E.lectronic supplementary information

Carboxylate free μ-oxo Bridged Ferric Wheel with a Record Exchange Coupling

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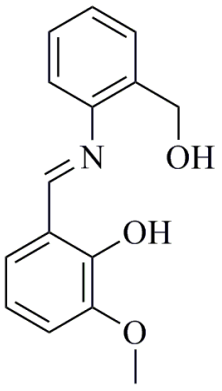
Unless otherwise mentioned all the reaction was carried out under aerobic condition. All the chemicals were purchased from commercially available source (Alfa Aesar) and used without further purification.

Synthesis of complex **1**:

The H_2L ligand (0.100g, 0.3889 mmol) was dissolved in 50 mL of MeOH and deprotonated using two equivalent of Et_3N. Into this deprotonated solution, methanolic solution of $Fe(NO_3)_3.9H_2O$ (0.157g, 0.3889 mmol in 10 mL) was added and stirred for 2hr at room temperature. The reddish brown solution was evaporated to dryness under reduced pressure. The obtained brown residue was washed with petroleum ether/MeOH mixture which was dissolved into 2 mL N,N-Dimethylformamide solvent immediately and filtered off. Red brown single crystals are grown in a week time upon slow evaporation at room temperature, which are suitable for single crystal X-ray diffraction. Yield (based on Fe): 40 mg (8%). FTIR-1620 cm^{-1} ($\nu_{C=N}$), 2930 cm^{-1} (ν_{Ar-H}). $_{)}$). Elemental analysis for **1.(n-hexane)$_{0.5}$((CH$_3$)$_2$NCHO)$_2$**: Calculated C, 55.02 %; H, 4.59 %; N, 5.55%. Found: C, 54.59%; H, 4.15 %; N, 5.68 %.



H_2L

Fig S1. The Schiff base ligand employed to reveal complex **1**.

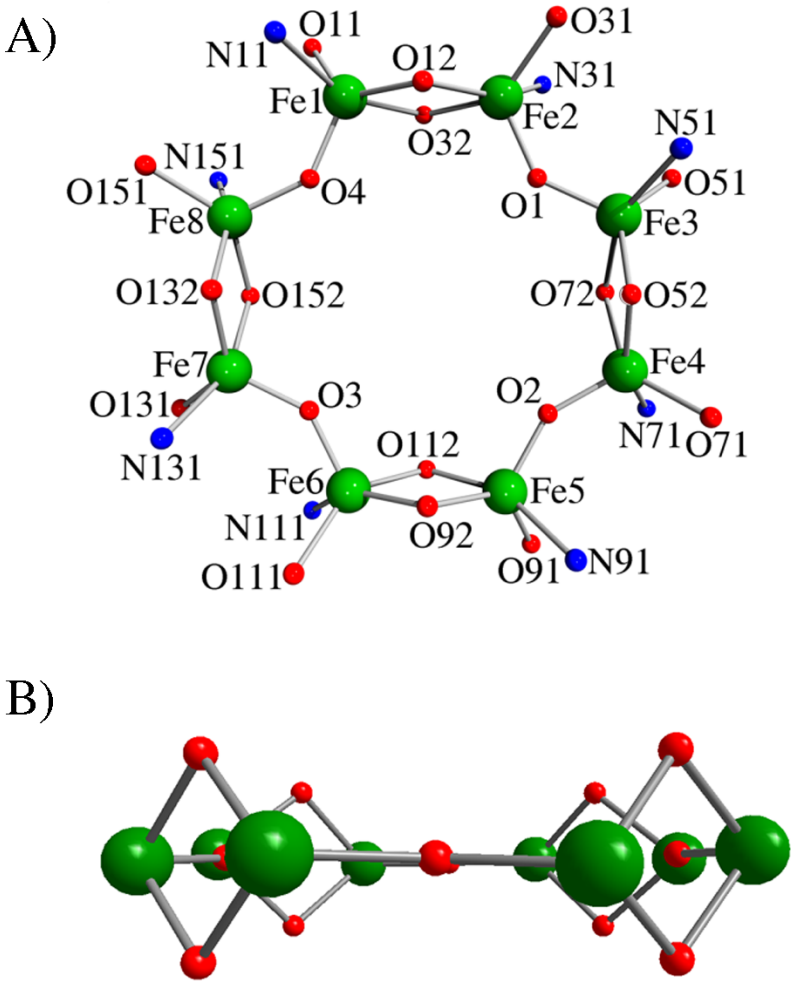


Fig S2. A) Metal core and its bridging motifs found in **1.** B) Core presenting molecular plane.

Table S1. Crystallographic data of complex **1**.

	1. (n-hexane)$_{0.5}$
Formula	$Fe_8C_{131.50}H_{133.25}N_{10.25}O_{32}$
Size [mm]	0.26 x 0.09 x 0.08
System	Monoclinic
Space group	$P2_1/n$
a [Å]	23.091(6)
b [Å]	24.427(6)
c [Å]	23.572(6)
β [°]	90.321(4)
V [Å^3]	13295(6)
Z	4
ρ_{calcd}[g/cm^{-3}]	1.407
$2\Theta_{max}$	56
radiation	MoK α
λ [Å]	0.71073
T [K]	100
reflns	140602
Ind. reflns	31723
reflns with $I>2\sigma(I)$	25879
$R1$	0.0841
$wR2$	0.2088

Table S2. Bond valence sum (BVS) calculation for metal ions in **1**.

Iron Center	Fe-O/N bond	s= exp(r_0-r)/B	BVS	Assigned O.S
1	Fe1-O4	0.87359785	3.053	**+3**
	Fe1-ON11	0.440908054		
	Fe1-O11	0.673953208		
	Fe1-O12	0.560807046		
	Fe1-O32	0.503341463		
2	Fe2-N31	0.440908054	3.094	**+3**
	Fe2-O1	0.892692133		
	Fe2-O12	0.519933659		
	Fe2-O31	0.670320046		
	Fe2-O32	0.569975351		
3	Fe3-N51	0.440908054	3.117	**+3**
	Fe3-O51	0.66670647		
	Fe3-O1	0.912203761		
	Fe3-O72	0.519933659		
	Fe3-O52	0.577729999		
4	Fe4-O2	0.944823863	3.175	**+3**
	Fe4-N71	0.465396818		
	Fe4-O71	0.684971273		
	Fe4-O72	0.544379803		
	Fe4-O52	0.535623214		
5	Fe5-N91	0.443297794	3.165	**+3**
	Fe5-O91	0.654211671		
	Fe5-O92	0.569975351		
	Fe5-O112	0.542910493		
	Fe5-O2	0.955093587		
6	Fe6-O92	0.526295787	3.12	**+3**
	Fe6-N111	0.464140687		
	Fe6-O111	0.631624972		
	Fe6-O112	0.568436957		
	Fe6-O3	0.929625955		
7	Fe7-N131	0.429151212	3.126	**+3**
	Fe7-O131	0.574615559		
	Fe7-O132	0.683122499		
	Fe7-O152	0.501982917		
	Fe7-O3	0.937194103		
8	Fe8-O131	0.511570297	3.096	**+3**
	Fe8-N151	0.437347578		
	Fe8-O151	0.677606062		
	Fe8-O152	0.584009612		
	Fe8-O4	0.885483353		

Table S3. Bond valence sum calculation for bridging oxygen in **1**.

Oxygen Center	**O-Fe bond**	**$S= (R/R_1)^{-N}$**	**BVS**	**Assigned O.S**
O1	O1-Fe2	0.917767224	1.859	-2
	O1-Fe3	0.941274692		
O2	O2-Fe4	0.981001615	1.975	-2
	O2-Fe5	0.993619543		
O3	O3-Fe6	0.962426079	1.934	-2
	O3-Fe7	0.971661672		
O4	O4-Fe1	0.914877578	1.824	-2
	O4-Fe8	0.909130308		

Table S4. Selected bond lengths and bond angles for **1**.

Fe(1)-O(4)	1.808(4)	Fe(6)-O(92)	2.005(4)
Fe(1)-O(11)	1.911(4)	Fe(6)-N(111)	2.097(5)
Fe(1)-O(12)	1.978(4)	Fe(7)-O(3)	1.789(4)
Fe(1)-O(32)	2.019(3)	Fe(7)-O(131)	1.906(4)
Fe(1)-N(11)	2.117(4)	Fe(7)-O(132)	1.970(4)
Fe(2)-O(1)	1.807(4)	Fe(7)-O(152)	2.021(4)
Fe(2)-O(31)	1.913(4)	Fe(7)-N(131)	2.127(5)
Fe(2)-O(32)	1.972(3)	Fe(8)-O(4)	1.809(3)
Fe(2)-O(12)	2.007(3)	Fe(8)-O(151)	1.909(4)
Fe(2)-N(31)	2.118(4)	Fe(8)-O(152)	1.965(4)
Fe(3)-O(1)	1.798(4)	Fe(8)-O(132)	2.012(4)
Fe(3)-O(51)	1.916(4)	Fe(8)-N(151)	2.121(5)
Fe(3)-O(52)	1.968(4)		
Fe(3)-O(72)	2.006(4)	**Bond angles (°)**	
Fe(3)-N(51)	2.118(5)		
Fe(4)-O(2)	1.786(4)	Fe(3)-O(1)-Fe(2)	138.9(2)
Fe(4)-O(71)	1.905(4)	Fe(5)-O(2)-Fe(4)	148.3(2)
Fe(4)-O(72)	1.991(4)	Fe(7)-O(3)-Fe(6)	142.2(2)
Fe(4)-O(52)	1.996(4)	Fe(1)-O(4)-Fe(8)	138.6(2)
Fe(4)-N(71)	2.098(5)	Fe(1)-O(12)-Fe(2)	104.52(17)
Fe(5)-O(2)	1.782(4)	Fe(2)-O(32)-Fe(1)	104.32(17)
Fe(5)-O(91)	1.922(5)	Fe(3)-O(52)-Fe(4)	104.73(19)
Fe(5)-O(92)	1.973(4)	Fe(4)-O(72)-Fe(3)	103.52(18)
Fe(5)-O(112)	1.992(4)	Fe(5)-O(92)-Fe(6)	103.5(2)
Fe(5)-N(91)	2.117(6)	Fe(6)-O(112)-Fe(5)	104.0(2)
Fe(6)-O(3)	1.792(4)	Fe(7)-O(132)-Fe(8)	103.7(2)
Fe(6)-O(111)	1.935(4)	Fe(8)-O(152)-Fe(7)	103.60(18)
Fe(6)-O(112)	1.973(4)		

