Supporting Information

2,5-Bis((*E*)-2-ferrocenylvinyl)-*N*,*N*,*N*′,*N*′-tetrapropylbenzene-1,4-diamine

Matthias Jochem, Igor Proz, Dieter Schollmeyer, and Heiner Detert *

[1] Johannes Gutenberg-Universität Mainz; *Correspondence: detert@uni-mainz.de

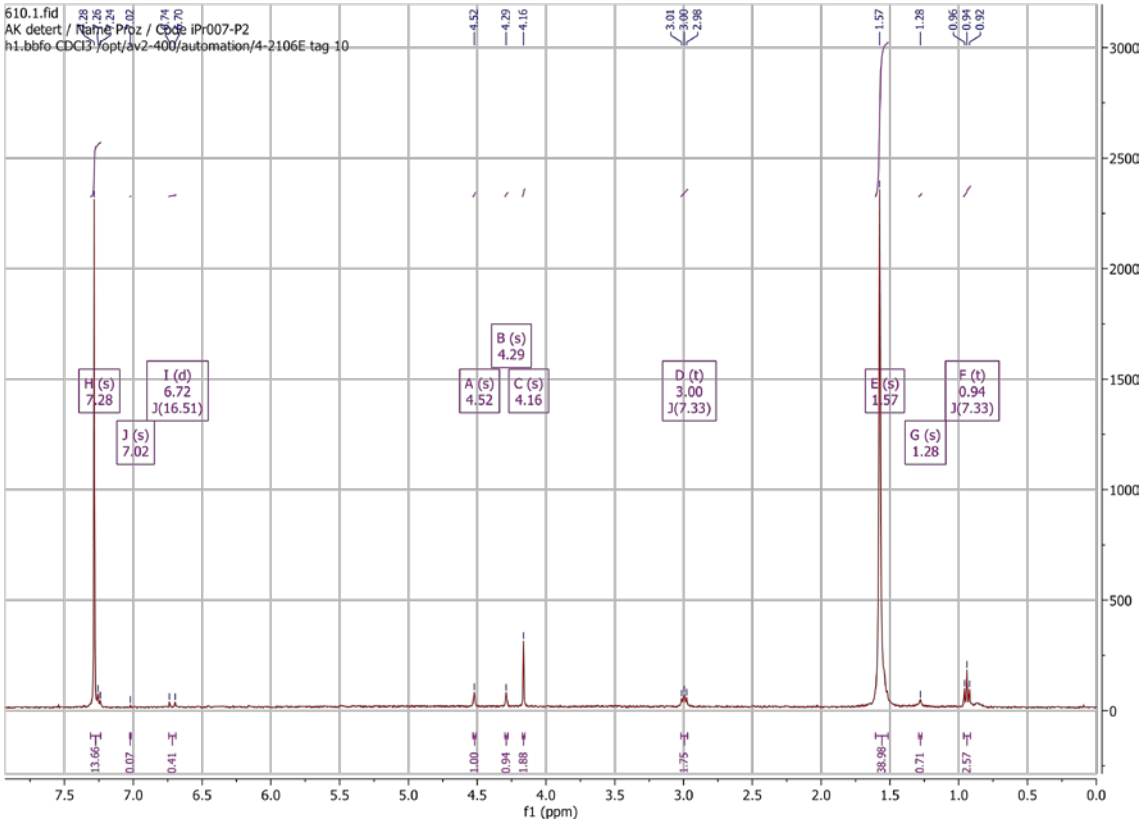

Figure S1: [1]H-NMR of **3** in $CDCl_3$, 400 MHz

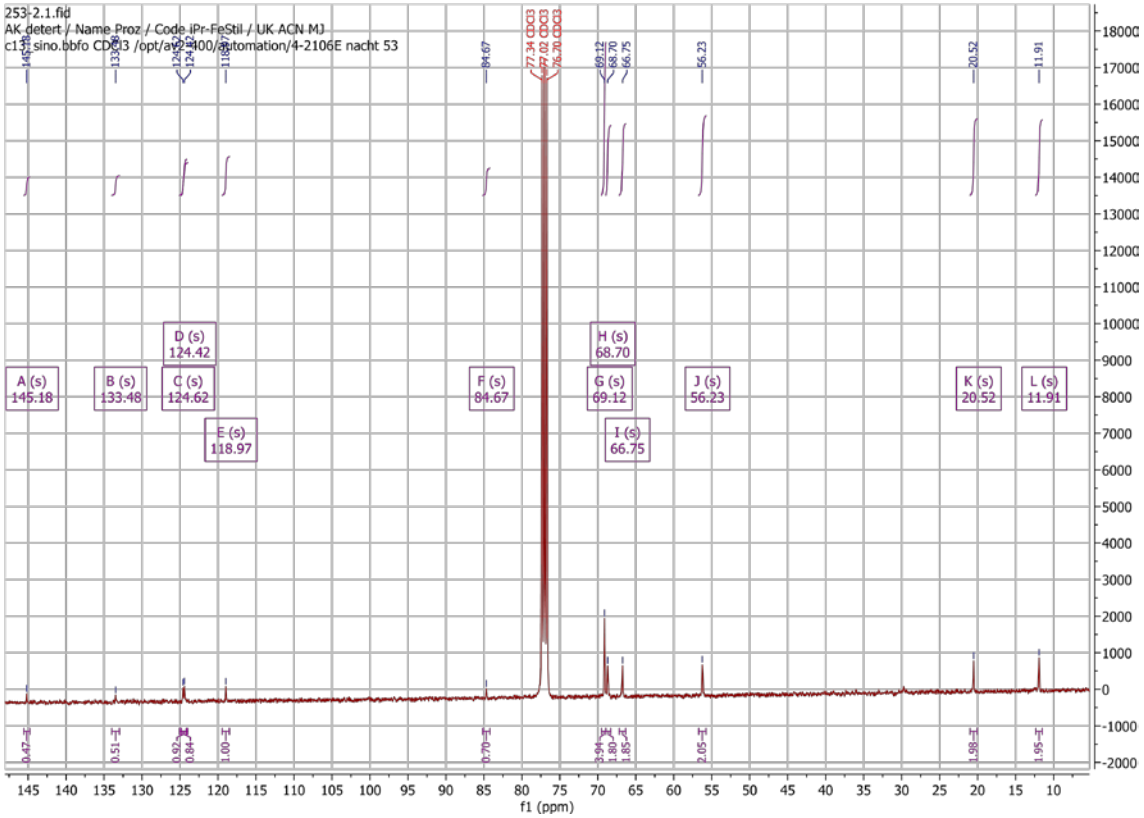

Figure S2: ^{13}C-NMR of **3** in $CDCl_3$, 100 MHz

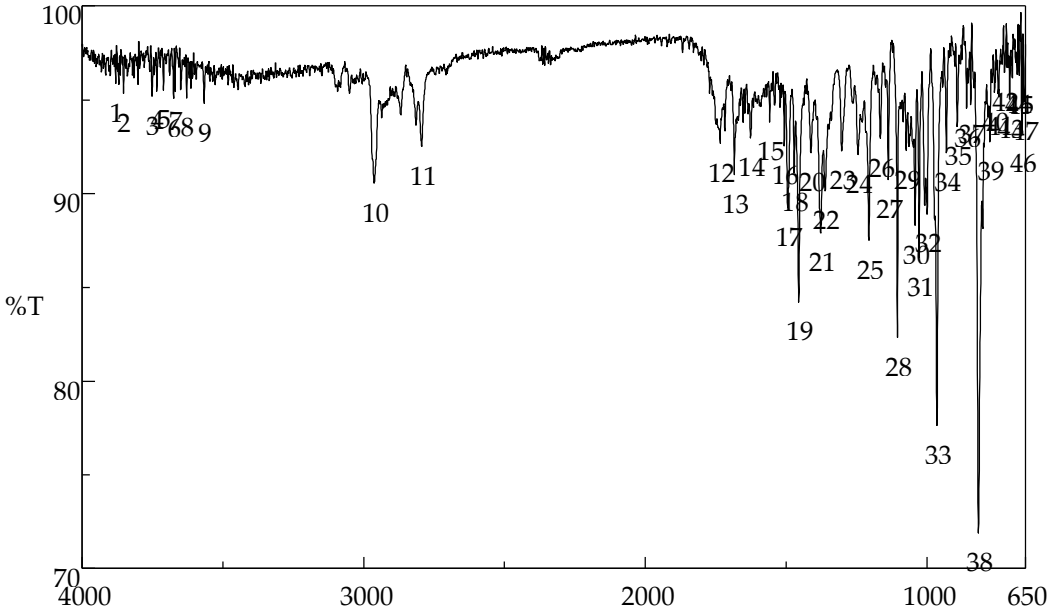

Figure S3: FT-IR of **3** , ATR

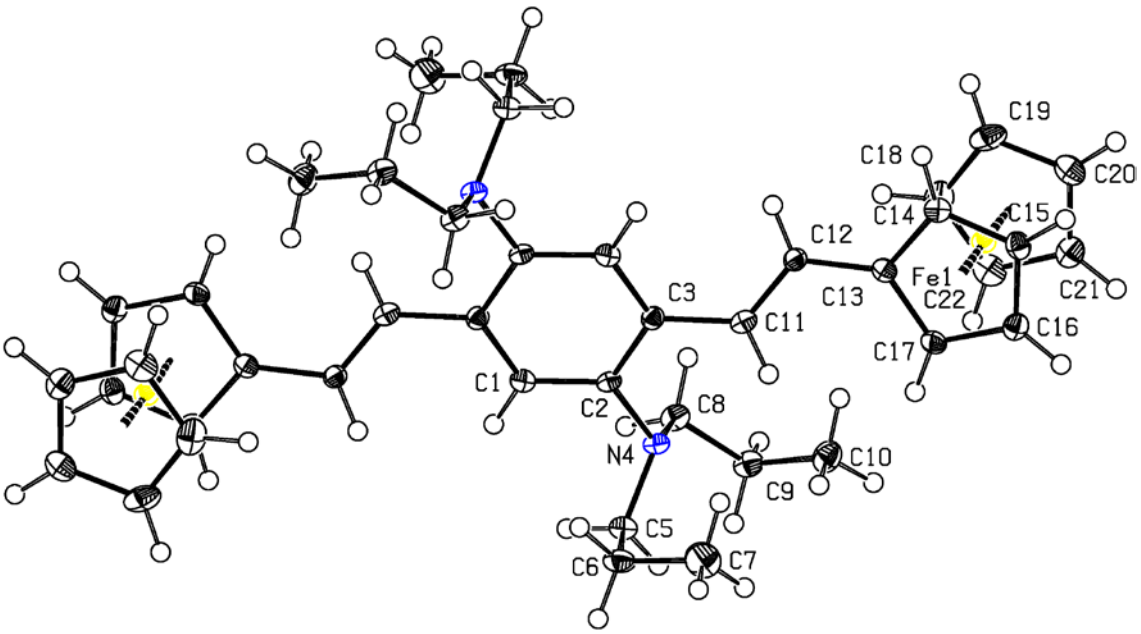

Figure S4: Displacement ellipsoid pot of **3**. Ecliptic conformer

