Supplementary Materials for

New ferrocene-based metalloligand with two triazole carboxamide pendant arms and its iron(II) complex: synthesis, crystal structure, ^{57}Fe Mössbauer spectroscopy, magnetic properties and theoretical calculations

Peter Antal [a], Ivan Nemec [a,b], Jiří Pechoušek [c], Radovan Herchel [a*]

[a] Department of Inorganic Chemistry, Faculty of Science, Palacký University Olomouc, 17. listopadu 12, Olomouc, 77146, Czech Republic

[b] Central European Institute of Technology, CEITEC BUT, Technická 3058/10, 61600, Brno, Czech Republic

[c] Department of Experimental Physics, Faculty of Science, Palacký University Olomouc, 17. listopadu 12, Olomouc, 77146, Czech Republic

* Correspondence: radovan.herchel@upol.cz

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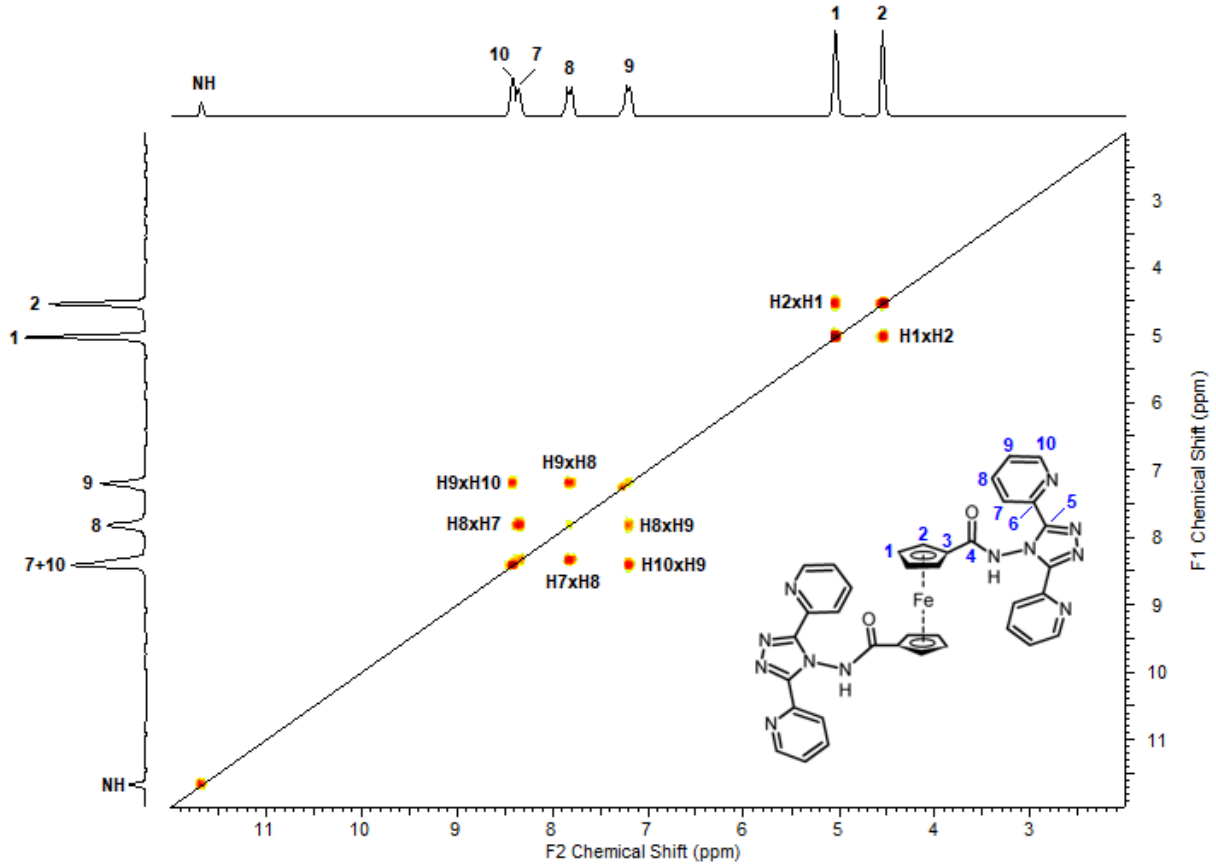


Figure S1: ^{1}H-^{1}H *gs*-COSY NMR spectrum (400 MHz, $CDCl_3$) of **L** (bis(*N*-4-[3,5-di-(2-pyridyl)-1,2,4-triazoyl])ferrocene carboxamide).

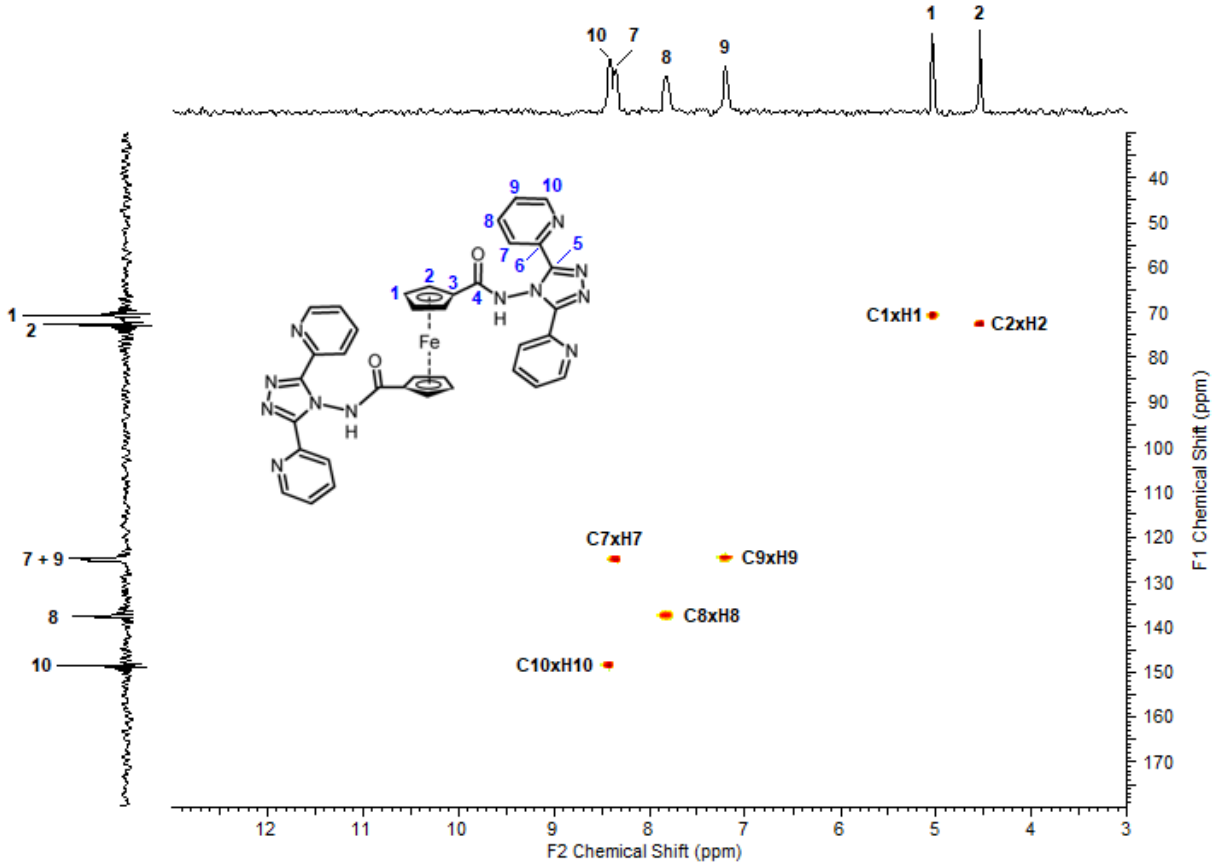


Figure S2: ^{1}H-^{13}C *gs*-HMQC NMR spectrum (400 MHz, $CDCl_3$) of **L** (bis(*N*-4-[3,5-di-(2-pyridyl)-1,2,4-triazoyl])ferrocene carboxamide).

