

Supporting Information

From Ylides to Doubly Yldiide-Bridged Iron(II) High Spin Dimers *via* Self Protolysis

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1. NMR Spectra of 2a-c, 4 and 6

SDB-MY-024-01 in C₆D₆ 1H, paramagn.

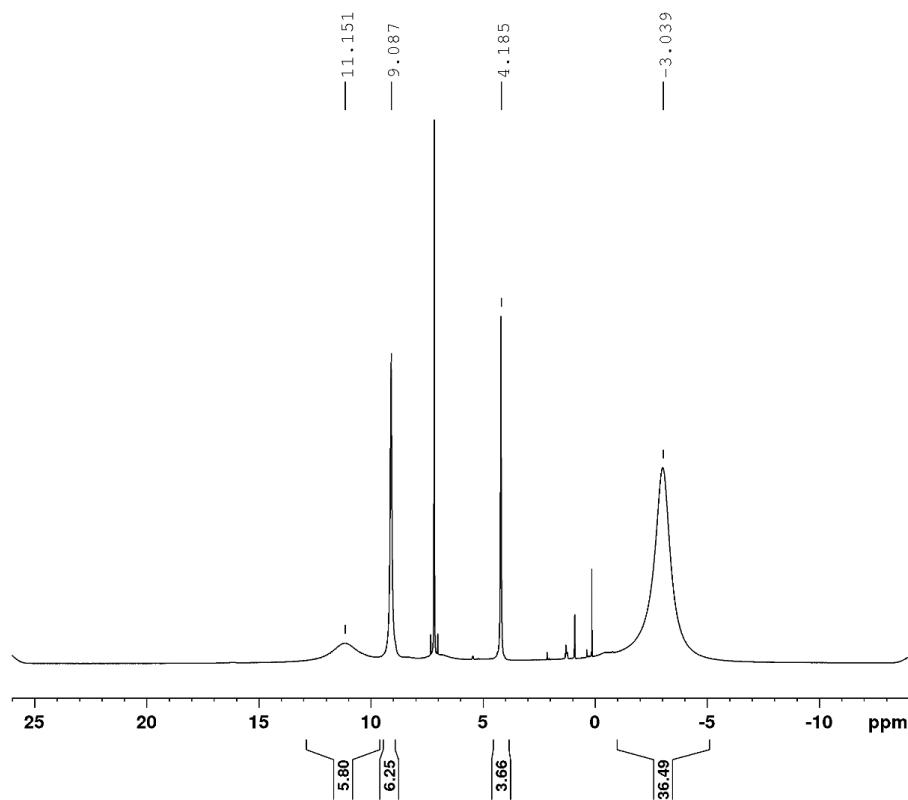


Figure S1. ¹H NMR spectrum of **2a** (C₆D₆, 298 K).

SDB-MY-024-01 in C₆D₆ 13C-BB, paramagn.

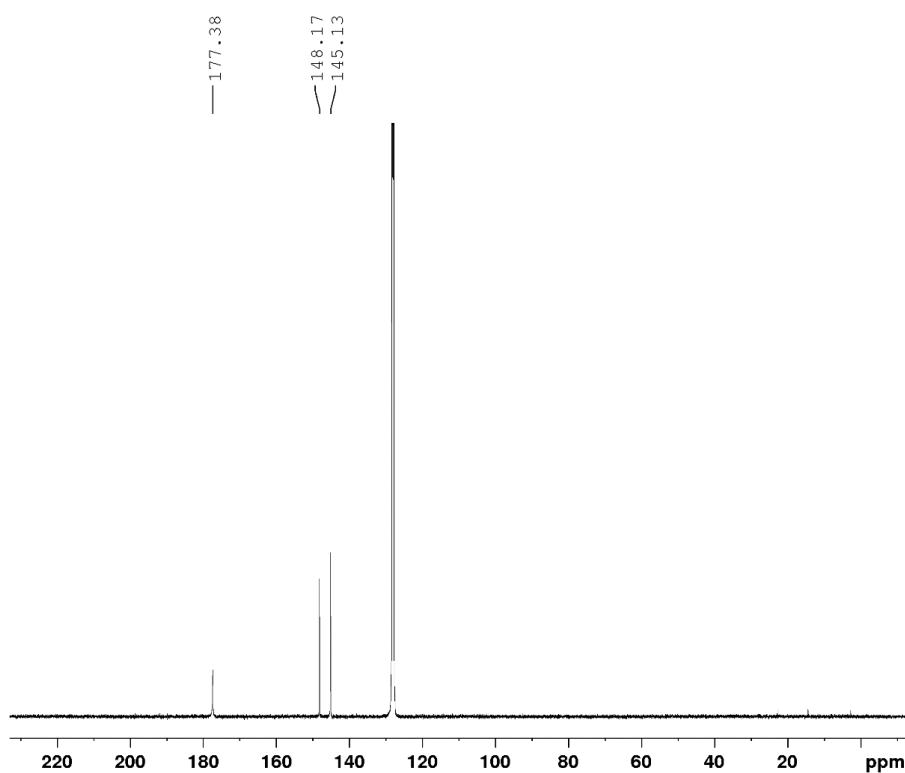


Figure S2. ¹³C{¹H} NMR spectrum of **2a** (C₆D₆, 298 K).

SDB-MY-060-02 in Toluol-d8, 1H paramagn. T=296K

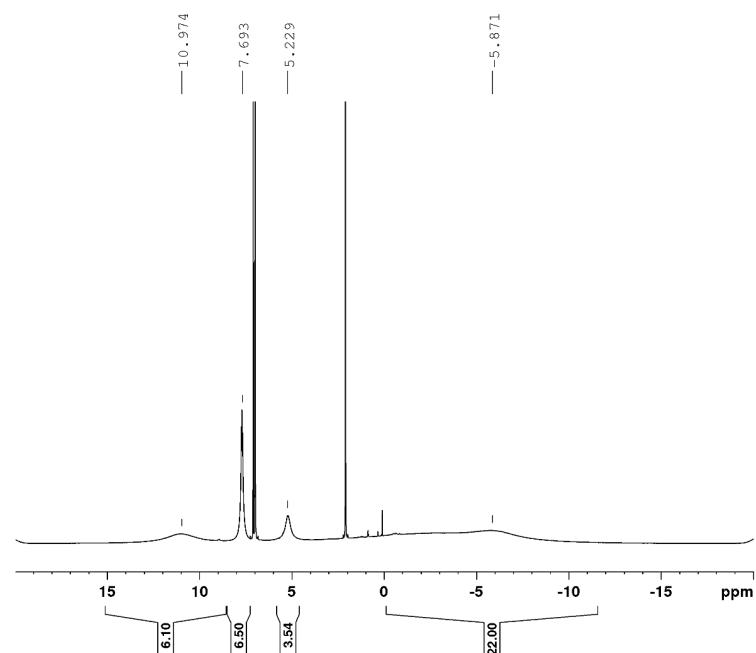


Figure S3. ¹H NMR spectrum of **2b** (toluene-d⁸, 298 K).

