Supporting Information

Table S1. Complete Crystallographic Details for [Fe(TMP)(2-MeHIm)$_2$]$_2$·[Fe(TMP)(2-MeHIm)]$_2$

formula	C$_{259.80}$H$_{259.85}$Cl$_{1.40}$Fe$_4$N$_{29.88}$O$_{0.76}$
unit cell content	8×{[Fe(TMP)(2-MeHIm)$_2$]$_2$·[Fe(TMP)(2-MeHIm)]$_2$
	·C$_6$H$_5$CH$_3$·0.94(2-MeHIm)·0.7CH$_2$Cl$_2$·0.34CH$_3$OH·0.42H$_2$O}
FW, amu	4085.99
a, Å	39.8634(3)
c, Å	28.1013(6)
V, Å^3	44655.5(11)
space group	$I\overline{4}$
Z	8
D$_c$, g/cm^3	1.216
F(000)	1729
μ, mm^{-1}	0.334
crystal dimensions, mm	0.33 × 0.26 × 0.20
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	0.72–26.37
index range	$-49 \leq$ h ≤ 49
	$-49 \leq$ k ≤ 41
	$-35 \leq$ l ≤ 34
total data collected	194984
absorption correction	Semi-empirical from equivalents
relative transmission coefficients (I)	0.9373 and 0.8985
unique data	44982 (R_{int} = 0.051)
unique observed data [I > 2σ(I)]	34716
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	44982/21/2649
goodness-of-fit (pased on F^2)	1.008
final R indices [I > 2σ(I)]	R_1 = 0.0632, wR_2 = 0.1728
final R indices (all data)	R_1 = 0.0882, wR_2 = 0.1903
absolute structure parameter	0.463(9)

Table S2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for $[\text{Fe}(\text{TMP})(2\text{-MeHIm})_2]_2 \cdot [\text{Fe}(\text{TMP})(2\text{-MeHIm})]_2$

atom	x	y	z	$U(\text{eq})$
Fe(1)	0.12793(1)	0.37151(1)	0.43599(2)	0.0184(1)
N(11)	0.10401(7)	0.35566(8)	0.49259(12)	0.0188(7)
N(12)	0.13027(8)	0.32544(8)	0.41136(12)	0.0215(7)
N(13)	0.15140(8)	0.38771(8)	0.37911(12)	0.0212(7)
N(14)	0.12538(8)	0.41770(8)	0.46077(13)	0.0235(7)
N(15)	0.08446(8)	0.37748(7)	0.39935(11)	0.0189(7)
C(11)	0.05585(10)	0.39228(10)	0.41045(15)	0.0240(9)
N(16)	0.03401(8)	0.38969(8)	0.37349(13)	0.0260(8)
C(12)	0.04935(10)	0.37251(10)	0.33758(16)	0.0276(9)
C(13)	0.08030(10)	0.36533(10)	0.35348(15)	0.0263(9)
C(14)	0.04649(11)	0.41080(12)	0.45465(17)	0.0353(11)
N(17)	0.17207(8)	0.36303(9)	0.47123(12)	0.0249(8)
C(15)	0.19922(10)	0.38136(11)	0.47788(16)	0.0301(10)
N(18)	0.22145(9)	0.36347(9)	0.50436(14)	0.0316(8)
C(16)	0.20841(12)	0.33295(13)	0.51413(19)	0.0405(12)
C(17)	0.17782(11)	0.33262(12)	0.49401(18)	0.0350(11)
C(18)	0.20565(11)	0.41564(11)	0.4603(2)	0.0409(12)
C(1a1)	0.09898(9)	0.37263(10)	0.53484(15)	0.0239(9)
C(1a2)	0.08937(9)	0.32453(9)	0.49887(14)	0.0182(8)
C(1a3)	0.11242(10)	0.29787(9)	0.42705(15)	0.0222(8)
C(1a4)	0.14956(9)	0.31390(9)	0.37422(14)	0.0212(8)
C(1a5)	0.16814(9)	0.36877(9)	0.34602(15)	0.0214(8)
C(1a6)	0.15231(10)	0.42039(9)	0.36285(14)	0.0215(8)
C(1a7)	0.12955(10)	0.44674(9)	0.43501(16)	0.0245(9)
C(1a8)	0.11895(10)	0.42748(10)	0.50672(14)	0.0232(9)
C(1b1)	0.08107(10)	0.35182(10)	0.56720(15)	0.0246(9)
C(1b2)	0.07409(10)	0.32310(10)	0.54503(15)	0.0241(9)
C(1b3)	0.12007(10)	0.26909(10)	0.39854(16)	0.0267(9)
C(1b4)	0.14361(10)	0.27878(9)	0.36638(15)	0.0249(9)
C(1b5)	0.18069(11)	0.39065(10)	0.30838(17)	0.0308(10)
C(1b6)	0.17009(11)	0.42161(10)	0.31804(15)	0.0285(10)
C(1b7)	0.12530(11)	0.47545(11)	0.46542(17)	0.0314(10)
C(1b8)	0.11938(11)	0.46345(11)	0.50990(16)	0.0324(10)
C(1m1)	0.09181(9)	0.29776(9)	0.46721(14)	0.0212(8)

Table S2. Continued

atom	x	y	z	U(eq)
C(1m2)	0.16940(9)	0.33400(10)	0.34428(15)	0.0231(9)
C(1m3)	0.14018(9)	0.44808(9)	0.38776(15)	0.0229(8)
C(1m4)	0.10774(10)	0.40591(10)	0.54245(16)	0.0281(9)
C(111)	0.07319(10)	0.26638(10)	0.47974(15)	0.0224(8)
C(112)	0.04044(10)	0.26127(10)	0.46198(14)	0.0222(8)
C(113)	0.02234(10)	0.23344(10)	0.47608(15)	0.0253(9)
C(114)	0.03600(11)	0.20979(10)	0.50762(15)	0.0265(9)
C(115)	0.06802(10)	0.21485(9)	0.52416(15)	0.0237(9)
C(116)	0.08722(10)	0.24262(10)	0.51066(15)	0.0238(9)
C(117)	0.02538(11)	0.28606(11)	0.42781(16)	0.0312(10)
C(118)	0.01614(12)	0.17964(11)	0.52272(17)	0.0355(11)
C(119)	0.12244(10)	0.24720(11)	0.52969(17)	0.0309(10)
C(121)	0.19023(9)	0.31777(9)	0.30766(15)	0.0206(8)
C(122)	0.17724(11)	0.31018(11)	0.26182(16)	0.0303(10)
C(123)	0.19812(12)	0.29607(12)	0.22793(17)	0.0368(11)
C(124)	0.23078(11)	0.28842(11)	0.23684(19)	0.0381(11)
C(125)	0.24359(11)	0.29492(11)	0.28237(18)	0.0366(11)
C(126)	0.22401(10)	0.30956(10)	0.31773(16)	0.0279(9)
C(127)	0.14205(12)	0.31963(14)	0.25000(18)	0.0454(13)
C(128)	0.25380(15)	0.27441(16)	0.1974(2)	0.0640(17)
C(129)	0.23912(12)	0.31720(14)	0.36478(19)	0.0474(13)
C(131)	0.13957(10)	0.48122(10)	0.36231(15)	0.0242(9)
C(132)	0.10900(10)	0.49242(10)	0.34292(15)	0.0270(9)
C(133)	0.10793(11)	0.52215(10)	0.31756(15)	0.0263(9)
C(134)	0.13709(11)	0.54186(10)	0.31132(15)	0.0285(9)
C(135)	0.16683(10)	0.53042(10)	0.33073(15)	0.0263(9)
C(136)	0.16899(10)	0.50101(10)	0.35702(15)	0.0262(9)
C(137)	0.07717(11)	0.47197(10)	0.34930(17)	0.0327(10)
C(138)	0.13564(13)	0.57464(11)	0.28524(17)	0.0384(11)
C(139)	0.20164(10)	0.49018(11)	0.37878(17)	0.0329(10)
C(141)	0.10356(11)	0.41873(11)	0.59263(16)	0.0319(10)
C(142)	0.07366(14)	0.43438(13)	0.60723(19)	0.0475(13)
C(143)	0.07079(17)	0.44452(16)	0.6548(2)	0.0647(18)
C(144)	0.09554(17)	0.43910(16)	0.6875(2)	0.0603(17)

Table S2. Continued

atom	x	y	z	$U(\text{eq})$
C(145)	0.12456(15)	0.42294(16)	0.6727(2)	0.0552(15)
C(146)	0.12911(12)	0.41266(13)	0.62617(17)	0.0398(12)
C(147)	0.04506(16)	0.44010(18)	0.5724(2)	0.072(2)
C(148)	0.0918(2)	0.4510(2)	0.7390(2)	0.094(3)
C(149)	0.16052(13)	0.39515(16)	0.6113(2)	0.0566(16)
Fe(2)	0.12392(1)	0.86653(1)	0.69748(2)	0.0180(1)
N(21)	0.12258(8)	0.82079(8)	0.67112(12)	0.0199(7)
N(22)	0.10029(8)	0.85157(8)	0.75477(12)	0.0198(7)
N(23)	0.12494(8)	0.91230(8)	0.72346(12)	0.0229(7)
N(24)	0.14730(8)	0.88164(8)	0.64031(12)	0.0217(7)
N(25)	0.16829(9)	0.85387(9)	0.72822(13)	0.0291(8)
C(21)	0.19817(12)	0.86735(14)	0.72821(18)	0.0439(13)
N(26)	0.22067(9)	0.84454(10)	0.74738(15)	0.0367(9)
C(22)	0.20333(13)	0.81621(14)	0.7622(2)	0.0488(13)
C(23)	0.17167(13)	0.82144(14)	0.75029(18)	0.0421(12)
C(24)	0.20759(14)	0.89958(14)	0.7093(2)	0.0553(15)
N(27)	0.08042(8)	0.87561(8)	0.66240(13)	0.0225(7)
C(25)	0.05309(10)	0.89361(10)	0.67293(16)	0.0286(9)
N(28)	0.03109(8)	0.89206(9)	0.63613(13)	0.0287(8)
C(26)	0.04415(11)	0.87282(11)	0.60004(17)	0.0321(10)
C(27)	0.07457(11)	0.86288(11)	0.61651(16)	0.0302(10)
C(28)	0.04619(11)	0.91325(12)	0.71579(18)	0.0367(11)
C(2a1)	0.14083(9)	0.80831(9)	0.63285(14)	0.0203(8)
C(2a2)	0.10348(9)	0.79433(10)	0.68737(15)	0.0221(8)
C(2a3)	0.08341(9)	0.82141(10)	0.76070(15)	0.0219(8)
C(2a4)	0.09614(9)	0.86835(10)	0.79730(15)	0.0217(8)
C(2a5)	0.11867(10)	0.92243(10)	0.76986(15)	0.0248(9)
C(2a6)	0.13018(10)	0.94134(9)	0.69783(15)	0.0239(9)
C(2a7)	0.15054(10)	0.91434(10)	0.62518(15)	0.0231(9)
C(2a8)	0.16297(9)	0.86245(10)	0.60628(14)	0.0214(8)
C(2b1)	0.13259(10)	0.77349(10)	0.62526(15)	0.0246(9)
C(2b2)	0.10883(10)	0.76526(10)	0.65854(15)	0.0258(9)
C(2b3)	0.06850(9)	0.81973(9)	0.80707(15)	0.0200(8)
C(2b4)	0.07706(9)	0.84857(9)	0.83007(15)	0.0217(8)

Table S2. Continued

atom	x	y	z	$U(\mathrm{eq})$
C(2b5)	0.12121(12)	0.95847(11)	0.77368(17)	0.0327(10)
C(2b6)	0.12700(11)	0.97010(10)	0.72944(16)	0.0282(9)
C(2b7)	0.16870(10)	0.91541(10)	0.58137(15)	0.0268(9)
C(2b8)	0.17778(10)	0.88372(10)	0.57076(16)	0.0254(9)
C(2m1)	0.08376(10)	0.79506(9)	0.72850(14)	0.0216(8)
C(2m2)	0.10691(10)	0.90154(9)	0.80596(15)	0.0225(8)
C(2m3)	0.14032(10)	0.94240(10)	0.65071(15)	0.0250(9)
C(2m4)	0.16150(9)	0.82721(9)	0.60355(14)	0.0212(8)
C(211)	0.06267(10)	0.76480(10)	0.74058(15)	0.0233(9)
C(212)	0.02928(10)	0.76394(10)	0.72447(14)	0.0234(8)
C(213)	0.00931(10)	0.73703(10)	0.73739(15)	0.0260(9)
C(214)	0.02127(11)	0.71119(10)	0.76590(15)	0.0280(9)
C(215)	0.05431(10)	0.71312(10)	0.78230(15)	0.0253(9)
C(216)	0.07537(10)	0.73967(9)	0.76913(15)	0.0248(9)
C(217)	0.01595(10)	0.79182(10)	0.69398(16)	0.0276(9)
C(218)	−0.00103(13)	0.68242(11)	0.78037(18)	0.0397(12)
C(219)	0.11085(10)	0.74040(10)	0.78616(16)	0.0287(9)
C(221)	0.10260(11)	0.91429(11)	0.85582(16)	0.0304(10)
C(222)	0.12848(12)	0.90925(13)	0.88842(19)	0.0428(12)
C(223)	0.12299(14)	0.91815(16)	0.93635(19)	0.0541(15)
C(224)	0.09373(14)	0.93224(14)	0.95206(19)	0.0483(13)
C(225)	0.06806(13)	0.93707(11)	0.91922(17)	0.0386(11)
C(226)	0.07214(12)	0.92831(11)	0.87081(17)	0.0343(10)
C(227)	0.16106(13)	0.89248(19)	0.8736(2)	0.0684(19)
C(228)	0.08759(17)	0.94113(18)	1.0030(2)	0.0683(19)
C(229)	0.04401(14)	0.93354(16)	0.8374(2)	0.0564(16)
C(231)	0.14061(10)	0.97575(10)	0.62499(15)	0.0266(9)
C(232)	0.16966(11)	0.99533(10)	0.62167(16)	0.0295(10)
C(233)	0.16861(12)	1.02487(10)	0.59491(17)	0.0344(11)
C(234)	0.14024(12)	1.03555(10)	0.57194(17)	0.0344(11)
C(235)	0.11150(12)	1.01564(10)	0.57540(16)	0.0339(10)
C(236)	0.11137(11)	0.98593(10)	0.60162(16)	0.0293(9)
C(237)	0.20154(11)	0.98467(12)	0.64782(19)	0.0377(11)
C(238)	0.13978(15)	1.06725(12)	0.5438(2)	0.0489(13)

Table S2. Continued

atom	x	y	z	$U(\mathrm{eq})$
C(239)	0.07976(11)	0.96499(11)	0.60368(18)	0.0358(11)
C(241)	0.18068(10)	0.81073(9)	0.56507(15)	0.0238(9)
C(242)	0.17009(11)	0.81249(12)	0.51797(17)	0.0324(10)
C(243)	0.19021(12)	0.80033(12)	0.48139(17)	0.0367(11)
C(244)	0.22085(11)	0.78551(12)	0.49079(18)	0.0355(11)
C(245)	0.23070(10)	0.78207(11)	0.53763(18)	0.0333(11)
C(246)	0.21097(10)	0.79418(10)	0.57574(16)	0.0262(9)
C(247)	0.13640(11)	0.82764(14)	0.50528(18)	0.0408(12)
C(248)	0.24316(14)	0.77428(16)	0.4500(2)	0.0583(16)
C(249)	0.22217(11)	0.78893(11)	0.62602(17)	0.0328(10)
Fe(3)	−0.10859(2)	0.11671(2)	0.16998(2)	0.0289(2)
N(35a)	−0.06338(12)	0.10477(12)	0.1338(2)	0.0345(19)
C(31a)	−0.05194(11)	0.07442(10)	0.12318(18)	0.050(3)
N(36a)	−0.02112(12)	0.07756(12)	0.1021(2)	0.040(2)
C(32a)	−0.01279(13)	0.11052(14)	0.0994(3)	0.060(3)
C(33a)	−0.03898(15)	0.12733(10)	0.1188(3)	0.054(3)
C(34a)	−0.06712(19)	0.04121(13)	0.1324(3)	0.061(3)
N(35b)	−0.06487(13)	0.08842(17)	0.1436(3)	0.032(2)
C(31b)	−0.03673(14)	0.10049(13)	0.1250(2)	0.047(3)
N(36b)	−0.01374(15)	0.07501(17)	0.1220(4)	0.052(3)
C(32b)	−0.0275(2)	0.04631(14)	0.1391(4)	0.097(6)
C(33b)	−0.05918(19)	0.05461(16)	0.1523(3)	0.061(4)
C(34b)	−0.0284(3)	0.13510(16)	0.1104(4)	0.073(5)
N(31)	−0.08908(9)	0.13321(8)	0.23394(12)	0.0266(8)
N(32)	−0.10583(9)	0.16603(8)	0.14568(13)	0.0315(9)
N(33)	−0.14378(8)	0.10734(8)	0.11768(12)	0.0239(7)
N(34)	−0.12565(8)	0.07399(8)	0.20507(12)	0.0246(7)
C(3a1)	−0.08360(10)	0.11334(10)	0.27343(15)	0.0251(9)
C(3a2)	−0.07465(10)	0.16381(10)	0.24283(16)	0.0280(10)
C(3a3)	−0.08910(11)	0.19227(10)	0.16640(16)	0.0308(10)
C(3a4)	−0.11706(11)	0.17749(11)	0.10248(15)	0.0286(9)
C(3a5)	−0.14987(10)	0.12704(10)	0.07857(14)	0.0232(9)
C(3a6)	−0.16198(9)	0.07872(9)	0.11199(15)	0.0231(9)
C(3a7)	−0.14634(10)	0.04971(10)	0.18693(15)	0.0260(9)

atom	x	y	z	$U(\text{eq})$
C(3a8)	−0.11556(10)	0.06263(10)	0.24902(16)	0.0264(9)
C(3b1)	−0.06430(9)	0.13265(9)	0.30817(16)	0.0244(9)
C(3b2)	−0.05914(10)	0.16352(10)	0.28922(15)	0.0247(9)
C(3b3)	−0.08958(12)	0.22087(11)	0.13521(17)	0.0355(11)
C(3b4)	−0.10654(11)	0.21171(11)	0.09614(17)	0.0332(10)
C(3b5)	−0.17280(10)	0.10995(10)	0.04725(15)	0.0261(9)
C(3b6)	−0.18031(10)	0.08050(10)	0.06743(15)	0.0252(9)
C(3b7)	−0.14850(11)	0.02214(10)	0.21971(16)	0.0291(9)
C(3b8)	−0.12988(11)	0.03022(10)	0.25802(16)	0.0283(10)
C(3m1)	−0.07384(11)	0.19104(10)	0.21174(16)	0.0297(10)
C(3m2)	−0.13696(10)	0.15951(10)	0.07055(14)	0.0247(9)
C(3m3)	−0.16329(9)	0.05121(10)	0.14352(15)	0.0230(8)
C(3m4)	−0.09519(10)	0.08072(10)	0.28139(15)	0.0243(9)
C(311)	−0.05720(11)	0.22257(10)	0.22996(15)	0.0277(9)
C(312)	−0.07626(11)	0.24608(11)	0.25551(18)	0.0350(11)
C(313)	−0.06032(12)	0.27379(11)	0.27474(19)	0.0368(11)
C(314)	−0.02574(11)	0.27927(10)	0.26905(17)	0.0324(10)
C(315)	−0.00760(11)	0.25589(10)	0.24291(16)	0.0320(10)
C(316)	−0.02300(12)	0.22792(11)	0.22295(17)	0.0340(10)
C(317)	−0.11377(13)	0.24147(13)	0.2602(3)	0.0607(18)
C(318)	−0.00855(13)	0.30975(12)	0.28969(19)	0.0435(12)
C(319)	−0.00249(14)	0.20329(13)	0.1943(2)	0.0526(14)
C(321)	−0.14432(11)	0.17461(9)	0.02228(15)	0.0256(9)
C(322)	−0.12032(12)	0.17170(13)	−0.01346(18)	0.0391(11)
C(323)	−0.12644(14)	0.18488(14)	−0.05813(19)	0.0494(14)
C(324)	−0.15615(15)	0.20051(13)	−0.06815(19)	0.0506(15)
C(325)	−0.17970(13)	0.20284(11)	−0.03275(19)	0.0404(12)
C(326)	−0.17475(12)	0.19007(11)	0.01302(17)	0.0347(11)
C(327)	−0.08690(13)	0.15353(17)	−0.0042(2)	0.0600(16)
C(328)	−0.1615(2)	0.21433(19)	−0.1185(2)	0.083(2)
C(329)	−0.20140(13)	0.19324(13)	0.0493(2)	0.0480(14)
C(331)	−0.18618(10)	0.02296(10)	0.13025(14)	0.0239(9)
C(332)	−0.17558(10)	−0.00221(10)	0.09824(15)	0.0256(9)
C(333)	−0.19802(10)	−0.02752(10)	0.08571(16)	0.0286(9)