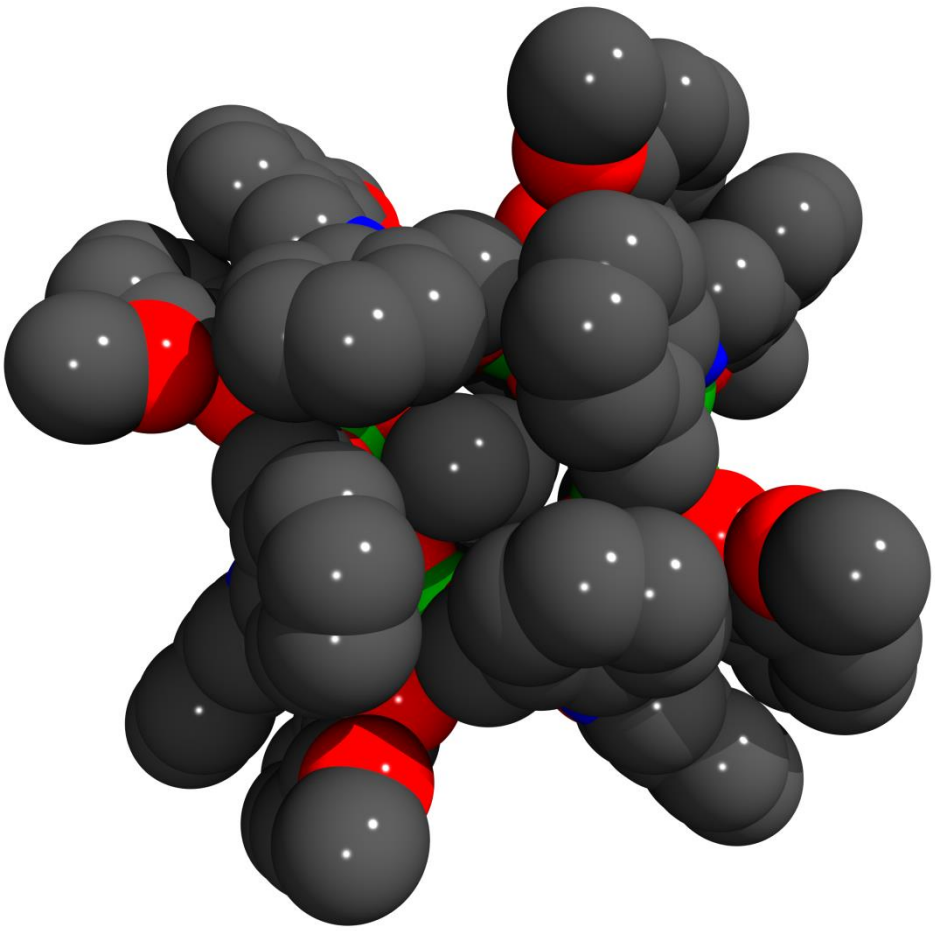


Fig S3. Space filling diagram of **1** viewing perpendicular to the plane of Fe(III) wheel, shows the presence of guest molecule (hexane) in cavity**.**

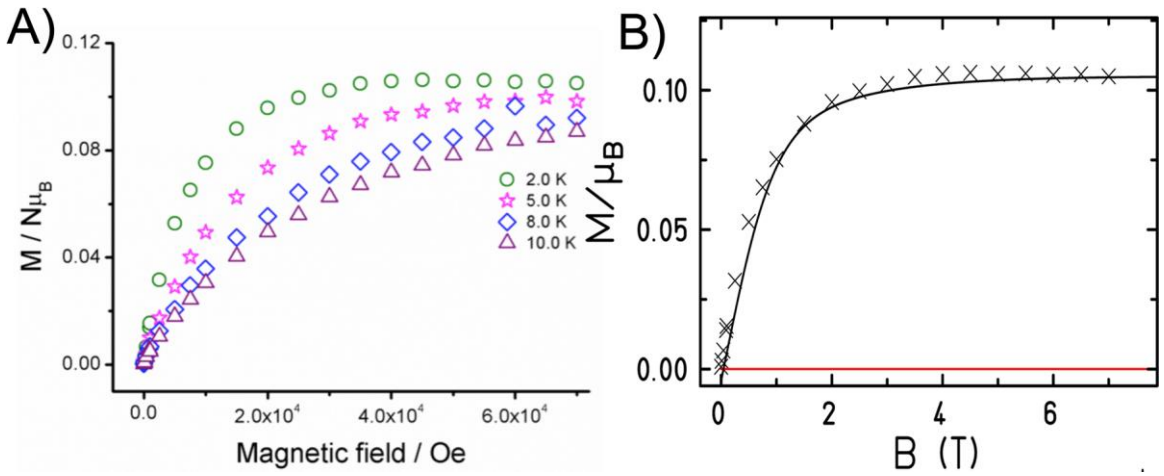


Fig S4. A) Field dependent magnetization data of polycrystalline sample of **1** measured at the indicated temperatures**.** B) Simulation of experimental magnetic data (symbols) obtained at 2.0 K and the black curve displays the contribution of a very small content of impurity spins (refer to main text for details); the contribution of **1** to the magnetization is virtually zero for these fields and temperature (red curve).

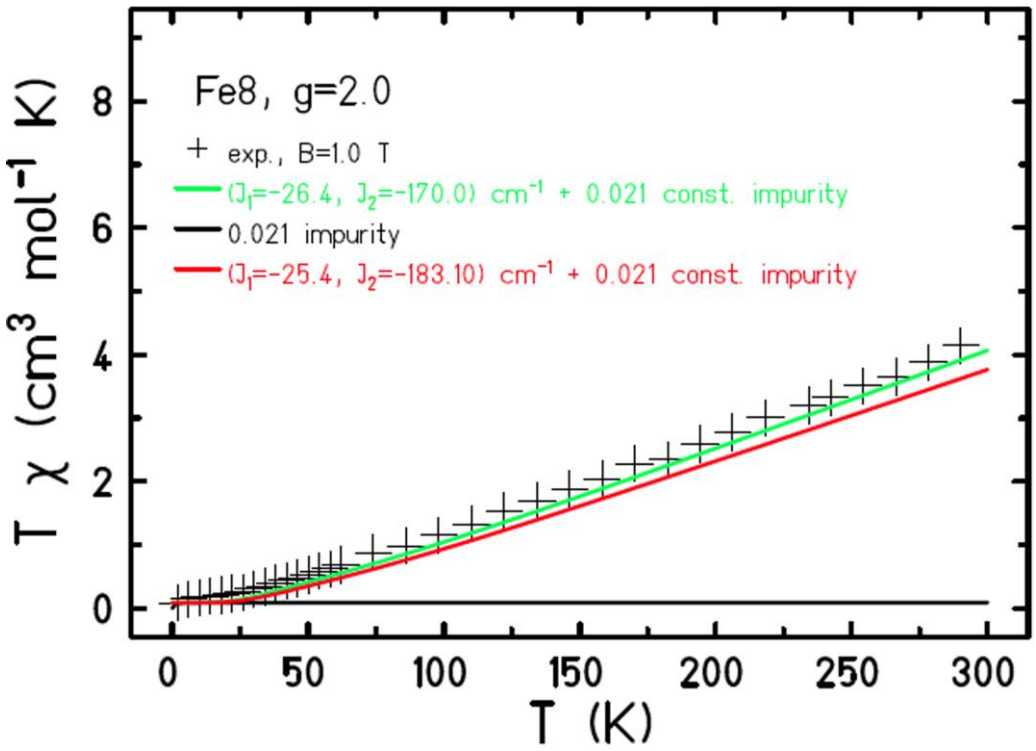


Fig S5. Temperature dependent magnetic susceptibility temperature product plot of complex **1** (symbols) and the solid curves (red and green) represents the simulation of experimental data using the parameters mentioned within the plot. Solid black curve: Contribution of 0.021 impurity to the $\chi_M T$ value of **1**.

Computational Details:

The exchange parameter values (*J*) between Fe^{III} ions in **1** are calculated using Noodleman's broken symmetry method.[1,2] B3LYP[3] functional along with TZV basis set[4] was employed in our calculations. For extracting *J* values (2*J* model- eqn1; 4*J* model- eqn2) the following Hamiltonian has been used:

$$\widehat{H}_{Ex} = -[J_1(\hat{S}_{Fe1}\ \hat{S}_{Fe2} + \hat{S}_{Fe3}\ \hat{S}_{Fe4} + \hat{S}_{Fe5}\ \hat{S}_{Fe6} + \hat{S}_{Fe7}\ \hat{S}_{Fe8}) + J_2(\ \hat{S}_{Fe2}\ \hat{S}_{Fe3} + \hat{S}_{Fe4}\ \hat{S}_{Fe5} + \hat{S}_{Fe6}\ \hat{S}_{Fe7} + \hat{S}_{Fe1}\ \hat{S}_{Fe8})] \ldots eqn\ 1$$

$$\widehat{H}_{Ex} = -[J_1(\hat{S}_{Fe1}\ \hat{S}_{Fe2} + \hat{S}_{Fe5}\ \hat{S}_{Fe6}) + J_2(\ \hat{S}_{Fe2}\ \hat{S}_{Fe3} + \hat{S}_{Fe1}\ \hat{S}_{Fe8}) + J_3(\ \hat{S}_{Fe3}\ \hat{S}_{Fe4} + \hat{S}_{Fe7}\ \hat{S}_{Fe8}) + J_4(\ \hat{S}_{Fe4}\ \hat{S}_{Fe5} + \hat{S}_{Fe6}\ \hat{S}_{Fe7})] \ldots eqn\ 2$$

The computed spin configurations for **1** is given in the ESI as Table ST1. From the energies of these spin configurations and expressing them by a pair-wise interaction model, the exchange coupling constants have been estimated using the Broken Symmetry (BS) approach developed by Noodleman. This method has previously been employed to compute reasonable estimates of exchange interactions in numerous polynuclear complexes including several {3d-4f} systems.[5] For extracting *J* values between two Fe^{III} ions in model dimers and diamgnetic substituted complexes following Hamiltonian has been employed,

$$\widehat{H}_{Ex} = -J(\hat{S}_{Fe1}\ \hat{S}_{Fe2})$$

All of our calculations have been performed using G09 suite of programs.[6] Corresponding orbital pair (COD) procedure has been followed to obtain well defined SOMO pairs and the overlap values between the corresponding orbital pairs have been computed using ORCA.[7]

Table S5. The different spin configurations employed in the calculations of the magnetic exchange

Configurations	Fe1	Fe2	Fe3	Fe4	Fe5	Fe6	Fe7	Fe8
HS	↑	↑	↑	↑	↑	↑	↑	↑
BS1	↓	↓	↑	↑	↑	↑	↑	↑
BS2	↓	↑	↑	↑	↑	↑	↑	↓
BS3	↓	↓	↓	↓	↑	↑	↑	↑
BS4	↓	↓	↓	↑	↑	↑	↑	↑

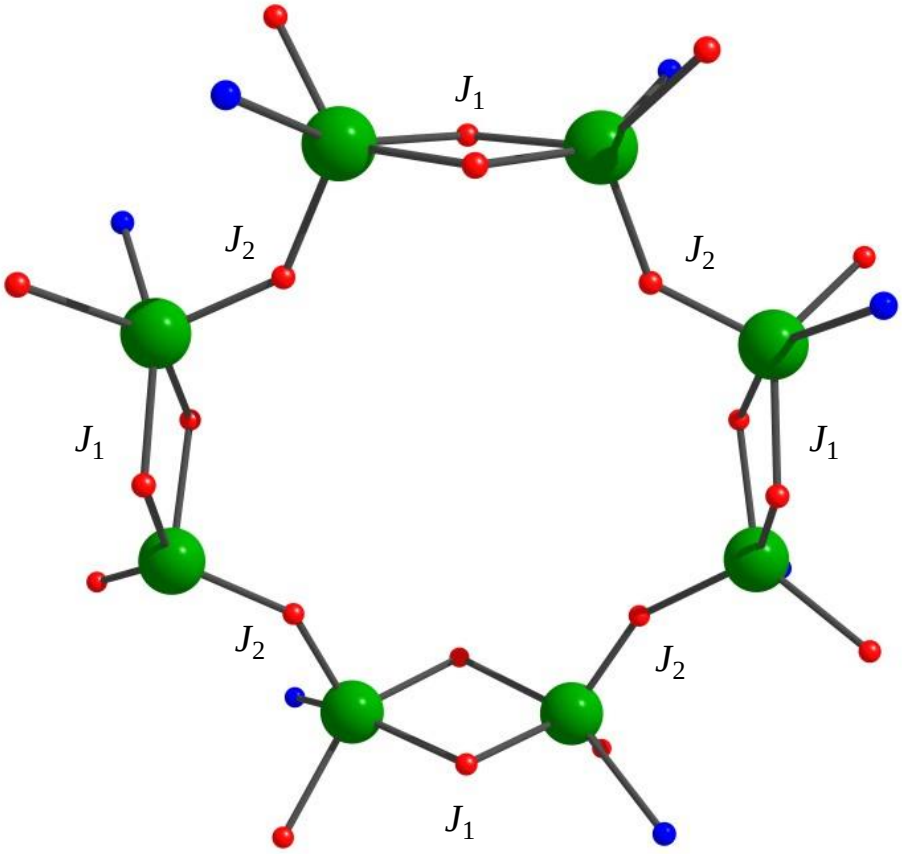


Fig S6. Schematic representation of two *J* model employed to compute exchange values in **1**.