SDB-MY-060-02 in Toluol-d8, 13C-BB paramagn. T=296K

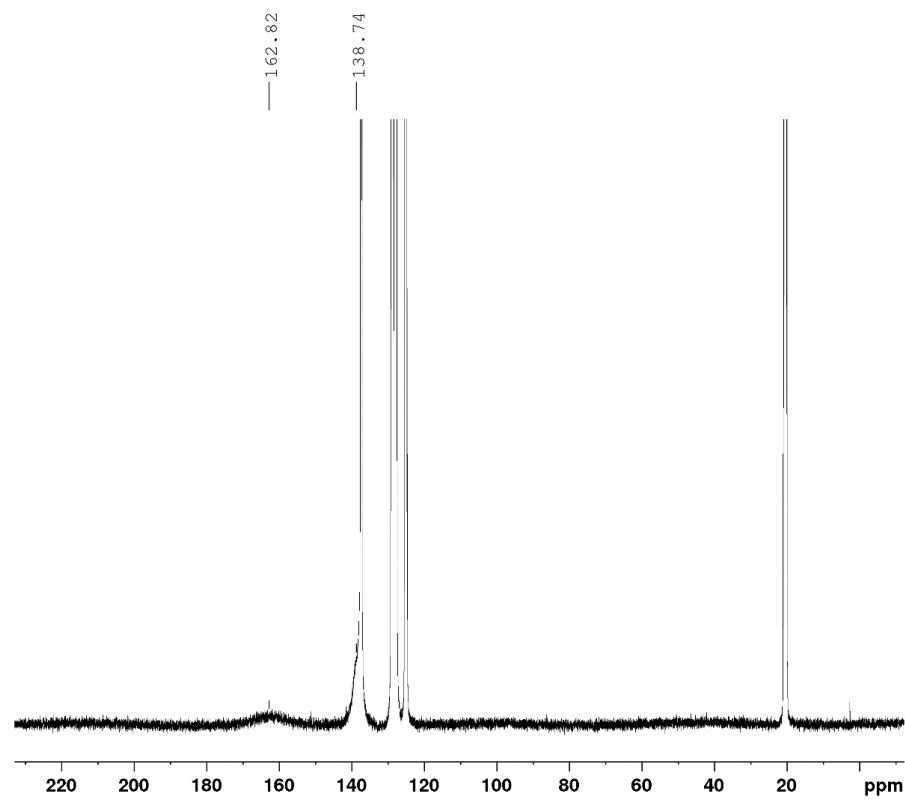


Figure S4. ¹³C{¹H} NMR spectrum of **2b** (toluene-d⁸, 298 K).

SDB-MY-188-01 in C₆D₆ 1H, paramagn.

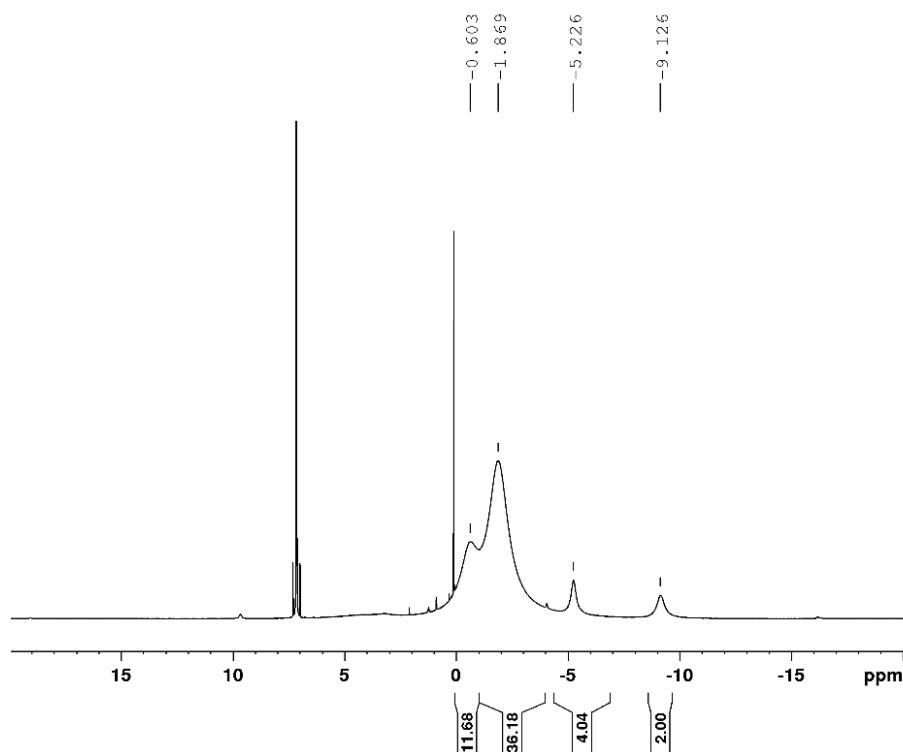


Figure S5. ¹H NMR spectrum of **2c** (C₆D₆, 298 K).

SDB-MY-193-01 in C₆D₆ 1H, paramagn.

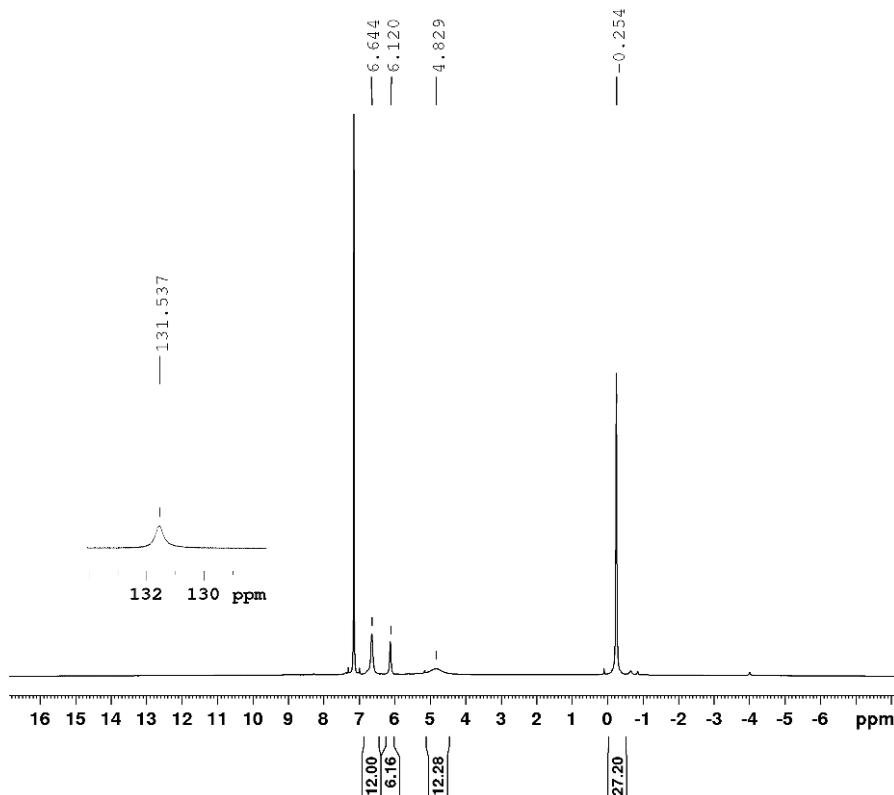


Figure S6. ¹H NMR spectrum of **4** (C₆D₆, 298 K).