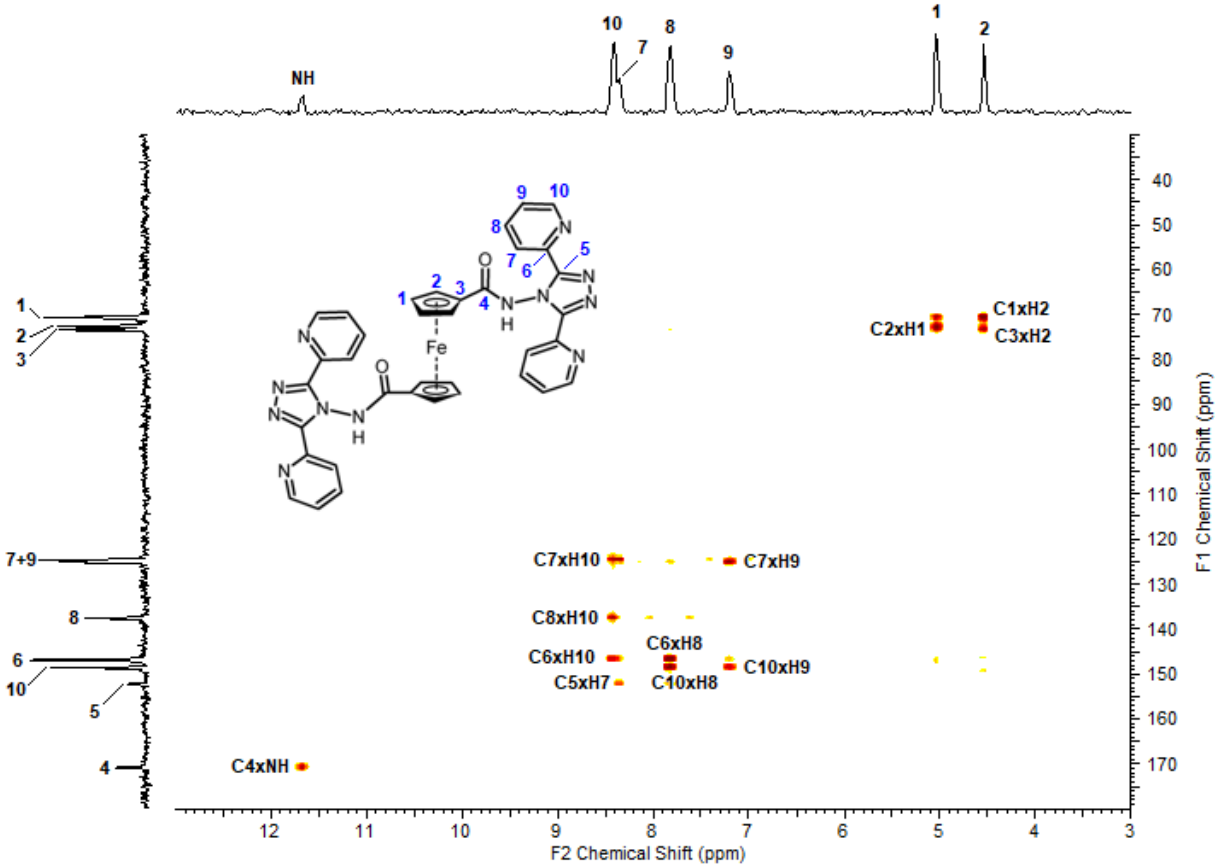


Figure S3: ^{1}H-^{13}C *g*-HMBC NMR spectrum 400 MHz, $CDCl_3$) of **L** (bis(*N*-4-[3,5-di-(2-pyridyl)-1,2,4-triazoyl])ferrocene carboxamide).

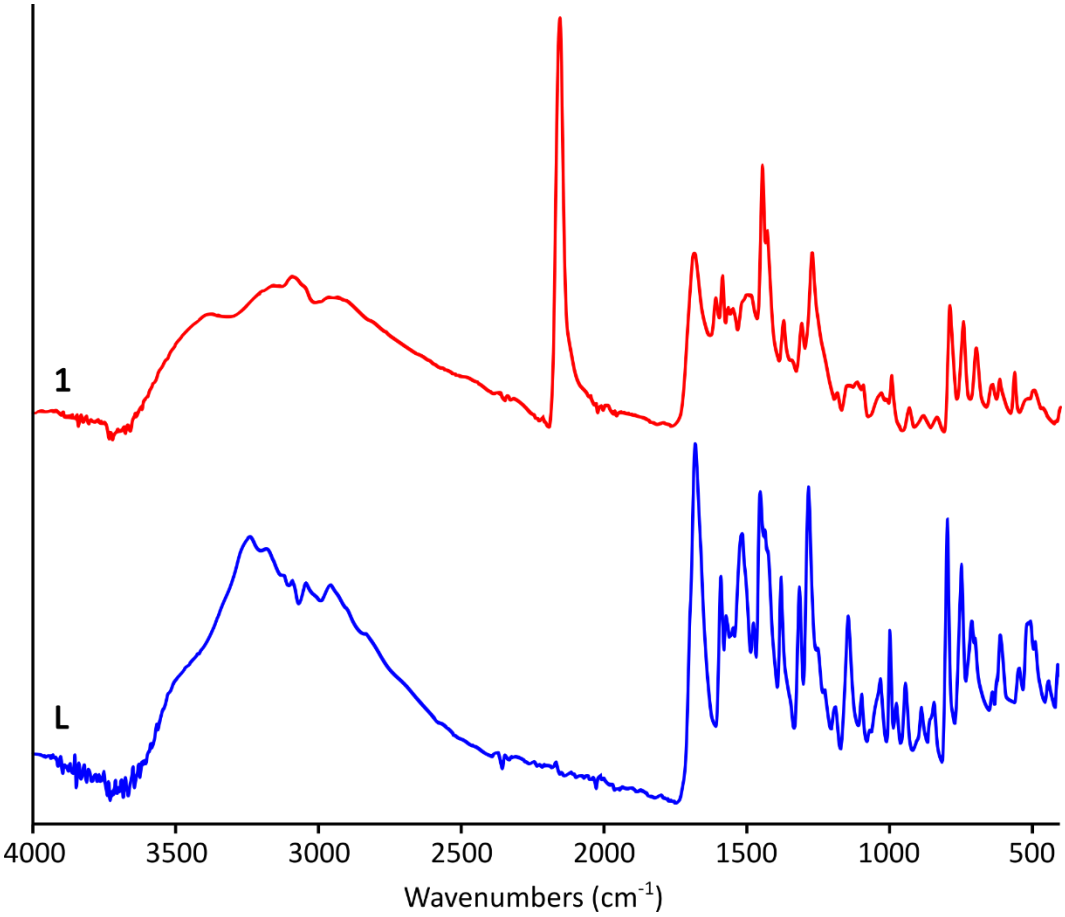
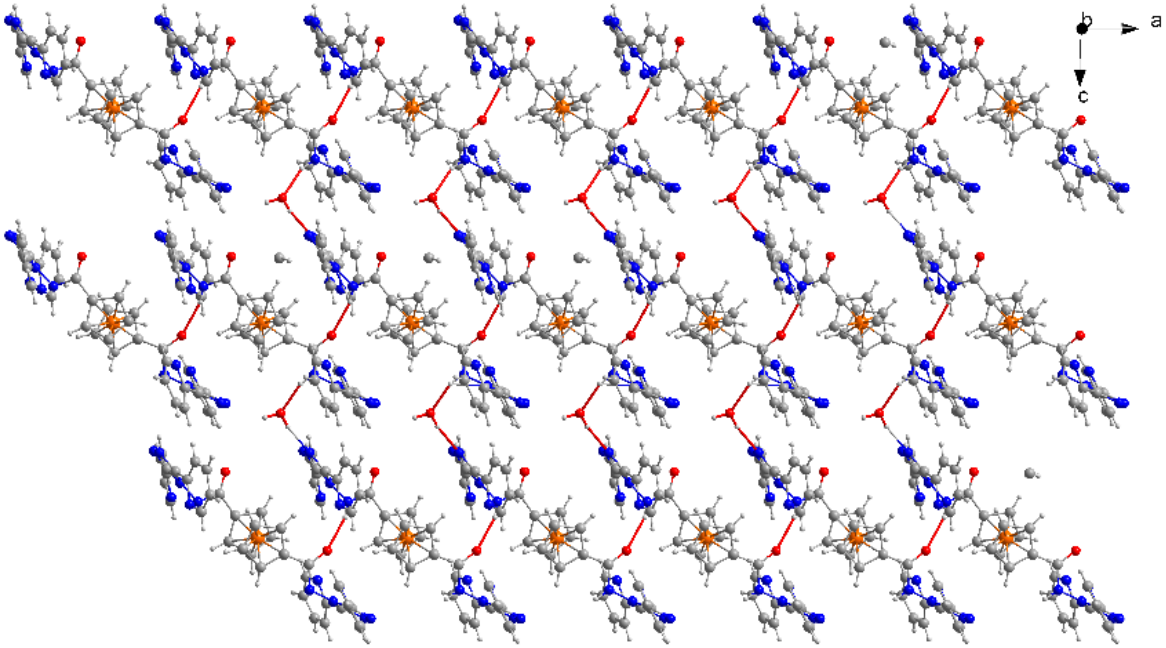
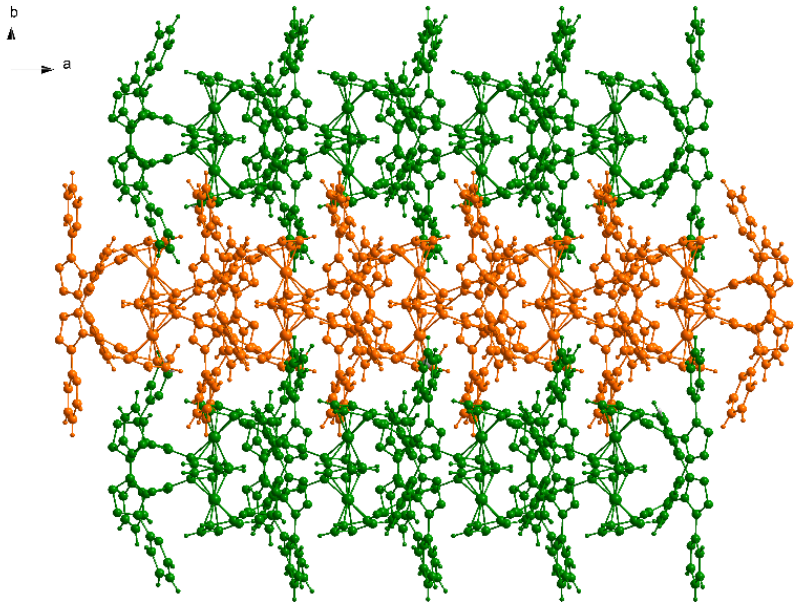


