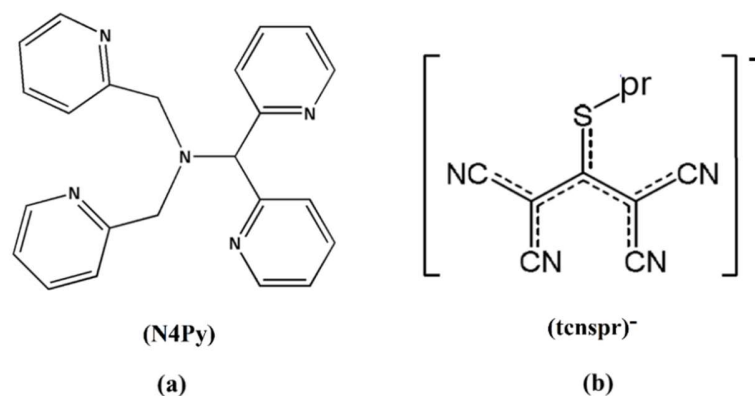


Figure 1. Schemes of (N4Py) (a) and (tcnspr) (b) molecules.

X-Ray Diffraction Analysis

Molecular and crystal structure of compound (**I**) was determined by single crystal X-ray diffraction technique. X-ray diffraction data collection was carried out on a STOE IPDS 2 [17] diffractometer with graphite monochromatized Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$). Semiempirical absorption correction was performed with SADABS [18]. Crystal structure was solved by direct method (SHELXS) [19] and refined by full matrix least squares techniques (SHELXL-2014/7) [20]. All non-hydrogen atoms were refined anisotropically. H atoms were located in difference-Fourier maps but introduced in calculated positions and treated as riding on their parent atoms, with C-H = 0.93 and 0.97 \AA with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The disordered (tcnspr) molecule was refined by splitting atoms over two positions (A and B parts) with occupancy factors of 0.681 (6) and 0.319 (6). Constraints EXYZ and EADP on bond lengths were applied. The structural diagrams were drawn with Diamond 3 [21]. Data collection and refinement parameters for the complex (**I**) are summarized in **Table 1**. CCDC 2042161 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif, or by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

RESULTS AND DISCUSSION

Crystal structure description

Complex (**I**) crystallizes in triclinic crystal system having space group $P-1$. The molecular structure of compound (**I**) is shown in **Fig. 2**. It contains one cation $[\text{Fe}(\text{N}_4\text{Py})(\text{tcnspr})]^+$ and one non-coordinated anion $(\text{tcnspr})^-$. The (tcnspr) molecule in the complex exhibits disorder over two sets of atomic sites with occupancies of 0.681 (6) and 0.319 (6), but the molecular conformations of the two disorder moieties are very similar and we comment in detail only on that of the major one (Solid bonds). The iron (II) center is six-coordinated by four N_{pyr} atoms and one tertiary nitrogen donor of N_4Py ligand, occupying the apical position. The sixth coordination site is occupied by (tcnspr) coordinated molecule. The four pyridine rings and (tcnspr) molecule are all positioned perpendicular to the basal plane of coordination (**Fig. 2**). The Fe-N ligand distances range from 1.957 (2) Å for Fe-N2 to 1.968 (2) Å for Fe-N4. The Fe-N6 bond of the polynitrile anion is the shorter than nitrogen atoms of N_4Py ligand (Table 2). Overall, the Fe-N bond lengths are comparable to those found for other low-spin iron(II) complexes [22-24]. The bond distances and angles within two different ligands are in good agreement with those observed in similar compounds [25,26].

The careful analysis of the shortest inter-molecular contacts (hydrogen bonding and π -stacking contacts) in (**I**) reveals that the moieties are linked together by weak $\text{C-H}\cdots\text{N}$ hydrogen bonds (Table 3) involving the carbons of tertiary amine and pyridine groups and the terminal nitrogen atoms from the adjacent (tcnspr) polynitrile anions, (**Figure 3b and d**). Another weak hydrogen bond $\text{C-H}\cdots\text{S}$ is also observed between C2 of amine groups and sulfur atom of adjacent coordinated (tcnspr) molecule within the cation (**Table 3**).

Furthermore, a remarkable supramolecular assembly is formed by means of a combination of common and uncommon π - π interactions, which is described by [27-29], where the donor π -system is a triple bond within the polynitrile anion $\pi(\text{C}\equiv\text{N})$. Thus, the polynitrile anions $(\text{tcnspr})^-$ chains are connected to each other through hydrogen bonds $\text{C-H}\cdots\text{N}$ (3.538 (2) Å) and by van der Waals contacts $\text{C-H}\cdots\pi$ (3.119 (2)-3.957 (3) Å), $\pi\cdots\pi$ (centroid-centroid distances = 4.210 (3) Å) and $\text{N}\cdots\pi$ interactions (3.389 (2) Å), see **Figure 3c**. The $[\text{Fe}(\text{N}_4\text{Py})(\text{tcnspr})]^+$ cations are interconnect to each other by weak $\text{C-H}\cdots\text{N}$ hydrogen bonding and by $\pi\cdots\pi$ interactions between coordinated (tcnspr) molecule (centroid-centroid distances \sim 4.3 (3) Å) (**Figure 2.d**).

There is also a single C-N... π (pyridine) interactions, with dimensions N12A...Cg4ⁱ ~ 3.1358(3)Å and N12B...Cg4ⁱ ~ 3.4836(3)Å, where Cg4 represents the centroid of the pyridine ring (N(5), C(19), C(20), C(21), C(22), C(23)) and the symmetry code i = (x, y, z) (**Figure 3b**). Such various intermolecular contacts lead to a supramolecular alternated chains oriented along the b axis (**Fig. 3a**).

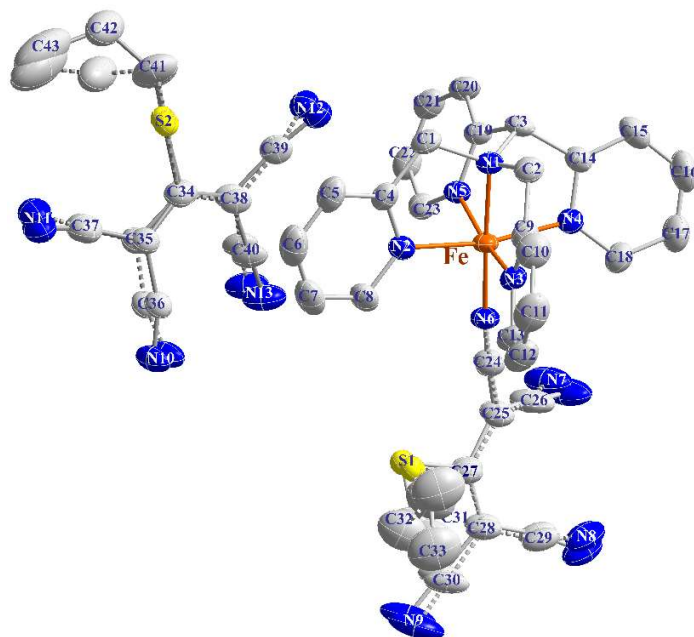


Figure 2. The molecular structure of (I), showing the atom-labelling scheme and the two disorder components, whose occupancies are 0.681(6) (solid bonds) and 0.319 (6) (broken bonds). Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms omitted for clarity.