2. Time- and Temperature Dependent Reaction of **1a** with $[\text{Fe}(\text{Mes})_2]_2$ Monitored by ^1H NMR Spectroscopy

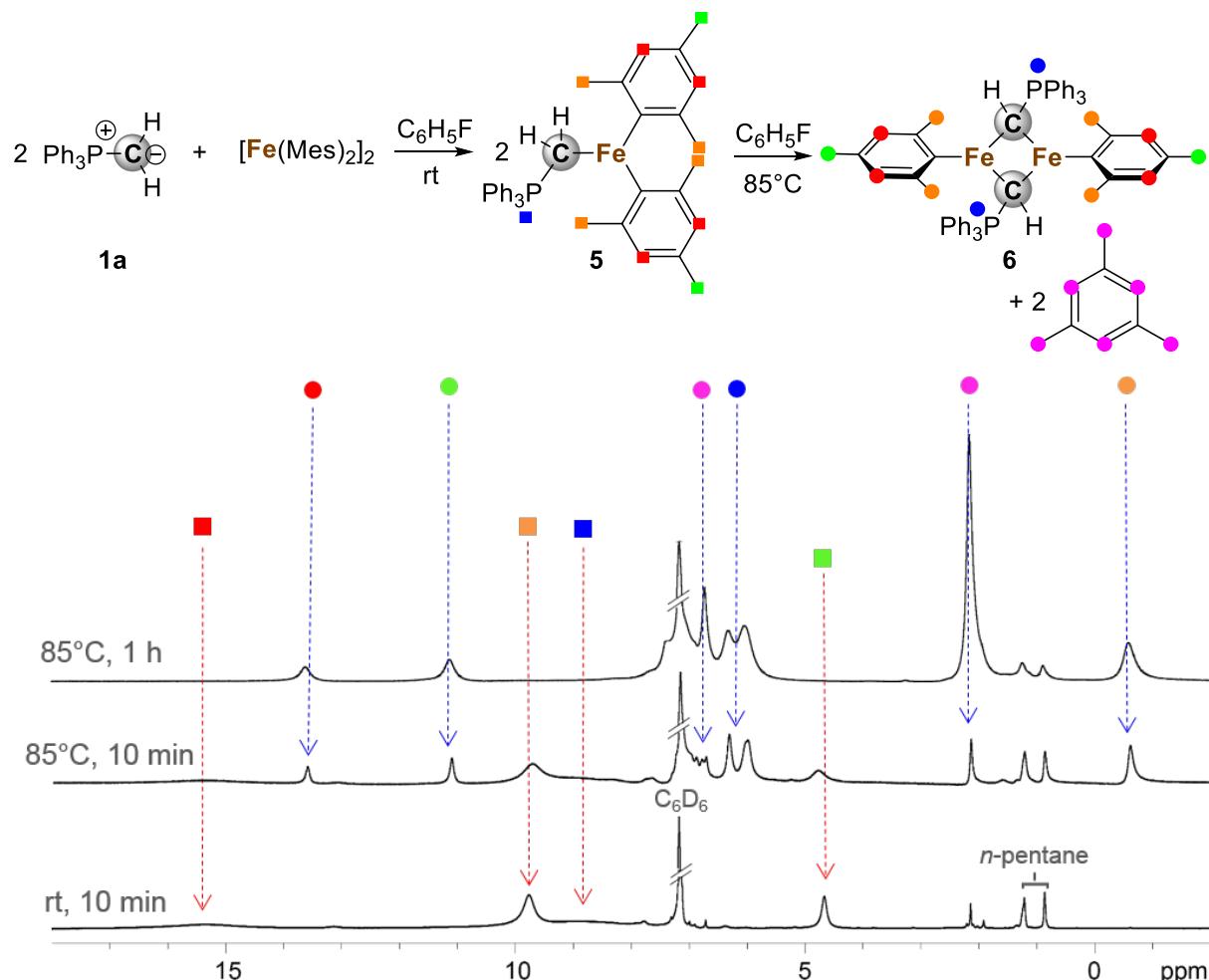


Figure S7. Stack of ^1H NMR spectra (298 K, C_6D_6): Time- and temperature dependent reaction of **1a** with $[\text{Fe}(\text{Mes})_2]_2$: Bottom (rt, 10 min): reaction mixture shows the presence of four broad resonances presumably due to the formation of the monomer **5** (for assignment, see colored squares); middle (85°C , 10 min): The resonances of **5** decrease in intensity accompanied by the appearance of eight new resonances assigned to **6** and mesitylene (for assignment, see colored dots). Top (85°C , 1 h): quantitative conversion to **6** is observed.

