

Supporting Information for

**Tuning Metal-Metal Interactions Through Reversible Ligand
Folding in a Series of Dinuclear Iron Complexes**

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1. Spectroscopic Data

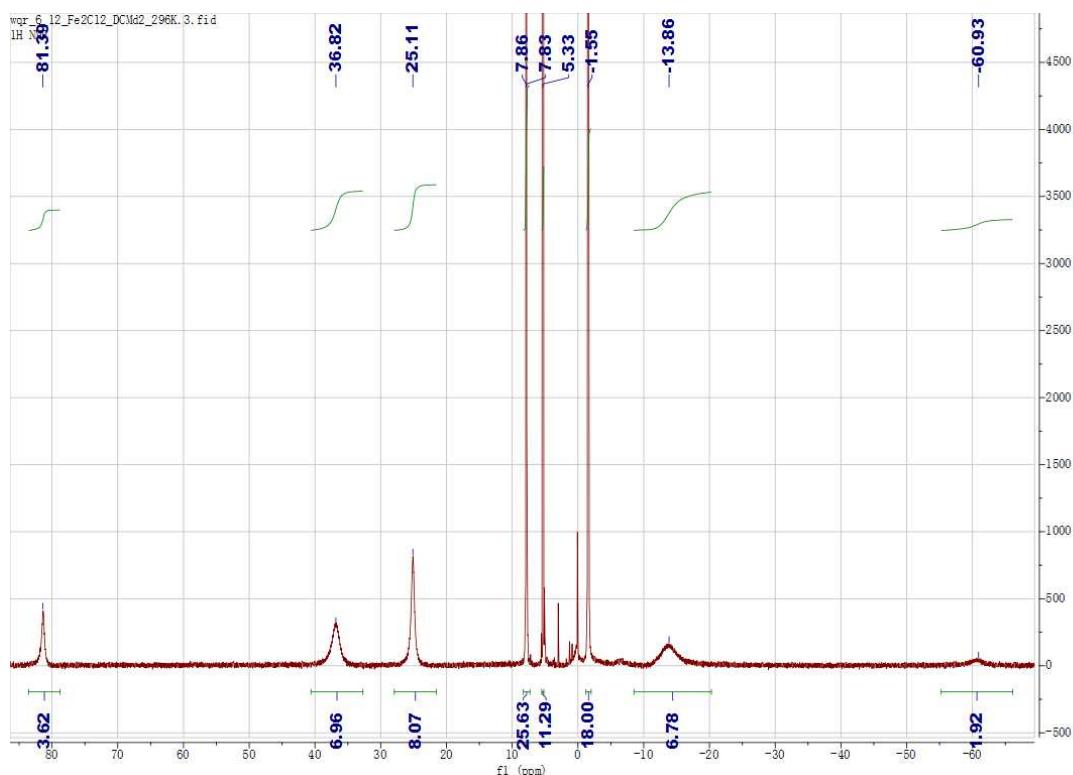


Figure S1. ¹H NMR spectrum of $[\text{Fe}_2\text{Cl}_2]\text{[BAr}^{\text{F}}_4\text{]}_2$ in CD_2Cl_2 (296 K).

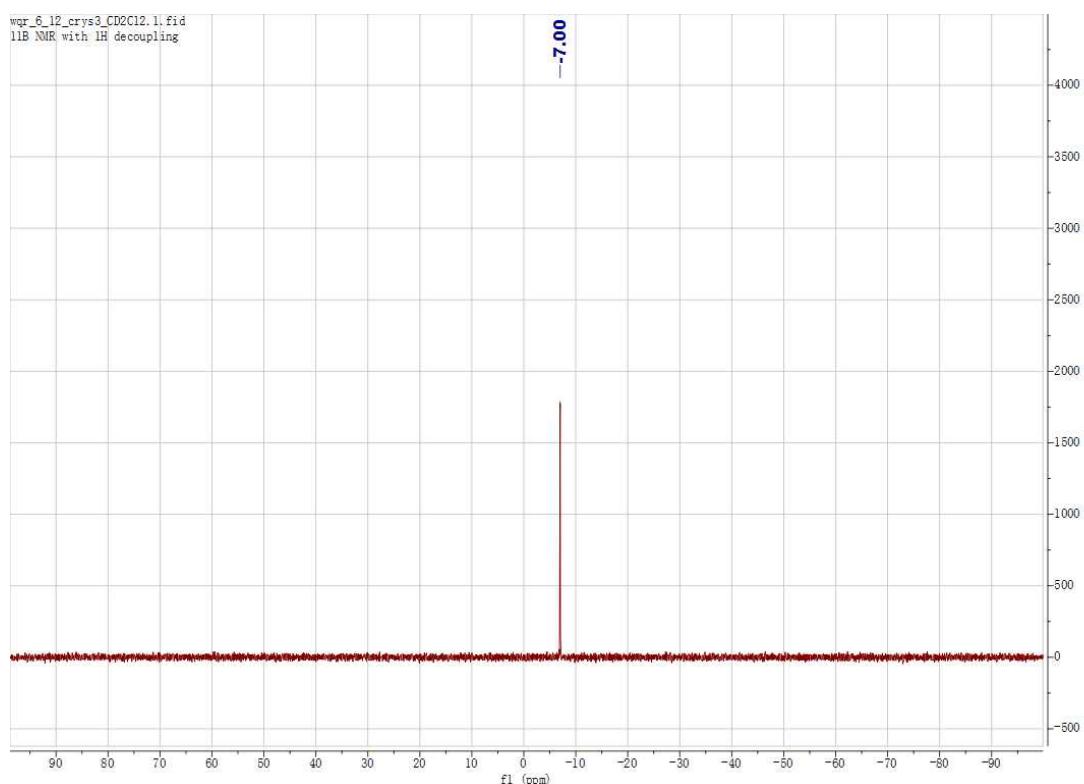


Figure S2. ¹¹B{¹H} NMR spectrum of $[\text{Fe}_2\text{Cl}_2]\text{[BAr}^{\text{F}}_4\text{]}_2$ in CD_2Cl_2 (298 K).

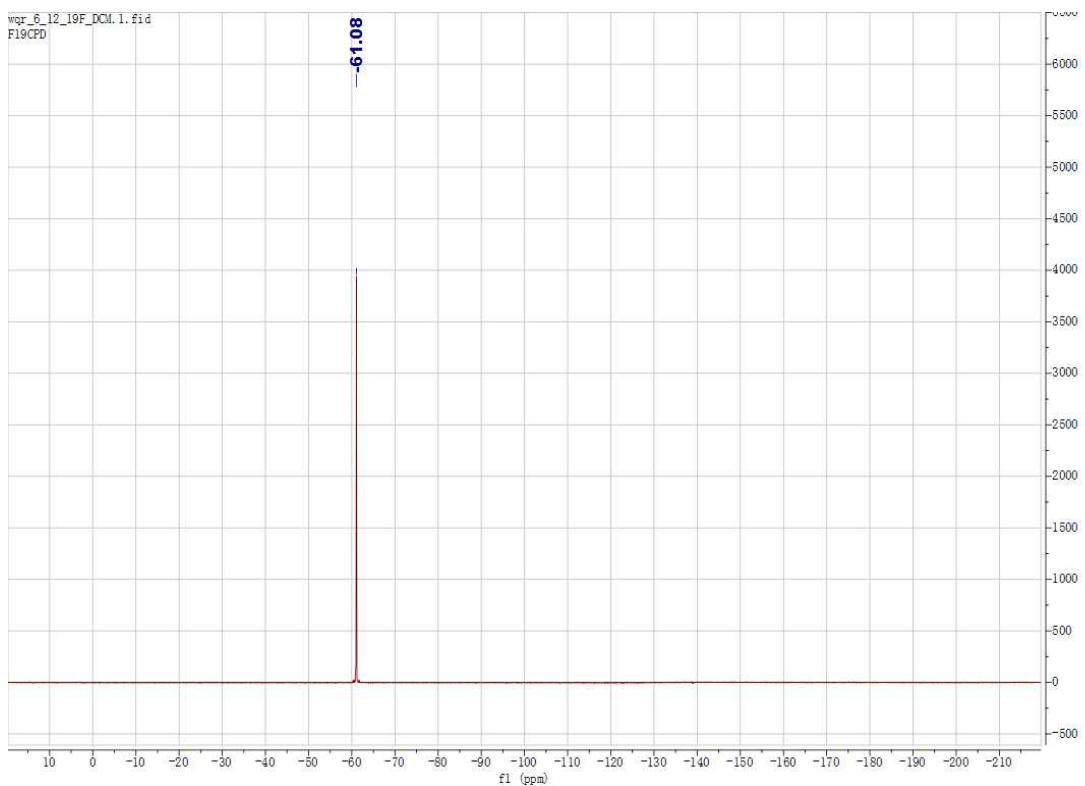


Figure S3. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of $[\text{Fe}_2\text{Cl}_2]\text{[BArF}_4]$ in CD_2Cl_2 (298 K).

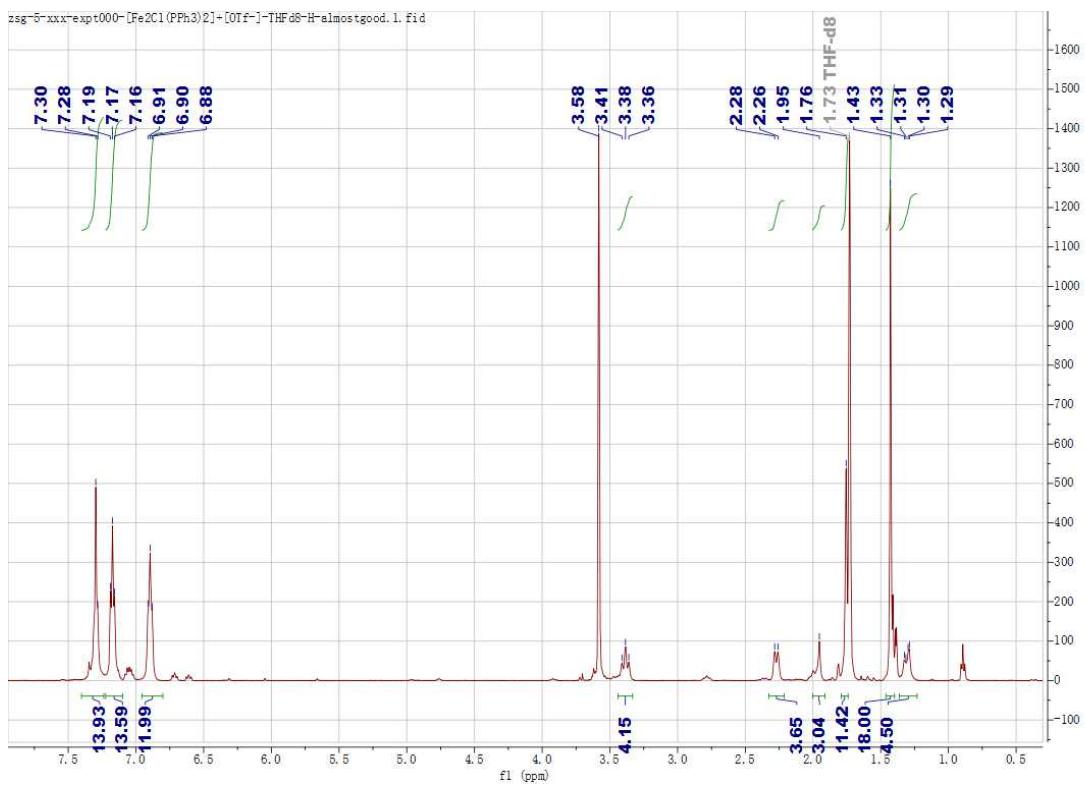


Figure S4. ^1H NMR spectrum of $[\text{Fe}_2\text{Cl}]\text{[OTf]}$ in $\text{THF}-d_8$ (298 K).

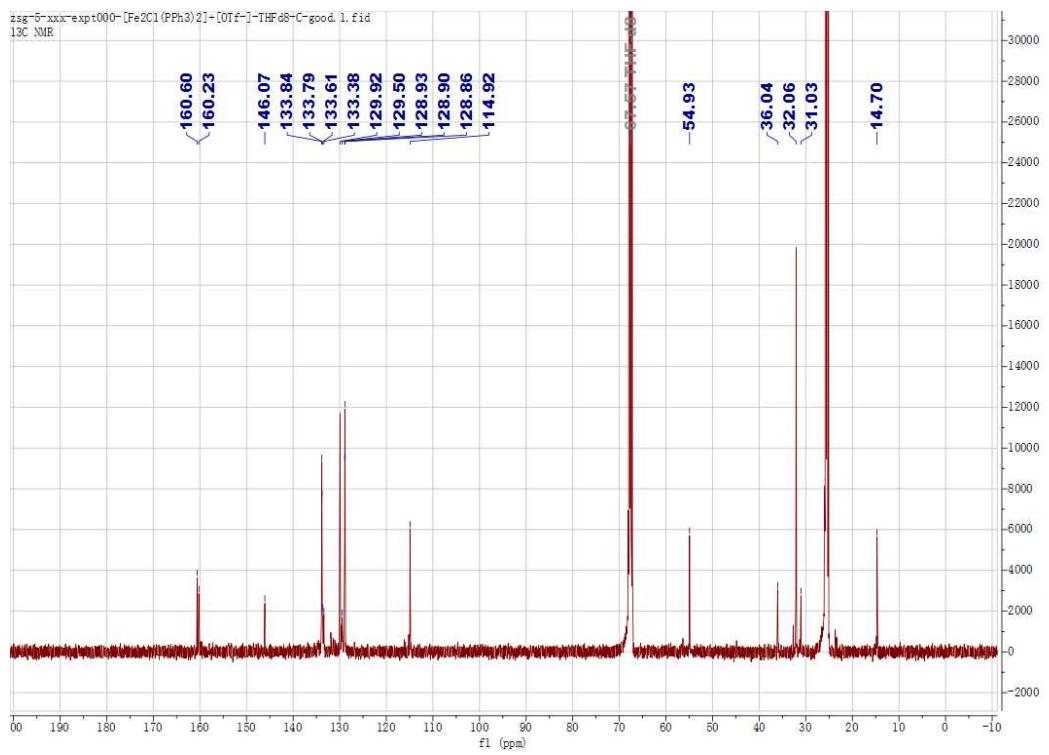


Figure S5. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of $[\text{Fe}_2\text{Cl}](\text{PPh}_3)_2\text{][OTf]}$ in $\text{THF}-d_8$ (298 K).