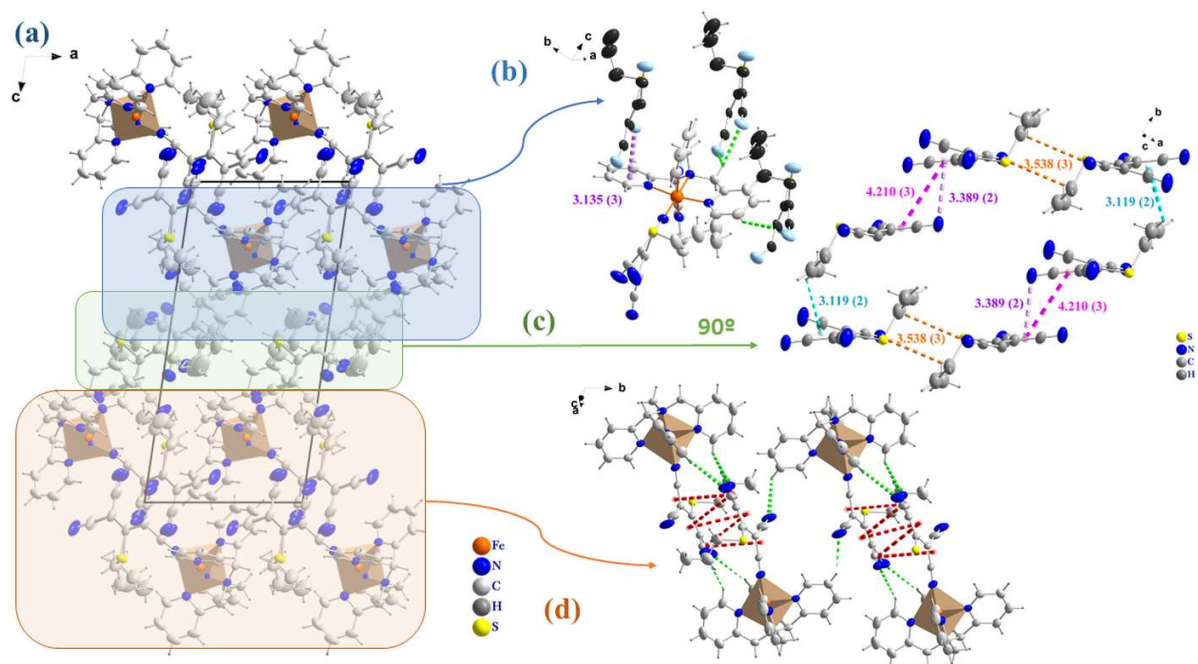


Figure 3: (a) View along b axis of the packing diagram, (b) Hydrogen bonding (green dashed line) and N... π (clear violet dashed line) interactions between $[\text{Fe}(\text{N}_4\text{Py})(\text{tcnspr})]^+$ cations and $(\text{tcnspr})^-$ anions, (c) A scheme of $(\text{tcnspr})^-$ anions formed by C-H...N hydrogen bonds (orange dashed line), C-H... π (Cyan dashed line), N... π (clear violet dashed line) and π ... π (pink dashed line) interactions, (d) A scheme of $[\text{Fe}(\text{N}_4\text{Py})(\text{tcnspr})]^+$ cations chains formed by C-H...N (green dashed line) and $\pi(\text{C}\equiv\text{N})\dots\pi(\text{C}\equiv\text{N})$ (red dashed line) interactions.

Table 1. Selected Single-Crystal Data and Structure Refinement Parameters for (I)

Empirical formula	C ₄₃ H ₃₅ FeN ₁₃ S ₂
Formula weight (g/mol)	853.81
Crystal system, space group	Triclinic, P-1
a (Å)	9.7573 (7)
b (Å)	11.3795 (9)
c (Å)	20.1483 (17)
α (°)	100.527 (7),
β (°)	96.823 (6),
γ (°)	97.529 (6)
V (Å ³)	2157.0 (3)
Z	2
μ (mm ⁻¹)	0.49
D _x (Mg m ⁻³)	1.315
F(000)	884
Crystal size (mm)	0.62 × 0.33 × 0.17
Crystal habit	Red Rod
θ _{min} / θ _{max} (deg)	1.8 / 26.6
Measured reflections	21644
Independent reflections	8910
Observed refl. with I > 2σ(I)	5964
R _{int}	0.033
Data/restraints/parameters	8910 / 62 / 625
R[F ² > 2σ(F ²)]	0.048
wR(F ²)	0.126
Goof=S	0.96
Δρ _{max} / Δρ _{min} (e.Å ⁻³)	0.60 / -0.29

Table 2: Selected bond lengths (Å) and angles (°) for (I)

Fe-N6B	1.907 (2)
Fe-N6A	1.907 (2)
Fe-N3	1.957 (2)
Fe-N5	1.958 (2)
Fe-N1	1.962 (2)
Fe-N2	1.967 (2)
Fe-N4	1.968 (2)
N6B-Fe-N3	97.32 (10)
N6A-Fe-N3	97.32 (10)
N6B-Fe-N5	94.24 (9)
N6A-Fe-N5	94.24 (9)
N3-Fe-N5	168.43 (9)
N6B-Fe-N1	175.79 (9)
N6A-Fe-N1	175.79 (9)
N3-Fe-N1	85.32 (9)
N5-Fe-N1	83.15 (8)
N6B-Fe-N2	98.64 (10)
N6A-Fe-N2	98.64 (10)
N3-Fe-N2	86.13 (9)
N5-Fe-N2	91.99 (9)
N1-Fe-N2	84.78 (9)
N6B-Fe-N4	93.93 (9)
N6A-Fe-N4	93.93 (9)
N3-Fe-N4	92.14 (9)
N5-Fe-N4	87.21 (9)
N1-Fe-N4	82.66 (9)
N2-Fe-N4	167.42 (9)

Table 3: Hydrogen-bond geometry in (I)

D-H...A	D-H	H...A/ Å	D...A/ Å	D-H...A/°
C1-H1A...N12A	0.97	2.59	3.37 (3)	137
C1-H1B...N10A ⁱ	0.97	2.70	3.64 (3)	163
C1-H1B...N10B ⁱ	0.97	2.59	3.52 (4)	162
C7-H7...N11A ⁱⁱ	0.93	2.50	3.30 (3)	145
C2-H2A...N10A ⁱ	0.97	2.69	3.626 (15)	162
C2-H2A...N10B ⁱ	0.97	2.44	3.39 (2)	168
C2-H2B...S1A ⁱ	0.97	3.02	3.745 (5)	133
C10-H10...N11A ⁱⁱⁱ	0.93	2.53	3.43 (6)	162
C10-H10...N11B ⁱⁱⁱ	0.93	2.50	3.37 (9)	155
C13-H13...N6A	0.93	2.69	3.156 (4)	112
C3-H3...N13B ⁱ	0.98	2.54	3.367 (16)	143
C15-H15...N7A ^{iv}	0.93	2.69	3.561 (12)	157
C15-H15...N7B ^{iv}	0.93	2.64	3.47 (3)	150
C22-H22...N7A ^v	0.93	2.65	3.404 (18)	138

Symmetry codes: (i) x+1, y, z; (ii) -x, -y+1, -z+1; (iii) -x+1, -y+1, -z+1; (iv) -x+1, -y+1, -z; (v) -x, -y+1, -z.

Hirshfeld Surface analysis

Analysis of Hirshfeld surface represents a major analysis tool enabling supramolecular chemists and crystal engineers to gain insight into understanding the crystal packing. The Hirshfeld surfaces are constructed based on the atomic electron densities.

The MoProViewer software [30] was used to quantify and visualize all intermolecular contacts in the main conformation of the molecular structure and compute the enrichment of contact types. The enrichment ratio E_{XY} for a pair of chemical elements (X,Y) is defined as the ratio between the percentage of actual contacts in the crystal (C_{XY}) and that of equi-distributed contacts R_{XY} . An enrichment ratio larger or smaller than unity reveals that the contact type is over or under-represented, respectively [31].

The Hirshfeld surface was computed around the $[\text{Fe}(\text{N}_4\text{Py})(\text{tcnspr})]^+$ complex cation and (tcnspr)⁻ anion (Table 4). Hydrogen is the most abundant species on the surface, followed by carbon and nitrogen.