Table S1. Crystal data and structure refinement for **3** **ecliptic conformer**

Empirical formula	$C_{42}H_{52}Fe_2N_2$
Empirical formula	$C_{42}H_{52}Fe_2N_2$
Formula weight	696.55
Temperature	120(2) K
Wavelength, radiation type	0.71073Å, MoKα
Diffractometer	STOE IPDS 2T
Crystal system	Monoklin
Space group name, number	P 21/n, (14)
Unit cell dimensions	a = 13.1109(8) Å
	b = 7.4274(4) Å
	β = 90.800(5)°
	c = 17.7619(11) Å
Volume	1729.48(18) $Å^3$
Number of reflections	11063
range used for lattice parameters	3.11° <=Θ<= 28.68°
Z	2
Density (calculated)	1.338 Mg/m^3
Absorption coefficient	0.871 mm^{-1}
Absorption correction	Integration
Max. and min. Transmission	0.9646 and 0.8825
F(000)	740
Crystal size, colour and form	0.070 x 0.080 x 0.190 mm^3, braune Nadel

Theta range for data collection	2.973 bis 28.188°.
Index ranges	-17<=h<=17, -9<=k<=9, -23<=l<=19
Number of reflections:	
collected	9156
independent	4211 [R_{int} = 0.0379]
observed [I>2sigma(I)]	3423
Completeness to theta = 25.2°	99.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4211 / 0 / 210
Goodness-of-fit on F^2	1.051
Final R indices R Werte [I>2sigma(I)]	R1 = 0.0542, wR2 = 0.1265
R indices (all data)	R1 = 0.0722, wR2 = 0.1405
Largest diff. peak and hole	0.486 und -0.866 $eÅ^{-3}$

Table S2. Anisotropic diffraction parameter (Å2) for compound **3** (ecliptic conformer)