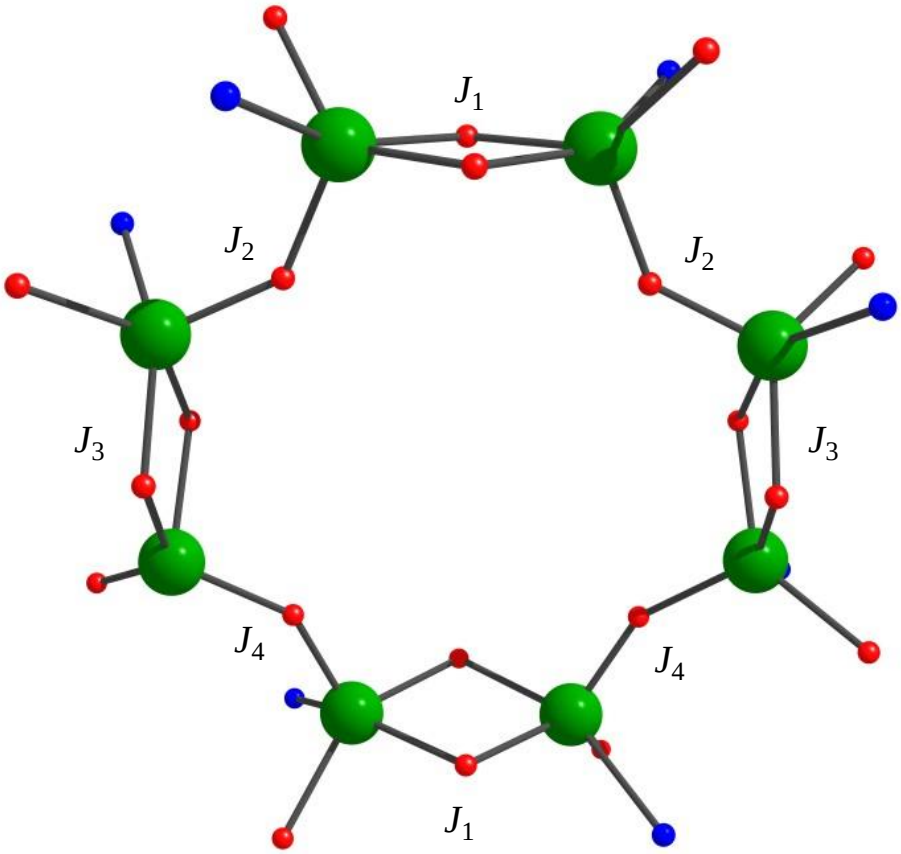


Fig S7. Schematic representation of four *J* model employed to compute exchange values in **1**.

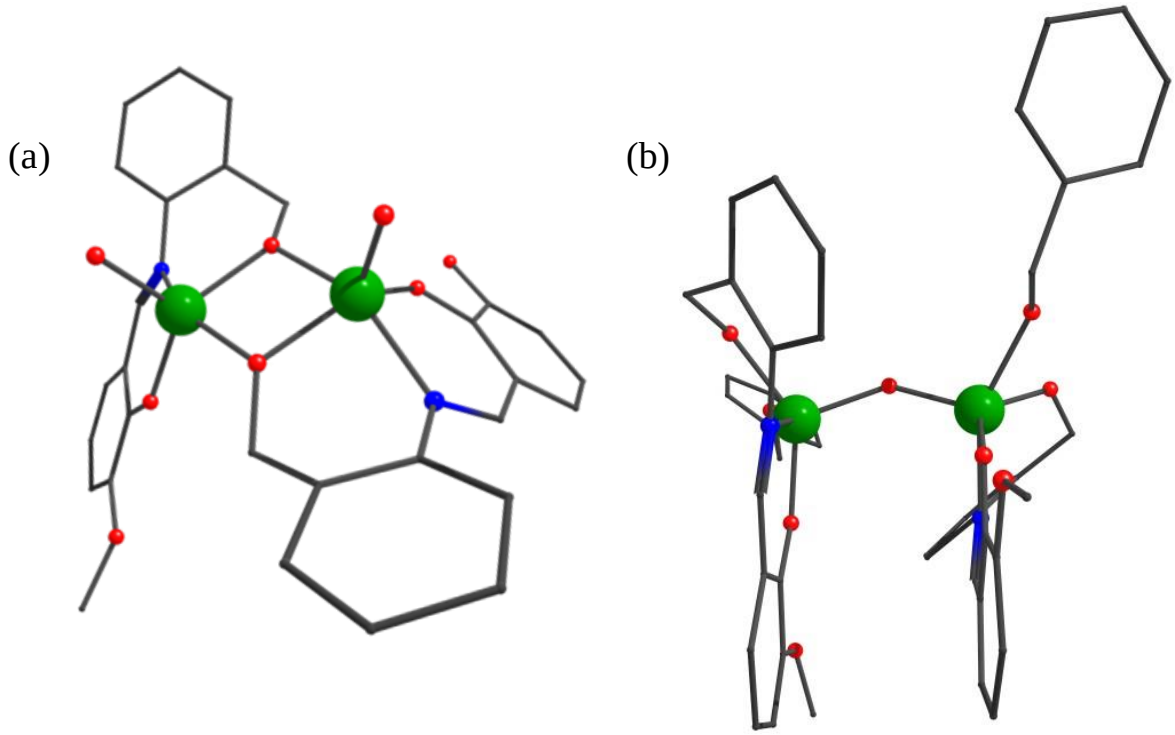


Fig S8. The dimeric models employed to compute J_1 (a) and J_2 (b) exchange values in **1**.

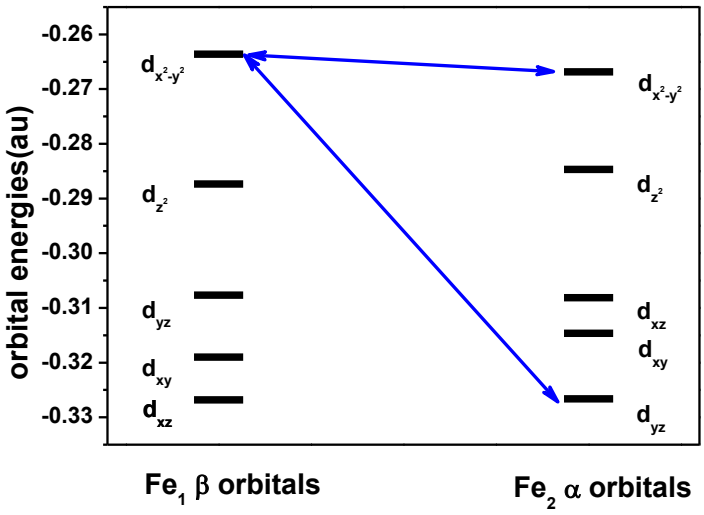


Fig S9. The J_{AF} interactions between the magnetic orbitals of Fe^{3+} ions in the dimer model (J_1 interaction). Cutoff value for overlap integral values is taken as 0.12.

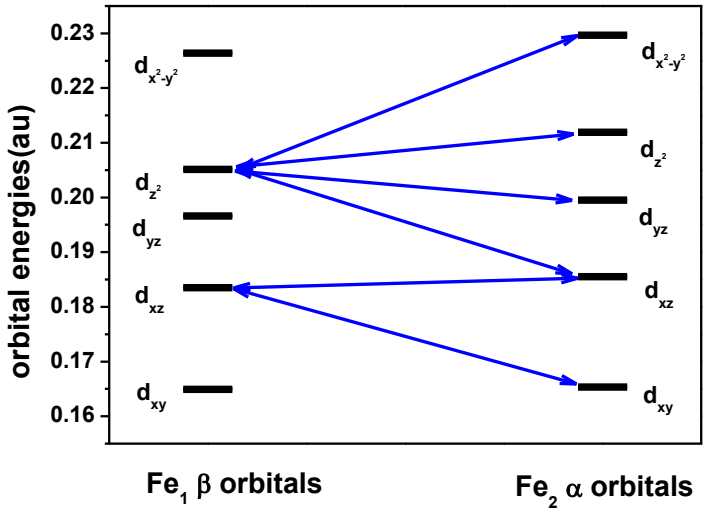


Fig S10. The J_{AF} interactions between the magnetic orbitals of Fe^{3+} ions in the dimer model (J_2 interaction). Cutoff value for overlap integral values is taken as 0.11.

Table S6. Computed overlap integrals values corresponding to J_1 interaction

Alpha/Beta	d_{xz}	d_{xy}	d_{yz}	d_z2	$d_x2_{-y}2$
d_{yz}	0.00964	0.02105	0.04528	-0.04285	-0.03775
d_{xy}	0.04239	-0.01548	-0.00009	0.0257	0.01442
d_{xz}	-0.03798	-0.02104	0.00445	0.06212	-0.00452
d_z2	0.0694	-0.05754	0.02445	-0.05634	-0.01246
$d_x2_{-y}2$	0.04621	-0.00672	-0.21656	-0.06413	0.11619

Table S7. Computed overlap integrals values corresponding to J_2 interaction

Alpha/Beta	d_{xy}	d_{xz}	d_{yz}	d_z2	$d_x2_{-y}2$
d_{xy}	-0.00399	0.11482	0.01857	0.02577	-0.00078
d_{xz}	-0.07298	0.09077	-0.05646	-0.05077	-0.03652
d_{yz}	0.01756	0.05239	0.04009	-0.18908	0.03282
d_z2	0.05872	0.20427	0.16308	0.44901	0.26484
$d_x2_{-y}2$	0.00035	-0.04959	-0.01454	-0.07682	0.00523

Table S8: Computed overlap integral values corresponding J_1 interaction

153: 0.99966

154: 0.99960

155: 0.99956

156: 0.99947

157: 0.99942

158: 0.99935

159: 0.99922

160: 0.99912

161: 0.99892

162: 0.99794

163: 0.99688

164: 0.15987 $d_x^2\text{-}_y^2 - d_x^2\text{-}_y^2$ overlap

165: 0.11052 $d_z^2\text{-}d_z^2$ overlap

166: 0.07976

167: 0.06883

168: 0.02507

Table S9: Computed overlap integral values corresponding J_2 interaction

206:	0.99986	
207:	0.99975	
208:	0.99974	
209:	0.99949	
210:	0.99949	
211:	0.99944	
212:	0.99920	
213:	0.99908	
214:	0.99826	
215:	0.99717	
216:	0.99629	
217:	0.29563	d_z^2-d_z^2 overlap (in phase)
218:	0.22293	d_z^2-d_z^2 overlap (out of phase)
219:	0.20461	d_{xz}-d_{xz} overlap
220:	0.00216	
221:	0.00017	

Discussion SD1: Orbitals are calculated following corresponding orbital transformation procedure and this procedure leads to three cases. Case1- orbital overlap close to unity for the doubly occupied αβ pairs. Case 2- non-negligible overlap values between the non-orthogonal magnetic orbital pairs. Case 3- overlap between the virtual states.