The surface is constituted a weak hydrogen bond donor (H-C) and three hydrogen bond acceptors of different strengths (C < S < N). The strongest N...H contacts are indeed the most enriched ($E_{\text{NH}}=1.7$) followed by S...H ($E_{\text{SH}}=1.7$) while the weakest H...C (H... π) are slightly disfavored in the crystal packing. The N...H and C...H hydrogen bonds are the most represented contacts in the crystal packing. Hydrophobic H...H and C...C self-contacts are the next well represented due to the abundance of these elements on the surface. Besides the H...N and H...S hydrogen bonds,

C...C represents the only significantly enriched contact at $E_{CC}=1.36$, due to interactions between the C-C \equiv N groups with the C₅N aromatic rings.

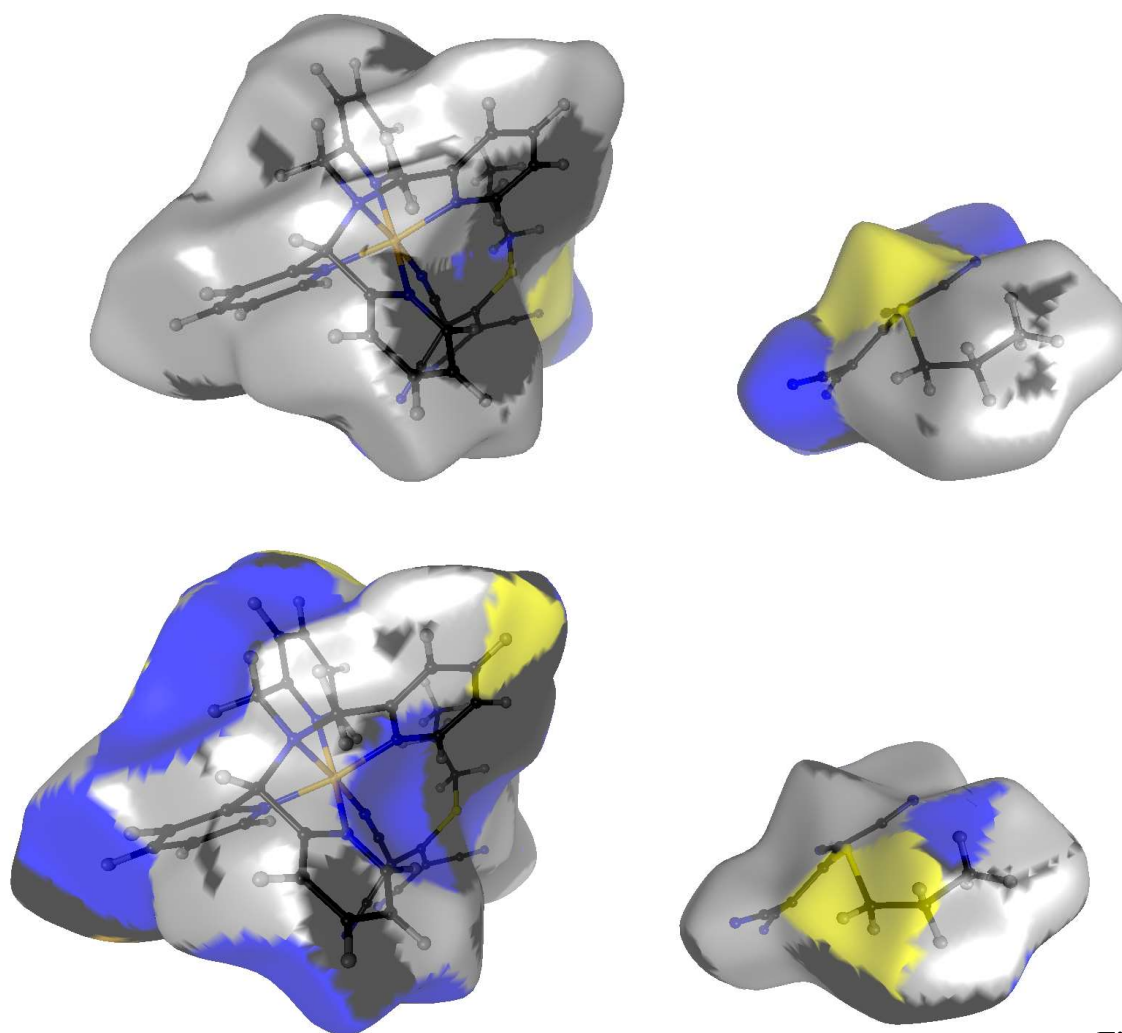


Figure 4. Hirshfeld surface around the $[\text{Fe}(\text{N}_4\text{Py})(\text{tenspr})]^+$ complex cation and $(\text{tenspr})^-$ anion. The surface is coloured according to the interior (a) and exterior (b) atom contributing most to the electron density. Carbon: dark grey; Hydrogen: grey; Sulphur: yellow; Nitrogen: blue.

Table 4: Hirshfeld contact surfaces and enrichment ratios for (I)

atom	C	N	S	H
surface%	29.6	19.7	4.3	46.2
C	12.0			
N	8.2	0.4		% contacts
S	2.9	0.2	0.0	
H	24.0	31.1	5.8	15.1
C	1.36			
N	0.68	0.10		enrichment
S	1.11	0.09	0.13	
H	0.89	1.70	1.42	0.73

Table 4. Chemical proportions on the Hirshfeld surface around the iron complex and the organic moiety in the crystal packing of the title compound. The actual contact C_{xy} by chemical types and their enrichment E_{xy} are then given. The major contacts and the most enriched are highlighted in bold.

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_exptl_transmission_factor_max  ?
_exptl_crystal_size_max        0.620
_exptl_crystal_size_mid        0.333
_exptl_crystal_size_min        0.170
_exptl_absorpt_coefficient_mu   0.494
_shelx_estimated_absorpt_T_min  0.749
_shelx_estimated_absorpt_T_max  0.921
_exptl_absorpt_correction_type  multi-scan
_exptl_absorpt_correction_T_min 0.796
_exptl_absorpt_correction_T_max 0.919
_exptl_absorpt_process_details  'SADABS (Sheldrick, 2003)'
_diffn_ambient_temperature      296(2)
_diffn_radiation_wavelength     0.71073
_diffn_radiation_type           MoK $\alpha$ 
_diffn_source
'fine focus sealed tube'
_diffn_measurement_device_type
'STOE IPDS 2'
_diffn_measurement_method       'rotation method'
_diffn_detector_area_resol_mean ?
_diffn_reflns_number            21644
_diffn_reflns_av_unetI/netI     0.0438
_diffn_reflns_av_R_equivalents  0.0332
_diffn_reflns_limit_h_min       -11
_diffn_reflns_limit_h_max       12
_diffn_reflns_limit_k_min       -14

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_diffrn_reflms_limit_k_max      14
_diffrn_reflms_limit_l_min     -25
_diffrn_reflms_limit_l_max      25
_diffrn_reflms_theta_min       1.843
_diffrn_reflms_theta_max       26.549
_diffrn_reflms_theta_full      25.242
_diffrn_measured_fraction_theta_max 0.990
_diffrn_measured_fraction_theta_full 0.993
_diffrn_reflms_Laue_measured_fraction_max 0.990
_diffrn_reflms_Laue_measured_fraction_full 0.993
_diffrn_reflms_point_group_measured_fraction_max 0.990
_diffrn_reflms_point_group_measured_fraction_full 0.993
_reflms_number_total           8910
_reflms_number_gt              5964
_reflms_threshold_expression    'I > 2\sigma(I)'
_reflms_Friedel_coverage       0.000
_reflms_Friedel_fraction_max   .
_reflms_Friedel_fraction_full  .

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```
_reflms_special_details
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Reflections were merged by SHELXL according to the crystal class for the calculation of statistics and refinement.

