Electronic Supplementary Material (ESI) for Polymer Chemistry.
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Supporting Information for

Atom Transfer Radical Polymerization by Solvent-stabilized (Me_3TACN)FeX_2: A Practical Access to Reusable Iron(II) Catalysts

So-ichiro Nakanishi,[b] Mitsunobu Kawamura,[a,] Yusuke Sunada,[a] and Hideo Nagashima*[a,b]

[a]*Institute for Materials Chemistry and Engineering,* [b]*Graduate School of Engineering Sciences, Kyushu University, Kasuga, Fukuoka, 816-8580, Japan.*

Contents:

1. Characterization of "(Me_3TACN)FeX_2" complexes, **4'**, **6**, and **7**.

Procedures for preparation of new compounds, **4'**, **6**, and **7**, are described in the experimental section. These complexes were characterized by X ray crystallography, ESI-MS, and elemental analysis.

ESI-MS measurement. Cationic and anionic modes of ESI-MS spectra of **4'** under the standard conditions were collected with cone voltage = 20V and the sample concentration = 0.1 mM. Under the standard conditions (cone voltage = 20V), the parent peak was clearly visible (**Fig. S-17** and **S-18**). Although no signal was observed in the ESI-MS spectra of **6** and **7** under the standard conditions, cationic mode measurement under the forced conditions (cone voltage = 90 V) gave fragment signals including the one due to "(Me_3TACN)$FeBr^+$" (**Fig. S-19** and **S-20**). Actual charts are shown in Actual charts of ESI-MS are shown in **Fig. S17~S20.**

NMR spectra. NMR analysis of these paramagnetic compounds did not give well-resolved spectra. Among them, the trinuclear complex **4'**, which was obtained by recrystallization from acetone and pentane, provided six broad ^{1}H resonances in a range of 0~200 ppm in acetone-d_6 (**Fig. S15**). The spectral pattern is similar to that of the trinuclear chloride homologue **1**, of which assignment was reported by Rauchfuss (ref. 11 in the manucript). When **4'** was dissolved in CD_3OD, only three ^{1}H singals were observed (**Fig. S16**); this is in coincidence with the ^{1}H NMR spectrum of the dinuclear complex **4**, of which crystals were obtained by recrystallization from CH_2Cl_2 and hexane. Attempted measurement of ^{1}H NMR spectra of the mononuclear complexes, **6** and **7**, in several solvents only gave broad bumps, which were unable to be assigned.

X-ray data collection and reduction. X-ray crystallography was performed on a Rigaku Saturn CCD area detector with graphite monochromated Mo-Kα radiation (λ = 0.71070A). The data were collected at 123(2) K using ω scan in the θ range of $2.14 \leq \theta \leq 30.90$ deg (**4'**), $2.95 \leq \theta \leq 30.54$ deg (**6**), $2.36 \leq \theta \leq 30.85$ deg (**7**). The data obtained were processed using Crystal-Clear (Rigaku) on a Pentium computer, and were corrected for Lorentz and polarization effects. The structures were solved by direct methods,[1] and expanded using Fourier techniques.[2] Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement on F2 was based on 9,597 observed reflections and 406 variable parameters for **4'**, 2,810 observed reflections and 163 variable parameters for **6**, 4,511 observed reflections and 202 variable parameters for **7**. Neutral atom scattering factors were taken from Cromer and Waber.[3] All calculations were performed using the Crystal Structure[4] crystallographic software package except for refinement, which was performed using SHELXL-97.[5] Details of final refinement as well as the bond lengths and angles are summarized in the supporting information, and the numbering scheme employed is also shown in the supporting information, which were drawn with ORTEP at 50% probability ellipsoid. The ORTEP drawings of the "(TACN)$FeBr_2$" complexes are shown in **Fig. S25 ~ S27**, and detailed data are summarized in **Table S2~S4**.

CCDC-1434140 (**6**), 1434139 (**7**) and 1434141 (**4'**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

References:

1) SIR2008: M. C. Burla, R. Caliandro, M. Camalli, B. Carrozzini, G. L. Cascarano, L. De Caro, C. Giacovazzo, G. Polidori, D. Siliqi, R. Spagna, *J. Appl. Crystallogr.* 2007, **40**, 609-613.

2) DIRDIF99: P. T. Beurskens, G. Admiraal, G. Beurskens, W. P. Bosman, R. de Gelder, R. Israel, J. M. M. Smits, The DIRDIF-99 program system; *Technical Report of the Crystallography Laboratory*; University of Nijmegen, Nijmegen, The Netherlands, 1999.

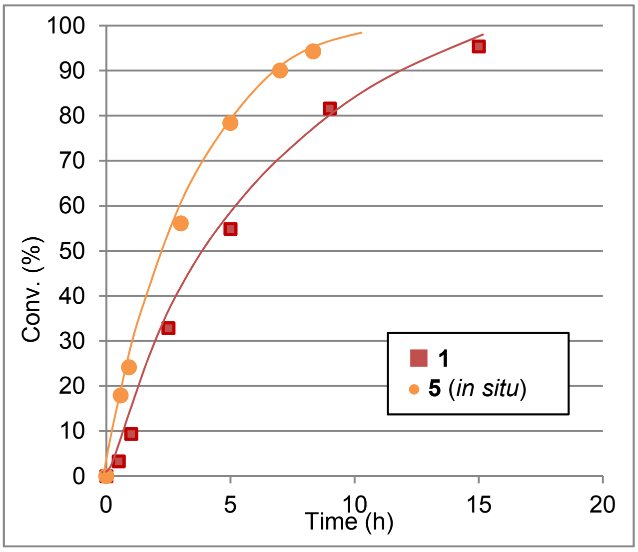
3) D. T. Cromer, J. T. Waber, *International Tables for X-ray Crystallography*; Kynoch Press: Birmingham, U.K., 1974, *Vol. 4*.

4) CrystalStructure 4.0: Crystal Structure Analysis Package, Rigaku Corporation (2000-2010). Tokyo 196-8666, Japan.

5) SHELX97: G. M. Sheldrick, *Acta Cryst.* 2008, **A64**, 112.

2. Reaction profiles and the conversion vs M_n plots

(1) Bulk polymerization of styrene using "(Me_3TACN)$FeCl_2$", **1** and **5** (in situ) [catalyst / initiator / monomer ratio = 1 / 1 / 250; initiator = 1-chloro-1-phenylethane; 120°C].



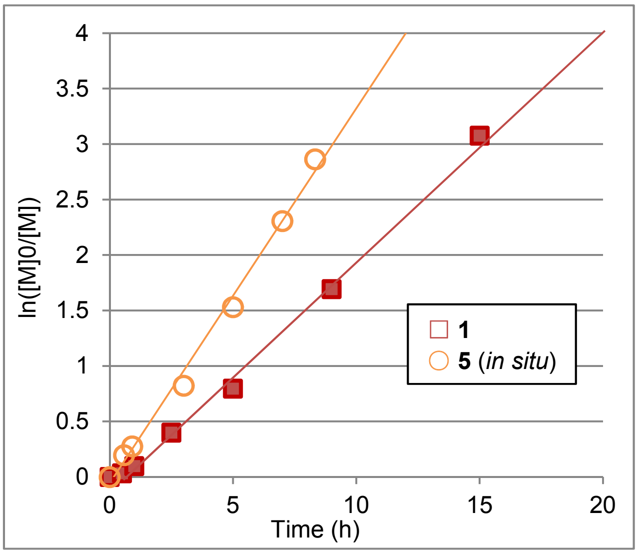


Fig.S1. The time vs conversion (%) plots (left) and time vs *ln([M]₀/[M])* plots (right) [1 (-■-) and 5 (*in situ*)] (-●-)]

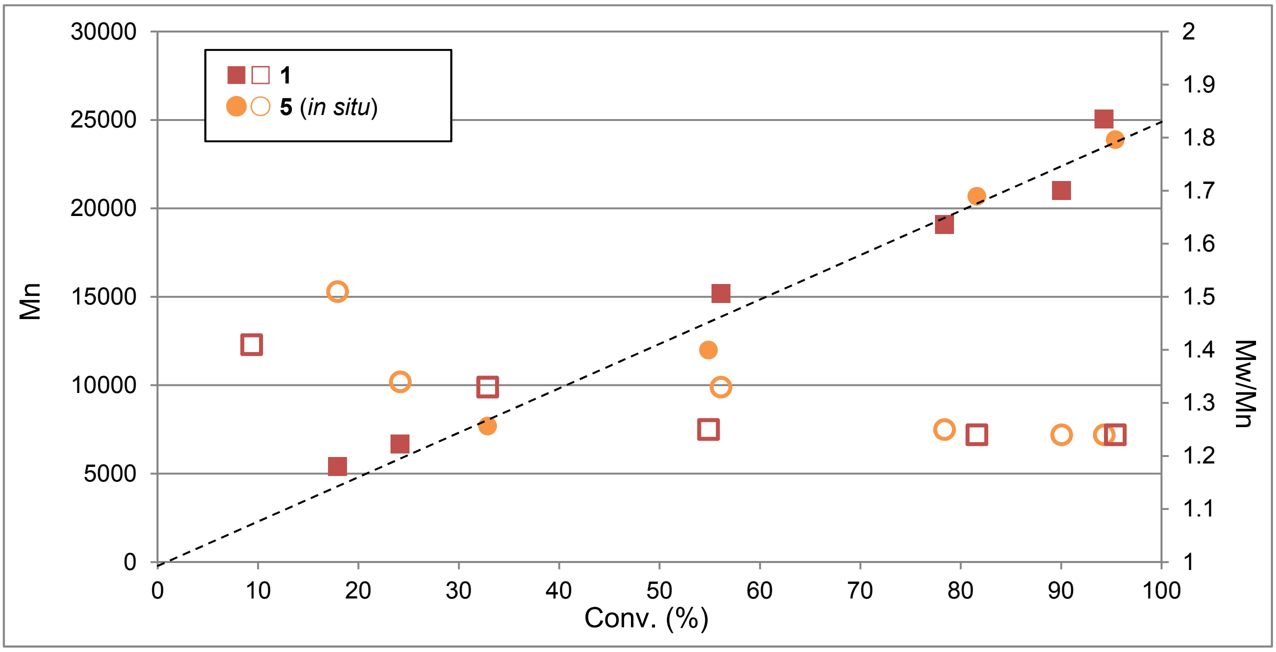


Fig.S2. The conversion vs M_n plots [**1** (-■-) and **5** (*in situ*) (-●-)] and conversion of M_w/M_n plots [**1** (-□) and **5** (*in situ*) (-○-).

(2) Bulk polymerization of styrene using “(Me_3TACN)$FeBr_2$”, **4**, **6** (*in situ*) and **6** (isolated). [catalyst / initiator / monomer ratio = 1 / 1 / 250; initiator = 1-bromo-1-phenylethane; 120^{o}C]

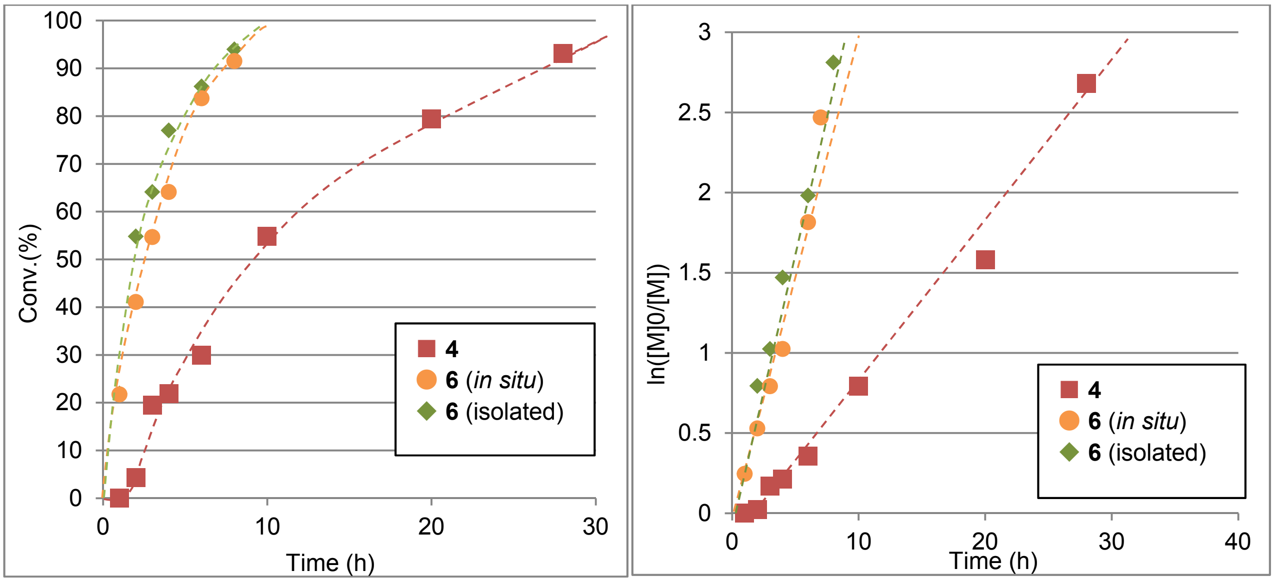


Fig.S3. The time vs conversion plots (left) and time vs *ln([M]₀/[M])* plots (right) [**4** (-■-), **6** (*in situ*) (-●-) and **6** (isolate) (-◆-)].

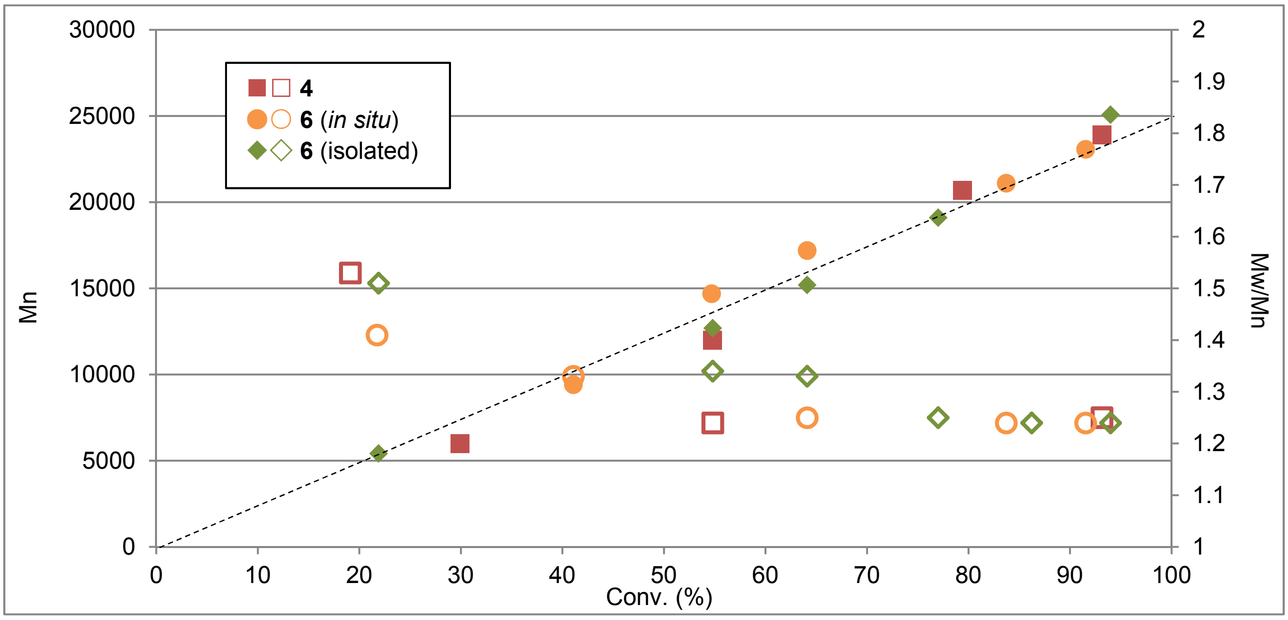


Fig.S4. The conversion vs M_n plots [**4** (-■-), **6** (*in situ*) (-●-) and **6** (isolate) (-◆-)] and M_w/M_n plots [**4** (-□-), **6** (*in situ*) (-○-) and **6** (isolate) (-◇-)].

(3) ATRP of styrene: Comparison of bulk polymerizations and solution polymerizations catalysed by **6** (*in situ*). [catalyst / initiator / monomer ratio = 1 / 1 / 250; initiator = 1-bromo-1-phenylethane; 120^{o}C;]

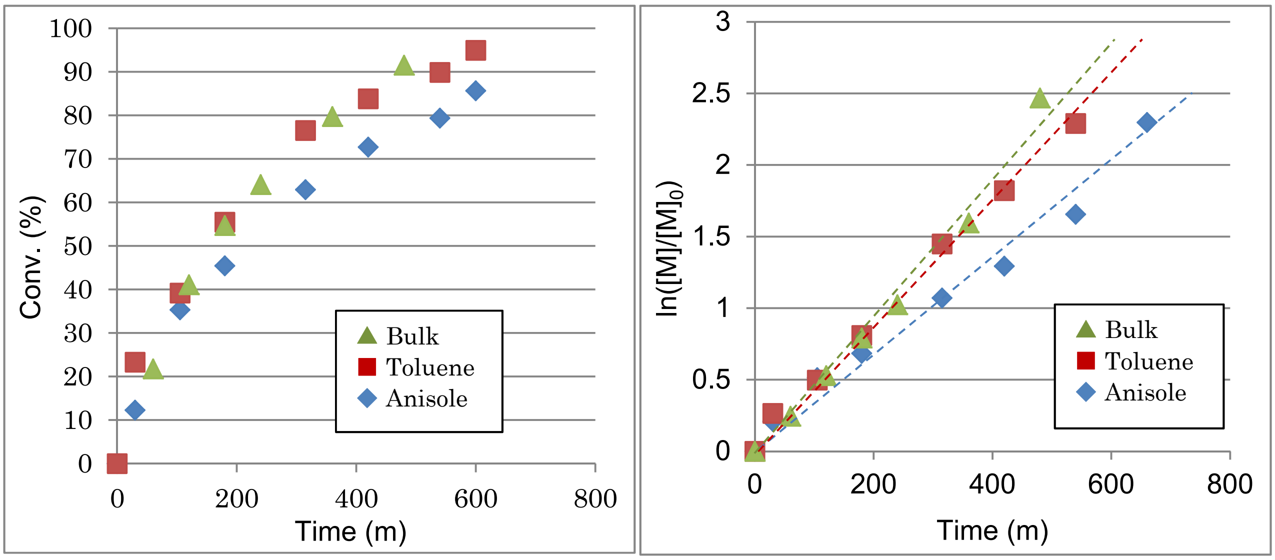


Fig.S5. The time vs conversion plot (right) and time vs *ln([M]$_0$/[M])* plot (left) [in a toluene solution (toluene / styrene = 1 / 1) (-■-), an anisole solution (anisole / styrene = 1 / 1) (-◆-), and bulk (-▲-).

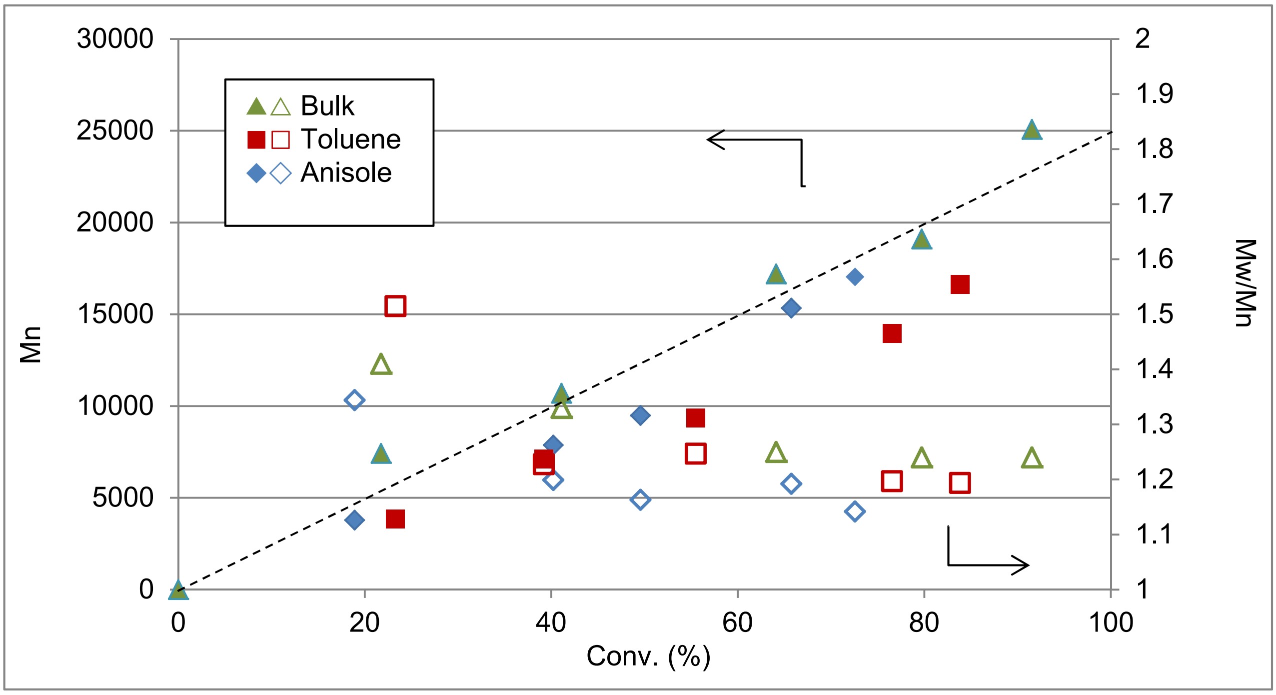


Fig.S6. The conversion vs M_n plots [in a toluene solution (toluene / styrene = 1 / 1) (-■-), in a anisole solution (anisole / styrene = 1 / 1) (-◆-), and bulk (-▲-)] and the conversion vs M_w/M_n plots [in a toluene solution (toluene / styrene = 1 / 1) (-□-), in a anisole solution (anisole / styrene = 1 / 1) (-◇-), and bulk (-△-)]

(4) Bulk polymerization of MMA using "($(Me_3TACN)FeCl_2$)", **1** and **5** (in situ) [catalyst / initiator / monomer ratio = 1 / 1 / 250; initiator = methyl trichloroacetate; 90^{o}C].