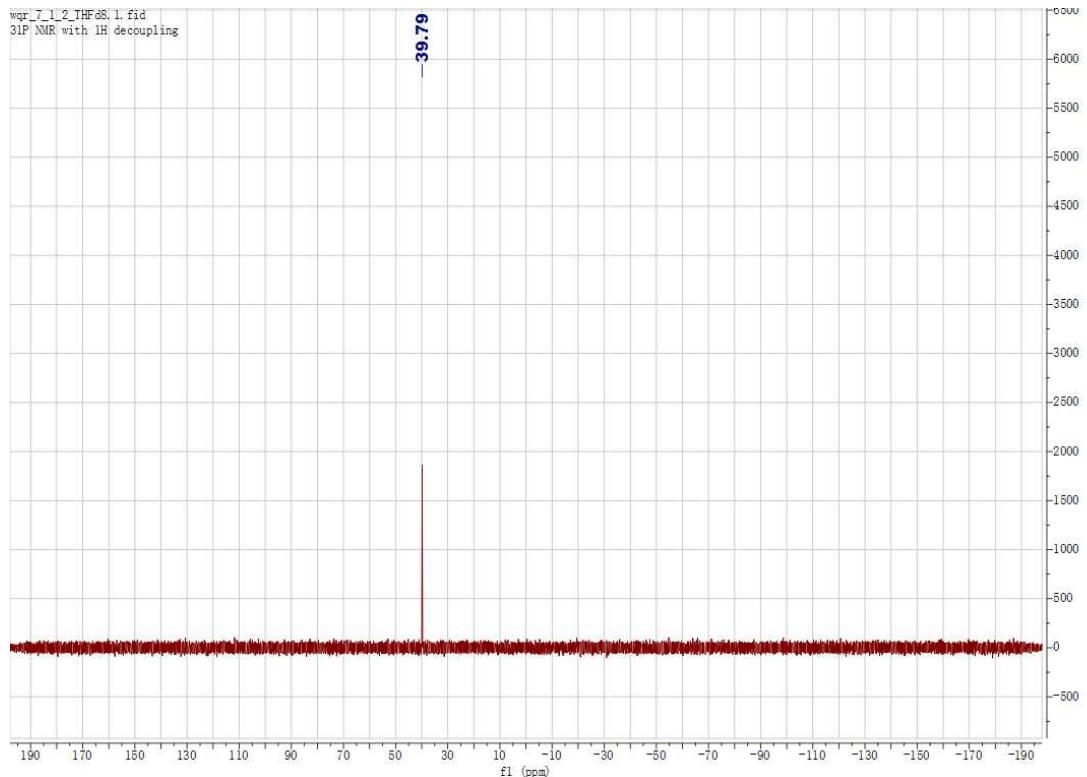


Figure S6. $^{31}\text{P}\{\text{H}\}$ NMR spectrum of $[\text{Fe}_2\text{Cl}](\text{PPh}_3)_2\text{][OTf]}$ in $\text{THF}-d_8$ (298 K).

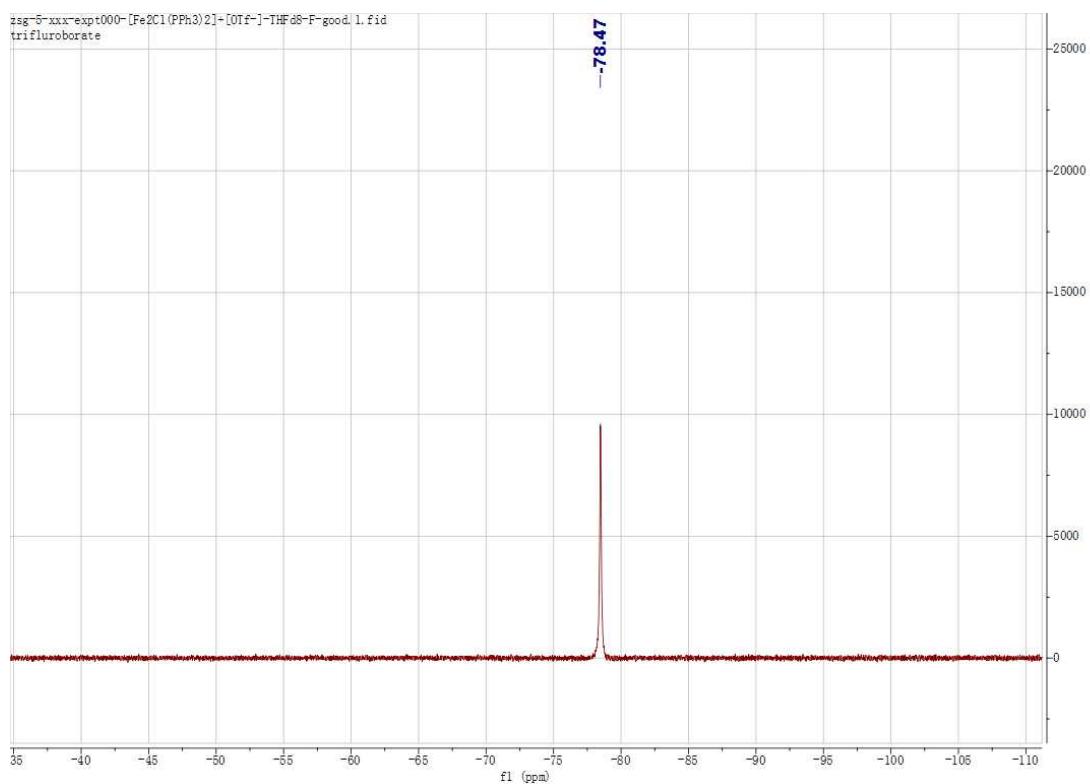


Figure S7. $^{19}\text{F}\{\text{H}\}$ NMR spectrum of $[\text{Fe}_2\text{Cl}]\text{[OTf]}$ in $\text{THF}-d_8$ (298 K).

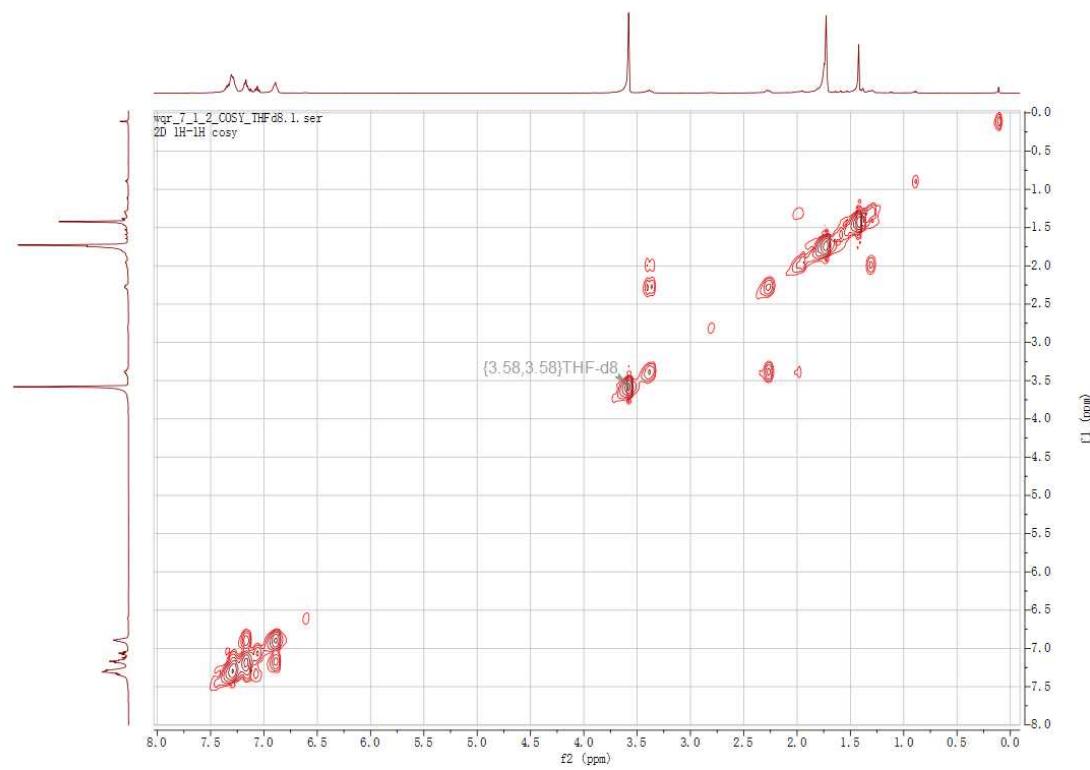


Figure S8. H-H COSY spectrum of $[\text{Fe}_2\text{Cl}]\text{[OTf]}$ in $\text{THF}-d_8$ (298 K).

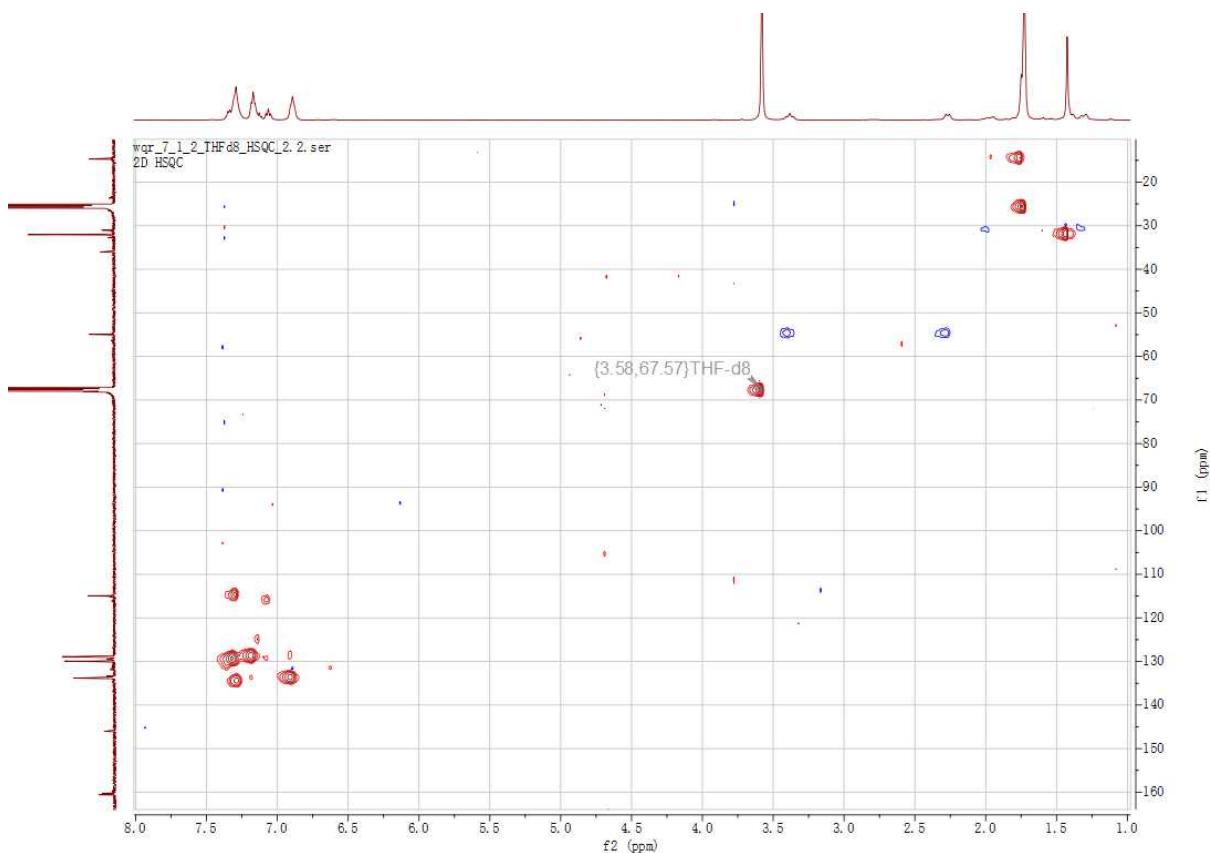


Figure S9. HSQC spectrum of $[\text{Fe}_2\text{Cl}]\text{[OTf]}$ in $\text{THF}-d_8$ (298 K).

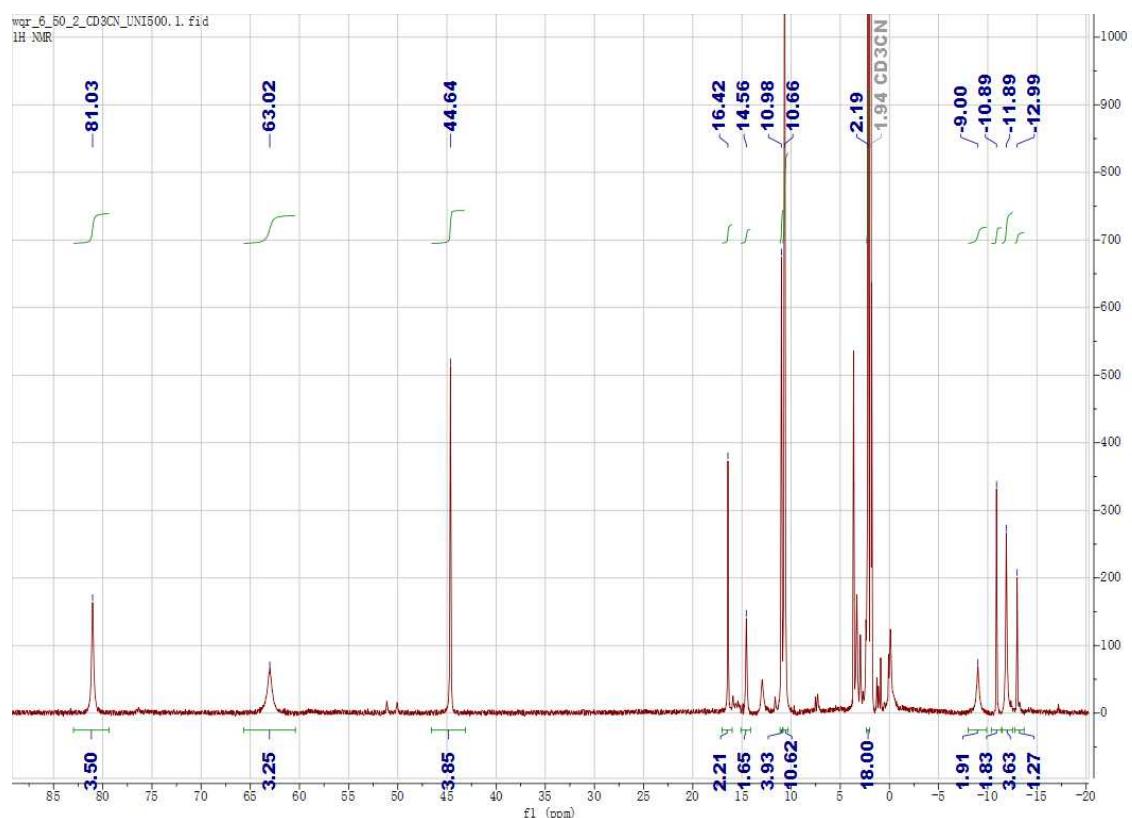


Figure S10. ^1H NMR spectrum of $[\text{Fe}_2(\text{SPh})_3]\text{[OTf]}$ in CD_3CN (298 K).