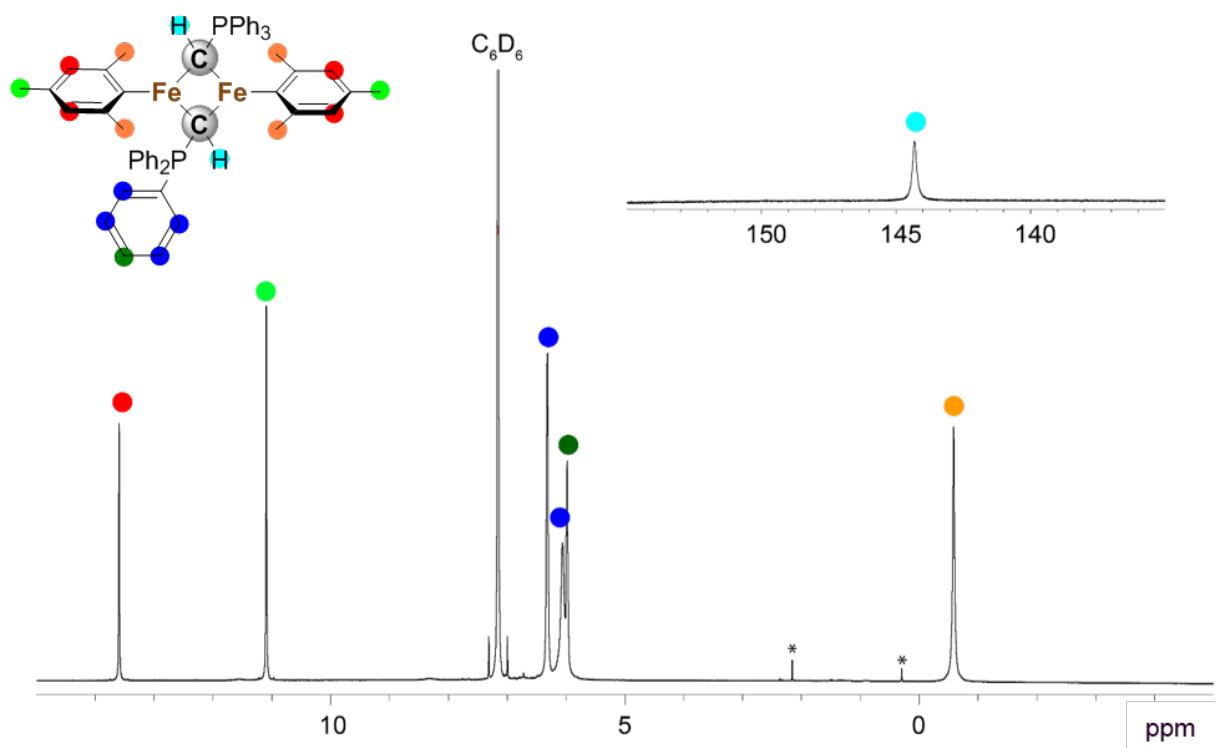


Figure S8. ^1H NMR spectrum (298 K, C_6D_6) of the isolated complex **6** (for assignment, see colored dots).

3. Reaction of **2a** with Benzonitrile

2a (72 mg, 0.11 mmol) was dissolved in benzonitrile (0.3 mL) and the reaction mixture was stirred for 12 h resulting in an orange-brown solution. *n*-Pentane (1 mL) was added and the reaction mixture was stored at –35 °C resulting in the formation of yellow crystals suitable for X-ray crystallography and are identified as **3** (see Table S4). The crystals decompose at ambient temperature to give a brown oil.

4. Mössbauer Spectra of **2a-c**

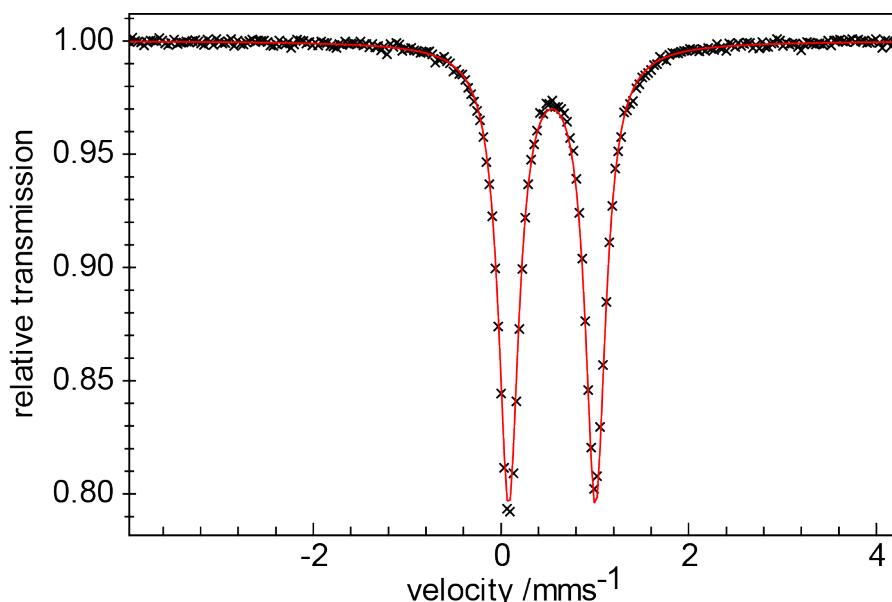


Figure S9. Zero field ⁵⁷Fe Mössbauer spectra of solid **2a** recorded at 80 K. The solid lines represent fits with $\delta = 0.54$ mm/s and $\Delta E_Q = 0.92$ mm/s.

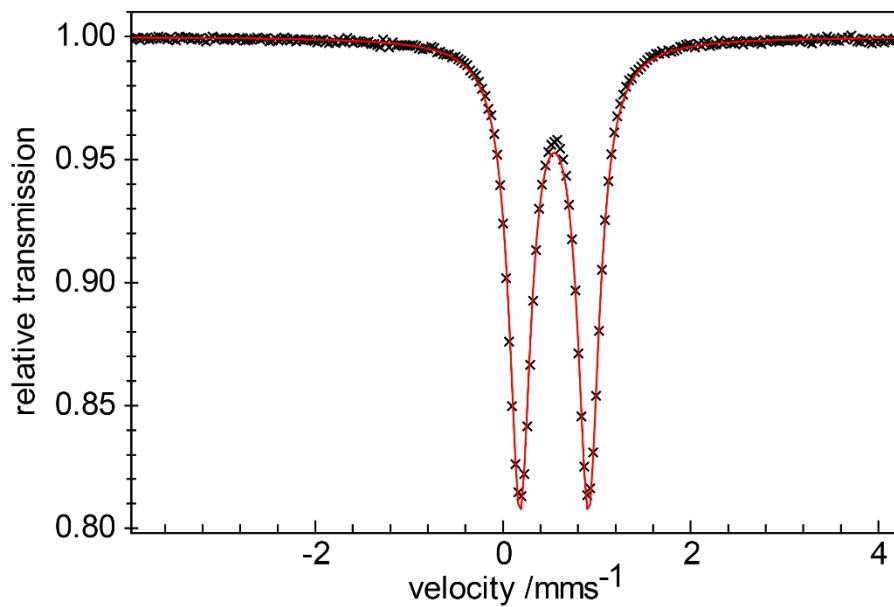


Figure S10. Zero field ^{57}Fe Mössbauer spectra of solid **2b** recorded at 80 K. The solid lines represent fits with $\delta = 0.55 \text{ mm/s}$ and $\Delta E_Q = 0.73 \text{ mm/s}$.

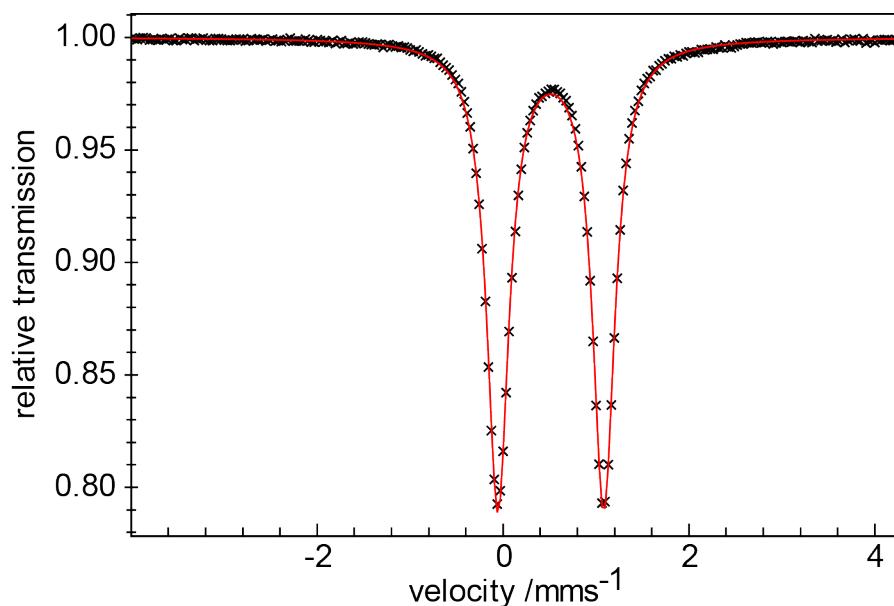


Figure S11. Zero field ^{57}Fe Mössbauer spectra of solid **2c** recorded at 80 K. The solid lines represent fits with $\delta = 0.51 \text{ mm/s}$ and $\Delta E_Q = 1.14 \text{ mm/s}$.