Figure S4: Comparison of FTIR spectra of studied ligand **L** (blue) and complex **1** (red).



a



b

Figure S5: a) Representation of the two-dimensional hydrogen-bonding network in the crystal structure of **L**. The network of interconnected neighboring molecules of **L** is parallel with the plane *ac*. b) Representation of the final three-dimensional network created by interconnection of layers by C–H···π interactions. The layers are colored for clarity (orange and green).

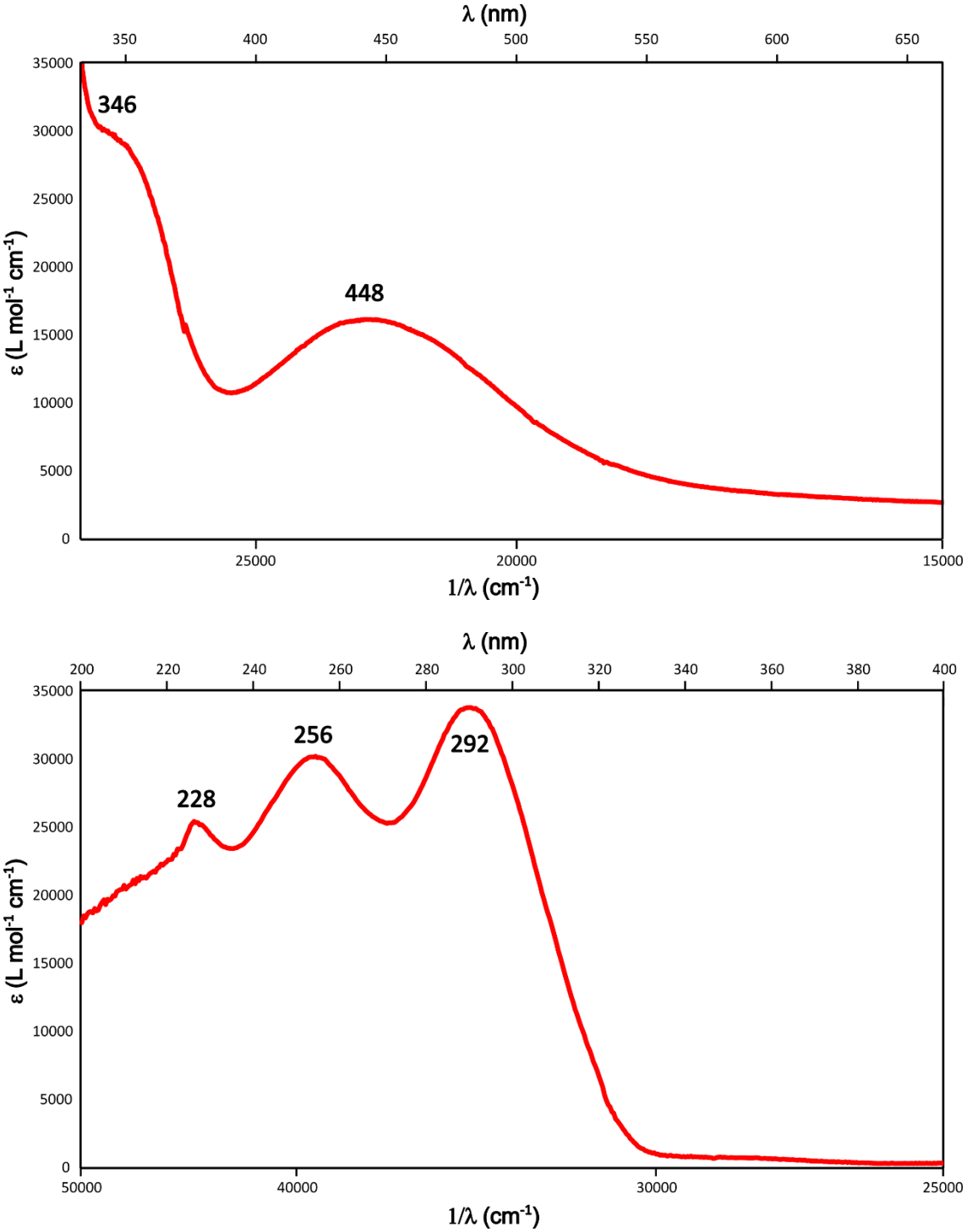


Figure S6: The UV-Vis absorption spectrum of ligand **L** in DCM solution with molar concentrations c = 2.1 mmol/dm^3 (*top*) and c = 43.2 µmol/dm^3 (*bottom*).

Table S1: Crystal data and structure refinements for **L**.

Formula	$C_{36}H_{28}Fe_1N_{12}O_3$
M_r	732.55
Color	light orange
Crystal system	monoclinic
Space group (space group no.)	$P2_1/c$ (14)
a (Å)	7.8354(3)
b (Å)	19.2990(7)
c (Å)	22.5050(12)
α (°)	90
β (°)	90.709(5)
γ (°)	90
U (Å^3)	3402.8(3)
Z	4
λ (Å), Cu Kα	1.54184
D_{calc} (g·cm^{-3})	1.430
μ (mm^{-1})	4.025
F (000)	1512
Reflection collected	15556
Independent reflections	5992 (R_{int} = 0.0435)
Data/restraints/parameters	5992/153/527
Goodness-of-fit on F^2	1.169
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0892 wR_2 = 0.1722
R indices (all data)	R_1 = 0.1597 wR_2 = 0.2007
CCDC no.	2177052

Table S2: The XYZ coordinates in Ångströms of the molecular structure of **L** optimized by DFT. The charge of the compound was 0, the spin multiplicity was 1.

Fe	3.26745108170459	12.60462299047482	4.65514021158902
O	6.28640965971098	12.75299190638555	7.13910726656723
O	0.51506224751068	12.40753380934100	1.87585988468957
N	-1.57911095098134	13.22977661850076	3.42915249222346
N	2.91552664165603	14.54275100744953	9.71648124241734
N	-0.35265257528073	12.85502189842584	3.96670960117574
H	-0.54394389513159	12.37394362869379	4.86756040617111
N	-3.16397951805303	14.13538024698879	2.20523186649533
N	4.84707079398555	12.42348680235383	9.43781555788381
N	4.24620239971401	12.70406653171155	8.21538527965241
H	3.43328989295767	13.32209002393469	8.40629222571350
N	-1.94606644345532	11.42416969905667	5.64508354619860
N	-3.74448169001279	13.20098339061902	3.01872711835081
N	6.10328554809402	11.58109250540997	11.03219391702422
N	5.47009417758244	12.68467383418114	11.53568012345860
N	0.19702382591695	15.45099046909754	2.46852876837388
C	2.07301601813388	15.58173506326349	9.80346777140212
H	1.35331757738421	15.68865945806041	8.98434137832695
C	3.83113081551598	14.36357686305105	10.69742927932560
C	-0.92274356308579	15.09663832518571	1.80470607735845
C	3.13610176513036	10.70395218413829	5.38809165100269
H	3.55556231231988	10.38912061039888	6.34650011920970
C	5.71874004016156	11.41122428095007	9.76590795065592
C	3.03824888347671	16.29999972827307	11.88974969764494
H	3.08555964480019	16.98837165503851	12.73933672412489
C	5.08364943011303	13.01374323907849	7.13865210507677
C	-2.97896967177723	11.62992769581689	4.79433709596574
C	2.09291097527261	16.48754982406692	10.87047404898608
H	1.38379859040368	17.31987462164958	10.89871141347104
C	1.83992168604081	11.28139752918662	5.19675282636225
H	1.09140865053300	11.43220655149404	5.97608340213325
C	-4.33424854684691	9.99500410983069	5.93047758551828
H	-5.26803125122117	9.43536783685210	6.04314772048734
C	2.79310014047840	14.58912686565220	4.58465059960992
H	1.84789696458080	14.97805782078785	4.19856338787542
C	0.78246645821744	16.89557951766147	0.62185913675813
H	1.49605203380646	17.60433041786991	0.19104467046359
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H	3.18161935796861	11.44369610535647	2.08737268204356
C	4.37774873118312	13.63017094325176	5.99302129728300
C	-2.78763330672791	12.64572471055713	3.75516600217398
C	-4.19705442928111	10.93209489850703	4.90327160507141
H	-5.00477831289329	11.12889916521923	4.19392588254170
C	3.02679777210333	14.15465868434609	5.92877080925978
H	2.30531399114828	14.20364567059873	6.74582172240857