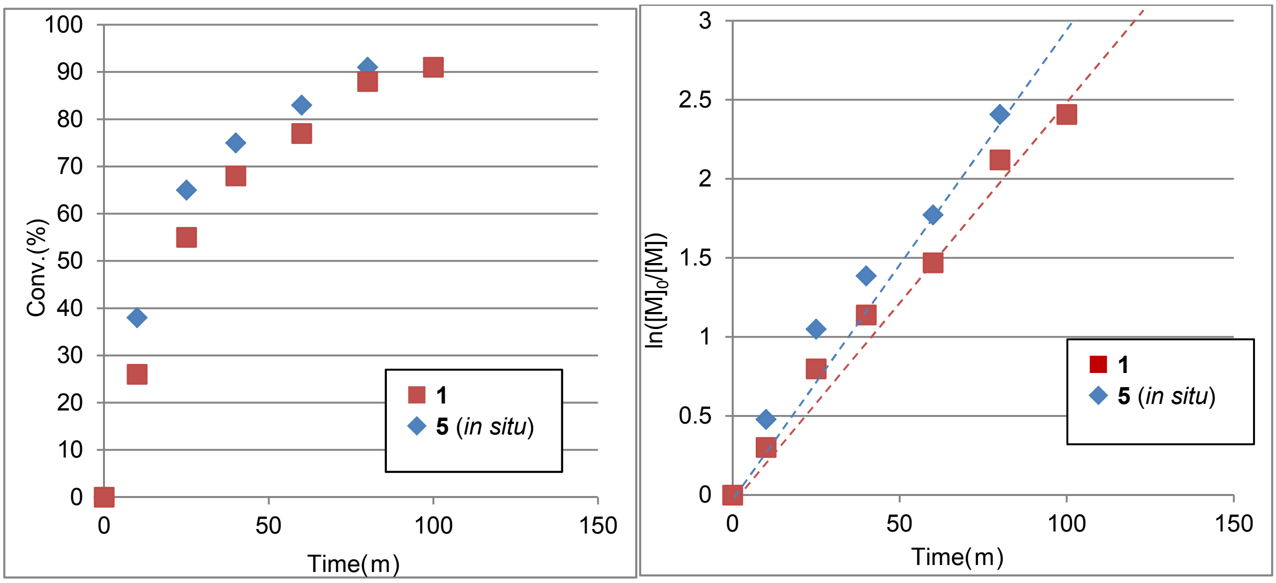


Fig.S7. The time vs Conversion plots (right) and time vs *ln([M]₀/[M])* plots (left) [1 (-■-) and 5 (*in situ*) (-◆-)].

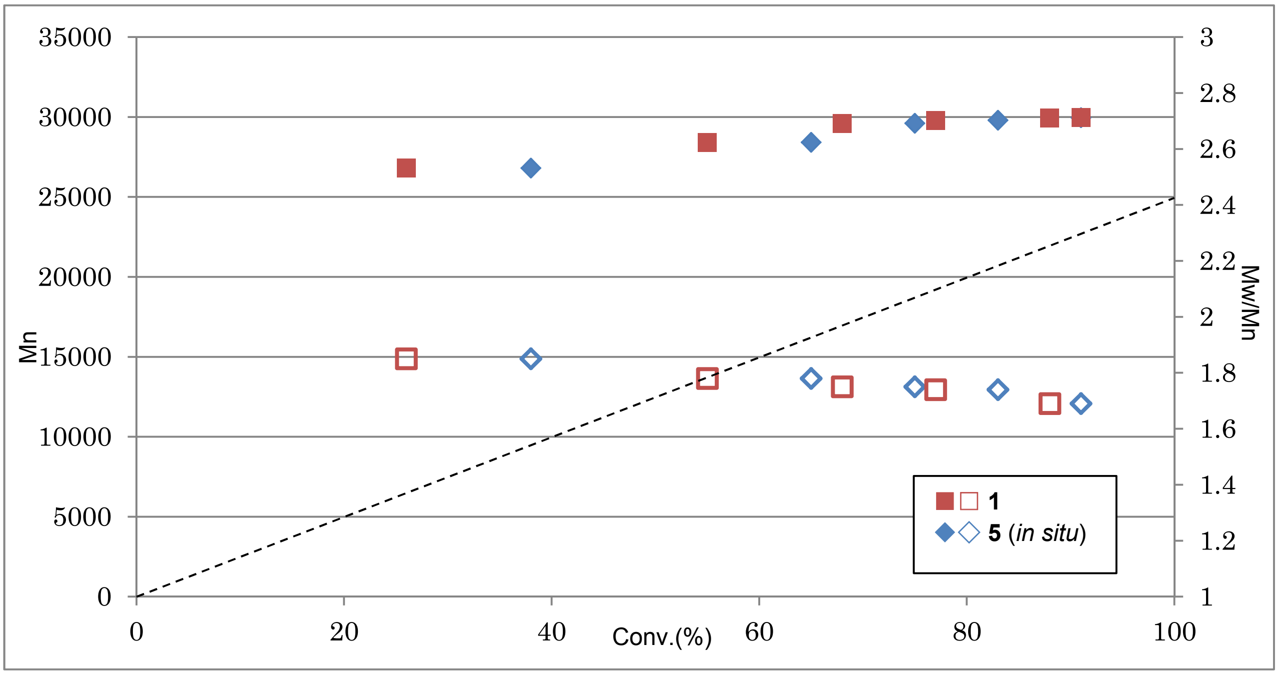


Fig.S8. The conversion vs M_n plots [1 (-■-) and 5 (*in situ*) (-◆-)] and the conversion vs M_w/M_n plots [1 (-□-) and 5 (*in situ*) (-◇-)]

(5) Bulk polymerization of MMA using "(Me3TACN)FeBr2" **4** and **6** (*in situ*). [catalyst / initiator / monomer ratio = 1 / 1 / 250; initiator =methyl 2-bromoisobutylate; 90^{o}C].

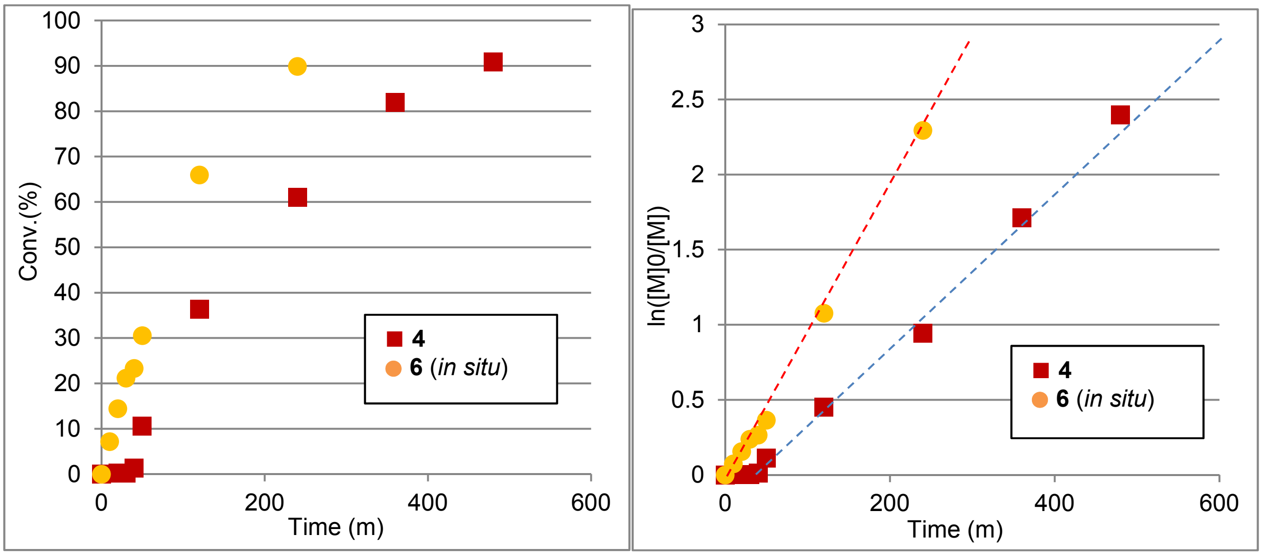


Fig.S9. The time vs conversion plots and time vs *ln([M]$_0$/[M])* plots [**4** (-■-) and **6** (*in situ*) (-●-)]

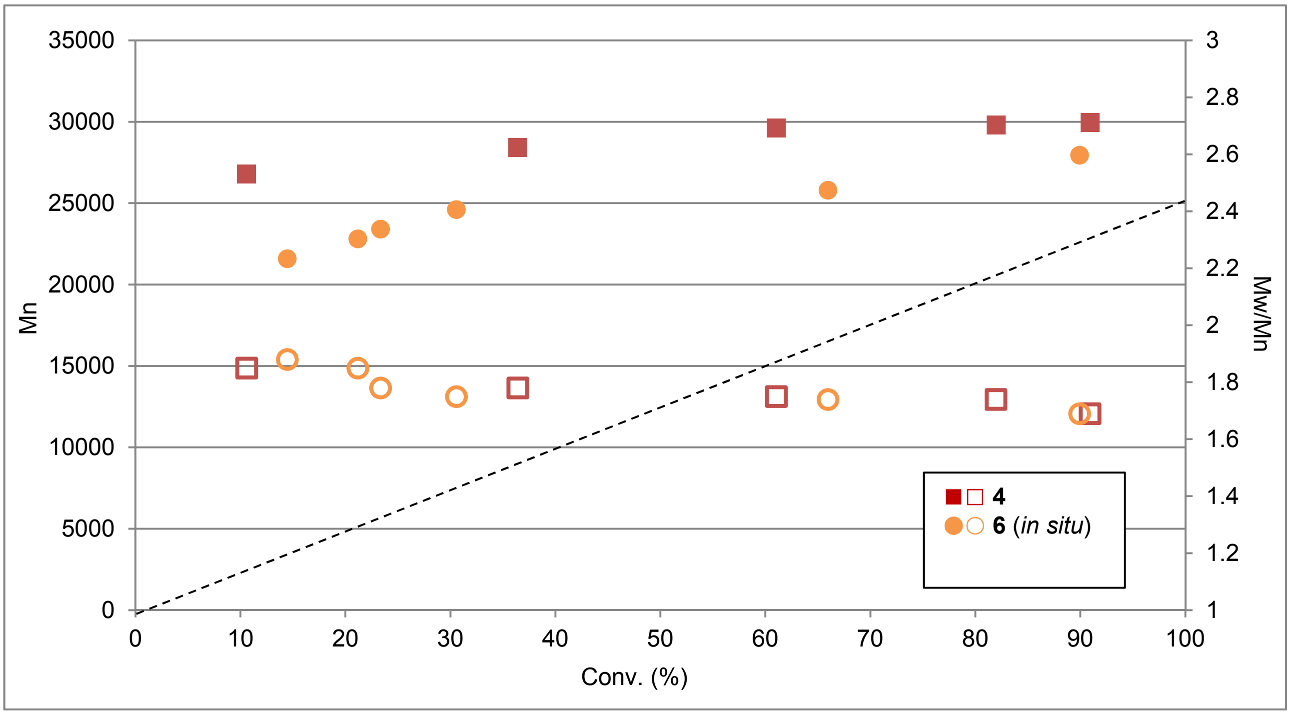


Fig. S10. The conversion vs M_n plots [**4** (-■-) and **6** (*in situ*) (-●-)] and the conversion vs M_w/M_n plots [**4** (-□-) and **6** (*in situ*) (-○-)].

(6) Solution polymerizations of MMA using (Me$_3$TACN)FeCl$_2$(κ-NCMe) [**5** (in situ)] and (Me$_3$TACN)FeBr$_2$(κ-NCMe) [**6** (*in situ*).] in MeCN (monomer / MMA = 1 / 0.2). [catalyst / initiator / monomer ratio = 1 / 1 / 250; initiator for **5** (*in situ*) = methyl trichloroacetate and that for **6** (*in situ*) = methyl 2-bromoisobutylate; 90^{o}C].

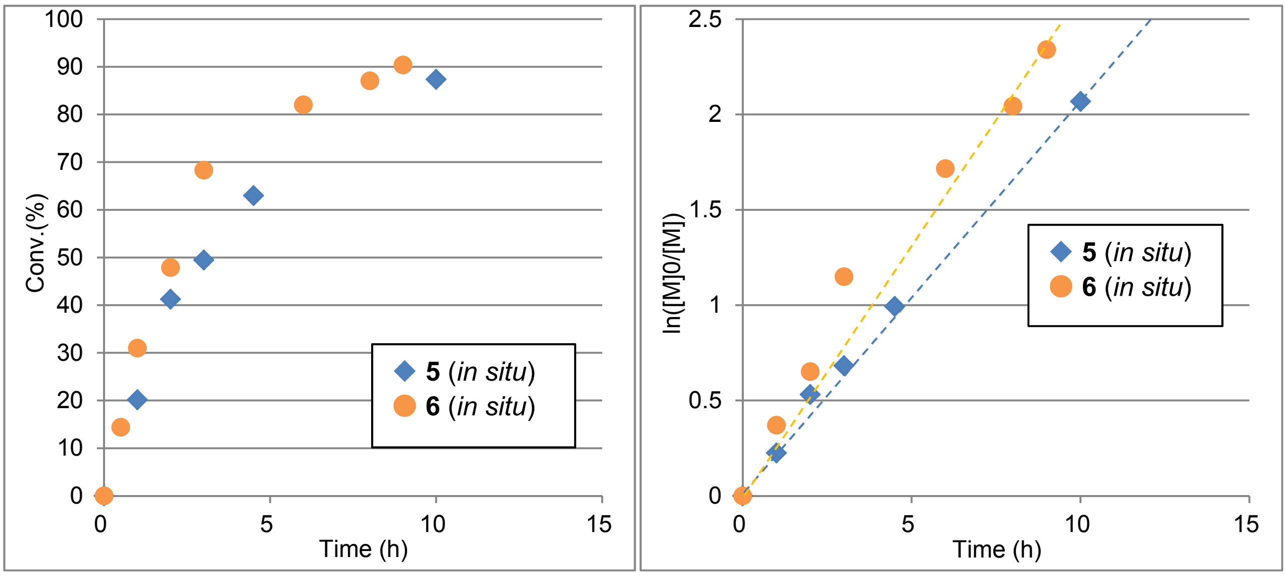


Fig.S11. The time vs Conversion plots (right) and time vs *ln([M]$_0$/[M])* plots (left) [**5** (*in situ*) (-◆-) and **6** (*in situ*) (-●-)]

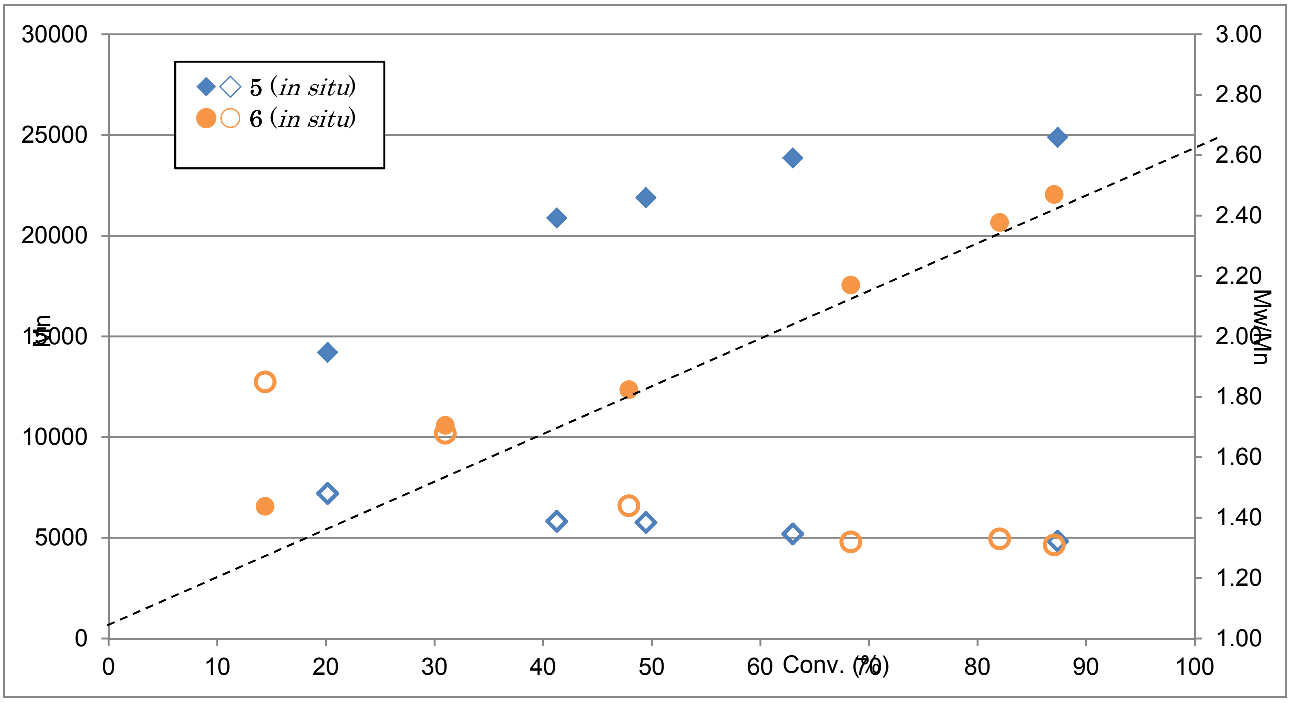


Fig. S12. The conv. vs M_n plots [**5** (*in situ*) (-◆-) and **6** (*in situ*) (-●-)]and the conversion vs M_w/M_n plots [**5** (*in situ*) (--◇-) and **6** (*in situ*) (-○-)]

(7) Solution polymerizations of BA using **6** (*in situ*). in MeCN (monomer / BA = 1 / 0.3). [catalyst / initiator / monomer ratio = 1 / 1 / 250; initiator = 2-bromoisobutylate; 90°C].

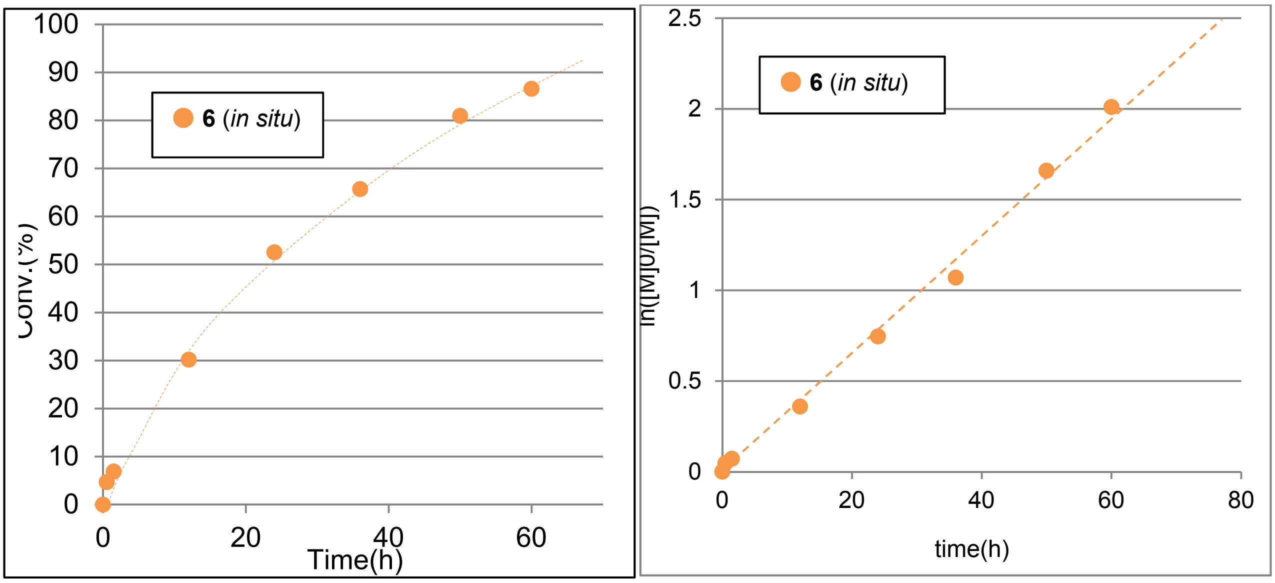


Fig.S13. The time vs conversion plot (left) and time vs *ln*($[M]_0/[M]$) plot (right).