5. Molecular Orbital Diagram for **6**

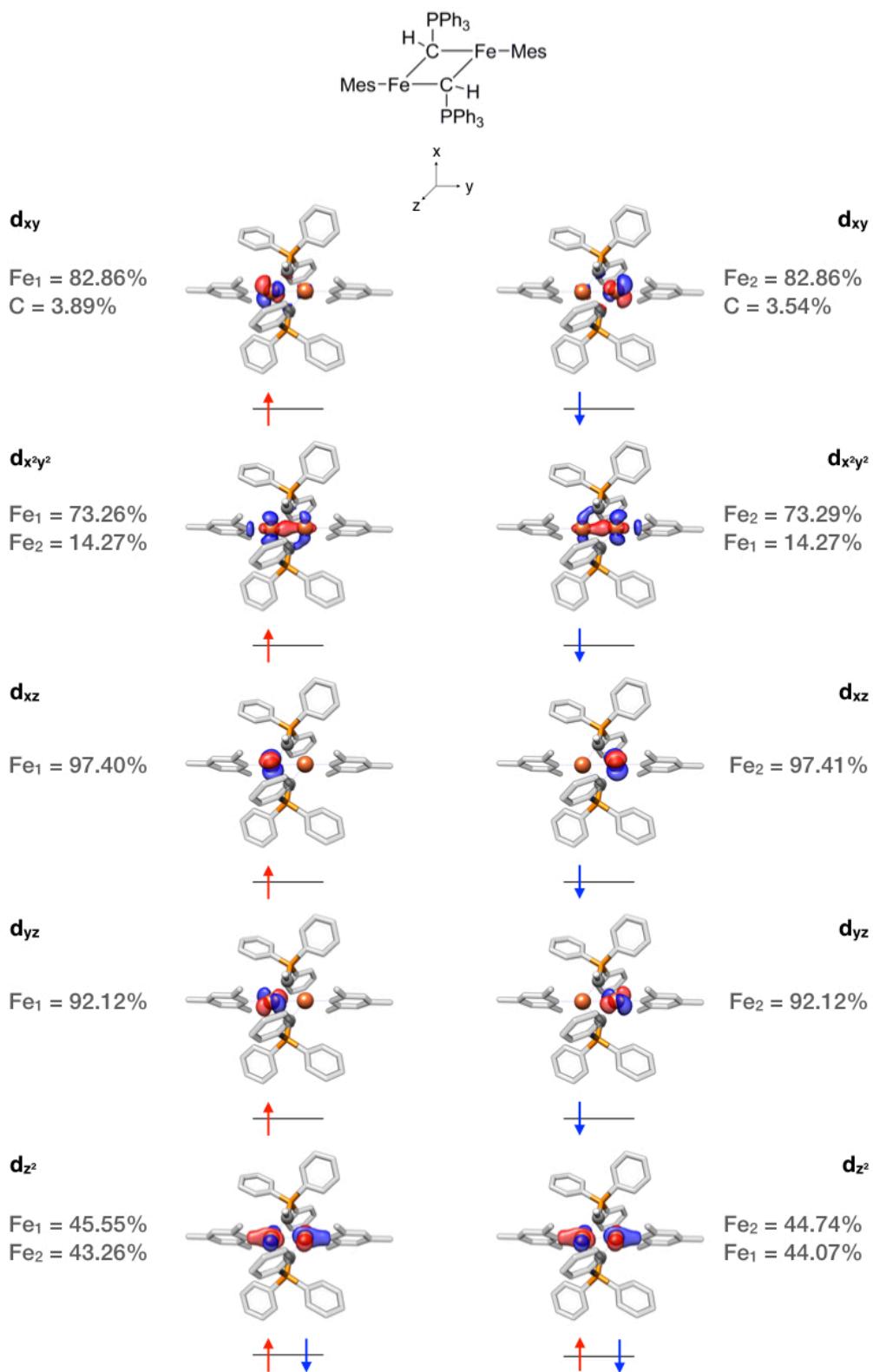


Figure S12. Localized magnetic molecular orbital (MO; isosurface-contour value = 0.05) diagram for complex **6**. For the localization, a threshold of 95% were chosen for strong localized MOs and 80% for bond MOs, respectively.

6. Mayer-Bond-Order-Analysis (MBOA) of complex 4 and 6

Table S1. Mayer-Bond-Order-Analysis (MBOA) of the antiferromagnetic coupled complex 4. The bonding

Bond	Order
Fe ₁ - Fe ₂	0.1764
Fe ₁ - C ₁	0.6545
Fe ₁ - C ₂	0.6355
Fe ₂ - C ₁	0.6353
Fe ₂ - C ₂	0.6549
Fe ₁ - N ₁	0.6545
Fe ₂ - N ₂	0.6373

Table S2. Mayer-Bond-Order-Analysis (MBOA) of the antiferromagnetic coupled complex 4.

Bond	Order
Fe ₁ - Fe ₂	0.2285
Fe ₁ - C ₁	0.6292
Fe ₁ - C ₂	0.6654
Fe ₂ - C ₁	0.6658
Fe ₂ - C ₂	0.6290
Fe ₁ - C ₃	0.9326
Fe ₂ - C ₄	0.9318

7. Orca DFT Input File for Full Geometry Optimization for 4 and 6 (Broken Symmetry)

```
!UKS TPSSH def2-TZVP def2/J RIJCOSX d3 Pal8 Grid5 GridX5 tightscf slowconv opt
```

```
%scf
DIISMAXEQ 30
MaxIter 600
Flipspin 0
FinalMs 0.0
end
*xyz 0 9
```

8. Orca DFT Input File for Localized Orbital Analysis for 4 and 6

```
!UKS TPSSH def2-TZVP def2/J RIJCOSX d3 Pal8 Grid5 GridX5 UCO UNO tightscf
slowconv noiter
```

```
!MORRead
%moinp "TPSSH_LO_pre.gbw"

%loc
locMet PM
T_Core -1000
Tol 1e-8
MaxIter 256
end

*xyzfile 0 1 TPSSH.xyz
```