C	1.71849572828312	11.63549509081697	3.79537046881531
C	-2.08728652329663	10.51763357785641	6.62248073586891
H	-1.22344883760336	10.38175256138692	7.28248749507914
C	0.59561279294517	12.30319965359237	3.09944795660250
C	1.02292865655308	16.32796570130219	1.88036738860508
H	1.92425503620703	16.59340581601791	2.44618415526663
C	4.71543416444398	13.20138233488881	10.57170516145215
C	4.95527235746101	13.73773413288807	4.67168249410034
H	5.95736428542707	13.40741248541401	4.39636034770723
C	-3.26150052965225	9.77854853323589	6.80814843650346
H	-3.33022013215167	9.05041401693576	7.62144802910135
C	-1.85462168883549	14.16621543931687	2.45980872298344
C	3.97567269355381	14.32886608747835	3.81066436711128
H	4.09460322580651	14.52045114151501	2.74291902574156
C	3.92614893402490	15.22432150625291	11.80760043244833
H	4.68144238279065	15.04272343726270	12.57631455678946
C	-0.38620464612855	16.53057791564718	-0.05932953475688
H	-0.61410460449202	16.94741211519434	-1.04551814189455
N	5.35239718034762	9.88185007426264	7.92545052312357
C	7.37986378888230	9.64941654204624	9.23145348116682
H	7.99856262683906	10.01832319767128	10.05336559107069
C	6.16059292143452	10.28678607545107	8.92705342275924
C	7.77257073831425	8.55557795177059	8.45519335686507
H	8.71730549843577	8.04257702770230	8.66150610132416
C	6.94085288471978	8.13540692423428	7.40884702116178
H	7.20925309857945	7.28671149687423	6.77261803449832
C	5.74463835964287	8.83186350855338	7.19000062610992
H	5.06542774013409	8.52919613637068	6.38372967527535

Table S3: The XYZ coordinates in Ångströms of the molecular structure of **1'** in the low-spin state optimized by DFT. The charge of the compound was 0, the spin multiplicity was 1.

Fe	1.79182146261960	14.45525408557916	-3.93444468329017
N	0.13628829290430	15.28954376618612	-3.53954125659527
N	3.44754433178615	13.62549527295553	-4.33628148363713
Fe	-0.61098378642670	18.13093021665578	2.38311893900849
C	-1.45708911013417	16.34397519025232	2.81023139561113
H	-2.26868655599978	15.87888370448432	2.24982723815220
C	-1.57832482780070	17.21439725069071	3.93899135423066
H	-2.51429014560801	17.54049331947162	4.39455866671430
C	-0.26230282157365	17.62643148528273	4.33866531207757
H	-0.02901080947579	18.32528108160748	5.14394054799616
C	0.69320310688944	17.01768706331238	3.46529531134456
H	1.77450010607213	17.15051810985397	3.51525126789708
C	-0.04537481554009	16.20565876313114	2.51441162868400
C	0.44126554425057	15.61260822903893	1.26475403718976
C	2.93104996776971	16.72885204234086	-0.72774243171989
C	2.04289776007177	14.77128803999378	-1.19624489802716
C	1.52152733842978	13.42533665521838	-1.27787789083344
C	1.25327122926487	12.56559777639385	-0.20728767755444
H	1.37022482083839	12.91593963809518	0.81966541360316
C	0.85224560117879	11.25583967100493	-0.48767474039753
H	0.63896268638539	10.55917771973219	0.32749209744120
C	0.73610655456769	10.85678944503954	-1.82431474909952
H	0.43063915603814	9.84213345781882	-2.09181608976188
C	1.01318736692559	11.77411586950016	-2.84215982593551
H	0.91762849682375	11.50628347672818	-3.89565261501944
C	3.41486115156696	17.87658680439178	0.03679273594506
C	3.74717857109605	19.08577912662624	-0.59930289597926
H	3.63811099136983	19.18815555723043	-1.68150122133334
C	4.20281116819248	20.14337177677814	0.19334645841343
H	4.46699469133531	21.10037466958021	-0.26567228184746
C	4.30333127557254	19.96385229447076	1.58049555167172
H	4.64559407828028	20.77049372915482	2.23416882506329
C	3.94527064971401	18.72384219815801	2.12461336841096
H	4.00185486846847	18.54343949224331	3.20278742594598
C	-1.78377000449699	19.72025550965124	1.93561951073963
H	-2.69500355709606	20.00296649691917	2.46339623219483
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H	0.10074779540515	18.10672314060125	-0.35777180149086
C	0.46789840547974	19.51602497331288	1.35500609417242
H	1.54975956500807	19.63130911864612	1.34072232511337
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C	-0.11204609313138	20.96867674866964	3.47070290826435
N	1.84557178265898	15.54423849616614	1.14272982031897
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N	2.31850851086365	15.62077455564017	-0.16615053713302
N	3.03323006883110	16.55125849624152	-2.04052178668451
N	2.46117289768584	15.35246078792707	-2.32519228696849

N	1.39176782002311	13.03910276268751	-2.58501660748766
N	3.52117295089350	17.69592691436669	1.37494869103695
O	-0.29294799343283	15.17722237429841	0.37148610823231
O	-1.00754809489734	21.44872686588296	4.20576133111832
N	1.20133468798265	21.19293468011344	3.70665085853778
H	-0.57937155924122	7.72799059087554	-7.69425023739468
C	-0.39111777933200	8.71262144046877	-8.13199162340820
H	-0.91295130274735	8.13071340268337	-10.16666705616704
C	-0.57668048442871	8.93243160711654	-9.50379879178038
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H	0.21902252115811	9.63745837529893	-6.25536756763005
H	1.16645004960992	12.77287197451602	-9.59649762045202
H	2.64282858362726	17.40990632978738	-3.95773833365335
C	2.52628309936359	17.15391894286562	-5.01183964379243
C	0.27759222131985	11.01297235624643	-7.93582368895618
C	3.64222333907922	12.93006248566086	-10.45032036998921
C	5.58282980255618	9.53318258981318	-10.07259275747237
C	3.29039326404026	9.42796742213828	-9.68736954445267
C	6.93384177947719	9.45856732582982	-10.68340651392824
H	6.02222518437243	10.83673223179365	-8.27979606079595
C	5.29046896712944	10.29464161119210	-8.87846907350825
N	2.16870178873749	15.88462332565516	-5.27783056499656
C	3.13678762196909	13.40947628042836	-9.15942714182439
H	3.34116111588466	10.71825982201107	-7.83768969320513
H	4.19412978285335	8.39901830768445	-11.47271277293711
C	2.01406303329846	15.51491457778639	-6.58656695289920
C	0.72019444171256	12.16820901021646	-7.15774310376575
C	1.52217826303185	14.15868857406787	-6.67602475525104
H	6.17562731060836	11.87612932842061	-12.41835753036487
N	0.09785210432224	11.23092893239561	-9.26017494397701
C	4.33174968998191	9.00313801213415	-10.57457600244380
C	3.88016562706903	10.22035848329518	-8.64604946958077
N	1.73368838819955	13.42599360295092	-9.02386396894079
C	2.23797528259536	16.39489543757052	-7.65096242658470
H	2.22949623400005	9.20519134970910	-9.80128085507051
C	5.22223417115395	12.12399482132693	-11.94846313655917
H	5.84797605120875	13.33492565600448	-10.14555085010121
H	3.72912985256169	11.06450308344065	-13.26599418021938
H	2.10162240535933	16.05699750152439	-8.67974848971616
Fe	4.29680402529192	11.02942644458936	-10.48518450435102
C	5.05940511886361	12.88421318287541	-10.74875265022619
C	2.75957933514707	18.09106368045981	-6.02254384649618
C	2.61905221933644	17.70864943292585	-7.36163384112638
N	0.61706679703163	12.32934334173427	-5.84328936153603
H	3.05044814521924	19.10800198996878	-5.74755325600096
N	1.27673409366711	13.30825248214117	-7.71284454547405
H	-0.43238635941540	10.41756680122874	-11.08907912517818
H	2.79736142118408	18.42114814058016	-8.17148282664990
N	1.13367204533328	13.55264388471188	-5.55047385208669
C	-0.31093702733801	10.20628643802302	-10.02169785828434
C	3.92888201243711	11.68779054189470	-12.39319583968587
C	2.94431602775051	12.17201197030728	-11.47358566829174