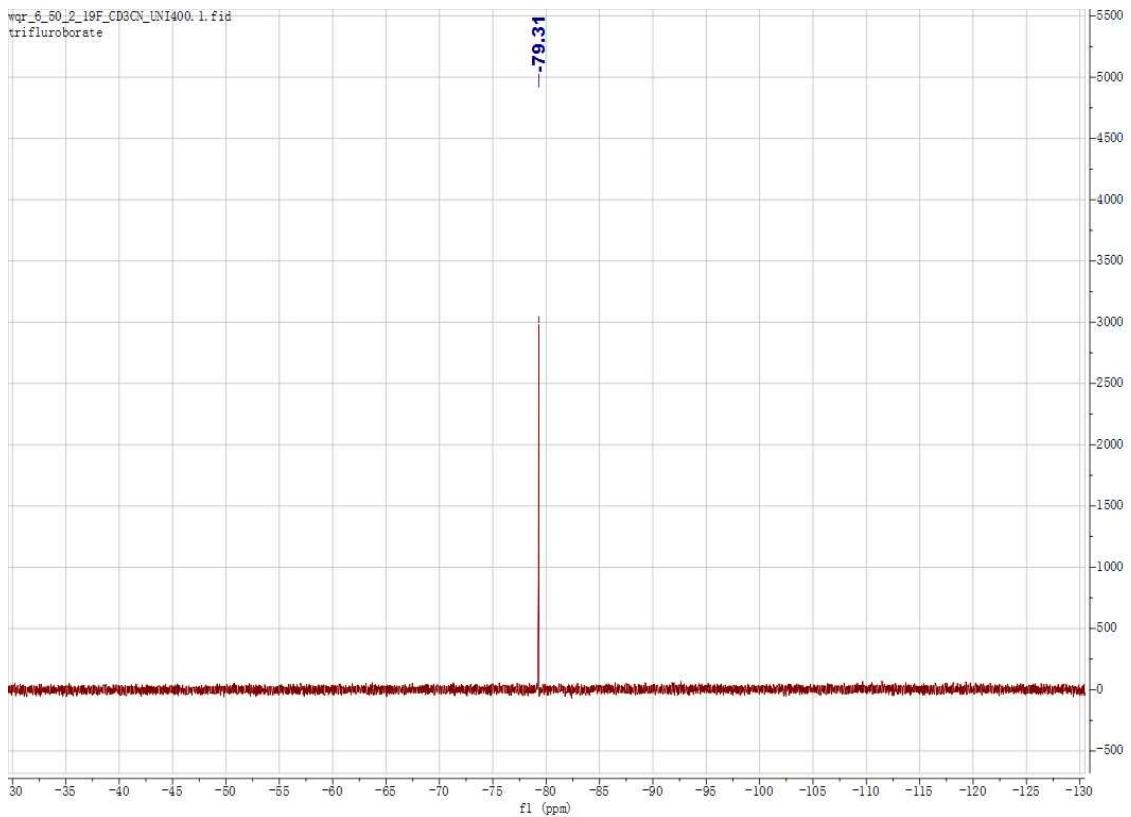


Figure S11. $^{19}\text{F}\{\text{H}\}$ NMR spectrum of $[\text{Fe}_2(\text{SPh})_3]\text{[OTf]}$ in CD_3CN (300 K).

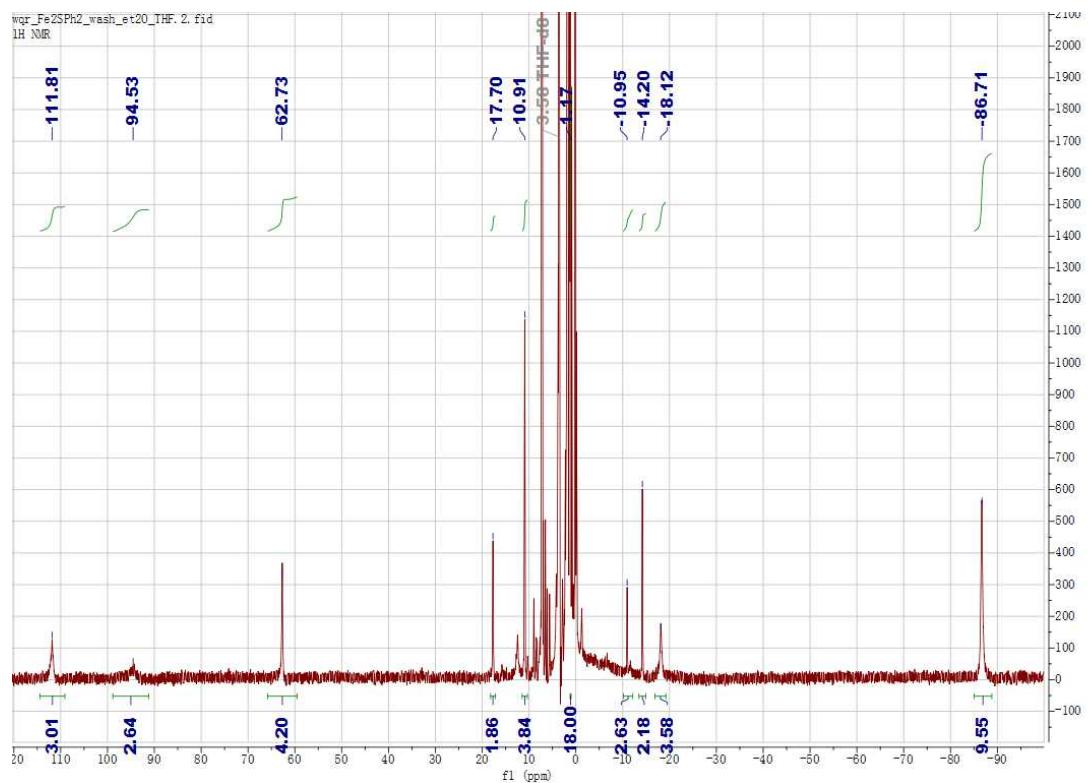


Figure S12. ^1H NMR spectrum of $[\text{Fe}_2(\text{SPh})_2]^0$ in $\text{THF}-d_8$ (298 K).

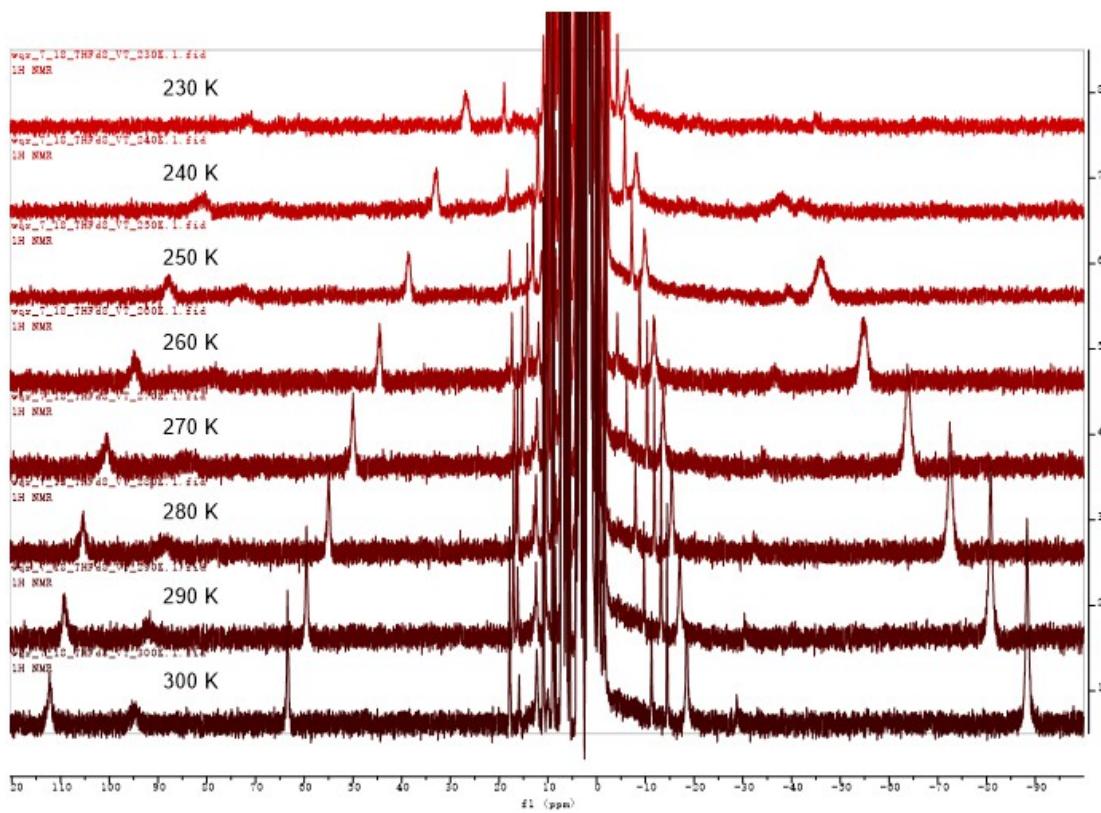


Figure S13. Variable-temperature ^1H NMR spectra of $[\text{Fe}_2(\text{SPh})_2]^0$ in THF- d_8 from 230 K to 300 K.

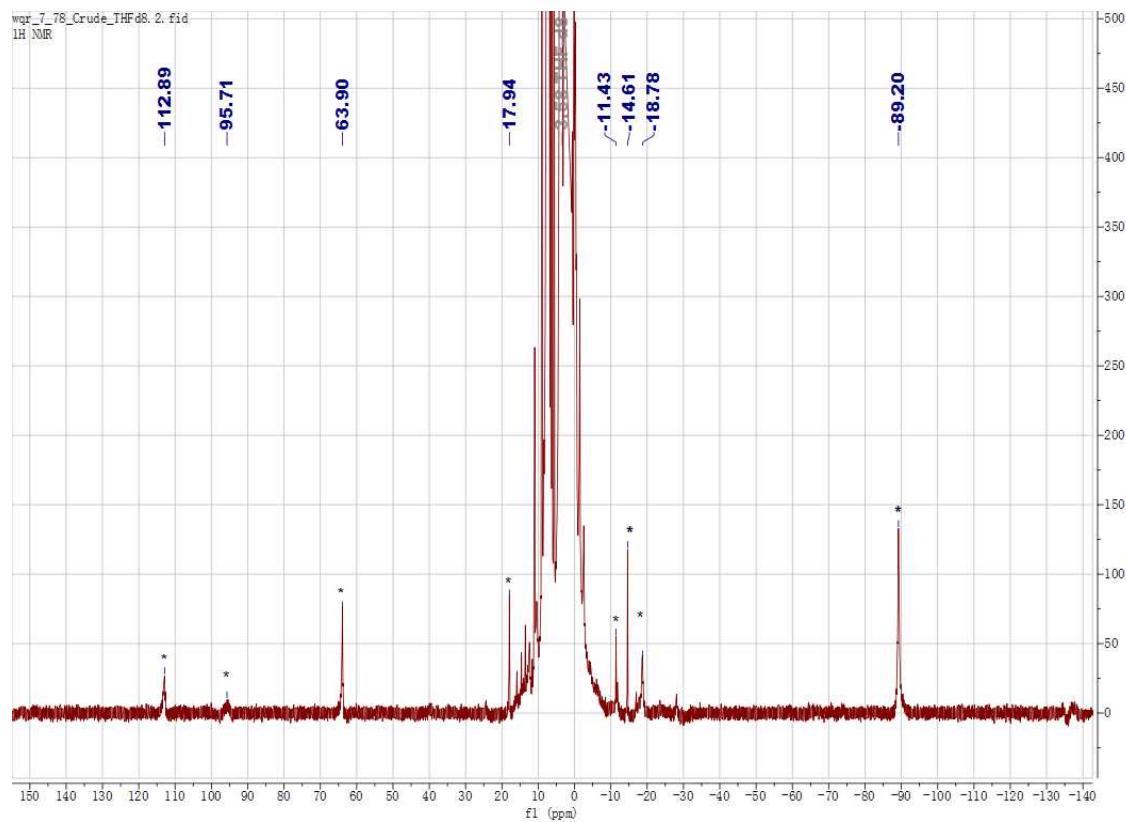


Figure S14. Crude ^1H NMR spectrum of the reaction mixture of $[\text{Fe}_2\text{Cl}]^+$ with 2.0 equivalents of NaSPh in THF- d_8 (298 K). Peaks assigned to $[\text{Fe}_2(\text{SPh})_2]^0$ are marked with *.