The large J_2 interaction is attributed towards overlap interaction between d_z^2-d_z^2 (in phase and out of phase), d_{xz}-d_{xz} orbitals (See Table S8) and this d_z^2-d_z^2 orbital overlap (See Table S9) gets diminished when it comes to J_1 interaction

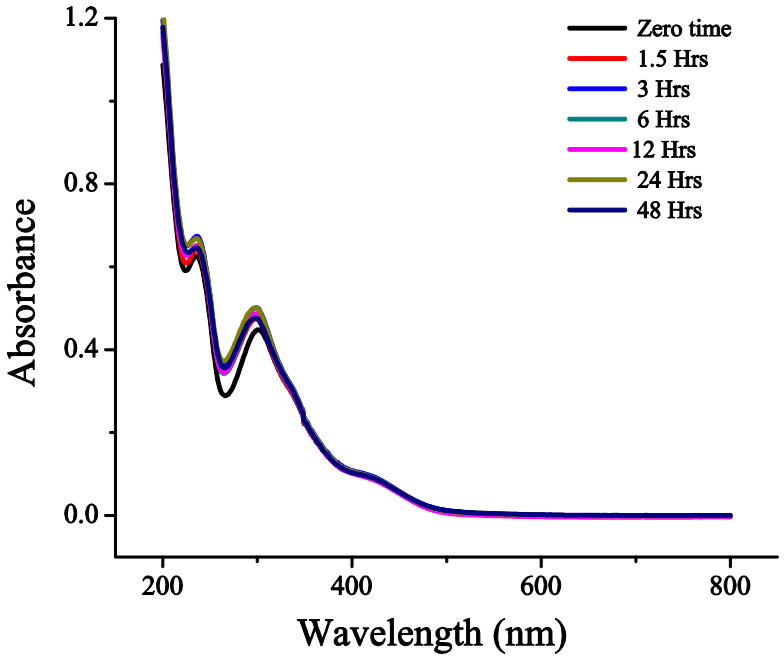


Fig S11. UV-Vis spectra of complex **1** in MeCN at the indicated time interval.

UV-Vis spectroscopic measurement was performed for complex **1** in CH_3CN solution at different time interval i.e. zero hrs, 1.5 hrs, 3 hrs, 6 hrs, 12 hrs, 24 hrs and 48 hrs. The spectrum remains unchanged over the period of two days indicative of its stability in solution and unambiguously confirms that the solid-state structure is maintained in solution.

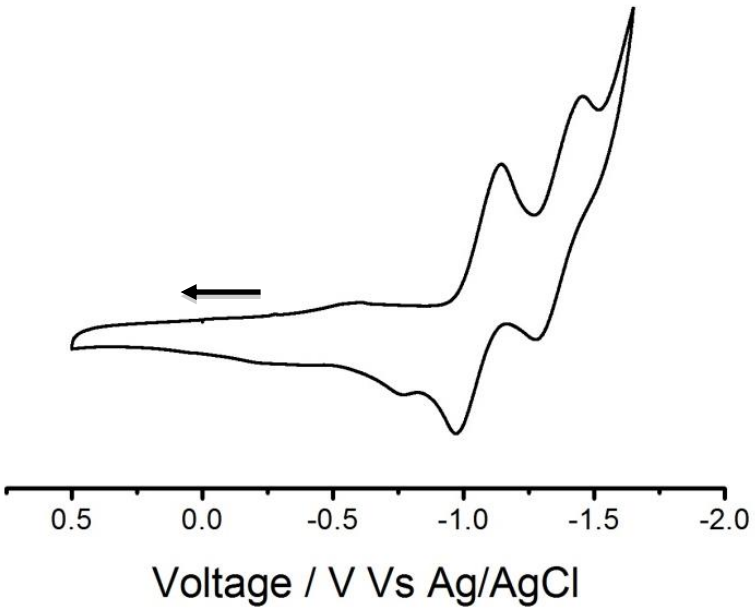


Fig S12. Cyclic voltammogram of 0.1×10^{-3} M complex **1** is recorded in DCM using TBAP as an electrolyte.

To confirm the obtained redox processes are metal based or ligand based, CV experiments were performed under identical condition as in **1**, for the free ligand (protonated, H_2L) and deprotonated ligand (L^{2-}). For the protonated ligand we observe only irreversible oxidation process, while featureless voltammogram obtained for the deprotonated ligand. Based on these experiments we conclude that the redox processes observed for **1** (Schiff base ligand is doubly deprotonated in **1**) is exclusively based on metal ions.

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Crystallographic information file

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Refinement of F^2^ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2^, conventional R-factors R are based on F, with F set to zero for negative F^2^. The threshold expression of F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2^ are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All non-hydrogen atoms exept the solvent molecule refined anisotropically and the hydrogen atoms refined as riding model.

For better convergence of disordered atoms and solvent molecules,restraints and constraints such as DFIX, SIMU, DELU, etc.were used.

Hydrogen atoms were not added in its geometrical position to the disordered hexane molecule, but in molecular formula.

The other solvate molecule in the crystal lattice (DMF and methanol) could not be modelled due to the diffused electron density, hence SQUZZEE routine was employed. The corresponding loop created by Platon is appended at the end of cif file.

The guest hexane molecule thermal parameters are in reasonably good agreement when it is refined with 50% occupancy.
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C84 C 0.7070(2) 0.6355(2) -0.0240(2) 0.0278(10) Uani 1 1 d . . .
H84A H 0.7212 0.6304 -0.0632 0.033 Uiso 1 1 calc R . .
H84B H 0.6701 0.6151 -0.0204 0.033 Uiso 1 1 calc R . .
C85 C 0.8819(2) 0.9338(3) -0.0957(3) 0.0491(16) Uani 1 1 d . . .
H85A H 0.9125 0.9411 -0.0677 0.074 Uiso 1 1 calc R . .
H85B H 0.8539 0.9639 -0.0956 0.074 Uiso 1 1 calc R . .

H85C H 0.8990 0.9305 -0.1335 0.074 Uiso 1 1 calc R . .
C91 C 0.93787(11) 0.78587(14) 0.09409(10) 0.0480(17) Uani 1 1 d G . .
C92 C 0.92398(11) 0.73937(14) 0.12516(12) 0.0414(15) Uani 1 1 d G A .
C93 C 0.96387(12) 0.69703(15) 0.13039(14) 0.0471(16) Uani 1 1 d G . .
C94 C 1.01765(12) 0.70119(17) 0.10455(14) 0.070(2) Uani 1 1 d G A .
H94 H 1.0449 0.6723 0.1081 0.084 Uiso 1 1 calc R . .
C95 C 1.03154(12) 0.74769(19) 0.07348(15) 0.081(3) Uani 1 1 d G . .
H95 H 1.0683 0.7505 0.0558 0.097 Uiso 1 1 calc R A .
C96 C 0.99165(13) 0.79003(17) 0.06824(14) 0.072(3) Uani 1 1 d G A .
H96 H 1.0011 0.8218 0.0470 0.087 Uiso 1 1 calc R . .
C97 C 0.9002(3) 0.8327(3) 0.08903(19) 0.0507(19) Uani 1 1 d . A .
H97 H 0.9151 0.8630 0.0685 0.061 Uiso 1 1 calc R . .
C98 C 0.81954(16) 0.88292(10) 0.09605(7) 0.021(2) Uani 0.573(14) 1 d PGU A 1
C99 C 0.78216(15) 0.90439(9) 0.13636(8) 0.024(2) Uani 0.573(14) 1 d PGU A 1
C100 C 0.74914(17) 0.95041(9) 0.12366(10) 0.026(2) Uani 0.573(14) 1 d PGU A 1
H100 H 0.7236 0.9651 0.1512 0.031 Uiso 0.573(14) 1 calc PR A 1
C101 C 0.7535(2) 0.97497(11) 0.07067(11) 0.026(2) Uani 0.573(14) 1 d PGU A 1
H101 H 0.7310 1.0064 0.0620 0.031 Uiso 0.573(14) 1 calc PR A 1
C102 C 0.7909(2) 0.95350(12) 0.03036(10) 0.026(2) Uani 0.573(14) 1 d PGU A 1
H102 H 0.7939 0.9703 -0.0059 0.031 Uiso 0.573(14) 1 calc PR A 1
C103 C 0.82392(19) 0.90748(12) 0.04305(8) 0.027(2) Uani 0.573(14) 1 d PGU A 1
H103 H 0.8495 0.8928 0.0155 0.033 Uiso 0.573(14) 1 calc PR A 1
C104 C 0.7757(3) 0.8804(2) 0.1982(2) 0.0398(13) Uani 1 1 d . . .
H10A H 0.8123 0.8858 0.2196 0.048 Uiso 1 1 calc R A 1
H10B H 0.7445 0.9001 0.2184 0.048 Uiso 1 1 calc R A 1
C105 C 0.9868(4) 0.6090(4) 0.1670(4) 0.075(2) Uiso 1 1 d . . .
H10G H 0.9939 0.5940 0.1291 0.113 Uiso 1 1 calc R A .
H10H H 0.9702 0.5805 0.1912 0.113 Uiso 1 1 calc R . .
H10I H 1.0233 0.6218 0.1836 0.113 Uiso 1 1 calc R . .
C111 C 0.79802(6) 0.77713(7) 0.39357(5) 0.0270(10) Uani 1 1 d G . .
C112 C 0.78675(6) 0.82691(6) 0.36715(6) 0.0295(11) Uani 1 1 d G . .
C113 C 0.79820(8) 0.87567(7) 0.39545(7) 0.0334(12) Uani 1 1 d G . .
C114 C 0.82092(9) 0.87467(8) 0.45017(7) 0.0369(13) Uani 1 1 d G . .
H114 H 0.8287 0.9080 0.4695 0.044 Uiso 1 1 calc R . .
C115 C 0.83219(9) 0.82489(9) 0.47659(6) 0.0413(14) Uani 1 1 d G . .
H115 H 0.8477 0.8242 0.5140 0.050 Uiso 1 1 calc R . .
C116 C 0.82074(7) 0.77612(8) 0.44829(6) 0.0345(12) Uani 1 1 d G . .
H116 H 0.8284 0.7421 0.4663 0.041 Uiso 1 1 calc R . .
C117 C 0.78395(5) 0.72488(6) 0.36981(5) 0.0273(11) Uani 1 1 d G . .
H117 H 0.7935 0.6937 0.3920 0.033 Uiso 1 1 calc R . .
C118 C 0.74040(6) 0.66005(6) 0.30736(6) 0.0247(10) Uani 1 1 d G . .
C119 C 0.74757(7) 0.63823(6) 0.25198(6) 0.0247(10) Uani 1 1 d G . .
C120 C 0.72858(8) 0.58423(7) 0.24340(8) 0.0306(11) Uani 1 1 d G . .
H120 H 0.7326 0.5679 0.2070 0.037 Uiso 1 1 calc R . .
C121 C 0.70376(9) 0.55388(6) 0.28763(9) 0.0406(13) Uani 1 1 d G . .
H121 H 0.6922 0.5170 0.2814 0.049 Uiso 1 1 calc R . .
C122 C 0.69617(8) 0.57755(7) 0.33991(8) 0.0386(13) Uani 1 1 d G . .
H122 H 0.6791 0.5570 0.3697 0.046 Uiso 1 1 calc R . .
C123 C 0.71295(7) 0.63037(6) 0.34941(7) 0.0289(11) Uani 1 1 d G . .
H123 H 0.7057 0.6469 0.3852 0.035 Uiso 1 1 calc R . .