O	3.86345589457492	13.80756230807581	-8.24250590550065
O	7.90899714688113	10.06833217163991	-10.18327695875933
N	7.06469614924309	8.69340487569211	-11.79004030329350
H	1.87034636535130	11.99403959580437	-11.54011109818189
C	-0.72151381551115	15.92477295091895	-3.05977151090451
C	4.30078075823101	13.01050329252301	-4.84975625131976
C	-1.73985889430700	16.71938471405237	-2.51456721146281
C	5.30851678818788	12.23557605500292	-5.44040229890213
C	6.31454417486092	12.84407300258288	-6.22529836595341
C	5.27176856462968	10.82970412363254	-5.29216533077646
C	-1.74024957175710	18.11000219546969	-2.77048322488067
C	-2.72191057863798	16.15248463284264	-1.67047989495864
N	-3.53987115629851	15.68519683899764	-0.97019587909724
N	-1.73467943776098	19.26348403025100	-2.98885979391783
N	7.15063445791492	13.34716436788036	-6.87785254773471
N	5.23392863563490	9.66364728931899	-5.16163373118956
H	7.96377929920681	8.65556439118233	-12.25824981484830
H	6.27637976213391	8.22020843056367	-12.21521433462809
H	1.93120819397879	20.75227050776756	3.15830319439581
H	1.46828953747361	21.71201511698955	4.53623650796093

Table S4: The XYZ coordinates in Ångströms of the molecular structure of **1'** in the high-spin state optimized by DFT. The charge of the compound was 0, the spin multiplicity was 5.

Fe	1.78042170464836	14.53280729019486	-3.99276394124730
N	0.04412847603938	15.71872672720887	-3.93219097055860
N	3.52877626923488	13.36637684424737	-4.04470474471824
Fe	-0.75167632997886	18.39803052308083	2.88849816062979
C	-1.71531657072353	16.62278752941332	3.01749925656698
H	-2.55909902486846	16.30732096673228	2.40338753840581
C	-1.77388159847156	17.29492701954034	4.27919509920305
H	-2.68433365317698	17.59813502590939	4.79802988907968
C	-0.43177638763326	17.54652580234831	4.72213490056108
H	-0.14762716396403	18.08339188899532	5.62906101989265
C	0.47685616215375	17.03361517443486	3.74310785439019
H	1.56447282091253	17.09110585385237	3.79897362275767
C	-0.31765443863161	16.44390055077771	2.68007689158955
C	0.12936536693271	15.97675187165065	1.36187338566650
C	2.70932450938033	16.97318817265619	-0.59515126900291
C	1.80873177604940	15.02262442044364	-1.09456258624610
C	1.18560582541083	13.70349976053715	-1.13620042467427
C	0.81691417878357	12.94313438436593	-0.01892474344190
H	0.95872999587544	13.33334593652507	0.99029463643369
C	0.28279501520571	11.66675433378361	-0.22932125878583
H	-0.01045035657528	11.04918035343485	0.62409840771258
C	0.13420528686556	11.19553465010957	-1.53918176197585
H	-0.27965631113641	10.20506620792641	-1.74484501327364
C	0.52738213461938	12.01643180581384	-2.60123075359898
H	0.43247231221601	11.69256005676734	-3.64138917926710
C	3.20711577470335	18.09152566250578	0.20962866923461
C	3.51616651462884	19.33316520746726	-0.36947171474135
H	3.34977298916207	19.50206815562160	-1.43574594427896
C	4.02949322900735	20.33583860667309	0.46006637108434
H	4.27892174101257	21.31726968988733	0.04658764055548
C	4.20946166769665	20.06839690128137	1.82412824824123
H	4.60146040959467	20.82857115990895	2.50511786272088
C	3.86229980007139	18.80179666988029	2.31193378274981
H	3.97564484212676	18.55476234340363	3.37237991648077
C	-1.76257389627541	20.15056788224192	2.77378282481637
H	-2.61937650167806	20.43159300511829	3.38681657448056
C	-1.80079741533072	19.48279689329866	1.50624300797265
H	-2.69834521964941	19.15298357793898	0.98207058798872
C	-0.44979842659574	19.27982724408086	1.06578052475442
H	-0.13506605816642	18.75561233693379	0.16254918673255
C	0.43287165984175	19.82027833414195	2.05289923212870
H	1.51968699296258	19.81449873626688	2.00350237632915
C	-0.37543088203586	20.36789853167148	3.11939608712555
C	0.08667109890366	20.93789443433478	4.40874633143345
N	1.52157649889362	15.82769984784372	1.23174490051900
H	2.15079170841814	16.39920772688554	1.82517118966547
N	2.01803514874860	15.89450197162551	-0.06589850402410
N	2.92093020683518	16.76127823019561	-1.88691840757579
N	2.35461526010932	15.55720491240351	-2.18899631548581

N	1.03875289910238	13.24259108706031	-2.40844371096758
N	3.37887040631629	17.82802346468164	1.52688686278034
O	-0.62916732808043	15.68392502698787	0.43065531230784
O	-0.72500550751783	21.34691554695074	5.27296453908692
N	1.42432356184157	21.00263651373262	4.59962869791249
H	-0.27776518039630	7.51185885001521	-7.77000306903079
C	-0.02724184759828	8.47072627727719	-8.23297535072654
H	-0.39216135071762	7.80850298114540	-10.27681379128448
C	-0.09149008809543	8.63183681042829	-9.62338980082323
C	0.36850917350755	9.55247335543596	-7.43984917144341
H	0.43956808180728	9.46956095807381	-6.35316381941767
H	1.73857108014423	12.43194033746925	-9.73282749777001
H	3.00248754099285	17.42573265269649	-4.39479106759806
C	2.94075714468941	17.07105231353061	-5.42721333304893
C	0.68239462342174	10.76139208401411	-8.08187514969914
C	4.24900962542922	12.60102003818710	-10.47491982920645
C	6.06029557694137	9.10836899097723	-10.39696372588967
C	3.74956940189398	9.05015484681270	-10.13451027068774
C	7.43641154841475	9.04908050544125	-10.95042939455247
H	6.44840491839424	10.18713840911376	-8.44750298873118
C	5.73341154262081	9.74193509171500	-9.13902633942453
N	2.49402431173824	15.81657465064402	-5.59650236688012
C	3.69103965760106	13.02896076468846	-9.18542288596016
H	3.74419617869960	10.13196840436789	-8.15759592657876
H	4.70726080621951	8.19425713518602	-11.98119798388717
C	2.38745693934640	15.31901295118019	-6.85886604237951
C	1.06339305604573	11.95128610322766	-7.31941536405316
C	1.82212785111417	13.97341634876171	-6.87419053415129
H	6.82872314852442	11.67408635472916	-12.44745329030369
N	0.62276968040239	10.92219154444040	-9.42486575263518
C	4.81968558965543	8.68744652980848	-11.01434354224927
C	4.31071530796959	9.69953160102796	-8.98400968052561
N	2.28748536310697	13.08041797339401	-9.13691171715709
C	2.73866552326674	16.06719501470633	-7.98981852238836
H	2.68910757906176	8.88402910995686	-10.32244115228746
C	5.86448627396044	11.90315800204049	-11.99026951138181
H	6.45111473845559	12.89781136956732	-10.04793127893307
H	4.39556141640711	11.04348169789146	-13.47080876124497
H	2.63090116003139	15.64613574742271	-8.99107101609503
Fe	4.84536779502638	10.69025870416567	-10.69449247411461
C	5.67467171814483	12.53623373391814	-10.72226566068112
C	3.31271162074812	17.88278629696761	-6.50385156383732
C	3.21006028591323	17.37182357821142	-7.80336192303884
N	0.76385633551682	12.21510079931832	-6.05495651519437
H	3.67516881654172	18.89694816335221	-6.31761989008688
N	1.72394938715482	13.04073982118618	-7.86551161599409
H	0.22283166721046	10.03942607687392	-11.25460878241423
H	3.48912401928802	17.98123187464038	-8.66734967641906
N	1.24196550114882	13.46405792160444	-5.78508481671884
C	0.24950756090776	9.87432894343477	-10.17268717568219
C	4.57797782531629	11.56270055530087	-12.52880745976272
C	3.57162250175244	11.98008542472174	-11.59944823949112

O	4.37504443504191	13.37748845353196	-8.21643052331230
O	8.40653956922098	9.56029926753133	-10.34163766778016
N	7.59517639906889	8.40715924139602	-12.12960258686854
H	2.49604696368721	11.84894522380137	-11.72485492652836
C	-0.37179794033904	16.63662724963941	-3.32466369820925
C	4.03680634233576	12.47208347660125	-4.61417284488241
C	-0.83309692645673	17.74473878941521	-2.61010797384010
C	4.61808890203208	11.39056508147994	-5.28196555774708
C	5.86733792796581	11.54831737534089	-5.92662554189397
C	3.93879277843268	10.14976309565953	-5.31266788580312
C	-2.02823334296370	17.65864004219433	-1.85684782230552
C	-0.08356529808506	18.94501057588820	-2.63988067795162
N	0.54443096504699	19.93519604896536	-2.66223770110416
N	-3.02859112494740	17.58745579122161	-1.24995428667087
N	6.91252109884254	11.68271476276522	-6.44063808406640
N	3.36920107666639	9.12502234869618	-5.33895146397741
H	6.81447069776016	8.00705887135319	-12.63612461779901
H	8.51478305646105	8.38243466327275	-12.55698823366381
H	2.08669976687050	20.64796046511950	3.91938646734205
H	1.77843207181376	21.35637862525196	5.48189120280583

Table S5: The XYZ coordinates in Ångströms of the molecular structure of $[Fe(DAPP)(abpt)]^{2+}$ in the low-spin state optimized by DFT. The charge of the compound was +2, the spin multiplicity was 1.