Table S2. Continued

atom	x	y	z	$U(\text{eq})$
C(334)	−0.23029(11)	−0.02879(10)	0.10436(15)	0.0286(10)
C(335)	−0.24044(10)	−0.00383(10)	0.13548(15)	0.0249(9)
C(336)	−0.21895(10)	0.02228(10)	0.14896(15)	0.0243(9)
C(337)	−0.14062(11)	−0.00220(11)	0.07737(18)	0.0357(11)
C(338)	−0.25332(12)	−0.05775(11)	0.09304(18)	0.0367(11)
C(339)	−0.23042(11)	0.04861(11)	0.18353(16)	0.0309(10)
C(341)	−0.08512(10)	0.06359(10)	0.32635(16)	0.0264(9)
C(342)	−0.10558(12)	0.06494(11)	0.36649(17)	0.0355(11)
C(343)	−0.09512(14)	0.04960(12)	0.40857(18)	0.0429(12)
C(344)	−0.06550(14)	0.03273(11)	0.41162(18)	0.0414(13)
C(345)	−0.04522(13)	0.03078(11)	0.3713(2)	0.0428(13)
C(346)	−0.05457(11)	0.04657(10)	0.32847(18)	0.0343(11)
C(347)	−0.13831(14)	0.08385(15)	0.3655(2)	0.0559(15)
C(348)	−0.05383(19)	0.01603(15)	0.4571(2)	0.072(2)
C(349)	−0.03156(13)	0.04442(13)	0.2862(2)	0.0473(13)
Fe(4a)	−0.12170(2)	0.36708(3)	0.55615(3)	0.0247(2)
N(45a)	−0.13832(9)	0.31952(9)	0.52756(17)	0.0379(14)
C(41a)	−0.16638(8)	0.30209(8)	0.53342(12)	0.0359(16)
N(46a)	−0.16161(10)	0.27038(8)	0.51579(19)	0.0529(17)
C(42a)	−0.13000(11)	0.26772(10)	0.4983(2)	0.061(2)
C(43a)	−0.11560(8)	0.29809(12)	0.50570(19)	0.052(2)
C(44a)	−0.19894(9)	0.31269(13)	0.5536(2)	0.0420(17)
Fe(4b)	−0.11264(5)	0.38494(6)	0.56732(7)	0.0229(4)
N(45b)	−0.0875(3)	0.4281(2)	0.5930(5)	0.058(4)
C(41b)	−0.0999(2)	0.4554(2)	0.6136(3)	0.064(5)
N(46b)	−0.0740(3)	0.4769(2)	0.6235(5)	0.062(4)
C(42b)	−0.0446(2)	0.4629(3)	0.6092(6)	0.096(8)
C(43b)	−0.0531(2)	0.4328(3)	0.5901(5)	0.054(5)
C(44b)	−0.1349(2)	0.4635(4)	0.6267(6)	0.059(5)
Cl(4)	−0.1153(3)	0.4716(3)	0.6338(4)	0.089(3)
Cl(5)	−0.0535(3)	0.4395(4)	0.6109(6)	0.124(5)
C(10s)	−0.0969(5)	0.4390(8)	0.6041(15)	0.091(12)
N(41)	−0.16310(9)	0.38547(9)	0.59234(13)	0.0296(8)
N(42)	−0.10312(8)	0.35051(8)	0.62057(12)	0.0235(7)

Table S2. Continued

atom	x	y	z	$U(\text{eq})$
N(43)	−0.07234(8)	0.36460(9)	0.52983(13)	0.0268(8)
N(44)	−0.13184(8)	0.40094(8)	0.50255(12)	0.0255(8)
C(4a1)	−0.18894(10)	0.40384(11)	0.57297(16)	0.0305(10)
C(4a2)	−0.17248(10)	0.37781(10)	0.63838(15)	0.0277(9)
C(4a3)	−0.12105(10)	0.34698(10)	0.66172(15)	0.0249(9)
C(4a4)	−0.07288(9)	0.33390(9)	0.62765(14)	0.0197(8)
C(4a5)	−0.04631(10)	0.34625(10)	0.54950(14)	0.0236(9)
C(4a6)	−0.06151(10)	0.37553(10)	0.48669(15)	0.0256(9)
C(4a7)	−0.11246(10)	0.40788(10)	0.46311(14)	0.0229(9)
C(4a8)	−0.16194(10)	0.41684(10)	0.49562(15)	0.0257(9)
C(4b1)	−0.21573(11)	0.40688(12)	0.60691(17)	0.0384(12)
C(4b2)	−0.20545(12)	0.39100(12)	0.64712(17)	0.0398(12)
C(4b3)	−0.10151(10)	0.32780(9)	0.69579(15)	0.0227(8)
C(4b4)	−0.07205(10)	0.31998(10)	0.67433(15)	0.0238(9)
C(4b5)	−0.01886(10)	0.34498(11)	0.51640(16)	0.0296(10)
C(4b6)	−0.02817(10)	0.36275(11)	0.47743(16)	0.0295(10)
C(4b7)	−0.13068(9)	0.42886(10)	0.43118(15)	0.0230(8)
C(4b8)	−0.16118(10)	0.43426(10)	0.45013(15)	0.0244(9)
C(4m1)	−0.15345(10)	0.35940(10)	0.67057(15)	0.0265(9)
C(4m2)	−0.04651(9)	0.33156(10)	0.59493(15)	0.0230(9)
C(4m3)	−0.07969(10)	0.39628(10)	0.45541(15)	0.0256(9)
C(4m4)	−0.18882(10)	0.41787(10)	0.52755(15)	0.0276(9)
C(411)	−0.16709(11)	0.35241(11)	0.71960(16)	0.0302(10)
C(412)	−0.16065(12)	0.37561(12)	0.75646(17)	0.0373(11)
C(413)	−0.17185(14)	0.36753(13)	0.80192(19)	0.0476(13)
C(414)	−0.18845(15)	0.33858(16)	0.8125(2)	0.0575(17)
C(415)	−0.19461(13)	0.31642(15)	0.7759(2)	0.0495(14)
C(416)	−0.18419(12)	0.32273(13)	0.72916(18)	0.0398(12)
C(417)	−0.14271(17)	0.40780(12)	0.7462(2)	0.0579(16)
C(418)	−0.20030(18)	0.32963(19)	0.8618(2)	0.074(2)
C(419)	−0.19048(15)	0.29751(15)	0.6904(2)	0.0561(15)
C(421)	−0.01587(9)	0.31236(10)	0.60996(14)	0.0214(8)
C(422)	−0.01228(10)	0.27885(10)	0.59544(15)	0.0252(9)
C(423)	0.01645(10)	0.26161(11)	0.61010(15)	0.0274(9)

Table S2. Continued

atom	x	y	z	U(eq)
C(424)	0.04073(10)	0.27613(11)	0.63795(15)	0.0273(9)
C(425)	0.03647(10)	0.30882(12)	0.65188(15)	0.0298(10)
C(426)	0.00871(10)	0.32782(10)	0.63780(14)	0.0239(9)
C(427)	−0.03878(11)	0.26176(11)	0.56615(17)	0.0315(10)
C(428)	0.07151(11)	0.25595(13)	0.65293(18)	0.0418(12)
C(429)	0.00593(11)	0.36425(11)	0.65277(18)	0.0344(10)
C(431)	−0.06217(10)	0.40840(10)	0.41130(15)	0.0249(9)
C(432)	−0.06425(11)	0.38992(11)	0.36879(16)	0.0302(10)
C(433)	−0.04759(10)	0.40188(11)	0.32853(16)	0.0300(10)
C(434)	−0.02903(10)	0.43123(12)	0.32917(17)	0.0331(10)
C(435)	−0.02754(11)	0.44918(11)	0.37166(17)	0.0337(10)
C(436)	−0.04396(10)	0.43827(10)	0.41276(16)	0.0276(9)
C(437)	−0.08412(14)	0.35799(12)	0.36660(19)	0.0456(13)
C(438)	−0.01032(12)	0.44327(14)	0.28634(18)	0.0461(13)
C(439)	−0.04213(12)	0.45874(12)	0.45753(18)	0.0395(11)
C(441)	−0.21964(10)	0.43673(11)	0.51113(15)	0.0272(9)
C(442)	−0.22106(12)	0.47141(12)	0.51568(18)	0.0363(11)
C(443)	−0.24803(14)	0.48859(14)	0.4956(2)	0.0482(14)
C(444)	−0.27354(13)	0.47223(15)	0.47257(18)	0.0470(14)
C(445)	−0.27211(11)	0.43756(15)	0.46947(18)	0.0446(13)
C(446)	−0.24578(11)	0.41909(12)	0.48910(17)	0.0345(11)
C(447)	−0.19401(12)	0.49023(13)	0.5408(2)	0.0498(14)
C(448)	−0.30335(16)	0.4911(2)	0.4515(2)	0.078(2)
C(449)	−0.24616(13)	0.38199(13)	0.4880(2)	0.0508(14)
C(1s)	0.1269(2)	0.26748(18)	1.1354(2)	0.074(2)
C(2s)	0.1284(3)	0.3013(2)	1.1194(3)	0.092(3)
C(3s)	0.1574(3)	0.3144(2)	1.0962(3)	0.101(3)
C(4s)	0.1876(2)	0.29390(18)	1.0869(3)	0.089(3)
C(5s)	0.1848(2)	0.2604(2)	1.1055(3)	0.080(2)
C(6s)	0.15433(18)	0.24731(17)	1.1293(2)	0.0689(19)
C(7s)	0.0948(2)	0.2541(2)	1.1601(3)	0.094(3)
Cl(1)	−0.06716(9)	0.26072(11)	0.40973(18)	0.0929(12)
Cl(2)	−0.1209(3)	0.2177(3)	0.3833(4)	0.128(4)
C(8s)	−0.1070(4)	0.2595(4)	0.3898(8)	0.051(5)

Table S2. Continued

atom	x	y	z	U(eq)
C(9s)	$-0.0982(5)$	$0.2428(6)$	$0.3806(10)$	$0.060(6)$
Cl(3)	$-0.1348(3)$	$0.2658(4)$	$0.3778(6)$	$0.159(5)$
O(1s)	0.0000	1.0000	$0.9412(3)$	$0.057(2)$
N(35s)	$-0.1725(2)$	$0.1615(3)$	$0.2459(4)$	$0.261(7)$
C(31s)	$-0.20170(17)$	$0.15387(14)$	$0.2259(3)$	$0.279(10)$
N(36s)	$-0.2234(2)$	$0.1434(3)$	$0.2607(3)$	$0.323(10)$
C(32s)	$-0.2077(3)$	$0.1443(3)$	$0.3035(3)$	$0.196(6)$
C(33s)	$-0.1762(3)$	$0.1556(3)$	$0.2943(4)$	$0.278(10)$
C(34s)	$-0.2116(2)$	$0.1545(2)$	$0.1752(3)$	$0.100(3)$
C(2os)	0.0000	0.5000	$0.6610(8)$	$0.150(10)$
O(2s)	$-0.0127(4)$	$0.4868(4)$	$0.7076(6)$	$0.106(6)$

[a] U(eq) is defined as one third of the trace of the orthogonalized $\mathbf{U}_{ij}$ tensor. The estimated standard deviations of the least significant digits are given in parentheses.

Table S3. Bond Lengths for [Fe(TMP)(2-MeHIm)$_2$]$_2$·[Fe(TMP)(2-MeHIm)]$_2$

bond	length (Å)	bond	length (Å)
Fe(1)–N(11)	1.959(3)	Fe(3)–N(34)	2.082(3)
Fe(1)–N(13)	1.961(3)	Fe(3)–N(32)	2.084(3)
Fe(1)–N(12)	1.965(3)	Fe(3)–N(35a)	2.123(4)
Fe(1)–N(14)	1.971(3)	Fe(3)–N(35b)	2.204(5)
Fe(1)–N(15)	2.030(3)	N(35a)–C(31a)	1.3268
Fe(1)–N(17)	2.047(3)	N(35a)–C(33a)	1.3896
N(11)–C(1a1)	1.381(5)	C(31a)–N(36a)	1.3696
N(11)–C(1a2)	1.383(5)	C(31a)–C(34a)	1.4782
N(12)–C(1a4)	1.375(5)	N(36a)–C(32a)	1.3574
N(12)–C(1a3)	1.382(5)	C(32a)–C(33a)	1.3559
N(13)–C(1a5)	1.371(5)	N(35b)–C(31b)	1.3271
N(13)–C(1a6)	1.381(5)	N(35b)–C(33b)	1.3884
N(14)–C(1a8)	1.373(5)	C(31b)–N(36b)	1.3707
N(14)–C(1a7)	1.375(5)	C(31b)–C(34b)	1.4778
N(15)–C(11)	1.321(5)	N(36b)–C(32b)	1.3568
N(15)–C(13)	1.387(5)	C(32b)–C(33b)	1.3565
C(11)–N(16)	1.359(5)	N(31)–C(3a2)	1.372(5)
C(11)–C(14)	1.492(6)	N(31)–C(3a1)	1.381(5)
N(16)–C(12)	1.365(5)	N(32)–C(3a3)	1.371(5)
N(16)–H(16n)	0.8800	N(32)–C(3a4)	1.372(5)
C(12)–C(13)	1.343(6)	N(33)–C(3a6)	1.361(5)
C(12)–H(12)	0.9500	N(33)–C(3a5)	1.372(5)
C(13)–H(13)	0.9500	N(34)–C(3a7)	1.370(5)
C(14)–H(14a)	0.9800	N(34)–C(3a8)	1.375(5)
C(14)–H(14b)	0.9800	C(3a1)–C(3m4)	1.398(6)
C(14)–H(14c)	0.9800	C(3a1)–C(3b1)	1.462(6)
N(17)–C(15)	1.319(5)	C(3a2)–C(3m1)	1.394(6)
N(17)–C(17)	1.390(6)	C(3a2)–C(3b2)	1.443(6)
C(15)–N(18)	1.359(6)	C(3a3)–C(3m1)	1.413(6)
C(15)–C(18)	1.476(6)	C(3a3)–C(3b3)	1.438(6)
N(18)–C(16)	1.352(6)	C(3a4)–C(3m2)	1.396(6)
N(18)–H(18n)	0.8800	C(3a4)–C(3b4)	1.438(6)
C(16)–C(17)	1.344(6)	C(3a5)–C(3m2)	1.411(5)
C(16)–H(16)	0.9500	C(3a5)–C(3b5)	1.440(6)

Table S3. Continued

bond	length (Å)	bond	length (Å)
C(17)–H(17)	0.9500	C(3a6)–C(3m3)	1.411(6)
C(18)–H(18a)	0.9800	C(3a6)–C(3b6)	1.452(6)
C(18)–H(18b)	0.9800	C(3a7)–C(3m3)	1.396(6)
C(18)–H(18c)	0.9800	C(3a7)–C(3b7)	1.436(6)
C(1a1)–C(1m4)	1.389(6)	C(3a8)–C(3m4)	1.417(6)
C(1a1)–C(1b1)	1.423(6)	C(3a8)–C(3b8)	1.435(5)
C(1a2)–C(1m1)	1.393(5)	C(3b1)–C(3b2)	1.356(6)
C(1a2)–C(1b2)	1.434(6)	C(3b1)–H(3b1)	0.9500
C(1a3)–C(1m1)	1.396(6)	C(3b2)–H(3b2)	0.9500
C(1a3)–C(1b3)	1.432(6)	C(3b3)–C(3b4)	1.340(6)
C(1a4)–C(1m2)	1.405(5)	C(3b3)–H(3b3)	0.9500
C(1a4)–C(1b4)	1.437(5)	C(3b4)–H(3b4)	0.9500
C(1a5)–C(1m2)	1.388(5)	C(3b5)–C(3b6)	1.338(6)
C(1a5)–C(1b5)	1.459(6)	C(3b5)–H(3b5)	0.9500
C(1a6)–C(1m3)	1.394(5)	C(3b6)–H(3b6)	0.9500
C(1a6)–C(1b6)	1.446(6)	C(3b7)–C(3b8)	1.347(6)
C(1a7)–C(1m3)	1.395(6)	C(3b7)–H(3b7)	0.9500
C(1a7)–C(1b7)	1.438(6)	C(3b8)–H(3b8)	0.9500
C(1a8)–C(1m4)	1.395(6)	C(3m1)–C(311)	1.511(5)
C(1a8)–C(1b8)	1.437(6)	C(3m2)–C(321)	1.513(6)
C(1b1)–C(1b2)	1.333(6)	C(3m3)–C(331)	1.497(5)
C(1b1)–H(1b1)	0.9500	C(3m4)–C(341)	1.491(6)
C(1b2)–H(1b2)	0.9500	C(311)–C(316)	1.394(6)
C(1b3)–C(1b4)	1.359(6)	C(311)–C(312)	1.404(7)
C(1b3)–H(1b3)	0.9500	C(312)–C(313)	1.384(6)
C(1b4)–H(1b4)	0.9500	C(312)–C(317)	1.512(7)
C(1b5)–C(1b6)	1.332(6)	C(313)–C(314)	1.405(7)
C(1b5)–H(1b5)	0.9500	C(313)–H(313)	0.9500
C(1b6)–H(1b6)	0.9500	C(314)–C(315)	1.390(7)
C(1b7)–C(1b8)	1.359(6)	C(314)–C(318)	1.511(6)
C(1b7)–H(1b7)	0.9500	C(315)–C(316)	1.391(6)
C(1b8)–H(1b8)	0.9500	C(315)–H(315)	0.9500
C(1m1)–C(111)	1.496(5)	C(316)–C(319)	1.510(7)
C(1m2)–C(121)	1.472(5)	C(317)–H(3d7)	0.9800

Table S3. Continued

bond	length (Å)	bond	length (Å)
C(1m3)–C(131)	1.503(5)	C(317)–H(3e7)	0.9800
C(1m4)–C(141)	1.509(6)	C(317)–H(3f7)	0.9800
C(111)–C(116)	1.402(6)	C(318)–H(3d8)	0.9800
C(111)–C(112)	1.413(5)	C(318)–H(3e8)	0.9800
C(112)–C(113)	1.381(6)	C(318)–H(3f8)	0.9800
C(112)–C(117)	1.503(6)	C(319)–H(3d9)	0.9800
C(113)–C(114)	1.404(6)	C(319)–H(3e9)	0.9800
C(113)–H(113)	0.9500	C(319)–H(3f9)	0.9800
C(114)–C(115)	1.373(6)	C(321)–C(326)	1.385(6)
C(114)–C(118)	1.501(6)	C(321)–C(322)	1.392(6)
C(115)–C(116)	1.399(5)	C(322)–C(323)	1.383(7)
C(115)–H(115)	0.9500	C(322)–C(327)	1.539(7)
C(116)–C(119)	1.513(6)	C(323)–C(324)	1.367(8)
C(117)–H(1d7)	0.9800	C(323)–H(323)	0.9500
C(117)–H(1e7)	0.9800	C(324)–C(325)	1.371(8)
C(117)–H(1f7)	0.9800	C(324)–C(328)	1.533(7)
C(118)–H(1d8)	0.9800	C(325)–C(326)	1.397(7)
C(118)–H(1e8)	0.9800	C(325)–H(325)	0.9500
C(118)–H(1f8)	0.9800	C(326)–C(329)	1.477(7)
C(119)–H(1d9)	0.9800	C(327)–H(3g7)	0.9800
C(119)–H(1e9)	0.9800	C(327)–H(3h7)	0.9800
C(119)–H(1f9)	0.9800	C(327)–H(3i7)	0.9800
C(121)–C(126)	1.414(5)	C(328)–H(3g8)	0.9800
C(121)–C(122)	1.421(6)	C(328)–H(3h8)	0.9800
C(122)–C(123)	1.384(6)	C(328)–H(3i8)	0.9800
C(122)–C(127)	1.490(6)	C(329)–H(3g9)	0.9800
C(123)–C(124)	1.360(7)	C(329)–H(3h9)	0.9800
C(123)–H(123)	0.9500	C(329)–H(3i9)	0.9800
C(124)–C(125)	1.402(7)	C(331)–C(336)	1.408(6)
C(124)–C(128)	1.543(7)	C(331)–C(332)	1.412(6)
C(125)–C(126)	1.392(6)	C(332)–C(333)	1.394(6)
C(125)–H(125)	0.9500	C(332)–C(337)	1.512(6)
C(126)–C(129)	1.484(7)	C(333)–C(334)	1.390(6)
C(127)–H(1g7)	0.9800	C(333)–H(333)	0.9500

Table S3. Continued

bond	length (Å)	bond	length (Å)
C(127)–H(1h7)	0.9800	C(334)–C(335)	1.385(6)
C(127)–H(1i7)	0.9800	C(334)–C(338)	1.509(6)
C(128)–H(1g8)	0.9800	C(335)–C(336)	1.400(6)
C(128)–H(1h8)	0.9800	C(335)–H(335)	0.9500
C(128)–H(1i8)	0.9800	C(336)–C(339)	1.501(6)
C(129)–H(1g9)	0.9800	C(337)–H(3j7)	0.9800
C(129)–H(1h9)	0.9800	C(337)–H(3k7)	0.9800
C(129)–H(1i9)	0.9800	C(337)–H(3l7)	0.9800
C(131)–C(132)	1.408(6)	C(338)–H(3j8)	0.9800
C(131)–C(136)	1.421(6)	C(338)–H(3k8)	0.9800
C(132)–C(133)	1.383(6)	C(338)–H(3l8)	0.9800
C(132)–C(137)	1.519(6)	C(339)–H(3j9)	0.9800
C(133)–C(134)	1.414(6)	C(339)–H(3k9)	0.9800
C(133)–H(133)	0.9500	C(339)–H(3l9)	0.9800
C(134)–C(135)	1.382(6)	C(341)–C(342)	1.393(6)
C(134)–C(138)	1.499(6)	C(341)–C(346)	1.395(6)
C(135)–C(136)	1.388(6)	C(342)–C(343)	1.395(7)
C(135)–H(135)	0.9500	C(342)–C(347)	1.507(7)
C(136)–C(139)	1.501(6)	C(343)–C(344)	1.362(8)
C(137)–H(1j7)	0.9800	C(343)–H(343)	0.9500
C(137)–H(1k7)	0.9800	C(344)–C(345)	1.394(8)
C(137)–H(1l7)	0.9800	C(344)–C(348)	1.514(7)
C(138)–H(1j8)	0.9800	C(345)–C(346)	1.409(7)
C(138)–H(1k8)	0.9800	C(345)–H(345)	0.9500
C(138)–H(1l8)	0.9800	C(346)–C(349)	1.503(7)
C(139)–H(1j9)	0.9800	C(347)–H(3m7)	0.9800
C(139)–H(1k9)	0.9800	C(347)–H(3n7)	0.9800
C(139)–H(1l9)	0.9800	C(347)–H(3p7)	0.9800
C(141)–C(142)	1.406(7)	C(348)–H(3m8)	0.9800
C(141)–C(146)	1.409(7)	C(348)–H(3n8)	0.9800
C(142)–C(143)	1.401(8)	C(348)–H(3p8)	0.9800
C(142)–C(147)	1.520(9)	C(349)–H(3m9)	0.9800
C(143)–C(144)	1.366(9)	C(349)–H(3n9)	0.9800
C(143)–H(143)	0.9500	C(349)–H(3l9)	0.9800