`_reflms_Friedel_fraction` is defined as the number of unique Friedel pairs measured divided by the number that would be possible theoretically, ignoring centric projections and systematic absences.

```
;
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_computing_data_collection    ?
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_computing_cell_refinement ?
 _computing_data_reduction ?
 _computing_structure_solution ?
 _computing_structure_refinement 'SHELXL-2014/7 (Sheldrick, 2014)'
 _computing_molecular_graphics ?
 _computing_publication_material ?
 _refine_special_details ?
 _refine_ls_structure_factor_coef Fsqd
 _refine_ls_matrix_type full
 _refine_ls_weighting_scheme calc
 _refine_ls_weighting_details
 'w=1/[s^2*(Fo^2)+(0.0727P)^2] where P=(Fo^2+2Fc^2)/3'
 _atom_sites_solution_primary ?
 _atom_sites_solution_secondary ?
 _atom_sites_solution_hydrogens geom
 _refine_ls_hydrogen_treatment constr
 _refine_ls_extinction_method none
 _refine_ls_extinction_coef .
 _refine_ls_number_reflns 8910
 _refine_ls_number_parameters 625
 _refine_ls_number_restraints 62
 _refine_ls_R_factor_all 0.0812
 _refine_ls_R_factor_gt 0.0482
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 _refine_ls_goodness_of_fit_ref 0.962
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 _refine_ls_shift/su_mean 0.000

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 Fe Fe 0.41487(4) 0.41810(3) 0.20229(2) 0.04771(12) Uani 1 1 d
 N1 N 0.5975(2) 0.50430(17) 0.24980(10) 0.0517(5) Uani 1 1 d
 C1 C 0.5796(3) 0.5817(2) 0.31517(13) 0.0622(7) Uani 1 1 d
 H1A H 0.5697 0.6625 0.3082 0.075 Uiso 1 1 calc R U . . .
 H1B H 0.6614 0.5879 0.3488 0.075 Uiso 1 1 calc R U . . .
 N2 N 0.3527(2) 0.45851(18) 0.29188(11) 0.0572(5) Uani 1 1 d
 C4 C 0.4527(3) 0.5280(2) 0.34050(13) 0.0599(7) Uani 1 1 d
 C5 C 0.4356(5) 0.5514(3) 0.40862(16) 0.0831(10) Uani 1 1 d
 H5 H 0.5066 0.5981 0.4414 0.100 Uiso 1 1 calc R U . . .
 C6 C 0.3126(6) 0.5050(4) 0.4271(2) 0.1037(14) Uani 1 1 d
 H6 H 0.2989 0.5201 0.4725 0.124 Uiso 1 1 calc R U . . .
 C7 C 0.2100(5) 0.4361(4) 0.3780(2) 0.1008(13) Uani 1 1 d
 H7 H 0.1255 0.4047 0.3898 0.121 Uiso 1 1 calc R U . . .
 C8 C 0.2327(4) 0.4134(3) 0.31091(18) 0.0773(9) Uani 1 1 d
 H8 H 0.1629 0.3656 0.2779 0.093 Uiso 1 1 calc R U . . .
 C2 C 0.6911(3) 0.4145(2) 0.26116(15) 0.0631(7) Uani 1 1 d

H2A H 0.7571 0.4461 0.3025 0.076 Uiso 1 1 calc R U . . .
H2B H 0.7435 0.3996 0.2233 0.076 Uiso 1 1 calc R U . . .
N3 N 0.4739(2) 0.27653(18) 0.23287(11) 0.0568(5) Uani 1 1 d
C9 C 0.6050(3) 0.2981(2) 0.26731(14) 0.0636(7) Uani 1 1 d
C10 C 0.6557(4) 0.2181(3) 0.30372(18) 0.0882(10) Uani 1 1 d
H10 H 0.7457 0.2353 0.3279 0.106 Uiso 1 1 calc R U . . .
C11 C 0.5699(6) 0.1115(3) 0.3035(2) 0.1035(14) Uani 1 1 d
H11 H 0.6017 0.0558 0.3278 0.124 Uiso 1 1 calc R U . . .
C12 C 0.4394(5) 0.0881(3) 0.2681(2) 0.0930(12) Uani 1 1 d
H12 H 0.3815 0.0161 0.2675 0.112 Uiso 1 1 calc R U . . .
C13 C 0.3931(4) 0.1711(2) 0.23304(16) 0.0748(9) Uani 1 1 d
H13 H 0.3033 0.1543 0.2087 0.090 Uiso 1 1 calc R U . . .
C3 C 0.6352(3) 0.5753(2) 0.19613(14) 0.0590(7) Uani 1 1 d
H3 H 0.7262 0.6275 0.2093 0.071 Uiso 1 1 calc R U . . .
N4 N 0.5174(2) 0.39486(19) 0.12367(11) 0.0552(5) Uani 1 1 d
C14 C 0.6283(3) 0.4829(3) 0.13189(14) 0.0597(7) Uani 1 1 d
C15 C 0.7184(4) 0.4852(4) 0.0841(2) 0.0851(10) Uani 1 1 d
H15 H 0.7942 0.5469 0.0903 0.102 Uiso 1 1 calc R U . . .
C16 C 0.6928(5) 0.3932(4) 0.0266(2) 0.1020(13) Uani 1 1 d
H16 H 0.7512 0.3930 -0.0067 0.122 Uiso 1 1 calc R U . . .
C17 C 0.5827(5) 0.3035(4) 0.01896(18) 0.0916(11) Uani 1 1 d
H17 H 0.5658 0.2409 -0.0192 0.110 Uiso 1 1 calc R U . . .
C18 C 0.4962(4) 0.3058(3) 0.06815(15) 0.0710(8) Uani 1 1 d
H18 H 0.4209 0.2439 0.0628 0.085 Uiso 1 1 calc R U . . .
N5 N 0.3915(2) 0.57706(18) 0.18252(10) 0.0510(5) Uani 1 1 d
C19 C 0.5165(3) 0.6449(2) 0.18421(13) 0.0556(6) Uani 1 1 d
C20 C 0.5281(4) 0.7607(2) 0.17154(15) 0.0681(8) Uani 1 1 d
H20 H 0.6154 0.8059 0.1731 0.082 Uiso 1 1 calc R U . . .
C21 C 0.4086(4) 0.8076(3) 0.15664(15) 0.0740(9) Uani 1 1 d
H21 H 0.4138 0.8848 0.1470 0.089 Uiso 1 1 calc R U . . .
C22 C 0.2816(4) 0.7402(3) 0.15607(15) 0.0711(8) Uani 1 1 d

H22 H 0.1997 0.7718 0.1469 0.085 Uiso 1 1 calc R U . . .
C23 C 0.2757(3) 0.6253(2) 0.16911(13) 0.0598(7) Uani 1 1 d
H23 H 0.1890 0.5798 0.1686 0.072 Uiso 1 1 calc R U . . .
C25A C 0.0186(7) 0.2447(11) 0.0661(3) 0.056(2) Uani 0.681(6) 1 d D . P A -1
C24A C 0.1379(10) 0.2991(10) 0.1134(5) 0.0536(19) Uani 0.681(6) 1 d D . P A -1
N6A N 0.2403(2) 0.33891(19) 0.15035(12) 0.0620(6) Uani 0.681(6) 1 d D . P A -1
C26A C 0.024(2) 0.262(3) -0.0014(6) 0.0866(18) Uani 0.681(6) 1 d D . P A -1
N7A N 0.030(2) 0.2797(11) -0.0556(4) 0.127(4) Uani 0.681(6) 1 d D . P A -1
C27A C -0.0903(10) 0.1694(12) 0.0848(3) 0.0598(11) Uani 0.681(6) 1 d D . P A -1
S1A S -0.0990(4) 0.1979(3) 0.1728(2) 0.0784(7) Uani 0.681(6) 1 d D . P A -1