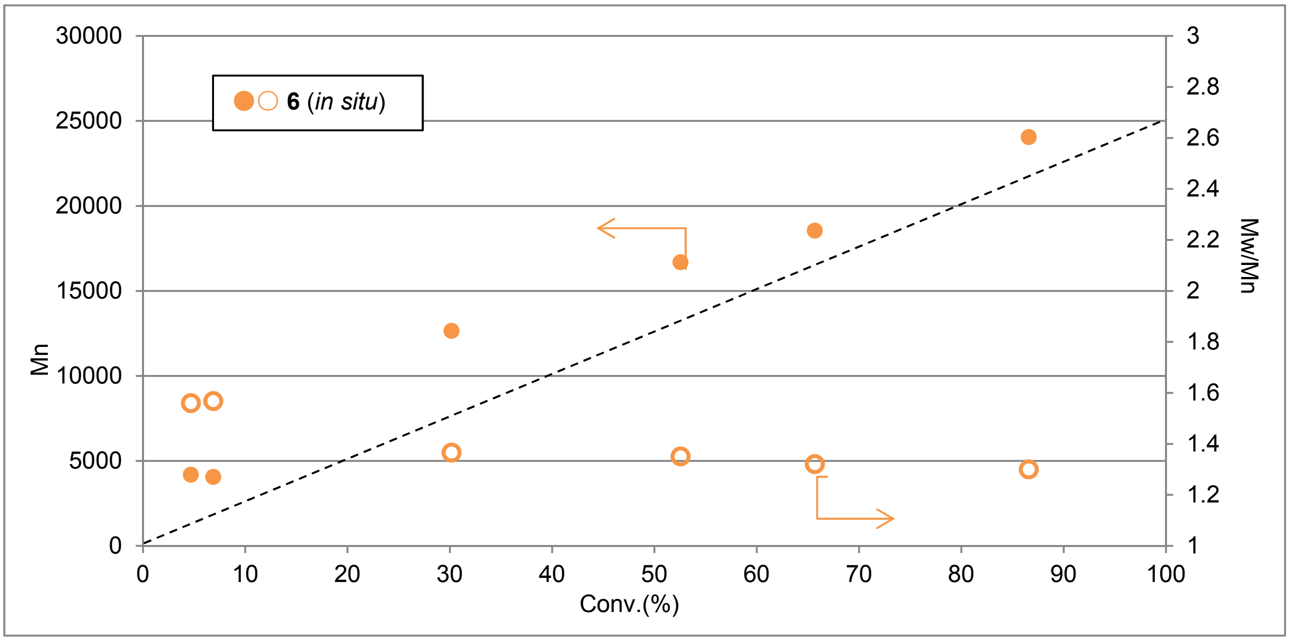


Fig. S14. The conversion vs M_n plot (-●-)and the conversion vs M_w/M_n plot (-○-).

3. Actual charts of spectral data and details of crystallographic data

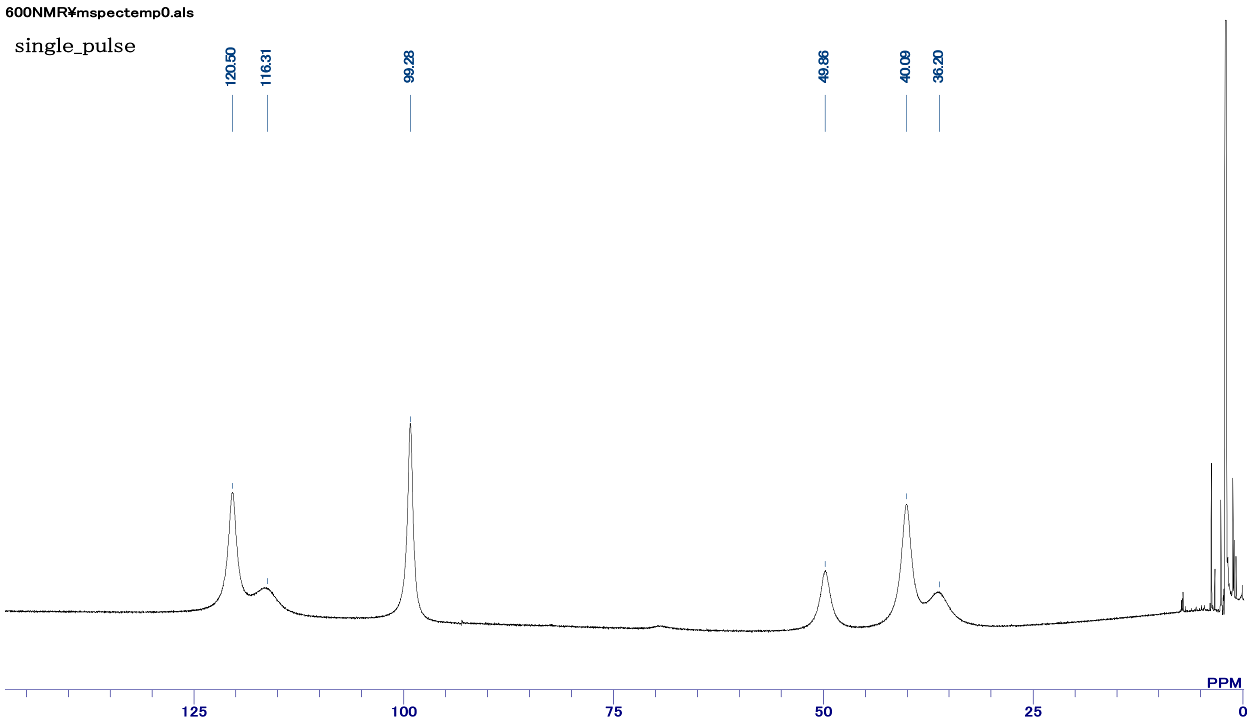


Fig. S15. ^{1}H-NMR spectrum of **4'** in acetone-d_6

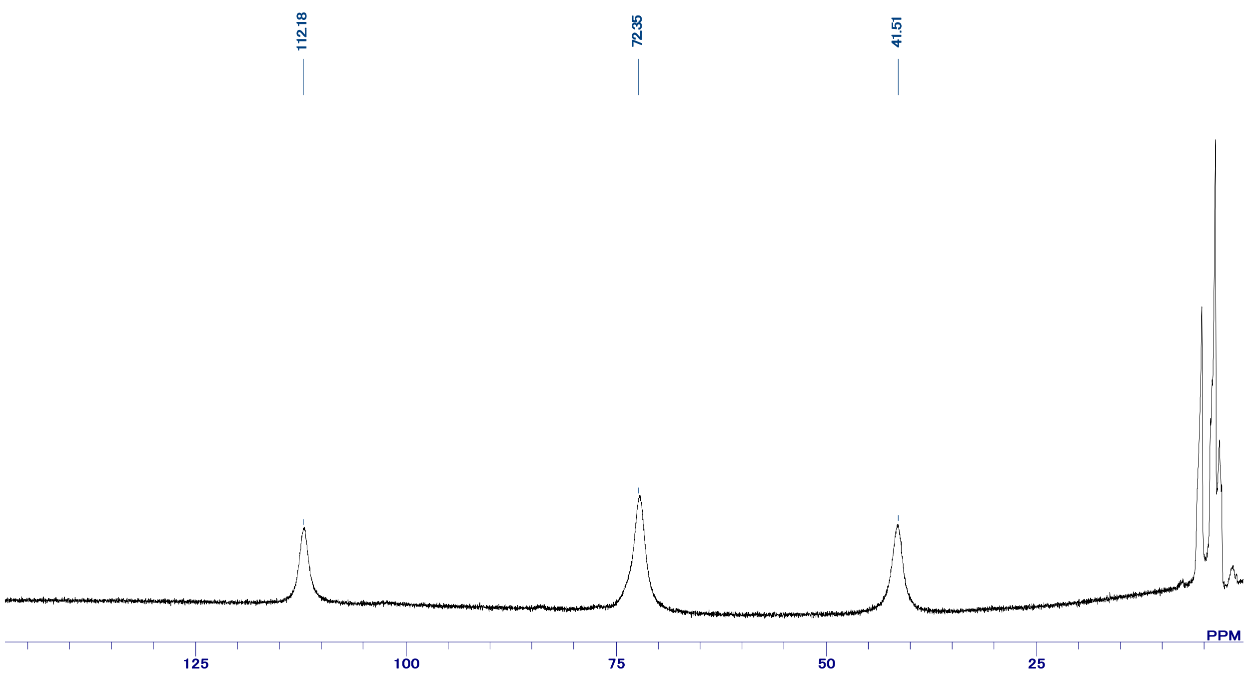


Fig. S16. ^{1}H-NMR spectrum of **4'** in CD_3OD.

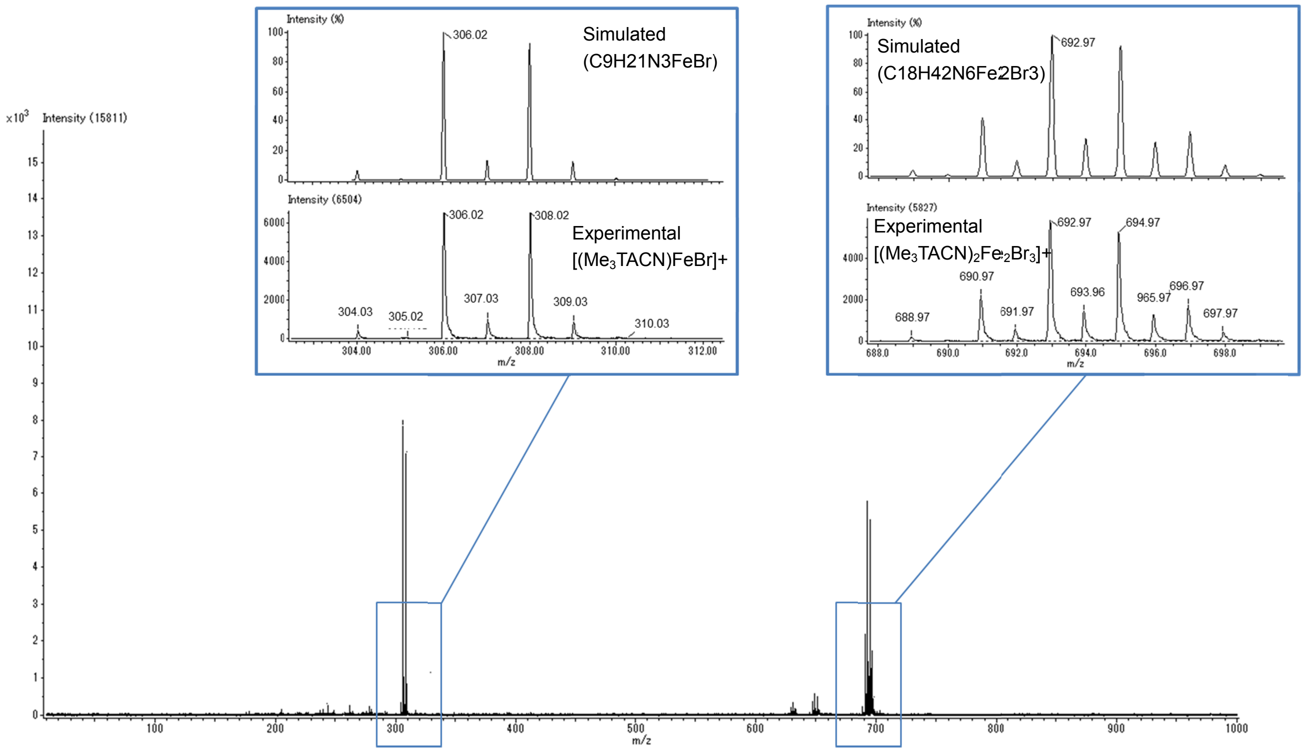


Fig. S17. ESI+ spectrum of 4’ (under the standard conditions)

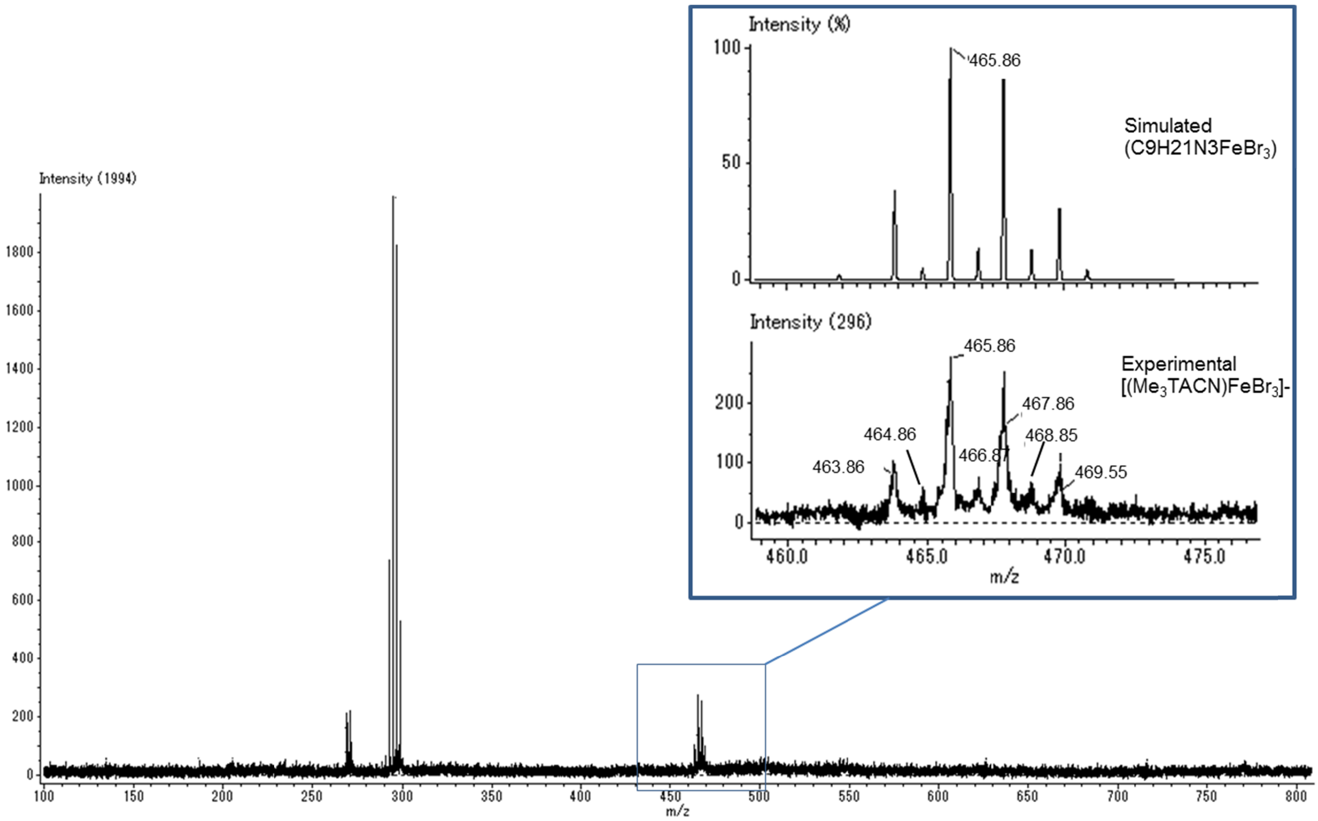


Fig. S18. ESI- spectrum of 4’ (under the standard conditions)

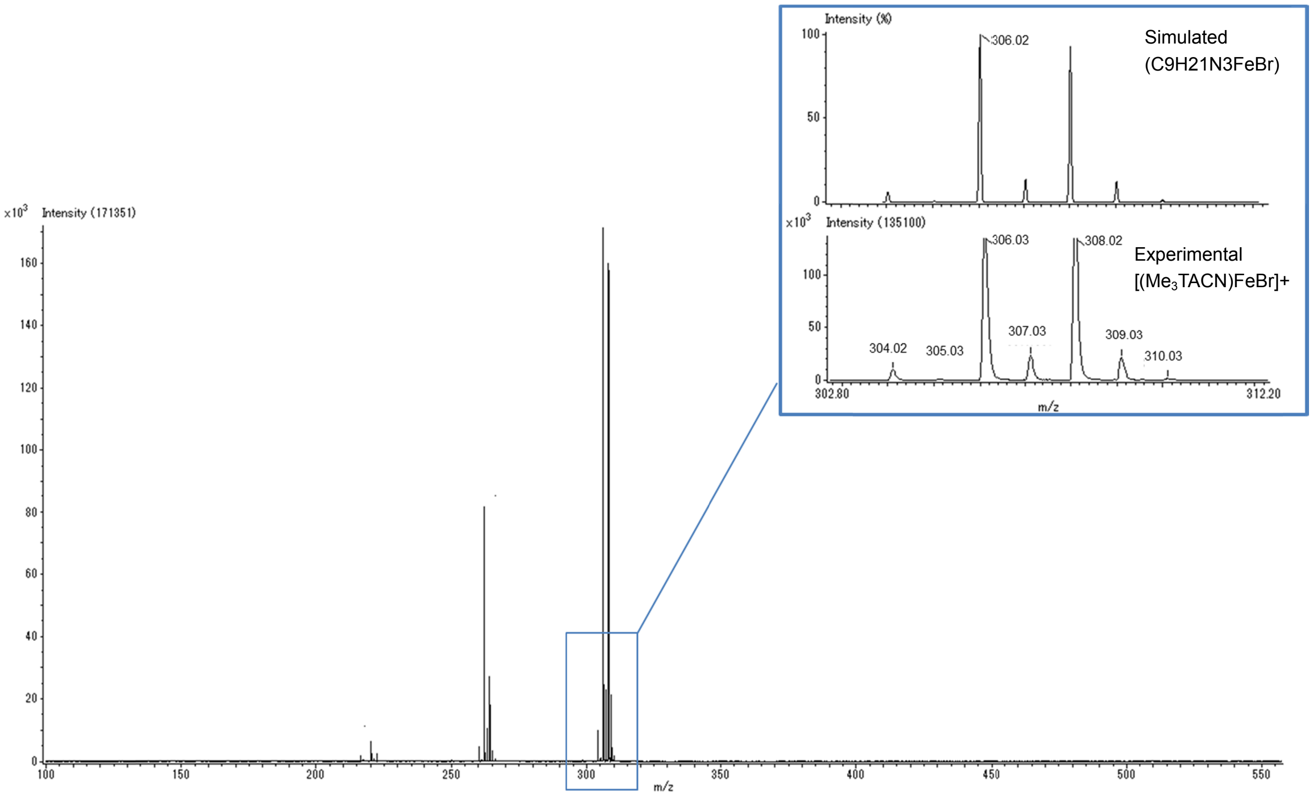


Fig. S19. ESI$^+$ spectrum of **6** (under the forced conditions)

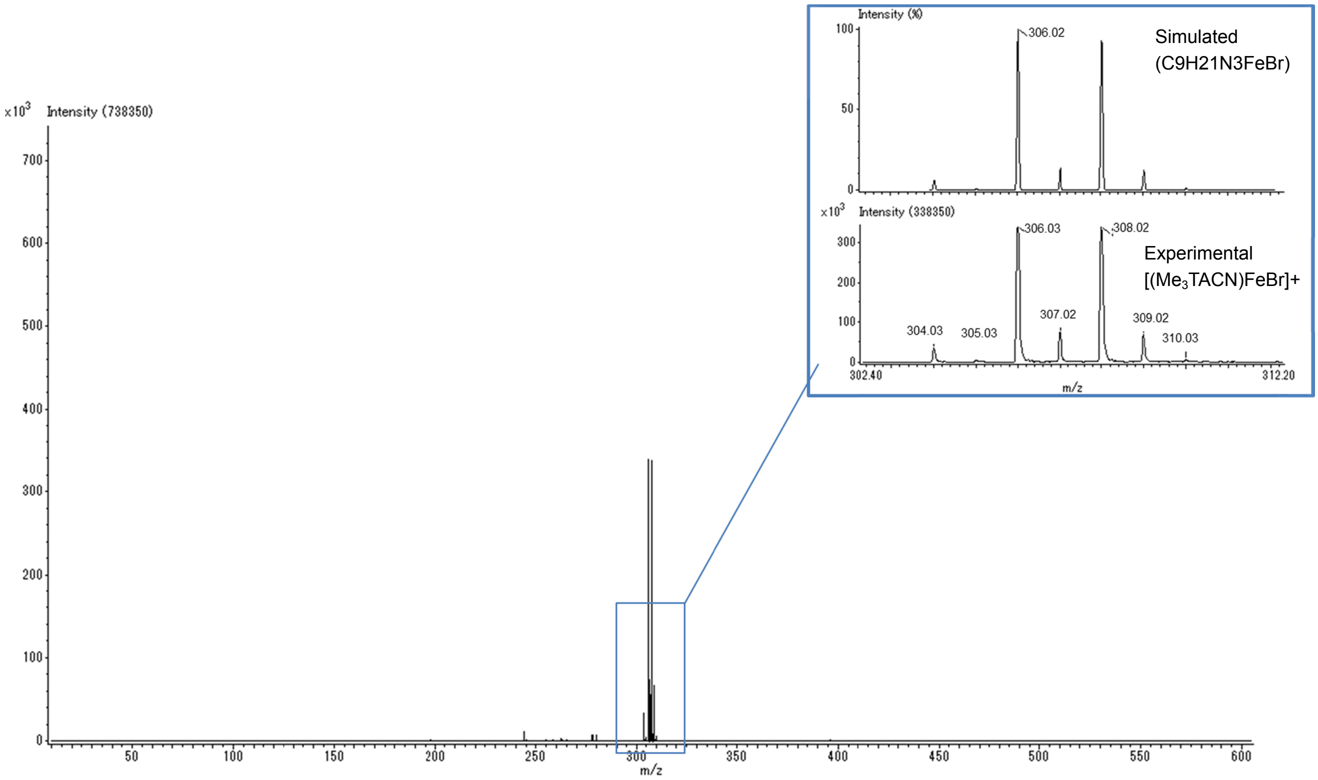


Fig. S20. ESI$^+$ spectrum of **7** (under the forced conditions)

The catalyst recycling experiments: evidence for the recovered species to be 4.