$$U_{äq}=(1/3)*\Sigma\Sigma_{ij}a_i^*a_j^*\,\mathbf{a}_i\mathbf{a}_j$$

Atom	x	y	z	Uäq
Fe1	0.39266(3)	0.63228(5)	0.86191(2)	0.02446(13)
C1	0.5926(2)	0.4324(4)	0.47737(15)	0.0236(5)
C2	0.56629(19)	0.4171(4)	0.55250(15)	0.0216(5)
C3	0.4710(2)	0.4854(4)	0.57608(15)	0.0232(5)
N4	0.63263(17)	0.3403(3)	0.60846(13)	0.0236(5)
C5	0.6913(2)	0.1820(4)	0.58635(17)	0.0267(6)
C6	0.6225(2)	0.0244(4)	0.56632(18)	0.0315(6)
C7	0.5523(3)	-0.0313(5)	0.6291(2)	0.0389(7)
C8	0.6914(2)	0.4758(4)	0.65057(16)	0.0270(6)
C9	0.7755(2)	0.5731(4)	0.60788(17)	0.0286(6)
C10	0.8273(2)	0.7146(4)	0.65744(18)	0.0349(7)
C11	0.4401(2)	0.4590(4)	0.65453(15)	0.0234(5)
C12	0.3660(2)	0.5445(4)	0.69085(15)	0.0243(5)
C13	0.33792(19)	0.5015(4)	0.76818(15)	0.0231(5)
C14	0.2558(2)	0.5838(4)	0.80853(16)	0.0272(6)
C15	0.2549(2)	0.5111(4)	0.88247(17)	0.0315(6)
C16	0.3356(2)	0.3844(4)	0.88893(16)	0.0289(6)
C17	0.3867(2)	0.3783(4)	0.81876(16)	0.0261(5)
C18	0.4545(3)	0.8703(5)	0.8285(2)	0.0505(10)
C19	0.4032(3)	0.8936(5)	0.8975(3)	0.0511(10)
C20	0.4490(3)	0.7779(5)	0.9513(2)	0.0401(8)
C21	0.5283(2)	0.6834(5)	0.91586(19)	0.0360(7)
C22	0.5318(3)	0.7416(5)	0.8398(2)	0.0448(9)

Table S3: Bond lengths [Å] and angles [°] for compound **3**..(ecliptic)

Atom	x	y	z	U(iso)
H1	0.656	0.385	0.462	0.028
H5A	0.738	0.147	0.628	0.032
H5B	0.734	0.213	0.542	0.032
H6A	0.581	0.057	0.522	0.038
H6B	0.666	-0.080	0.553	0.038
H7A	0.514	-0.139	0.614	0.058
H7B	0.505	0.067	0.640	0.058
H7C	0.593	-0.058	0.675	0.058
H8A	0.723	0.416	0.695	0.032
H8B	0.643	0.567	0.669	0.032
H9A	0.827	0.484	0.591	0.034
H9B	0.746	0.632	0.563	0.034
H10A	0.854	0.658	0.703	0.052
H10B	0.778	0.808	0.671	0.052
H10C	0.884	0.770	0.630	0.052
H11	0.477	0.371	0.683	0.028
H12	0.330	0.637	0.665	0.029
H14	0.210	0.672	0.789	0.033
H15	0.208	0.542	0.921	0.038
H16	0.353	0.316	0.932	0.035
H17	0.444	0.305	0.808	0.031
H18	0.439	0.931	0.783	0.061
H19	0.348	0.973	0.906	0.061
H20	0.430	0.766	1.002	0.048
H21	0.572	0.596	0.939	0.043
H22	0.578	0.701	0.803	0.054

Table S4: Bond lengths [Å] and angles [°] for compound **3 (ecliptic)**.

C1-C2	1.388(4)	C12-H12	0.9500
C1-C3#1	1.395(4)	C13-C17	1.427(4)
C1-H1	0.9500	C13-C14	1.438(4)
C2-C3	1.417(4)	C14-C15	1.420(4)
C2-N4	1.430(3)	C14-H14	0.9500
C3-C11	1.470(4)	C15-C16	1.420(4)
N4-C5	1.462(4)	C15-H15	0.9500
N4-C8	1.466(4)	C16-C17	1.424(4)
C5-C6	1.518(4)	C16-H16	0.9500
C5-H5A	0.9900	C17-H17	0.9500
C5-H5B	0.9900	C18-C22	1.406(6)
C6-C7	1.514(5)	C18-C19	1.417(6)
C6-H6A	0.9900	C18-H18	0.9500
C6-H6B	0.9900	C19-C20	1.413(5)
C7-H7A	0.9800	C19-H19	0.9500
C7-H7B	0.9800	C20-C21	1.410(5)
C7-H7C	0.9800	C20-H20	0.9500
C8-C9	1.528(4)	C21-C22	1.420(5)
C8-H8A	0.9900	C21-H21	0.9500
C8-H8B	0.9900	C22-H22	0.9500
C9-C10	1.525(4)		
C9-H9A	0.9900	C2-C1-C3#1	122.4(2)
C9-H9B	0.9900	C2-C1-H1	118.8
C10-H10A	0.9800	C3#1-C1-H1	118.8
C10-H10B	0.9800	C1-C2-C3	119.1(2)
C10-H10C	0.9800	C1-C2-N4	123.0(2)
C11-C12	1.335(4)	C3-C2-N4	117.9(2)
C11-H11	0.9500	C1#1-C3-C2	118.4(2)
C12-C13	1.462(4)	C1#1-C3-C11	122.2(2)