C31A C -0.1238(13) 0.0478(7) 0.1935(6) 0.112(3) Uani 0.681(6) 1 d D . P A -1
H24 H -0.2005 0.0414 0.2198 0.134 Uiso 0.681(6) 1 calc R U P A -1
H25 H -0.1487 -0.0127 0.1516 0.134 Uiso 0.681(6) 1 calc R U P A -1
C32A C -0.0005(9) 0.0239(8) 0.2318(5) 0.145(3) Uani 0.681(6) 1 d D . P A -1
H26 H 0.0296 0.0886 0.2715 0.174 Uiso 0.681(6) 1 calc R U P A -1
H27 H 0.0738 0.0225 0.2038 0.174 Uiso 0.681(6) 1 calc R U P A -1
C33A C -0.0253(12) -0.0946(8) 0.2546(5) 0.165(4) Uani 0.681(6) 1 d D . P A -1
H28 H -0.1032 -0.0958 0.2796 0.248 Uiso 0.681(6) 1 calc R U P A -1
H29 H 0.0566 -0.1040 0.2834 0.248 Uiso 0.681(6) 1 calc R U P A -1
H30 H -0.0451 -0.1597 0.2155 0.248 Uiso 0.681(6) 1 calc R U P A -1
C28A C -0.1965(15) 0.0910(17) 0.0393(3) 0.067(2) Uani 0.681(6) 1 d D . P A -1
C30A C -0.3231(7) 0.0475(7) 0.0613(6) 0.085(2) Uani 0.681(6) 1 d D . P A -1
N9A N -0.4223(16) 0.010(2) 0.0800(19) 0.136(5) Uani 0.681(6) 1 d D . P A -1
C29A C -0.1893(15) 0.0534(10) -0.0310(4) 0.074(2) Uani 0.681(6) 1 d D . P A -1
N8A N -0.193(2) 0.007(2) -0.0875(5) 0.106(3) Uani 0.681(6) 1 d D . P A -1
C25B C 0.0249(17) 0.224(3) 0.0688(6) 0.056(2) Uani 0.319(6) 1 d D . P A -2
C24B C 0.142(2) 0.277(3) 0.1179(11) 0.0536(19) Uani 0.319(6) 1 d D . P A -2
N6B N 0.2403(2) 0.33891(19) 0.15035(12) 0.0620(6) Uani 0.319(6) 1 d D . P A -2
C26B C 0.021(4) 0.265(6) 0.0065(14) 0.0866(18) Uani 0.319(6) 1 d D . P A -2
N7B N 0.026(5) 0.316(3) -0.0380(10) 0.127(4) Uani 0.319(6) 1 d D . P A -2
C27B C -0.092(2) 0.158(3) 0.0877(5) 0.0598(11) Uani 0.319(6) 1 d D . P A -2

S1B S -0.0811(11) 0.1658(7) 0.1761(5) 0.0784(7) Uani 0.319(6) 1 d D . P A -2
C31B C -0.116(3) 0.0081(12) 0.1842(13) 0.112(3) Uani 0.319(6) 1 d D . P A -2
H31 H -0.2150 -0.0219 0.1709 0.134 Uiso 0.319(6) 1 calc R U P A -2
H32 H -0.0657 -0.0400 0.1535 0.134 Uiso 0.319(6) 1 calc R U P A -2
C32B C -0.0745(17) -0.0060(18) 0.2526(10) 0.145(3) Uani 0.319(6) 1 d D . P A -2
H33 H -0.1250 -0.0810 0.2596 0.174 Uiso 0.319(6) 1 calc R U P A -2
H34 H -0.0990 0.0601 0.2844 0.174 Uiso 0.319(6) 1 calc R U P A -2
C33B C 0.0797(18) -0.0076(18) 0.2669(11) 0.165(4) Uani 0.319(6) 1 d D . P A -2
H35 H 0.1295 0.0723 0.2701 0.248 Uiso 0.319(6) 1 calc R U P A -2
H36 H 0.1072 -0.0625 0.2306 0.248 Uiso 0.319(6) 1 calc R U P A -2
H37 H 0.1009 -0.0335 0.3092 0.248 Uiso 0.319(6) 1 calc R U P A -2
C28B C -0.195(3) 0.076(4) 0.0426(7) 0.067(2) Uani 0.319(6) 1 d D . P A -2
C30B C -0.3127(16) 0.019(2) 0.0664(14) 0.085(2) Uani 0.319(6) 1 d D . P A -2
N9B N -0.417(4) -0.021(6) 0.080(4) 0.136(5) Uani 0.319(6) 1 d D . P A -2
C29B C -0.183(3) 0.032(3) -0.0266(9) 0.074(2) Uani 0.319(6) 1 d D . P A -2
N8B N -0.163(6) 0.022(6) -0.0829(12) 0.106(3) Uani 0.319(6) 1 d D . P A -2
C35A C 0.066(3) 0.711(3) 0.4785(8) 0.065(4) Uani 0.574(7) 1 d D . P B -3
C37A C 0.049(5) 0.762(5) 0.5462(13) 0.0844(12) Uani 0.574(7) 1 d D . P B -3
N11A N 0.028(5) 0.784(4) 0.6022(12) 0.111(5) Uani 0.574(7) 1 d D . P B -3
C36A C -0.0337(15) 0.6063(14) 0.4477(11) 0.060(3) Uani 0.574(7) 1 d D . P B -3
N10A N -0.134(3) 0.532(2) 0.4344(7) 0.083(2) Uani 0.574(7) 1 d D . P B -3
C34A C 0.162(2) 0.770(3) 0.4445(6) 0.0633(8) Uani 0.574(7) 1 d D . P B -3
S2A S 0.2943(14) 0.8784(7) 0.4981(6) 0.0818(11) Uani 0.574(7) 1 d D . P B -3
C41A C 0.286(3) 1.0110(12) 0.4629(10) 0.134(5) Uani 0.574(7) 1 d D . P B -3
H38 H 0.3565 1.0163 0.4331 0.161 Uiso 0.574(7) 1 calc R U P B -3
H39 H 0.1955 1.0018 0.4350 0.161 Uiso 0.574(7) 1 calc R U P B -3
C42A C 0.3054(11) 1.1234(9) 0.5122(6) 0.145(3) Uani 0.574(7) 1 d D . P B -3
H40 H 0.2765 1.1856 0.4890 0.175 Uiso 0.574(7) 1 calc R U P B -3
H41 H 0.4045 1.1465 0.5290 0.175 Uiso 0.574(7) 1 calc R U P B -3
C43A C 0.226(4) 1.122(3) 0.5742(14) 0.232(8) Uani 0.574(7) 1 d D . P B -3
H42 H 0.1316 1.0837 0.5588 0.348 Uiso 0.574(7) 1 calc R U P B -3

H43 H 0.2274 1.2038 0.5976 0.348 Uiso 0.574(7) 1 calc R U P B -3
H44 H 0.2712 1.0785 0.6047 0.348 Uiso 0.574(7) 1 calc R U P B -3
C38A C 0.1620(12) 0.7547(11) 0.3740(5) 0.055(2) Uani 0.574(7) 1 d D . P B -3
C39A C 0.2844(13) 0.7914(17) 0.3468(7) 0.058(3) Uani 0.574(7) 1 d D . P B -3
N12A N 0.387(2) 0.807(2) 0.3224(9) 0.073(3) Uani 0.574(7) 1 d D . P B -3
C40A C 0.0582(14) 0.6639(7) 0.3267(6) 0.067(2) Uani 0.574(7) 1 d D . P B -3
N13A N -0.0260(16) 0.6097(8) 0.2838(8) 0.100(3) Uani 0.574(7) 1 d D . P B -3
C35B C 0.048(4) 0.725(4) 0.4804(11) 0.065(4) Uani 0.426(7) 1 d D . P B -4
C37B C 0.049(7) 0.765(7) 0.5515(18) 0.0844(12) Uani 0.426(7) 1 d D . P B -4
N11B N 0.043(8) 0.814(5) 0.6063(17) 0.111(5) Uani 0.426(7) 1 d D . P B -4
C36B C -0.060(2) 0.627(2) 0.4497(16) 0.060(3) Uani 0.426(7) 1 d D . P B -4
N10B N -0.123(4) 0.534(3) 0.4177(10) 0.083(2) Uani 0.426(7) 1 d D . P B -4
C34B C 0.158(3) 0.767(3) 0.4481(8) 0.0633(8) Uani 0.426(7) 1 d D . P B -4
S2B S 0.303(2) 0.8571(9) 0.5039(9) 0.0818(11) Uani 0.426(7) 1 d D . P B -4
C41B C 0.314(4) 0.9995(17) 0.4778(15) 0.134(5) Uani 0.426(7) 1 d D . P B -4