ATRP of styrene was performed by treatment of styrene 1.09 ml (9.49 mmol), 1-bromo-1-phenylethane 5.2 μl (0.038 mmol) in the presence of **6** in situ prepared from **4** 14.7 mg (0.019 mmol) at 120°C for 8 h. After the reaction was over, the polymer was dissolved in THF (5 ml), and the solution was slowly added dropwise into MeOH (60 ml) with stirring. The polymer was collected by filtration and the filtrate was concentrated. As shown in Fig. **S-21**, The ESI-MS spectrum of a CH_2Cl_2 solution of the residue recovered from the filtrate indicated the iron species to be $[(Me_3TACN)Fe(\mu\text{-}Br)_2Fe(Me_3TACN)]^+Br^-$ (**4**). This was supported by polymerizations by the recovered iron species. Entry 1 of **Table S-2** shows ATRP of styrene by **6** (in situ) described above. When the recovered iron species was used for another run of ATRP, the reaction was significantly slower (entry 1). The rate was similar to the polymerization using **4** (entry 3). In contrast, the rate of the polymerization was similar to that shown in the initial ATRP described above (entry 4), when the recovered iron species was reactivated by treatment with MeCN at room temperature (entry 2).

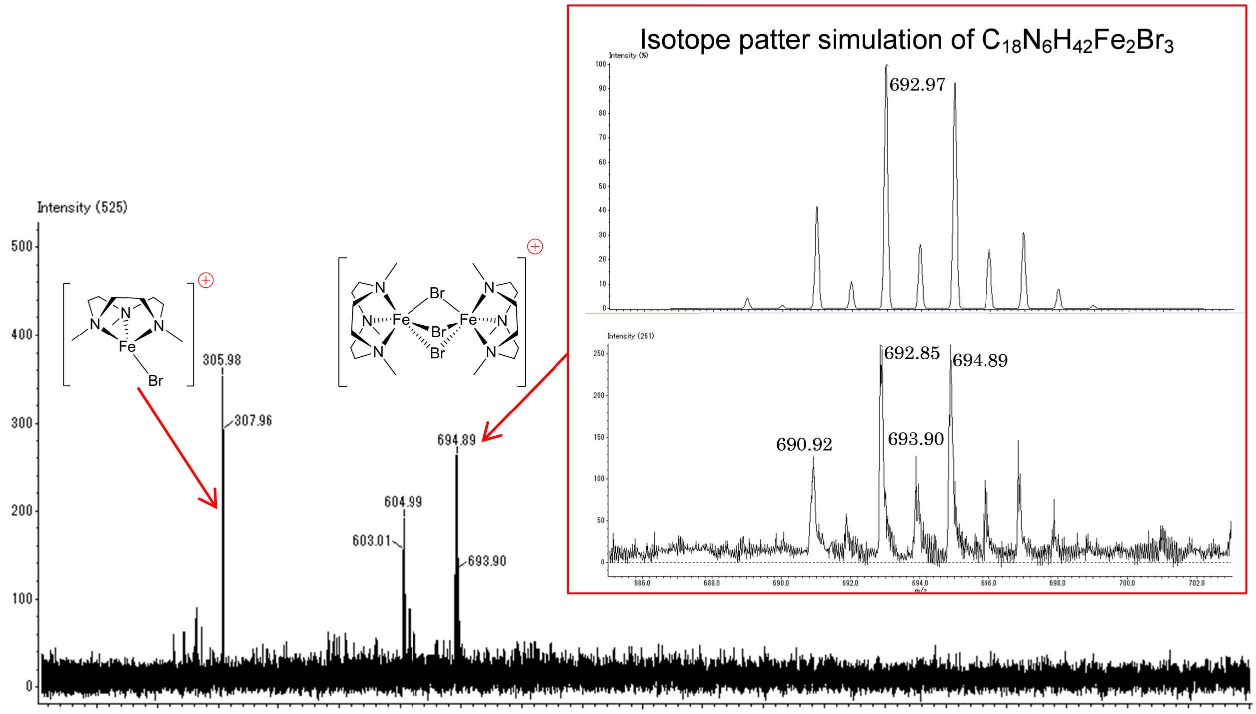


Fig. S21. ESI-MS spectra of recovered iron residue (CH_2Cl_2, standard condition)

Table S1. Comparison of polymerization behavior catalyzed by recovered iron species with ATRPs of **6** (in situ) and 4.

Entry	Monomer	catalyst	Time (h)	Conv. (%)	M_n (exp.)	M_n (calc.)	M_w/M_n
1	styrene	Non activated by MeCN before reuse	8	48	13,658	12,000	1.28
			20	92	26,584	23,000	1.26
2	styrene	**4**	28	93	23,900	23,300	1.25
3	styrene	Activated by MeCN before reuse	8	>95	27,062	25,000	1.25
4	styrene	**6** (*in situ*)	8	>95	24,000	25,000	1.20

Reaction condition: catalyst : 1-bromo-1phenylethane : styrene = 1 : 1 : 250. Polymerization was performed at 120 ^{o}C. In entry 1, recovered iron residue was used for catalyst without activation by MeCN.(entry 1) Recovered iron residue was activated in MeCN (1 ml) at room temperature for 1 h and dried in vacuo, then used as a catalyst for next polymerization (entry 3).

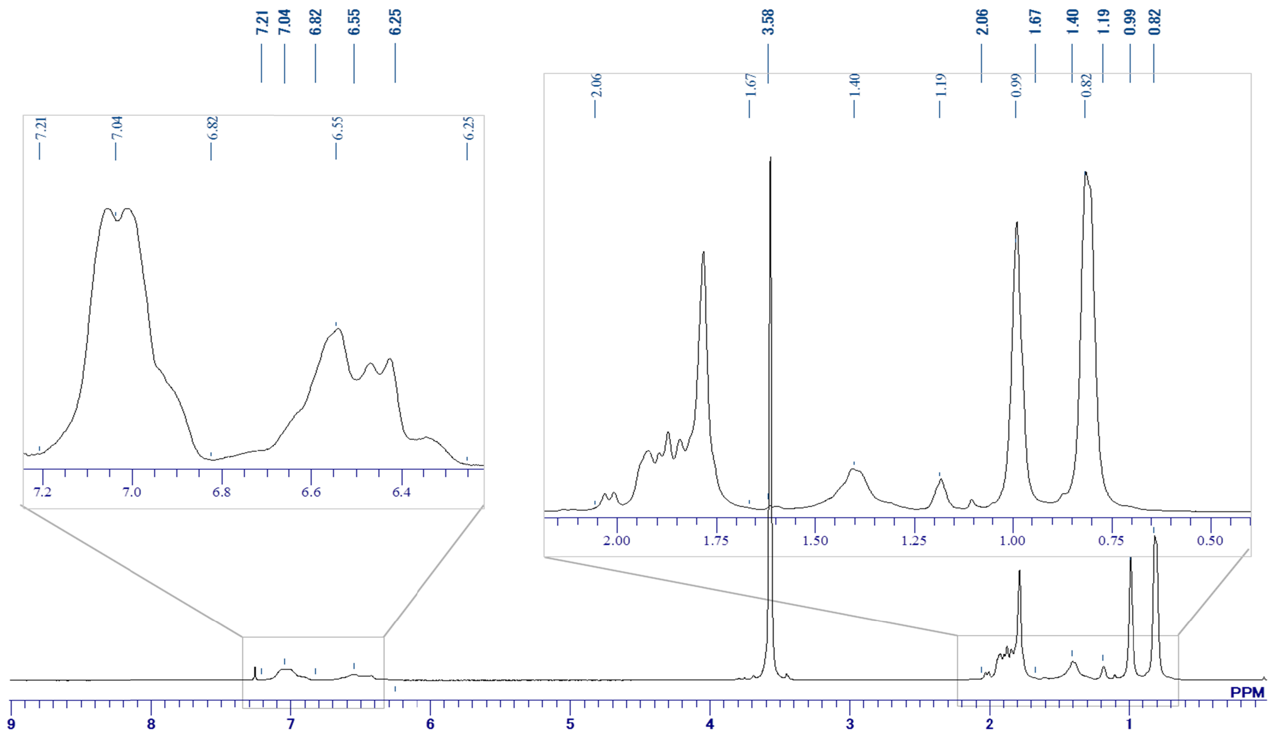


Fig. S22 ^{1}H-NMR of pSt$_{100}$-*b*-pMMA$_{500}$ by **6** (*in situ*)

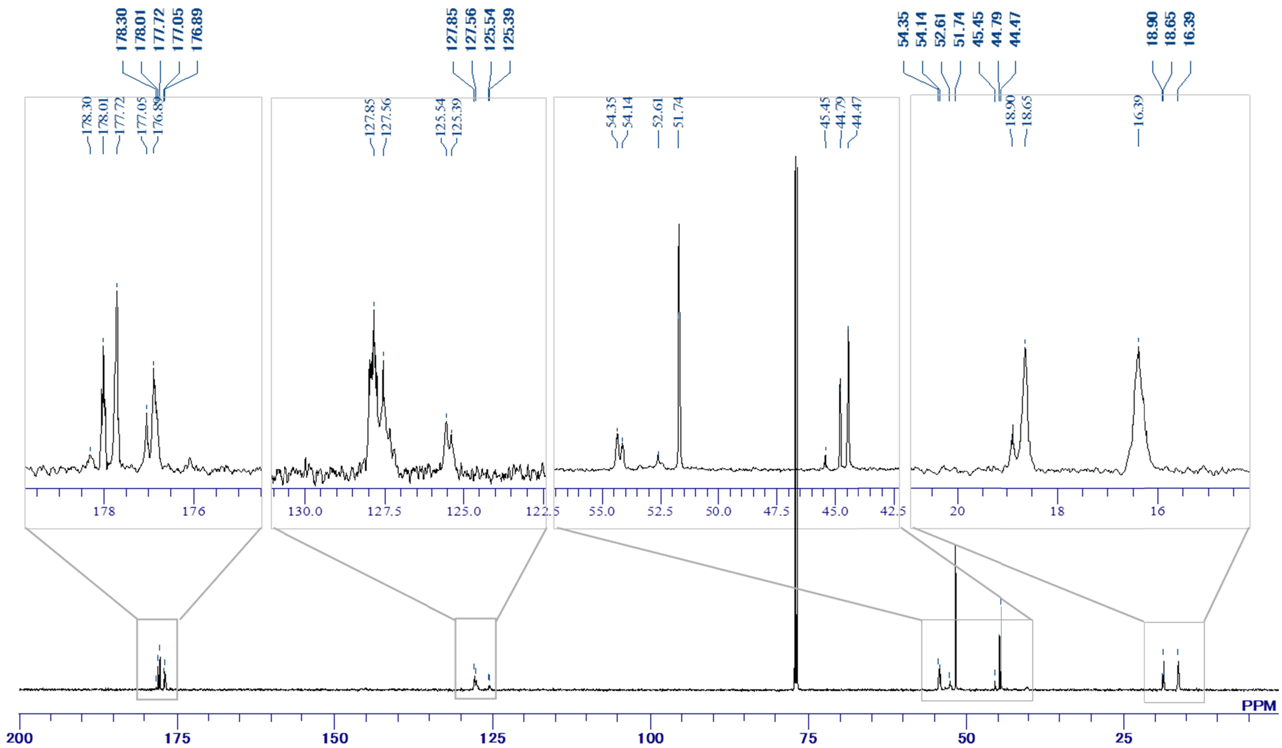


Fig. S23 ^{13}C-NMR of pSt$_{100}$-*b*-pMMA$_{500}$ by **6** (*in situ*)

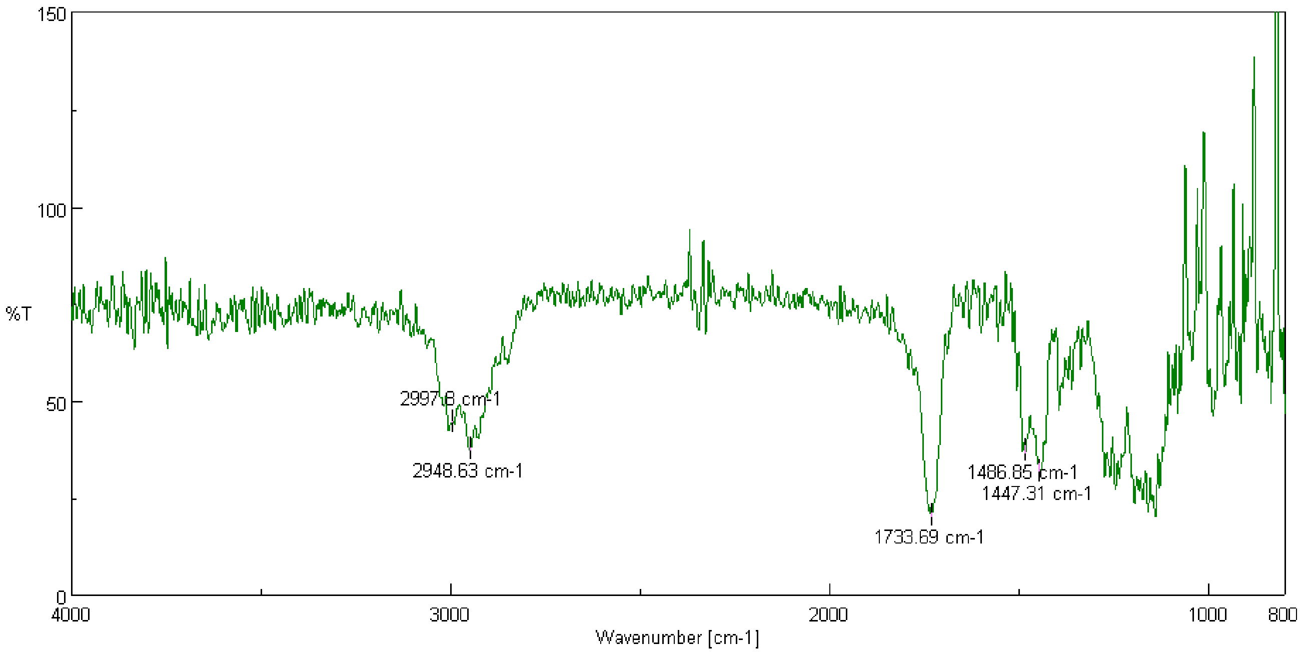


Fig. S24 FT-IR spectra of pSt_{100}-*b*-$pMMA_{500}$ by **6** (*in situ*)

4. Details of Crystallographic data

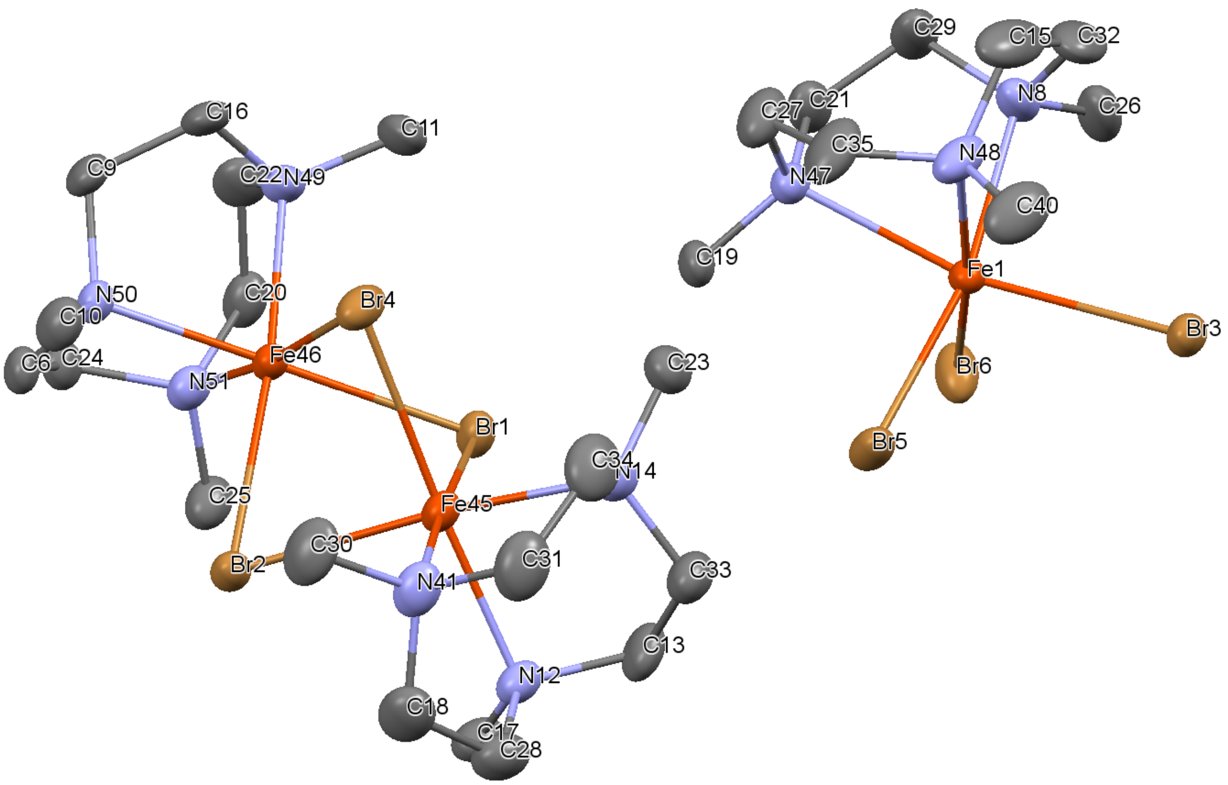


Fig. S25.ORTEP drawing of **4’**

Table S2-1. Crystal data and structure refinement for **4’**

Empirical Formula	$C_{27}H_{63}Br_6Fe_3N_9$
Formula Weight	1160.82
Crystal Color, Habit	colorless, prism
Crystal Dimensions	0.200 X 0.200 X 0.200 mm
Crystal System	orthorhombic
Lattice Type	Primitive
Lattice Parameters	a = 22.0243(16) Å
	b = 16.0659(11) Å
	c = 23.6931(17) Å
	V = 8383.6(10) Å^3
Space Group	Pbca (#61)
Z value	8
D_{calc}	1.839 g/cm^3
F_{000}	4608.00
μ(MoKα)	67.911 cm^{-1}
Diffractometer	Saturn724
Radiation	MoKα (λ = 0.71075 Å)
	multi-layer mirror monochromated
Voltage, Current	50kV, 40mA
Temperature	-159.8^{o}C
Detector Aperture	72.8 x 72.8 mm
Data Images	720 exposures
ω oscillation Range (χ=45.0, ϕ=90.0)	-105.0 - 75.0^o
Exposure Rate	10.0 sec./^{o}
Detector Swing Angle	-14.80^o

Detector Position	40.16 mm
Pixel Size	0.070 mm
$2\theta_{max}$	55.0^{o}
No. of Reflections Measured	Total: 76991 Unique: 9597 (R_{int} = 0.0597)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.154 - 0.257)
Structure Solution	Direct Methods (SIR2008)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	w = 1/ [$\sigma^2(Fo^2)$ + $(0.0464 \cdot P)^2$ + 37.1650 · P] where P = (Max(Fo^2,0) + $2Fc^2$)/3
$2\theta_{max}$ cutoff	55.0^{o}
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	9597
No. Variables	406
Reflection/Parameter Ratio	23.64
Residuals: R1 (I>2.00σ(I))	0.0623
Residuals: R (All reflections)	0.0661
Residuals: wR2 (All reflections)	0.1391
Goodness of Fit Indicator	1.300
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	1.52 $e^-/Å^3$
Minimum peak in Final Diff. Map	-1.11 $e^-/Å^3$