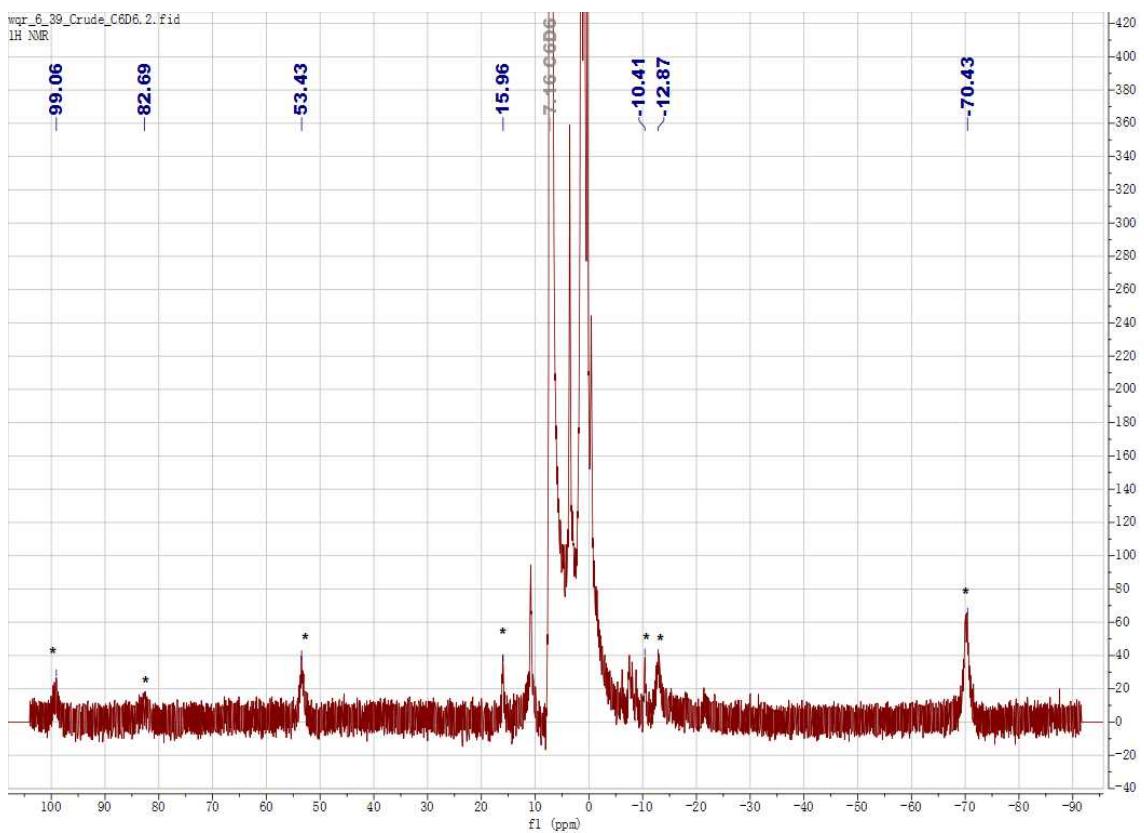


Figure S15. Crude ^1H NMR spectrum of the reaction mixture of $[\text{Fe}_2(\text{SPh})_3]^+$ with 2.0 equivalents of KC_8 in C_6D_6 (298 K). Reaction was done in THF, then the solvent was removed under vacuum before C_6D_6 was added to the mixture. Peaks assigned to $[\text{Fe}_2(\text{SPh})_2]^0$ are marked with *.

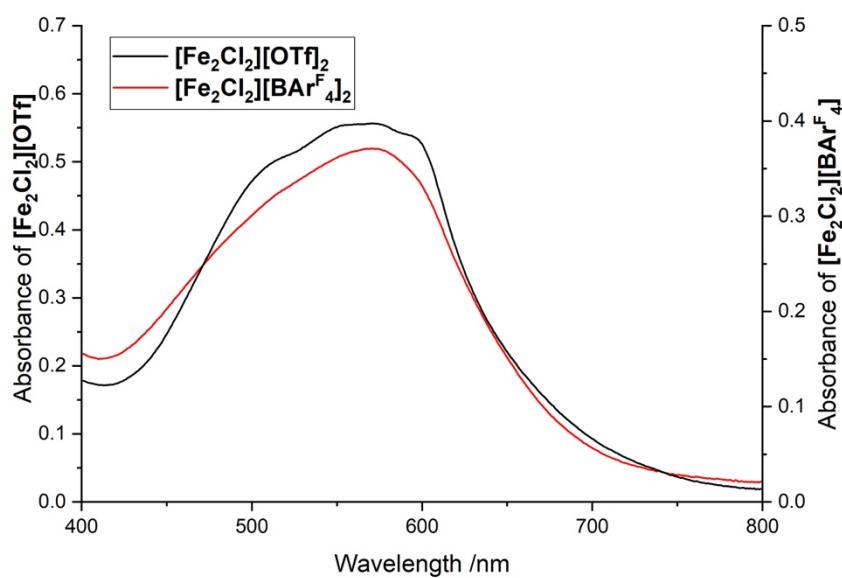


Figure S16. UV-Vis spectra of $[\text{Fe}_2\text{Cl}_2]\text{[OTf]}_2$ and $[\text{Fe}_2\text{Cl}_2]\text{[BAr}^{\text{F}}\text{]}_2$ in THF in the range of 400 nm to 800 nm.

2. Variable Temperature Solid-state Magnetometry Data

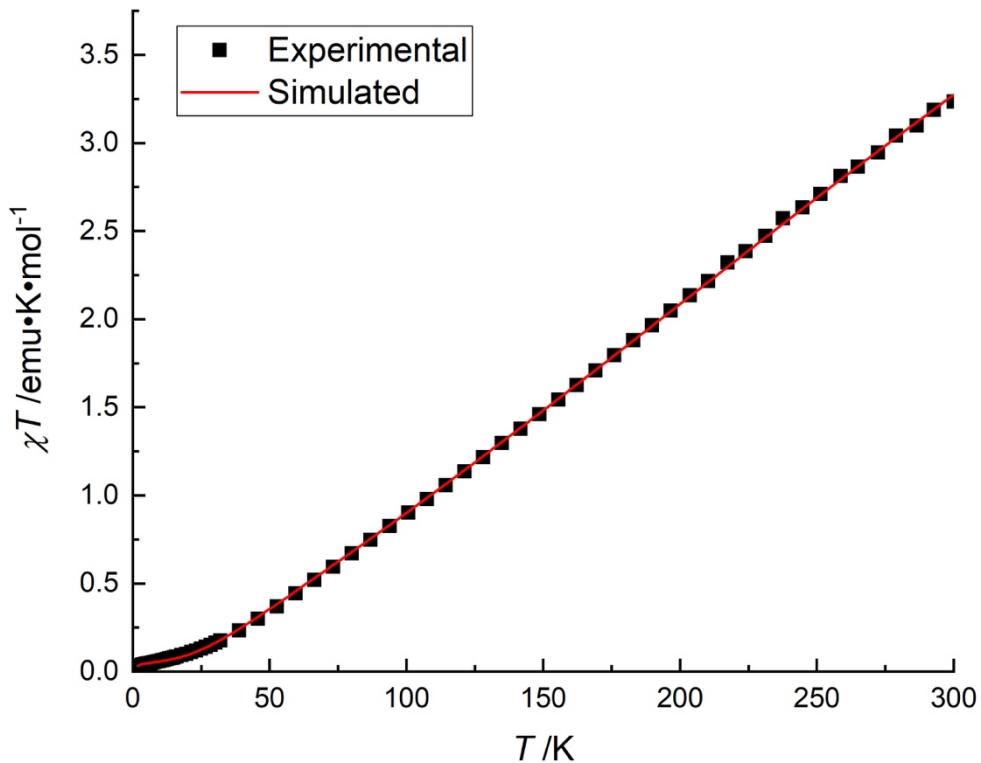


Figure S17. Variable temperature solid-state χT vs. T data for $[\text{Fe}_2(\text{SPh})_3]\text{[OTf]}$. The measured data were plotted as black squares. Simulated data were plotted as a red line.

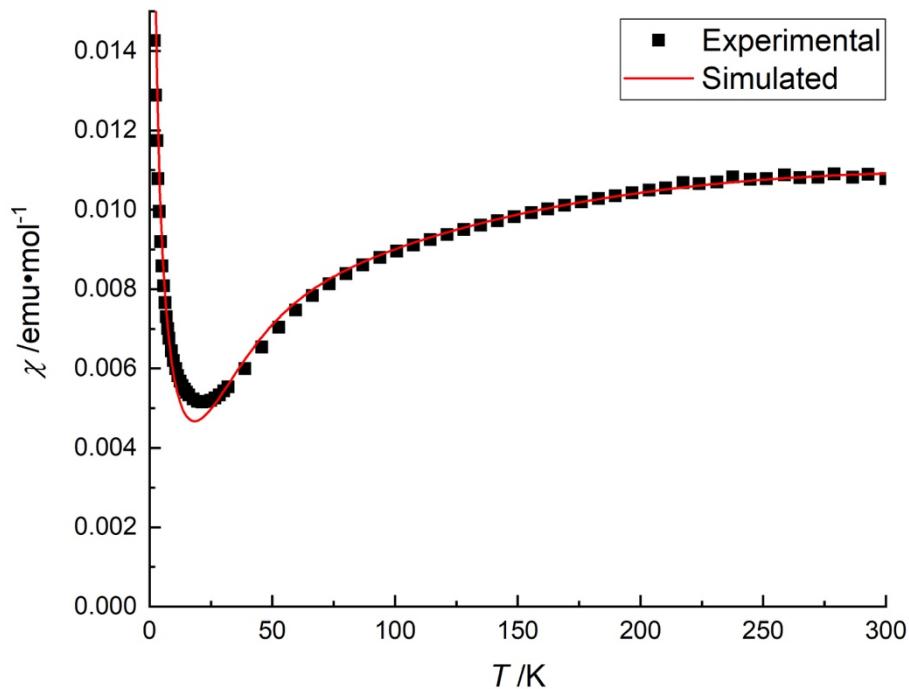


Figure S18. Variable temperature solid-state χ vs. T data for $[\text{Fe}_2(\text{SPh})_3]\text{[OTf]}$. The measured data were plotted as black squares. Simulated data were plotted as a red line.

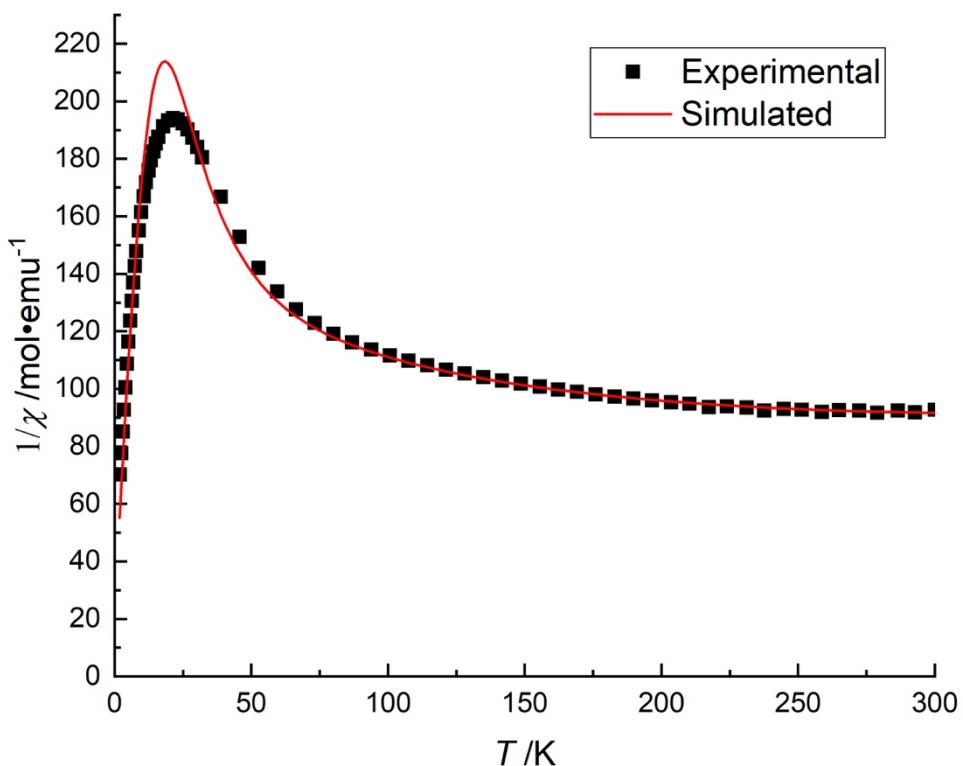


Figure S19. Variable temperature solid-state $1/\chi$ vs. T data for $[\text{Fe}_2(\text{SPh})_3]\text{[OTf]}$. The measured data were plotted as black squares. Simulated data were plotted as a red line.

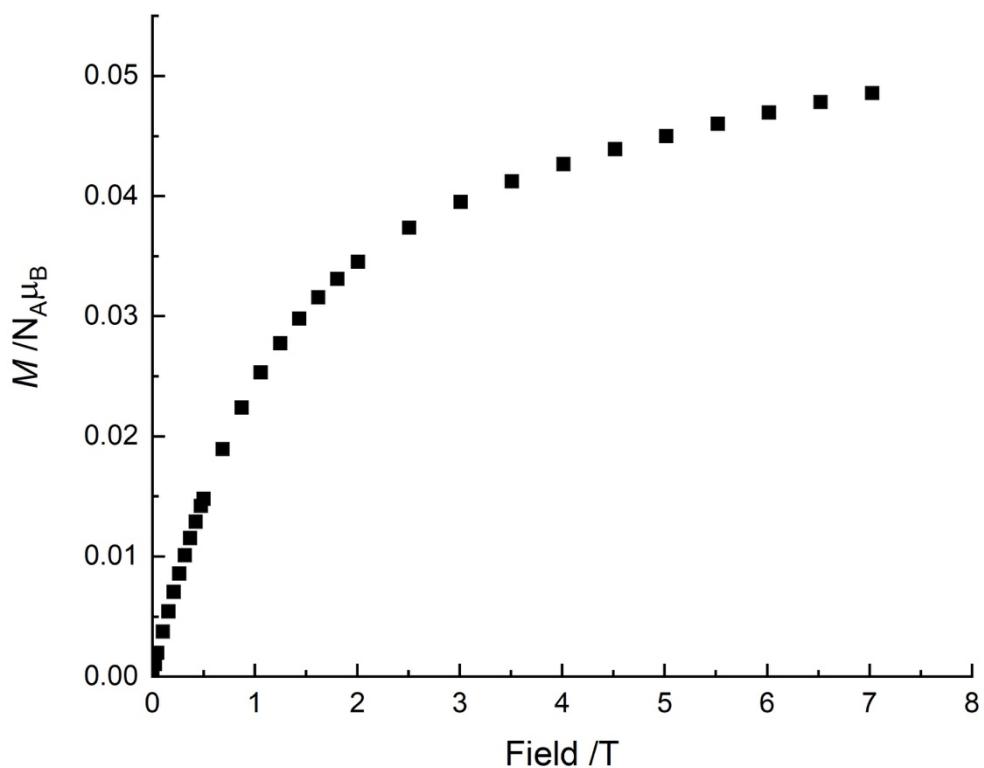


Figure S20. M vs. H plot data for $[\text{Fe}_2(\text{SPh})_3]\text{[OTf]}$ collected at 2 K.