C124 C 0.77754(8) 0.66710(7) 0.20453(6) 0.0227(9) Uani 1 1 d G . .
H12A H 0.8197 0.6606 0.2080 0.027 Uiso 1 1 calc R . .
H12B H 0.7645 0.6511 0.1681 0.027 Uiso 1 1 calc R . .
C125 C 0.83322(10) 0.94545(7) 0.33547(9) 0.0433(14) Uani 1 1 d G . .
H12C H 0.8681 0.9524 0.3583 0.065 Uiso 1 1 calc R . .
H12D H 0.8210 0.9795 0.3169 0.065 Uiso 1 1 calc R . .
H12E H 0.8417 0.9178 0.3066 0.065 Uiso 1 1 calc R . .
C131 C 0.65153(19) 0.8016(2) 0.43433(19) 0.0287(10) Uani 1 1 d . . .
C132 C 0.63589(17) 0.7472(2) 0.42300(17) 0.0243(10) Uani 1 1 d . B .
C133 C 0.6438(2) 0.7076(2) 0.46601(19) 0.0328(12) Uani 1 1 d . . .
C134 C 0.6705(2) 0.7218(3) 0.5171(2) 0.0394(14) Uani 1 1 d . B .
H134 H 0.6767 0.6946 0.5454 0.047 Uiso 1 1 calc R . .
C135 C 0.6878(2) 0.7749(3) 0.5271(2) 0.0437(15) Uani 1 1 d . . .
H135 H 0.7063 0.7842 0.5619 0.052 Uiso 1 1 calc R B .
C136 C 0.6785(2) 0.8142(3) 0.4869(2) 0.0373(13) Uani 1 1 d . B .
H136 H 0.6902 0.8508 0.4944 0.045 Uiso 1 1 calc R . .
C137 C 0.6411(2) 0.8456(2) 0.39597(19) 0.0296(11) Uani 1 1 d . B .
H137 H 0.6539 0.8809 0.4074 0.036 Uiso 1 1 calc R . .
C138 C 0.61157(9) 0.88976(9) 0.31188(10) 0.0315(10) Uani 1 1 d GU B 1
C139 C 0.55844(9) 0.89927(9) 0.28567(11) 0.0378(12) Uani 1 1 d GU B 1
C140 C 0.54954(11) 0.94710(10) 0.25490(13) 0.0556(16) Uani 1 1 d GU B 1
H140 H 0.5132 0.9536 0.2370 0.067 Uiso 1 1 calc R B 1
C141 C 0.59376(13) 0.98543(10) 0.25033(13) 0.0624(17) Uani 1 1 d GU B 1
H141 H 0.5877 1.0181 0.2293 0.075 Uiso 1 1 calc R B 1
C142 C 0.64689(12) 0.97592(11) 0.27653(14) 0.0487(14) Uani 1 1 d GU B 1
H142 H 0.6771 1.0021 0.2734 0.058 Uiso 1 1 calc R B 1
C143 C 0.65580(10) 0.92809(11) 0.30731(13) 0.0370(11) Uani 1 1 d GU B 1
H143 H 0.6921 0.9216 0.3252 0.044 Uiso 1 1 calc R B 1
C144 C 0.50960(11) 0.85464(12) 0.28557(16) 0.0365(12) Uani 1 1 d G . .
H14A H 0.4923 0.8526 0.3239 0.044 Uiso 1 1 calc R B 1
H14B H 0.4787 0.8657 0.2586 0.044 Uiso 1 1 calc R B 1
C145 C 0.6172(3) 0.6187(2) 0.4969(3) 0.084(3) Uiso 1 1 d G . .
H14C H 0.6546 0.6010 0.5044 0.126 Uiso 1 1 calc R B .
H14D H 0.5885 0.5908 0.4866 0.126 Uiso 1 1 calc R . .
H14E H 0.6045 0.6381 0.5310 0.126 Uiso 1 1 calc R . .
C151 C 0.34409(18) 0.7055(2) 0.29446(18) 0.0261(10) Uani 1 1 d . . .
C152 C 0.36160(19) 0.7611(2) 0.29453(17) 0.0262(10) Uani 1 1 d . . .
C153 C 0.3213(2) 0.8011(2) 0.31445(19) 0.0314(11) Uani 1 1 d . . .
C154 C 0.2668(2) 0.7858(2) 0.3315(2) 0.0346(12) Uani 1 1 d . . .
H154 H 0.2406 0.8130 0.3446 0.042 Uiso 1 1 calc R . .
C155 C 0.2495(2) 0.7314(3) 0.3299(2) 0.0372(13) Uani 1 1 d . . .
H155 H 0.2115 0.7216 0.3414 0.045 Uiso 1 1 calc R . .
C156 C 0.2869(2) 0.6920(2) 0.3119(2) 0.0333(11) Uani 1 1 d . . .
H156 H 0.2746 0.6549 0.3109 0.040 Uiso 1 1 calc R . .
C157 C 0.38098(18) 0.6617(2) 0.27719(17) 0.0246(9) Uani 1 1 d . . .
H157 H 0.3645 0.6260 0.2773 0.030 Uiso 1 1 calc R . .
C158 C 0.46294(19) 0.61663(19) 0.24377(17) 0.0221(9) Uani 1 1 d . . .
C159 C 0.52198(19) 0.6083(2) 0.25736(17) 0.0232(9) Uani 1 1 d . . .
C160 C 0.5486(2) 0.5597(2) 0.24054(19) 0.0282(10) Uani 1 1 d . . .
H160 H 0.5880 0.5534 0.2505 0.034 Uiso 1 1 calc R . .

C161 C 0.5188(2) 0.5206(2) 0.2096(2) 0.0330(11) Uani 1 1 d . . .
H161 H 0.5375 0.4876 0.1990 0.040 Uiso 1 1 calc R . .
C162 C 0.4614(2) 0.5295(2) 0.1940(2) 0.0303(11) Uani 1 1 d . . .
H162 H 0.4411 0.5028 0.1724 0.036 Uiso 1 1 calc R . .
C163 C 0.43390(19) 0.5778(2) 0.21027(18) 0.0265(10) Uani 1 1 d . . .
H163 H 0.3951 0.5844 0.1985 0.032 Uiso 1 1 calc R . .
C164 C 0.55707(18) 0.6489(2) 0.29299(18) 0.0238(9) Uani 1 1 d . . .
H16A H 0.5458 0.6450 0.3333 0.029 Uiso 1 1 calc R . .
H16B H 0.5987 0.6396 0.2901 0.029 Uiso 1 1 calc R . .
C165 C 0.3023(4) 0.8949(4) 0.3277(4) 0.102(3) Uiso 1 1 d . . .
H16C H 0.3186 0.9306 0.3177 0.152 Uiso 1 1 calc R . .
H16D H 0.2935 0.8941 0.3683 0.152 Uiso 1 1 calc R . .
H16E H 0.2667 0.8887 0.3058 0.152 Uiso 1 1 calc R . .
C1 C 0.6133(7) 0.6452(7) 0.1273(7) 0.072(4) Uiso 0.50 1 d PU . .
C2 C 0.6288(3) 0.6999(3) 0.1337(3) 0.0089(13) Uiso 0.50 1 d PU . .
C3 C 0.5928(3) 0.7440(3) 0.1166(3) 0.0077(12) Uiso 0.50 1 d PU . .
C4 C 0.6151(3) 0.8012(3) 0.1229(3) 0.0077(12) Uiso 0.50 1 d PU . .
C5 C 0.5787(6) 0.8423(6) 0.1151(6) 0.057(3) Uiso 0.50 1 d PU . .
C6 C 0.6002(9) 0.8950(8) 0.1285(8) 0.089(5) Uiso 0.50 1 d PU . .

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Fe1 0.0128(3) 0.0230(3) 0.0110(2) -0.0004(2) 0.0026(2) 0.0010(2)
Fe2 0.0120(3) 0.0218(3) 0.0102(2) -0.0006(2) 0.0017(2) 0.0002(2)
Fe3 0.0105(3) 0.0269(3) 0.0143(3) -0.0017(2) -0.0004(2) -0.0009(2)
Fe4 0.0099(3) 0.0306(4) 0.0137(3) -0.0001(2) 0.0003(2) -0.0026(2)
Fe5 0.0231(3) 0.0413(4) 0.0118(3) -0.0006(3) -0.0002(2) -0.0110(3)
Fe6 0.0154(3) 0.0347(4) 0.0134(3) -0.0016(3) -0.0004(2) -0.0009(3)
Fe7 0.0130(3) 0.0315(4) 0.0166(3) -0.0051(3) -0.0033(2) -0.0002(2)
Fe8 0.0118(3) 0.0299(3) 0.0139(3) -0.0013(2) -0.0011(2) -0.0006(2)
O1 0.0122(13) 0.0320(18) 0.0176(13) -0.0024(12) -0.0015(11) -0.0020(12)
O2 0.0284(17) 0.0376(19) 0.0142(14) -0.0010(13) -0.0003(12) -0.0080(15)
O3 0.0181(14) 0.039(2) 0.0177(14) -0.0035(13) -0.0007(12) 0.0018(14)
O4 0.0146(13) 0.0269(16) 0.0132(13) -0.0020(12) -0.0006(11) -0.0008(12)
O11 0.0130(13) 0.0268(17) 0.0217(14) -0.0009(12) 0.0027(11) 0.0006(12)
O12 0.0235(15) 0.0214(16) 0.0116(12) -0.0004(11) 0.0059(11) 0.0035(12)
O13 0.0199(16) 0.0307(19) 0.052(2) -0.0048(17) 0.0044(15) -0.0033(14)
O31 0.0180(14) 0.0242(16) 0.0141(13) 0.0005(12) -0.0028(11) 0.0027(12)
O32 0.0191(14) 0.0234(16) 0.0117(12) 0.0007(11) 0.0047(11) 0.0023(12)
O33 0.0242(15) 0.0277(17) 0.0209(14) 0.0013(13) -0.0042(12) 0.0018(13)
O51 0.0243(15) 0.0279(17) 0.0162(13) -0.0020(12) -0.0011(12) 0.0035(13)
O52 0.0117(13) 0.0282(17) 0.0244(15) -0.0009(13) -0.0037(11) -0.0004(12)
O53 0.0335(18) 0.036(2) 0.0212(15) -0.0083(14) 0.0051(13) 0.0027(15)
O71 0.0152(14) 0.041(2) 0.0358(18) 0.0144(16) 0.0085(13) 0.0001(14)