Table S2-2. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Br1	0.09356(3)	0.25897(4)	0.44709(2)	2.189(11)
Br2	-0.03442(3)	0.36274(4)	0.51525(2)	2.158(11)
Br3	0.25007(3)	-0.00141(4)	0.17681(3)	2.541(12)
Br4	-0.01335(3)	0.13580(4)	0.53168(3)	2.655(12)
Br5	0.15038(3)	0.13925(5)	0.27874(3)	2.963(13)
Br6	0.31925(3)	0.18147(4)	0.25873(3)	3.036(13)
Fe1	0.25139(4)	0.05498(5)	0.28235(3)	1.703(13)
Fe45	-0.02602(4)	0.23440(5)	0.44472(3)	1.818(14)
Fe46	0.05571(4)	0.26869(5)	0.55203(3)	1.667(13)
N8	0.3332(3)	-0.0273(3)	0.3060(2)	2.85(10)
N12	-0.0406(2)	0.3088(3)	0.3677(2)	2.19(8)
N14	-0.0287(2)	0.1321(3)	0.3822(2)	2.42(9)
N41	-0.1261(2)	0.2203(4)	0.4369(2)	2.64(9)
N47	0.2605(2)	0.0747(3)	0.3796(2)	2.02(8)
N48	0.2059(3)	-0.0597(3)	0.3186(2)	2.89(10)
N49	0.1291(2)	0.1953(3)	0.5916(2)	2.37(9)
N50	0.0270(2)	0.2806(3)	0.6406(2)	1.96(8)
N51	0.1168(2)	0.3712(3)	0.5763(2)	2.18(8)
C6	0.0379(3)	0.3703(4)	0.6523(3)	2.24(10)
C9	0.0672(3)	0.2264(4)	0.6763(3)	2.45(10)
C10	-0.0376(3)	0.2609(5)	0.6514(3)	2.80(11)
C11	0.1527(3)	0.1268(4)	0.5554(3)	3.25(13)
C13	-0.0097(4)	0.2569(5)	0.3237(3)	3.29(13)
C15	0.2514(4)	-0.1279(4)	0.3270(4)	4.54(19)
C16	0.0990(3)	0.1592(4)	0.6418(3)	2.70(11)
C17	-0.0104(3)	0.3909(4)	0.3684(3)	2.61(11)
C18	-0.1434(3)	0.2992(5)	0.4087(3)	3.58(14)
C19	0.2436(3)	0.1595(4)	0.3972(3)	2.51(10)
C20	0.1780(3)	0.3322(4)	0.5749(3)	2.66(11)
C21	0.3263(3)	0.0641(5)	0.3899(3)	3.03(12)
C22	0.1793(3)	0.2524(5)	0.6081(3)	3.04(12)
C23	0.0222(3)	0.0722(4)	0.3879(3)	3.03(12)
C24	0.1009(3)	0.3984(4)	0.6350(3)	2.30(10)
C25	0.1164(3)	0.4432(4)	0.5375(3)	2.84(11)
C26	0.3850(3)	-0.0130(5)	0.2673(3)	3.77(15)
C27	0.2241(4)	0.0123(5)	0.4101(3)	3.42(13)
C28	-0.1060(3)	0.3176(5)	0.3576(3)	3.27(13)
C29	0.3522(4)	-0.0131(5)	0.3654(3)	3.82(15)
C30	-0.1579(3)	0.2157(5)	0.4916(3)	3.52(14)
C31	-0.1393(3)	0.1474(5)	0.4007(3)	3.74(15)
C32	0.3099(4)	-0.1130(4)	0.2975(4)	4.24(17)
C33	-0.0292(4)	0.1683(5)	0.3250(3)	3.25(13)
C34	-0.0866(4)	0.0887(5)	0.3963(3)	3.75(14)
C35	0.1790(4)	-0.0308(5)	0.3736(3)	3.91(15)
C40	0.1557(4)	-0.0873(5)	0.2821(3)	3.96(16)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S2-3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br1	0.0233(3)	0.0377(3)	0.0222(3)	0.0016(2)	0.0015(2)	-0.0028(2)
Br2	0.0268(3)	0.0323(3)	0.0229(3)	0.0068(2)	-0.0038(2)	-0.0014(2)
Br3	0.0410(3)	0.0330(3)	0.0226(3)	0.0066(3)	-0.0033(2)	-0.0025(2)
Br4	0.0448(4)	0.0305(3)	0.0256(3)	-0.0075(3)	-0.0062(3)	0.0042(2)
Br5	0.0341(3)	0.0547(4)	0.0238(3)	0.0172(3)	-0.0028(2)	0.0026(3)
Br6	0.0478(4)	0.0309(3)	0.0366(4)	-0.0109(3)	0.0177(3)	-0.0048(3)
Fe1	0.0253(4)	0.0197(4)	0.0197(4)	0.0016(3)	-0.0004(3)	0.0018(3)
Fe45	0.0221(4)	0.0287(4)	0.0184(4)	-0.0024(3)	-0.0010(3)	0.0007(3)
Fe46	0.0207(4)	0.0249(4)	0.0177(4)	0.0021(3)	-0.0012(3)	0.0004(3)
N8	0.040(3)	0.036(3)	0.033(3)	0.015(2)	-0.010(2)	-0.008(2)
N12	0.028(2)	0.033(3)	0.022(2)	-0.005(2)	-0.0027(19)	0.004(2)
N14	0.031(3)	0.032(3)	0.029(3)	-0.001(2)	-0.007(2)	-0.002(2)
N41	0.021(2)	0.049(3)	0.030(3)	-0.008(2)	-0.001(2)	-0.002(2)
N47	0.029(2)	0.026(2)	0.022(2)	0.001(2)	-0.0013(19)	-0.0011(19)
N48	0.050(3)	0.034(3)	0.026(3)	-0.013(3)	-0.008(2)	0.007(2)
N49	0.030(3)	0.035(3)	0.025(2)	0.011(2)	-0.002(2)	0.003(2)
N50	0.025(2)	0.030(2)	0.019(2)	0.0001(19)	-0.0009(19)	-0.0023(19)
N51	0.025(2)	0.034(3)	0.024(2)	-0.003(2)	-0.003(2)	0.000(2)
C6	0.031(3)	0.033(3)	0.021(3)	0.001(2)	0.004(2)	-0.005(2)
C9	0.036(3)	0.038(3)	0.018(3)	0.002(3)	-0.000(2)	0.006(2)
C10	0.027(3)	0.052(4)	0.028(3)	-0.002(3)	0.005(3)	0.002(3)
C11	0.046(4)	0.041(4)	0.037(4)	0.023(3)	0.005(3)	0.005(3)
C13	0.052(4)	0.051(4)	0.022(3)	-0.004(3)	0.009(3)	0.000(3)
C15	0.092(7)	0.024(3)	0.057(5)	-0.010(4)	-0.029(5)	0.006(3)
C16	0.041(3)	0.036(3)	0.025(3)	0.008(3)	-0.007(3)	0.010(3)
C17	0.037(3)	0.034(3)	0.029(3)	-0.006(3)	-0.004(3)	0.009(3)
C18	0.026(3)	0.064(5)	0.045(4)	0.009(3)	-0.003(3)	0.000(4)
C19	0.040(3)	0.031(3)	0.024(3)	0.007(3)	0.004(3)	-0.005(2)
C20	0.021(3)	0.051(4)	0.028(3)	-0.005(3)	0.001(2)	-0.005(3)
C21	0.035(3)	0.048(4)	0.032(3)	0.008(3)	-0.012(3)	-0.012(3)
C22	0.019(3)	0.054(4)	0.042(4)	0.007(3)	-0.008(3)	0.000(3)
C23	0.045(4)	0.033(3)	0.037(4)	0.006(3)	-0.002(3)	-0.004(3)
C24	0.029(3)	0.031(3)	0.027(3)	-0.003(2)	-0.002(2)	-0.007(2)
C25	0.044(4)	0.034(3)	0.029(3)	-0.010(3)	0.001(3)	0.000(3)
C26	0.042(4)	0.062(5)	0.040(4)	0.024(4)	-0.004(3)	-0.015(3)
C27	0.059(5)	0.044(4)	0.027(3)	-0.015(3)	0.005(3)	0.002(3)
C28	0.039(4)	0.045(4)	0.040(4)	0.001(3)	-0.011(3)	0.006(3)
C29	0.048(4)	0.064(5)	0.033(4)	0.025(4)	-0.017(3)	-0.011(3)
C30	0.026(3)	0.070(5)	0.038(4)	-0.015(3)	0.009(3)	0.000(4)
C31	0.035(4)	0.063(5)	0.045(4)	-0.019(3)	-0.001(3)	-0.009(4)
C32	0.089(6)	0.025(3)	0.048(4)	0.017(4)	-0.004(4)	0.005(3)
C33	0.055(4)	0.041(4)	0.027(3)	0.000(3)	-0.000(3)	0.000(3)
C34	0.051(4)	0.042(4)	0.049(4)	-0.022(3)	0.001(3)	-0.008(3)
C35	0.059(5)	0.059(5)	0.031(4)	-0.024(4)	0.007(3)	0.007(3)
C40	0.056(5)	0.049(4)	0.046(4)	-0.030(4)	-0.012(4)	0.007(3)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S2-4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Br1	Fe45	2.6637(11)	Br1	Fe46	2.6270(9)
Br2	Fe45	2.6605(10)	Br2	Fe46	2.6425(11)
Br3	Fe1	2.6598(10)	Br4	Fe45	2.6139(10)
Br4	Fe46	2.6654(11)	Br5	Fe1	2.6057(11)

Br6	Fe1	2.5839(11)	Fe1	N8	2.303(6)
Fe1	N47	2.334(5)	Fe1	N48	2.266(6)
Fe45	N12	2.205(5)	Fe45	N14	2.214(5)
Fe45	N41	2.223(5)	Fe46	N49	2.210(5)
Fe46	N50	2.199(5)	Fe46	N51	2.203(5)
N8	C26	1.481(9)	N8	C29	1.485(9)
N8	C32	1.484(9)	N12	C13	1.499(9)
N12	C17	1.477(8)	N12	C28	1.466(8)
N14	C23	1.482(9)	N14	C33	1.475(9)
N14	C34	1.492(9)	N41	C18	1.483(10)
N41	C30	1.475(9)	N41	C31	1.480(10)
N47	C19	1.472(8)	N47	C21	1.480(8)
N47	C27	1.474(9)	N48	C15	1.497(10)
N48	C35	1.505(9)	N48	C40	1.472(10)
N49	C11	1.490(9)	N49	C16	1.481(8)
N49	C22	1.488(8)	N50	C6	1.488(8)
N50	C9	1.503(8)	N50	C10	1.479(8)
N51	C20	1.487(8)	N51	C24	1.500(8)
N51	C25	1.476(8)	C6	C24	1.515(8)
C9	C16	1.524(9)	C13	C33	1.488(10)
C15	C32	1.485(13)	C18	C28	1.493(10)
C20	C22	1.504(10)	C21	C29	1.484(11)
C27	C35	1.488(11)	C31	C34	1.498(11)

Table S2-5. Bond angles (o)

atom	atom	atom	angle	atom	atom	atom	angle
Fe45	Br1	Fe46	73.44(3)	Fe45	Br2	Fe46	73.25(3)
Fe45	Br4	Fe46	73.62(3)	Br3	Fe1	Br5	97.86(3)
Br3	Fe1	Br6	94.05(3)	Br3	Fe1	N8	92.39(14)
Br3	Fe1	N47	167.19(12)	Br3	Fe1	N48	94.26(14)
Br5	Fe1	Br6	94.48(3)	Br5	Fe1	N8	166.87(14)
Br5	Fe1	N47	92.02(12)	Br5	Fe1	N48	93.29(15)
Br6	Fe1	N8	92.95(14)	Br6	Fe1	N47	93.28(12)
Br6	Fe1	N48	167.75(15)	N8	Fe1	N47	76.74(18)
N8	Fe1	N48	77.7(2)	N47	Fe1	N48	76.98(18)
Br1	Fe45	Br2	86.60(3)	Br1	Fe45	Br4	88.15(3)
Br1	Fe45	N12	94.65(13)	Br1	Fe45	N14	98.64(14)
Br1	Fe45	N41	175.54(14)	Br2	Fe45	Br4	88.97(3)
Br2	Fe45	N12	95.13(13)	Br2	Fe45	N14	173.74(14)
Br2	Fe45	N41	93.59(15)	Br4	Fe45	N12	175.17(14)
Br4	Fe45	N14	94.61(14)	Br4	Fe45	N41	96.32(14)
N12	Fe45	N14	81.09(19)	N12	Fe45	N41	80.89(19)
N14	Fe45	N41	80.9(2)	Br1	Fe46	Br2	87.72(3)
Br1	Fe46	Br4	87.84(3)	Br1	Fe46	N49	97.91(13)
Br1	Fe46	N50	177.65(13)	Br1	Fe46	N51	95.58(13)
Br2	Fe46	Br4	88.26(3)	Br2	Fe46	N49	174.05(13)
Br2	Fe46	N50	92.80(13)	Br2	Fe46	N51	96.72(13)
Br4	Fe46	N49	93.85(14)	Br4	Fe46	N50	94.47(13)
Br4	Fe46	N51	174.05(13)	N49	Fe46	N50	81.50(18)
N49	Fe46	N51	80.87(19)	N50	Fe46	N51	82.08(18)
Fe1	N8	C26	111.3(4)	Fe1	N8	C29	111.3(4)
Fe1	N8	C32	103.2(5)	C26	N8	C29	110.1(6)
C26	N8	C32	109.1(6)	C29	N8	C32	111.6(6)
Fe45	N12	C13	102.0(4)	Fe45	N12	C17	114.2(4)
Fe45	N12	C28	109.3(4)	C13	N12	C17	107.4(5)
C13	N12	C28	112.7(5)	C17	N12	C28	111.0(5)
Fe45	N14	C23	113.6(4)	Fe45	N14	C33	108.8(4)
Fe45	N14	C34	102.6(4)	C23	N14	C33	110.3(5)
C23	N14	C34	108.8(5)	C33	N14	C34	112.6(5)

Fe45	N41	C18	101.9(4)	Fe45	N41	C30	113.7(4)
Fe45	N41	C31	108.9(4)	C18	N41	C30	108.4(5)
C18	N41	C31	111.4(5)	C30	N41	C31	112.1(6)
Fe1	N47	C19	112.5(4)	Fe1	N47	C21	103.4(4)
Fe1	N47	C27	110.2(4)	C19	N47	C21	107.9(5)
C19	N47	C27	110.7(5)	C21	N47	C27	111.9(5)
Fe1	N48	C15	110.5(5)	Fe1	N48	C35	104.5(4)
Fe1	N48	C40	110.8(4)	C15	N48	C35	111.9(6)
C15	N48	C40	111.1(6)	C35	N48	C40	107.7(6)
Fe46	N49	C11	113.9(4)	Fe46	N49	C16	102.8(4)
Fe46	N49	C22	109.0(4)	C11	N49	C16	109.2(5)
C11	N49	C22	110.4(5)	C16	N49	C22	111.3(5)
Fe46	N50	C6	102.5(3)	Fe46	N50	C9	108.5(3)
Fe46	N50	C10	115.1(4)	C6	N50	C9	111.1(4)
C6	N50	C10	109.3(5)	C9	N50	C10	110.2(5)
Fe46	N51	C20	103.5(4)	Fe46	N51	C24	108.4(3)
Fe46	N51	C25	114.8(4)	C20	N51	C24	110.7(5)
C20	N51	C25	108.9(5)	C24	N51	C25	110.4(5)
N50	C6	C24	112.6(5)	N50	C9	C16	112.3(5)
N12	C13	C33	112.8(6)	N48	C15	C32	113.6(6)
N49	C16	C9	111.0(5)	N41	C18	C28	113.1(6)
N51	C20	C22	111.5(5)	N47	C21	C29	114.1(6)
N49	C22	C20	112.0(5)	N51	C24	C6	112.3(5)
N47	C27	C35	113.2(6)	N12	C28	C18	113.0(6)
N8	C29	C21	113.0(6)	N41	C31	C34	112.7(6)
N8	C32	C15	112.7(6)	N14	C33	C13	113.2(6)
N14	C34	C31	112.6(6)	N48	C35	C27	112.6(6)

Table S2-6. Torsion Angles(°)
(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Fe45	Br1	Fe46	Br2	-45.08(3)	Fe45	Br1	Fe46	Br4	43.26(3)
Fe45	Br1	Fe46	N49	136.86(3)	Fe45	Br1	Fe46	N51	-141.62(3)
Fe46	Br1	Fe45	Br2	44.75(2)	Fe46	Br1	Fe45	Br4	-44.33(2)
Fe46	Br1	Fe45	N12	139.62(3)	Fe46	Br1	Fe45	N14	-138.71(3)
Fe45	Br2	Fe46	Br1	45.21(2)	Fe45	Br2	Fe46	Br4	-42.69(2)
Fe45	Br2	Fe46	N50	-137.08(3)	Fe45	Br2	Fe46	N51	140.57(3)
Fe46	Br2	Fe45	Br1	-44.48(2)	Fe46	Br2	Fe45	Br4	43.73(3)
Fe46	Br2	Fe45	N12	-138.85(4)	Fe46	Br2	Fe45	N41	139.99(3)
Fe45	Br4	Fe46	Br1	-44.25(3)	Fe45	Br4	Fe46	Br2	43.54(3)
Fe45	Br4	Fe46	N49	-142.03(3)	Fe45	Br4	Fe46	N50	136.21(4)
Fe46	Br4	Fe45	Br1	43.48(3)	Fe46	Br4	Fe45	Br2	-43.15(3)
Fe46	Br4	Fe45	N14	142.00(4)	Fe46	Br4	Fe45	N41	-136.65(3)
Br3	Fe1	N8	C26	54.9(3)	Br3	Fe1	N8	C29	178.2(3)
Br3	Fe1	N8	C32	-62.0(3)	Br3	Fe1	N48	C15	81.2(3)
Br3	Fe1	N48	C35	-158.2(3)	Br3	Fe1	N48	C40	-42.4(3)
Br5	Fe1	N47	C19	-40.6(3)	Br5	Fe1	N47	C21	-156.8(2)
Br5	Fe1	N47	C27	83.5(2)	Br5	Fe1	N48	C15	179.4(3)
Br5	Fe1	N48	C35	-60.0(3)	Br5	Fe1	N48	C40	55.8(3)
Br6	Fe1	N8	C26	-39.3(3)	Br6	Fe1	N8	C29	84.0(3)
Br6	Fe1	N8	C32	-156.2(2)	Br6	Fe1	N47	C19	54.0(3)
Br6	Fe1	N47	C21	-62.2(2)	Br6	Fe1	N47	C27	178.1(2)
N8	Fe1	N47	C19	146.3(3)	N8	Fe1	N47	C21	30.1(2)
N8	Fe1	N47	C27	-89.7(3)	N47	Fe1	N8	C26	-132.0(3)
N47	Fe1	N8	C29	-8.7(3)	N47	Fe1	N8	C32	111.2(3)
N8	Fe1	N48	C15	-10.3(3)	N8	Fe1	N48	C35	110.3(3)
N8	Fe1	N48	C40	-133.9(3)	N48	Fe1	N8	C26	148.7(3)
N48	Fe1	N8	C29	-88.0(3)	N48	Fe1	N8	C32	31.9(3)
N47	Fe1	N48	C15	-89.3(3)	N47	Fe1	N48	C35	31.3(3)