H45 H 0.4045 1.0469 0.4974 0.161 Uiso 0.426(7) 1 calc R U P B -4
H46 H 0.3094 0.9850 0.4285 0.161 Uiso 0.426(7) 1 calc R U P B -4
C42B C 0.2067(14) 1.0699(12) 0.4967(9) 0.145(3) Uani 0.426(7) 1 d D . P B -4
H47 H 0.1171 1.0257 0.4731 0.175 Uiso 0.426(7) 1 calc R U P B -4
H48 H 0.2225 1.1449 0.4805 0.175 Uiso 0.426(7) 1 calc R U P B -4
C43B C 0.197(7) 1.101(4) 0.5737(14) 0.232(8) Uani 0.426(7) 1 d D . P B -4
H49 H 0.2176 1.0344 0.5943 0.348 Uiso 0.426(7) 1 calc R U P B -4
H49A H 0.1043 1.1159 0.5799 0.348 Uiso 0.426(7) 1 calc R U P B -4
H49B H 0.2631 1.1719 0.5948 0.348 Uiso 0.426(7) 1 calc R U P B -4
C38B C 0.1753(16) 0.7306(16) 0.3796(7) 0.055(2) Uani 0.426(7) 1 d D . P B -4
C39B C 0.2998(18) 0.776(3) 0.3564(10) 0.058(3) Uani 0.426(7) 1 d D . P B -4
N12B N 0.395(3) 0.830(3) 0.3389(13) 0.073(3) Uani 0.426(7) 1 d D . P B -4
C40B C 0.0523(19) 0.7011(11) 0.3267(9) 0.067(2) Uani 0.426(7) 1 d D . P B -4
N13B N -0.043(2) 0.6562(12) 0.2877(12) 0.100(3) Uani 0.426(7) 1 d D . P B -4

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 N1 0.0477(12) 0.0509(11) 0.0520(12) 0.0110(9) -0.0011(9) -0.0020(9)
 C1 0.0663(18) 0.0575(14) 0.0519(15) 0.0037(12) -0.0100(13) -0.0022(13)
 N2 0.0595(14) 0.0530(11) 0.0604(13) 0.0166(10) 0.0130(11) 0.0028(10)
 C4 0.078(2) 0.0509(13) 0.0510(15) 0.0116(11) 0.0081(13) 0.0122(13)
 C5 0.124(3) 0.078(2) 0.0517(17) 0.0137(15) 0.0169(18) 0.028(2)
 C6 0.158(4) 0.097(3) 0.078(3) 0.033(2) 0.054(3) 0.045(3)
 C7 0.115(3) 0.095(3) 0.117(3) 0.048(3) 0.066(3) 0.025(2)
 C8 0.080(2) 0.0705(18) 0.088(2) 0.0247(16) 0.0356(18) 0.0032(16)
 C2 0.0551(17) 0.0676(16) 0.0610(16) 0.0105(13) -0.0061(13) 0.0061(13)
 N3 0.0679(15) 0.0488(11) 0.0491(12) 0.0066(9) 0.0053(10) 0.0000(10)
 C9 0.075(2) 0.0602(15) 0.0542(15) 0.0102(12) 0.0058(14) 0.0124(14)
 C10 0.104(3) 0.090(2) 0.078(2) 0.0336(18) -0.0004(19) 0.028(2)
 C11 0.160(5) 0.077(2) 0.090(3) 0.040(2) 0.023(3) 0.039(3)
 C12 0.145(4) 0.0556(17) 0.082(2) 0.0213(16) 0.026(2) 0.007(2)
 C13 0.101(3) 0.0493(14) 0.0697(19) 0.0113(13) 0.0153(17) -0.0067(15)
 C3 0.0438(15) 0.0617(15) 0.0662(16) 0.0168(13) 0.0017(12) -0.0111(12)
 N4 0.0538(13) 0.0599(12) 0.0493(12) 0.0106(10) 0.0028(10) 0.0045(10)
 C14 0.0502(16) 0.0716(16) 0.0591(16) 0.0201(13) 0.0095(12) 0.0046(12)
 C15 0.067(2) 0.106(3) 0.094(3) 0.039(2) 0.0302(19) 0.0129(18)
 C16 0.116(3) 0.133(3) 0.077(2) 0.034(2) 0.048(2) 0.045(3)
 C17 0.110(3) 0.106(3) 0.064(2) 0.0115(18) 0.025(2) 0.030(2)
 C18 0.081(2) 0.0733(18) 0.0550(16) 0.0050(14) 0.0027(15) 0.0149(15)
 N5 0.0474(13) 0.0529(11) 0.0479(11) 0.0096(9) -0.0007(9) -0.0025(9)

C19 0.0555(16) 0.0548(13) 0.0518(14) 0.0130(11) 0.0023(12) -0.0063(12)
C20 0.079(2) 0.0557(15) 0.0658(18) 0.0177(13) 0.0086(15) -0.0083(14)
C21 0.105(3) 0.0580(16) 0.0603(18) 0.0176(13) 0.0111(17) 0.0111(17)
C22 0.088(2) 0.0727(18) 0.0553(17) 0.0146(14) 0.0003(15) 0.0283(17)
C23 0.0568(17) 0.0667(16) 0.0528(15) 0.0088(12) 0.0027(12) 0.0069(13)
C25A 0.0434(16) 0.047(5) 0.0719(19) 0.0141(15) -0.0059(13) -0.003(2)
C24A 0.0507(17) 0.039(5) 0.067(2) 0.012(2) 0.0030(14) -0.003(2)
N6A 0.0543(14) 0.0594(12) 0.0635(14) 0.0068(10) 0.0027(11) -0.0103(11)
C26A 0.063(2) 0.100(3) 0.082(4) 0.027(4) -0.011(3) -0.030(2)
N7A 0.120(3) 0.152(9) 0.079(5) 0.031(6) -0.021(6) -0.065(7)
C27A 0.0469(16) 0.052(3) 0.0770(19) 0.0173(14) -0.0031(14) -0.0002(14)
S1A 0.0670(13) 0.0794(18) 0.0872(8) 0.0242(12) 0.0089(8) -0.0023(12)
C31A 0.096(4) 0.117(6) 0.128(5) 0.072(5) -0.011(3) -0.007(5)
C32A 0.127(8) 0.163(7) 0.160(8) 0.087(5) 0.007(6) 0.017(6)
C33A 0.195(10) 0.127(6) 0.180(8) 0.071(6) -0.019(7) 0.033(6)
C28A 0.0507(17) 0.053(5) 0.091(2) 0.026(2) -0.0120(16) -0.007(2)
C30A 0.061(2) 0.075(5) 0.118(4) 0.062(3) -0.028(2) -0.021(3)
N9A 0.076(3) 0.161(15) 0.168(4) 0.104(10) -0.028(3) -0.051(5)
C29A 0.068(3) 0.043(5) 0.099(3) 0.015(2) -0.026(2) 0.000(3)
N8A 0.101(10) 0.084(7) 0.104(3) -0.011(3) -0.034(4) 0.002(6)
C25B 0.0434(16) 0.047(5) 0.0719(19) 0.0141(15) -0.0059(13) -0.003(2)
C24B 0.0507(17) 0.039(5) 0.067(2) 0.012(2) 0.0030(14) -0.003(2)
N6B 0.0543(14) 0.0594(12) 0.0635(14) 0.0068(10) 0.0027(11) -0.0103(11)
C26B 0.063(2) 0.100(3) 0.082(4) 0.027(4) -0.011(3) -0.030(2)
N7B 0.120(3) 0.152(9) 0.079(5) 0.031(6) -0.021(6) -0.065(7)
C27B 0.0469(16) 0.052(3) 0.0770(19) 0.0173(14) -0.0031(14) -0.0002(14)
S1B 0.0670(13) 0.0794(18) 0.0872(8) 0.0242(12) 0.0089(8) -0.0023(12)
C31B 0.096(4) 0.117(6) 0.128(5) 0.072(5) -0.011(3) -0.007(5)
C32B 0.127(8) 0.163(7) 0.160(8) 0.087(5) 0.007(6) 0.017(6)
C33B 0.195(10) 0.127(6) 0.180(8) 0.071(6) -0.019(7) 0.033(6)
C28B 0.0507(17) 0.053(5) 0.091(2) 0.026(2) -0.0120(16) -0.007(2)

C30B 0.061(2) 0.075(5) 0.118(4) 0.062(3) -0.028(2) -0.021(3)
N9B 0.076(3) 0.161(15) 0.168(4) 0.104(10) -0.028(3) -0.051(5)
C29B 0.068(3) 0.043(5) 0.099(3) 0.015(2) -0.026(2) 0.000(3)
N8B 0.101(10) 0.084(7) 0.104(3) -0.011(3) -0.034(4) 0.002(6)
C35A 0.048(6) 0.072(7) 0.071(2) 0.012(2) 0.0014(19) 0.007(6)