9. Cartesian Coordinates of the Fully Geometry Optimized Structure of 4 (Broken Symmetry)

Fe	3.01219641153941	7.23160080614720	5.66394019308723
C	2.92414529583934	9.26890573523151	5.75607892670562
H	3.74744798172458	9.75969240704335	5.22677533052778
P	1.46520400780184	10.11166671613693	5.52374169368122
C	0.15683123785816	9.52047654488760	6.62768761661331
C	-0.56068285738531	10.37716228648380	7.46312087755656
H	-0.31850384687417	11.43157329245778	7.49317672987571
C	-1.58571529055320	9.87634587350994	8.26051877538490
H	-2.12594146734846	10.54577588105073	8.91934338105405
C	-1.91021163537909	8.52550108146753	8.21673030338960
H	-2.70735324772299	8.13865413248574	8.84062267084366
C	-1.20815823963696	7.66858103862111	7.37157775861376
H	-1.45694843979443	6.61520770909628	7.32778340732387
C	-0.18308683400665	8.16474066341202	6.57984097500833

H	0.36162968390987	7.50473801865071	5.91449981620818
C	0.71097600257915	9.96518208582001	3.87358804748966
C	1.52637533903110	9.66862103701166	2.78245192217848
H	2.58187824774485	9.48764669280471	2.94464516102581
C	0.98167783082196	9.58325419550127	1.50634703343771
H	1.62036631020194	9.35961983674073	0.66038469072004
C	-0.38440178915766	9.76772511900380	1.31879473044990
H	-0.81066216311674	9.68376095216660	0.32593198648507
C	-1.20676984423094	10.04503898842122	2.40764333993189
H	-2.27317491323676	10.17540303527850	2.26514498020389
C	-0.66130873975019	10.14971933537288	3.68120198473587
H	-1.30180898583400	10.36308587879094	4.52923737433702
C	1.58469696292640	11.90166108451693	5.80411488149334
C	2.12471774145294	12.33898113834517	7.01974003547758
H	2.45995811235840	11.61049443272062	7.75249969253997
C	2.23558340192589	13.69858177516818	7.27975246319199
H	2.64171575677264	14.03117940090464	8.22728046812904
C	1.83205755660789	14.63039343424318	6.32638473441712
H	1.92753251579128	15.69075137966852	6.53013541113651
C	1.31115277594832	14.19935849301615	5.11083762873823
H	1.00288104120289	14.92136483764005	4.36358033483845
C	1.17998236361816	12.83887934692402	4.85061271902256
H	0.76717600300376	12.50713263796158	3.90615815648290
N	2.76949069896274	6.05285542861317	4.15720671834268
Si	1.30045969723443	5.16231354509343	4.10100192117310
Si	3.92493718365858	6.16330598011318	2.88986551811392
C	0.74794515838883	4.66037062717503	5.83755765928845
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H	-0.26103676304924	4.23474808419463	5.80691810501979
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C	-0.08655076321887	6.14093140269929	3.27962069116865
H	-0.24997722854931	7.10910690817660	3.75945257946971
H	-1.03346166553108	5.59092110572230	3.30137447387700
H	0.15890658488726	6.34208661689675	2.23287551729579
C	1.46622582796116	3.54526046103449	3.13709085677073
H	1.75485172492100	3.70765435748411	2.09527897644799
H	0.51133604160158	3.00890863297481	3.13263577069508
H	2.21196460029115	2.88521412109992	3.58827282149054
C	5.01150763458206	4.62319789850309	2.78949101721183
H	5.54286529583132	4.44678669353878	3.72725365292139
H	5.75996879315616	4.72238577595030	1.99597975953092
H	4.41455700022528	3.73287283006139	2.57291149775376
C	5.05973109541449	7.64294230454503	3.16321427807842
H	4.52671578214774	8.59129931782820	3.05553279385388
H	5.87944706848260	7.63953957112973	2.43689696746183
H	5.50774436150886	7.63152808504772	4.16032304455018
C	3.13012997430112	6.37137638101333	1.18971420329116
H	2.54171565806920	5.49541816720030	0.90275099959825
H	3.89427418571181	6.51945526549618	0.41904003666561
H	2.46102905507200	7.23449925515541	1.17269531111235
Fe	3.31917417208979	8.76491530183302	7.70090529318378
C	3.40711017464034	6.72761445624394	7.60880407943095
H	2.58367953488268	6.23699836253381	8.13807507257791
P	4.86576792188249	5.88430232327810	7.84093897620748
C	6.17409826124445	6.47496826521286	6.73667712758823
C	6.89117950765698	5.61805859559227	5.90109523874484
H	6.64859789081298	4.56373892029686	5.87100494309484
C	7.91630116387491	6.11854559357217	5.10360332436157
H	8.45619873819659	5.44895592508347	4.44467124125513
C	8.24132863050760	7.46926189020653	5.14746517242423
H	9.03855279539308	7.85584923454572	4.52351591111234

C	7.53971775347991	8.32639206081867	5.99277052157874
H	7.78895456000821	9.37965706997607	6.03663741392927
C	6.51453548227477	7.83057652492344	6.78458355319097
H	5.97017654870025	8.49073586685715	7.45007060948116
C	5.62049188950403	6.03056325129292	9.49088980266231
C	4.80549441722957	6.32708679486437	10.58232220782814
H	3.7499613493144	6.50819624676635	10.42048524564449
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H	4.71226277448278	6.63563794043434	12.70449745427432
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C	7.53873384350857	5.95027174958163	10.95616059042780
H	8.60516658493760	5.81973177325965	11.09829477160082
C	6.99281613671125	5.84579338595809	9.68278506289767
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C	4.74539227860302	4.09435959133529	7.56071486969565
C	4.20499676725630	3.65711321758400	6.34522665796229
H	3.87009059086431	4.38563670464413	5.61235065898029
C	4.09314436164797	2.29752874772824	6.08556512659484
H	3.68673716328672	1.96498880741700	5.13813426520521
C	4.49598132964078	1.36566339408425	7.03917811659522
H	4.39971208025272	0.30532396230763	6.83570831945819
C	5.01717290373051	1.79664217082293	8.25461985413493
H	5.32486684449932	1.07461250977957	9.00209326838860
C	5.14935739275887	3.15709211775670	8.51448133212194
H	5.56237864664868	3.48877760982960	9.45886318013449
N	3.56180468656514	9.94372358978746	9.20761041984367
Si	5.03104613640802	10.83388726155272	9.26389736751348
Si	2.40608140403064	9.83353395176604	10.47470911069451
C	5.58394785030424	11.33567728286051	7.52742405269967
H	4.91534319476018	12.09525559495563	7.11380597060839
H	6.59293138539783	11.76127954800232	7.55832383540481
H	5.59355188470114	10.50501007391709	6.81770983403165
C	6.41775070266087	9.85497988439743	10.08546186623695
H	6.58100123604646	8.88674361697592	9.60567722910549
H	7.36478473602346	10.40478016568037	10.06375997166215
H	6.17216617500458	9.65391311033844	11.13218959178628
C	4.86549141599450	12.45101781902598	10.22771554882758
H	4.57677194320454	12.28872798385221	11.26951700425393
H	5.82044746052556	12.98724825096529	10.23219520925018
H	4.11986500219817	13.11113755951455	9.77645130049724
C	1.31973925308252	11.37380058763254	10.57469828781967
H	0.78866279946152	11.55030896145773	9.63680351889094
H	0.57107407200990	11.27474521604713	11.36803355159969
H	1.91679402299826	12.26402591360239	10.79141119857119
C	1.27112547003819	8.35403283159616	10.20126498315564
H	1.80386368686003	7.40558983117562	10.30953172795162
H	0.45104447309869	8.35784859546676	10.92716793108730
H	0.82359704289091	8.36521835354251	9.20393660589006
C	3.20042960721187	9.62564632806328	12.17509864965405
H	3.78893292561234	10.50155487551230	12.46202471001129
H	2.43605677867119	9.47788071160249	12.94560707962199
H	3.86935604594769	8.76241101902224	12.19249061454998