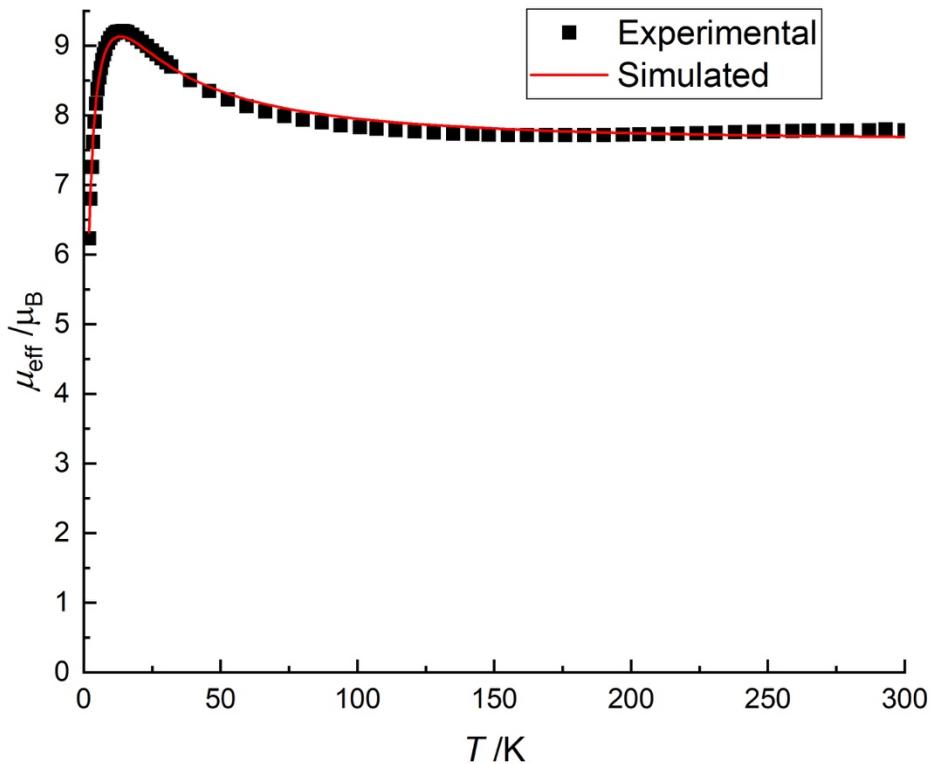


Figure S21. Variable temperature solid-state μ_{eff} vs. T data for $[\text{Fe}_2\text{Cl}_2]\text{BAr}^{\text{F}}_4]_2$. The measured data were plotted as black squares. Simulated data were plotted as a red line.

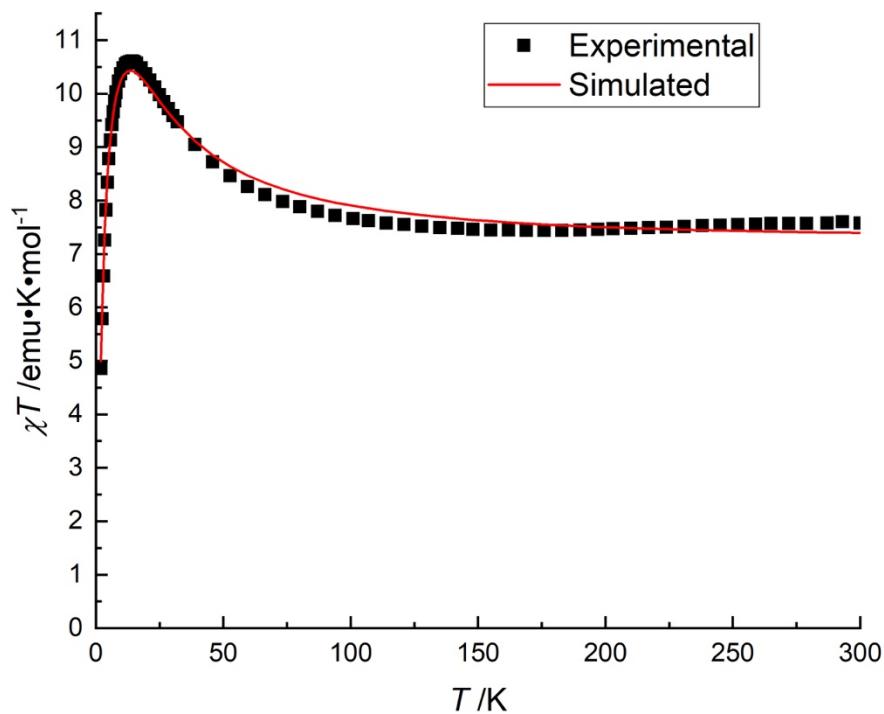


Figure S22. Variable temperature solid-state χT vs. T data for $[\text{Fe}_2\text{Cl}_2]\text{BAr}^{\text{F}}_4]_2$. The measured data were plotted as black squares. Simulated data were plotted as a red line.

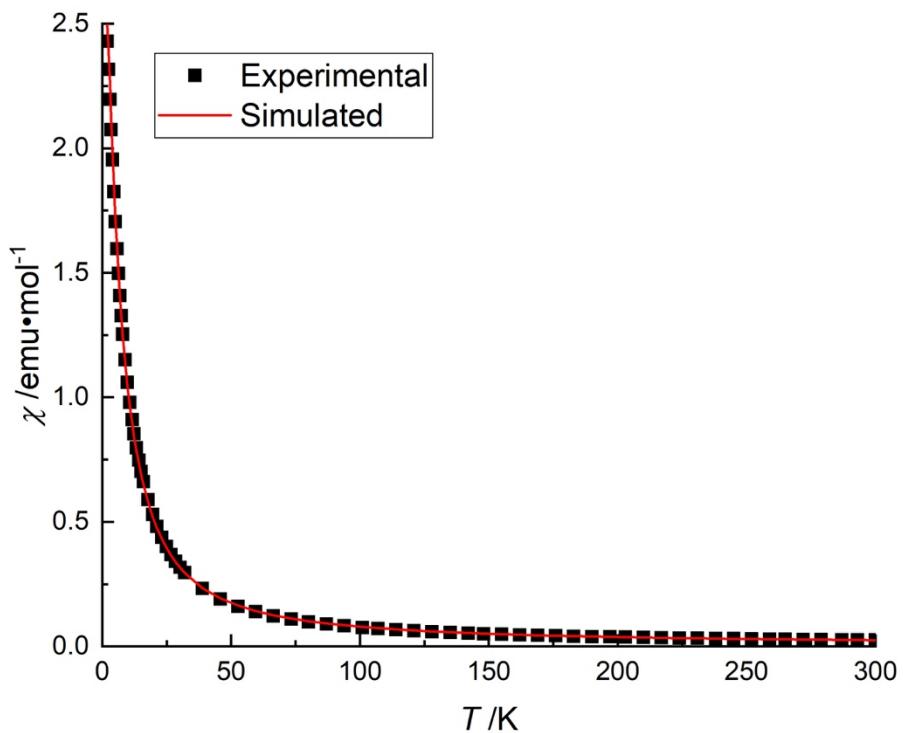


Figure S23. Variable temperature solid-state χ vs. T data for $[\text{Fe}_2\text{Cl}_2]\text{[BAr}^{\text{F}}_4\text{]}_2$. The measured data were plotted as black squares. Simulated data were plotted as a red line.

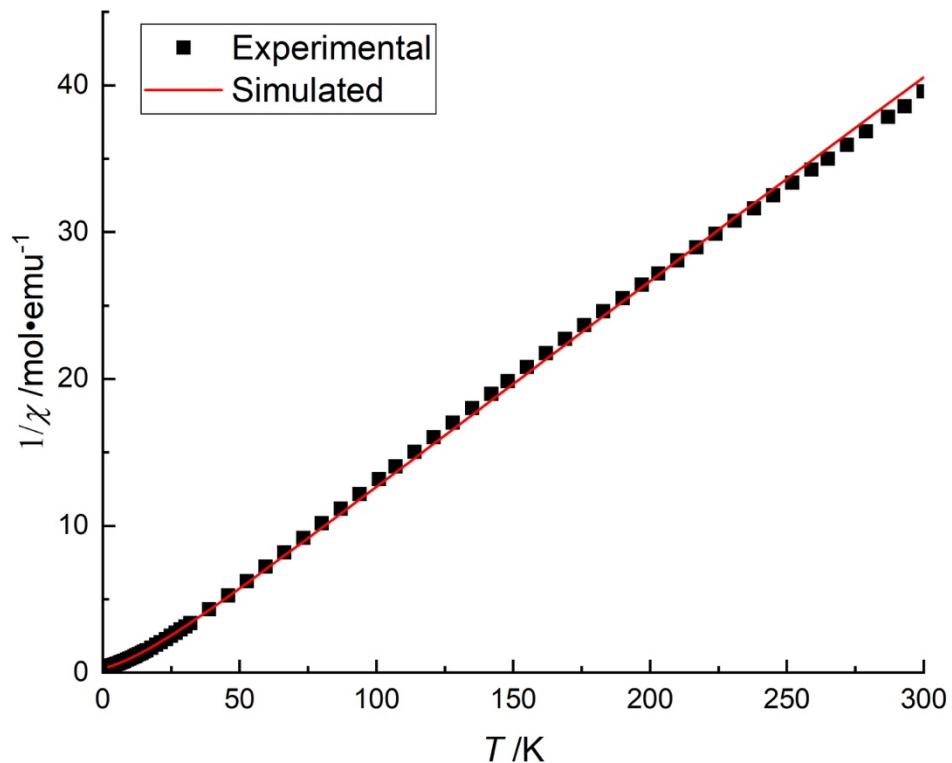


Figure S24. Variable temperature solid-state $1/\chi$ vs. T data for $[\text{Fe}_2\text{Cl}_2]\text{[BAr}^{\text{F}}_4\text{]}_2$. The measured data were plotted as black squares. Simulated data were plotted as a red line.

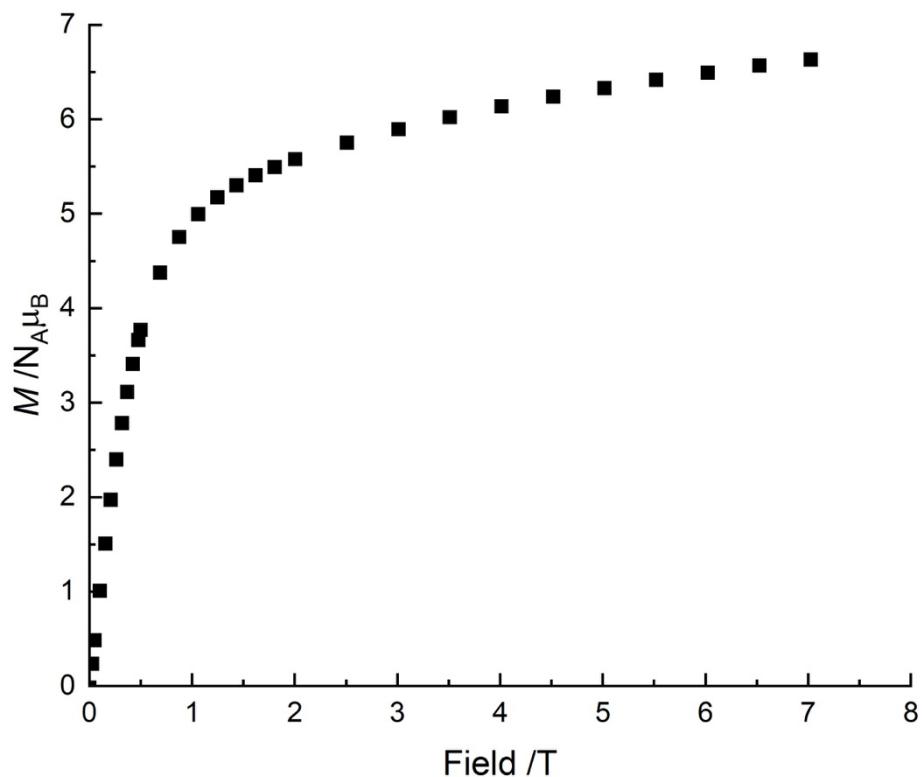


Figure S25. M vs. H plot data for $[\text{Fe}_2\text{Cl}_2][\text{BAr}^{\text{F}}_4]_2$ collected at 2 K.

3. X-ray Crystallography

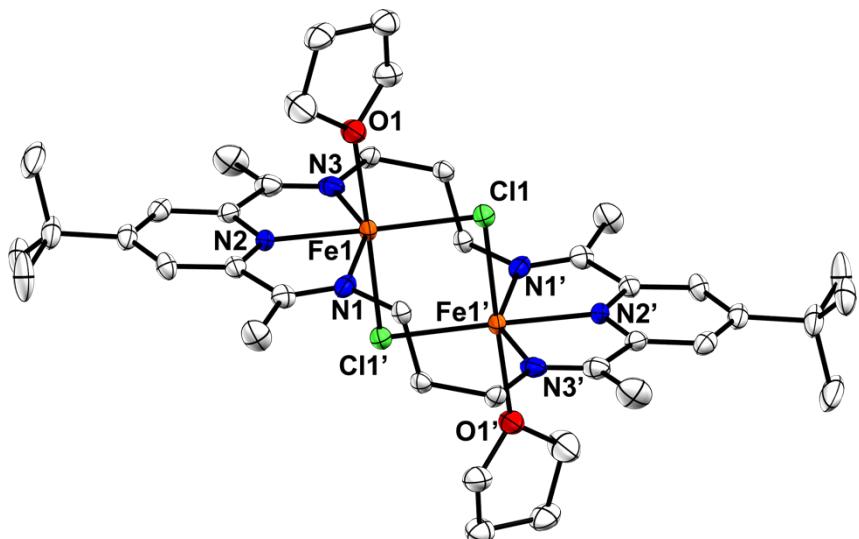


Figure S26. Crystallographic structure of the dicationic portion of $[\text{Fe}_2\text{Cl}_2]\text{[BAr}^{\text{F}}_4\text{]}_2$, with thermal ellipsoids at the 50% probability level. The $\text{BAr}^{\text{F}}_4^-$ counterions and hydrogen atoms were omitted for clarity.