Table S3. Continued

bond	length (Å)	bond	length (Å)
C(144)–C(145)	1.388(9)	Fe(4a)–N(44)	2.062(3)
C(144)–C(148)	1.531(8)	Fe(4a)–N(42)	2.065(4)
C(145)–C(146)	1.381(7)	Fe(4a)–N(41)	2.073(3)
C(145)–H(145)	0.9500	Fe(4a)–N(43)	2.104(3)
C(146)–C(149)	1.493(8)	Fe(4a)–N(45a)	2.163(3)
C(147)–H(1m7)	0.9800	N(45a)–C(41a)	1.3271
C(147)–H(1n7)	0.9800	N(45a)–C(43a)	1.3883
C(147)–H(1p7)	0.9800	C(41a)–N(46a)	1.3709
C(148)–H(1m8)	0.9800	C(41a)–C(44a)	1.4781
C(148)–H(1n8)	0.9800	N(46a)–C(42a)	1.3569
C(148)–H(1p8)	0.9800	C(42a)–C(43a)	1.3560
C(149)–H(1m9)	0.9800	Fe(4b)–N(42)	2.066(4)
C(149)–H(1n9)	0.9800	Fe(4b)–N(44)	2.075(4)
C(149)–H(1p9)	0.9800	Fe(4b)–N(43)	2.085(4)
Fe(2)–N(24)	1.953(3)	Fe(4b)–N(45b)	2.117(9)
Fe(2)–N(22)	1.958(3)	Fe(4b)–N(41)	2.131(4)
Fe(2)–N(23)	1.965(3)	N(45b)–C(41b)	1.3262
Fe(2)–N(21)	1.969(3)	N(45b)–C(43b)	1.3898
Fe(2)–N(27)	2.028(3)	C(41b)–N(46b)	1.3703
Fe(2)–N(25)	2.032(3)	C(41b)–C(44b)	1.4782
N(21)–C(2a2)	1.379(5)	N(46b)–C(42b)	1.3572
N(21)–C(2a1)	1.391(5)	C(42b)–C(43b)	1.3562
N(22)–C(2a4)	1.380(5)	Cl(4)–C(10s)	1.710(19)
N(22)–C(2a3)	1.388(5)	Cl(5)–C(10s)	1.743(19)
N(23)–C(2a6)	1.379(5)	N(41)–C(4a1)	1.376(5)
N(23)–C(2a5)	1.388(5)	N(41)–C(4a2)	1.381(5)
N(24)–C(2a8)	1.375(5)	N(42)–C(4a3)	1.366(5)
N(24)–C(2a7)	1.377(5)	N(42)–C(4a4)	1.390(5)
N(25)–C(21)	1.307(6)	N(43)–C(4a6)	1.359(5)
N(25)–C(23)	1.440(6)	N(43)–C(4a5)	1.385(5)
C(21)–N(26)	1.386(7)	N(44)–C(4a8)	1.371(5)
C(21)–C(24)	1.440(8)	N(44)–C(4a7)	1.379(5)
N(26)–C(22)	1.388(6)	C(4a1)–C(4m4)	1.394(6)
N(26)–H(26n)	0.8800	C(4a1)–C(4b1)	1.437(6)

bond	length (Å)	bond	length (Å)
C(22)–C(23)	1.322(7)	C(4a2)–C(4m1)	1.390(6)
C(22)–H(22)	0.9500	C(4a2)–C(4b2)	1.437(6)
C(23)–H(23)	0.9500	C(4a3)–C(4m1)	1.405(6)
C(24)–H(24a)	0.9800	C(4a3)–C(4b3)	1.452(6)
C(24)–H(24b)	0.9800	C(4a4)–C(4m2)	1.400(5)
C(24)–H(24c)	0.9800	C(4a4)–C(4b4)	1.425(6)
N(27)–C(25)	1.338(5)	C(4a5)–C(4m2)	1.405(6)
N(27)–C(27)	1.405(6)	C(4a5)–C(4b5)	1.437(6)
C(25)–N(28)	1.357(6)	C(4a6)–C(4m3)	1.407(6)
C(25)–C(28)	1.463(6)	C(4a6)–C(4b6)	1.447(6)
N(28)–C(26)	1.374(6)	C(4a7)–C(4m3)	1.402(5)
N(28)–H(28n)	0.8800	C(4a7)–C(4b7)	1.426(6)
C(26)–C(27)	1.357(6)	C(4a8)–C(4m4)	1.398(6)
C(26)–H(26)	0.9500	C(4a8)–C(4b8)	1.455(6)
C(27)–H(27)	0.9500	C(4b1)–C(4b2)	1.358(6)
C(28)–H(28a)	0.9800	C(4b1)–H(4b1)	0.9500
C(28)–H(28b)	0.9800	C(4b2)–H(4b2)	0.9500
C(28)–H(28c)	0.9800	C(4b3)–C(4b4)	1.356(6)
C(2a1)–C(2m4)	1.387(6)	C(4b3)–H(4b3)	0.9500
C(2a1)–C(2b1)	1.442(5)	C(4b4)–H(4b4)	0.9500
C(2a2)–C(2m1)	1.398(6)	C(4b5)–C(4b6)	1.356(6)
C(2a2)–C(2b2)	1.430(6)	C(4b5)–H(4b5)	0.9500
C(2a3)–C(2m1)	1.387(6)	C(4b6)–H(4b6)	0.9500
C(2a3)–C(2b3)	1.434(6)	C(4b7)–C(4b8)	1.345(5)
C(2a4)–C(2m2)	1.412(5)	C(4b7)–H(4b7)	0.9500
C(2a4)–C(2b4)	1.431(6)	C(4b8)–H(4b8)	0.9500
C(2a5)–C(2m2)	1.394(6)	C(4m1)–C(411)	1.507(6)
C(2a5)–C(2b5)	1.444(6)	C(4m2)–C(421)	1.502(5)
C(2a6)–C(2m3)	1.385(6)	C(4m3)–C(431)	1.503(6)
C(2a6)–C(2b6)	1.456(6)	C(4m4)–C(441)	1.512(6)
C(2a7)–C(2m3)	1.390(6)	C(411)–C(416)	1.392(7)
C(2a7)–C(2b7)	1.429(6)	C(411)–C(412)	1.412(7)
C(2a8)–C(2m4)	1.408(5)	C(412)–C(413)	1.391(7)
C(2a8)–C(2b8)	1.436(6)	C(412)–C(417)	1.497(7)

Table S3. Continued

bond	length (Å)	bond	length (Å)
C(2b1)–C(2b2)	1.371(6)	C(413)–C(414)	1.363(8)
C(2b1)–H(2b1)	0.9500	C(413)–H(413)	0.9500
C(2b2)–H(2b2)	0.9500	C(414)–C(415)	1.378(9)
C(2b3)–C(2b4)	1.362(5)	C(414)–C(418)	1.505(7)
C(2b3)–H(2b3)	0.9500	C(415)–C(416)	1.402(7)
C(2b4)–H(2b4)	0.9500	C(415)–H(415)	0.9500
C(2b5)–C(2b6)	1.347(6)	C(416)–C(419)	1.503(8)
C(2b5)–H(2b5)	0.9500	C(417)–H(4d7)	0.9800
C(2b6)–H(2b6)	0.9500	C(417)–H(4e7)	0.9800
C(2b7)–C(2b8)	1.348(6)	C(417)–H(4f7)	0.9800
C(2b7)–H(2b7)	0.9500	C(418)–H(4d8)	0.9800
C(2b8)–H(2b8)	0.9500	C(418)–H(4e8)	0.9800
C(2m1)–C(211)	1.509(5)	C(418)–H(4f8)	0.9800
C(2m2)–C(221)	1.500(6)	C(419)–H(4d9)	0.9800
C(2m3)–C(231)	1.513(6)	C(419)–H(4e9)	0.9800
C(2m4)–C(241)	1.478(6)	C(419)–H(4f9)	0.9800
C(211)–C(216)	1.380(6)	C(421)–C(426)	1.397(6)
C(211)–C(212)	1.406(6)	C(421)–C(422)	1.404(6)
C(212)–C(213)	1.384(6)	C(422)–C(423)	1.398(6)
C(212)–C(217)	1.501(6)	C(422)–C(427)	1.503(6)
C(213)–C(214)	1.389(6)	C(423)–C(424)	1.373(6)
C(213)–H(213)	0.9500	C(423)–H(423)	0.9500
C(214)–C(215)	1.397(6)	C(424)–C(425)	1.371(6)
C(214)–C(218)	1.507(6)	C(424)–C(428)	1.527(6)
C(215)–C(216)	1.401(5)	C(425)–C(426)	1.398(6)
C(215)–H(215)	0.9500	C(425)–H(425)	0.9500
C(216)–C(219)	1.493(6)	C(426)–C(429)	1.516(6)
C(217)–H(2d7)	0.9800	C(427)–H(4g7)	0.9800
C(217)–H(2e7)	0.9800	C(427)–H(4h7)	0.9800
C(217)–H(2f7)	0.9800	C(427)–H(4i7)	0.9800
C(218)–H(2d8)	0.9800	C(428)–H(4g8)	0.9800
C(218)–H(2e8)	0.9800	C(428)–H(4h8)	0.9800
C(218)–H(2f8)	0.9800	C(428)–H(4i8)	0.9800
C(219)–H(2d9)	0.9800	C(429)–H(4g9)	0.9800

Table S3. Continued

bond	length (Å)	bond	length (Å)
C(219)–H(2e9)	0.9800	C(429)–H(4h9)	0.9800
C(219)–H(2f9)	0.9800	C(429)–H(4i9)	0.9800
C(221)–C(222)	1.394(7)	C(431)–C(436)	1.395(6)
C(221)–C(226)	1.402(6)	C(431)–C(432)	1.406(6)
C(222)–C(223)	1.410(7)	C(432)–C(433)	1.396(6)
C(222)–C(227)	1.519(8)	C(432)–C(437)	1.501(7)
C(223)–C(224)	1.368(8)	C(433)–C(434)	1.384(6)
C(223)–H(223)	0.9500	C(433)–H(433)	0.9500
C(224)–C(225)	1.391(8)	C(434)–C(435)	1.393(7)
C(224)–C(228)	1.496(7)	C(434)–C(438)	1.495(6)
C(225)–C(226)	1.414(7)	C(435)–C(436)	1.397(6)
C(225)–H(225)	0.9500	C(435)–H(435)	0.9500
C(226)–C(229)	1.477(7)	C(436)–C(439)	1.501(6)
C(227)–H(2g7)	0.9800	C(437)–H(4j7)	0.9800
C(227)–H(2h7)	0.9800	C(437)–H(4k7)	0.9800
C(227)–H(2i7)	0.9800	C(437)–H(4l7)	0.9800
C(228)–H(2g8)	0.9800	C(438)–H(4j8)	0.9800
C(228)–H(2h8)	0.9800	C(438)–H(4k8)	0.9800
C(228)–H(2i8)	0.9800	C(438)–H(4l8)	0.9800
C(229)–H(2g9)	0.9800	C(439)–H(4j9)	0.9800
C(229)–H(2h9)	0.9800	C(439)–H(4k9)	0.9800
C(229)–H(2i9)	0.9800	C(439)–H(4l9)	0.9800
C(231)–C(236)	1.398(6)	C(441)–C(442)	1.390(6)
C(231)–C(232)	1.399(6)	C(441)–C(446)	1.401(6)
C(232)–C(233)	1.398(6)	C(442)–C(443)	1.394(7)
C(232)–C(237)	1.528(7)	C(442)–C(447)	1.492(7)
C(233)–C(234)	1.370(7)	C(443)–C(444)	1.370(8)
C(233)–H(233)	0.9500	C(443)–H(443)	0.9500
C(234)–C(235)	1.397(7)	C(444)–C(445)	1.386(8)
C(234)–C(238)	1.491(6)	C(444)–C(448)	1.526(7)
C(235)–C(236)	1.395(6)	C(445)–C(446)	1.396(7)
C(235)–H(235)	0.9500	C(445)–H(445)	0.9500
C(236)–C(239)	1.513(6)	C(446)–C(449)	1.479(7)
C(237)–H(2j7)	0.9800	C(447)–H(4m7)	0.9800

Table S3. Continued

bond	length (Å)	bond	length (Å)
C(237)–H(2k7)	0.9800	C(447)–H(4n7)	0.9800
C(237)–H(2l7)	0.9800	C(447)–H(4p7)	0.9800
C(238)–H(2j8)	0.9800	C(448)–H(4m8)	0.9800
C(238)–H(2k8)	0.9800	C(448)–H(4n8)	0.9800
C(238)–H(2l8)	0.9800	C(448)–H(4p8)	0.9800
C(239)–H(2j9)	0.9800	C(449)–H(4m9)	0.9800
C(239)–H(2k9)	0.9800	C(449)–H(4n9)	0.9800
C(239)–H(2l9)	0.9800	C(449)–H(4p9)	0.9800
C(241)–C(242)	1.391(6)	C(1s)–C(6s)	1.368(9)
C(241)–C(246)	1.408(5)	C(1s)–C(2s)	1.422(11)
C(242)–C(243)	1.391(6)	C(1s)–C(7s)	1.552(12)
C(242)–C(247)	1.515(6)	C(2s)–C(3s)	1.425(13)
C(243)–C(244)	1.382(6)	C(3s)–C(4s)	1.479(13)
C(243)–H(243)	0.9500	C(4s)–C(5s)	1.437(11)
C(244)–C(245)	1.380(7)	C(5s)–C(6s)	1.481(10)
C(244)–C(248)	1.518(7)	Cl(1)–C(9s)	1.65(2)
C(245)–C(246)	1.414(6)	Cl(1)–C(8s)	1.685(16)
C(245)–H(245)	0.9500	Cl(2)–C(8s)	1.767(16)
C(246)–C(249)	1.497(6)	C(9s)–Cl(3)	1.725(17)
C(247)–H(2m7)	0.9800	N(35s)–C(31s)	1.3272
C(247)–H(2n7)	0.9800	N(35s)–C(33s)	1.3887
C(247)–H(2p7)	0.9800	C(31s)–N(36s)	1.3703
C(248)–H(2m8)	0.9800	C(31s)–C(34s)	1.4782
C(248)–H(2n8)	0.9800	N(36s)–C(32s)	1.3574
C(248)–H(2p8)	0.9800	C(32s)–C(33s)	1.3557
C(249)–H(2m9)	0.9800	C(2os)–O(2s)#1	1.498(17)
C(249)–H(2n9)	0.9800	C(2os)–O(2s)	1.498(17)
C(249)–H(2p9)	0.9800	O(2s)–O(2s)#1	1.46(3)
Fe(3)–N(31)	2.066(3)		
Fe(3)–N(33)	2.066(3)		

[a]The estimated standard deviations of the least significant digits are given in parentheses.

Table S4. Bond Angles for [Fe(TMP)(2-MeHIm)$_2$]$_2$·[Fe(TMP)(2-MeHIm)]$_2$

angle	degree	angle	degree
N(11)–Fe(1)–N(13)	179.29(14)	H(2m9)–C(249)–H(2n9)	109.5
N(11)–Fe(1)–N(12)	90.45(13)	C(246)–C(249)–H(2p9)	109.5
N(13)–Fe(1)–N(12)	89.89(13)	H(2m9)–C(249)–H(2p9)	109.5
N(11)–Fe(1)–N(14)	89.38(13)	H(2n9)–C(249)–H(2p9)	109.5
N(13)–Fe(1)–N(14)	90.28(14)	N(31)–Fe(3)–N(33)	158.76(14)
N(12)–Fe(1)–N(14)	179.76(15)	N(31)–Fe(3)–N(34)	88.35(13)
N(11)–Fe(1)–N(15)	91.95(13)	N(33)–Fe(3)–N(34)	88.12(13)
N(13)–Fe(1)–N(15)	87.44(13)	N(31)–Fe(3)–N(32)	87.98(13)
N(12)–Fe(1)–N(15)	88.36(13)	N(33)–Fe(3)–N(32)	88.47(13)
N(14)–Fe(1)–N(15)	91.47(13)	N(34)–Fe(3)–N(32)	160.72(15)
N(11)–Fe(1)–N(17)	88.42(13)	N(31)–Fe(3)–N(35a)	99.72(19)
N(13)–Fe(1)–N(17)	92.21(14)	N(33)–Fe(3)–N(35a)	101.25(19)
N(12)–Fe(1)–N(17)	88.58(13)	N(34)–Fe(3)–N(35a)	108.72(18)
N(14)–Fe(1)–N(17)	91.59(14)	N(32)–Fe(3)–N(35a)	90.56(18)
N(15)–Fe(1)–N(17)	176.93(13)	N(31)–Fe(3)–N(35b)	99.1(2)
C(1a1)–N(11)–C(1a2)	105.6(3)	N(33)–Fe(3)–N(35b)	101.8(2)
C(1a1)–N(11)–Fe(1)	127.6(3)	N(34)–Fe(3)–N(35b)	90.0(2)
C(1a2)–N(11)–Fe(1)	126.7(3)	N(32)–Fe(3)–N(35b)	109.3(2)
C(1a4)–N(12)–C(1a3)	105.3(3)	N(35a)–Fe(3)–N(35b)	18.77(19)
C(1a4)–N(12)–Fe(1)	127.3(3)	C(31a)–N(35a)–C(33a)	106.4
C(1a3)–N(12)–Fe(1)	127.4(3)	C(31a)–N(35a)–Fe(3)	127.1(3)
C(1a5)–N(13)–C(1a6)	106.4(3)	C(33a)–N(35a)–Fe(3)	126.4(3)
C(1a5)–N(13)–Fe(1)	127.1(3)	N(35a)–C(31a)–N(36a)	108.8
C(1a6)–N(13)–Fe(1)	126.4(3)	N(35a)–C(31a)–C(34a)	129.6
C(1a8)–N(14)–C(1a7)	106.2(3)	N(36a)–C(31a)–C(34a)	121.6
C(1a8)–N(14)–Fe(1)	127.4(3)	C(32a)–N(36a)–C(31a)	109.4
C(1a7)–N(14)–Fe(1)	126.4(3)	C(33a)–C(32a)–N(36a)	105.5
C(11)–N(15)–C(13)	105.8(3)	C(32a)–C(33a)–N(35a)	109.9
C(11)–N(15)–Fe(1)	132.0(3)	C(31b)–N(35b)–C(33b)	106.4
C(13)–N(15)–Fe(1)	122.2(3)	C(31b)–N(35b)–Fe(3)	127.9(4)
N(15)–C(11)–N(16)	109.8(4)	C(33b)–N(35b)–Fe(3)	124.5(4)
N(15)–C(11)–C(14)	129.3(4)	N(35b)–C(31b)–N(36b)	108.7
N(16)–C(11)–C(14)	120.9(4)	N(35b)–C(31b)–C(34b)	129.6
C(11)–N(16)–C(12)	108.4(3)	N(36b)–C(31b)–C(34b)	121.6

Table S4. Continued

angle	degree	angle	degree
C(11)–N(16)–H(16n)	125.8	C(32b)–N(36b)–C(31b)	109.4
C(12)–N(16)–H(16n)	125.8	C(33b)–C(32b)–N(36b)	105.5
C(13)–C(12)–N(16)	105.8(4)	C(32b)–C(33b)–N(35b)	109.9
C(13)–C(12)–H(12)	127.1	C(3a2)–N(31)–C(3a1)	107.3(3)
N(16)–C(12)–H(12)	127.1	C(3a2)–N(31)–Fe(3)	126.9(3)
C(12)–C(13)–N(15)	110.2(4)	C(3a1)–N(31)–Fe(3)	125.2(3)
C(12)–C(13)–H(13)	124.9	C(3a3)–N(32)–C(3a4)	106.3(3)
N(15)–C(13)–H(13)	124.9	C(3a3)–N(32)–Fe(3)	127.3(3)
C(11)–C(14)–H(14a)	109.5	C(3a4)–N(32)–Fe(3)	125.9(3)
C(11)–C(14)–H(14b)	109.5	C(3a6)–N(33)–C(3a5)	106.9(3)
H(14a)–C(14)–H(14b)	109.5	C(3a6)–N(33)–Fe(3)	126.7(3)
C(11)–C(14)–H(14c)	109.5	C(3a5)–N(33)–Fe(3)	125.9(3)
H(14a)–C(14)–H(14c)	109.5	C(3a7)–N(34)–C(3a8)	106.1(3)
H(14b)–C(14)–H(14c)	109.5	C(3a7)–N(34)–Fe(3)	126.7(3)
C(15)–N(17)–C(17)	106.4(4)	C(3a8)–N(34)–Fe(3)	126.8(3)
C(15)–N(17)–Fe(1)	133.0(3)	N(31)–C(3a1)–C(3m4)	127.6(4)
C(17)–N(17)–Fe(1)	120.6(3)	N(31)–C(3a1)–C(3b1)	108.5(3)
N(17)–C(15)–N(18)	108.8(4)	C(3m4)–C(3a1)–C(3b1)	123.9(4)
N(17)–C(15)–C(18)	127.4(4)	N(31)–C(3a2)–C(3m1)	126.0(4)
N(18)–C(15)–C(18)	123.8(4)	N(31)–C(3a2)–C(3b2)	109.7(3)
C(16)–N(18)–C(15)	109.4(4)	C(3m1)–C(3a2)–C(3b2)	124.2(4)
C(16)–N(18)–H(18n)	125.3	N(32)–C(3a3)–C(3m1)	124.5(4)
C(15)–N(18)–H(18n)	125.3	N(32)–C(3a3)–C(3b3)	109.9(4)
C(17)–C(16)–N(18)	105.8(4)	C(3m1)–C(3a3)–C(3b3)	125.7(4)
C(17)–C(16)–H(16)	127.1	N(32)–C(3a4)–C(3m2)	125.7(4)
N(18)–C(16)–H(16)	127.1	N(32)–C(3a4)–C(3b4)	109.3(4)
C(16)–C(17)–N(17)	109.6(4)	C(3m2)–C(3a4)–C(3b4)	125.0(4)
C(16)–C(17)–H(17)	125.2	N(33)–C(3a5)–C(3m2)	126.0(4)
N(17)–C(17)–H(17)	125.2	N(33)–C(3a5)–C(3b5)	109.3(3)
C(15)–C(18)–H(18a)	109.5	C(3m2)–C(3a5)–C(3b5)	124.6(4)
C(15)–C(18)–H(18b)	109.5	N(33)–C(3a6)–C(3m3)	126.7(4)
H(18a)–C(18)–H(18b)	109.5	N(33)–C(3a6)–C(3b6)	109.2(3)
C(15)–C(18)–H(18c)	109.5	C(3m3)–C(3a6)–C(3b6)	124.1(3)
H(18a)–C(18)–H(18c)	109.5	N(34)–C(3a7)–C(3m3)	125.9(4)