10. Cartesian Coordinates of the Fully Geometry Optimized Structure of 6 (Broken Symmetry)

Fe 5.93900146750661 2.54334905573165 4.84743857148267

C	6.87426956937295	1.52640309130527	6.34286485772119
H	7.96606096073409	1.53789911896844	6.40904611149536
P	6.24192719972701	-0.04994029232764	6.46409632157174
C	4.48547030812901	-0.08130865332144	6.01248207499548
C	3.60265263191737	0.68012410661415	6.78823760514160
H	3.98742131968135	1.25797349344512	7.62215592437547
C	2.24761680884146	0.69870784484412	6.49145915631294
H	1.57561350820588	1.30208848543689	7.09056559896275
C	1.75620521060282	-0.06377555922190	5.43384138168955
H	0.69751236293746	-0.05144082839767	5.20232965584181
C	2.62486087361755	-0.84217150357333	4.67724345359422
H	2.24646285294380	-1.43603526375169	3.85361966549872
C	3.98664795325701	-0.85377972026654	4.96269379693739
H	4.65861336356872	-1.45492801992979	4.36409680084469
C	6.23990350341859	-0.77114772328097	8.13489288218329
C	5.56148931688771	-1.96018385314064	8.42441229030746
H	5.05560747203005	-2.50359201022118	7.63358412341527
C	5.51899499320093	-2.43347187646587	9.72915986495501
H	4.99032719366629	-3.35287783828820	9.95303673997581
C	6.13983020101923	-1.71745634421824	10.75260488871153
H	6.09096696353600	-2.08242302143804	11.77217272297223
C	6.80331006909696	-0.52863099899810	10.47050357563483
H	7.26304551754578	0.04764299086045	11.26460515348588
C	6.85434017974650	-0.05846045474750	9.16242699334842
H	7.33002212034789	0.88624769481097	8.93382119093482
C	7.08886871009323	-1.24095186870865	5.38935266388019
C	7.71242638751046	-2.39267396748661	5.87343505017088
H	7.66031839171790	-2.63552557417681	6.92763409980405
C	8.41356796164319	-3.22240153442467	5.00312523770386
H	8.90186498828380	-4.11115402138790	5.38593814481204
C	8.49068327886996	-2.91139868937807	3.64932211307947
H	9.03811463966429	-3.56033745651750	2.97524720597127
C	7.87051757965854	-1.76249817900398	3.16251265976568
H	7.92845914897833	-1.50855208105724	2.11035471930013
C	7.17869054632329	-0.92620749059669	4.02751751619668
H	6.71123836068041	-0.02044555309778	3.65289146220072
C	5.84324798993117	2.20581297637969	2.84912845009144
C	7.00012278964540	2.10640376675017	2.04549620129564
C	6.90708668935094	1.89840613679449	0.67029103099139
H	7.81633615157114	1.81861411705382	0.07756271442936
C	5.66969097063648	1.78765880814150	0.03505682389711
C	4.52319892188261	1.88737942670559	0.81875300249494
H	3.54911421292891	1.79331015684395	0.34300265702977
C	4.59853339210138	2.09358248436474	2.19856265110707
C	8.36926581620966	2.24099307551757	2.66881713470424
H	9.11296458055579	1.62815522730464	2.15204473352812
H	8.34785331254944	1.94023802015203	3.72142649182357
H	8.71752851939945	3.27928282436831	2.62602142552044
C	5.58126961343229	1.55317488077054	-1.45048102738602
H	4.54252866269502	1.55626421981486	-1.78683648723311
H	6.02136162002802	0.59005943915216	-1.72798893976891
H	6.12041307085412	2.32571556516378	-2.00693945673882
C	3.31334778500370	2.22097857793129	2.98100574514969
H	2.54137706597308	1.54644143122355	2.60255503517067
H	2.90924041893699	3.23886186737165	2.92072554396843
H	3.47228863039763	1.99472810831957	4.03790742923575
Fe	5.95217524034320	3.02045265798737	7.35935258180505
C	5.01715707823431	4.03755436072554	5.86403257828150
H	3.92534043536472	4.02639632672395	5.79799662950036
P	5.65002571857599	5.61363347354781	5.74154120103439
C	7.40602298972808	5.64518280246789	6.19481285770432

C	8.28952876353632	4.88307773307504	5.42051626597402
H	7.90556924367512	4.30462282503104	4.58666856300844
C	9.64424970270066	4.86448672529202	5.71875888822292
H	10.31679597270471	4.26062275946956	5.12075799480084
C	10.13462306415436	5.62751018245633	6.77647144300227
H	11.19305992374295	5.61517158636515	7.00913813547620
C	9.26524465934541	6.40636479218405	7.53177760736368
H	9.64283022565433	7.00058848332931	8.35551552727401
C	7.90377882152278	6.41801462641600	7.24483374709817
H	7.23121878189671	7.01945097383511	7.84246349255986
C	5.65389192563365	6.33227125287871	4.06965802443100
C	6.33493149193950	7.51933819003889	3.77821620716412
H	6.84177124339654	8.06306133149049	4.56821157451499
C	6.37898455667945	7.99009458470605	2.47260083068584
H	6.90970670993803	8.90795182717287	2.24723220478927
C	5.75717648737272	7.27343018867967	1.45020109933364
H	5.80735523295449	7.63634579410600	0.42996573553688
C	5.09109438527311	6.08651970480719	1.73421127335488
H	4.63074130563638	5.50955051988787	0.94096987671241
C	5.03843279483892	5.61897660471391	3.04315546353409
H	4.56070093906686	4.67570260477495	3.27329886355804
C	4.80249648493582	6.80631320062674	6.81395812849358
C	4.18095685715443	7.95843323433017	6.32819623261062
H	4.23466815188820	8.20040790348051	5.27388673733536
C	3.47970730556326	8.78965816731291	7.19696846275026
H	2.99298684435060	9.67870789067589	6.81283907743280
C	3.40038656550212	8.47975532228255	8.55090203214464
H	2.85287030972755	9.12988416596938	9.22376012205984
C	4.01849788144773	7.33047734193779	9.03939108983861
H	3.95887821876640	7.07737748838215	10.09165179375523
C	4.71046195955566	6.49270397845233	8.17591042853863
H	5.17650023651336	5.58678235646195	8.55187248253541
C	6.04762917591669	3.35883469274486	9.35746624885963
C	4.89057213621498	3.46015796970158	10.16062232497105
C	4.98335603278564	3.67044907433432	11.53551299037271
H	4.07398838232375	3.75165740096529	12.12787407932754
C	6.22063237914953	3.78163234930617	12.17088500990661
C	7.36729893186791	3.67984000314098	11.38770488311983
H	8.34130138927975	3.77416088959143	11.86355559064693
C	7.29223037787477	3.47134750908340	10.00823928713923
C	3.52151789913844	3.32529526501558	9.53720515421386
H	2.77778666653804	3.93866222362903	10.05329535741307
H	3.54315592126909	3.62517953182206	8.48434173273789
H	3.17317072825441	2.28705217692141	9.58076288035397
C	6.30879398718940	4.01890882847575	13.65599628657433
H	7.34734626805602	4.01426717336608	13.99289713730611
H	5.87068175042183	4.98356423975678	13.93128446880306
H	5.76765448340419	3.24870512985539	14.21375077577826
C	8.57748889399521	3.34168880463668	9.22628572274371
H	9.35086249799781	4.01420877962232	9.60543221244259
H	8.97920601652677	2.32283413151414	9.28608115493668
H	8.41947744343570	3.56890324972528	8.16943901355082