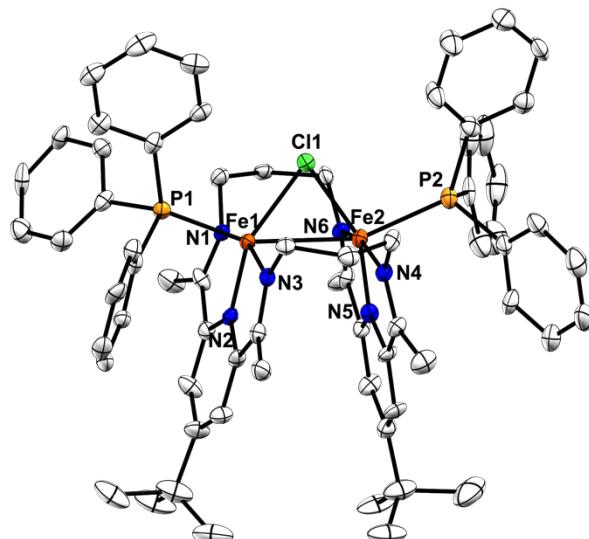


Figure S27. Crystallographic structure of the cationic portion of $[\text{Fe}_2\text{Cl}]\text{[OTf]}$, with thermal ellipsoids at the 50% probability level. The triflate counterions, disordered *tert*-butyl carbons and hydrogen atoms were omitted for clarity.

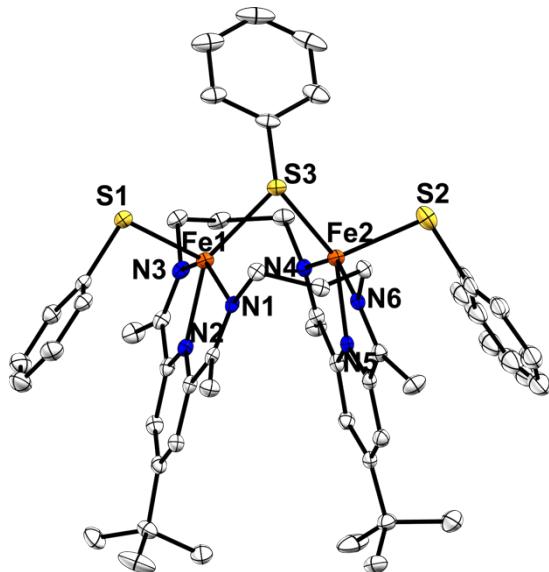


Figure S28. Crystallographic structure of the cationic portion of $[\text{Fe}_2(\text{SPh})_3]\text{[OTf]}$, with thermal ellipsoids at the 50% probability level. The triflate counterions and hydrogen atoms were omitted for clarity.

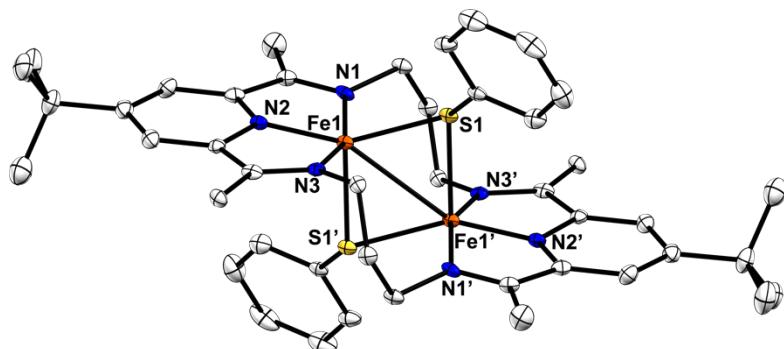


Figure S29. Molecular structure of $[\text{Fe}_2(\text{SPh})_2]^0$, with thermal ellipsoids at the 50% probability level. All hydrogen atoms were omitted for clarity.

4. Crystallographic Bond Lengths (Å) and Angles (°)

Table S1.

	[Fe ₂ Cl ₂][BAr ^F ₄] ₂	[Fe ₂ Cl][OTf]	[Fe ₂ (SPh) ₃][OTf]	[Fe ₂ (SPh) ₂] ⁰
Fe–Fe	3.3262(5)	2.7096(17)	3.1733(5)	2.7320(11)
Fe–(μ-X)	2.3667(7)	2.287(2)	2.3536(5)	2.2647(10)
	2.5028(7)	2.303(3)	2.3557(5)	2.2422(11)
Fe–N_{imine}	2.264(2)	1.943(7)	2.1840(14)	1.978(3)
	2.200(2)	1.952(8)	2.1812(14)	1.962(3)
		1.953(7)	2.1738(14)	
		1.941(7)	2.1741(14)	
Fe–N_{py}	2.0781(19)	1.816(7)	2.0577(14)	1.826(3)
		1.823(7)	2.0699(14)	
N_{imine}–C_{imine}	1.272(4)	1.310(11)	1.287(2)	1.328(5)
	1.284(3)	1.317(12)	1.288(2)	1.333(5)
		1.297(11)	1.285(2)	
		1.310(11)	1.287(2)	
C_{imine}–C_{py}	1.500(3)	1.453(13)	1.486(2)	1.435(5)
	1.496(3)	1.456(12)	1.491(2)	1.430(5)
		1.456(12)	1.493(2)	
		1.459(12)	1.491(2)	
∠Fe–X–Fe	86.12(2)	72.34(8)	84.727(17)	74.63(4)
Δ	0.192	0.119	0.176	0.075
FSR	1.42	1.16	1.36	1.17

5. Supplementary Computational Details

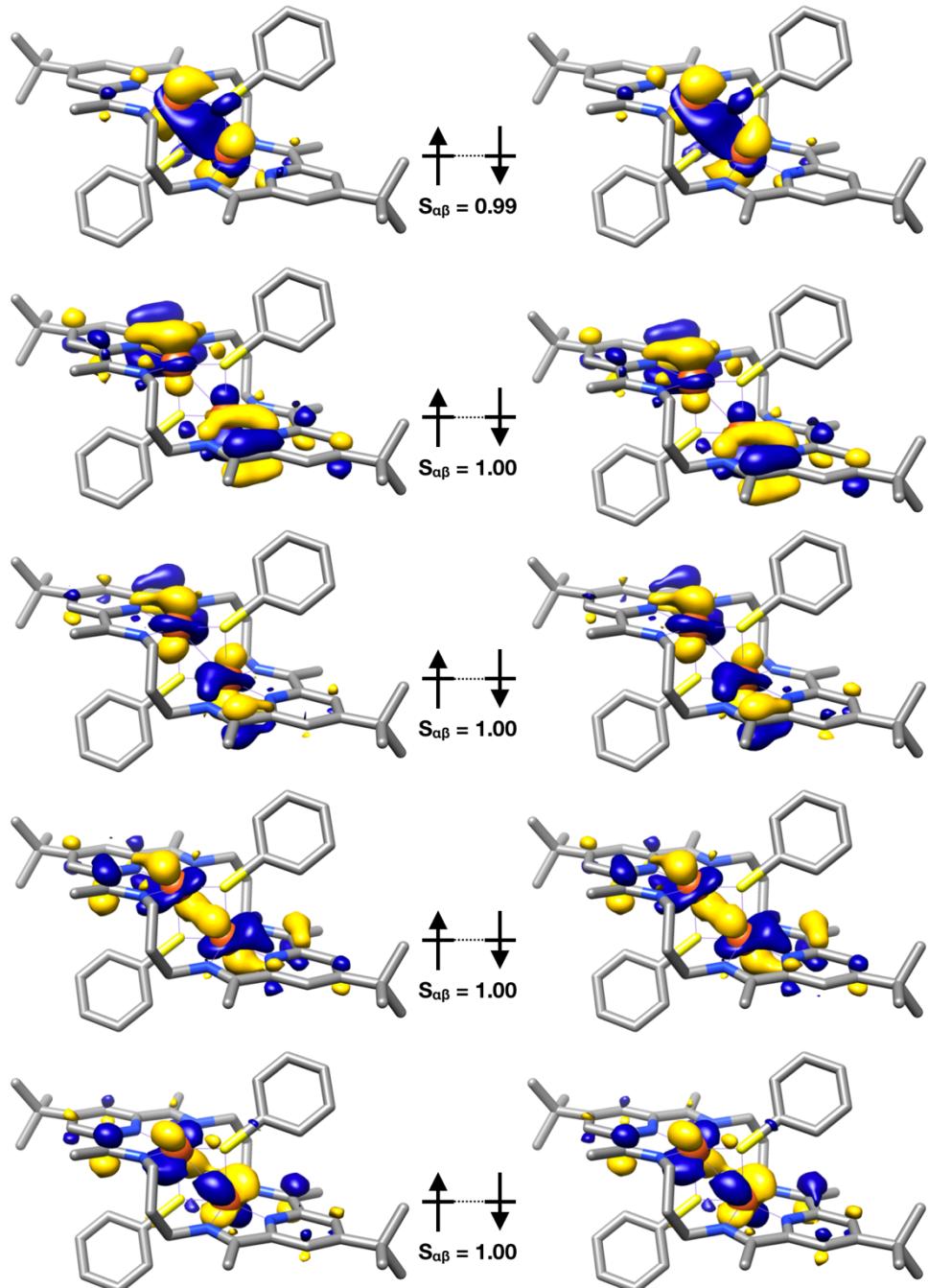


Figure S30. Plots of the highest-lying α -spin (left) and β -spin (right) UCOs for the geometry optimized singlet state of $[\text{Fe}_2(\text{SPh})_2]^0$.

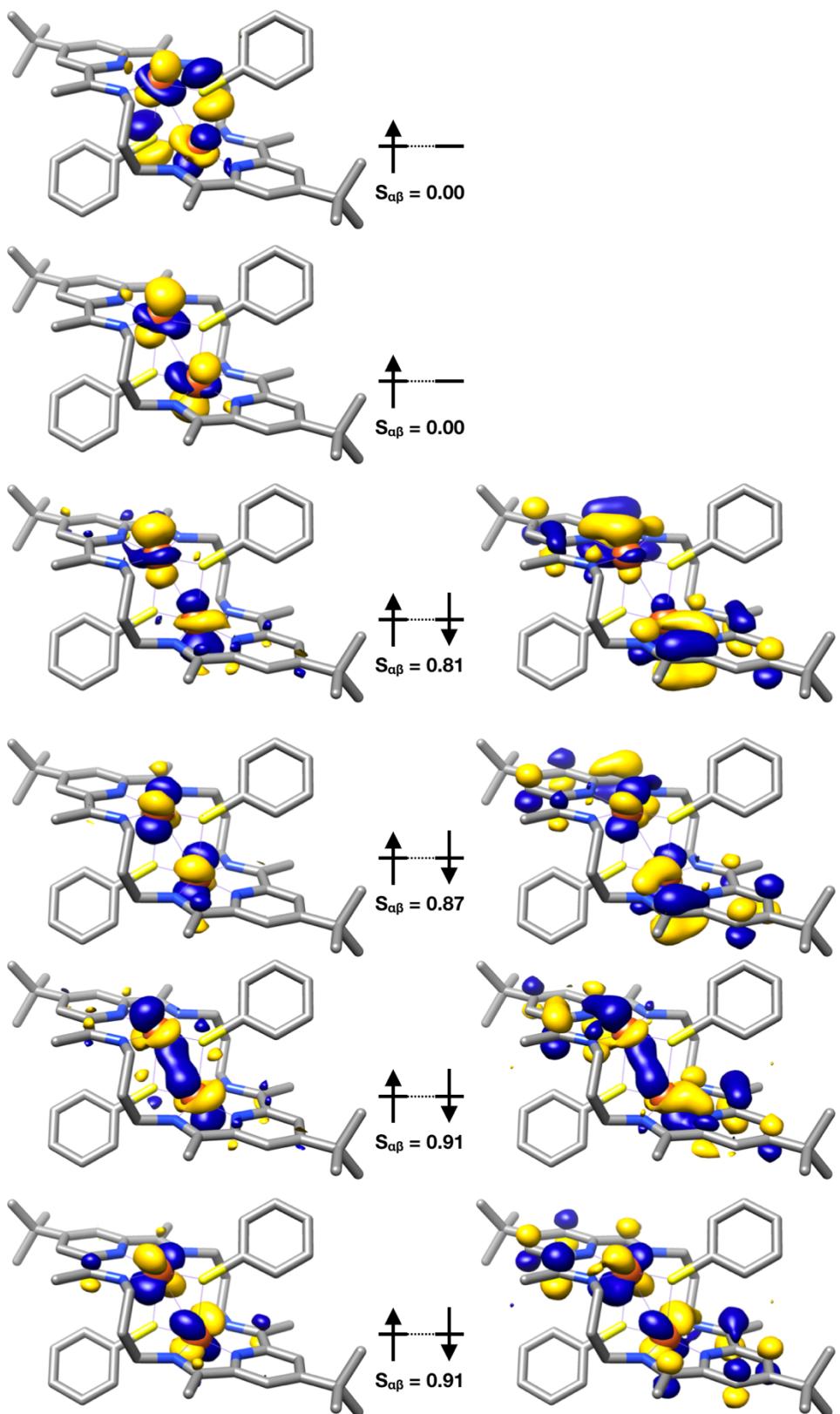


Figure S31. Plots of the highest-lying α -spin (left) and β -spin (right) UCOs for the geometry optimized triplet state of $[\text{Fe}_2(\text{SPh})_2]^0$.