Fe	0.46144985010774	3.80254145683909	10.50853020181794
N	2.06139887674299	3.54375220461022	11.82571028566010
N	-0.78179419619453	4.68910956227892	11.85579639229291
H	-0.92218370285676	5.63375287564888	11.48474225316091
H	-1.69695639713516	4.23462017275131	11.79513658984822
N	-0.36239121541499	2.02626986903868	11.01974437023971
H	-0.84053885035214	2.13622398579004	11.91983487271064
H	-1.10045239191821	1.82032323720892	10.34042100734731
N	1.27247999836270	5.54633120613317	10.19999317067203
N	-0.95575548054016	3.99021927844194	9.11350938967106
N	1.41599197908807	3.01953606050881	9.00173196626121
N	1.46762792440075	2.37240485503132	6.90306387145006
N	2.66339585718219	2.53564761247081	8.75846894673243
N	3.68435299361299	1.07355858511481	5.56976536327904
N	1.04576011301690	2.04798775228563	5.59589773704109
H	0.88506334985394	2.93600542539357	5.10685947941297
H	1.87876936573143	1.59854568934197	5.17478481630185
C	1.87225364237014	3.93809136010366	13.26925027795359
H	2.88061279851396	4.08465148129162	13.69539943280056
H	1.41945274174133	3.07729733157632	13.78224019107357
C	0.99479157429727	5.15285479782475	13.53178030386865
H	1.13058565598223	5.42290351461776	14.59320361716578
H	1.30463896146097	6.03310795194288	12.94206630045249
C	-0.47303492956728	4.83329908029516	13.30752751292287
H	-0.72486770242359	3.87915580253240	13.79781307109837
H	-1.12248862593679	5.61606901350398	13.73436087500969
C	0.52897405514555	0.83852783050836	11.11847683028751
H	0.97950424263621	0.67407985973874	10.12750138916161
H	-0.07404979547653	-0.05165979104096	11.36857605744453
C	1.60027821306397	1.04956878122394	12.17906150843423
H	1.11908690877401	1.22783453900100	13.15791683287547
H	2.16828606999016	0.10888895744628	12.28324986903295
C	2.61461707486972	2.13872761686453	11.84483886032448
H	3.44408497344509	2.11798175303085	12.57567457760812
H	3.03723255606162	1.94948591647758	10.84960500794943
C	0.66874900223139	6.62009712977552	9.64030178105869
H	-0.34124378508809	6.46736728221862	9.25596813538414
C	1.29305666126326	7.86434024064134	9.55011520405772
H	0.76017906095333	8.69884967799661	9.08680408745754
C	2.58877090367694	8.01506069835081	10.06022900294142
H	3.10296439646859	8.97918440725156	10.01024641895811
C	3.21284441488588	6.90410869306478	10.64234143758761
H	4.22083728392635	6.97150633872133	11.06036142139607
C	2.53246574001373	5.68558226718555	10.69262691270432
C	3.12431545478535	4.41967407723075	11.22564414651993
H	3.92601844339039	4.62015673549692	11.95568296785112
H	3.56193135208471	3.86125600286432	10.38257765184214
C	-2.18619438361345	4.53946223725552	9.23856158477269

H	-2.43289149962524	5.00306524906132	10.19287208319053
C	-3.13567452063126	4.55231652437612	8.21633016038695
H	-4.10605479843741	5.01980508006157	8.40161772681268
C	-2.82628268657490	3.96899037724584	6.98128440647829
H	-3.55070042318600	3.95792428002516	6.16266093520015
C	-1.56045577186527	3.40282380326134	6.81640590950215
H	-1.26860725602306	2.93833957096727	5.87354695032357
C	-0.65591456782415	3.43093896784325	7.88730482890805
C	0.68671858143175	2.91878350827302	7.87902844495289
C	2.69560571758660	2.14385523211649	7.48189043802660
C	3.86247267280370	1.55952480647201	6.82165855086580
C	4.74146869450321	0.53388088064929	4.94369195114439
H	4.55794471259917	0.15529203539830	3.93257504494592
C	6.01135335601220	0.44307125319913	5.52401579276150
H	6.83748673470439	-0.01012912187504	4.96938216231429
C	6.19104235559414	0.94373412207030	6.82125081876281
H	7.16880649361791	0.89264001131053	7.30944370289400
C	5.10332452408902	1.51445425709303	7.48587515036596
H	5.20192764761050	1.92190474856921	8.49462696026483

Table S6: The XYZ coordinates in Ångströms of the molecular structure of $[Fe(DAPP)(abpt)]^{2+}$ in the high-spin state optimized by DFT. The charge of the compound was +2, the spin multiplicity was 5.

Fe	0.29194250978439	3.60373689959227	10.64880460015837
N	2.12274634373492	3.52261929943690	11.91219547836122
N	-1.00055919364701	4.73450785320366	11.98109828819051
H	-1.09570694576346	5.66490045446364	11.56349227335291
H	-1.94637321221975	4.34486112859768	12.01321010042365
N	-0.41500461843056	1.75551628977741	11.52265629541827
H	-0.78706345028662	1.93632368017266	12.45978812175326
H	-1.20483178919023	1.42721930144534	10.96176060915168
N	1.24050617407984	5.48215560957184	10.11599256380286
N	-1.12541601049334	3.79184564521924	8.98360108873518
N	1.31210017239773	2.71756875528123	8.93976123507668
N	1.52457878511662	2.54502617513270	6.76386865111497
N	2.52417123405878	2.15279947044043	8.69699515589692
N	3.73969906026954	1.31584279455463	5.35454059867514
N	1.22853377919305	2.56523748451314	5.38454685347823
H	1.20412444841477	3.55092889443731	5.09969405809357
H	2.05800864785887	2.12375871529246	4.94773003604056
C	1.92568941698725	4.06815577013553	13.29882610215025
H	2.92481001795658	4.34170565320545	13.68768305955792
H	1.54936510129206	3.24195086504612	13.91982633016295
C	0.96586588348833	5.24927794801127	13.46327712672054
H	1.14791143070586	5.63860833520081	14.48029856512708
H	1.20045780433672	6.07994127769444	12.77558516738593
C	-0.51716562347054	4.88731105398376	13.38369040070115
H	-0.69717859851906	3.92917846666122	13.89854009762155
H	-1.11801436929083	5.65869247820202	13.89577877447880
C	0.60235368677319	0.67188058108716	11.61745740307497
H	0.97334857549099	0.47134802200705	10.59977868534514
H	0.13371678687770	-0.25528326829361	11.99240610709952
C	1.75279005162191	1.06122487477040	12.54323472073702
H	1.34843400251093	1.32691827962522	13.53710893643226
H	2.37032565946722	0.15969333804574	12.70081116111981
C	2.70392761527200	2.13934364306530	12.02044105957513
H	3.59643649337237	2.19000368616668	12.67392358314331
H	3.04339594026526	1.86381903017807	11.01077230334564
C	0.62995120660003	6.54341048069323	9.55492556955994
H	-0.38198038169732	6.37755988350001	9.17387405799804
C	1.24392264240427	7.79426223319870	9.46006319487972
H	0.71107968986149	8.62944765404996	8.99766360802301
C	2.54035442555306	7.94519712685193	9.96915778151664
H	3.05127989957440	8.91134483181531	9.91733129044703
C	3.17206018119870	6.84047547552789	10.55471690163122
H	4.17978496535967	6.91795365076695	10.97225607633998
C	2.49160049301110	5.61941268719681	10.61113018421949
C	3.10860469173179	4.36433366917650	11.16842518818316
H	3.97574351457150	4.60519748650718	11.80860198908002
H	3.47332113083655	3.75929727336047	10.32128066201491
C	-2.37076821742700	4.29140769413806	9.08471617125153

H	-2.73647355802456	4.49483143991091	10.09281657902259
C	-3.18381990650860	4.54514919625590	7.97808668176076
H	-4.18784318158935	4.95089974753087	8.12579974988027
C	-2.68290045299603	4.27395444888254	6.69834246517382
H	-3.28736285010225	4.46382153702720	5.80709360162782
C	-1.39229745982297	3.75268974299796	6.57216650086602
H	-0.97708027324357	3.52270609419651	5.59068999521733
C	-0.63972679776938	3.51727295950827	7.73454053866643
C	0.69352254276138	2.94616312516378	7.77308316257621
C	2.65833044317576	2.05229193226517	7.37365806710505
C	3.82970370684083	1.49585822940026	6.69339715399223
C	4.80121316461262	0.80680050319817	4.71028319464058
H	4.69007906339492	0.68005585160372	3.62821504022154
C	5.98838608929165	0.44687615706156	5.35711786548406
H	6.82190883295796	0.03198840370558	4.78381929206197
C	6.07709018256416	0.63169235101799	6.74382053360166
H	6.98890134604746	0.36434456336363	7.28609886521720
C	4.98387237312924	1.16698147750431	7.42898600674904
H	5.01405768368568	1.33326060669407	8.50812243947799

Table S7: The list of calculated frequencies for DFT optimized molecular structures in Tables S2-S7.