C37A 0.065(2) 0.097(4) 0.081(4) 0.009(4) 0.004(4) -0.004(2)
N11A 0.095(10) 0.124(19) 0.088(4) -0.016(5) 0.015(5) -0.024(10)
C36A 0.045(5) 0.074(5) 0.064(2) 0.019(4) 0.003(4) 0.012(5)
N10A 0.079(4) 0.111(2) 0.051(7) 0.026(5) 0.006(6) -0.028(2)
C34A 0.0530(19) 0.0630(17) 0.072(2) 0.0177(18) -0.0007(16) 0.0063(13)
S2A 0.0715(16) 0.078(2) 0.0819(19) 0.005(2) -0.0036(11) -0.012(2)
C41A 0.153(11) 0.076(3) 0.156(10) 0.015(3) 0.006(9) -0.017(4)
C42A 0.090(6) 0.121(6) 0.201(9) -0.023(6) 0.007(6) 0.018(4)
C43A 0.22(2) 0.119(11) 0.313(13) -0.037(7) -0.053(10) 0.046(14)
C38A 0.054(3) 0.046(5) 0.066(2) 0.028(2) -0.0090(18) 0.009(3)
C39A 0.069(3) 0.053(5) 0.054(4) 0.027(3) -0.007(3) 0.013(3)
N12A 0.085(3) 0.070(8) 0.058(8) 0.004(5) 0.010(5) -0.001(3)
C40A 0.077(3) 0.048(6) 0.073(2) 0.029(4) -0.0067(18) -0.007(4)
N13A 0.102(5) 0.090(7) 0.091(3) 0.030(6) -0.026(3) -0.028(6)
C35B 0.048(6) 0.072(7) 0.071(2) 0.012(2) 0.0014(19) 0.007(6)
C37B 0.065(2) 0.097(4) 0.081(4) 0.009(4) 0.004(4) -0.004(2)
N11B 0.095(10) 0.124(19) 0.088(4) -0.016(5) 0.015(5) -0.024(10)
C36B 0.045(5) 0.074(5) 0.064(2) 0.019(4) 0.003(4) 0.012(5)
N10B 0.079(4) 0.111(2) 0.051(7) 0.026(5) 0.006(6) -0.028(2)
C34B 0.0530(19) 0.0630(17) 0.072(2) 0.0177(18) -0.0007(16) 0.0063(13)
S2B 0.0715(16) 0.078(2) 0.0819(19) 0.005(2) -0.0036(11) -0.012(2)
C41B 0.153(11) 0.076(3) 0.156(10) 0.015(3) 0.006(9) -0.017(4)
C42B 0.090(6) 0.121(6) 0.201(9) -0.023(6) 0.007(6) 0.018(4)
C43B 0.22(2) 0.119(11) 0.313(13) -0.037(7) -0.053(10) 0.046(14)
C38B 0.054(3) 0.046(5) 0.066(2) 0.028(2) -0.0090(18) 0.009(3)
C39B 0.069(3) 0.053(5) 0.054(4) 0.027(3) -0.007(3) 0.013(3)

N12B 0.085(3) 0.070(8) 0.058(8) 0.004(5) 0.010(5) -0.001(3)
C40B 0.077(3) 0.048(6) 0.073(2) 0.029(4) -0.0067(18) -0.007(4)
N13B 0.102(5) 0.090(7) 0.091(3) 0.030(6) -0.026(3) -0.028(6)

_geom_special_details

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All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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_geom_bond_atom_site_label_2

_geom_bond_distance

_geom_bond_site_symmetry_2

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Fe N6B 1.907(2) . ?

Fe N6A 1.907(2) . ?

Fe N3 1.957(2) . ?

Fe N5 1.958(2) . ?

Fe N1 1.962(2) . ?

Fe N2 1.967(2) . ?

Fe N4 1.968(2) . ?

N1 C2 1.487(4) . ?

N1 C1 1.488(3) . ?

N1 C3 1.514(3) . ?

C1 C4 1.494(4) . ?

C1 H1A 0.9700 . ?
C1 H1B 0.9700 . ?
N2 C8 1.342(4) . ?
N2 C4 1.351(3) . ?
C4 C5 1.384(4) . ?
C5 C6 1.367(6) . ?
C5 H5 0.9300 . ?
C6 C7 1.367(6) . ?
C6 H6 0.9300 . ?
C7 C8 1.379(5) . ?
C7 H7 0.9300 . ?
C8 H8 0.9300 . ?
C2 C9 1.506(4) . ?
C2 H2A 0.9700 . ?
C2 H2B 0.9700 . ?
N3 C13 1.347(3) . ?
N3 C9 1.351(4) . ?
C9 C10 1.374(4) . ?
C10 C11 1.380(5) . ?
C10 H10 0.9300 . ?
C11 C12 1.351(6) . ?
C11 H11 0.9300 . ?
C12 C13 1.369(5) . ?
C12 H12 0.9300 . ?
C13 H13 0.9300 . ?
C3 C14 1.500(4) . ?
C3 C19 1.507(4) . ?
C3 H3 0.9800 . ?
N4 C18 1.340(4) . ?
N4 C14 1.347(3) . ?
C14 C15 1.379(4) . ?

C15 C16 1.387(6) . ?
C15 H15 0.9300 . ?
C16 C17 1.355(6) . ?
C16 H16 0.9300 . ?
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C17 H17 0.9300 . ?
C18 H18 0.9300 . ?
N5 C23 1.339(4) . ?
N5 C19 1.349(3) . ?
C19 C20 1.380(4) . ?
C20 C21 1.369(5) . ?
C20 H20 0.9300 . ?
C21 C22 1.367(5) . ?
C21 H21 0.9300 . ?
C22 C23 1.376(4) . ?
C22 H22 0.9300 . ?
C23 H23 0.9300 . ?
C25A C24A 1.407(4) . ?
C25A C27A 1.407(4) . ?
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C24A N6A 1.157(4) . ?
C26A N7A 1.154(8) . ?
C27A C28A 1.393(4) . ?
C27A S1A 1.757(4) . ?
S1A C31A 1.825(5) . ?
C31A C32A 1.435(11) . ?
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C28A C29A 1.416(6) . ?
C28A C30A 1.420(6) . ?
C30A N9A 1.140(5) . ?
C29A N8A 1.160(8) . ?
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C25B C24B 1.410(5) . ?
C25B C26B 1.417(7) . ?
C24B N6B 1.160(5) . ?
C26B N7B 1.155(10) . ?
C27B C28B 1.393(5) . ?
C27B S1B 1.757(5) . ?
S1B C31B 1.823(6) . ?
C31B C32B 1.433(12) . ?
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C31B H32 0.9700 . ?
C32B C33B 1.501(10) . ?
C32B H33 0.9700 . ?
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C33B H37 0.9600 . ?
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C28B C30B 1.421(7) . ?
C30B N9B 1.141(6) . ?
C29B N8B 1.161(9) . ?
C35A C34A 1.398(7) . ?
C35A C37A 1.420(10) . ?
C35A C36A 1.424(5) . ?

C37A N11A 1.157(10) . ?
C36A N10A 1.180(9) . ?
C34A C38A 1.399(6) . ?
C34A S2A 1.768(5) . ?
S2A C41A 1.787(6) . ?
C41A C42A 1.445(17) . ?
C41A H38 0.9700 . ?
C41A H39 0.9700 . ?
C42A C43A 1.545(8) . ?
C42A H40 0.9700 . ?
C42A H41 0.9700 . ?
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C43A H44 0.9600 . ?
C38A C39A 1.417(5) . ?
C38A C40A 1.463(6) . ?
C39A N12A 1.171(8) . ?
C40A N13A 1.143(5) . ?
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C35B C37B 1.420(11) . ?
C35B C36B 1.423(5) . ?
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C36B N10B 1.180(10) . ?