11.X-Ray Crystallographic Data Collection and Refinement of the Structures.

Table S3. Crystallographic data of complexes **2a-c**.

	2a	2b	2c
Formula	C ₃₁ H ₅₃ FeN ₂ PSi ₄	C ₃₄ H ₆₁ FeN ₂ PSi ₅	C ₂₆ H ₅₆ FeN ₄ Si ₄
M _r in g mol ⁻¹	652.93	725.11	592.95
Color, habit	yellow, prism	colorless, prism	colorless, prism
Crystal system	monoclinic	orthorhombic	monoclinic
Space group	P2 ₁ /n	Pca2 ₁	P2 ₁ /c
a in Å	9.2297(13)	20.157(2)	23.796(4)
b in Å	21.680(3)	11.7867(13)	15.220(3)
c in Å	19.105(3)	17.463(2)	19.864(3)
α in °	90	90	90
β in °	99.468(3)	90	103.112(12)
γ in °	90	90	90
V in Å ³	3770.8(10)	4148.9(8)	7007(2)
Z	4	4	8
T in K	100(2)	100(2)	100(2)
Crystal size in mm ³	0.132 × 0.084 × 0.041	0.228 × 0.110 × 0.100	0.170 × 0.080 × 0.070
ρ _c in g cm ⁻³	1.150	1.161	1.124
F(000)	1400	1560	2576.0
Diffractometer	Bruker-AXS Kappa Mach3 APEX-II	Bruker-AXS Kappa Mach3 APEX-II	Bruker AXS Enraf-Nonius KappaCCD
λ _{XKα} in Å	X = Mo 0.71073	X = Mo 0.71073	X = Mo 0.71073
θ _{min} in °	2.640	2.333	2.800
θ _{max} in °	27.499	31.543	27.500
Index range	-11 ≤ h ≤ 11 -28 ≤ k ≤ 28 -24 ≤ l ≤ 24	-29 ≤ h ≤ 29 -17 ≤ k ≤ 17 -25 ≤ l ≤ 25	-30 ≤ h ≤ 30 -19 ≤ k ≤ 19 -25 ≤ l ≤ 25
μ in mm ⁻¹	0.591	0.571	0.587
Abs. correction	gaussian	gaussian	gaussian
Reflections collected	87083	122059	91835
Reflections unique	8647	13803	16082
R _{int}	0.0481	0.0379	0.1096
Reflections obs. [F>2σ(F)]	6875	13081	10691
Residual density in e Å ⁻³	1.418, -1.162	0.463, -0.487	0.750, -0.766
Parameters	413	406	679
GOOF	1.036	1.044	1.041
R ₁ [I>2σ(I)]	0.0697	0.0217	0.0642
wR ₂ (all data)	0.1956	0.0572	0.1532
CCDC	1901690	1901692	1901691

Table S4. Crystallographic data of complexes **3**, **4**, and **6**.

	3	4	6
Formula	C ₃₈ H ₅₈ FeN ₃ PSi ₄	C ₅₀ H ₆₈ Fe ₂ N ₂ P ₂ Si ₄	C ₅₆ H ₅₄ Fe ₂ P ₂
M _r in g mol ⁻¹	756.05	983.06	900.63
Color, habit	yellow, plate	orange-red, plate	orange, prism
Crystal system	monoclinic	monoclinic	triclinic
Space group	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> - <i>I</i>
a in Å	9.0849(8)	12.111(2)	8.7466(4)
b in Å	19.771(2)	15.996(3)	12.3605(11)
c in Å	23.879(3)	14.561(2)	13.7778(10)
α in °	90	90	64.446(6)
β in °	96.210(7)	113.388(15)	76.804(5)
γ in °	90	90	82.119(6)
V in Å ³	4263.9(8)	2589.1(8)	1307.09(17)
Z	4	2	1
T in K	100(2)	100(2)	100(2)
Crystal size in mm ³	0.260 × 0.170 × 0.050	0.090 × 0.050 × 0.030	0.270 × 0.140 × 0.110
ρ _c in g cm ⁻³	1.178	1.261	1.144
F(000)	1616	1040	472.0
Diffractometer	Bruker AXS Enraf-Nonius KappaCCD	Bruker AXS Enraf-Nonius KappaCCD	Bruker AXS Enraf-Nonius KappaCCD
λ _{XKα} in Å	X = Mo 0.71073	X = Mo 0.71073	X = Mo 0.71073
θ _{min} in °	3.055	2.866	2.943
θ _{max} in °	32.993	27.493	29.999
Index range	−13 ≤ h ≤ 13 −30 ≤ k ≤ 30 −36 ≤ l ≤ 36	−15 ≤ h ≤ 15 −20 ≤ k ≤ 20 −18 ≤ l ≤ 17	−12 ≤ h ≤ 12 −17 ≤ k ≤ 17 −19 ≤ l ≤ 19
μ in mm ⁻¹	0.532	0.749	0.649
Abs. correction	gaussian	gaussian	gaussian
Reflections collected	95803	21948	23751
Reflections unique	16040	5912	7602
R _{int}	0.0723	0.1070	0.0291
Reflections obs. [F>2σ(F)]	11662	4174	6410
Residual density in e Å ⁻³	0.520, −0.456	0.844, −1.921	0.407, −0.404
Parameters	442	277	274
GOOF	1.078	1.043	1.065
R ₁ [I>2σ(I)]	0.0886	0.0750	0.0408
wR ₂ (all data)	0.0994	0.2058	0.1240
CCDC	1901689	1901687	1901688