L	**1´** (LS)	**1´** (HS)	$[Fe(DAPP)(abpt)]^{2+}$ (LS)	$[Fe(DAPP)(abpt)]^{2+}$ (HS)
6.52	7.56	8.82	15.83	12.61
10.01	10.46	10.13	22.66	20.44
18.60	14.85	15.16	39.17	35.28
26.27	15.59	17.92	52.23	44.93
33.46	25.22	23.78	57.06	50.03
35.51	26.45	25.76	63.86	58.32
37.33	30.20	28.61	80.52	68.34
40.43	33.28	34.29	101.49	74.93
40.79	37.91	35.94	108.81	88.57
46.51	38.11	37.98	114.83	100.06
47.78	41.74	41.45	126.96	103.62
51.78	44.62	45.27	134.17	106.92
64.20	45.16	46.67	156.51	127.12
81.43	48.07	47.27	178.93	131.32
86.60	49.01	50.29	189.16	143.11
97.24	49.86	52.29	191.54	155.07
98.62	50.96	55.07	211.12	161.58
102.97	54.11	56.15	212.68	175.66
105.54	54.76	57.83	226.49	185.57
124.82	58.04	59.85	237.11	191.85
127.67	60.95	60.71	256.79	203.39
154.81	61.75	63.58	266.23	212.06
156.52	67.34	64.68	281.66	223.73
164.22	67.82	66.21	289.88	230.19
171.06	72.28	66.82	298.15	266.23
183.28	73.73	68.42	300.59	269.59
197.61	81.22	74.12	314.40	277.96
199.14	82.94	79.22	328.65	291.99
211.36	87.50	83.03	333.07	307.45
246.07	91.06	84.60	342.98	308.76
247.29	99.05	88.96	352.62	323.99
283.71	102.04	90.73	354.00	328.50
286.62	111.33	95.78	362.72	328.90
296.29	113.15	97.21	374.07	351.79
304.70	117.88	100.38	396.83	367.16
322.69	118.93	105.38	400.88	369.11
323.74	121.48	112.74	406.47	388.73
334.56	127.59	119.02	430.60	393.56
342.36	131.29	124.50	442.91	407.38
351.15	137.35	126.52	452.00	414.09
386.34	143.29	129.06	460.28	418.20
391.86	145.09	137.67	466.17	425.96
398.82	152.38	141.21	479.33	443.96
401.42	155.55	151.28	486.93	445.16
404.50	163.48	154.53	497.15	461.12
405.01	168.53	159.29	504.80	492.41
405.86	169.42	166.17	518.87	492.56

409.77	172.77	169.16	530.62	519.99
427.49	191.22	170.36	555.19	528.74
428.10	197.94	173.12	610.95	561.27
460.60	210.43	179.37	618.23	578.32
481.35	211.94	189.22	634.47	601.02
500.48	215.92	192.27	636.97	616.36
503.61	217.49	197.38	648.54	625.42
508.08	217.95	203.42	670.88	631.59
518.84	229.89	205.33	675.54	636.46
519.24	231.80	207.72	683.73	672.96
542.06	236.84	210.11	688.09	693.94
543.05	246.82	217.30	702.21	700.14
582.21	268.60	219.78	727.73	724.35
583.02	276.82	221.72	732.63	730.31
586.43	278.97	227.17	747.78	744.07
592.55	282.52	244.03	749.73	747.07
600.01	287.28	257.32	757.85	748.93
603.16	296.77	262.59	766.34	758.34
616.16	302.71	264.76	780.70	768.92
616.25	306.18	269.54	784.36	793.08
630.88	308.79	290.92	799.23	802.15
631.21	310.39	293.68	816.10	802.95
651.09	318.94	301.74	847.69	843.70
657.39	323.74	302.72	865.10	850.64
692.40	327.28	303.67	890.40	874.39
693.70	351.84	312.72	892.91	886.51
698.17	353.35	321.55	898.42	899.44
699.25	356.44	322.83	901.02	902.40
704.82	365.51	347.41	911.91	908.52
704.99	369.56	348.43	917.70	913.19
735.26	372.33	358.48	928.58	921.42
735.64	375.65	359.56	964.88	954.92
742.44	379.21	372.03	968.18	971.71
743.25	386.01	372.86	976.74	972.32
748.97	392.60	378.89	979.04	973.96
749.04	402.53	388.21	982.24	981.43
751.21	403.63	399.71	987.41	988.05
751.84	409.85	399.93	989.12	988.86
757.34	414.40	402.51	993.51	989.63
759.66	415.12	404.26	994.84	992.34
798.75	424.59	406.95	1014.98	1007.19
798.92	429.22	408.22	1015.44	1018.18
800.01	437.82	417.34	1020.83	1022.17
800.49	447.03	419.67	1024.62	1023.90
816.19	449.69	424.83	1026.51	1023.98
817.94	452.92	435.58	1032.87	1027.35
827.89	461.42	443.89	1041.39	1028.09
838.69	463.64	445.47	1048.61	1044.38
846.57	464.90	447.44	1062.58	1048.34
852.02	466.74	468.13	1068.67	1059.22

865.87	467.76	469.44	1075.15	1062.64
867.15	470.36	469.96	1078.16	1063.90
888.94	474.79	479.11	1080.41	1074.88
890.56	478.45	480.96	1094.74	1080.44
910.92	485.05	484.74	1097.01	1085.36
911.28	495.62	495.35	1098.51	1098.16
911.42	503.89	504.02	1107.29	1104.41
911.86	507.47	506.17	1114.01	1110.00
915.33	508.82	510.13	1134.70	1110.80
915.85	511.18	511.58	1140.62	1122.98
940.70	521.67	518.68	1143.37	1140.75
941.57	526.81	519.53	1143.73	1143.71
973.92	528.18	526.61	1151.06	1144.99
974.09	537.00	537.46	1156.80	1152.78
984.14	543.01	544.01	1165.03	1160.75
984.55	543.26	546.49	1175.45	1165.90
985.56	553.24	554.54	1202.58	1194.79
985.60	557.72	558.02	1225.89	1226.19
985.93	563.40	575.56	1253.41	1250.70
986.05	563.53	576.29	1264.10	1264.86
994.05	591.77	591.46	1268.31	1266.06
994.81	592.39	591.76	1278.16	1273.28
1018.76	595.61	596.38	1278.77	1274.11
1021.47	596.11	597.25	1280.89	1285.42
1021.69	597.69	598.61	1293.86	1291.89
1022.04	600.23	601.02	1297.25	1295.27
1025.17	605.70	603.67	1304.47	1303.60
1025.89	608.67	604.17	1309.09	1309.28
1037.66	609.29	605.32	1312.82	1311.48
1039.59	609.75	606.57	1317.69	1312.65
1039.93	613.02	608.77	1330.28	1322.61
1042.19	614.40	610.07	1337.54	1328.25
1052.16	621.01	622.85	1345.24	1336.31
1052.32	624.83	624.99	1355.10	1356.73
1058.94	632.06	629.02	1357.53	1358.21
1060.02	636.82	629.40	1368.14	1369.00
1067.38	641.33	630.46	1392.92	1387.25
1073.33	642.79	631.07	1403.93	1400.25
1095.26	652.06	652.63	1408.17	1407.54
1095.73	653.14	653.59	1417.58	1409.99
1098.12	678.64	662.48	1420.20	1414.13
1098.20	682.22	664.04	1423.02	1422.47
1104.84	687.14	674.84	1433.74	1431.44
1106.91	687.78	678.32	1434.77	1432.31
1127.59	688.86	693.89	1436.14	1436.01
1128.62	695.24	694.16	1440.43	1436.30
1143.15	696.79	698.32	1451.63	1450.70
1143.49	699.39	700.42	1460.20	1457.10
1144.88	702.42	702.00	1462.19	1457.96
1145.03	707.26	702.29	1464.05	1462.40