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S2B C41B 1.787(6) . ?
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C41B H46 0.9700 . ?
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C42B H47 0.9700 . ?

C42B H48 0.9700 . ?
C43B H49 0.9600 . ?
C43B H49A 0.9600 . ?
C43B H49B 0.9600 . ?
C38B C39B 1.421(5) . ?
C38B C40B 1.466(7) . ?
C39B N12B 1.171(9) . ?
C40B N13B 1.143(5) . ?

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N6B Fe N3 97.32(10) . . ?
N6A Fe N3 97.32(10) . . ?
N6B Fe N5 94.24(9) . . ?
N6A Fe N5 94.24(9) . . ?
N3 Fe N5 168.43(9) . . ?
N6B Fe N1 175.79(9) . . ?
N6A Fe N1 175.79(9) . . ?
N3 Fe N1 85.32(9) . . ?
N5 Fe N1 83.15(8) . . ?
N6B Fe N2 98.64(10) . . ?
N6A Fe N2 98.64(10) . . ?
N3 Fe N2 86.13(9) . . ?
N5 Fe N2 91.99(9) . . ?
N1 Fe N2 84.78(9) . . ?

N6B Fe N4 93.93(9) . . ?
N6A Fe N4 93.93(9) . . ?
N3 Fe N4 92.14(9) . . ?
N5 Fe N4 87.21(9) . . ?
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N2 Fe N4 167.42(9) . . ?
C2 N1 C1 111.7(2) . . ?
C2 N1 C3 113.9(2) . . ?
C1 N1 C3 113.6(2) . . ?
C2 N1 Fe 109.03(15) . . ?
C1 N1 Fe 109.62(16) . . ?
C3 N1 Fe 98.04(14) . . ?
N1 C1 C4 109.7(2) . . ?
N1 C1 H1A 109.7 . . ?
C4 C1 H1A 109.7 . . ?
N1 C1 H1B 109.7 . . ?
C4 C1 H1B 109.7 . . ?
H1A C1 H1B 108.2 . . ?
C8 N2 C4 118.2(3) . . ?
C8 N2 Fe 127.6(2) . . ?
C4 N2 Fe 113.55(18) . . ?
N2 C4 C5 122.0(3) . . ?
N2 C4 C1 115.4(2) . . ?
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C6 C5 C4 119.0(4) . . ?
C6 C5 H5 120.5 . . ?
C4 C5 H5 120.5 . . ?
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C6 C7 H7 120.2 . . ?
C8 C7 H7 120.2 . . ?
N2 C8 C7 121.9(4) . . ?
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C7 C8 H8 119.1 . . ?
N1 C2 C9 109.5(2) . . ?
N1 C2 H2A 109.8 . . ?
C9 C2 H2A 109.8 . . ?
N1 C2 H2B 109.8 . . ?
C9 C2 H2B 109.8 . . ?
H2A C2 H2B 108.2 . . ?
C13 N3 C9 118.2(3) . . ?
C13 N3 Fe 127.3(2) . . ?
C9 N3 Fe 113.54(17) . . ?
N3 C9 C10 122.0(3) . . ?
N3 C9 C2 114.8(2) . . ?
C10 C9 C2 123.2(3) . . ?
C9 C10 C11 118.4(4) . . ?
C9 C10 H10 120.8 . . ?
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C12 C11 H11 120.0 . . ?
C10 C11 H11 120.0 . . ?
C11 C12 C13 119.6(3) . . ?
C11 C12 H12 120.2 . . ?
C13 C12 H12 120.2 . . ?
N3 C13 C12 121.9(4) . . ?
N3 C13 H13 119.1 . . ?
C12 C13 H13 119.1 . . ?
C14 C3 C19 106.3(2) . . ?
C14 C3 N1 105.7(2) . . ?

C19 C3 N1 105.6(2) . . ?
C14 C3 H3 112.9 . . ?
C19 C3 H3 112.9 . . ?
N1 C3 H3 112.9 . . ?
C18 N4 C14 118.8(3) . . ?
C18 N4 Fe 130.3(2) . . ?
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N4 C14 C3 111.7(2) . . ?
C15 C14 C3 126.5(3) . . ?
C14 C15 C16 118.2(3) . . ?
C14 C15 H15 120.9 . . ?
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C17 C16 C15 119.9(3) . . ?
C17 C16 H16 120.1 . . ?
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C16 C17 C18 119.4(4) . . ?
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N4 C18 C17 121.8(3) . . ?
N4 C18 H18 119.1 . . ?
C17 C18 H18 119.1 . . ?
C23 N5 C19 118.4(2) . . ?
C23 N5 Fe 130.72(17) . . ?
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N5 C19 C3 111.7(2) . . ?
C20 C19 C3 126.1(2) . . ?
C21 C20 C19 118.7(3) . . ?
C21 C20 H20 120.7 . . ?
C19 C20 H20 120.7 . . ?

C22 C21 C20 119.5(3) . . ?
C22 C21 H21 120.2 . . ?
C20 C21 H21 120.2 . . ?
C21 C22 C23 119.5(3) . . ?
C21 C22 H22 120.3 . . ?
C23 C22 H22 120.3 . . ?
N5 C23 C22 121.8(3) . . ?
N5 C23 H23 119.1 . . ?
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C24A C25A C27A 120.9(3) . . ?
C24A C25A C26A 115.1(4) . . ?
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N6A C24A C25A 175.9(17) . . ?
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N7A C26A C25A 178(2) . . ?
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C28A C27A S1A 120.4(3) . . ?
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S1A C31A H24 109.2 . . ?
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S1A C31A H25 109.2 . . ?
H24 C31A H25 107.9 . . ?
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C32A C33A H29 109.5 .. ?
H28 C33A H29 109.5 .. ?
C32A C33A H30 109.5 .. ?
H28 C33A H30 109.5 .. ?
H29 C33A H30 109.5 .. ?
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N9A C30A C28A 177.5(15) .. ?
N8A C29A C28A 170.2(14) .. ?
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N6B C24B C25B 166(2) .. ?
C24B N6B Fe 171.1(19) .. ?
N7B C26B C25B 170(4) .. ?
C28B C27B C25B 124.9(6) .. ?
C28B C27B S1B 120.4(6) .. ?
C25B C27B S1B 113.6(6) .. ?
C27B S1B C31B 104.1(5) .. ?
C32B C31B S1B 111.7(9) .. ?
C32B C31B H31 109.3 .. ?
S1B C31B H31 109.3 .. ?
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S1B C31B H32 109.3 .. ?
H31 C31B H32 107.9 .. ?
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C31B C32B H33 109.3 .. ?
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C31B C32B H34 109.3 .. ?

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