N47	Fe1	N48	C40	147.1(3)	N48	Fe1	N47	C19	-133.5(3)
N48	Fe1	N47	C21	110.3(3)	N48	Fe1	N47	C27	-9.5(3)
Br1	Fe45	N12	C13	67.8(2)	Br1	Fe45	N12	C17	-47.8(3)
Br1	Fe45	N12	C28	-172.7(2)	Br1	Fe45	N14	C23	38.1(3)
Br1	Fe45	N14	C33	-85.1(3)	Br1	Fe45	N14	C34	155.4(2)
Br2	Fe45	N12	C13	154.8(2)	Br2	Fe45	N12	C17	39.2(3)
Br2	Fe45	N12	C28	-85.8(3)	Br2	Fe45	N41	C18	65.2(2)
Br2	Fe45	N41	C30	-51.3(3)	Br2	Fe45	N41	C31	-177.0(3)
Br4	Fe45	N14	C23	-50.7(3)	Br4	Fe45	N14	C33	-173.9(2)
Br4	Fe45	N14	C34	66.6(2)	Br4	Fe45	N41	C18	154.5(2)
Br4	Fe45	N41	C30	38.1(3)	Br4	Fe45	N41	C31	-87.7(3)
N12	Fe45	N14	C23	131.5(3)	N12	Fe45	N14	C33	8.3(3)
N12	Fe45	N14	C34	-111.2(3)	N14	Fe45	N12	C13	-30.3(2)
N14	Fe45	N12	C17	-145.8(3)	N14	Fe45	N12	C28	89.2(3)
N12	Fe45	N41	C18	-29.5(3)	N12	Fe45	N41	C30	-145.9(4)
N12	Fe45	N41	C31	88.3(3)	N41	Fe45	N12	C13	-112.4(3)
N41	Fe45	N12	C17	132.0(3)	N41	Fe45	N12	C28	7.1(3)
N14	Fe45	N41	C18	-111.8(3)	N14	Fe45	N41	C30	131.8(4)
N14	Fe45	N41	C31	6.0(3)	N41	Fe45	N14	C23	-146.4(3)
N41	Fe45	N14	C33	90.4(3)	N41	Fe45	N14	C34	-29.1(3)
Br1	Fe46	N49	C11	-33.5(3)	Br1	Fe46	N49	C16	-151.5(2)
Br1	Fe46	N49	C22	90.3(3)	Br1	Fe46	N51	C20	-68.5(2)
Br1	Fe46	N51	C24	173.9(2)	Br1	Fe46	N51	C25	50.0(3)
Br2	Fe46	N50	C6	-67.0(2)	Br2	Fe46	N50	C9	175.4(2)
Br2	Fe46	N50	C10	51.5(3)	Br2	Fe46	N51	C20	-156.8(2)
Br2	Fe46	N51	C24	85.6(2)	Br2	Fe46	N51	C25	-38.3(3)
Br4	Fe46	N49	C11	54.8(3)	Br4	Fe46	N49	C16	-63.1(2)
Br4	Fe46	N49	C22	178.7(2)	Br4	Fe46	N50	C6	-155.5(2)
Br4	Fe46	N50	C9	87.0(2)	Br4	Fe46	N50	C10	-36.9(3)
N49	Fe46	N50	C6	111.3(3)	N49	Fe46	N50	C9	-6.3(3)
N49	Fe46	N50	C10	-130.2(3)	N50	Fe46	N49	C11	148.8(3)
N50	Fe46	N49	C16	30.8(3)	N50	Fe46	N49	C22	-87.4(3)
N49	Fe46	N51	C20	28.7(2)	N49	Fe46	N51	C24	-88.9(3)
N49	Fe46	N51	C25	147.2(3)	N51	Fe46	N49	C11	-127.9(3)
N51	Fe46	N49	C16	114.1(3)	N51	Fe46	N49	C22	-4.1(3)
N50	Fe46	N51	C20	111.3(3)	N50	Fe46	N51	C24	-6.3(3)
N50	Fe46	N51	C25	-130.2(3)	N51	Fe46	N50	C6	29.4(2)
N51	Fe46	N50	C9	-88.2(3)	N51	Fe46	N50	C10	147.9(3)
Fe1	N8	C29	C21	-15.4(7)	Fe1	N8	C32	C15	-51.4(6)
C26	N8	C29	C21	108.5(6)	C26	N8	C32	C15	-169.8(5)
C29	N8	C32	C15	68.2(8)	C32	N8	C29	C21	-130.2(6)
Fe45	N12	C13	C33	50.5(5)	Fe45	N12	C28	C18	18.0(6)
C17	N12	C13	C33	170.8(5)	C13	N12	C28	C18	130.7(5)
C28	N12	C13	C33	-66.6(7)	C17	N12	C28	C18	-108.8(6)
Fe45	N14	C33	C13	17.1(6)	Fe45	N14	C34	C31	50.2(6)
C23	N14	C33	C13	-108.1(6)	C23	N14	C34	C31	170.8(5)
C33	N14	C34	C31	-66.6(7)	C34	N14	C33	C13	130.1(6)
Fe45	N41	C18	C28	49.9(5)	Fe45	N41	C31	C34	19.6(6)
C30	N41	C18	C28	170.1(5)	C18	N41	C31	C34	131.1(5)
C31	N41	C18	C28	-66.1(6)	C30	N41	C31	C34	-107.1(6)
Fe1	N47	C21	C29	-50.8(5)	Fe1	N47	C27	C35	-15.6(6)
C19	N47	C21	C29	-170.2(4)	C19	N47	C27	C35	109.4(6)
C21	N47	C27	C35	-130.1(5)	C27	N47	C21	C29	67.8(6)
Fe1	N48	C15	C32	-14.2(7)	Fe1	N48	C35	C27	-52.1(6)
C15	N48	C35	C27	67.5(7)	C35	N48	C15	C32	-130.3(6)
C40	N48	C15	C32	109.2(7)	C40	N48	C35	C27	-170.0(5)
Fe46	N49	C16	C9	-51.6(5)	Fe46	N49	C22	C20	-22.1(6)
C11	N49	C16	C9	-172.8(5)	C11	N49	C22	C20	103.7(5)
C16	N49	C22	C20	-134.9(5)	C22	N49	C16	C9	65.0(6)
Fe46	N50	C6	C24	-50.0(4)	Fe46	N50	C9	C16	-20.0(5)

C6	N50	C9	C16	-131.9(5)	C9	N50	C6	C24	65.7(5)
C10	N50	C6	C24	-172.5(4)	C10	N50	C9	C16	106.9(5)
Fe46	N51	C20	C22	-50.6(5)	Fe46	N51	C24	C6	-18.9(5)
C20	N51	C24	C6	-131.7(5)	C24	N51	C20	C22	65.4(6)
C25	N51	C20	C22	-173.1(4)	C25	N51	C24	C6	107.7(5)
N50	C6	C24	N51	48.7(6)	N50	C9	C16	N49	50.4(6)
N12	C13	C33	N14	-47.9(8)	N48	C15	C32	N8	46.3(9)
N41	C18	C28	N12	-48.5(8)	N51	C20	C22	N49	50.9(7)
N47	C21	C29	N8	46.9(8)	N47	C27	C35	N48	46.8(8)
N41	C31	C34	N14	-49.3(8)					

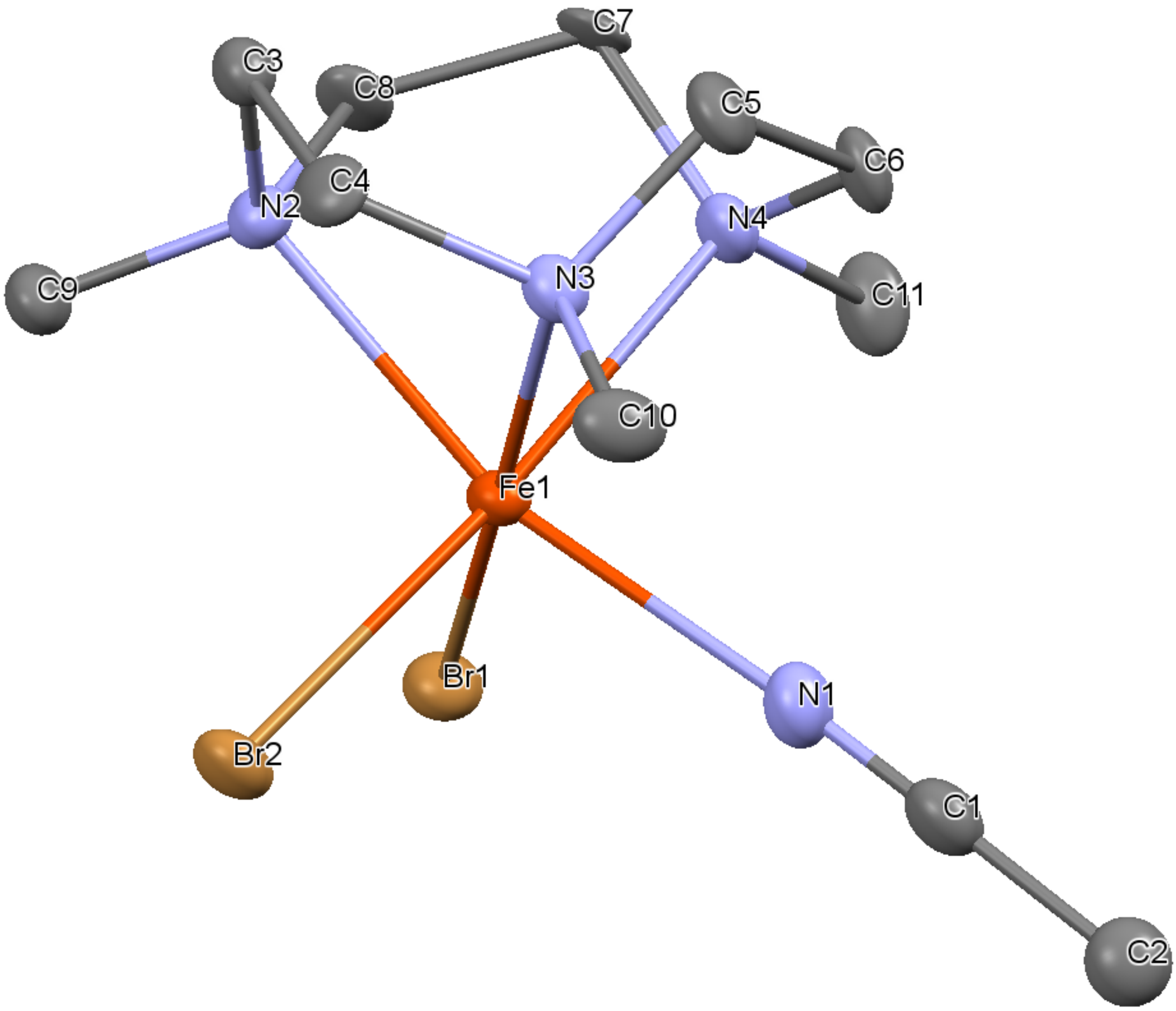


Figure S26. ORTEP drawing of **6** (50% probability of the thermal ellipsoids)

Table S3-1. Crystal data and structure refinement for **6**

Empirical Formula	$C_{11}H_{24}Br_2FeN_4$
Formula Weight	427.99
Crystal Color, Habit	pink-red, block
Crystal Dimensions	0.200 X 0.200 X 0.100 mm
Crystal System	orthorhombic
Lattice Type	Primitive
Lattice Parameters	*a* = 16.354(2) Å
	b = 12.5257(13) Å
	c = 7.6117(8) Å
	V = 1559.2(3) $Å^3$
Space Group	$Pna2_1$ (#33)
Z value	4
D_{calc}	1.823 g/cm^3
F_{000}	856.00
μ(MoKα)	60.973 cm^{-1}
Diffractometer	Saturn724
Radiation	MoKα (λ = 0.71075 Å)
	multi-layer mirror monochromated
Voltage, Current	50kV, 40mA
Temperature	-159.8^{o}C
Detector Aperture	70 x 70 mm
Data Images	420 exposures
ω oscillation Range	-60.0 - -15.0^o
Exposure Rate	10.0 sec./^{o}
Detector Swing Angle	-14.83^o
Detector Position	40.12 mm
Pixel Size	0.070 mm
$2\theta_{max}$	55.0^o
No. of Reflections Measured	Total: 8301
	Unique: 2810 (R_{int} = 0.1235)
	Friedel pairs: 894
Corrections	Lorentz-polarization
	Absorption
	(trans. factors: 0.372 - 0.543)
Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\ \omega\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$\omega = 1/ [\ \sigma^2(Fo^2) + (0.1366 \cdot P)^2$
	$+ 9.6946 \cdot\ P\ ]$
	where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	55.0^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	2810
No. Variables	163
Reflection/Parameter Ratio	17.24
Residuals: R1 (I>2.00σ(I))	0.0643
Residuals: R (All reflections)	0.0664
Residuals: wR2 (All reflections)	0.1631
Goodness of Fit Indicator	0.886
Flack Parameter (Friedel pairs = 894)	0.01(3)
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	1.30 $e^-/Å^3$
Minimum peak in Final Diff. Map	-2.14 $e^-/Å^3$

Table S3-2. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Br1	0.95004(5)	0.62272(6)	0.31676(12)	1.54(2)
Br2	0.89758(5)	0.91545(6)	0.33886(13)	1.62(2)
Fe1	0.86807(7)	0.74335(9)	0.5196(2)	1.12(3)

N1	0.7505(4)	0.7114(6)	0.3752(11)	1.75(13)
N2	0.9648(4)	0.7647(6)	0.7268(10)	1.24(11)
N3	0.7991(4)	0.8376(5)	0.7298(10)	1.24(11)
N4	0.8345(5)	0.6129(5)	0.7144(11)	1.33(12)
C1	0.6913(6)	0.6998(7)	0.2972(12)	1.7(2)
C2	0.6159(6)	0.6863(8)	0.197(2)	2.0(2)
C3	0.9375(5)	0.8379(7)	0.8692(12)	1.4(2)
C4	0.8653(5)	0.9051(6)	0.808(2)	1.5(2)
C5	0.7642(5)	0.7643(7)	0.8628(13)	1.7(2)
C6	0.7563(5)	0.6514(6)	0.7913(12)	1.5(2)
C7	0.8993(5)	0.6036(7)	0.8548(13)	1.26(13)
C8	0.9789(5)	0.6541(7)	0.7924(13)	1.6(2)
C9	1.0420(5)	0.8041(8)	0.6496(13)	1.6(2)
C10	0.7355(6)	0.9074(7)	0.653(2)	1.8(2)
C11	0.8209(6)	0.5092(7)	0.632(2)	2.0(2)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S3-3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br1	0.0251(4)	0.0157(4)	0.0178(5)	0.0032(3)	0.0021(4)	-0.0024(4)
Br2	0.0270(4)	0.0144(4)	0.0200(5)	0.0019(3)	0.0040(4)	0.0047(4)
Fe1	0.0177(5)	0.0127(5)	0.0122(6)	0.0003(4)	0.0004(5)	-0.0000(5)
N1	0.020(3)	0.017(3)	0.029(5)	0.000(3)	0.002(3)	-0.000(3)
N2	0.019(3)	0.012(3)	0.016(4)	0.000(3)	-0.002(3)	-0.002(3)
N3	0.018(3)	0.011(3)	0.018(4)	0.002(3)	0.003(3)	-0.001(3)
N4	0.020(3)	0.011(3)	0.020(4)	-0.002(3)	0.001(3)	0.003(3)
C1	0.027(4)	0.015(4)	0.023(6)	0.001(3)	0.006(4)	0.003(4)
C2	0.027(4)	0.019(4)	0.031(6)	0.006(4)	0.002(4)	-0.002(4)
C3	0.019(4)	0.015(4)	0.018(5)	-0.002(3)	0.002(4)	-0.001(4)
C4	0.028(4)	0.011(4)	0.019(5)	-0.001(3)	-0.001(4)	-0.007(4)
C5	0.020(4)	0.018(4)	0.025(5)	0.000(3)	0.009(4)	0.000(4)
C6	0.017(3)	0.010(3)	0.029(6)	-0.002(3)	0.007(4)	0.003(4)
C7	0.024(4)	0.014(4)	0.010(4)	0.001(3)	0.002(3)	0.008(4)
C8	0.022(4)	0.018(4)	0.021(5)	0.003(3)	-0.002(4)	0.011(4)
C9	0.019(4)	0.024(4)	0.019(5)	-0.003(3)	0.003(4)	-0.000(4)
C10	0.026(4)	0.020(4)	0.021(5)	0.011(4)	0.003(4)	-0.000(4)
C11	0.025(4)	0.010(4)	0.040(6)	0.001(4)	0.007(4)	-0.005(4)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S3-4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Br1	Fe1	2.5424(15)	Br2	Fe1	2.6024(15)
Fe1	N1	2.251(8)	Fe1	N2	2.250(8)
Fe1	N3	2.287(7)	Fe1	N4	2.274(8)
N1	C1	1.145(12)	N2	C3	1.488(11)
N2	C8	1.491(11)	N2	C9	1.478(11)
N3	C4	1.498(11)	N3	C5	1.480(12)
N3	C10	1.480(12)	N4	C6	1.487(11)
N4	C7	1.510(12)	N4	C11	1.461(11)
C1	C2	1.462(13)	C3	C4	1.522(12)
C5	C6	1.521(12)	C7	C8	1.522(12)

Table S3-5. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Br1	Fe1	Br2	94.21(5)	Br1	Fe1	N1	92.8(2)
Br1	Fe1	N2	97.23(19)	Br1	Fe1	N3	172.80(18)
Br1	Fe1	N4	95.52(19)	Br2	Fe1	N1	92.7(2)
Br2	Fe1	N2	98.15(18)	Br2	Fe1	N3	91.93(17)
Br2	Fe1	N4	170.0(2)	N1	Fe1	N2	164.6(3)
N1	Fe1	N3	90.7(3)	N1	Fe1	N4	89.1(3)
N2	Fe1	N3	78.2(3)	N2	Fe1	N4	78.3(3)
N3	Fe1	N4	78.2(3)	Fe1	N1	C1	176.6(7)
Fe1	N2	C3	111.9(5)	Fe1	N2	C8	103.5(5)
Fe1	N2	C9	111.2(6)	C3	N2	C8	112.0(7)
C3	N2	C9	109.9(7)	C8	N2	C9	108.1(7)
Fe1	N3	C4	102.3(5)	Fe1	N3	C5	110.4(5)
Fe1	N3	C10	111.9(6)	C4	N3	C5	110.9(7)
C4	N3	C10	109.5(6)	C5	N3	C10	111.6(7)
Fe1	N4	C6	103.3(5)	Fe1	N4	C7	110.3(5)
Fe1	N4	C11	113.2(7)	C6	N4	C7	110.5(7)
C6	N4	C11	109.1(7)	C7	N4	C11	110.1(7)
N1	C1	C2	179.3(9)	N2	C3	C4	110.6(7)
N3	C4	C3	111.7(6)	N3	C5	C6	111.4(8)
N4	C6	C5	111.7(7)	N4	C7	C8	110.3(8)
N2	C8	C7	111.0(7)				

Table S3-6. Torsion Angles(°)
(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Br1	Fe1	N2	C3	177.7(4)	Br1	Fe1	N2	C8	-61.5(4)
Br1	Fe1	N2	C9	54.3(4)	Br1	Fe1	N4	C6	-153.0(4)
Br1	Fe1	N4	C7	88.8(4)	Br1	Fe1	N4	C11	-35.1(4)
Br2	Fe1	N2	C3	82.3(4)	Br2	Fe1	N2	C8	-156.9(3)
Br2	Fe1	N2	C9	-41.0(4)	Br2	Fe1	N3	C4	-65.9(3)
Br2	Fe1	N3	C5	176.0(4)	Br2	Fe1	N3	C10	51.2(4)
N1	Fe1	N3	C4	-158.7(4)	N1	Fe1	N3	C5	83.3(4)
N1	Fe1	N3	C10	-41.6(4)	N1	Fe1	N4	C6	-60.3(4)
N1	Fe1	N4	C7	-178.5(4)	N1	Fe1	N4	C11	57.6(5)
N2	Fe1	N3	C4	32.0(4)	N2	Fe1	N3	C5	-86.0(4)
N2	Fe1	N3	C10	149.1(4)	N3	Fe1	N2	C3	-7.9(4)
N3	Fe1	N2	C8	112.9(4)	N3	Fe1	N2	C9	-131.3(4)
N2	Fe1	N4	C6	110.7(4)	N2	Fe1	N4	C7	-7.5(4)
N2	Fe1	N4	C11	-131.4(5)	N4	Fe1	N2	C3	-88.1(4)
N4	Fe1	N2	C8	32.6(4)	N4	Fe1	N2	C9	148.5(4)
N3	Fe1	N4	C6	30.6(4)	N3	Fe1	N4	C7	-87.6(4)
N3	Fe1	N4	C11	148.4(5)	N4	Fe1	N3	C4	112.4(4)
N4	Fe1	N3	C5	-5.7(4)	N4	Fe1	N3	C10	-130.5(4)
Fe1	N2	C3	C4	-18.5(7)	Fe1	N2	C8	C7	-55.5(7)
C3	N2	C8	C7	65.3(8)	C8	N2	C3	C4	-134.1(6)
C9	N2	C3	C4	105.6(7)	C9	N2	C8	C7	-173.5(7)
Fe1	N3	C4	C3	-54.0(7)	Fe1	N3	C5	C6	-20.9(7)
C4	N3	C5	C6	-133.5(6)	C5	N3	C4	C3	63.7(9)
C10	N3	C4	C3	-172.8(7)	C10	N3	C5	C6	104.2(7)
Fe1	N4	C6	C5	-53.3(7)	Fe1	N4	C7	C8	-19.5(7)
C6	N4	C7	C8	-133.2(6)	C7	N4	C6	C5	64.8(8)
C11	N4	C6	C5	-174.0(7)	C11	N4	C7	C8	106.2(7)
N2	C3	C4	N3	50.7(9)	N3	C5	C6	N4	51.9(9)
N4	C7	C8	N2	51.8(9)					