C2-C3-C11	119.2(2)	H10B-C10-H10C	109.5
C2-N4-C5	116.8(2)	C12-C11-C3	127.4(3)
C2-N4-C8	113.0(2)	C12-C11-H11	116.3
C5-N4-C8	114.4(2)	C3-C11-H11	116.3
N4-C5-C6	111.7(2)	C11-C12-C13	123.0(3)
N4-C5-H5A	109.3	C11-C12-H12	118.5
C6-C5-H5A	109.3	C13-C12-H12	118.5
N4-C5-H5B	109.3	C17-C13-C14	106.9(2)
C6-C5-H5B	109.3	C17-C13-C12	127.9(2)
H5A-C5-H5B	107.9	C14-C13-C12	125.1(2)
C7-C6-C5	113.8(3)	C15-C14-C13	108.4(3)
C7-C6-H6A	108.8	C15-C14-H14	125.8
C5-C6-H6A	108.8	C13-C14-H14	125.8
C7-C6-H6B	108.8	C16-C15-C14	108.1(3)
C5-C6-H6B	108.8	C16-C15-H15	125.9
H6A-C6-H6B	107.7	C14-C15-H15	125.9
C6-C7-H7A	109.5	C15-C16-C17	108.1(2)
C6-C7-H7B	109.5	C15-C16-H16	126.0
H7A-C7-H7B	109.5	C17-C16-H16	126.0
C6-C7-H7C	109.5	C16-C17-C13	108.5(2)
H7A-C7-H7C	109.5	C16-C17-H17	125.7
H7B-C7-H7C	109.5	C13-C17-H17	125.7
N4-C8-C9	116.7(2)	C22-C18-C19	108.0(3)
N4-C8-H8A	108.1	C22-C18-H18	126.0
C9-C8-H8A	108.1	C19-C18-H18	126.0
N4-C8-H8B	108.1	C20-C19-C18	108.0(3)
C9-C8-H8B	108.1	C20-C19-H19	126.0
H8A-C8-H8B	107.3	C18-C19-H19	126.0
C10-C9-C8	111.0(3)	C21-C20-C19	108.1(3)
C10-C9-H9A	109.4	C21-C20-H20	126.0
C8-C9-H9A	109.4	C19-C20-H20	126.0
C10-C9-H9B	109.4	C20-C21-C22	107.9(3)
C8-C9-H9B	109.4	C20-C21-H21	126.1
H9A-C9-H9B	108.0	C22-C21-H21	126.1
C9-C10-H10A	109.5	C18-C22-C21	108.1(3)
C9-C10-H10B	109.5	C18-C22-H22	126.0
H10A-C10-H10B	109.5	C21-C22-H22	126.0
C9-C10-H10C	109.5		
H10A-C10-H10C	109.5		

Symmetrie transformation for equivalent atoms : #1 -x+1,-y+1,-z+1

Table S5: Torsion angles [°] for compound **3** (ecliptic)

C3#1-C1-C2-C3	0.7(4)	C11-C12-C13-C14	-177.0(3)
C3#1-C1-C2-N4	-177.2(2)	C17-C13-C14-C15	-0.1(3)
C1-C2-C3-C1#1	-0.7(4)	C12-C13-C14-C15	-178.1(3)
N4-C2-C3-C1#1	177.3(2)	C13-C14-C15-C16	0.1(3)
C1-C2-C3-C11	176.1(2)	C14-C15-C16-C17	-0.1(3)
N4-C2-C3-C11	-5.9(4)	C15-C16-C17-C13	0.0(3)
C1-C2-N4-C5	-39.6(4)	C14-C13-C17-C16	0.0(3)
C3-C2-N4-C5	142.5(2)	C12-C13-C17-C16	178.0(3)
C1-C2-N4-C8	96.4(3)	C22-C18-C19-C20	-0.2(4)
C3-C2-N4-C8	-81.5(3)	C18-C19-C20-C21	0.0(4)
C2-N4-C5-C6	-63.0(3)	C19-C20-C21-C22	0.3(4)
C8-N4-C5-C6	161.6(2)	C19-C18-C22-C21	0.4(4)
N4-C5-C6-C7	-57.6(3)	C20-C21-C22-C18	-0.4
C2-N4-C8-C9	-70.6(3)		
C5-N4-C8-C9	66.5(3)		
N4-C8-C9-C10	177.8(2)		
C1#1-C3-C11-C12	-19.0(4)		
C2-C3-C11-C12	164.3(3)		
C3-C11-C12-C13	176.8(3)		
C11-C12-C13-C17	5.4(5)		