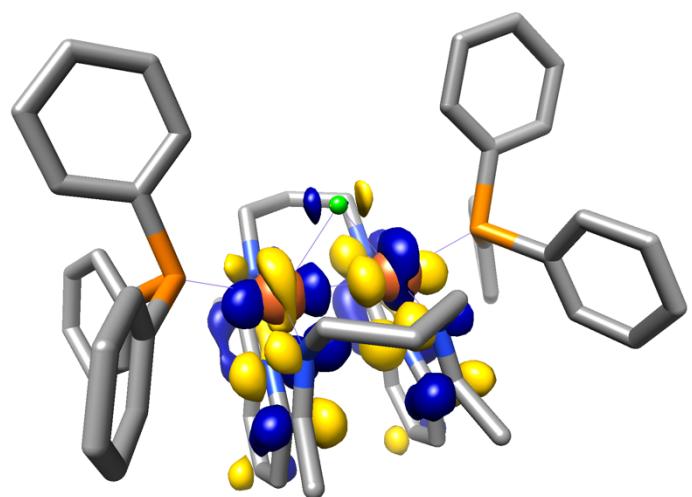


Figure S32. Plot of the LUMO+1 of $[\text{Fe}_2\text{Cl}]^{+}/2^{+}$.

6. DFT Energies and Optimized Coordinates

$[\text{Fe}_2\text{Cl}]^+, S_{\text{tot}} = 1$

$G = -6318.31613787 \text{ E}_h$

Fe	0.07283763246288	0.01606246468668	0.00206187274959
Fe	0.06735000052480	-0.00647418330891	2.68185032691289
Cl	1.90869769554677	-0.40104237948311	1.34079581809806
P	0.84922258834719	-0.03557491541957	-2.10092394430408
P	0.82902661134308	-0.13526534568977	4.78635411870935
N	-0.56182110111196	-1.80511565152767	-0.10368273824159
N	-1.68783405701202	0.35956105526771	-0.26857219000327
N	0.15736056593210	1.95609014708682	-0.02069343162899
N	0.17875148819424	1.92678141460197	2.77178687149041
N	-1.69045720962951	0.35485762638799	2.95078976556452
N	-0.59600600371848	-1.82285258357175	2.71829794208399
C	-1.85146722104847	-1.95286953310175	-0.38288161792561
C	-2.55887626720486	-0.69278834962218	-0.42739771320759
C	-3.92725551252776	-0.44179420532711	-0.61897339893595
H	-4.62680160634717	-1.27790695103760	-0.73169415238059
C	-4.38731324034032	0.88704279696478	-0.64710950618301
C	-3.47577660336500	1.94750310562562	-0.51515821320005
H	-3.81539416720796	2.98854327608319	-0.55412105237913
C	-2.11251344357402	1.66271457156543	-0.33760888744813
C	-0.99251129049328	2.57401666382852	-0.25544921681873
C	1.39763895216981	2.73192006057483	0.09163492977407
H	1.50457656472399	3.40277268629422	-0.78363831684832
H	2.23045562914088	2.01564209414807	0.05539355306277
C	1.50056229906636	3.54584998139627	1.38976404993292
H	2.47972327491428	4.06733823265497	1.38642067966922
H	0.72476036066649	4.33212011431426	1.41388718520437
C	1.42490696947576	2.69115893526330	2.66284920136795
H	2.25098047411520	1.96620495811833	2.66096187821792
H	1.55338895311674	3.33513909428186	3.55553152649721
C	-0.96067665325505	2.55511237186082	3.03252338478824
C	-2.09521677674502	1.66024317754358	3.07549820715585
C	-3.45637044780722	1.95788244565352	3.25211621175599
H	-3.78076016519183	3.00130199639470	3.33551328410676
C	-4.38617559897769	0.90780523698248	3.32107068899610
C	-3.94712693136937	-0.42583404761620	3.23085901952709
H	-4.66068575328736	-1.25532645182000	3.29306635587957
C	-2.58080463349531	-0.68795006685092	3.04489186104241
C	-1.89458996050828	-1.95717289791827	2.95595926796508
C	0.25723275607665	-3.01119233581672	2.60375098233977
H	0.08119382562441	-3.68357313912405	3.46437504565084
H	1.30023588687541	-2.66511502216289	2.66824904197517
C	0.05655972987625	-3.79244977839962	1.29770877495816
H	0.77070139281854	-4.64163344608818	1.30141915941829
H	-0.95467365139303	-4.23816657496365	1.27665932123151
C	0.29834767605496	-2.98663763138402	0.01427606328946
H	1.33997084281233	-2.63203893581154	-0.00822006199560

H	0.15546292118190	-3.64538185712366	-0.86243951944778
C	-2.55337003658407	-3.24653440527900	-0.68909316189300
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H	-3.32742901660872	-3.08306636034659	-1.46253451953022
H	-3.06757718497636	-3.67060226384278	0.19773484419037
C	-1.19341141558880	4.03717390918617	-0.53313644729206
H	-1.75545090586754	4.53777732799702	0.28150073011018
H	-1.78960347964760	4.15438770834040	-1.45914194699519
H	-0.24770498000486	4.58193690313826	-0.68212046421793
C	-1.12986898047658	4.01474054159871	3.34618831214488
H	-0.18327753615386	4.49484036970009	3.64294772875757
H	-1.83216361778950	4.13088742124547	4.19335092653593
H	-1.54626166362829	4.58189871261464	2.48877170419390
C	-2.64329350481355	-3.24120825241577	3.18140808182755
H	-3.29266276454625	-3.49370141116553	2.31809227547498
H	-3.30718812281059	-3.14093558533715	4.06185430532829
H	-1.97671586284912	-4.09760481608772	3.37072430660695
C	2.62673417922289	0.08619818487608	-2.55219325672732
C	2.98394447096811	0.05584786672039	-3.92032529999552
H	2.20285472846208	-0.02681597045935	-4.68643159606281
C	4.32747392155225	0.13119038573276	-4.30388441610228
H	4.59248730794213	0.10844677328824	-5.36960381661078
C	5.33520910620477	0.23163855264952	-3.32760829128640
H	6.38962539831727	0.28800712160779	-3.62992117560596
C	4.98902900641809	0.25322957717298	-1.96965789212900
H	5.77095893502479	0.32280769928367	-1.20145394581521
C	3.63957808865893	0.17977686549270	-1.58268736445875
H	3.37878497246720	0.17789938832023	-0.52032323675833
C	0.39193454333099	-1.58197939419530	-2.98835496988003
C	-0.91202647886483	-1.85151027721730	-3.45416504421224
H	-1.69257592210456	-1.08936320635740	-3.41022169115482
C	-1.23627559610714	-3.10440486342791	-3.99519865350560
H	-2.25655344090283	-3.28615204856613	-4.35952305453579
C	-0.26865801384946	-4.11714683419891	-4.07508497418440
H	-0.52377532479564	-5.09562672373249	-4.50342270015088
C	1.03117115317560	-3.86336367407324	-3.60977703036723
H	1.80191962499925	-4.64365917027754	-3.67018762181161
C	1.35651702184651	-2.61211491391120	-3.06865992998678
H	2.37411275205387	-2.43832769376934	-2.70059928977478
C	0.12274757770962	1.37054960295060	-3.04239345813923
C	0.93576834278574	2.46007380007130	-3.42972718829478
H	2.01687259398868	2.42469270968476	-3.25912752779867
C	0.38074118466344	3.59421700656106	-4.03958456724472
H	1.03794878947375	4.42200788603268	-4.33890201021100
C	-1.00037276860193	3.66765623139175	-4.27907028017318
H	-1.43302907175830	4.55113417167322	-4.76725121704138
C	-1.82217980534229	2.60418713400983	-3.87890875190850
H	-2.90780694786759	2.65081272883628	-4.03839706585410
C	-1.26929666623311	1.47833365884261	-3.25193466768578
H	-1.94709670205316	0.69433488770889	-2.90783616742126

C	2.60464574051179	-0.04697071098302	5.25129828817955
C	3.62462886117903	0.04987832569628	4.28967241199113
H	3.37051082061238	0.06901537403407	3.22596500130385
C	4.97213160219610	0.10609705465923	4.68626849850442
H	5.75953096003597	0.17962061896615	3.92404193931514
C	5.30943965356426	0.06322639107449	6.04591070229725
H	6.36234058041983	0.10614974384997	6.35562356352563
C	4.29449694694097	-0.04019695040321	7.01439176557318
H	4.55220548050505	-0.07846108666082	8.08145328579717
C	2.95286147915656	-0.09685176050424	6.62132265869504
H	2.16608517438649	-0.18012947264905	7.38148139530108
C	0.33348497156389	-1.69710459839194	5.62333211798700
C	1.29410965927247	-2.7068618929630	5.78570246558989
H	2.33911045048886	-2.54005787140539	5.51062881163895
C	0.93071901127991	-3.97574599310717	6.29426031966181
H	1.69852739812147	-4.75115820307301	6.41962734917975
C	-0.40234901865613	-4.23886279844472	6.64540734947121
H	-0.68670778603274	-5.21910370924986	7.05068990349627
C	-1.36792371710583	-3.23475353453317	6.47611547628875
H	-2.41556075850046	-3.42571770795462	6.74580954308698
C	-1.00657291716567	-1.98133851409685	5.96251838246546
H	-1.78909526513012	-1.23315232769236	5.82223370461912
C	0.12487815921569	1.26033409676475	5.76402379968489
C	-1.26129109314526	1.38062232815776	6.00085774653698
H	-1.95525257461446	0.60689345176334	5.66637414202696
C	-1.79052948784723	2.50643000670988	6.64839732064014
H	-2.87272556164936	2.56322914136642	6.82690712392512
C	-0.95049182770516	3.55575430415430	7.04717575847332
H	-1.36494765074893	4.43854368873206	7.55208789948885
C	0.42575708321850	3.46829748573903	6.78558073812317
H	1.09805376247369	4.28398978974271	7.08469244687750
C	0.95659001387502	2.33592412323851	6.15157282655135
H	2.03412924964284	2.29086844686402	5.96245708534926
H	-5.45320517526428	1.12614594329410	3.45147381029421
H	-5.45626840381922	1.09428255908885	-0.77985630543568

[Fe₂(SPh)₃]⁺, BS(4,4)

G = -5676.23511792 E_h

Fe	-0.27733371251705	-0.05242629411961	0.12801183023554
Fe	-0.22957547474833	-0.09057267566005	2.97068716590512
S	-0.24537428649605	-0.87725882660962	-1.97199294907510
S	-0.12552886466702	-0.97912246954547	5.04205399219996
S	-0.33563608615579	-1.88280423775055	1.52563771191062
N	-2.44220892070052	0.36881238105207	0.16577752066814
N	-0.42940303508673	1.96292594659588	-0.06045165562687
N	1.74494876310903	0.63842157968371	0.10570572666517
N	1.79491992914945	0.60005545271587	2.94443952858395
N	-2.39134646053987	0.32908306325728	3.02725086172362
N	-0.37165054601292	1.91723471035058	3.22732403853899
C	-2.77312239818020	1.58967650436868	-0.11179189877956

C	-1.64759497669110	2.54592896384581	-0.15037986741735
C	-1.77603214933577	3.93328827164162	-0.28779276547208
H	-2.76520423588272	4.39883451039470	-0.35152645637173
C	-0.61420855872028	4.72240616426670	-0.35047572192172
C	0.63730812910698	4.09783918785062	-0.31282599941085
H	1.55481643932224	4.69002873880125	-0.39485628644670
C	0.70340377301593	2.70057845003826	-0.17276388626048
C	1.93059021346692	1.90120538591946	-0.16010417108279
C	2.85069025579859	-0.31160062056026	0.19333120163481
H	3.52150950194587	-0.21230403007355	-0.68463706516475
H	2.41817081867287	-1.32346500665686	0.14926847842347
C	3.68056095057588	-0.16681127043387	1.48085269398877
H	4.47188888697352	-0.94294194689045	1.45658821769459
H	4.19482979249159	0.81301803550814	1.48564863341085
C	2.89555352079308	-0.34749575131923	2.79185325171372
H	2.46286788019216	-1.35986747038753	2.82211815474959
H	3.59648426593903	-0.27374256383705	3.64856894076362
C	1.99028440045855	1.85486364588435	3.23815851425022
C	0.76448371463293	2.65252756507951	3.31886481616158
C	0.70415368292919	4.04470870860327	3.50321457535423
H	1.62432050196973	4.63490820933884	3.56858289425119
C	-0.54499575717378	4.66666017695196	3.60784876661720
C	-1.70836693593793	3.87867218020687	3.56567951107355
H	-2.69424647462256	4.34101179715255	3.68203601109395
C	-1.58559042922998	2.49619939503587	3.38116884443492
C	-2.71152523973148	1.54041058500597	3.35549704148977
C	-3.37126616623348	-0.74748019393285	2.90263185575149
H	-4.05114642839232	-0.76355642057695	3.77817070698835
H	-2.81077209181166	-1.69799054846162	2.91240387417664
C	-4.20965278077864	-0.65255120271359	1.61482186975467
H	-4.82221896296660	0.26928199780408	1.63896834481463
H	-4.91882131591107	-1.50461374040017	1.61546853328273
C	-3.41831789440617	-0.71076115173309	0.29542155047403
H	-2.85984909363000	-1.66077387981492	0.23816816920422
H	-4.12966634993583	-0.70159900221288	-0.55490359624230
C	-4.16298227190127	2.09072212718050	-0.41222144596336
H	-4.88747887096941	1.27228676729966	-0.55253784226010
H	-4.15693052844106	2.70490581697888	-1.33338209596387
H	-4.53500015575921	2.73850104208195	0.40710070613002
C	3.24625663450757	2.56536936127992	-0.47415188156253
H	3.57233079576432	3.22916338938496	0.35199271972429
H	3.14651748446129	3.19342332831629	-1.37997858390083
H	4.05235374675607	1.83646563733697	-0.65754128505369
C	3.31638146906593	2.51093536757237	3.52458608917322
H	4.13152249067416	1.77887511686268	3.64369959072899
H	3.25233374010855	3.10152053812475	4.45852799785858
H	3.60534065246456	3.20974396862126	2.71372882693379
C	-4.08913790306650	2.03024477879800	3.72279119736880
H	-4.48997604986918	2.70483981942481	2.93947860947145
H	-4.04847025969351	2.61344211947223	4.66303497937776