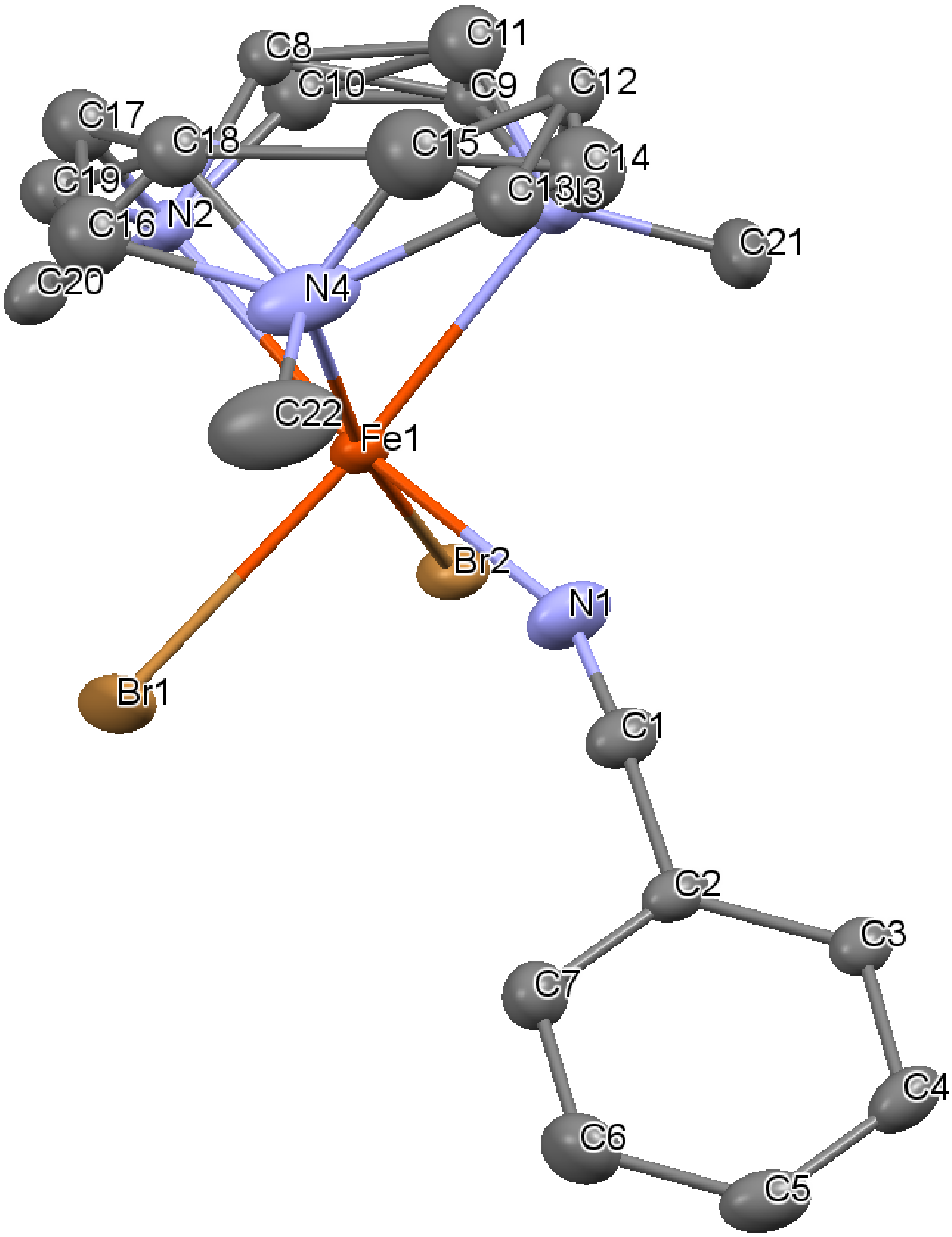


Figure S27. ORTEP drawing of **7** (50% probability of the thermal ellipsoids). The site occupancy factors for C8 ~ C20 were defined as 0.5.

Table S4-1. Crystal data and structure refinement for **7**

Empirical Formula	$C_{16}H_{26}Br_2FeN_4$
Formula Weight	490.06
Crystal Color, Habit	colorless, block
Crystal Dimensions	0.120 X 0.100 X 0.100 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 7.7264(17) Å
	b = 17.285(3) Å
	c = 14.927(3) Å
	β = 94.081(7) ^{o}
	V = 1988.4(7) $Å^3$
Space Group	$P2_1/c$ (#14)
Z value	4
D_{calc}	1.637 g/cm^3
F_{000}	984.00
μ(MoKα)	47.928 cm^{-1}
Diffractometer	Saturn724
Radiation	MoKα (λ = 0.71075 Å)
	multi-layer mirror monochromated
Voltage, Current	50kV, 40mA
Temperature	-159.8 ^{o}C
Detector Aperture	72.8 x 72.8 mm
Data Images	510 exposures
ω oscillation Range (χ=45.0, ϕ=90.0)	-30.0 - 45.0 ^{o}
Exposure Rate	10.0 sec./ ^{o}
Detector Swing Angle	-14.70 ^{o}
Detector Position	40.12 mm
Pixel Size	0.070 mm
$2\theta_{max}$	55.0 ^{o}
No. of Reflections Measured	Total: 12908
	Unique: 4511 (R_{int} = 0.0452)
Corrections	Lorentz-polarization
	Absorption
	(trans. factors: 0.480 - 0.619)
Structure Solution	Direct Methods (SIR2008)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma w (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.0794 \cdot P)^2$
	$+ 2.9899 \cdot P]$
	where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	55.0 ^{o}
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	4511
No. Variables	202
Reflection/Parameter Ratio	22.33
Residuals: R1 (I>2.00σ(I))	0.0572
Residuals: R (All reflections)	0.0593
Residuals: wR2 (All reflections)	0.1458
Goodness of Fit Indicator	1.245
Max Shift/Error in Final Cycle	0.002
Maximum peak in Final Diff. Map	1.02 $e^-/Å^3$
Minimum peak in Final Diff. Map	-2.11 $e^-/Å^3$

Table S4-2. Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Br1	0.74170(6)	0.29817(3)	1.09346(3)	2.912(13)	1
Br2	0.81199(4)	0.11497(2)	0.96796(3)	1.821(11)	1

Fe1	0.57413(6)	0.21855(3)	0.97032(3)	1.375(12)	1
N1	0.6850(5)	0.2878(2)	0.8663(3)	2.55(6)	1
N2	0.3963(4)	0.15739(19)	1.0583(2)	1.59(5)	1
N3	0.3950(4)	0.1568(2)	0.8658(2)	2.32(6)	1
N4	0.3350(5)	0.2974(2)	0.9593(3)	3.15(8)	1
C1	0.7638(5)	0.3373(2)	0.8391(3)	2.01(6)	1
C2	0.8607(5)	0.4031(2)	0.8112(3)	1.62(5)	1
C3	0.9203(5)	0.4062(2)	0.7250(3)	1.66(5)	1
C4	1.0143(5)	0.4707(2)	0.7016(3)	2.12(6)	1
C5	1.0510(5)	0.5296(2)	0.7636(3)	2.46(7)	1
C6	0.9918(6)	0.5253(3)	0.8492(3)	2.60(7)	1
C7	0.8962(5)	0.4621(3)	0.8733(3)	2.24(6)	1
C8	0.2857(11)	0.1015(5)	1.0084(5)	1.37(11)	1/2
C9	0.3601(9)	0.0798(4)	0.9187(5)	1.36(10)	1/2
C10	0.3428(13)	0.0856(5)	1.0013(6)	2.15(14)	1/2
C11	0.2752(13)	0.1081(6)	0.9067(6)	2.68(15)	1/2
C12	0.2421(11)	0.1941(5)	0.8370(5)	2.00(12)	1/2
C13	0.2637(12)	0.2788(5)	0.8541(6)	2.24(13)	1/2
C14	0.2832(14)	0.2320(7)	0.8278(7)	3.31(17)	1/2
C15	0.2089(16)	0.2804(7)	0.8956(8)	3.69(19)	1/2
C16	0.2699(14)	0.2864(6)	1.0606(7)	2.98(16)	1/2
C17	0.2437(13)	0.2013(6)	1.0783(7)	2.41(15)	1/2
C18	0.2031(11)	0.2707(5)	1.0152(6)	2.28(13)	1/2
C19	0.2869(12)	0.2235(5)	1.0917(6)	1.89(13)	1/2
C20	0.4919(5)	0.1249(3)	1.1386(3)	2.54(7)	1
C21	0.4861(6)	0.1274(3)	0.7897(3)	3.13(9)	1
C22	0.3776(8)	0.3807(3)	0.9631(5)	4.35(13)	1

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S4-3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br1	0.0295(3)	0.0381(3)	0.0443(3)	-0.01494(17)	0.01106(19)	-0.02308(19)
Br2	0.0158(2)	0.0216(2)	0.0321(2)	0.00074(12)	0.00376(15)	-0.00343(13)
Fe1	0.0145(3)	0.0168(3)	0.0213(3)	-0.00242(17)	0.00335(19)	0.00167(18)
N1	0.0276(18)	0.0332(18)	0.037(2)	-0.0043(14)	0.0064(15)	0.0146(15)
N2	0.0167(14)	0.0266(15)	0.0171(13)	-0.0040(12)	0.0025(11)	0.0009(12)
N3	0.0202(15)	0.050(2)	0.0177(15)	-0.0073(15)	0.0023(12)	0.0000(15)
N4	0.0240(18)	0.0231(17)	0.073(3)	0.0054(14)	0.0101(18)	0.0151(18)
C1	0.0192(17)	0.0292(19)	0.0278(19)	-0.0007(15)	0.0014(14)	0.0091(16)
C2	0.0148(15)	0.0236(17)	0.0232(17)	-0.0001(13)	0.0013(13)	0.0086(14)
C3	0.0174(16)	0.0236(17)	0.0219(17)	0.0010(14)	0.0015(13)	0.0040(14)
C4	0.0217(18)	0.0301(19)	0.0297(19)	0.0017(15)	0.0080(14)	0.0102(16)
C5	0.0231(19)	0.0242(18)	0.046(2)	-0.0023(15)	0.0032(17)	0.0083(17)
C6	0.033(2)	0.028(2)	0.037(2)	-0.0043(17)	0.0004(17)	-0.0052(17)
C7	0.0277(19)	0.034(2)	0.0234(18)	-0.0032(17)	0.0019(14)	0.0018(16)
C20	0.0230(19)	0.053(3)	0.0204(18)	-0.0071(18)	0.0016(15)	0.0110(18)
C21	0.028(2)	0.067(3)	0.024(2)	-0.009(2)	0.0036(16)	-0.012(2)
C22	0.040(3)	0.022(2)	0.105(5)	0.0094(19)	0.014(3)	0.007(3)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S4-4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Br1	Fe1	2.5710(7)	Br2	Fe1	2.5678(7)

Fe1	N1	2.183(4)	Fe1	N2	2.233(3)
Fe1	N3	2.277(3)	Fe1	N4	2.292(4)
N1	C1	1.142(6)	N2	C8	1.459(8)
N2	C10	1.544(10)	N2	C17	1.452(11)
N2	C19	1.526(10)	N2	C20	1.473(5)
N3	C9	1.580(8)	N3	C11	1.421(10)
N3	C12	1.387(9)	N3	C14	1.640(12)
N3	C21	1.468(6)	N4	C13	1.659(10)
N4	C15	1.344(13)	N4	C16	1.638(12)
N4	C18	1.438(10)	N4	C22	1.478(6)
C1	C2	1.438(6)	C2	C3	1.398(5)
C2	C7	1.392(6)	C3	C4	1.388(5)
C4	C5	1.392(6)	C5	C6	1.389(7)
C6	C7	1.381(6)	C8	C9	1.540(10)
C8	C10	0.536(13)	C8	C11	1.519(12)
C9	C10	1.253(11)	C9	C11	0.827(12)
C10	C11	1.521(13)	C11	C12	1.822(13)
C12	C13	1.493(12)	C12	C14	0.745(14)
C12	C15	1.757(14)	C13	C14	0.915(14)
C13	C15	0.776(16)	C14	C15	1.461(17)
C15	C18	1.797(15)	C16	C17	1.510(14)
C16	C18	0.866(13)	C16	C19	1.186(13)
C17	C18	1.543(13)	C17	C19	0.537(13)
C18	C19	1.512(12)			

Table S4-5. Bond angles (^{o})

atom	atom	atom	angle	atom	atom	atom	angle
Br1	Fe1	Br2	93.36(2)	Br1	Fe1	N1	90.66(10)
Br1	Fe1	N2	97.63(8)	Br1	Fe1	N3	172.63(9)
Br1	Fe1	N4	95.48(11)	Br2	Fe1	N1	93.16(10)
Br2	Fe1	N2	98.56(8)	Br2	Fe1	N3	93.68(10)
Br2	Fe1	N4	170.93(10)	N1	Fe1	N2	165.18(13)
N1	Fe1	N3	91.14(13)	N1	Fe1	N4	88.76(15)
N2	Fe1	N3	79.14(12)	N2	Fe1	N4	78.28(14)
N3	Fe1	N4	77.41(14)	Fe1	N1	C1	155.6(4)
Fe1	N2	C8	112.1(4)	Fe1	N2	C10	102.0(4)
Fe1	N2	C17	114.6(4)	Fe1	N2	C19	102.5(4)
Fe1	N2	C20	111.4(2)	C8	N2	C10	20.3(5)
C8	N2	C17	89.8(5)	C8	N2	C19	110.2(5)
C8	N2	C20	113.8(4)	C10	N2	C17	110.1(6)
C10	N2	C19	130.5(5)	C10	N2	C20	103.9(4)
C17	N2	C19	20.6(5)	C17	N2	C20	113.6(5)
C19	N2	C20	106.0(4)	Fe1	N3	C9	99.7(3)
Fe1	N3	C11	111.5(4)	Fe1	N3	C12	117.1(4)
Fe1	N3	C14	98.3(4)	Fe1	N3	C21	113.0(3)
C9	N3	C11	31.4(5)	C9	N3	C12	112.0(5)
C9	N3	C14	137.4(5)	C9	N3	C21	101.8(4)
C11	N3	C12	80.9(5)	C11	N3	C14	105.9(6)
C11	N3	C21	119.4(5)	C12	N3	C14	26.9(5)
C12	N3	C21	111.5(4)	C14	N3	C21	106.1(5)
Fe1	N4	C13	99.5(4)	Fe1	N4	C15	117.5(6)
Fe1	N4	C16	99.4(4)	Fe1	N4	C18	111.7(4)
Fe1	N4	C22	113.6(3)	C13	N4	C15	27.5(6)
C13	N4	C16	138.5(5)	C13	N4	C18	106.7(5)
C13	N4	C22	106.4(5)	C15	N4	C16	111.9(7)
C15	N4	C18	80.4(7)	C15	N4	C22	112.8(6)
C16	N4	C18	31.8(5)	C16	N4	C22	99.2(5)
C18	N4	C22	117.1(5)	N1	C1	C2	175.4(4)
C1	C2	C3	120.6(3)	C1	C2	C7	117.9(4)

C3	C2	C7	121.4(4)	C2	C3	C4	118.4(4)
C3	C4	C5	120.3(4)	C4	C5	C6	120.5(4)
C5	C6	C7	120.0(4)	C2	C7	C6	119.3(4)
N2	C8	C9	111.3(6)	N2	C8	C10	88.8(14)
N2	C8	C11	116.6(7)	C9	C8	C10	48.7(11)
C9	C8	C11	31.4(5)	C10	C8	C11	80.0(13)
N3	C9	C8	108.6(5)	N3	C9	C10	117.3(7)
N3	C9	C11	63.6(8)	C8	C9	C10	18.8(6)
C8	C9	C11	72.9(9)	C10	C9	C11	91.6(10)
N2	C10	C8	70.8(12)	N2	C10	C9	124.3(8)
N2	C10	C11	111.5(7)	C8	C10	C9	112.5(14)
C8	C10	C11	79.7(13)	C9	C10	C11	32.9(5)
N3	C11	C8	119.0(7)	N3	C11	C9	85.0(9)
N3	C11	C10	111.1(7)	N3	C11	C12	48.8(4)
C8	C11	C9	75.7(9)	C8	C11	C10	20.3(5)
C8	C11	C12	128.8(7)	C9	C11	C10	55.4(8)
C9	C11	C12	133.1(11)	C10	C11	C12	139.8(7)
N3	C12	C11	50.3(4)	N3	C12	C13	108.7(6)
N3	C12	C14	95.8(11)	N3	C12	C15	113.1(6)
C11	C12	C13	133.9(7)	C11	C12	C14	141.1(12)
C11	C12	C15	115.4(7)	C13	C12	C14	29.0(10)
C13	C12	C15	26.0(6)	C14	C12	C15	54.8(11)
N4	C13	C12	112.1(6)	N4	C13	C14	121.5(10)
N4	C13	C15	53.1(10)	C12	C13	C14	23.2(8)
C12	C13	C15	96.4(12)	C14	C13	C15	119.3(15)
N3	C14	C12	57.3(10)	N3	C14	C13	130.7(11)
N3	C14	C15	116.0(8)	C12	C14	C13	127.8(17)
C12	C14	C15	100.5(13)	C13	C14	C15	27.6(8)
N4	C15	C12	114.3(8)	N4	C15	C13	99.4(13)
N4	C15	C14	108.3(9)	N4	C15	C18	52.1(5)
C12	C15	C13	57.6(10)	C12	C15	C14	24.6(6)
C12	C15	C18	115.4(7)	C13	C15	C14	33.1(9)
C13	C15	C18	147.6(14)	C14	C15	C18	132.3(9)
N4	C16	C17	109.1(7)	N4	C16	C18	61.2(9)
N4	C16	C19	115.8(9)	C17	C16	C18	75.6(10)
C17	C16	C19	18.4(6)	C18	C16	C19	93.6(11)
N2	C17	C16	110.6(8)	N2	C17	C18	114.5(7)
N2	C17	C19	87.5(15)	C16	C17	C18	32.9(5)
C16	C17	C19	44.3(13)	C18	C17	C19	76.6(14)
N4	C18	C15	47.5(5)	N4	C18	C16	86.9(10)
N4	C18	C17	118.8(7)	N4	C18	C19	109.2(7)
C15	C18	C16	133.9(11)	C15	C18	C17	131.3(8)
C15	C18	C19	139.6(8)	C16	C18	C17	71.4(9)
C16	C18	C19	51.5(9)	C17	C18	C19	20.2(5)
N2	C19	C16	127.4(9)	N2	C19	C17	71.9(14)
N2	C19	C18	112.0(6)	C16	C19	C17	117.3(16)
C16	C19	C18	34.9(6)	C17	C19	C18	83.2(14)

Table S4-6. Torsion Angles(o)
(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Br1	Fe1	N1	C1	-6.0(7)	Br1	Fe1	N2	C8	-176.34(15)
Br1	Fe1	N2	C10	-157.85(12)	Br1	Fe1	N2	C17	83.18(17)
Br1	Fe1	N2	C19	65.54(13)	Br1	Fe1	N2	C20	-47.48(18)
Br1	Fe1	N4	C13	153.83(15)	Br1	Fe1	N4	C15	175.9(3)
Br1	Fe1	N4	C16	-63.28(16)	Br1	Fe1	N4	C18	-93.9(2)
Br1	Fe1	N4	C22	41.2(3)	Br2	Fe1	N1	C1	-99.4(7)
Br2	Fe1	N2	C8	-81.75(17)	Br2	Fe1	N2	C10	-63.27(14)