Symmetrie transformation for equivalent atoms: #1 -x+1,-y+1,-

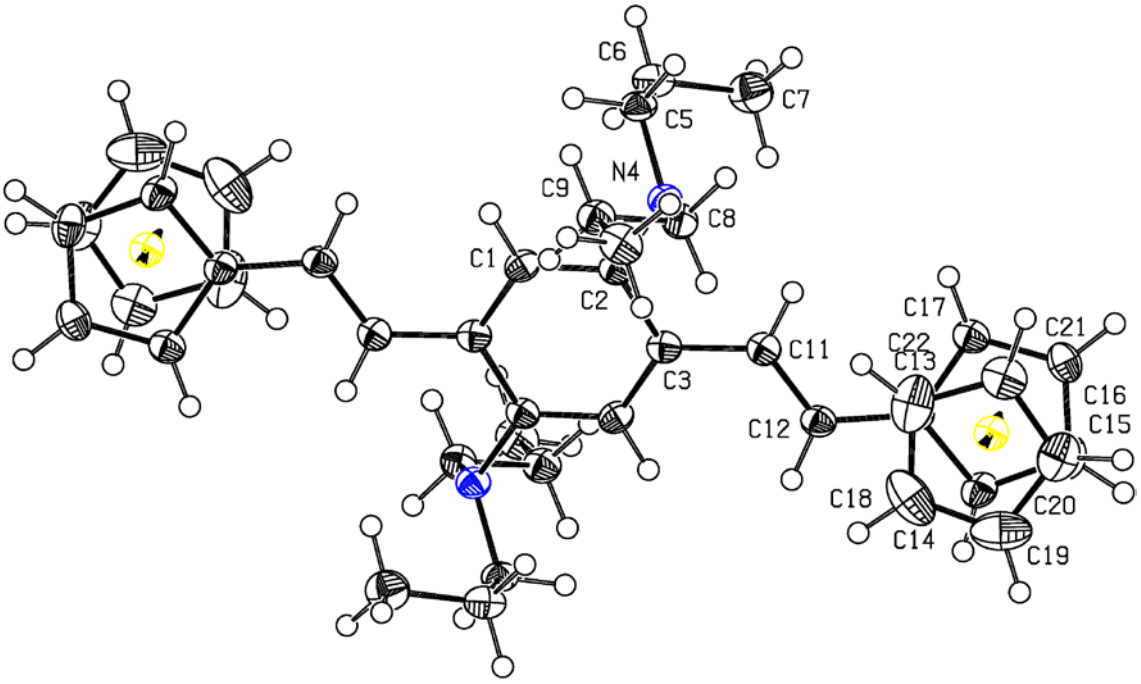

Figure S5: Displacement ellipsoid pot of **3**. Staggered conformer

Table S6. Crystal data and structure refinement for **3** **staggered conformer**

Empirical formula	$C_{42}H_{52}Fe_2N_2$
Empirical formula	$C_{42}H_{52}Fe_2N_2$
Formula weight	696.55
Temperature	120(2) K
Wavelength, radiation type	0.71073Å, MoKα
Diffractometer	STOE IPDS 2T
Crystal system	MonoklinKristallsystem Monoklin
Space group name, number	P 21/c, (14)
Unit cell dimensions	a = 18.3397(12) Å b = 7.4111(3) Å, β = 110.424(5)° c = 13.3820(9) Å
Volume	1704.51(18) $Å^3$
Number of reflections	9002
range used for lattice parameters	2.99° <=Θ<= 28.33°
Z	2
Density (calculated)	1.357 Mg/m^3
Absorption coefficient	0.884 mm^{-1}
Absorption correction	Integration
Max. und min. Transmission	0.9725 und 0.7879
F(000)	740
Crystal size, colour and form	0.030 x 0.160 x 0.350 mm^3, brown needle

Theta range for data collection	2.993 bis 27.908°.
Index ranges	-24<=h<=24, -8<=k<=9, -17<=l<=17
Number of reflections:	
collected	8157
independent	4008 [R_{int} = 0.0340]
observed [I>2sigma(I)]	3190
Completeness to theta = 25.2°	98.8 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4008 / 0 / 210
Goodness-of-fit on F^2	1.064
Final R indices R Werte [I>2sigma(I)]	R1 = 0.0461, wR2 = 0.1044
R indices (all data)	R1 = 0.0659, wR2 = 0.1162
Largest diff. peak and hole	0.473 und -0.415 $eÅ^{-3}$

Table S7. Anisotropic diffraction parameter (Å2) for compound 3 (staggered conformer)