O72 0.0148(13) 0.0250(17) 0.0248(15) -0.0051(13) -0.0045(12) -0.0003(12)
O73 0.0328(19) 0.043(2) 0.046(2) 0.0190(18) 0.0131(17) -0.0044(17)
O91 0.0224(16) 0.061(3) 0.0248(16) -0.0016(17) 0.0021(13) -0.0087(17)
O92 0.0377(19) 0.0332(19) 0.0199(15) -0.0014(14) 0.0002(14) -0.0081(16)
O93 0.0271(19) 0.085(4) 0.049(2) -0.008(2) -0.0055(18) 0.010(2)
O111 0.0261(16) 0.042(2) 0.0174(14) -0.0053(14) -0.0061(12) 0.0035(15)
O112 0.0246(15) 0.0334(18) 0.0149(13) -0.0011(13) 0.0067(12) 0.0020(14)
O113 0.0278(18) 0.044(2) 0.040(2) -0.0129(17) -0.0020(15) 0.0014(16)
O131 0.0252(16) 0.046(2) 0.0153(14) -0.0029(14) -0.0022(12) -0.0020(15)
O132 0.0151(14) 0.0342(19) 0.0322(17) -0.0027(15) -0.0091(13) -0.0004(13)
O133 0.057(2) 0.055(3) 0.0188(16) 0.0065(17) 0.0084(16) -0.011(2)
O151 0.0200(15) 0.0339(19) 0.0220(15) -0.0011(13) 0.0074(12) -0.0007(13)
O152 0.0153(14) 0.0269(17) 0.0236(15) 0.0003(13) -0.0071(12) 0.0023(12)
O153 0.038(2) 0.039(2) 0.045(2) -0.0039(17) 0.0240(17) 0.0039(17)
N11 0.0156(16) 0.0249(19) 0.0133(15) 0.0032(14) -0.0014(13) 0.0036(14)
N31 0.0126(15) 0.0202(18) 0.0167(15) -0.0004(14) 0.0019(12) -0.0017(13)
N51 0.0130(15) 0.029(2) 0.0167(16) -0.0013(15) 0.0015(13) -0.0039(14)
N71 0.0160(16) 0.034(2) 0.0146(15) -0.0002(15) -0.0004(13) -0.0026(15)
N91 0.053(3) 0.058(3) 0.0122(17) 0.0024(19) -0.0039(18) -0.025(2)
N111 0.0111(15) 0.039(2) 0.0140(15) 0.0021(15) 0.0018(13) 0.0024(15)
N131 0.0150(17) 0.035(2) 0.0271(19) -0.0127(17) -0.0030(15) 0.0027(16)
N151 0.0160(16) 0.037(2) 0.0135(15) 0.0007(15) -0.0009(13) -0.0036(16)
C10A 0.051(7) 0.050(7) 0.014(5) -0.004(5) 0.004(5) -0.021(5)
C10F 0.048(7) 0.051(7) 0.019(5) 0.000(5) 0.004(5) -0.020(5)
C10E 0.056(8) 0.051(7) 0.024(5) 0.004(5) 0.000(5) -0.023(6)
C10D 0.059(8) 0.051(7) 0.029(5) -0.006(5) -0.003(6) -0.024(6)
C10C 0.056(7) 0.054(7) 0.029(5) -0.005(5) 0.005(5) -0.023(5)
C10B 0.054(7) 0.050(7) 0.015(4) -0.002(5) 0.009(5) -0.025(5)
C11 0.0148(19) 0.033(2) 0.0110(17) 0.0003(17) 0.0021(15) 0.0035(17)
C12 0.0132(18) 0.035(3) 0.0162(18) 0.0017(18) 0.0049(15) 0.0002(17)
C13 0.019(2) 0.031(3) 0.024(2) 0.0013(19) 0.0027(17) 0.0020(19)
C14 0.017(2) 0.040(3) 0.040(3) 0.005(2) 0.0037(19) -0.005(2)
C15 0.018(2) 0.042(3) 0.027(2) 0.003(2) 0.0074(18) 0.008(2)
C16 0.0149(19) 0.039(3) 0.020(2) -0.0008(19) 0.0024(16) 0.0030(19)
C17 0.0157(19) 0.032(2) 0.0147(18) -0.0011(17) -0.0002(15) 0.0038(17)
C18 0.0150(18) 0.029(2) 0.0164(18) -0.0004(17) 0.0040(15) -0.0019(17)
C19 0.029(2) 0.024(2) 0.020(2) 0.0010(18) 0.0023(18) 0.0025(19)
C20 0.027(2) 0.031(3) 0.023(2) 0.0037(19) 0.0093(18) 0.004(2)
C21 0.035(3) 0.025(2) 0.031(2) 0.001(2) -0.002(2) -0.004(2)
C22 0.034(2) 0.030(3) 0.022(2) -0.0020(19) -0.0020(19) 0.008(2)
C23 0.0176(19) 0.027(2) 0.0182(19) -0.0021(17) 0.0018(16) 0.0033(17)
C24 0.036(3) 0.024(2) 0.020(2) 0.0035(18) 0.0059(19) 0.006(2)
C31 0.0143(18) 0.025(2) 0.0157(18) -0.0003(16) 0.0018(15) -0.0018(16)
C32 0.0081(16) 0.032(2) 0.0124(17) -0.0038(16) 0.0008(14) -0.0013(16)
C33 0.0153(19) 0.029(2) 0.0184(19) -0.0016(17) -0.0025(16) 0.0011(17)
C34 0.021(2) 0.033(3) 0.019(2) 0.0045(19) -0.0035(17) 0.0017(19)
C35 0.034(3) 0.039(3) 0.016(2) -0.004(2) -0.0063(18) -0.004(2)
C36 0.028(2) 0.029(3) 0.020(2) -0.0063(18) -0.0020(18) -0.0002(19)
C37 0.0158(18) 0.024(2) 0.0165(18) -0.0032(16) 0.0026(15) -0.0029(16)
C38 0.0119(17) 0.021(2) 0.0202(19) -0.0028(16) -0.0004(15) 0.0003(16)

C39 0.020(2) 0.024(2) 0.0151(18) -0.0030(16) -0.0018(16) 0.0024(17)
C40 0.029(2) 0.025(2) 0.020(2) 0.0039(18) -0.0024(18) 0.0014(19)
C41 0.026(2) 0.025(2) 0.033(2) -0.003(2) -0.0052(19) 0.0078(19)
C42 0.019(2) 0.022(2) 0.038(3) -0.009(2) 0.0004(19) 0.0018(18)
C43 0.0154(19) 0.030(2) 0.021(2) -0.0064(18) 0.0036(16) 0.0005(17)
C44 0.024(2) 0.023(2) 0.0202(19) 0.0024(17) 0.0097(17) 0.0028(18)
C45 0.034(3) 0.031(3) 0.030(2) 0.004(2) -0.010(2) 0.003(2)
C51 0.018(2) 0.033(3) 0.0181(19) -0.0039(18) 0.0028(16) -0.0035(18)
C52 0.0128(18) 0.034(3) 0.0189(19) -0.0057(18) 0.0052(15) -0.0034(17)
C53 0.021(2) 0.036(3) 0.022(2) -0.0007(19) 0.0033(17) -0.0070(19)
C54 0.033(3) 0.037(3) 0.021(2) -0.007(2) 0.0035(19) -0.005(2)
C55 0.034(3) 0.056(4) 0.014(2) -0.009(2) -0.0009(19) -0.007(2)
C56 0.024(2) 0.039(3) 0.028(2) 0.001(2) -0.0043(19) -0.002(2)
C57 0.0103(17) 0.033(3) 0.023(2) 0.0052(18) -0.0023(16) -0.0032(17)
C58 0.020(2) 0.024(2) 0.0180(19) 0.0016(17) 0.0024(16) -0.0033(17)
C59 0.022(2) 0.021(2) 0.027(2) -0.0035(18) -0.0003(18) -0.0002(18)
C60 0.030(2) 0.028(3) 0.028(2) -0.004(2) -0.0088(19) -0.004(2)
C61 0.031(2) 0.021(2) 0.032(2) -0.0025(19) 0.004(2) 0.0022(19)
C62 0.021(2) 0.022(2) 0.026(2) 0.0080(18) 0.0029(17) 0.0041(18)
C63 0.0180(19) 0.030(2) 0.0171(19) 0.0039(17) 0.0008(16) -0.0038(18)
C64 0.0124(19) 0.029(3) 0.036(2) -0.005(2) -0.0038(18) -0.0038(18)
C65 0.054(3) 0.042(3) 0.030(3) -0.007(2) 0.005(2) 0.002(3)
C71 0.0145(19) 0.049(3) 0.0146(18) -0.0027(19) 0.0021(16) -0.0051(19)
C72 0.017(2) 0.046(3) 0.0133(18) 0.0013(19) 0.0043(16) -0.006(2)
C73 0.021(2) 0.048(3) 0.017(2) 0.005(2) 0.0036(17) -0.007(2)
C74 0.024(2) 0.056(4) 0.020(2) 0.006(2) 0.0048(18) -0.016(2)
C75 0.012(2) 0.075(4) 0.031(2) 0.008(3) 0.0091(19) -0.009(2)
C76 0.021(2) 0.053(3) 0.027(2) -0.005(2) 0.0046(19) 0.000(2)
C77 0.019(2) 0.039(3) 0.021(2) -0.004(2) -0.0014(17) 0.0031(19)
C78 0.018(2) 0.030(2) 0.023(2) -0.0006(18) 0.0046(17) 0.0026(18)
C79 0.018(2) 0.027(2) 0.033(2) -0.002(2) 0.0001(18) 0.0026(18)
C80 0.025(2) 0.032(3) 0.047(3) 0.005(2) 0.000(2) -0.002(2)
C81 0.032(3) 0.029(3) 0.054(3) 0.015(2) -0.001(2) 0.002(2)
C82 0.034(3) 0.041(3) 0.035(3) 0.011(2) -0.008(2) 0.006(2)
C83 0.021(2) 0.040(3) 0.024(2) 0.002(2) -0.0013(18) -0.002(2)
C84 0.022(2) 0.027(3) 0.033(2) -0.003(2) -0.0090(19) -0.0014(19)
C85 0.034(3) 0.052(4) 0.062(4) 0.022(3) 0.012(3) -0.011(3)
C91 0.037(3) 0.085(5) 0.021(2) -0.007(3) -0.003(2) -0.027(3)
C92 0.022(2) 0.082(5) 0.020(2) -0.018(3) 0.0004(19) -0.021(3)
C93 0.021(2) 0.085(5) 0.036(3) -0.022(3) -0.007(2) -0.004(3)
C94 0.025(3) 0.129(7) 0.056(4) -0.035(5) 0.011(3) -0.017(4)
C95 0.032(3) 0.162(9) 0.050(4) -0.029(5) 0.017(3) -0.030(5)
C96 0.053(4) 0.133(8) 0.031(3) -0.013(4) 0.007(3) -0.052(5)
C97 0.064(4) 0.078(5) 0.010(2) -0.004(2) -0.001(2) -0.052(4)
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C99 0.024(4) 0.024(4) 0.024(4) -0.003(3) -0.002(3) -0.009(3)
C100 0.025(4) 0.029(4) 0.023(4) -0.006(3) 0.002(3) -0.002(3)
C101 0.029(4) 0.027(4) 0.023(4) 0.003(3) -0.001(3) -0.003(3)
C102 0.029(4) 0.030(4) 0.019(4) -0.002(3) -0.002(3) -0.007(4)
C103 0.031(4) 0.032(4) 0.019(4) -0.005(3) 0.004(3) -0.006(3)