Br2	Fe1	N2	C17	177.76(15)	Br2	Fe1	N2	C19	160.12(12)
Br2	Fe1	N2	C20	47.11(18)	Br2	Fe1	N3	C9	63.24(15)
Br2	Fe1	N3	C11	93.6(2)	Br2	Fe1	N3	C12	-175.8(2)
Br2	Fe1	N3	C14	-155.58(13)	Br2	Fe1	N3	C21	-44.1(2)
N1	Fe1	N3	C9	156.48(17)	N1	Fe1	N3	C11	-173.2(2)
N1	Fe1	N3	C12	-82.6(2)	N1	Fe1	N3	C14	-62.34(17)
N1	Fe1	N3	C21	49.2(2)	N3	Fe1	N1	C1	166.8(7)
N1	Fe1	N4	C13	63.29(19)	N1	Fe1	N4	C15	85.3(3)
N1	Fe1	N4	C16	-153.83(19)	N1	Fe1	N4	C18	175.6(3)
N1	Fe1	N4	C22	-49.4(3)	N4	Fe1	N1	C1	89.4(7)
N2	Fe1	N3	C9	-34.79(15)	N2	Fe1	N3	C11	-4.4(2)
N2	Fe1	N3	C12	86.2(2)	N2	Fe1	N3	C14	106.39(16)
N2	Fe1	N3	C21	-142.1(2)	N3	Fe1	N2	C8	10.38(18)
N3	Fe1	N2	C10	28.87(15)	N3	Fe1	N2	C17	-90.11(19)
N3	Fe1	N2	C19	-107.74(16)	N3	Fe1	N2	C20	139.2(2)
N2	Fe1	N4	C13	-109.49(18)	N2	Fe1	N4	C15	-87.5(3)
N2	Fe1	N4	C16	33.40(16)	N2	Fe1	N4	C18	2.8(2)
N2	Fe1	N4	C22	137.9(3)	N4	Fe1	N2	C8	89.6(2)
N4	Fe1	N2	C10	108.10(18)	N4	Fe1	N2	C17	-10.88(19)
N4	Fe1	N2	C19	-28.51(16)	N4	Fe1	N2	C20	-141.5(2)
N3	Fe1	N4	C13	-28.16(16)	N3	Fe1	N4	C15	-6.1(3)
N3	Fe1	N4	C16	114.72(19)	N3	Fe1	N4	C18	84.1(2)
N3	Fe1	N4	C22	-140.8(3)	N4	Fe1	N3	C9	-115.05(19)
N4	Fe1	N3	C11	-84.7(2)	N4	Fe1	N3	C12	5.9(2)
N4	Fe1	N3	C14	26.13(16)	N4	Fe1	N3	C21	137.6(2)
Fe1	N2	C8	C9	19.0(6)	Fe1	N2	C8	C10	63.3(9)
Fe1	N2	C8	C11	-14.9(7)	Fe1	N2	C10	C8	-122.2(9)
Fe1	N2	C10	C9	-17.5(9)	Fe1	N2	C10	C11	-52.1(6)
Fe1	N2	C17	C16	-18.7(7)	Fe1	N2	C17	C18	16.8(8)
Fe1	N2	C17	C19	-57.2(11)	Fe1	N2	C19	C16	17.5(9)
Fe1	N2	C19	C17	128.4(8)	Fe1	N2	C19	C18	53.9(6)
C8	N2	C10	C8	0.0(9)	C8	N2	C10	C9	104.7(15)
C8	N2	C10	C11	70.1(12)	C10	N2	C8	C9	-44.3(11)
C10	N2	C8	C10	0.0(9)	C10	N2	C8	C11	-78.2(13)
C8	N2	C17	C16	-133.0(6)	C8	N2	C17	C18	-97.5(7)
C8	N2	C17	C19	-171.6(11)	C17	N2	C8	C9	135.6(6)
C17	N2	C8	C10	179.9(9)	C17	N2	C8	C11	101.7(7)
C8	N2	C19	C16	-101.9(9)	C8	N2	C19	C17	9.0(10)
C8	N2	C19	C18	-65.5(7)	C19	N2	C8	C9	132.5(5)
C19	N2	C8	C10	176.7(8)	C19	N2	C8	C11	98.5(6)
C20	N2	C8	C9	-108.6(5)	C20	N2	C8	C10	-64.3(9)
C20	N2	C8	C11	-142.5(5)	C10	N2	C17	C16	-133.0(6)
C10	N2	C17	C18	-97.5(7)	C10	N2	C17	C19	-171.5(10)
C17	N2	C10	C8	-0.1(11)	C17	N2	C10	C9	104.6(9)
C17	N2	C10	C11	69.9(8)	C10	N2	C19	C16	-100.4(10)
C10	N2	C19	C17	10.5(12)	C10	N2	C19	C18	-64.0(9)
C19	N2	C10	C8	-4.0(13)	C19	N2	C10	C9	100.7(10)
C19	N2	C10	C11	66.0(9)	C20	N2	C10	C8	121.9(9)
C20	N2	C10	C9	-133.4(8)	C20	N2	C10	C11	-168.1(5)
C17	N2	C19	C16	-110.9(17)	C17	N2	C19	C17	-0.0(11)
C17	N2	C19	C18	-74.5(14)	C19	N2	C17	C16	38.6(12)
C19	N2	C17	C18	74.1(14)	C19	N2	C17	C19	0.0(9)
C20	N2	C17	C16	110.9(6)	C20	N2	C17	C18	146.4(5)
C20	N2	C17	C19	72.4(11)	C20	N2	C19	C16	134.5(7)
C20	N2	C19	C17	-114.6(9)	C20	N2	C19	C18	170.9(5)
Fe1	N3	C9	C8	56.4(4)	Fe1	N3	C9	C10	38.3(5)
Fe1	N3	C9	C11	115.6(4)	Fe1	N3	C11	C8	-2.2(8)
Fe1	N3	C11	C9	-72.8(7)	Fe1	N3	C11	C10	-22.9(7)
Fe1	N3	C11	C12	115.7(3)	Fe1	N3	C12	C11	-109.5(3)
Fe1	N3	C12	C13	22.6(7)	Fe1	N3	C12	C14	49.2(8)

Fe1	N3	C12	C15	-5.0(7)	Fe1	N3	C14	C12	-137.1(7)
Fe1	N3	C14	C13	-23.0(13)	Fe1	N3	C14	C15	-51.2(7)
C9	N3	C11	C8	70.6(9)	C9	N3	C11	C9	-0.0(5)
C9	N3	C11	C10	49.9(7)	C9	N3	C11	C12	-171.5(8)
C11	N3	C9	C8	-59.2(8)	C11	N3	C9	C10	-77.2(9)
C11	N3	C9	C11	0.0(7)	C9	N3	C12	C11	4.8(3)
C9	N3	C12	C13	136.9(5)	C9	N3	C12	C14	163.5(6)
C9	N3	C12	C15	109.3(5)	C12	N3	C9	C8	-68.2(6)
C12	N3	C9	C10	-86.3(6)	C12	N3	C9	C11	-9.1(6)
C9	N3	C14	C12	-22.9(12)	C9	N3	C14	C13	91.2(14)
C9	N3	C14	C15	63.0(11)	C14	N3	C9	C8	-57.3(8)
C14	N3	C9	C10	-75.4(9)	C14	N3	C9	C11	1.9(9)
C21	N3	C9	C8	172.5(4)	C21	N3	C9	C10	154.5(5)
C21	N3	C9	C11	-128.3(5)	C11	N3	C12	C11	0.0(4)
C11	N3	C12	C13	132.1(6)	C11	N3	C12	C14	158.7(8)
C11	N3	C12	C15	104.6(6)	C12	N3	C11	C8	-117.9(8)
C12	N3	C11	C9	171.5(8)	C12	N3	C11	C10	-138.6(7)
C12	N3	C11	C12	0.0(3)	C11	N3	C14	C12	-21.9(9)
C11	N3	C14	C13	92.2(14)	C11	N3	C14	C15	64.0(9)
C14	N3	C11	C8	-108.1(7)	C14	N3	C11	C9	-178.7(7)
C14	N3	C11	C10	-128.8(6)	C14	N3	C11	C12	9.8(4)
C21	N3	C11	C8	132.4(6)	C21	N3	C11	C9	61.8(8)
C21	N3	C11	C10	111.7(6)	C21	N3	C11	C12	-109.7(4)
C12	N3	C14	C12	0.0(7)	C12	N3	C14	C13	114.1(19)
C12	N3	C14	C15	85.9(12)	C14	N3	C12	C11	-158.7(11)
C14	N3	C12	C13	-26.6(9)	C14	N3	C12	C14	-0.0(8)
C14	N3	C12	C15	-54.1(10)	C21	N3	C12	C11	118.1(4)
C21	N3	C12	C13	-109.8(5)	C21	N3	C12	C14	-83.2(8)
C21	N3	C12	C15	-137.4(5)	C21	N3	C14	C12	105.9(8)
C21	N3	C14	C13	-139.9(12)	C21	N3	C14	C15	-168.2(6)
Fe1	N4	C13	C12	52.8(6)	Fe1	N4	C13	C14	28.9(9)
Fe1	N4	C13	C15	133.9(6)	Fe1	N4	C15	C12	5.3(10)
Fe1	N4	C15	C13	-53.3(11)	Fe1	N4	C15	C14	-20.4(10)
Fe1	N4	C15	C18	109.5(4)	Fe1	N4	C16	C17	-55.6(6)
Fe1	N4	C16	C18	-116.2(6)	Fe1	N4	C16	C19	-36.9(8)
Fe1	N4	C18	C15	-115.9(3)	Fe1	N4	C18	C16	72.2(6)
Fe1	N4	C18	C17	5.4(7)	Fe1	N4	C18	C19	24.9(6)
C13	N4	C15	C12	58.6(11)	C13	N4	C15	C13	-0.0(6)
C13	N4	C15	C14	32.9(8)	C13	N4	C15	C18	162.8(12)
C15	N4	C13	C12	-81.1(13)	C15	N4	C13	C14	-104.9(16)
C15	N4	C13	C15	-0.0(11)	C13	N4	C16	C17	60.5(10)
C13	N4	C16	C18	-0.2(11)	C13	N4	C16	C19	79.2(11)
C16	N4	C13	C12	-63.2(10)	C16	N4	C13	C14	-87.1(11)
C16	N4	C13	C15	17.8(11)	C13	N4	C18	C15	-8.2(4)
C13	N4	C18	C16	179.9(6)	C13	N4	C18	C17	113.1(6)
C13	N4	C18	C19	132.6(5)	C18	N4	C13	C12	-63.3(7)
C18	N4	C13	C14	-87.2(10)	C18	N4	C13	C15	17.7(7)
C22	N4	C13	C12	171.0(5)	C22	N4	C13	C14	147.1(8)
C22	N4	C13	C15	-108.0(6)	C15	N4	C16	C17	69.3(8)
C15	N4	C16	C18	8.6(9)	C15	N4	C16	C19	87.9(9)
C16	N4	C15	C12	-108.8(8)	C16	N4	C15	C13	-167.4(9)
C16	N4	C15	C14	-134.5(7)	C16	N4	C15	C18	-4.6(5)
C15	N4	C18	C15	0.0(5)	C15	N4	C18	C16	-171.9(8)
C15	N4	C18	C17	121.3(8)	C15	N4	C18	C19	140.8(7)
C18	N4	C15	C12	-104.2(8)	C18	N4	C15	C13	-162.8(11)
C18	N4	C15	C14	-129.9(8)	C18	N4	C15	C18	0.0(3)
C22	N4	C15	C12	140.3(6)	C22	N4	C15	C13	81.8(11)
C22	N4	C15	C14	114.7(7)	C22	N4	C15	C18	-115.5(5)
C16	N4	C18	C15	171.9(9)	C16	N4	C18	C16	0.0(7)
C16	N4	C18	C17	-66.8(9)	C16	N4	C18	C19	-47.3(8)

C18	N4	C16	C17	60.7(9)	C18	N4	C16	C18	0.0(7)
C18	N4	C16	C19	79.3(10)	C22	N4	C16	C17	-171.5(5)
C22	N4	C16	C18	127.8(6)	C22	N4	C16	C19	-152.9(7)
C22	N4	C18	C15	110.8(5)	C22	N4	C18	C16	-61.1(8)
C22	N4	C18	C17	-128.0(6)	C22	N4	C18	C19	-108.5(6)
C1	C2	C3	C4	-179.6(3)	C1	C2	C7	C6	178.8(3)
C3	C2	C7	C6	0.2(5)	C7	C2	C3	C4	-1.0(5)
C2	C3	C4	C5	1.4(5)	C3	C4	C5	C6	-1.0(6)
C4	C5	C6	C7	0.1(6)	C5	C6	C7	C2	0.2(6)
N2	C8	C9	N3	-52.9(7)	N2	C8	C9	C11	-106.5(6)
N2	C8	C10	N2	-0.00(12)	N2	C8	C10	C9	-120.1(10)
N2	C8	C10	C11	-117.3(4)	N2	C8	C11	N3	11.8(11)
N2	C8	C11	C9	87.7(8)	N2	C8	C11	C10	83.6(10)
N2	C8	C11	C12	-46.7(11)	C9	C8	C10	N2	120.1(10)
C9	C8	C10	C9	0.0(3)	C9	C8	C10	C11	2.8(9)
C10	C8	C9	N3	-121.1(17)	C10	C8	C9	C11	-174.7(18)
C9	C8	C11	N3	-75.9(9)	C9	C8	C11	C9	0.0(5)
C9	C8	C11	C10	-4.0(10)	C9	C8	C11	C12	-134.4(13)
C11	C8	C9	N3	53.6(8)	C11	C8	C9	C11	-0.0(7)
C10	C8	C11	N3	-71.8(15)	C10	C8	C11	C9	4.0(14)
C10	C8	C11	C10	0.0(10)	C10	C8	C11	C12	-130.4(14)
C11	C8	C10	N2	117.3(6)	C11	C8	C10	C9	-2.8(10)
C11	C8	C10	C11	0.0(4)	N3	C9	C10	N2	-15.5(12)
N3	C9	C10	C8	66.0(15)	N3	C9	C10	C11	60.9(5)
N3	C9	C11	N3	-0.00(13)	N3	C9	C11	C8	-121.6(5)
N3	C9	C11	C10	-119.9(5)	N3	C9	C11	C12	8.8(8)
C8	C9	C11	N3	121.6(6)	C8	C9	C11	C8	0.0(3)
C8	C9	C11	C10	1.7(4)	C8	C9	C11	C12	130.4(12)
C10	C9	C11	N3	119.9(6)	C10	C9	C11	C8	-1.7(5)
C10	C9	C11	C10	0.0(4)	C10	C9	C11	C12	128.7(11)
C11	C9	C10	N2	-76.4(12)	C11	C9	C10	C8	5.1(16)
C11	C9	C10	C11	0.0(7)	N2	C10	C11	N3	52.5(9)
N2	C10	C11	C8	-64.5(9)	N2	C10	C11	C9	120.3(9)
N2	C10	C11	C12	2.2(15)	C8	C10	C11	N3	117.0(14)
C8	C10	C11	C8	0.0(9)	C8	C10	C11	C9	-175.2(16)
C8	C10	C11	C12	66.7(18)	C9	C10	C11	N3	-67.7(9)
C9	C10	C11	C8	175.2(15)	C9	C10	C11	C9	0.0(6)
C9	C10	C11	C12	-118.0(15)	N3	C11	C12	N3	0.00(18)
N3	C11	C12	C13	-77.4(8)	N3	C11	C12	C14	-35.2(13)
N3	C11	C12	C15	-99.9(6)	C8	C11	C12	N3	97.0(9)
C8	C11	C12	C13	19.6(14)	C8	C11	C12	C14	61.8(18)
C8	C11	C12	C15	-2.9(12)	C9	C11	C12	N3	-11.6(12)
C9	C11	C12	C13	-89.0(16)	C9	C11	C12	C14	-47(2)
C9	C11	C12	C15	-111.5(14)	C10	C11	C12	N3	72.8(12)
C10	C11	C12	C13	-4.6(17)	C10	C11	C12	C14	38(2)
C10	C11	C12	C15	-27.1(14)	N3	C12	C13	N4	-51.9(8)
N3	C12	C13	C14	67.0(10)	N3	C12	C13	C15	-104.5(8)
N3	C12	C14	N3	-0.00(13)	N3	C12	C14	C13	-118.8(15)
N3	C12	C14	C15	-114.3(7)	N3	C12	C15	N4	-0.2(11)
N3	C12	C15	C13	85.5(10)	N3	C12	C15	C14	80.5(8)
N3	C12	C15	C18	-58.1(9)	C11	C12	C13	N4	0.6(12)
C11	C12	C13	C14	119.5(14)	C11	C12	C13	C15	-52.0(12)
C11	C12	C14	N3	26.5(14)	C11	C12	C14	C13	-92(2)
C11	C12	C14	C15	-87.8(18)	C11	C12	C15	N4	55.3(11)
C11	C12	C15	C13	141.1(9)	C11	C12	C15	C14	136.0(10)
C11	C12	C15	C18	-2.6(10)	C13	C12	C14	N3	118.8(17)
C13	C12	C14	C13	0.0(7)	C13	C12	C14	C15	4.5(12)
C14	C12	C13	N4	-119(2)	C14	C12	C13	C14	-0.0(17)
C14	C12	C13	C15	-172(2)	C13	C12	C15	N4	-85.7(13)
C13	C12	C15	C13	0.0(8)	C13	C12	C15	C14	-5.0(10)

C13	C12	C15	C18	-143.6(15)	C15	C12	C13	N4	52.6(10)
C15	C12	C13	C14	171.5(17)	C15	C12	C13	C15	0.0(9)
C14	C12	C15	N4	-80.7(14)	C14	C12	C15	C13	5.0(12)
C14	C12	C15	C14	-0.0(10)	C14	C12	C15	C18	-138.6(14)
C15	C12	C14	N3	114.3(8)	C15	C12	C14	C13	-4.5(11)
C15	C12	C14	C15	-0.0(5)	N4	C13	C14	N3	-4(2)
N4	C13	C14	C12	72(2)	N4	C13	C14	C15	62.4(10)
N4	C13	C15	N4	-0.00(17)	N4	C13	C15	C12	-112.9(7)
N4	C13	C15	C14	-109.1(12)	N4	C13	C15	C18	-25.8(17)
C12	C13	C14	N3	-76.4(19)	C12	C13	C14	C12	-0.0(8)
C12	C13	C14	C15	-10(3)	C12	C13	C15	N4	112.9(8)
C12	C13	C15	C12	0.0(3)	C12	C13	C15	C14	3.8(8)
C12	C13	C15	C18	87(2)	C14	C13	C15	N4	109.1(14)
C14	C13	C15	C12	-3.8(10)	C14	C13	C15	C14	-0.0(8)
C14	C13	C15	C18	83(3)	C15	C13	C14	N3	-67(2)
C15	C13	C14	C12	10(3)	C15	C13	C14	C15	-0.0(10)
N3	C14	C15	N4	50.2(11)	N3	C14	C15	C12	-58.6(9)
N3	C14	C15	C13	129.2(14)	N3	C14	C15	C18	-4.8(16)
C12	C14	C15	N4	108.8(13)	C12	C14	C15	C12	0.0(6)
C12	C14	C15	C13	-172.2(18)	C12	C14	C15	C18	53.8(17)
C13	C14	C15	N4	-79.0(17)	C13	C14	C15	C12	172(2)
C13	C14	C15	C13	-0.0(12)	C13	C14	C15	C18	-134(2)
N4	C15	C18	N4	0.0(2)	N4	C15	C18	C16	11.2(11)
N4	C15	C18	C17	-93.7(9)	N4	C15	C18	C19	-67.1(10)
C12	C15	C18	N4	102.0(9)	C12	C15	C18	C16	113.3(12)
C12	C15	C18	C17	8.4(13)	C12	C15	C18	C19	34.9(14)
C13	C15	C18	N4	33(2)	C13	C15	C18	C16	44(3)
C13	C15	C18	C17	-61(3)	C13	C15	C18	C19	-34(3)
C14	C15	C18	N4	80.1(12)	C14	C15	C18	C16	91.4(16)
C14	C15	C18	C17	-13.5(17)	C14	C15	C18	C19	13.0(19)
N4	C16	C17	N2	51.4(9)	N4	C16	C17	C18	-52.1(6)
N4	C16	C17	C19	114.5(14)	N4	C16	C18	N4	0.00(15)
N4	C16	C18	C15	-8.3(9)	N4	C16	C18	C17	121.8(5)
N4	C16	C18	C19	117.5(7)	N4	C16	C19	N2	14.6(14)
N4	C16	C19	C17	-72.7(16)	N4	C16	C19	C18	-59.7(7)
C17	C16	C18	N4	-121.8(6)	C17	C16	C18	C15	-130.0(12)
C17	C16	C18	C17	0.0(4)	C17	C16	C18	C19	-4.2(6)
C18	C16	C17	N2	103.5(10)	C18	C16	C17	C18	-0.0(6)
C18	C16	C17	C19	166.6(18)	C18	C16	C19	N2	74.3(13)
C18	C16	C19	C17	-13.0(18)	C18	C16	C19	C18	0.0(6)
C19	C16	C18	N4	-117.5(8)	C19	C16	C18	C15	-125.8(12)
C19	C16	C18	C17	4.2(6)	C19	C16	C18	C19	0.0(4)
N2	C17	C18	N4	-15.0(11)	N2	C17	C18	C15	42.1(12)
N2	C17	C18	C16	-90.5(8)	N2	C17	C18	C19	-80.9(11)
N2	C17	C19	N2	-0.00(12)	N2	C17	C19	C16	123.3(11)
N2	C17	C19	C18	115.9(5)	C16	C17	C18	N4	75.6(10)
C16	C17	C18	C15	132.7(13)	C16	C17	C18	C16	-0.0(7)
C16	C17	C18	C19	9.6(13)	C16	C17	C19	N2	-123.3(13)
C16	C17	C19	C16	-0.0(6)	C16	C17	C19	C18	-7.5(12)
C18	C17	C19	N2	-115.9(6)	C18	C17	C19	C16	7.5(11)
C18	C17	C19	C18	0.0(3)	C19	C17	C18	N4	66.0(16)
C19	C17	C18	C15	123.1(15)	C19	C17	C18	C16	-9.6(14)
C19	C17	C18	C19	-0.0(10)	N4	C18	C19	N2	-54.8(8)
N4	C18	C19	C16	69.6(7)	N4	C18	C19	C17	-122.1(10)
C15	C18	C19	N2	-8.8(14)	C15	C18	C19	C16	115.6(13)
C15	C18	C19	C17	-76.1(15)	C16	C18	C19	N2	-124.4(12)
C16	C18	C19	C16	0.0(9)	C16	C18	C19	C17	168.3(16)
C17	C18	C19	N2	67.3(14)	C17	C18	C19	C16	-168.3(17)
C17	C18	C19	C17	-0.0(11)					