$U_{äq}=(1/3)*\Sigma\Sigma_{ij}a_i^*a_j^*\ \mathbf{a}_i\mathbf{a}_j$

Atom	x	y	z	$U_{äq}$
Fe1	0.88551(2)	0.35103(5)	0.57141(3)	0.01387(11)
C1	0.47265(14)	0.5726(4)	0.57513(19)	0.0152(5)
C2	0.55178(14)	0.5815(3)	0.59222(19)	0.0133(5)
C3	0.58018(14)	0.5083(3)	0.5155(2)	0.0142(5)
N4	0.60738(12)	0.6562(3)	0.68781(16)	0.0143(4)
C5	0.58175(15)	0.8172(4)	0.7293(2)	0.0172(5)
C6	0.56405(17)	0.9739(4)	0.6511(2)	0.0221(6)
C7	0.6326(2)	1.0254(5)	0.6178(3)	0.0337(7)
C8	0.63872(15)	0.5166(4)	0.7697(2)	0.0185(5)
C9	0.71605(15)	0.5689(4)	0.8553(2)	0.0197(5)
C10	0.77819(16)	0.6168(4)	0.8084(2)	0.0248(6)
C11	0.66273(15)	0.5285(4)	0.5290(2)	0.0156(5)
C12	0.70232(14)	0.4353(4)	0.4788(2)	0.0146(5)
C13	0.78202(14)	0.4786(3)	0.4859(2)	0.0142(5)
C14	0.81989(15)	0.4096(4)	0.4164(2)	0.0163(5)
C15	0.89461(15)	0.4920(4)	0.4449(2)	0.0180(5)
C16	0.90400(15)	0.6092(4)	0.5322(2)	0.0175(5)
C17	0.83520(15)	0.6007(3)	0.5588(2)	0.0165(5)
C18	0.86190(17)	0.1485(4)	0.6597(2)	0.0258(6)
C19	0.89572(17)	0.0775(4)	0.5871(2)	0.0258(6)
C20	0.97078(16)	0.1570(4)	0.6108(2)	0.0220(6)
C21	0.98244(16)	0.2783(4)	0.6973(2)	0.0208(6)
C22	0.91534(17)	0.2730(4)	0.7274(2)	0.0234(6)

Table S8. Coordinates and isotropic diffraction parameter of hydrogen atoms (Å2) for compound **3** (staggered)..

Atom	x	y	z	U(iso)
H1	0.454	0.623	0.627	0.018
H5A	0.623	0.854	0.797	0.021
H5B	0.534	0.788	0.746	0.021
H6A	0.549	1.080	0.684	0.027
H6B	0.519	0.941	0.587	0.027
H7A	0.621	1.137	0.576	0.050
H7B	0.642	0.929	0.574	0.050
H7C	0.679	1.043	0.682	0.050
H8A	0.646	0.404	0.735	0.022
H8B	0.600	0.492	0.804	0.022
H9A	0.708	0.674	0.896	0.024
H9B	0.735	0.467	0.906	0.024
H10A	0.784	0.517	0.763	0.037
H10B	0.828	0.637	0.866	0.037
H10C	0.763	0.727	0.765	0.037
H11	0.691	0.617	0.579	0.019
H12	0.677	0.335	0.436	0.018
H14	0.799	0.324	0.361	0.020
H15	0.932	0.472	0.411	0.022
H16	0.949	0.681	0.567	0.021
H17	0.826	0.665	0.615	0.020
H18	0.812	0.118	0.662	0.031
H19	0.872	-0.008	0.532	0.031
H20	1.006	0.133	0.575	0.026
H21	1.027	0.351	0.730	0.025
H22	0.908	0.341	0.783	0.028

Table S9: Bond lengths [Å] and angles [°] for compound **3** (staggered).

C1-C2	1.390(3)	C10-H10A 0.9800
C1-C3#1	1.396(3)	C10-H10B 0.9800
C1-H1	0.9500	C10-H10C 0.9800
C2-C3	1.411(3)	C11-C12 1.341(4)
C2-N4	1.439(3)	C11-H11 0.9500
C3-C11	1.468(3)	C12-C13 1.466(3)
N4-C5	1.461(3)	C12-H12 0.9500
N4-C8	1.470(3)	C13-C17 1.434(4)
C5-C6	1.520(4)	C13-C14 1.436(3)
C5-H5A	0.9900	C14-C15 1.425(4)
C5-H5B	0.9900	C14-H14 0.9500
C6-C7	1.521(4)	C15-C16 1.417(4)
C6-H6A	0.9900	C15-H15 0.9500
C6-H6B	0.9900	C16-C17 1.427(4)
C7-H7A	0.9800	C16-H16 0.9500
C7-H7B	0.9800	C17-H17 0.9500
C7-H7C	0.9800	C18-C22 1.418(4)
C8-C9	1.530(4)	C18-C19 1.424(4)
C8-H8A	0.9900	C18-H18 0.9500
C8-H8B	0.9900	C19-C20 1.428(4)
C9-C10	1.523(4)	C19-H19 0.9500
C9-H9A	0.9900	C20-C21 1.421(4)
C9-H9B	0.9900	C20-H20 0.9500