Table S4. Continued

angle	degree	angle	degree
H(18b)–C(18)–H(18c)	109.5	N(34)–C(3a7)–C(3b7)	109.8(4)
N(11)–C(1a1)–C(1m4)	124.3(4)	C(3m3)–C(3a7)–C(3b7)	124.3(4)
N(11)–C(1a1)–C(1b1)	109.7(3)	N(34)–C(3a8)–C(3m4)	125.2(4)
C(1m4)–C(1a1)–C(1b1)	125.8(4)	N(34)–C(3a8)–C(3b8)	109.8(4)
N(11)–C(1a2)–C(1m1)	125.2(4)	C(3m4)–C(3a8)–C(3b8)	125.0(4)
N(11)–C(1a2)–C(1b2)	109.3(3)	C(3b2)–C(3b1)–C(3a1)	107.2(4)
C(1m1)–C(1a2)–C(1b2)	125.2(4)	C(3b2)–C(3b1)–H(3b1)	126.4
N(12)–C(1a3)–C(1m1)	124.3(4)	C(3a1)–C(3b1)–H(3b1)	126.4
N(12)–C(1a3)–C(1b3)	110.4(3)	C(3b1)–C(3b2)–C(3a2)	107.3(4)
C(1m1)–C(1a3)–C(1b3)	125.1(4)	C(3b1)–C(3b2)–H(3b2)	126.4
N(12)–C(1a4)–C(1m2)	125.3(3)	C(3a2)–C(3b2)–H(3b2)	126.4
N(12)–C(1a4)–C(1b4)	110.5(3)	C(3b4)–C(3b3)–C(3a3)	106.9(4)
C(1m2)–C(1a4)–C(1b4)	123.8(4)	C(3b4)–C(3b3)–H(3b3)	126.6
N(13)–C(1a5)–C(1m2)	126.3(4)	C(3a3)–C(3b3)–H(3b3)	126.6
N(13)–C(1a5)–C(1b5)	109.2(3)	C(3b3)–C(3b4)–C(3a4)	107.7(4)
C(1m2)–C(1a5)–C(1b5)	124.0(4)	C(3b3)–C(3b4)–H(3b4)	126.1
N(13)–C(1a6)–C(1m3)	124.9(4)	C(3a4)–C(3b4)–H(3b4)	126.1
N(13)–C(1a6)–C(1b6)	109.4(3)	C(3b6)–C(3b5)–C(3a5)	107.3(4)
C(1m3)–C(1a6)–C(1b6)	125.5(4)	C(3b6)–C(3b5)–H(3b5)	126.3
N(14)–C(1a7)–C(1m3)	124.7(4)	C(3a5)–C(3b5)–H(3b5)	126.3
N(14)–C(1a7)–C(1b7)	110.1(4)	C(3b5)–C(3b6)–C(3a6)	107.2(4)
C(1m3)–C(1a7)–C(1b7)	124.8(4)	C(3b5)–C(3b6)–H(3b6)	126.4
N(14)–C(1a8)–C(1m4)	124.2(4)	C(3a6)–C(3b6)–H(3b6)	126.4
N(14)–C(1a8)–C(1b8)	109.8(4)	C(3b8)–C(3b7)–C(3a7)	107.3(3)
C(1m4)–C(1a8)–C(1b8)	125.0(4)	C(3b8)–C(3b7)–H(3b7)	126.4
C(1b2)–C(1b1)–C(1a1)	107.9(4)	C(3a7)–C(3b7)–H(3b7)	126.4
C(1b2)–C(1b1)–H(1b1)	126.1	C(3b7)–C(3b8)–C(3a8)	107.1(4)
C(1a1)–C(1b1)–H(1b1)	126.1	C(3b7)–C(3b8)–H(3b8)	126.5
C(1b1)–C(1b2)–C(1a2)	107.5(4)	C(3a8)–C(3b8)–H(3b8)	126.5
C(1b1)–C(1b2)–H(1b2)	126.3	C(3a2)–C(3m1)–C(3a3)	125.6(4)
C(1a2)–C(1b2)–H(1b2)	126.3	C(3a2)–C(3m1)–C(311)	116.5(4)
C(1b4)–C(1b3)–C(1a3)	107.0(4)	C(3a3)–C(3m1)–C(311)	117.7(4)
C(1b4)–C(1b3)–H(1b3)	126.5	C(3a4)–C(3m2)–C(3a5)	125.2(4)
C(1a3)–C(1b3)–H(1b3)	126.5	C(3a4)–C(3m2)–C(321)	118.8(3)

Table S4. Continued

angle	degree	angle	degree
C(1b3)–C(1b4)–C(1a4)	106.8(4)	C(3a5)–C(3m2)–C(321)	115.9(3)
C(1b3)–C(1b4)–H(1b4)	126.6	C(3a7)–C(3m3)–C(3a6)	124.3(4)
C(1a4)–C(1b4)–H(1b4)	126.6	C(3a7)–C(3m3)–C(331)	118.7(3)
C(1b6)–C(1b5)–C(1a5)	107.3(4)	C(3a6)–C(3m3)–C(331)	116.8(3)
C(1b6)–C(1b5)–H(1b5)	126.4	C(3a1)–C(3m4)–C(3a8)	124.1(4)
C(1a5)–C(1b5)–H(1b5)	126.4	C(3a1)–C(3m4)–C(341)	118.2(4)
C(1b5)–C(1b6)–C(1a6)	107.6(4)	C(3a8)–C(3m4)–C(341)	117.7(3)
C(1b5)–C(1b6)–H(1b6)	126.2	C(316)–C(311)–C(312)	120.0(4)
C(1a6)–C(1b6)–H(1b6)	126.2	C(316)–C(311)–C(3m1)	120.6(4)
C(1b8)–C(1b7)–C(1a7)	106.7(4)	C(312)–C(311)–C(3m1)	119.4(4)
C(1b8)–C(1b7)–H(1b7)	126.7	C(313)–C(312)–C(311)	118.9(4)
C(1a7)–C(1b7)–H(1b7)	126.7	C(313)–C(312)–C(317)	121.1(5)
C(1b7)–C(1b8)–C(1a8)	107.2(4)	C(311)–C(312)–C(317)	119.9(4)
C(1b7)–C(1b8)–H(1b8)	126.4	C(312)–C(313)–C(314)	122.0(4)
C(1a8)–C(1b8)–H(1b8)	126.4	C(312)–C(313)–H(313)	119.0
C(1a2)–C(1m1)–C(1a3)	123.7(4)	C(314)–C(313)–H(313)	119.0
C(1a2)–C(1m1)–C(111)	117.1(3)	C(315)–C(314)–C(313)	117.8(4)
C(1a3)–C(1m1)–C(111)	119.0(3)	C(315)–C(314)–C(318)	120.4(4)
C(1a5)–C(1m2)–C(1a4)	121.9(4)	C(313)–C(314)–C(318)	121.8(4)
C(1a5)–C(1m2)–C(121)	118.9(3)	C(314)–C(315)–C(316)	121.4(4)
C(1a4)–C(1m2)–C(121)	119.0(3)	C(314)–C(315)–H(315)	119.3
C(1a6)–C(1m3)–C(1a7)	123.6(4)	C(316)–C(315)–H(315)	119.3
C(1a6)–C(1m3)–C(131)	117.6(4)	C(315)–C(316)–C(311)	119.8(4)
C(1a7)–C(1m3)–C(131)	118.8(3)	C(315)–C(316)–C(319)	119.8(4)
C(1a1)–C(1m4)–C(1a8)	123.9(4)	C(311)–C(316)–C(319)	120.4(4)
C(1a1)–C(1m4)–C(141)	116.1(4)	C(312)–C(317)–H(3d7)	109.5
C(1a8)–C(1m4)–C(141)	119.9(4)	C(312)–C(317)–H(3e7)	109.5
C(116)–C(111)–C(112)	119.4(4)	H(3d7)–C(317)–H(3e7)	109.5
C(116)–C(111)–C(1m1)	120.8(3)	C(312)–C(317)–H(3f7)	109.5
C(112)–C(111)–C(1m1)	119.7(4)	H(3d7)–C(317)–H(3f7)	109.5
C(113)–C(112)–C(111)	119.8(4)	H(3e7)–C(317)–H(3f7)	109.5
C(113)–C(112)–C(117)	120.2(4)	C(314)–C(318)–H(3d8)	109.5
C(111)–C(112)–C(117)	120.0(4)	C(314)–C(318)–H(3e8)	109.5
C(112)–C(113)–C(114)	121.2(4)	H(3d8)–C(318)–H(3e8)	109.5

Table S4. Continued

angle	degree	angle	degree
C(112)–C(113)–H(113)	119.4	C(314)–C(318)–H(3f8)	109.5
C(114)–C(113)–H(113)	119.4	H(3d8)–C(318)–H(3f8)	109.5
C(115)–C(114)–C(113)	118.4(4)	H(3e8)–C(318)–H(3f8)	109.5
C(115)–C(114)–C(118)	120.8(4)	C(316)–C(319)–H(3d9)	109.5
C(113)–C(114)–C(118)	120.8(4)	C(316)–C(319)–H(3e9)	109.5
C(114)–C(115)–C(116)	122.2(4)	H(3d9)–C(319)–H(3e9)	109.5
C(114)–C(115)–H(115)	118.9	C(316)–C(319)–H(3f9)	109.5
C(116)–C(115)–H(115)	118.9	H(3d9)–C(319)–H(3f9)	109.5
C(115)–C(116)–C(111)	119.0(4)	H(3e9)–C(319)–H(3f9)	109.5
C(115)–C(116)–C(119)	120.5(4)	C(326)–C(321)–C(322)	120.2(4)
C(111)–C(116)–C(119)	120.5(4)	C(326)–C(321)–C(3m2)	121.0(4)
C(112)–C(117)–H(1d7)	109.5	C(322)–C(321)–C(3m2)	118.7(4)
C(112)–C(117)–H(1e7)	109.5	C(323)–C(322)–C(321)	120.2(5)
H(1d7)–C(117)–H(1e7)	109.5	C(323)–C(322)–C(327)	119.0(5)
C(112)–C(117)–H(1f7)	109.5	C(321)–C(322)–C(327)	120.8(4)
H(1d7)–C(117)–H(1f7)	109.5	C(324)–C(323)–C(322)	120.8(5)
H(1e7)–C(117)–H(1f7)	109.5	C(324)–C(323)–H(323)	119.6
C(114)–C(118)–H(1d8)	109.5	C(322)–C(323)–H(323)	119.6
C(114)–C(118)–H(1e8)	109.5	C(323)–C(324)–C(325)	118.3(5)
H(1d8)–C(118)–H(1e8)	109.5	C(323)–C(324)–C(328)	118.4(6)
C(114)–C(118)–H(1f8)	109.5	C(325)–C(324)–C(328)	123.3(6)
H(1d8)–C(118)–H(1f8)	109.5	C(324)–C(325)–C(326)	123.1(5)
H(1e8)–C(118)–H(1f8)	109.5	C(324)–C(325)–H(325)	118.4
C(116)–C(119)–H(1d9)	109.5	C(326)–C(325)–H(325)	118.4
C(116)–C(119)–H(1e9)	109.5	C(321)–C(326)–C(325)	117.3(5)
H(1d9)–C(119)–H(1e9)	109.5	C(321)–C(326)–C(329)	122.6(4)
C(116)–C(119)–H(1f9)	109.5	C(325)–C(326)–C(329)	120.1(4)
H(1d9)–C(119)–H(1f9)	109.5	C(322)–C(327)–H(3g7)	109.5
H(1e9)–C(119)–H(1f9)	109.5	C(322)–C(327)–H(3h7)	109.5
C(126)–C(121)–C(122)	118.6(4)	H(3g7)–C(327)–H(3h7)	109.5
C(126)–C(121)–C(1m2)	119.9(4)	C(322)–C(327)–H(3i7)	109.5
C(122)–C(121)–C(1m2)	121.4(3)	H(3g7)–C(327)–H(3i7)	109.5
C(123)–C(122)–C(121)	119.4(4)	H(3h7)–C(327)–H(3i7)	109.5
C(123)–C(122)–C(127)	121.0(4)	C(324)–C(328)–H(3g8)	109.5

angle	degree	angle	degree
C(121)–C(122)–C(127)	119.4(4)	C(324)–C(328)–H(3h8)	109.5
C(124)–C(123)–C(122)	122.7(5)	H(3g8)–C(328)–H(3h8)	109.5
C(124)–C(123)–H(123)	118.7	C(324)–C(328)–H(3i8)	109.5
C(122)–C(123)–H(123)	118.7	H(3g8)–C(328)–H(3i8)	109.5
C(123)–C(124)–C(125)	118.4(4)	H(3h8)–C(328)–H(3i8)	109.5
C(123)–C(124)–C(128)	121.2(5)	C(326)–C(329)–H(3g9)	109.5
C(125)–C(124)–C(128)	120.4(4)	C(326)–C(329)–H(3h9)	109.5
C(126)–C(125)–C(124)	121.6(4)	H(3g9)–C(329)–H(3h9)	109.5
C(126)–C(125)–H(125)	119.2	C(326)–C(329)–H(3i9)	109.5
C(124)–C(125)–H(125)	119.2	H(3g9)–C(329)–H(3i9)	109.5
C(125)–C(126)–C(121)	119.2(4)	H(3h9)–C(329)–H(3i9)	109.5
C(125)–C(126)–C(129)	119.6(4)	C(336)–C(331)–C(332)	120.1(4)
C(121)–C(126)–C(129)	121.1(4)	C(336)–C(331)–C(3m3)	119.1(4)
C(122)–C(127)–H(1g7)	109.5	C(332)–C(331)–C(3m3)	120.7(4)
C(122)–C(127)–H(1h7)	109.5	C(333)–C(332)–C(331)	118.9(4)
H(1g7)–C(127)–H(1h7)	109.5	C(333)–C(332)–C(337)	119.6(4)
C(122)–C(127)–H(1i7)	109.5	C(331)–C(332)–C(337)	121.5(4)
H(1g7)–C(127)–H(1i7)	109.5	C(334)–C(333)–C(332)	121.7(4)
H(1h7)–C(127)–H(1i7)	109.5	C(334)–C(333)–H(333)	119.2
C(124)–C(128)–H(1g8)	109.5	C(332)–C(333)–H(333)	119.2
C(124)–C(128)–H(1h8)	109.5	C(335)–C(334)–C(333)	118.8(4)
H(1g8)–C(128)–H(1h8)	109.5	C(335)–C(334)–C(338)	120.3(4)
C(124)–C(128)–H(1i8)	109.5	C(333)–C(334)–C(338)	120.8(4)
H(1g8)–C(128)–H(1i8)	109.5	C(334)–C(335)–C(336)	121.7(4)
H(1h8)–C(128)–H(1i8)	109.5	C(334)–C(335)–H(335)	119.1
C(126)–C(129)–H(1g9)	109.5	C(336)–C(335)–H(335)	119.1
C(126)–C(129)–H(1h9)	109.5	C(335)–C(336)–C(331)	118.7(4)
H(1g9)–C(129)–H(1h9)	109.5	C(335)–C(336)–C(339)	120.6(4)
C(126)–C(129)–H(1i9)	109.5	C(331)–C(336)–C(339)	120.7(4)
H(1g9)–C(129)–H(1i9)	109.5	C(332)–C(337)–H(3j7)	109.5
H(1h9)–C(129)–H(1i9)	109.5	C(332)–C(337)–H(3k7)	109.5
C(132)–C(131)–C(136)	119.9(4)	H(3j7)–C(337)–H(3k7)	109.5
C(132)–C(131)–C(1m3)	118.5(3)	C(332)–C(337)–H(3l7)	109.5
C(136)–C(131)–C(1m3)	121.6(4)	H(3j7)–C(337)–H(3l7)	109.5

angle	degree	angle	degree
C(133)–C(132)–C(131)	119.8(4)	H(3k7)–C(337)–H(3l7)	109.5
C(133)–C(132)–C(137)	119.7(4)	C(334)–C(338)–H(3j8)	109.5
C(131)–C(132)–C(137)	120.5(4)	C(334)–C(338)–H(3k8)	109.5
C(132)–C(133)–C(134)	121.0(4)	H(3j8)–C(338)–H(3k8)	109.5
C(132)–C(133)–H(133)	119.5	C(334)–C(338)–H(3l8)	109.5
C(134)–C(133)–H(133)	119.5	H(3j8)–C(338)–H(3l8)	109.5
C(135)–C(134)–C(133)	118.2(4)	H(3k8)–C(338)–H(3l8)	109.5
C(135)–C(134)–C(138)	120.9(4)	C(336)–C(339)–H(3j9)	109.5
C(133)–C(134)–C(138)	120.9(4)	C(336)–C(339)–H(3k9)	109.5
C(134)–C(135)–C(136)	122.8(4)	H(3j9)–C(339)–H(3k9)	109.5
C(134)–C(135)–H(135)	118.6	C(336)–C(339)–H(3l9)	109.5
C(136)–C(135)–H(135)	118.6	H(3j9)–C(339)–H(3l9)	109.5
C(135)–C(136)–C(131)	118.3(4)	H(3k9)–C(339)–H(3l9)	109.5
C(135)–C(136)–C(139)	120.9(4)	C(342)–C(341)–C(346)	119.7(4)
C(131)–C(136)–C(139)	120.9(4)	C(342)–C(341)–C(3m4)	120.7(4)
C(132)–C(137)–H(1j7)	109.5	C(346)–C(341)–C(3m4)	119.6(4)
C(132)–C(137)–H(1k7)	109.5	C(341)–C(342)–C(343)	119.6(5)
H(1j7)–C(137)–H(1k7)	109.5	C(341)–C(342)–C(347)	120.8(4)
C(132)–C(137)–H(1l7)	109.5	C(343)–C(342)–C(347)	119.6(5)
H(1j7)–C(137)–H(1l7)	109.5	C(344)–C(343)–C(342)	122.0(5)
H(1k7)–C(137)–H(1l7)	109.5	C(344)–C(343)–H(343)	119.0
C(134)–C(138)–H(1j8)	109.5	C(342)–C(343)–H(343)	119.0
C(134)–C(138)–H(1k8)	109.5	C(343)–C(344)–C(345)	118.7(4)
H(1j8)–C(138)–H(1k8)	109.5	C(343)–C(344)–C(348)	122.5(6)
C(134)–C(138)–H(1l8)	109.5	C(345)–C(344)–C(348)	118.9(5)
H(1j8)–C(138)–H(1l8)	109.5	C(344)–C(345)–C(346)	121.1(5)
H(1k8)–C(138)–H(1l8)	109.5	C(344)–C(345)–H(345)	119.5
C(136)–C(139)–H(1j9)	109.5	C(346)–C(345)–H(345)	119.5
C(136)–C(139)–H(1k9)	109.5	C(341)–C(346)–C(345)	119.0(5)
H(1j9)–C(139)–H(1k9)	109.5	C(341)–C(346)–C(349)	121.8(4)
C(136)–C(139)–H(1l9)	109.5	C(345)–C(346)–C(349)	119.2(4)
H(1j9)–C(139)–H(1l9)	109.5	C(342)–C(347)–H(3m7)	109.5
H(1k9)–C(139)–H(1l9)	109.5	C(342)–C(347)–H(3n7)	109.5
C(142)–C(141)–C(146)	119.6(4)	H(3m7)–C(347)–H(3n7)	109.5

Table S4. Continued

angle	degree	angle	degree
C(142)–C(141)–C(1m4)	121.1(4)	C(342)–C(347)–H(3p7)	109.5
C(146)–C(141)–C(1m4)	119.2(4)	H(3m7)–C(347)–H(3p7)	109.5
C(143)–C(142)–C(141)	118.4(5)	H(3n7)–C(347)–H(3p7)	109.5
C(143)–C(142)–C(147)	120.7(5)	C(344)–C(348)–H(3m8)	109.5
C(141)–C(142)–C(147)	120.9(5)	C(344)–C(348)–H(3n8)	109.5
C(144)–C(143)–C(142)	122.5(6)	H(3m8)–C(348)–H(3n8)	109.5
C(144)–C(143)–H(143)	118.7	C(344)–C(348)–H(3p8)	109.5
C(142)–C(143)–H(143)	118.7	H(3m8)–C(348)–H(3p8)	109.5
C(143)–C(144)–C(145)	118.2(5)	H(3n8)–C(348)–H(3p8)	109.5
C(143)–C(144)–C(148)	121.1(6)	C(346)–C(349)–H(3m9)	109.5
C(145)–C(144)–C(148)	120.6(6)	C(346)–C(349)–H(3n9)	109.5
C(146)–C(145)–C(144)	122.1(6)	H(3m9)–C(349)–H(3n9)	109.5
C(146)–C(145)–H(145)	119.0	C(346)–C(349)–H(3l9)	109.5
C(144)–C(145)–H(145)	119.0	H(3m9)–C(349)–H(3l9)	109.5
C(145)–C(146)–C(141)	119.2(5)	H(3n9)–C(349)–H(3l9)	109.5
C(145)–C(146)–C(149)	120.9(5)	N(44)–Fe(4a)–N(42)	156.96(15)
C(141)–C(146)–C(149)	120.0(4)	N(44)–Fe(4a)–N(41)	88.32(14)
C(142)–C(147)–H(1m7)	109.5	N(42)–Fe(4a)–N(41)	88.20(14)
C(142)–C(147)–H(1n7)	109.5	N(44)–Fe(4a)–N(43)	87.56(13)
H(1m7)–C(147)–H(1n7)	109.5	N(42)–Fe(4a)–N(43)	87.58(13)
C(142)–C(147)–H(1p7)	109.5	N(41)–Fe(4a)–N(43)	159.02(16)
H(1m7)–C(147)–H(1p7)	109.5	N(44)–Fe(4a)–N(45a)	104.01(17)
H(1n7)–C(147)–H(1p7)	109.5	N(42)–Fe(4a)–N(45a)	98.92(17)
C(144)–C(148)–H(1m8)	109.5	N(41)–Fe(4a)–N(45a)	104.38(15)
C(144)–C(148)–H(1n8)	109.5	N(43)–Fe(4a)–N(45a)	96.58(14)
H(1m8)–C(148)–H(1n8)	109.5	C(41a)–N(45a)–C(43a)	106.4
C(144)–C(148)–H(1p8)	109.5	C(41a)–N(45a)–Fe(4a)	132.1(2)
H(1m8)–C(148)–H(1p8)	109.5	C(43a)–N(45a)–Fe(4a)	120.3(2)
H(1n8)–C(148)–H(1p8)	109.5	N(45a)–C(41a)–N(46a)	108.7
C(146)–C(149)–H(1m9)	109.5	N(45a)–C(41a)–C(44a)	129.6
C(146)–C(149)–H(1n9)	109.5	N(46a)–C(41a)–C(44a)	121.6
H(1m9)–C(149)–H(1n9)	109.5	C(42a)–N(46a)–C(41a)	109.4
C(146)–C(149)–H(1p9)	109.5	C(43a)–C(42a)–N(46a)	105.5
H(1m9)–C(149)–H(1p9)	109.5	C(42a)–C(43a)–N(45a)	110.0