C104 0.054(3) 0.037(3) 0.029(2) -0.002(2) -0.006(2) -0.011(3)
C111 0.0129(19) 0.049(3) 0.019(2) -0.008(2) 0.0018(16) 0.0036(19)
C112 0.0120(19) 0.053(3) 0.023(2) -0.012(2) 0.0013(17) 0.004(2)
C113 0.015(2) 0.054(4) 0.031(2) -0.010(2) 0.0000(18) -0.002(2)
C114 0.020(2) 0.062(4) 0.029(2) -0.014(3) 0.0003(19) -0.003(2)
C115 0.026(2) 0.078(5) 0.020(2) -0.016(3) 0.0004(19) -0.004(3)
C116 0.022(2) 0.060(4) 0.022(2) -0.006(2) 0.0003(18) 0.004(2)
C117 0.016(2) 0.049(3) 0.0165(19) 0.005(2) 0.0011(16) 0.010(2)
C118 0.0141(19) 0.039(3) 0.020(2) 0.0003(19) -0.0027(16) 0.0034(19)
C119 0.0122(18) 0.038(3) 0.024(2) 0.005(2) -0.0018(16) -0.0007(18)
C120 0.021(2) 0.037(3) 0.034(2) 0.004(2) -0.0021(19) 0.003(2)
C121 0.029(3) 0.034(3) 0.059(4) 0.021(3) -0.009(2) 0.001(2)
C122 0.025(2) 0.052(4) 0.040(3) 0.024(3) 0.005(2) 0.006(2)
C123 0.019(2) 0.046(3) 0.022(2) 0.015(2) 0.0035(17) 0.007(2)
C124 0.018(2) 0.035(3) 0.0148(18) -0.0021(18) -0.0004(16) 0.0030(18)
C125 0.034(3) 0.054(4) 0.042(3) 0.001(3) 0.000(2) -0.002(3)
C131 0.018(2) 0.045(3) 0.023(2) -0.008(2) -0.0002(17) 0.001(2)
C132 0.0119(18) 0.046(3) 0.0145(18) -0.0039(19) 0.0034(15) 0.0035(18)
C133 0.024(2) 0.056(3) 0.018(2) -0.005(2) 0.0078(18) -0.005(2)
C134 0.028(3) 0.073(4) 0.017(2) 0.007(2) -0.0006(19) -0.006(3)
C135 0.033(3) 0.079(5) 0.019(2) -0.007(3) -0.006(2) -0.011(3)
C136 0.020(2) 0.059(4) 0.033(3) -0.016(3) -0.005(2) -0.007(2)
C137 0.025(2) 0.037(3) 0.027(2) -0.019(2) 0.0001(19) -0.001(2)
C138 0.025(2) 0.029(2) 0.040(3) -0.006(2) -0.004(2) -0.0002(19)
C139 0.031(2) 0.027(3) 0.055(3) -0.002(2) -0.014(2) 0.002(2)
C140 0.048(3) 0.039(3) 0.080(4) 0.006(3) -0.035(3) -0.005(3)
C141 0.065(4) 0.037(3) 0.084(4) 0.010(3) -0.035(3) -0.018(3)
C142 0.048(3) 0.031(3) 0.067(4) -0.007(3) -0.014(3) -0.015(2)
C143 0.029(2) 0.033(3) 0.050(3) -0.013(2) -0.010(2) -0.004(2)
C144 0.023(2) 0.032(3) 0.054(3) -0.010(2) -0.010(2) 0.004(2)
C151 0.0152(19) 0.046(3) 0.0172(19) 0.002(2) -0.0013(16) -0.004(2)
C152 0.018(2) 0.049(3) 0.0124(18) 0.0005(19) 0.0007(16) -0.001(2)
C153 0.026(2) 0.048(3) 0.020(2) 0.003(2) 0.0056(18) 0.007(2)
C154 0.024(2) 0.050(3) 0.031(2) 0.000(2) 0.009(2) 0.005(2)
C155 0.018(2) 0.060(4) 0.034(3) -0.004(3) 0.010(2) 0.000(2)
C156 0.022(2) 0.046(3) 0.031(2) 0.002(2) 0.0062(19) -0.009(2)
C157 0.019(2) 0.035(3) 0.020(2) 0.0007(19) 0.0001(16) -0.0032(19)
C158 0.024(2) 0.027(2) 0.0156(18) 0.0029(17) 0.0047(16) 0.0012(18)
C159 0.021(2) 0.032(3) 0.0157(18) 0.0050(18) -0.0001(16) -0.0064(19)
C160 0.027(2) 0.029(3) 0.028(2) 0.002(2) -0.0034(19) 0.004(2)
C161 0.044(3) 0.027(3) 0.027(2) 0.005(2) 0.001(2) 0.005(2)
C162 0.036(3) 0.030(3) 0.025(2) 0.005(2) -0.001(2) -0.006(2)
C163 0.019(2) 0.041(3) 0.019(2) 0.010(2) -0.0044(17) -0.008(2)
C164 0.019(2) 0.034(3) 0.0183(19) -0.0033(18) -0.0020(16) 0.0044(19)

_geom_special_details
;
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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Fe1 N11 2.117(4) . ?
Fe2 O1 1.804(3) . ?
Fe2 O31 1.913(3) . ?
Fe2 O32 1.974(3) . ?
Fe2 O12 2.007(3) . ?
Fe2 N31 2.117(4) . ?
Fe3 O1 1.801(3) . ?
Fe3 O51 1.916(3) . ?
Fe3 O52 1.967(3) . ?
Fe3 O72 2.004(3) . ?
Fe3 N51 2.122(4) . ?
Fe4 O2 1.787(3) . ?
Fe4 O71 1.904(3) . ?
Fe4 O72 1.991(3) . ?
Fe4 O52 1.997(3) . ?
Fe4 N71 2.098(4) . ?
Fe5 O2 1.782(3) . ?
Fe5 O91 1.920(4) . ?
Fe5 O92 1.972(3) . ?
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Fe5 N91 2.116(4) . ?
Fe6 O3 1.792(3) . ?
Fe6 O111 1.935(3) . ?
Fe6 O112 1.973(3) . ?
Fe6 O92 2.003(3) . ?
Fe6 N111 2.100(4) . ?
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Fe7 O131 1.903(3) . ?
Fe7 O132 1.968(3) . ?
Fe7 O152 2.021(3) . ?
Fe7 N131 2.124(4) . ?
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Fe8 O152 1.968(3) . ?
Fe8 O132 2.014(3) . ?

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O11 C12 1.325(5) . ?
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N71 C78 1.433(6) . ?
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H45A C45 H45B 109.5 . . ?
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H14D C145 H14E 109.5 . . ?
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C163 C158 N151 120.8(4) . . ?
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C163 C162 H162 120.2 . . ?
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C158 C163 H163 119.7 . . ?
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C159 C164 H16A 108.9 . . ?
O152 C164 H16B 108.9 . . ?
C159 C164 H16B 108.9 . . ?
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O153 C165 H16D 109.5 . . ?
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O153 C165 H16E 109.5 . . ?
H16C C165 H16E 109.5 . . ?
H16D C165 H16E 109.5 . . ?
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C5 C4 C3 118.5(8) . . ?
C4 C5 C6 116.0(13) . . ?

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O52 Fe4 O72 Fe3 5.83(12) . . . . ?
N71 Fe4 O72 Fe3 -154.18(14) . . . . ?
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O91 Fe5 N91 C98 -179.4(3) . . . . ?
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O92 Fe5 N91 C97 148.8(4) . . . . ?
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O131 Fe7 N131 C138 -179.9(2) . . . . ?
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O152 Fe8 N151 C157 145.7(3) . . . . ?
O132 Fe8 N151 C157 94.6(4) . . . . ?
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O151 Fe8 N151 C158 177.6(3) . . . . ?
O152 Fe8 N151 C158 -44.5(3) . . . . ?
O132 Fe8 N151 C158 -95.6(4) . . . . ?
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C97 N91 C10A C10F 36.8(5) . . . . ?

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C98 N91 C10A C10B -163.0(15) . . . . ?
C97 N91 C10A C10B -144.8(4) . . . . ?
Fe5 N91 C10A C10B 47.6(3) . . . . ?
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C10F C10E C10D C10C 0.0 . . . . ?
C10E C10D C10C C10B 0.0 . . . . ?
C10D C10C C10B C10A 0.0 . . . . ?
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C10F C10A C10B C104 -173.6(4) . . . . ?
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Fe1 O11 C12 C11 -0.9(6) . . . . ?
C16 C11 C12 O11 -177.4(4) . . . . ?
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C16 C11 C12 C13 3.6(6) . . . . ?
C17 C11 C12 C13 -173.5(4) . . . . ?
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C25 O13 C13 C12 -160.4(4) . . . . ?
O11 C12 C13 O13 -2.9(6) . . . . ?
C11 C12 C13 O13 176.1(4) . . . . ?
O11 C12 C13 C14 178.3(4) . . . . ?
C11 C12 C13 C14 -2.7(6) . . . . ?
O13 C13 C14 C15 -178.7(4) . . . . ?
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C17 N11 C18 C23 41.2(6) . . . . ?
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C17 N11 C18 C19 -141.6(4) . . . . ?
Fe1 N11 C18 C19 49.0(5) . . . . ?
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N11 C18 C19 C20 -179.7(4) . . . . ?
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C19 C20 C21 C22 0.8(7) . . . . ?
C20 C21 C22 C23 0.2(7) . . . . ?
C21 C22 C23 C18 -2.4(7) . . . . ?

C19 C18 C23 C22 3.6(7) . . . . ?
N11 C18 C23 C22 -179.3(4) . . . . ?
Fe1 O12 C24 C19 38.5(5) . . . . ?
Fe2 O12 C24 C19 -162.4(3) . . . . ?
C20 C19 C24 O12 132.8(4) . . . . ?
C18 C19 C24 O12 -51.3(6) . . . . ?
Fe2 O31 C32 C33 -177.1(3) . . . . ?
Fe2 O31 C32 C31 2.6(6) . . . . ?
C36 C31 C32 O31 -179.5(4) . . . . ?
C37 C31 C32 O31 -1.0(6) . . . . ?
C36 C31 C32 C33 0.1(5) . . . . ?
C37 C31 C32 C33 178.6(4) . . . . ?
C45 O33 C33 C34 -13.3(6) . . . . ?
C45 O33 C33 C32 167.0(4) . . . . ?
O31 C32 C33 O33 -1.6(5) . . . . ?
C31 C32 C33 O33 178.7(3) . . . . ?
O31 C32 C33 C34 178.7(4) . . . . ?
C31 C32 C33 C34 -1.0(6) . . . . ?
O33 C33 C34 C35 -178.8(4) . . . . ?
C32 C33 C34 C35 1.0(6) . . . . ?
C33 C34 C35 C36 0.0(7) . . . . ?
C34 C35 C36 C31 -0.9(7) . . . . ?
C32 C31 C36 C35 0.8(6) . . . . ?
C37 C31 C36 C35 -177.8(4) . . . . ?
C38 N31 C37 C31 -173.3(4) . . . . ?
Fe2 N31 C37 C31 -3.2(5) . . . . ?
C36 C31 C37 N31 -179.8(4) . . . . ?
C32 C31 C37 N31 1.6(6) . . . . ?
C37 N31 C38 C43 41.7(5) . . . . ?
Fe2 N31 C38 C43 -129.3(4) . . . . ?
C37 N31 C38 C39 -139.5(4) . . . . ?
Fe2 N31 C38 C39 49.4(4) . . . . ?
C43 C38 C39 C40 -2.4(6) . . . . ?
N31 C38 C39 C40 178.9(4) . . . . ?
C43 C38 C39 C44 -177.5(4) . . . . ?
N31 C38 C39 C44 3.8(6) . . . . ?
C38 C39 C40 C41 -0.4(7) . . . . ?
C44 C39 C40 C41 174.7(4) . . . . ?
C39 C40 C41 C42 1.2(7) . . . . ?
C40 C41 C42 C43 0.8(7) . . . . ?
C41 C42 C43 C38 -3.7(7) . . . . ?
C39 C38 C43 C42 4.4(7) . . . . ?
N31 C38 C43 C42 -176.9(4) . . . . ?
Fe2 O32 C44 C39 42.1(5) . . . . ?
Fe1 O32 C44 C39 -163.5(3) . . . . ?
C40 C39 C44 O32 132.9(4) . . . . ?
C38 C39 C44 O32 -52.1(6) . . . . ?
Fe3 O51 C52 C51 -3.0(6) . . . . ?
Fe3 O51 C52 C53 175.3(3) . . . . ?
C56 C51 C52 O51 -179.5(4) . . . . ?