C21-C22	1.423(4)	H9A-C9-H9B	107.8
C21-H21	0.9500	C9-C10-H10A	109.5
C22-H22	0.9500	C9-C10-H10B	109.5
		H10A-C10-H10B	109.5
C2-C1-C3#1	122.1(2)	C9-C10-H10C	109.5
C2-C1-H1	118.9	H10A-C10-H10C	109.5
C3#1-C1-H1	118.9	H10B-C10-H10C	109.5
C1-C2-C3	119.4(2)	C12-C11-C3	127.0(2)
C1-C2-N4	122.7(2)	C12-C11-H11	116.5
C3-C2-N4	117.9(2)	C3-C11-H11	116.5
C1#1-C3-C2	118.5(2)	C11-C12-C13	123.8(2)
C1#1-C3-C11	121.6(2)	C11-C12-H12	118.1
C2-C3-C11	119.9(2)	C13-C12-H12	118.1
C2-N4-C5	115.4(2)	C17-C13-C14	107.3(2)
C2-N4-C8	111.3(2)	C17-C13-C12	127.5(2)
C5-N4-C8	112.7(2)	C14-C13-C12	125.2(2)
N4-C5-C6	112.5(2)	C15-C14-C13	108.1(2)
N4-C5-H5A	109.1	C15-C14-H14	125.9
C6-C5-H5A	109.1	C13-C14-H14	125.9
N4-C5-H5B	109.1	C16-C15-C14	108.2(2)
C6-C5-H5B	109.1	C16-C15-H15	125.9
H5A-C5-H5B	107.8	C14-C15-H15	125.9
C5-C6-C7	113.2(2)	C15-C16-C17	108.3(2)
C5-C6-H6A	108.9	C15-C16-H16	125.8
C7-C6-H6A	108.9	C17-C16-H16	125.8
C5-C6-H6B	108.9	C16-C17-C13	108.0(2)
C7-C6-H6B	108.9	C16-C17-H17	126.0
H6A-C6-H6B	107.8	C13-C17-H17	126.0
C6-C7-H7A	109.5	C22-C18-C19	107.9(3)
C6-C7-H7B	109.5	C22-C18-H18	126.0
H7A-C7-H7B	109.5	C19-C18-H18	126.0
C6-C7-H7C	109.5	C18-C19-C20	108.1(3)
H7A-C7-H7C	109.5	C18-C19-H19	125.9
H7B-C7-H7C	109.5	C20-C19-H19	125.9
N4-C8-C9	113.5(2)	C21-C20-C19	107.5(3)
N4-C8-H8A	108.9	C21-C20-H20	126.2
C9-C8-H8A	108.9	C19-C20-H20	126.2
N4-C8-H8B	108.9	C20-C21-C22	108.3(3)
C9-C8-H8B	108.9	C20-C21-H21	125.9
H8A-C8-H8B	107.7	C22-C21-H21	125.9
C10-C9-C8	112.5(2)	C18-C22-C21	108.1(3)
C10-C9-H9A	109.1	C18-C22-H22	126.0
C8-C9-H9A	109.1	C21-C22-H22	126.0
C10-C9-H9B	109.1		
C8-C9-H9B	109.1		

Symmetrie transformation for equivalent atoms 1 -x+1,-y+1,-z+1

Table S10: Torsion angles [°] for compound **3** (staggered).

C3#1-C1-C2-C3	0.6(4)	C2-N4-C8-C9	159.9(2)
C3#1-C1-C2-N4	-176.7(2)	C5-N4-C8-C9	-68.6(3)
C1-C2-C3-C1#1	-0.6(4)	N4-C8-C9-C10	-56.3(3)
N4-C2-C3-C1#1	176.9(2)	C1#1-C3-C11-C12	-20.2(4)
C1-C2-C3-C11	175.6(2)	C2-C3-C11-C12	163.7(3)
N4-C2-C3-C11	-6.9(4)	C3-C11-C12-C13	171.8(2)
C1-C2-N4-C5	-39.5(3)	C11-C12-C13-C17	11.8(4)
C3-C2-N4-C5	143.1(2)	C11-C12-C13-C14	-165.4(3)
C1-C2-N4-C8	90.6(3)	C17-C13-C14-C15	-1.3(3)
C3-C2-N4-C8	-86.8(3)	C12-C13-C14-C15	176.3(2)
C2-N4-C5-C6	-61.6(3)	C13-C14-C15-C16	0.8(3)
C8-N4-C5-C6	169.0(2)	C14-C15-C16-C17	0.0(3)
N4-C5-C6-C7	-56.9(3)	C15-C16-C17-C13	-0.9(3)

C14-C13-C17-C16	1.4(3)	C19-C18-C22-C21	-0.4(3)
C12-C13-C17-C16	-176.2(2)	C20-C21-C22-C18	0.0(3)
C22-C18-C19-C20	0.6(3)		
C18-C19-C20-C21	-0.6(3)		
C19-C20-C21-C22	0.4(3)		

Symmetrie transformation for equivalent atoms:

#1 -x+1,-y+1,-z+1