Table S4. Continued

angle	degree	angle	degree
H(1n9)–C(149)–H(1p9)	109.5	N(42)–Fe(4b)–N(44)	155.14(19)
N(24)–Fe(2)–N(22)	179.68(15)	N(42)–Fe(4b)–N(43)	88.06(15)
N(24)–Fe(2)–N(23)	90.54(13)	N(44)–Fe(4b)–N(43)	87.75(15)
N(22)–Fe(2)–N(23)	89.27(13)	N(42)–Fe(4b)–N(45b)	101.9(4)
N(24)–Fe(2)–N(21)	89.37(13)	N(44)–Fe(4b)–N(45b)	102.9(4)
N(22)–Fe(2)–N(21)	90.82(13)	N(43)–Fe(4b)–N(45b)	97.1(3)
N(23)–Fe(2)–N(21)	179.52(15)	N(42)–Fe(4b)–N(41)	86.61(15)
N(24)–Fe(2)–N(27)	87.31(14)	N(44)–Fe(4b)–N(41)	86.45(15)
N(22)–Fe(2)–N(27)	92.44(14)	N(43)–Fe(4b)–N(41)	153.87(19)
N(23)–Fe(2)–N(27)	91.87(14)	N(45b)–Fe(4b)–N(41)	109.0(3)
N(21)–Fe(2)–N(27)	87.65(13)	C(41b)–N(45b)–C(43b)	106.4
N(24)–Fe(2)–N(25)	90.63(14)	C(41b)–N(45b)–Fe(4b)	129.8(5)
N(22)–Fe(2)–N(25)	89.64(14)	C(43b)–N(45b)–Fe(4b)	123.8(5)
N(23)–Fe(2)–N(25)	93.15(14)	N(45b)–C(41b)–N(46b)	108.8
N(21)–Fe(2)–N(25)	87.33(14)	N(45b)–C(41b)–C(44b)	129.6
N(27)–Fe(2)–N(25)	174.60(14)	N(46b)–C(41b)–C(44b)	121.6
C(2a2)–N(21)–C(2a1)	105.7(3)	C(42b)–N(46b)–C(41b)	109.4
C(2a2)–N(21)–Fe(2)	126.8(3)	C(43b)–C(42b)–N(46b)	105.5
C(2a1)–N(21)–Fe(2)	127.5(3)	C(42b)–C(43b)–N(45b)	109.9
C(2a4)–N(22)–C(2a3)	104.9(3)	Cl(4)–C(10s)–Cl(5)	111.4(15)
C(2a4)–N(22)–Fe(2)	128.5(2)	C(4a1)–N(41)–C(4a2)	106.6(3)
C(2a3)–N(22)–Fe(2)	126.6(3)	C(4a1)–N(41)–Fe(4a)	126.2(3)
C(2a6)–N(23)–C(2a5)	105.9(3)	C(4a2)–N(41)–Fe(4a)	126.7(3)
C(2a6)–N(23)–Fe(2)	126.0(3)	C(4a1)–N(41)–Fe(4b)	125.5(3)
C(2a5)–N(23)–Fe(2)	128.0(3)	C(4a2)–N(41)–Fe(4b)	124.2(3)
C(2a8)–N(24)–C(2a7)	105.6(3)	Fe(4a)–N(41)–Fe(4b)	23.49(7)
C(2a8)–N(24)–Fe(2)	128.1(3)	C(4a3)–N(42)–C(4a4)	106.5(3)
C(2a7)–N(24)–Fe(2)	126.2(3)	C(4a3)–N(42)–Fe(4a)	126.0(3)
C(21)–N(25)–C(23)	106.5(4)	C(4a4)–N(42)–Fe(4a)	126.1(3)
C(21)–N(25)–Fe(2)	133.7(3)	C(4a3)–N(42)–Fe(4b)	125.8(3)
C(23)–N(25)–Fe(2)	119.2(3)	C(4a4)–N(42)–Fe(4b)	125.4(3)
N(25)–C(21)–N(26)	108.7(4)	Fe(4a)–N(42)–Fe(4b)	23.97(7)
N(25)–C(21)–C(24)	127.2(5)	C(4a6)–N(43)–C(4a5)	106.7(3)
N(26)–C(21)–C(24)	124.0(4)	C(4a6)–N(43)–Fe(4b)	124.8(3)

angle	degree	angle	degree
C(21)–N(26)–C(22)	109.1(4)	C(4a5)–N(43)–Fe(4b)	125.5(3)
C(21)–N(26)–H(26n)	125.4	C(4a6)–N(43)–Fe(4a)	126.5(3)
C(22)–N(26)–H(26n)	125.4	C(4a5)–N(43)–Fe(4a)	125.8(3)
C(23)–C(22)–N(26)	105.7(5)	Fe(4b)–N(43)–Fe(4a)	23.62(7)
C(23)–C(22)–H(22)	127.1	C(4a8)–N(44)–C(4a7)	106.5(3)
N(26)–C(22)–H(22)	127.1	C(4a8)–N(44)–Fe(4a)	125.3(3)
C(22)–C(23)–N(25)	109.9(5)	C(4a7)–N(44)–Fe(4a)	127.5(3)
C(22)–C(23)–H(23)	125.1	C(4a8)–N(44)–Fe(4b)	126.1(3)
N(25)–C(23)–H(23)	125.1	C(4a7)–N(44)–Fe(4b)	124.0(3)
C(21)–C(24)–H(24a)	109.5	Fe(4a)–N(44)–Fe(4b)	23.93(7)
C(21)–C(24)–H(24b)	109.5	N(41)–C(4a1)–C(4m4)	125.0(4)
H(24a)–C(24)–H(24b)	109.5	N(41)–C(4a1)–C(4b1)	109.8(4)
C(21)–C(24)–H(24c)	109.5	C(4m4)–C(4a1)–C(4b1)	125.2(4)
H(24a)–C(24)–H(24c)	109.5	N(41)–C(4a2)–C(4m1)	125.4(4)
H(24b)–C(24)–H(24c)	109.5	N(41)–C(4a2)–C(4b2)	109.1(4)
C(25)–N(27)–C(27)	105.2(3)	C(4m1)–C(4a2)–C(4b2)	125.5(4)
C(25)–N(27)–Fe(2)	133.2(3)	N(42)–C(4a3)–C(4m1)	126.5(4)
C(27)–N(27)–Fe(2)	121.6(3)	N(42)–C(4a3)–C(4b3)	109.4(3)
N(27)–C(25)–N(28)	109.5(4)	C(4m1)–C(4a3)–C(4b3)	124.2(4)
N(27)–C(25)–C(28)	128.5(4)	N(42)–C(4a4)–C(4m2)	126.1(4)
N(28)–C(25)–C(28)	122.0(4)	N(42)–C(4a4)–C(4b4)	109.7(3)
C(25)–N(28)–C(26)	110.0(3)	C(4m2)–C(4a4)–C(4b4)	124.2(4)
C(25)–N(28)–H(28n)	125.0	N(43)–C(4a5)–C(4m2)	125.4(3)
C(26)–N(28)–H(28n)	125.0	N(43)–C(4a5)–C(4b5)	109.3(3)
C(27)–C(26)–N(28)	104.5(4)	C(4m2)–C(4a5)–C(4b5)	125.3(4)
C(27)–C(26)–H(26)	127.8	N(43)–C(4a6)–C(4m3)	125.6(4)
N(28)–C(26)–H(26)	127.8	N(43)–C(4a6)–C(4b6)	109.8(4)
C(26)–C(27)–N(27)	110.8(4)	C(4m3)–C(4a6)–C(4b6)	124.6(4)
C(26)–C(27)–H(27)	124.6	N(44)–C(4a7)–C(4m3)	125.4(4)
N(27)–C(27)–H(27)	124.6	N(44)–C(4a7)–C(4b7)	109.8(3)
C(25)–C(28)–H(28a)	109.5	C(4m3)–C(4a7)–C(4b7)	124.8(4)
C(25)–C(28)–H(28b)	109.5	N(44)–C(4a8)–C(4m4)	126.4(4)
H(28a)–C(28)–H(28b)	109.5	N(44)–C(4a8)–C(4b8)	109.1(3)
C(25)–C(28)–H(28c)	109.5	C(4m4)–C(4a8)–C(4b8)	124.5(4)

angle	degree	angle	degree
H(28a)–C(28)–H(28c)	109.5	C(4b2)–C(4b1)–C(4a1)	106.8(4)
H(28b)–C(28)–H(28c)	109.5	C(4b2)–C(4b1)–H(4b1)	126.6
C(2m4)–C(2a1)–N(21)	125.1(3)	C(4a1)–C(4b1)–H(4b1)	126.6
C(2m4)–C(2a1)–C(2b1)	124.8(4)	C(4b1)–C(4b2)–C(4a2)	107.7(4)
N(21)–C(2a1)–C(2b1)	109.8(3)	C(4b1)–C(4b2)–H(4b2)	126.1
N(21)–C(2a2)–C(2m1)	124.6(4)	C(4a2)–C(4b2)–H(4b2)	126.1
N(21)–C(2a2)–C(2b2)	110.5(3)	C(4b4)–C(4b3)–C(4a3)	107.0(4)
C(2m1)–C(2a2)–C(2b2)	124.7(4)	C(4b4)–C(4b3)–H(4b3)	126.5
C(2m1)–C(2a3)–N(22)	125.0(4)	C(4a3)–C(4b3)–H(4b3)	126.5
C(2m1)–C(2a3)–C(2b3)	124.2(4)	C(4b3)–C(4b4)–C(4a4)	107.4(4)
N(22)–C(2a3)–C(2b3)	110.5(3)	C(4b3)–C(4b4)–H(4b4)	126.3
N(22)–C(2a4)–C(2m2)	124.5(4)	C(4a4)–C(4b4)–H(4b4)	126.3
N(22)–C(2a4)–C(2b4)	110.7(3)	C(4b6)–C(4b5)–C(4a5)	107.2(4)
C(2m2)–C(2a4)–C(2b4)	124.5(4)	C(4b6)–C(4b5)–H(4b5)	126.4
N(23)–C(2a5)–C(2m2)	124.8(4)	C(4a5)–C(4b5)–H(4b5)	126.4
N(23)–C(2a5)–C(2b5)	110.3(4)	C(4b5)–C(4b6)–C(4a6)	106.9(4)
C(2m2)–C(2a5)–C(2b5)	124.3(4)	C(4b5)–C(4b6)–H(4b6)	126.6
N(23)–C(2a6)–C(2m3)	124.7(4)	C(4a6)–C(4b6)–H(4b6)	126.6
N(23)–C(2a6)–C(2b6)	109.2(4)	C(4b8)–C(4b7)–C(4a7)	107.8(4)
C(2m3)–C(2a6)–C(2b6)	125.8(4)	C(4b8)–C(4b7)–H(4b7)	126.1
N(24)–C(2a7)–C(2m3)	125.1(4)	C(4a7)–C(4b7)–H(4b7)	126.1
N(24)–C(2a7)–C(2b7)	110.0(3)	C(4b7)–C(4b8)–C(4a8)	106.9(4)
C(2m3)–C(2a7)–C(2b7)	124.7(4)	C(4b7)–C(4b8)–H(4b8)	126.6
N(24)–C(2a8)–C(2m4)	125.0(4)	C(4a8)–C(4b8)–H(4b8)	126.6
N(24)–C(2a8)–C(2b8)	110.0(3)	C(4a2)–C(4m1)–C(4a3)	124.9(4)
C(2m4)–C(2a8)–C(2b8)	124.6(4)	C(4a2)–C(4m1)–C(411)	119.7(4)
C(2b2)–C(2b1)–C(2a1)	106.7(4)	C(4a3)–C(4m1)–C(411)	115.4(4)
C(2b2)–C(2b1)–H(2b1)	126.7	C(4a4)–C(4m2)–C(4a5)	125.0(3)
C(2a1)–C(2b1)–H(2b1)	126.7	C(4a4)–C(4m2)–C(421)	117.4(3)
C(2b1)–C(2b2)–C(2a2)	107.2(3)	C(4a5)–C(4m2)–C(421)	117.6(3)
C(2b1)–C(2b2)–H(2b2)	126.4	C(4a7)–C(4m3)–C(4a6)	125.2(4)
C(2a2)–C(2b2)–H(2b2)	126.4	C(4a7)–C(4m3)–C(431)	117.0(3)
C(2b4)–C(2b3)–C(2a3)	106.7(3)	C(4a6)–C(4m3)–C(431)	117.7(3)
C(2b4)–C(2b3)–H(2b3)	126.6	C(4a1)–C(4m4)–C(4a8)	125.4(4)

Table S4. Continued

angle	degree	angle	degree
C(2a3)–C(2b3)–H(2b3)	126.6	C(4a1)–C(4m4)–C(441)	118.4(4)
C(2b3)–C(2b4)–C(2a4)	107.0(4)	C(4a8)–C(4m4)–C(441)	116.2(4)
C(2b3)–C(2b4)–H(2b4)	126.5	C(416)–C(411)–C(412)	120.3(4)
C(2a4)–C(2b4)–H(2b4)	126.5	C(416)–C(411)–C(4m1)	120.7(4)
C(2b6)–C(2b5)–C(2a5)	106.6(4)	C(412)–C(411)–C(4m1)	119.0(4)
C(2b6)–C(2b5)–H(2b5)	126.7	C(413)–C(412)–C(411)	117.6(5)
C(2a5)–C(2b5)–H(2b5)	126.7	C(413)–C(412)–C(417)	121.9(5)
C(2b5)–C(2b6)–C(2a6)	107.9(4)	C(411)–C(412)–C(417)	120.5(4)
C(2b5)–C(2b6)–H(2b6)	126.1	C(414)–C(413)–C(412)	123.5(5)
C(2a6)–C(2b6)–H(2b6)	126.1	C(414)–C(413)–H(413)	118.2
C(2b8)–C(2b7)–C(2a7)	107.4(4)	C(412)–C(413)–H(413)	118.2
C(2b8)–C(2b7)–H(2b7)	126.3	C(413)–C(414)–C(415)	117.8(5)
C(2a7)–C(2b7)–H(2b7)	126.3	C(413)–C(414)–C(418)	123.6(6)
C(2b7)–C(2b8)–C(2a8)	106.8(4)	C(415)–C(414)–C(418)	118.6(6)
C(2b7)–C(2b8)–H(2b8)	126.6	C(414)–C(415)–C(416)	122.1(5)
C(2a8)–C(2b8)–H(2b8)	126.6	C(414)–C(415)–H(415)	118.9
C(2a3)–C(2m1)–C(2a2)	124.1(4)	C(416)–C(415)–H(415)	118.9
C(2a3)–C(2m1)–C(211)	117.0(4)	C(411)–C(416)–C(415)	118.6(5)
C(2a2)–C(2m1)–C(211)	118.8(3)	C(411)–C(416)–C(419)	120.7(4)
C(2a5)–C(2m2)–C(2a4)	122.5(4)	C(415)–C(416)–C(419)	120.6(5)
C(2a5)–C(2m2)–C(221)	121.0(4)	C(412)–C(417)–H(4d7)	109.5
C(2a4)–C(2m2)–C(221)	116.3(4)	C(412)–C(417)–H(4e7)	109.5
C(2a6)–C(2m3)–C(2a7)	123.7(4)	H(4d7)–C(417)–H(4e7)	109.5
C(2a6)–C(2m3)–C(231)	119.0(3)	C(412)–C(417)–H(4f7)	109.5
C(2a7)–C(2m3)–C(231)	117.3(4)	H(4d7)–C(417)–H(4f7)	109.5
C(2a1)–C(2m4)–C(2a8)	122.3(4)	H(4e7)–C(417)–H(4f7)	109.5
C(2a1)–C(2m4)–C(241)	120.0(3)	C(414)–C(418)–H(4d8)	109.5
C(2a8)–C(2m4)–C(241)	117.5(3)	C(414)–C(418)–H(4e8)	109.5
C(216)–C(211)–C(212)	121.1(4)	H(4d8)–C(418)–H(4e8)	109.5
C(216)–C(211)–C(2m1)	120.5(4)	C(414)–C(418)–H(4f8)	109.5
C(212)–C(211)–C(2m1)	118.3(3)	H(4d8)–C(418)–H(4f8)	109.5
C(213)–C(212)–C(211)	118.6(4)	H(4e8)–C(418)–H(4f8)	109.5
C(213)–C(212)–C(217)	121.3(4)	C(416)–C(419)–H(4d9)	109.5
C(211)–C(212)–C(217)	120.1(4)	C(416)–C(419)–H(4e9)	109.5

Table S4. Continued

angle	degree	angle	degree
C(212)–C(213)–C(214)	121.9(4)	H(4d9)–C(419)–H(4e9)	109.5
C(212)–C(213)–H(213)	119.0	C(416)–C(419)–H(4f9)	109.5
C(214)–C(213)–H(213)	119.0	H(4d9)–C(419)–H(4f9)	109.5
C(213)–C(214)–C(215)	118.2(4)	H(4e9)–C(419)–H(4f9)	109.5
C(213)–C(214)–C(218)	121.2(4)	C(426)–C(421)–C(422)	120.7(4)
C(215)–C(214)–C(218)	120.6(4)	C(426)–C(421)–C(4m2)	120.2(4)
C(214)–C(215)–C(216)	121.3(4)	C(422)–C(421)–C(4m2)	119.1(4)
C(214)–C(215)–H(215)	119.3	C(423)–C(422)–C(421)	117.8(4)
C(216)–C(215)–H(215)	119.3	C(423)–C(422)–C(427)	121.0(4)
C(211)–C(216)–C(215)	118.8(4)	C(421)–C(422)–C(427)	121.3(4)
C(211)–C(216)–C(219)	121.3(4)	C(424)–C(423)–C(422)	122.6(4)
C(215)–C(216)–C(219)	119.9(4)	C(424)–C(423)–H(423)	118.7
C(212)–C(217)–H(2d7)	109.5	C(422)–C(423)–H(423)	118.7
C(212)–C(217)–H(2e7)	109.5	C(425)–C(424)–C(423)	118.4(4)
H(2d7)–C(217)–H(2e7)	109.5	C(425)–C(424)–C(428)	121.4(4)
C(212)–C(217)–H(2f7)	109.5	C(423)–C(424)–C(428)	120.1(4)
H(2d7)–C(217)–H(2f7)	109.5	C(424)–C(425)–C(426)	122.1(4)
H(2e7)–C(217)–H(2f7)	109.5	C(424)–C(425)–H(425)	118.9
C(214)–C(218)–H(2d8)	109.5	C(426)–C(425)–H(425)	118.9
C(214)–C(218)–H(2e8)	109.5	C(421)–C(426)–C(425)	118.3(4)
H(2d8)–C(218)–H(2e8)	109.5	C(421)–C(426)–C(429)	121.8(4)
C(214)–C(218)–H(2f8)	109.5	C(425)–C(426)–C(429)	119.9(4)
H(2d8)–C(218)–H(2f8)	109.5	C(422)–C(427)–H(4g7)	109.5
H(2e8)–C(218)–H(2f8)	109.5	C(422)–C(427)–H(4h7)	109.5
C(216)–C(219)–H(2d9)	109.5	H(4g7)–C(427)–H(4h7)	109.5
C(216)–C(219)–H(2e9)	109.5	C(422)–C(427)–H(4i7)	109.5
H(2d9)–C(219)–H(2e9)	109.5	H(4g7)–C(427)–H(4i7)	109.5
C(216)–C(219)–H(2f9)	109.5	H(4h7)–C(427)–H(4i7)	109.5
H(2d9)–C(219)–H(2f9)	109.5	C(424)–C(428)–H(4g8)	109.5
H(2e9)–C(219)–H(2f9)	109.5	C(424)–C(428)–H(4h8)	109.5
C(222)–C(221)–C(226)	120.1(4)	H(4g8)–C(428)–H(4h8)	109.5
C(222)–C(221)–C(2m2)	118.7(4)	C(424)–C(428)–H(4i8)	109.5
C(226)–C(221)–C(2m2)	121.0(4)	H(4g8)–C(428)–H(4i8)	109.5
C(221)–C(222)–C(223)	118.5(5)	H(4h8)–C(428)–H(4i8)	109.5

angle	degree	angle	degree
C(221)–C(222)–C(227)	121.1(5)	C(426)–C(429)–H(4g9)	109.5
C(223)–C(222)–C(227)	120.3(5)	C(426)–C(429)–H(4h9)	109.5
C(224)–C(223)–C(222)	123.0(5)	H(4g9)–C(429)–H(4h9)	109.5
C(224)–C(223)–H(223)	118.5	C(426)–C(429)–H(4i9)	109.5
C(222)–C(223)–H(223)	118.5	H(4g9)–C(429)–H(4i9)	109.5
C(223)–C(224)–C(225)	118.0(5)	H(4h9)–C(429)–H(4i9)	109.5
C(223)–C(224)–C(228)	123.1(6)	C(436)–C(431)–C(432)	120.2(4)
C(225)–C(224)–C(228)	118.8(5)	C(436)–C(431)–C(4m3)	119.5(4)
C(224)–C(225)–C(226)	121.3(5)	C(432)–C(431)–C(4m3)	120.3(4)
C(224)–C(225)–H(225)	119.4	C(433)–C(432)–C(431)	118.8(4)
C(226)–C(225)–H(225)	119.4	C(433)–C(432)–C(437)	120.5(4)
C(221)–C(226)–C(225)	119.2(5)	C(431)–C(432)–C(437)	120.7(4)
C(221)–C(226)–C(229)	121.5(4)	C(434)–C(433)–C(432)	122.2(4)
C(225)–C(226)–C(229)	119.3(4)	C(434)–C(433)–H(433)	118.9
C(222)–C(227)–H(2g7)	109.5	C(432)–C(433)–H(433)	118.9
C(222)–C(227)–H(2h7)	109.5	C(433)–C(434)–C(435)	117.9(4)
H(2g7)–C(227)–H(2h7)	109.5	C(433)–C(434)–C(438)	121.8(5)
C(222)–C(227)–H(2i7)	109.5	C(435)–C(434)–C(438)	120.3(4)
H(2g7)–C(227)–H(2i7)	109.5	C(434)–C(435)–C(436)	121.9(4)
H(2h7)–C(227)–H(2i7)	109.5	C(434)–C(435)–H(435)	119.0
C(224)–C(228)–H(2g8)	109.5	C(436)–C(435)–H(435)	119.0
C(224)–C(228)–H(2h8)	109.5	C(431)–C(436)–C(435)	119.0(4)
H(2g8)–C(228)–H(2h8)	109.5	C(431)–C(436)–C(439)	120.9(4)
C(224)–C(228)–H(2i8)	109.5	C(435)–C(436)–C(439)	120.1(4)
H(2g8)–C(228)–H(2i8)	109.5	C(432)–C(437)–H(4j7)	109.5
H(2h8)–C(228)–H(2i8)	109.5	C(432)–C(437)–H(4k7)	109.5
C(226)–C(229)–H(2g9)	109.5	H(4j7)–C(437)–H(4k7)	109.5
C(226)–C(229)–H(2h9)	109.5	C(432)–C(437)–H(4l7)	109.5
H(2g9)–C(229)–H(2h9)	109.5	H(4j7)–C(437)–H(4l7)	109.5
C(226)–C(229)–H(2i9)	109.5	H(4k7)–C(437)–H(4l7)	109.5
H(2g9)–C(229)–H(2i9)	109.5	C(434)–C(438)–H(4j8)	109.5
H(2h9)–C(229)–H(2i9)	109.5	C(434)–C(438)–H(4k8)	109.5
C(236)–C(231)–C(232)	119.8(4)	H(4j8)–C(438)–H(4k8)	109.5
C(236)–C(231)–C(2m3)	118.2(4)	C(434)–C(438)–H(4l8)	109.5