C57 C51 C52 O51 2.1(6) . . . . ?
C56 C51 C52 C53 2.1(6) . . . . ?
C57 C51 C52 C53 -176.2(4) . . . . ?
C65 O53 C53 C54 4.0(6) . . . . ?
C65 O53 C53 C52 -175.0(4) . . . . ?
O51 C52 C53 C54 -177.7(4) . . . . ?
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O51 C52 C53 O53 1.3(6) . . . . ?
C51 C52 C53 O53 179.7(4) . . . . ?
O53 C53 C54 C55 178.8(4) . . . . ?
C52 C53 C54 C55 -2.3(7) . . . . ?
C53 C54 C55 C56 1.0(7) . . . . ?
C54 C55 C56 C51 1.9(7) . . . . ?
C52 C51 C56 C55 -3.5(7) . . . . ?
C57 C51 C56 C55 174.9(4) . . . . ?
C58 N51 C57 C51 -179.2(4) . . . . ?
Fe3 N51 C57 C51 -10.7(6) . . . . ?
C52 C51 C57 N51 5.4(7) . . . . ?
C56 C51 C57 N51 -173.0(4) . . . . ?
C57 N51 C58 C63 41.3(5) . . . . ?
Fe3 N51 C58 C63 -128.3(3) . . . . ?
C57 N51 C58 C59 -140.2(4) . . . . ?
Fe3 N51 C58 C59 50.2(4) . . . . ?
C63 C58 C59 C60 -1.1(6) . . . . ?
N51 C58 C59 C60 -179.6(4) . . . . ?
C63 C58 C59 C64 -178.3(4) . . . . ?
N51 C58 C59 C64 3.2(6) . . . . ?
C58 C59 C60 C61 -1.3(7) . . . . ?
C64 C59 C60 C61 176.0(4) . . . . ?
C59 C60 C61 C62 1.9(7) . . . . ?
C60 C61 C62 C63 -0.2(7) . . . . ?
C59 C58 C63 C62 2.7(6) . . . . ?
N51 C58 C63 C62 -178.8(4) . . . . ?
C61 C62 C63 C58 -2.0(6) . . . . ?
Fe3 O52 C64 C59 38.7(5) . . . . ?
Fe4 O52 C64 C59 -166.8(3) . . . . ?
C60 C59 C64 O52 132.3(4) . . . . ?
C58 C59 C64 O52 -50.5(6) . . . . ?
Fe4 O71 C72 C71 6.4(7) . . . . ?
Fe4 O71 C72 C73 -172.2(3) . . . . ?
C76 C71 C72 O71 -178.9(4) . . . . ?
C77 C71 C72 O71 -0.4(7) . . . . ?
C76 C71 C72 C73 -0.3(6) . . . . ?
C77 C71 C72 C73 178.2(4) . . . . ?
C85 O73 C73 C74 -12.3(7) . . . . ?
C85 O73 C73 C72 169.4(5) . . . . ?
O71 C72 C73 O73 -4.2(6) . . . . ?
C71 C72 C73 O73 177.1(4) . . . . ?
O71 C72 C73 C74 177.5(4) . . . . ?
C71 C72 C73 C74 -1.2(7) . . . . ?

O73 C73 C74 C75 -177.2(5) . . . . ?
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C73 C74 C75 C76 0.8(8) . . . . ?
C74 C75 C76 C71 -2.3(8) . . . . ?
C72 C71 C76 C75 2.1(7) . . . . ?
C77 C71 C76 C75 -176.5(4) . . . . ?
C78 N71 C77 C71 -173.4(4) . . . . ?
Fe4 N71 C77 C71 -5.3(6) . . . . ?
C72 C71 C77 N71 0.5(7) . . . . ?
C76 C71 C77 N71 179.1(4) . . . . ?
C77 N71 C78 C83 44.5(6) . . . . ?
Fe4 N71 C78 C83 -124.7(4) . . . . ?
C77 N71 C78 C79 -139.6(4) . . . . ?
Fe4 N71 C78 C79 51.2(5) . . . . ?
C83 C78 C79 C80 -2.2(7) . . . . ?
N71 C78 C79 C80 -178.1(4) . . . . ?
C83 C78 C79 C84 177.7(4) . . . . ?
N71 C78 C79 C84 1.8(6) . . . . ?
C78 C79 C80 C81 0.3(8) . . . . ?
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C79 C80 C81 C82 2.0(8) . . . . ?
C80 C81 C82 C83 -2.3(8) . . . . ?
C81 C82 C83 C78 0.4(8) . . . . ?
C79 C78 C83 C82 1.9(7) . . . . ?
N71 C78 C83 C82 177.7(4) . . . . ?
Fe4 O72 C84 C79 39.9(5) . . . . ?
Fe3 O72 C84 C79 -167.6(3) . . . . ?
C80 C79 C84 O72 129.6(5) . . . . ?
C78 C79 C84 O72 -50.3(6) . . . . ?
Fe5 O91 C92 C91 9.7(5) . . . . ?
Fe5 O91 C92 C93 -167.4(2) . . . . ?
C96 C91 C92 O91 -177.1(3) . . . . ?
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C97 C91 C92 C93 -176.7(3) . . . . ?
C105 O93 C93 C94 -3.7(6) . . . . ?
C105 O93 C93 C92 177.9(4) . . . . ?
O91 C92 C93 O93 -4.4(3) . . . . ?
C91 C92 C93 O93 178.4(3) . . . . ?
O91 C92 C93 C94 177.2(3) . . . . ?
C91 C92 C93 C94 0.0 . . . . ?
O93 C93 C94 C95 -178.3(4) . . . . ?
C92 C93 C94 C95 0.0 . . . . ?
C93 C94 C95 C96 0.0 . . . . ?
C94 C95 C96 C91 0.0 . . . . ?
C92 C91 C96 C95 0.0 . . . . ?
C97 C91 C96 C95 176.9(3) . . . . ?
C98 N91 C97 C91 -174.8(4) . . . . ?
C10A N91 C97 C91 -178.4(4) . . . . ?
Fe5 N91 C97 C91 -12.2(6) . . . . ?

C92 C91 C97 N91 -3.4(6) . . . . ?
C96 C91 C97 N91 179.7(4) . . . . ?
C97 N91 C98 C99 -146.6(3) . . . . ?
C10A N91 C98 C99 17.1(14) . . . . ?
Fe5 N91 C98 C99 50.1(3) . . . . ?
C97 N91 C98 C103 36.6(5) . . . . ?
C10A N91 C98 C103 -159.8(15) . . . . ?
Fe5 N91 C98 C103 -126.81(18) . . . . ?
N91 C98 C99 C100 -177.0(3) . . . . ?
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C103 C98 C99 C104 -178.0(3) . . . . ?
C98 C99 C100 C101 0.0 . . . . ?
C104 C99 C100 C101 178.2(2) . . . . ?
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C100 C101 C102 C103 0.0 . . . . ?
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Fe5 O92 C104 C10B 58.2(6) . . . . ?
Fe6 O92 C104 C10B -153.6(3) . . . . ?
Fe5 O92 C104 C99 42.2(6) . . . . ?
Fe6 O92 C104 C99 -169.6(3) . . . . ?
C10C C10B C104 O92 121.7(4) . . . . ?
C10A C10B C104 O92 -65.2(5) . . . . ?
C10C C10B C104 C99 -160.5(12) . . . . ?
C10A C10B C104 C99 12.5(9) . . . . ?
C98 C99 C104 O92 -54.7(5) . . . . ?
C100 C99 C104 O92 127.2(3) . . . . ?
C98 C99 C104 C10B -163.0(11) . . . . ?
C100 C99 C104 C10B 18.9(11) . . . . ?
Fe6 O111 C112 C111 2.8(4) . . . . ?
Fe6 O111 C112 C113 -176.44(19) . . . . ?
C116 C111 C112 O111 -179.21(17) . . . . ?
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C114 C115 C116 C111 0.0 . . . . ?
C112 C111 C116 C115 0.0 . . . . ?
C117 C111 C116 C115 -175.7 . . . . ?
C118 N111 C117 C111 -170.85(12) . . . . ?

Fe6 N111 C117 C111 3.8(3) . . . . ?
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C117 N111 C118 C119 -140.77(18) . . . . ?
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N111 C118 C119 C120 -179.77(16) . . . . ?
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N111 C118 C123 C122 -178.59(16) . . . . ?
Fe6 O112 C124 C119 16.7(3) . . . . ?
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C131 C132 C133 C134 -4.5(6) . . . . ?
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C132 C133 C134 C135 2.0(7) . . . . ?
C133 C134 C135 C136 0.6(8) . . . . ?
C134 C135 C136 C131 -0.7(8) . . . . ?
C132 C131 C136 C135 -1.9(7) . . . . ?
C137 C131 C136 C135 177.2(5) . . . . ?
C138 N131 C137 C131 -176.5(4) . . . . ?
Fe7 N131 C137 C131 -12.9(6) . . . . ?
C132 C131 C137 N131 0.9(7) . . . . ?
C136 C131 C137 N131 -178.2(4) . . . . ?
C137 N131 C138 C139 -135.7(3) . . . . ?
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C137 N131 C138 C143 38.8(4) . . . . ?
Fe7 N131 C138 C143 -126.53(17) . . . . ?
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C143 C138 C139 C144 174.6 . . . . ?
N131 C138 C139 C144 -10.7(2) . . . . ?
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C141 C142 C143 C138 0.0 . . . . ?
C139 C138 C143 C142 0.0 . . . . ?
N131 C138 C143 C142 -174.3(2) . . . . ?
Fe7 O132 C144 C139 49.9(3) . . . . ?
Fe8 O132 C144 C139 -164.53(16) . . . . ?
C138 C139 C144 O132 -47.2(2) . . . . ?
C140 C139 C144 O132 127.4(2) . . . . ?
Fe8 O151 C152 C151 1.8(6) . . . . ?
Fe8 O151 C152 C153 -178.7(3) . . . . ?
C156 C151 C152 O151 -178.1(4) . . . . ?
C157 C151 C152 O151 1.4(7) . . . . ?
C156 C151 C152 C153 2.5(6) . . . . ?
C157 C151 C152 C153 -178.1(4) . . . . ?
C165 O153 C153 C154 -8.6(8) . . . . ?
C165 O153 C153 C152 172.4(6) . . . . ?
O151 C152 C153 O153 -2.1(6) . . . . ?
C151 C152 C153 O153 177.4(4) . . . . ?
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C153 C154 C155 C156 0.9(8) . . . . ?
C154 C155 C156 C151 0.0(8) . . . . ?
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C157 C151 C156 C155 178.8(5) . . . . ?
C158 N151 C157 C151 -177.7(4) . . . . ?
Fe8 N151 C157 C151 -8.0(6) . . . . ?
C152 C151 C157 N151 2.4(7) . . . . ?
C156 C151 C157 N151 -178.1(4) . . . . ?
C157 N151 C158 C163 40.5(5) . . . . ?
Fe8 N151 C158 C163 -129.9(3) . . . . ?
C157 N151 C158 C159 -143.0(4) . . . . ?
Fe8 N151 C158 C159 46.5(5) . . . . ?
C163 C158 C159 C160 -4.6(6) . . . . ?
N151 C158 C159 C160 178.9(4) . . . . ?
C163 C158 C159 C164 179.2(4) . . . . ?
N151 C158 C159 C164 2.7(6) . . . . ?
C158 C159 C160 C161 1.9(7) . . . . ?
C164 C159 C160 C161 178.2(4) . . . . ?
C159 C160 C161 C162 0.8(7) . . . . ?
C160 C161 C162 C163 -0.7(7) . . . . ?
C161 C162 C163 C158 -2.2(7) . . . . ?
C159 C158 C163 C162 4.8(6) . . . . ?
N151 C158 C163 C162 -178.8(4) . . . . ?

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Fe7 O152 C164 C159 -168.8(2) . . . . ?
C160 C159 C164 O152 137.8(4) . . . . ?
C158 C159 C164 O152 -46.0(5) . . . . ?
C1 C2 C3 C4 -177.0(9) . . . . ?
C2 C3 C4 C5 -170.0(9) . . . . ?
C3 C4 C5 C6 172.4(11) . . . . ?

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_refine_diff_density_rms    0.123
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  _platon_squeeze_void_average_x
  _platon_squeeze_void_average_y
  _platon_squeeze_void_average_z
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  _platon_squeeze_void_count_electrons
  _platon_squeeze_void_content
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   2 -0.007  0.500 -0.007      1260       264 ' '
   3  0.098  0.496  0.596         6         1 ' '
   4  0.402  0.996  0.904         6         1 ' '
   5  0.598  0.004  0.096         6         1 ' '
   6  0.902  0.504  0.404         6         1 ' '
_platon_squeeze_details                    ?
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