1183.60	737.39	737.88	1467.75	1465.97
1183.99	738.65	738.74	1468.98	1467.70
1223.68	742.39	739.45	1472.27	1472.06
1228.93	745.01	740.64	1488.16	1482.37
1261.77	749.04	748.18	1489.42	1487.47
1262.47	750.09	750.60	1527.81	1519.51
1272.49	757.12	754.83	1539.39	1533.02
1272.95	757.95	755.75	1552.33	1549.14
1277.23	758.48	756.63	1576.96	1574.90
1283.17	763.53	757.26	1580.62	1586.36
1285.36	766.25	766.21	1587.01	1587.94
1287.54	768.90	766.43	1609.08	1588.67
1308.26	785.73	793.96	1612.02	1611.03
1308.42	786.27	795.17	1621.95	1616.37
1313.51	796.97	799.34	1628.51	1623.83
1313.80	798.29	799.70	1638.31	1628.89
1325.65	805.59	810.42	3002.32	2982.14
1326.00	815.67	819.15	3012.82	2992.06
1356.42	820.71	822.62	3016.52	3009.00
1363.21	821.86	822.81	3022.34	3012.55
1396.87	824.60	825.62	3026.30	3018.08
1404.46	825.41	825.89	3026.94	3019.47
1404.68	827.10	830.83	3032.33	3029.84
1404.77	831.52	834.10	3064.99	3061.55
1417.31	840.38	840.81	3071.25	3065.97
1420.31	843.07	843.09	3078.35	3068.13
1429.62	845.86	846.67	3087.01	3078.17
1429.91	848.69	851.18	3090.21	3082.04
1439.95	862.55	864.64	3095.71	3087.63
1440.20	866.87	868.07	3113.03	3095.60
1452.65	871.75	874.44	3155.08	3148.88
1453.13	875.92	876.20	3163.27	3162.09
1463.24	892.50	889.79	3173.21	3166.54
1463.52	892.84	891.85	3174.58	3172.07
1463.93	901.62	902.69	3183.34	3176.22
1464.96	906.45	904.35	3184.15	3182.02
1501.43	909.88	910.79	3189.12	3182.84
1501.79	910.35	911.60	3189.40	3190.12
1518.52	910.64	912.80	3194.49	3191.14
1518.71	912.23	913.70	3196.04	3192.30
1581.84	912.71	915.06	3198.57	3195.85
1582.29	914.54	916.16	3211.92	3201.91
1588.38	919.60	920.26	3223.36	3215.92
1588.50	922.00	921.03	3353.94	3367.66
1589.79	955.49	948.55	3356.99	3368.20
1590.00	961.69	949.55	3374.81	3381.08
1608.64	985.88	979.94	3418.67	3436.17
1608.80	987.39	982.03	3422.72	3437.31
1614.49	988.03	987.05		
1614.66	988.52	989.27		

1672.11	993.10	992.80		
1675.70	993.83	993.19		
3094.14	996.22	993.44		
3099.95	998.01	1000.04		
3135.87	1007.75	1001.82		
3136.33	1011.54	1002.15		
3152.29	1020.48	1017.15		
3152.41	1023.03	1021.96		
3165.00	1023.13	1022.71		
3165.08	1024.70	1024.36		
3169.64	1024.86	1025.03		
3169.81	1025.15	1027.67		
3179.42	1026.96	1028.59		
3179.53	1027.26	1030.54		
3179.72	1029.13	1035.51		
3180.80	1035.30	1037.16		
3184.83	1042.79	1043.12		
3185.11	1043.39	1043.51		
3188.06	1043.81	1044.11		
3188.46	1045.33	1044.78		
3190.86	1046.61	1049.68		
3190.99	1049.69	1050.28		
3205.84	1049.94	1052.78		
3207.32	1053.35	1054.98		
3208.57	1058.22	1056.27		
3211.97	1061.46	1059.49		
3222.44	1071.24	1067.91		
3222.76	1072.84	1069.02		
	1073.69	1071.06		
	1078.39	1089.63		
	1098.37	1096.89		
	1099.48	1098.18		
	1099.81	1103.37		
	1105.95	1104.58		
	1112.92	1111.18		
	1114.28	1114.71		
	1144.32	1139.54		
	1146.53	1140.13		
	1146.63	1145.81		
	1147.26	1146.66		
	1149.25	1149.66		
	1149.40	1150.02		
	1181.61	1181.84		
	1182.39	1182.19		
	1187.59	1183.96		
	1189.19	1185.40		
	1214.91	1218.63		
	1220.92	1222.36		
	1221.61	1224.52		
	1226.79	1234.62		

	1240.34	1241.06		
	1240.61	1243.28		
	1266.40	1267.23		
	1267.61	1267.86		
	1268.52	1268.94		
	1271.83	1269.60		
	1278.61	1275.68		
	1280.34	1277.02		
	1285.90	1287.57		
	1290.72	1288.90		
	1297.82	1295.50		
	1300.58	1295.85		
	1309.51	1310.94		
	1310.10	1311.36		
	1313.88	1312.12		
	1314.44	1313.60		
	1344.13	1334.68		
	1345.02	1335.75		
	1347.63	1347.85		
	1349.07	1349.03		
	1354.13	1356.11		
	1357.98	1358.59		
	1369.20	1369.91		
	1372.56	1376.08		
	1397.54	1397.94		
	1401.62	1401.77		
	1407.22	1407.36		
	1408.13	1410.10		
	1412.18	1410.94		
	1413.59	1411.43		
	1414.84	1415.45		
	1415.07	1415.65		
	1418.00	1417.21		
	1418.35	1418.43		
	1437.89	1435.62		
	1438.72	1435.98		
	1445.22	1444.29		
	1447.75	1448.74		
	1455.69	1454.65		
	1456.43	1455.79		
	1457.80	1460.60		
	1461.96	1461.61		
	1475.02	1474.25		
	1476.12	1475.23		
	1476.99	1475.58		
	1477.25	1479.27		
	1493.33	1490.98		
	1500.31	1499.50		
	1531.52	1526.71		
	1532.95	1528.22		

	1558.35	1558.22		
	1561.43	1562.04		
	1576.71	1574.37		
	1579.01	1580.48		
	1585.92	1587.11		
	1587.79	1588.80		
	1590.29	1589.29		
	1592.25	1591.04		
	1596.54	1596.86		
	1596.85	1600.48		
	1612.62	1613.57		
	1613.90	1615.05		
	1632.07	1624.55		
	1632.89	1624.88		
	1638.87	1633.52		
	1639.47	1634.74		
	2137.38	2128.81		
	2137.69	2134.59		
	2160.47	2153.85		
	2162.54	2154.27		
	2227.63	2203.56		
	2233.60	2205.33		
	3108.07	3127.09		
	3141.36	3145.72		
	3165.28	3165.68		
	3166.84	3166.50		
	3178.11	3167.12		
	3179.13	3172.51		
	3180.45	3178.80		
	3181.72	3179.40		
	3186.56	3183.91		
	3187.96	3184.24		
	3190.12	3192.09		
	3191.33	3192.73		
	3196.03	3197.52		
	3196.80	3197.61		
	3197.50	3197.66		
	3197.74	3199.09		
	3199.93	3203.89		
	3201.04	3204.15		
	3204.24	3205.01		
	3204.91	3205.86		
	3205.21	3206.44		
	3205.61	3208.66		
	3208.77	3210.78		
	3211.56	3211.83		
	3213.50	3214.47		
	3214.40	3219.81		
	3218.60	3219.93		
	3221.19	3221.84		

	3223.08	3222.82		
	3225.72	3227.04		
	3226.49	3227.91		
	3226.73	3228.03		
	3226.88	3231.75		
	3238.45	3274.17		
	3476.80	3479.58		
	3480.43	3482.47		
	3601.00	3606.03		
	3606.56	3608.93		

Table S8: The list of TPSSh calculated values of the electron density at the iron nucleus (ρ_0^{TPSSh}) and the quadrupole splitting (ΔE_Q^{TPSSh}) for DFT optimized molecular structures in Tables S3-S7[a]

	{Fe(abpt)}^{LS}		**{Fe(abpt)}^{HS}**		**{Fe(Cp)}**	
	ρ_0^{TPSSh}	ΔE_Q^{TPSSh}	ρ_0^{TPSSh}	ΔE_Q^{TPSSh}	ρ_0^{TPSSh}	ΔE_Q^{TPSSh}
1′(LS)	11820.072272201	-0.490			11819.948596626 11819.948505317	2.291 2.302
1′(HS)			11818.924826778	3.300	11819.951281692 11819.948057032	2.290 2.301
[Fe(DAPP)(abpt)]$^{2+}$ (LS)	11819.926867403	0.367				
[Fe(DAPP)(abpt)]$^{2+}$ (HS)			11819.071137816	-3.173		

[a] values of ρ_0^{TPSSh} are in au^{-3} and values of the quadrupole splitting (ΔE_Q^{TPSSh}) are in mms^{-1}.