angle	degree	angle	degree
C(232)–C(231)–C(2m3)	121.9(4)	H(4j8)–C(438)–H(4l8)	109.5
C(233)–C(232)–C(231)	118.7(4)	H(4k8)–C(438)–H(4l8)	109.5
C(233)–C(232)–C(237)	121.2(4)	C(436)–C(439)–H(4j9)	109.5
C(231)–C(232)–C(237)	120.1(4)	C(436)–C(439)–H(4k9)	109.5
C(234)–C(233)–C(232)	122.7(4)	H(4j9)–C(439)–H(4k9)	109.5
C(234)–C(233)–H(233)	118.7	C(436)–C(439)–H(4l9)	109.5
C(232)–C(233)–H(233)	118.7	H(4j9)–C(439)–H(4l9)	109.5
C(233)–C(234)–C(235)	117.9(4)	H(4k9)–C(439)–H(4l9)	109.5
C(233)–C(234)–C(238)	121.6(4)	C(442)–C(441)–C(446)	120.6(4)
C(235)–C(234)–C(238)	120.5(5)	C(442)–C(441)–C(4m4)	120.0(4)
C(236)–C(235)–C(234)	121.5(4)	C(446)–C(441)–C(4m4)	119.3(4)
C(236)–C(235)–H(235)	119.3	C(441)–C(442)–C(443)	118.9(5)
C(234)–C(235)–H(235)	119.3	C(441)–C(442)–C(447)	120.9(4)
C(235)–C(236)–C(231)	119.4(4)	C(443)–C(442)–C(447)	120.2(5)
C(235)–C(236)–C(239)	119.5(4)	C(444)–C(443)–C(442)	122.0(5)
C(231)–C(236)–C(239)	121.1(4)	C(444)–C(443)–H(443)	119.0
C(232)–C(237)–H(2j7)	109.5	C(442)–C(443)–H(443)	119.0
C(232)–C(237)–H(2k7)	109.5	C(443)–C(444)–C(445)	118.3(5)
H(2j7)–C(237)–H(2k7)	109.5	C(443)–C(444)–C(448)	121.7(6)
C(232)–C(237)–H(2l7)	109.5	C(445)–C(444)–C(448)	120.0(6)
H(2j7)–C(237)–H(2l7)	109.5	C(444)–C(445)–C(446)	122.1(5)
H(2k7)–C(237)–H(2l7)	109.5	C(444)–C(445)–H(445)	118.9
C(234)–C(238)–H(2j8)	109.5	C(446)–C(445)–H(445)	118.9
C(234)–C(238)–H(2k8)	109.5	C(445)–C(446)–C(441)	118.0(4)
H(2j8)–C(238)–H(2k8)	109.5	C(445)–C(446)–C(449)	120.8(5)
C(234)–C(238)–H(2l8)	109.5	C(441)–C(446)–C(449)	121.2(4)
H(2j8)–C(238)–H(2l8)	109.5	C(442)–C(447)–H(4m7)	109.5
H(2k8)–C(238)–H(2l8)	109.5	C(442)–C(447)–H(4n7)	109.5
C(236)–C(239)–H(2j9)	109.5	H(4m7)–C(447)–H(4n7)	109.5
C(236)–C(239)–H(2k9)	109.5	C(442)–C(447)–H(4p7)	109.5
H(2j9)–C(239)–H(2k9)	109.5	H(4m7)–C(447)–H(4p7)	109.5
C(236)–C(239)–H(2l9)	109.5	H(4n7)–C(447)–H(4p7)	109.5
H(2j9)–C(239)–H(2l9)	109.5	C(444)–C(448)–H(4m8)	109.5
H(2k9)–C(239)–H(2l9)	109.5	C(444)–C(448)–H(4n8)	109.5

Table S4. Continued

angle	degree	angle	degree
C(242)–C(241)–C(246)	119.1(4)	H(4m8)–C(448)–H(4n8)	109.5
C(242)–C(241)–C(2m4)	121.1(4)	C(444)–C(448)–H(4p8)	109.5
C(246)–C(241)–C(2m4)	119.7(4)	H(4m8)–C(448)–H(4p8)	109.5
C(241)–C(242)–C(243)	120.7(4)	H(4n8)–C(448)–H(4p8)	109.5
C(241)–C(242)–C(247)	120.9(4)	C(446)–C(449)–H(4m9)	109.5
C(243)–C(242)–C(247)	118.4(4)	C(446)–C(449)–H(4n9)	109.5
C(244)–C(243)–C(242)	121.2(4)	H(4m9)–C(449)–H(4n9)	109.5
C(244)–C(243)–H(243)	119.4	C(446)–C(449)–H(4p9)	109.5
C(242)–C(243)–H(243)	119.4	H(4m9)–C(449)–H(4p9)	109.5
C(245)–C(244)–C(243)	118.4(4)	H(4n9)–C(449)–H(4p9)	109.5
C(245)–C(244)–C(248)	121.6(4)	C(6s)–C(1s)–C(2s)	118.9(8)
C(243)–C(244)–C(248)	120.0(5)	C(6s)–C(1s)–C(7s)	120.9(7)
C(244)–C(245)–C(246)	122.0(4)	C(2s)–C(1s)–C(7s)	120.1(7)
C(244)–C(245)–H(245)	119.0	C(1s)–C(2s)–C(3s)	121.8(7)
C(246)–C(245)–H(245)	119.0	C(2s)–C(3s)–C(4s)	122.5(8)
C(241)–C(246)–C(245)	118.4(4)	C(5s)–C(4s)–C(3s)	112.7(8)
C(241)–C(246)–C(249)	121.5(4)	C(4s)–C(5s)–C(6s)	123.7(7)
C(245)–C(246)–C(249)	120.1(4)	C(1s)–C(6s)–C(5s)	120.3(7)
C(242)–C(247)–H(2m7)	109.5	C(9s)–Cl(1)–C(8s)	27.5(8)
C(242)–C(247)–H(2n7)	109.5	Cl(1)–C(8s)–Cl(2)	111.0(11)
H(2m7)–C(247)–H(2n7)	109.5	Cl(1)–C(9s)–Cl(3)	115.4(15)
C(242)–C(247)–H(2p7)	109.5	C(31s)–N(35s)–C(33s)	106.4
H(2m7)–C(247)–H(2p7)	109.5	N(35s)–C(31s)–N(36s)	108.7
H(2n7)–C(247)–H(2p7)	109.5	N(35s)–C(31s)–C(34s)	129.6
C(244)–C(248)–H(2m8)	109.5	N(36s)–C(31s)–C(34s)	121.6
C(244)–C(248)–H(2n8)	109.5	C(32s)–N(36s)–C(31s)	109.4
H(2m8)–C(248)–H(2n8)	109.5	C(33s)–C(32s)–N(36s)	105.5
C(244)–C(248)–H(2p8)	109.5	C(32s)–C(33s)–N(35s)	110.0
H(2m8)–C(248)–H(2p8)	109.5	O(2s)#1–C(2os)–O(2s)	58.3(15)
H(2n8)–C(248)–H(2p8)	109.5	O(2s)#1–O(2s)–C(2os)	60.9(8)
C(246)–C(249)–H(2m9)	109.5		
C(246)–C(249)–H(2n9)	109.5		

[a]The estimated standard deviations of the least significant digits are given in parentheses.

Table S5. Anisotropic Displacement Parameters (Å^2) for [Fe(TMP)(2-MeHIm)$_2$]$_2$·[Fe(TMP)-(2-MeHIm)]$_2$

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0189(3)	0.0182(3)	0.0183(3)	0.0008(2)	0.0014(2)	−0.0005(2)
N(11)	0.0156(15)	0.0192(16)	0.0216(18)	0.0001(14)	−0.0016(13)	−0.0005(12)
N(12)	0.0218(16)	0.0216(17)	0.0210(18)	0.0019(14)	0.0041(14)	0.0019(13)
N(13)	0.0232(17)	0.0200(16)	0.0202(18)	0.0022(14)	0.0025(14)	−0.0021(13)
N(14)	0.0219(17)	0.0214(17)	0.027(2)	0.0003(14)	0.0022(14)	−0.0024(13)
N(15)	0.0224(16)	0.0152(15)	0.0191(18)	0.0000(13)	0.0013(13)	−0.0017(13)
C(11)	0.024(2)	0.024(2)	0.024(2)	0.0028(17)	0.0064(17)	−0.0018(16)
N(16)	0.0182(16)	0.0315(18)	0.028(2)	−0.0023(15)	−0.0024(14)	0.0019(14)
C(12)	0.028(2)	0.031(2)	0.025(2)	0.0004(18)	−0.0066(18)	0.0001(17)
C(13)	0.031(2)	0.023(2)	0.024(2)	−0.0015(17)	−0.0015(18)	0.0016(17)
C(14)	0.025(2)	0.044(3)	0.037(3)	−0.008(2)	0.001(2)	0.0020(19)
N(17)	0.0190(16)	0.0342(19)	0.0216(19)	−0.0040(15)	0.0026(14)	−0.0030(14)
C(15)	0.025(2)	0.037(2)	0.028(2)	−0.0024(19)	0.0041(18)	0.0035(18)
N(18)	0.0239(18)	0.038(2)	0.033(2)	0.0060(17)	0.0000(16)	−0.0014(16)
C(16)	0.032(2)	0.047(3)	0.042(3)	0.015(2)	0.001(2)	0.002(2)
C(17)	0.028(2)	0.038(3)	0.039(3)	0.011(2)	0.001(2)	0.0026(19)
C(18)	0.024(2)	0.038(3)	0.061(3)	0.001(2)	−0.003(2)	0.0011(19)
C(1a1)	0.0195(19)	0.030(2)	0.023(2)	−0.0023(17)	−0.0003(16)	−0.0015(16)
C(1a2)	0.0147(17)	0.0203(19)	0.019(2)	0.0023(15)	−0.0007(15)	−0.0005(14)
C(1a3)	0.024(2)	0.0181(19)	0.025(2)	0.0036(16)	0.0007(17)	0.0029(15)
C(1a4)	0.0208(19)	0.0209(19)	0.022(2)	0.0016(16)	0.0033(16)	−0.0004(15)
C(1a5)	0.0203(19)	0.0222(19)	0.022(2)	0.0028(16)	0.0024(16)	−0.0008(15)
C(1a6)	0.025(2)	0.023(2)	0.016(2)	0.0000(16)	0.0011(16)	−0.0011(16)
C(1a7)	0.024(2)	0.0202(19)	0.030(2)	0.0018(17)	0.0006(18)	−0.0021(15)
C(1a8)	0.026(2)	0.026(2)	0.018(2)	−0.0075(17)	0.0022(16)	−0.0035(16)
C(1b1)	0.025(2)	0.032(2)	0.017(2)	−0.0037(17)	0.0030(17)	−0.0044(16)
C(1b2)	0.0204(19)	0.030(2)	0.022(2)	0.0045(17)	0.0042(16)	−0.0007(16)
C(1b3)	0.026(2)	0.021(2)	0.033(3)	0.0006(18)	0.0008(18)	−0.0007(16)
C(1b4)	0.033(2)	0.0173(19)	0.024(2)	−0.0004(16)	0.0027(18)	0.0025(16)
C(1b5)	0.035(2)	0.025(2)	0.032(3)	0.0055(19)	0.014(2)	0.0018(18)
C(1b6)	0.038(2)	0.024(2)	0.024(2)	0.0041(17)	0.0076(18)	−0.0026(18)
C(1b7)	0.036(2)	0.023(2)	0.035(3)	−0.0019(19)	0.005(2)	−0.0010(18)
C(1b8)	0.042(3)	0.029(2)	0.026(2)	−0.0081(19)	0.005(2)	−0.0070(19)
C(1m1)	0.0223(19)	0.0195(19)	0.022(2)	0.0016(16)	0.0012(16)	0.0005(15)

Table S5. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1m2)	0.0173(18)	0.028(2)	0.024(2)	0.0041(17)	0.0004(16)	0.0033(16)
C(1m3)	0.0210(19)	0.0217(19)	0.026(2)	0.0020(17)	0.0001(17)	−0.0017(15)
C(1m4)	0.026(2)	0.030(2)	0.029(2)	−0.0066(19)	0.0055(18)	−0.0019(17)
C(111)	0.023(2)	0.022(2)	0.022(2)	−0.0034(16)	0.0007(16)	−0.0010(16)
C(112)	0.0232(19)	0.023(2)	0.020(2)	−0.0037(16)	0.0023(16)	−0.0021(16)
C(113)	0.022(2)	0.029(2)	0.025(2)	−0.0090(18)	0.0053(17)	−0.0030(16)
C(114)	0.036(2)	0.022(2)	0.022(2)	−0.0044(17)	0.0130(18)	−0.0073(17)
C(115)	0.032(2)	0.0176(19)	0.021(2)	0.0023(16)	0.0077(17)	−0.0009(16)
C(116)	0.027(2)	0.022(2)	0.022(2)	0.0002(17)	0.0040(17)	−0.0008(16)
C(117)	0.029(2)	0.034(2)	0.031(3)	0.0013(19)	−0.0035(19)	0.0000(18)
C(118)	0.042(3)	0.031(2)	0.034(3)	0.002(2)	0.009(2)	−0.009(2)
C(119)	0.027(2)	0.030(2)	0.036(3)	0.0010(19)	−0.0072(19)	−0.0033(17)
C(121)	0.0208(19)	0.0160(18)	0.025(2)	0.0049(16)	0.0044(17)	0.0028(14)
C(122)	0.033(2)	0.030(2)	0.029(3)	0.0037(19)	0.0062(19)	0.0053(18)
C(123)	0.043(3)	0.040(3)	0.027(3)	−0.006(2)	0.008(2)	0.006(2)
C(124)	0.033(2)	0.033(2)	0.048(3)	−0.002(2)	0.016(2)	0.0045(19)
C(125)	0.025(2)	0.036(2)	0.048(3)	0.002(2)	0.011(2)	0.0071(18)
C(126)	0.022(2)	0.028(2)	0.034(3)	0.0049(18)	0.0050(18)	0.0048(16)
C(127)	0.039(3)	0.068(4)	0.029(3)	−0.008(2)	−0.007(2)	0.013(2)
C(128)	0.054(3)	0.074(4)	0.064(4)	−0.010(3)	0.023(3)	0.014(3)
C(129)	0.033(3)	0.061(3)	0.049(3)	−0.003(3)	−0.010(2)	0.000(2)
C(131)	0.030(2)	0.0212(19)	0.021(2)	0.0013(16)	0.0028(17)	−0.0001(16)
C(132)	0.030(2)	0.024(2)	0.027(2)	−0.0018(17)	0.0020(18)	−0.0018(17)
C(133)	0.031(2)	0.025(2)	0.023(2)	−0.0021(17)	0.0005(17)	0.0007(17)
C(134)	0.046(3)	0.0176(19)	0.021(2)	−0.0020(16)	0.0077(19)	0.0005(17)
C(135)	0.031(2)	0.021(2)	0.027(2)	−0.0037(17)	0.0069(18)	−0.0061(16)
C(136)	0.032(2)	0.021(2)	0.025(2)	−0.0056(17)	0.0031(18)	−0.0010(17)
C(137)	0.033(2)	0.025(2)	0.041(3)	0.0069(19)	−0.004(2)	−0.0036(18)
C(138)	0.058(3)	0.023(2)	0.034(3)	0.0062(19)	0.001(2)	0.001(2)
C(139)	0.029(2)	0.031(2)	0.039(3)	0.004(2)	0.005(2)	−0.0050(18)
C(141)	0.036(2)	0.036(2)	0.023(2)	−0.0073(19)	0.0055(19)	−0.0160(19)
C(142)	0.059(3)	0.047(3)	0.036(3)	−0.014(2)	0.011(3)	0.000(3)
C(143)	0.075(4)	0.078(4)	0.041(4)	−0.027(3)	0.016(3)	0.005(3)
C(144)	0.081(4)	0.070(4)	0.031(3)	−0.019(3)	0.010(3)	−0.025(3)

Table S5. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(145)	0.059(4)	0.077(4)	0.029(3)	−0.013(3)	−0.002(3)	−0.030(3)
C(146)	0.038(3)	0.058(3)	0.024(3)	−0.012(2)	0.002(2)	−0.028(2)
C(147)	0.062(4)	0.098(5)	0.056(4)	−0.021(4)	0.014(3)	0.037(4)
C(148)	0.106(6)	0.133(7)	0.042(4)	−0.047(4)	0.014(4)	−0.022(5)
C(149)	0.036(3)	0.090(4)	0.044(3)	−0.004(3)	−0.010(2)	−0.017(3)
Fe(2)	0.0177(3)	0.0178(3)	0.0186(3)	−0.0006(2)	0.0013(2)	−0.0001(2)
N(21)	0.0206(16)	0.0199(16)	0.0192(17)	−0.0031(14)	−0.0002(14)	−0.0022(13)
N(22)	0.0197(16)	0.0171(16)	0.0226(19)	−0.0028(13)	0.0005(14)	−0.0026(12)
N(23)	0.0226(17)	0.0247(17)	0.0216(19)	−0.0005(14)	0.0058(14)	−0.0062(13)
N(24)	0.0187(16)	0.0203(16)	0.0262(19)	0.0002(14)	0.0001(14)	−0.0025(13)
N(25)	0.0252(18)	0.042(2)	0.0205(19)	0.0004(16)	−0.0010(15)	0.0059(15)
C(21)	0.029(2)	0.072(4)	0.031(3)	0.002(3)	−0.006(2)	−0.016(2)
N(26)	0.0180(17)	0.054(2)	0.038(2)	0.0070(19)	−0.0055(16)	−0.0043(17)
C(22)	0.043(3)	0.059(3)	0.044(3)	0.012(3)	−0.009(2)	0.001(2)
C(23)	0.039(3)	0.058(3)	0.028(3)	0.002(2)	−0.004(2)	0.001(2)
C(24)	0.048(3)	0.060(4)	0.058(4)	0.001(3)	−0.004(3)	−0.006(3)
N(27)	0.0173(16)	0.0214(16)	0.029(2)	0.0019(14)	0.0002(14)	0.0000(13)
C(25)	0.027(2)	0.027(2)	0.032(2)	0.0059(19)	0.0090(19)	−0.0018(17)
N(28)	0.0140(16)	0.0347(19)	0.037(2)	0.0027(17)	−0.0053(15)	0.0038(14)
C(26)	0.031(2)	0.037(2)	0.028(2)	−0.005(2)	−0.0070(19)	0.0004(19)
C(27)	0.033(2)	0.033(2)	0.025(2)	−0.0009(19)	−0.0061(19)	0.0005(18)
C(28)	0.025(2)	0.046(3)	0.039(3)	0.004(2)	0.000(2)	0.005(2)
C(2a1)	0.0199(18)	0.0224(19)	0.019(2)	−0.0016(16)	−0.0021(16)	0.0009(15)
C(2a2)	0.0207(19)	0.0219(19)	0.024(2)	0.0014(16)	−0.0009(16)	−0.0024(15)
C(2a3)	0.0200(19)	0.0219(19)	0.024(2)	0.0037(16)	0.0013(16)	0.0017(15)
C(2a4)	0.0162(18)	0.026(2)	0.023(2)	0.0007(17)	−0.0014(16)	−0.0006(15)
C(2a5)	0.025(2)	0.025(2)	0.024(2)	−0.0032(17)	0.0020(17)	−0.0048(16)
C(2a6)	0.028(2)	0.0159(18)	0.028(2)	0.0005(17)	0.0026(18)	−0.0004(15)
C(2a7)	0.023(2)	0.024(2)	0.022(2)	0.0051(17)	0.0046(17)	−0.0028(16)
C(2a8)	0.0213(19)	0.024(2)	0.019(2)	−0.0014(16)	0.0025(16)	−0.0004(15)
C(2b1)	0.028(2)	0.022(2)	0.023(2)	−0.0024(17)	−0.0001(17)	0.0036(16)
C(2b2)	0.028(2)	0.0204(19)	0.029(2)	−0.0025(17)	0.0015(18)	−0.0020(16)
C(2b3)	0.0176(18)	0.0199(18)	0.022(2)	−0.0006(16)	0.0040(16)	−0.0011(14)
C(2b4)	0.025(2)	0.0222(19)	0.018(2)	−0.0024(16)	0.0007(16)	−0.0004(16)

Table S5. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(2b5)	0.043(3)	0.026(2)	0.029(3)	$-0.0090(19)$	0.012(2)	$-0.0077(19)$
C(2b6)	0.036(2)	0.021(2)	0.028(2)	$-0.0037(17)$	0.0081(19)	$-0.0060(17)$
C(2b7)	0.027(2)	0.028(2)	0.026(2)	$-0.0021(18)$	0.0048(18)	$-0.0001(17)$
C(2b8)	0.0194(19)	0.031(2)	0.026(2)	0.0008(18)	0.0028(17)	$-0.0013(16)$
C(2m1)	0.0233(19)	0.0179(19)	0.023(2)	$-0.0004(16)$	$-0.0011(16)$	$-0.0016(15)$
C(2m2)	0.027(2)	0.0208(19)	0.020(2)	$-0.0019(17)$	0.0045(17)	$-0.0021(15)$
C(2m3)	0.023(2)	0.022(2)	0.030(2)	0.0007(17)	0.0040(17)	$-0.0013(16)$
C(2m4)	0.0182(18)	0.0221(19)	0.023(2)	$-0.0019(16)$	$-0.0028(16)$	0.0033(15)
C(211)	0.025(2)	0.022(2)	0.023(2)	$-0.0034(16)$	0.0013(17)	$-0.0009(16)$
C(212)	0.027(2)	0.024(2)	0.019(2)	$-0.0055(16)$	0.0004(17)	$-0.0020(16)$
C(213)	0.023(2)	0.028(2)	0.027(2)	$-0.0045(18)$	$-0.0021(17)$	$-0.0043(17)$
C(214)	0.038(2)	0.024(2)	0.022(2)	0.0001(17)	0.0046(18)	$-0.0051(18)$
C(215)	0.031(2)	0.023(2)	0.022(2)	0.0016(17)	0.0006(17)	$-0.0024(17)$
C(216)	0.035(2)	0.0175(19)	0.022(2)	$-0.0026(16)$	0.0064(18)	$-0.0046(16)$
C(217)	0.027(2)	0.029(2)	0.027(2)	$-0.0004(18)$	$-0.0020(18)$	0.0014(17)
C(218)	0.049(3)	0.031(2)	0.039(3)	$-0.001(2)$	0.005(2)	$-0.017(2)$
C(219)	0.033(2)	0.028(2)	0.025(2)	0.0033(18)	$-0.0039(18)$	$-0.0014(18)$
C(221)	0.035(2)	0.028(2)	0.028(2)	$-0.0054(19)$	0.0023(19)	$-0.0093(18)$
C(222)	0.038(3)	0.057(3)	0.034(3)	$-0.015(2)$	0.002(2)	$-0.011(2)$
C(223)	0.048(3)	0.086(4)	0.028(3)	$-0.016(3)$	$-0.007(2)$	$-0.014(3)$
C(224)	0.057(3)	0.055(3)	0.033(3)	$-0.016(2)$	0.005(3)	$-0.015(3)$
C(225)	0.053(3)	0.032(2)	0.032(3)	$-0.008(2)$	0.012(2)	$-0.006(2)$
C(226)	0.042(3)	0.027(2)	0.034(3)	$-0.002(2)$	0.011(2)	$-0.0027(19)$
C(227)	0.034(3)	0.128(6)	0.043(3)	$-0.022(4)$	$-0.006(3)$	$-0.004(3)$
C(228)	0.077(4)	0.091(5)	0.037(3)	$-0.030(3)$	0.007(3)	$-0.014(4)$
C(229)	0.059(3)	0.076(4)	0.034(3)	$-0.002(3)$	0.006(3)	0.034(3)
C(231)	0.034(2)	0.0197(19)	0.026(2)	$-0.0062(17)$	0.0081(18)	$-0.0004(16)$
C(232)	0.038(2)	0.027(2)	0.024(2)	$-0.0035(18)$	0.0103(19)	0.0016(18)
C(233)	0.045(3)	0.023(2)	0.036(3)	$-0.0083(19)$	0.021(2)	$-0.0075(19)$
C(234)	0.053(3)	0.022(2)	0.029(3)	$-0.0016(18)$	0.016(2)	0.0051(19)
C(235)	0.048(3)	0.024(2)	0.030(3)	0.0002(18)	0.006(2)	0.0112(19)
C(236)	0.038(2)	0.024(2)	0.026(2)	$-0.0029(18)$	0.0076(19)	0.0043(18)
C(237)	0.030(2)	0.036(2)	0.047(3)	$-0.004(2)$	0.006(2)	$-0.0131(19)$
C(238)	0.073(4)	0.030(2)	0.044(3)	0.005(2)	0.007(3)	$-0.006(2)$

Table S5. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(239)	0.032(2)	0.033(2)	0.043(3)	0.007(2)	−0.004(2)	−0.0026(19)
C(241)	0.024(2)	0.0218(19)	0.026(2)	0.0037(17)	0.0047(17)	0.0021(15)
C(242)	0.024(2)	0.044(3)	0.030(3)	−0.005(2)	−0.0031(18)	0.0091(19)
C(243)	0.038(3)	0.050(3)	0.023(2)	−0.010(2)	−0.003(2)	0.006(2)
C(244)	0.024(2)	0.040(3)	0.042(3)	−0.010(2)	0.009(2)	0.0057(19)
C(245)	0.020(2)	0.031(2)	0.049(3)	−0.012(2)	0.005(2)	0.0009(17)
C(246)	0.022(2)	0.022(2)	0.035(3)	−0.0057(18)	−0.0008(18)	−0.0003(16)
C(247)	0.029(2)	0.065(3)	0.028(3)	−0.007(2)	−0.005(2)	0.018(2)
C(248)	0.048(3)	0.077(4)	0.051(4)	−0.022(3)	0.011(3)	0.014(3)
C(249)	0.028(2)	0.032(2)	0.038(3)	0.003(2)	−0.001(2)	0.0042(18)
Fe(3)	0.0325(3)	0.0257(3)	0.0285(4)	0.0053(3)	−0.0086(3)	−0.0063(3)
N(31)	0.035(2)	0.0232(17)	0.0219(19)	0.0021(15)	−0.0105(15)	−0.0053(15)
N(32)	0.043(2)	0.0231(18)	0.028(2)	0.0041(15)	−0.0152(17)	−0.0107(15)
N(33)	0.0275(17)	0.0205(16)	0.0239(19)	0.0060(14)	−0.0052(15)	−0.0018(14)
N(34)	0.0300(18)	0.0210(17)	0.0229(19)	0.0029(14)	−0.0073(15)	−0.0043(14)
C(3a1)	0.027(2)	0.022(2)	0.026(2)	0.0025(17)	−0.0022(17)	−0.0007(16)
C(3a2)	0.026(2)	0.022(2)	0.036(3)	0.0060(18)	−0.0117(19)	−0.0019(16)
C(3a3)	0.037(2)	0.025(2)	0.031(3)	0.0041(19)	−0.012(2)	−0.0113(18)
C(3a4)	0.032(2)	0.031(2)	0.023(2)	0.0103(18)	−0.0055(18)	−0.0088(18)
C(3a5)	0.027(2)	0.024(2)	0.019(2)	0.0025(16)	0.0013(16)	−0.0059(16)
C(3a6)	0.0217(19)	0.0202(19)	0.027(2)	−0.0006(17)	−0.0041(17)	−0.0037(15)
C(3a7)	0.026(2)	0.025(2)	0.027(2)	0.0008(17)	−0.0055(17)	−0.0030(16)
C(3a8)	0.025(2)	0.023(2)	0.031(2)	0.0078(18)	−0.0071(18)	−0.0014(16)
C(3b1)	0.0221(19)	0.0221(19)	0.029(2)	0.0056(17)	−0.0084(17)	−0.0053(15)
C(3b2)	0.022(2)	0.025(2)	0.027(2)	−0.0016(17)	−0.0076(17)	−0.0014(16)
C(3b3)	0.047(3)	0.024(2)	0.035(3)	0.0080(19)	−0.015(2)	−0.0161(19)
C(3b4)	0.043(3)	0.027(2)	0.030(3)	0.0086(19)	−0.011(2)	−0.0121(19)
C(3b5)	0.031(2)	0.028(2)	0.020(2)	0.0020(17)	−0.0088(17)	−0.0016(17)
C(3b6)	0.023(2)	0.031(2)	0.021(2)	−0.0008(18)	−0.0056(17)	−0.0021(16)
C(3b7)	0.034(2)	0.0182(19)	0.035(3)	0.0048(18)	−0.0041(19)	−0.0067(17)
C(3b8)	0.036(2)	0.020(2)	0.029(2)	0.0099(17)	−0.0096(19)	−0.0063(17)
C(3m1)	0.032(2)	0.024(2)	0.034(3)	0.0036(18)	−0.0149(19)	−0.0081(17)
C(3m2)	0.031(2)	0.026(2)	0.018(2)	0.0068(17)	−0.0050(17)	−0.0057(16)
C(3m3)	0.0214(19)	0.0215(19)	0.026(2)	0.0004(17)	−0.0019(17)	−0.0022(15)

Table S5. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(3m4)	0.025(2)	0.024(2)	0.024(2)	0.0025(17)	−0.0058(17)	−0.0042(16)
C(311)	0.039(2)	0.0178(19)	0.026(2)	0.0064(17)	−0.0140(19)	−0.0064(17)
C(312)	0.032(2)	0.029(2)	0.044(3)	0.005(2)	−0.015(2)	−0.0024(18)
C(313)	0.041(3)	0.021(2)	0.048(3)	0.001(2)	−0.009(2)	0.0038(19)
C(314)	0.042(3)	0.024(2)	0.031(3)	0.0056(19)	−0.013(2)	−0.0107(19)
C(315)	0.036(2)	0.026(2)	0.034(3)	0.0068(19)	−0.003(2)	−0.0079(18)
C(316)	0.040(3)	0.027(2)	0.035(3)	0.0006(19)	−0.003(2)	−0.0068(19)
C(317)	0.043(3)	0.030(3)	0.109(6)	−0.009(3)	−0.004(3)	−0.004(2)
C(318)	0.058(3)	0.029(2)	0.043(3)	−0.007(2)	−0.009(2)	−0.014(2)
C(319)	0.054(3)	0.044(3)	0.059(4)	−0.010(3)	0.012(3)	−0.013(2)
C(321)	0.037(2)	0.0171(19)	0.023(2)	0.0040(16)	−0.0085(18)	−0.0079(17)
C(322)	0.037(3)	0.049(3)	0.032(3)	0.011(2)	−0.002(2)	−0.010(2)
C(323)	0.053(3)	0.062(3)	0.034(3)	0.013(3)	−0.005(2)	−0.023(3)
C(324)	0.073(4)	0.048(3)	0.031(3)	0.020(2)	−0.019(3)	−0.025(3)
C(325)	0.051(3)	0.026(2)	0.044(3)	0.007(2)	−0.024(3)	−0.002(2)
C(326)	0.045(3)	0.024(2)	0.035(3)	0.0010(19)	−0.013(2)	−0.0061(19)
C(327)	0.037(3)	0.086(4)	0.058(4)	0.019(3)	0.012(3)	−0.001(3)
C(328)	0.100(5)	0.101(5)	0.049(4)	0.038(4)	−0.034(4)	−0.034(4)
C(329)	0.053(3)	0.045(3)	0.047(3)	−0.017(2)	−0.007(3)	0.020(2)
C(331)	0.032(2)	0.022(2)	0.018(2)	0.0045(16)	−0.0065(17)	−0.0032(17)
C(332)	0.030(2)	0.027(2)	0.020(2)	0.0012(17)	−0.0065(17)	−0.0046(17)
C(333)	0.032(2)	0.027(2)	0.027(2)	−0.0006(18)	−0.0031(19)	−0.0021(17)
C(334)	0.036(2)	0.029(2)	0.021(2)	0.0084(18)	−0.0115(18)	−0.0087(18)
C(335)	0.024(2)	0.027(2)	0.024(2)	0.0057(17)	−0.0014(17)	−0.0080(16)
C(336)	0.025(2)	0.025(2)	0.023(2)	0.0062(17)	−0.0053(17)	−0.0001(16)
C(337)	0.035(2)	0.032(2)	0.040(3)	−0.002(2)	0.004(2)	−0.0050(19)
C(338)	0.044(3)	0.031(2)	0.035(3)	0.000(2)	−0.010(2)	−0.014(2)
C(339)	0.030(2)	0.032(2)	0.030(3)	0.0037(19)	0.0023(19)	0.0027(18)
C(341)	0.031(2)	0.0206(19)	0.027(2)	0.0038(17)	−0.0050(18)	−0.0052(16)
C(342)	0.045(3)	0.030(2)	0.031(3)	0.008(2)	−0.004(2)	−0.008(2)
C(343)	0.060(3)	0.042(3)	0.027(3)	0.005(2)	−0.008(2)	−0.020(2)
C(344)	0.064(3)	0.030(2)	0.031(3)	0.008(2)	−0.028(3)	−0.023(2)
C(345)	0.045(3)	0.029(2)	0.055(4)	0.015(2)	−0.028(3)	−0.005(2)
C(346)	0.038(2)	0.024(2)	0.040(3)	0.007(2)	−0.016(2)	−0.0023(18)

Table S5. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(347)	0.049(3)	0.069(4)	0.049(4)	0.008(3)	0.017(3)	0.008(3)
C(348)	0.118(6)	0.052(3)	0.048(4)	0.023(3)	−0.053(4)	−0.029(4)
C(349)	0.040(3)	0.043(3)	0.058(4)	0.013(3)	0.003(3)	0.012(2)
Fe(4a)	0.0196(5)	0.0340(6)	0.0204(5)	0.0110(4)	0.0066(4)	0.0060(4)
Fe(4b)	0.0226(10)	0.0249(11)	0.0211(11)	0.0046(9)	0.0048(8)	0.0017(8)
N(41)	0.0267(18)	0.038(2)	0.024(2)	0.0078(16)	0.0107(15)	0.0112(15)
N(42)	0.0277(18)	0.0236(17)	0.0193(18)	0.0057(14)	0.0079(14)	0.0052(14)
N(43)	0.0242(18)	0.0339(19)	0.022(2)	0.0080(15)	0.0047(15)	0.0080(15)
N(44)	0.0229(17)	0.0294(18)	0.0242(19)	0.0055(15)	0.0086(14)	0.0057(14)
C(4a1)	0.027(2)	0.038(2)	0.026(2)	0.0058(19)	0.0062(18)	0.0092(18)
C(4a2)	0.028(2)	0.030(2)	0.025(2)	0.0097(18)	0.0095(18)	0.0100(17)
C(4a3)	0.031(2)	0.026(2)	0.018(2)	0.0041(17)	0.0058(17)	0.0043(17)
C(4a4)	0.0205(19)	0.0199(18)	0.019(2)	0.0021(16)	0.0014(16)	0.0025(15)
C(4a5)	0.023(2)	0.028(2)	0.020(2)	0.0047(17)	0.0062(16)	0.0027(16)
C(4a6)	0.024(2)	0.026(2)	0.027(2)	0.0024(18)	0.0070(17)	0.0037(16)
C(4a7)	0.027(2)	0.024(2)	0.017(2)	0.0034(17)	0.0058(17)	0.0014(16)
C(4a8)	0.026(2)	0.027(2)	0.024(2)	0.0021(17)	0.0061(17)	0.0050(17)
C(4b1)	0.031(2)	0.050(3)	0.034(3)	0.013(2)	0.011(2)	0.017(2)
C(4b2)	0.041(3)	0.046(3)	0.032(3)	0.020(2)	0.022(2)	0.018(2)
C(4b3)	0.029(2)	0.024(2)	0.014(2)	0.0030(16)	0.0033(17)	0.0020(16)
C(4b4)	0.025(2)	0.024(2)	0.022(2)	0.0004(17)	0.0009(17)	−0.0002(16)
C(4b5)	0.025(2)	0.035(2)	0.029(2)	0.0062(19)	0.0066(18)	0.0076(18)
C(4b6)	0.027(2)	0.037(2)	0.024(2)	0.0056(19)	0.0103(18)	0.0080(18)
C(4b7)	0.024(2)	0.026(2)	0.019(2)	0.0038(17)	0.0054(16)	−0.0019(16)
C(4b8)	0.026(2)	0.024(2)	0.023(2)	0.0013(17)	−0.0010(17)	0.0031(16)
C(4m1)	0.030(2)	0.032(2)	0.018(2)	0.0024(18)	0.0046(18)	0.0053(17)
C(4m2)	0.0213(19)	0.026(2)	0.021(2)	−0.0001(17)	0.0013(16)	0.0082(16)
C(4m3)	0.028(2)	0.029(2)	0.020(2)	0.0062(17)	0.0084(17)	0.0063(17)
C(4m4)	0.028(2)	0.030(2)	0.025(2)	0.0019(18)	0.0062(18)	0.0066(17)
C(411)	0.031(2)	0.035(2)	0.025(2)	0.0149(19)	0.0102(19)	0.0123(18)
C(412)	0.049(3)	0.039(3)	0.024(2)	0.004(2)	0.008(2)	0.020(2)
C(413)	0.069(4)	0.045(3)	0.029(3)	0.008(2)	0.015(3)	0.027(3)
C(414)	0.063(4)	0.072(4)	0.037(3)	0.021(3)	0.028(3)	0.032(3)
C(415)	0.043(3)	0.063(3)	0.042(3)	0.025(3)	0.021(2)	0.006(3)

Table S5. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(416)	0.036(3)	0.047(3)	0.036(3)	0.016(2)	0.011(2)	0.010(2)
C(417)	0.096(5)	0.031(3)	0.047(3)	−0.008(2)	0.009(3)	0.012(3)
C(418)	0.079(4)	0.106(5)	0.038(4)	0.023(4)	0.027(3)	0.026(4)
C(419)	0.057(3)	0.059(3)	0.052(4)	0.012(3)	0.006(3)	−0.021(3)
C(421)	0.0195(19)	0.029(2)	0.015(2)	0.0089(16)	0.0049(15)	0.0076(16)
C(422)	0.027(2)	0.031(2)	0.018(2)	0.0043(17)	0.0093(17)	0.0025(17)
C(423)	0.027(2)	0.032(2)	0.023(2)	0.0072(18)	0.0063(18)	0.0087(18)
C(424)	0.023(2)	0.038(2)	0.021(2)	0.0109(18)	0.0067(17)	0.0037(17)
C(425)	0.027(2)	0.047(3)	0.016(2)	0.0051(19)	−0.0010(17)	0.0002(19)
C(426)	0.022(2)	0.032(2)	0.018(2)	0.0046(17)	0.0052(16)	0.0029(16)
C(427)	0.032(2)	0.030(2)	0.032(3)	−0.0030(19)	0.003(2)	0.0058(18)
C(428)	0.031(2)	0.059(3)	0.035(3)	0.014(2)	0.004(2)	0.018(2)
C(429)	0.028(2)	0.036(2)	0.040(3)	−0.005(2)	0.000(2)	−0.0039(19)
C(431)	0.025(2)	0.027(2)	0.023(2)	0.0060(17)	0.0060(17)	0.0112(16)
C(432)	0.032(2)	0.032(2)	0.026(2)	0.0060(19)	0.0066(19)	0.0076(18)
C(433)	0.029(2)	0.037(2)	0.024(2)	0.0040(19)	0.0049(18)	0.0149(18)
C(434)	0.025(2)	0.045(3)	0.029(3)	0.015(2)	0.0040(19)	0.0162(19)
C(435)	0.029(2)	0.035(2)	0.038(3)	0.016(2)	0.006(2)	0.0064(18)
C(436)	0.020(2)	0.031(2)	0.032(2)	0.0085(18)	0.0053(18)	0.0089(17)
C(437)	0.058(3)	0.037(3)	0.042(3)	−0.002(2)	0.008(3)	−0.005(2)
C(438)	0.038(3)	0.064(3)	0.036(3)	0.024(3)	0.009(2)	0.011(2)
C(439)	0.033(2)	0.042(3)	0.043(3)	−0.008(2)	0.005(2)	−0.004(2)
C(441)	0.028(2)	0.034(2)	0.019(2)	0.0099(18)	0.0076(17)	0.0083(18)
C(442)	0.037(3)	0.036(2)	0.036(3)	0.008(2)	0.015(2)	0.011(2)
C(443)	0.051(3)	0.048(3)	0.046(3)	0.014(3)	0.017(3)	0.024(2)
C(444)	0.039(3)	0.072(4)	0.030(3)	0.021(3)	0.013(2)	0.029(3)
C(445)	0.023(2)	0.083(4)	0.028(3)	0.006(3)	0.0042(19)	0.006(2)
C(446)	0.024(2)	0.045(3)	0.034(3)	0.009(2)	0.0082(19)	0.0003(19)
C(447)	0.038(3)	0.042(3)	0.069(4)	−0.010(3)	0.012(3)	0.006(2)
C(448)	0.058(4)	0.133(6)	0.044(4)	0.020(4)	0.003(3)	0.059(4)
C(449)	0.036(3)	0.057(3)	0.060(4)	−0.005(3)	0.009(3)	−0.006(2)
C(1s)	0.098(5)	0.074(5)	0.050(4)	−0.024(3)	−0.024(4)	0.034(4)
C(2s)	0.132(7)	0.074(5)	0.069(5)	−0.017(4)	−0.039(5)	0.045(5)
C(3s)	0.157(9)	0.082(6)	0.063(5)	−0.006(4)	−0.055(6)	−0.004(6)

Table S5. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(4s)	0.131(7)	0.059(4)	0.078(5)	−0.023(4)	−0.041(5)	0.023(4)
C(5s)	0.099(6)	0.086(5)	0.054(4)	−0.012(4)	−0.001(4)	−0.001(4)
C(6s)	0.084(5)	0.075(4)	0.047(4)	−0.019(3)	−0.020(3)	0.027(4)
C(7s)	0.098(6)	0.082(5)	0.102(7)	−0.026(5)	−0.032(5)	0.029(4)
Cl(1)	0.060(2)	0.097(3)	0.122(4)	−0.016(3)	0.007(2)	0.0091(19)

[a]The estimated standard deviations of the least significant digits are given in parentheses. The anisotropic displacement factor exponent takes the form: -2π [h^2 U_{11} +...+ 2 h k a* b* U_{12}].

Table S6. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters ($\mathrm{\mathring{A}}^2$) for $[\mathrm{Fe(TMP)(2\text{-}MeHIm)_2}]_2 \cdot [\mathrm{Fe(TMP)(2\text{-}MeHIm)}]_2$

atom	x	y	z	U(eq)
H(16n)	0.0135	0.3977	0.3728	0.031
H(12)	0.0401	0.3668	0.3075	0.033
H(13)	0.0969	0.3536	0.3359	0.032
H(14a)	0.0530	0.3976	0.4825	0.053
H(14b)	0.0222	0.4145	0.4551	0.053
H(14c)	0.0581	0.4325	0.4553	0.053
H(14n)	0.2413	0.3706	0.5137	0.038
H(16)	0.2187	0.3153	0.5316	0.049
H(17)	0.1625	0.3144	0.4952	0.042
H(18a)	0.2013	0.4166	0.4260	0.061
H(18b)	0.2291	0.4217	0.4664	0.061
H(18c)	0.1909	0.4315	0.4767	0.061
H(1b1)	0.0751	0.3574	0.5990	0.030
H(1b2)	0.0613	0.3050	0.5575	0.029
H(1b3)	0.1105	0.2474	0.4015	0.032
H(1b4)	0.1541	0.2650	0.3432	0.030
H(1b5)	0.1940	0.3840	0.2819	0.037
H(1b6)	0.1736	0.4410	0.2989	0.034
H(1b7)	0.1264	0.4984	0.4562	0.038
H(1b8)	0.1161	0.4764	0.5379	0.039
H(113)	0.0003	0.2302	0.4642	0.030
H(115)	0.0774	0.1989	0.5455	0.028
H(1d7)	0.0390	0.2870	0.3988	0.047
H(1e7)	0.0248	0.3083	0.4426	0.047
H(1f7)	0.0025	0.2791	0.4197	0.047
H(1d8)	0.0236	0.1600	0.5047	0.053
H(1e8)	−0.0077	0.1836	0.5166	0.053
H(1f8)	0.0195	0.1756	0.5568	0.053
H(1d9)	0.1276	0.2291	0.5521	0.046
H(1e9)	0.1241	0.2689	0.5460	0.046
H(1f9)	0.1385	0.2466	0.5032	0.046
H(123)	0.1893	0.2915	0.1972	0.044
H(125)	0.2662	0.2892	0.2893	0.044
H(1g7)	0.1378	0.3153	0.2162	0.068

Table S6. Continued

atom	x	y	z	$U(\text{eq})$
H(1h7)	0.1386	0.3435	0.2567	0.068
H(1i7)	0.1265	0.3063	0.2693	0.068
H(1g8)	0.2476	0.2511	0.1906	0.096
H(1h8)	0.2772	0.2753	0.2081	0.096
H(1i8)	0.2512	0.2879	0.1685	0.096
H(1g9)	0.2597	0.3041	0.3688	0.071
H(1h9)	0.2232	0.3114	0.3900	0.071
H(1i9)	0.2444	0.3412	0.3666	0.071
H(133)	0.0873	0.5294	0.3041	0.032
H(135)	0.1866	0.5432	0.3259	0.032
H(1j7)	0.0587	0.4827	0.3319	0.049
H(1k7)	0.0715	0.4708	0.3832	0.049
H(1l7)	0.0807	0.4493	0.3369	0.049
H(1j8)	0.1344	0.5931	0.3082	0.058
H(1k8)	0.1158	0.5751	0.2647	0.058
H(1l8)	0.1558	0.5772	0.2657	0.058
H(1j9)	0.2086	0.4687	0.3649	0.049
H(1k9)	0.1988	0.4876	0.4132	0.049
H(1l9)	0.2188	0.5072	0.3724	0.049
H(143)	0.0509	0.4556	0.6647	0.078
H(145)	0.1418	0.4188	0.6952	0.066
H(1m7)	0.0275	0.4535	0.5877	0.109
H(1n7)	0.0357	0.4184	0.5625	0.109
H(1p7)	0.0535	0.4521	0.5444	0.109
H(1m8)	0.1108	0.4428	0.7579	0.141
H(1n8)	0.0708	0.4423	0.7523	0.141
H(1p8)	0.0915	0.4756	0.7398	0.141
H(1m9)	0.1731	0.3883	0.6396	0.085
H(1n9)	0.1743	0.4104	0.5921	0.085
H(1p9)	0.1548	0.3753	0.5925	0.085
H(26n)	0.2425	0.8475	0.7498	0.044
H(22)	0.2123	0.7970	0.7776	0.059
H(23)	0.1538	0.8061	0.7555	0.051
H(24a)	0.2064	0.8990	0.6745	0.083

atom	x	y	z	$U(\text{eq})$
H(24b)	0.2306	0.9049	0.7192	0.083
H(24c)	0.1922	0.9168	0.7214	0.083
H(28n)	0.0113	0.9019	0.6355	0.034
H(26)	0.0341	0.8676	0.5703	0.039
H(27)	0.0898	0.8492	0.5993	0.036
H(28a)	0.0494	0.8991	0.7440	0.055
H(28b)	0.0230	0.9214	0.7149	0.055
H(28c)	0.0616	0.9324	0.7172	0.055
H(2b1)	0.1418	0.7591	0.6018	0.030
H(2b2)	0.0979	0.7442	0.6618	0.031
H(2b3)	0.0552	0.8020	0.8194	0.024
H(2b4)	0.0714	0.8544	0.8618	0.026
H(2b5)	0.1192	0.9714	0.8019	0.039
H(2b6)	0.1287	0.9930	0.7204	0.034
H(2b7)	0.1735	0.9349	0.5631	0.032
H(2b8)	0.1914	0.8768	0.5448	0.031
H(213)	−0.0132	0.7362	0.7264	0.031
H(215)	0.0626	0.6961	0.8028	0.030
H(2d7)	0.0276	0.7918	0.6633	0.041
H(2e7)	0.0197	0.8134	0.7099	0.041
H(2f7)	−0.0081	0.7886	0.6888	0.041
H(2d8)	−0.0209	0.6912	0.7967	0.060
H(2e8)	0.0113	0.6675	0.8019	0.060
H(2f8)	−0.0079	0.6699	0.7520	0.060
H(2d9)	0.1260	0.7406	0.7587	0.043
H(2e9)	0.1153	0.7205	0.8056	0.043
H(2f9)	0.1145	0.7606	0.8053	0.043
H(223)	0.1404	0.9142	0.9587	0.065
H(225)	0.0474	0.9464	0.9295	0.046
H(2g7)	0.1561	0.8730	0.8534	0.103
H(2h7)	0.1733	0.8851	0.9020	0.103
H(2i7)	0.1749	0.9085	0.8558	0.103
H(2g8)	0.1037	0.9292	1.0233	0.103
H(2h8)	0.0647	0.9346	1.0119	0.103

atom	x	y	z	$U(\text{eq})$
H(2i8)	0.0903	0.9654	1.0073	0.103
H(2g9)	0.0512	0.9486	0.8117	0.085
H(2h9)	0.0250	0.9436	0.8544	0.085
H(2i9)	0.0372	0.9119	0.8239	0.085
H(233)	0.1884	1.0381	0.5925	0.041
H(235)	0.0916	1.0225	0.5595	0.041
H(2j7)	0.1961	0.9794	0.6810	0.057
H(2k7)	0.2179	1.0030	0.6469	0.057
H(2l7)	0.2111	0.9648	0.6324	0.057
H(2j8)	0.1412	1.0865	0.5654	0.073
H(2k8)	0.1189	1.0686	0.5255	0.073
H(2l8)	0.1589	1.0675	0.5219	0.073
H(2j9)	0.0631	0.9741	0.5815	0.054
H(2k9)	0.0707	0.9655	0.6361	0.054
H(2l9)	0.0850	0.9418	0.5948	0.054
H(243)	0.1828	0.8022	0.4494	0.044
H(245)	0.2514	0.7712	0.5445	0.040
H(2m7)	0.1189	0.8176	0.5252	0.061
H(2n7)	0.1315	0.8232	0.4717	0.061
H(2p7)	0.1370	0.8519	0.5107	0.061
H(2m8)	0.2606	0.7912	0.4444	0.088
H(2n8)	0.2296	0.7716	0.4212	0.088
H(2p8)	0.2537	0.7528	0.4581	0.088
H(2m9)	0.2163	0.8086	0.6451	0.049
H(2n9)	0.2465	0.7856	0.6267	0.049
H(2p9)	0.2110	0.7691	0.6392	0.049
H(3b1)	−0.0568	0.1250	0.3384	0.029
H(3b2)	−0.0475	0.1816	0.3038	0.030
H(3b3)	−0.0798	0.2422	0.1412	0.043
H(3b4)	−0.1108	0.2254	0.0691	0.040
H(3b5)	−0.1811	0.1181	0.0177	0.031
H(3b6)	−0.1949	0.0639	0.0549	0.030
H(3b7)	−0.1608	0.0020	0.2152	0.035
H(3b8)	−0.1268	0.0170	0.2858	0.034

Table S6. Continued

atom	x	y	z	$U(\text{eq})$
H(313)	−0.0732	0.2896	0.2923	0.044
H(315)	0.0158	0.2591	0.2386	0.038
H(3d7)	−0.1230	0.2593	0.2804	0.091
H(3e7)	−0.1185	0.2196	0.2747	0.091
H(3f7)	−0.1242	0.2425	0.2287	0.091
H(3d8)	0.0131	0.3032	0.3032	0.065
H(3e8)	−0.0226	0.3194	0.3148	0.065
H(3f8)	−0.0050	0.3264	0.2645	0.065
H(3d9)	0.0201	0.2123	0.1896	0.079
H(3e9)	−0.0132	0.1997	0.1633	0.079
H(3f9)	−0.0011	0.1819	0.2115	0.079
H(323)	−0.1098	0.1831	−0.0822	0.059
H(325)	−0.2004	0.2136	−0.0397	0.048
H(3g7)	−0.0771	0.1464	−0.0346	0.090
H(3h7)	−0.0909	0.1338	0.0158	0.090
H(3i7)	−0.0714	0.1688	0.0120	0.090
H(3g8)	−0.1492	0.2355	−0.1220	0.125
H(3h8)	−0.1855	0.2183	−0.1237	0.125
H(3i8)	−0.1533	0.1981	−0.1418	0.125
H(3g9)	−0.2124	0.1715	0.0537	0.072
H(3h9)	−0.2180	0.2098	0.0387	0.072
H(3i9)	−0.1915	0.2006	0.0794	0.072
H(333)	−0.1911	−0.0443	0.0639	0.034
H(335)	−0.2626	−0.0044	0.1480	0.030
H(3j7)	−0.1379	−0.0217	0.0564	0.054
H(3k7)	−0.1241	−0.0033	0.1031	0.054
H(3l7)	−0.1372	0.0184	0.0590	0.054
H(3j8)	−0.2558	−0.0598	0.0585	0.055
H(3k8)	−0.2753	−0.0538	0.1075	0.055
H(3l8)	−0.2438	−0.0785	0.1058	0.055
H(3j9)	−0.2547	0.0468	0.1881	0.046
H(3k9)	−0.2250	0.0709	0.1710	0.046
H(3l9)	−0.2190	0.0454	0.2141	0.046
H(343)	−0.1091	0.0510	0.4359	0.052

Table S6. Continued

atom	x	y	z	U(eq)
H(345)	−0.0248	0.0186	0.3728	0.051
H(3m7)	−0.1554	0.0702	0.3497	0.084
H(3n7)	−0.1353	0.1049	0.3481	0.084
H(3p7)	−0.1454	0.0887	0.3982	0.084
H(3m8)	−0.0685	0.0228	0.4834	0.109
H(3n8)	−0.0307	0.0229	0.4640	0.109
H(3p8)	−0.0547	−0.0084	0.4533	0.109
H(3m9)	−0.0446	0.0388	0.2578	0.071
H(3n9)	−0.0146	0.0270	0.2918	0.071
H(3l9)	−0.0204	0.0661	0.2815	0.071
H(4b1)	−0.2366	0.4179	0.6021	0.046
H(4b2)	−0.2178	0.3890	0.6759	0.048
H(4b3)	−0.1081	0.3218	0.7272	0.027
H(4b4)	−0.0541	0.3075	0.6879	0.029
H(4b5)	0.0019	0.3338	0.5210	0.036
H(4b6)	−0.0153	0.3662	0.4494	0.035
H(4b7)	−0.1227	0.4375	0.4018	0.028
H(4b8)	−0.1789	0.4470	0.4364	0.029
H(413)	−0.1677	0.3830	0.8269	0.057
H(415)	−0.2063	0.2962	0.7826	0.059
H(4d7)	−0.1574	0.4226	0.7278	0.087
H(4e7)	−0.1223	0.4031	0.7279	0.087
H(4f7)	−0.1367	0.4187	0.7763	0.087
H(4d8)	−0.2249	0.3290	0.8623	0.111
H(4e8)	−0.1923	0.3465	0.8845	0.111
H(4f8)	−0.1914	0.3076	0.8706	0.111
H(4d9)	−0.2022	0.3084	0.6639	0.084
H(4e9)	−0.2043	0.2792	0.7029	0.084
H(4f9)	−0.1690	0.2885	0.6791	0.084
H(423)	0.0193	0.2390	0.6004	0.033
H(425)	0.0529	0.3189	0.6717	0.036
H(4g7)	−0.0376	0.2699	0.5333	0.047
H(4h7)	−0.0610	0.2668	0.5794	0.047
H(4i7)	−0.0351	0.2375	0.5667	0.047

Table S6. Continued

atom	x	y	z	$U(\text{eq})$
H(4h8)	0.0896	0.2596	0.6299	0.063
H(4h8)	0.0658	0.2320	0.6539	0.063
H(4i8)	0.0789	0.2633	0.6846	0.063
H(4g9)	0.0046	0.3785	0.6244	0.052
H(4h9)	0.0257	0.3705	0.6715	0.052
H(4i9)	−0.0143	0.3673	0.6721	0.052
H(433)	−0.0490	0.3895	0.2997	0.036
H(435)	−0.0150	0.4694	0.3727	0.040
H(4j7)	−0.0875	0.3516	0.3333	0.068
H(4k7)	−0.1060	0.3614	0.3819	0.068
H(4l7)	−0.0719	0.3402	0.3832	0.068
H(4j8)	0.0137	0.4391	0.2906	0.069
H(4k8)	−0.0141	0.4674	0.2822	0.069
H(4l8)	−0.0183	0.4313	0.2581	0.069
H(4j9)	−0.0647	0.4660	0.4666	0.059
H(4k9)	−0.0280	0.4785	0.4521	0.059
H(4l9)	−0.0325	0.4451	0.4831	0.059
H(443)	−0.2487	0.5124	0.4979	0.058
H(445)	−0.2896	0.4260	0.4535	0.054
H(4m7)	−0.1967	0.5143	0.5348	0.075
H(4n7)	−0.1721	0.4828	0.5291	0.075
H(4p7)	−0.1955	0.4859	0.5751	0.075
H(4m8)	−0.3147	0.4768	0.4282	0.117
H(4n8)	−0.2954	0.5116	0.4359	0.117
H(4p8)	−0.3191	0.4970	0.4770	0.117
H(4m9)	−0.2244	0.3737	0.4767	0.076
H(4n9)	−0.2639	0.3743	0.4665	0.076
H(4p9)	−0.2504	0.3734	0.5202	0.076

[a] $U(\text{eq})$ is defined as one third of the trace of the orthogonalized $\mathbf{U}_{ij}$ tensor the estimated standard deviations of the least significant digits are given in parentheses.

Captions for Supporting Information Figures

Figure S1. ORTEP diagram of [Fe(TMP)(2-MeHIm)] (mol 3) showing the two orientations of the imidazole ligand. The major (55%) orientation is drawn with heavy bonds, while the minor orientation is depicted with open bonds. 50% probability ellipsoids are depicted.
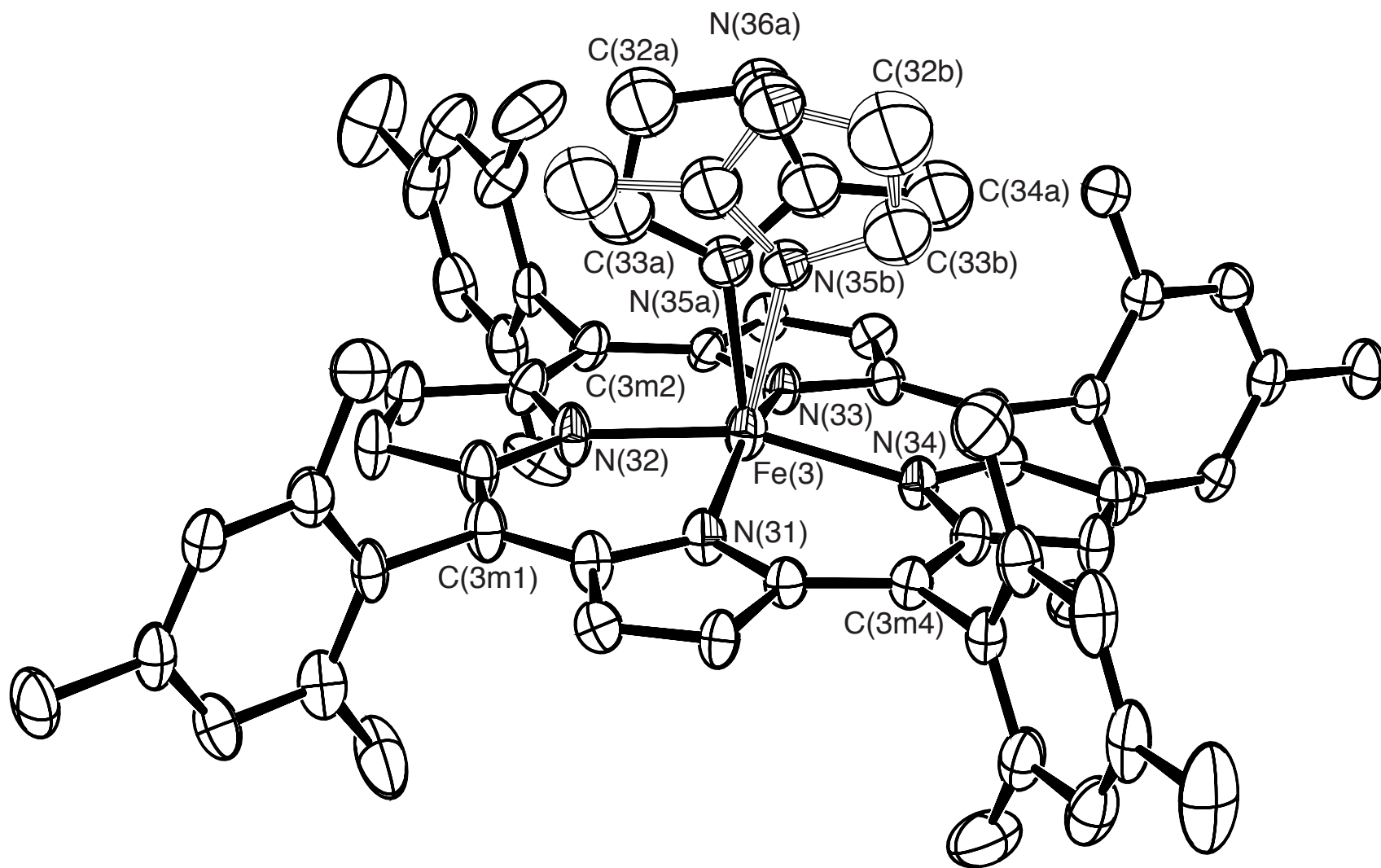
Figure S2. ORTEP diagram of [Fe(TMP)(2-MeHIm)] (mol 4) showing the two disordered parts of both iron and imidazole ligands. The major (68%) orientation is drawn with heavy bonds, while the minor orientation is depicted with open bonds. 50% probability ellipsoids are depicted.
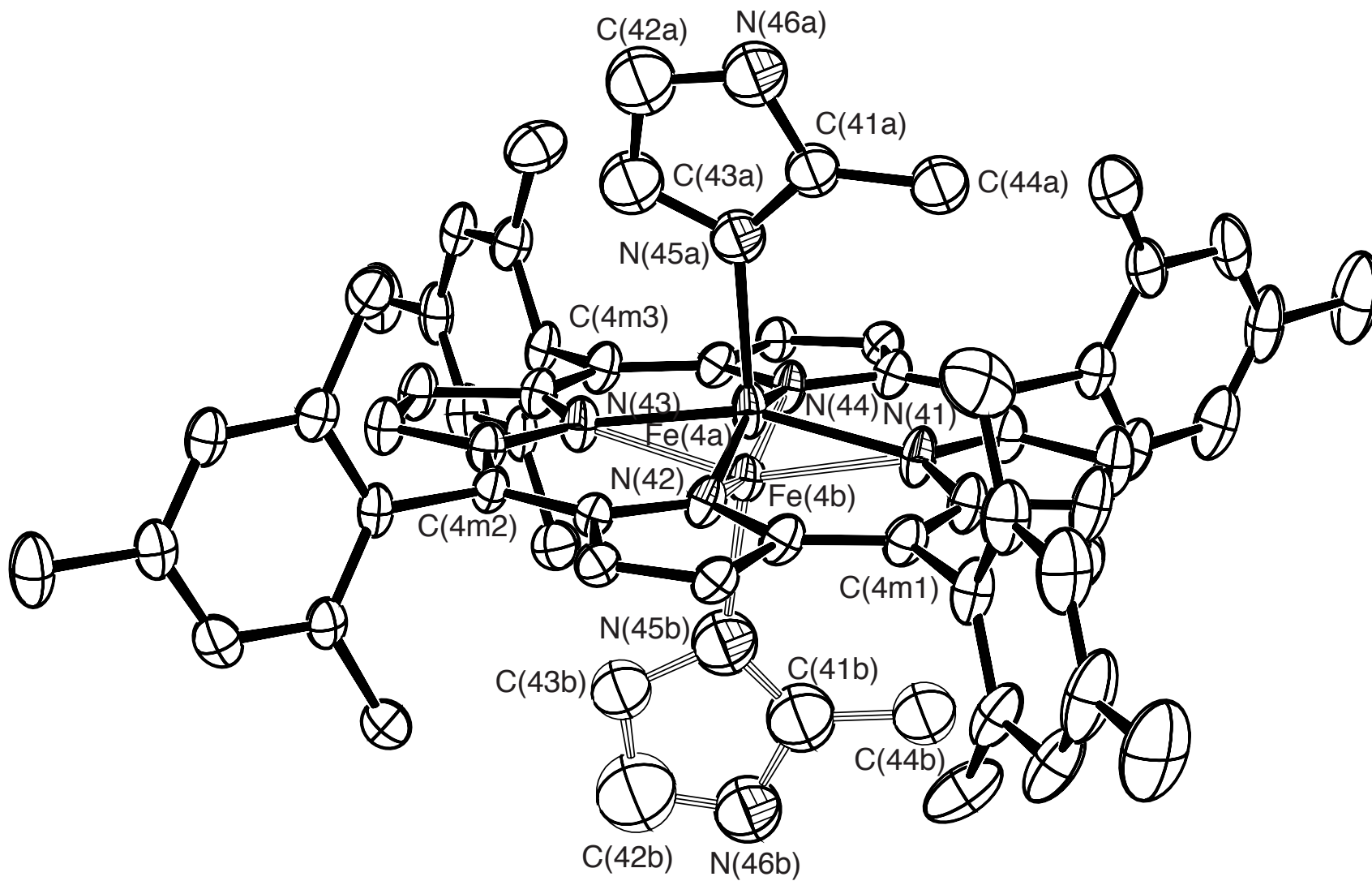
Figure S1

Figure S2