H	-4.80881870717103	1.20739113117305	3.86200940731942
C	-0.07961975348558	0.65313638745461	-2.84474130032160
C	-1.22565256685371	1.40174428536081	-3.19654019512202
H	-2.21937085389175	0.98837612046297	-2.98161381748299
C	-1.09401028826868	2.65592461304545	-3.80603078487651
H	-1.99362958238906	3.22847213747333	-4.07191901493248
C	0.17929448919211	3.17958542523053	-4.08842622673323
H	0.27909957627968	4.16058702870999	-4.57134406338644
C	1.32115582893566	2.42585602173709	-3.77296681803662
H	2.32027463893850	2.81378577572986	-4.01683753820463
C	1.19669561250142	1.17351217509561	-3.15465706801430
H	2.08819545543294	0.58273948476970	-2.91075762318814
C	0.04033191448202	0.52588105235287	5.95720365843605
C	1.31586886686857	1.06341335820123	6.24026708996131
H	2.21028785478025	0.49927009324706	5.94869098543191
C	1.43581107216292	2.29878758110663	6.89244350313113
H	2.43454716982863	2.70089712880169	7.11399193314534
C	0.29033611771337	3.01777274226883	7.27025639773681
H	0.38691156238737	3.98554018715991	7.77978141307081
C	-0.98097196697807	2.47551329127336	7.01576764520883
H	-1.88235054131504	3.01985919879741	7.33055278060943
C	-1.10794449866811	1.23825410046265	6.37153099602362
H	-2.09975077836176	0.80991038151297	6.17819277279895
C	0.91998183467180	-3.13621752447164	1.48877683082815
C	1.38457561188137	-3.62806832870275	0.25215455072826
H	0.97765070667270	-3.22713442433876	-0.68423333460061
C	2.37060102984327	-4.62464553098722	0.23014563262540
H	2.73200150891183	-5.00433139504040	-0.73500430447466
C	2.88955124755214	-5.13834657332146	1.43015521038720
H	3.66079985303269	-5.91934872525669	1.40724395096769
C	2.40875150768350	-4.65830567724968	2.65958119021538
H	2.80004850044390	-5.06441494462805	3.60204932963355
C	1.42292543894330	-3.66199657741972	2.69611138476272
H	1.04575188856369	-3.28789340840786	3.65568414944775
H	-0.68876931035349	5.81185069021362	-0.45175456064462
H	-0.61539120811736	5.75243123578407	3.74514674677498

[Fe₂(SPh)₃]⁺, S_{tot} = 3

G = -5676.21460823 E_h

Fe	-0.06990757729040	0.15349827232405	0.07004594200154
Fe	-0.02969848194422	0.11163186942246	3.01763590575773
S	-0.01682572250510	-0.76044334583549	-1.93905896572146
S	0.05691397417022	-0.87372505529177	4.99267414206957
S	-0.19476891649013	-1.60892045921204	1.52040927506089
N	-1.99766454098581	0.52400869978140	0.08472669349570
N	-0.03499996285843	2.02263501039755	-0.20591911598713
N	2.04211454863524	0.59025485148616	0.07071572552211
N	2.08071279516726	0.54588333129362	2.98633847454015
N	-1.95982603208898	0.48671174284278	3.05192090701163
N	0.01311889474210	1.97101120309330	3.35154784468796

C	-2.35788673484888	1.76681380031329	-0.21064407489708
C	-1.23786814315974	2.67439981133265	-0.32795068748572
C	-1.27560484658059	4.06387300853167	-0.53335974270837
H	-2.23909419791899	4.57821584637523	-0.61728879676016
C	-0.07578856297623	4.77882795364116	-0.62116059776624
C	1.14762799073064	4.09133977915025	-0.52063668208941
H	2.09616829998997	4.63316769173629	-0.60262387944017
C	1.14385202408525	2.70635539374343	-0.31801251134430
C	2.31523428989838	1.83499454596655	-0.22095530184762
C	3.09139704055859	-0.42054071577289	0.19894087175676
H	3.77490553362186	-0.37051803593594	-0.67226682225193
H	2.60501480858484	-1.40479138504336	0.16595781743010
C	3.91421216529874	-0.30280472949124	1.49216013930812
H	4.67288932935306	-1.11113659674366	1.46967605749599
H	4.47135855261381	0.65311689488834	1.50062125480046
C	3.12415822254196	-0.46175198041170	2.80134733242872
H	2.63660333058779	-1.44589266849307	2.81497572496121
H	3.82981474900958	-0.44066296667660	3.65597741812246
C	2.36248077254215	1.78002753020034	3.31311058721462
C	1.19547447517803	2.64971223391010	3.46018259935571
C	1.20663615256169	4.02814601864784	3.70236350691799
H	2.15801202049521	4.56537948907991	3.78175610726613
C	-0.01282083292403	4.71500757361269	3.84541075422989
C	-1.21582816639508	4.00507196850830	3.75907254226146
H	-2.17617801887997	4.51916023500387	3.87501526939383
C	-1.18554186487277	2.62208532851794	3.51391139752376
C	-2.30988885132125	1.72048732787179	3.39280971899070
C	-2.97903966388968	-0.55721424293240	2.87174327895300
H	-3.66645770857081	-0.55496900763600	3.74063345909401
H	-2.45718025633996	-1.52565491371010	2.87908997711599
C	-3.79982489202866	-0.41430130017500	1.57916153604504
H	-4.36999939157164	0.53280633654068	1.59781462815155
H	-4.55067699800898	-1.23063451690991	1.57874990234723
C	-3.01195373907512	-0.52512096998517	0.26333178538768
H	-2.49035627293462	-1.49273913457677	0.21843532946918
H	-3.72112546114069	-0.50082621580070	-0.58744072506414
C	-3.76222809072617	2.25472610087229	-0.43318872503142
H	-4.47202634271622	1.43406327445378	-0.62605686901594
H	-3.78673227824691	2.92822970415668	-1.31060683174815
H	-4.13899711500704	2.83033723433243	0.43767142052240
C	3.68298751654833	2.40528103902058	-0.49572853736674
H	4.00196674052020	3.08485249461204	0.32052155738264
H	3.66306443622945	3.00575659087737	-1.42602629224143
H	4.45576653854459	1.62899500291837	-0.61152333258119
C	3.73680523824941	2.33849926328748	3.57864315006715
H	4.51069745203199	1.55791584153887	3.64939752398156
H	3.73802849391133	2.90518019448662	4.53016288722598
H	4.03876904546638	3.04669632659719	2.78047265638087
C	-3.70804278791721	2.20342356717895	3.66087638382041
H	-4.10103796371678	2.80747009096109	2.81682699211912

H	-3.71283364958265	2.84871830697521	4.55959568268943
H	-4.41592112889044	1.37826361066498	3.84124642878377
C	-0.57732777212529	0.60540117820034	-2.92043507253394
C	-1.94878733184701	0.77841791635551	-3.20532920404417
H	-2.66429107396018	0.01494043560650	-2.87552635743793
C	-2.39075560906099	1.91081783801263	-3.90581996585583
H	-3.46051726026930	2.02919507879305	-4.12805391801759
C	-1.47315301215707	2.88658231361009	-4.32585451109816
H	-1.82042678821299	3.77308064001517	-4.87299189590623
C	-0.10377531796411	2.71251205314361	-4.05875713543815
H	0.62159604079289	3.46493381299643	-4.39759084151991
C	0.34326824779205	1.57930657922436	-3.36886233799446
H	1.41147655351075	1.44056524647524	-3.15918485506839
C	-0.43182371336556	0.47776625741876	6.02998783071846
C	0.53265476917380	1.40413635352239	6.48687679956934
H	1.59058356778752	1.23387306541789	6.24993348218858
C	0.14130703713420	2.53083756359169	7.22001645543310
H	0.90032123786362	3.24600222473253	7.56588774230407
C	-1.21511039645553	2.74583597723145	7.52116236933453
H	-1.51872444738171	3.62747021201913	8.10109482277790
C	-2.17593065958279	1.81646558984624	7.09264381380907
H	-3.23585022259695	1.96623962134752	7.34163524931223
C	-1.79012744557855	0.69052427708131	6.34994869190939
H	-2.53923503057617	-0.03704042021417	6.01369321498703
C	0.99390046889639	-2.92188540811992	1.48395623425026
C	1.41093900021895	-3.46501310443741	0.24947013248848
H	1.03895029461859	-3.03578894584863	-0.68887731344072
C	2.28978265796024	-4.55668353162539	0.22610344756850
H	2.60862142211821	-4.97225795568843	-0.73939557380628
C	2.75537136802894	-5.12099987138124	1.42541247344797
H	3.44356794886068	-5.97610579278612	1.40258895145931
C	2.32212522221428	-4.59545399112252	2.65405396074431
H	2.66633231717359	-5.04154124935010	3.59696565772176
C	1.44332089946537	-3.50399400064599	2.68887915371389
H	1.09662044561065	-3.10532804491270	3.65013483543032
H	-0.08793792318492	5.86429130080221	-0.77636031326494
H	-0.01953573236549	5.79562263017477	4.03154387846462

[Fe₂(SPh)₃]⁺, S_{tot} = 5

G = -5676.22350973 E_h

Fe	-0.22483668094613	-0.09675928262161	-0.14731378757318
Fe	-0.23321848597010	0.10031669173648	2.82551288117321
S	-0.12404379825968	-1.13037912273805	-2.15700953441093
S	-0.21575109176690	-0.77182399522872	4.88174777276252
S	-0.36345216664098	-1.73732159198269	1.57189342283727
N	-2.34946079245784	0.32327520047566	-0.05398703026745
N	-0.39125243473846	1.96770673698042	-0.06258358635396
N	1.78605970872447	0.64391677447868	0.04798344929086
N	1.70670116107342	0.58820578143382	2.92828778064719
N	-2.34798736824711	0.35504311941416	2.82007103758789

N	-0.38578908127528	1.93075769522628	3.19065775030544
C	-2.71265419664820	1.55561109277796	-0.24548230727907
C	-1.61219806482196	2.53236147131822	-0.17461702809756
C	-1.75529144658714	3.92937882659228	-0.21776518140345
H	-2.74765484599356	4.38696923818464	-0.28720605236981
C	-0.60422272458841	4.72907045749068	-0.16962538174987
C	0.65742708877534	4.11986491027030	-0.13395160229513
H	1.56835322182188	4.72742579974075	-0.13453261304450
C	0.73224760977486	2.71659307218375	-0.10019684122174
C	1.96912331077910	1.92286546899500	-0.10779025020463
C	2.90337326922125	-0.28981602064087	0.16534705291413
H	3.61723310743589	-0.15496437856177	-0.67348801489446
H	2.49272831705976	-1.30707965051264	0.07598889971108
C	3.65640164202133	-0.15871916463187	1.50061210575453
H	4.45073747092675	-0.93219261788237	1.50945041883103
H	4.16834094969570	0.82051152902073	1.54910139291588
C	2.80494308305510	-0.37157899857407	2.76289974243902
H	2.36013515996650	-1.37398003282376	2.73992968116876
H	3.46315066770644	-0.33752065993682	3.65371301204916
C	1.95124903063671	1.83652462008979	3.28317004795451
C	0.75743942023786	2.66239162577338	3.38524573156530
C	0.68886848460866	4.03845312128947	3.64432441723385
H	1.60749364932177	4.61279430504923	3.80468939062945
C	-0.56413078073006	4.66705465412812	3.69227364678098
C	-1.72649699355090	3.90281557314595	3.50846606048461
H	-2.71408490304769	4.37415695543381	3.55837555905637
C	-1.61798392230325	2.52541416434796	3.26892368452989
C	-2.71883788372043	1.57632072545372	3.11731014880823
C	-3.31495006802062	-0.73751123024173	2.66861251993662
H	-4.01467841654907	-0.74140281237247	3.52752546653114
H	-2.74416165461106	-1.67847175621290	2.71682238887127
C	-4.12898183974014	-0.69665155032702	1.36079100133423
H	-4.77162103083150	0.20348908017913	1.34878202491047
H	-4.81199036053206	-1.56996046100639	1.37497610410014
C	-3.31752915444020	-0.76563822370482	0.05371862365478
H	-2.75217822982759	-1.71117158123132	0.01116637214722
H	-4.01478108131634	-0.76361081369854	-0.80940693148600
C	-4.10385163036091	2.04642072743439	-0.55202462033265
H	-4.79871792110416	1.22405801876714	-0.78781882824352
H	-4.07499776443569	2.72798239454653	-1.42466824885765
H	-4.52993881919856	2.62127724851350	0.29444856697671
C	3.28335731399634	2.62508802029789	-0.32868355037040
H	3.55171280644979	3.26812413369092	0.53356099167727
H	3.20776079699900	3.28709174753496	-1.21375417113148
H	4.11523775908539	1.92342435165713	-0.50140363331008
C	3.29742604353487	2.42630756434353	3.60221570181586
H	4.07773231409723	1.66150026321707	3.74201150003884
H	3.23088215788817	3.01509260123636	4.53681961627862
H	3.63795573125236	3.11546903203759	2.80258926065243
C	-4.12854332380028	2.04392435881442	3.37230304998804

H	-4.44983046907301	2.77898684515513	2.60707944029745
H	-4.18232626385848	2.55874509554286	4.35213534242957
H	-4.86126982726952	1.22202038010639	3.38166428669133
C	-0.16676206004022	0.48716406378494	-2.89213981118667
C	-1.40254851660020	1.09378475576168	-3.22046856621497
H	-2.32975364538466	0.52856848747117	-3.06740123701790
C	-1.44039197313341	2.39920674897356	-3.72649054539808
H	-2.40811648428081	2.85726745732835	-3.97485616122912
C	-0.25077013389181	3.11995353874076	-3.92559871013075
H	-0.28365146571627	4.14394748760360	-4.32023664251242
C	0.98262701403959	2.50985127245300	-3.64097168294594
H	1.91971367700159	3.05443954627474	-3.82338438729747
C	1.02851903325619	1.20541142092651	-3.13314510710559
H	1.99020840906344	0.72699795288308	-2.91287987489133
C	0.11901630106265	0.63535014302592	5.89765668811164
C	1.44544604379490	0.95431850859079	6.26270121711490
H	2.25787387458979	0.28170081779107	5.96024893730095
C	1.72007165484643	2.11226477429076	7.00511948423786
H	2.75569802333470	2.34308685189066	7.29148446746322
C	0.67749293291018	2.97240427496132	7.38465362074174
H	0.89332795158673	3.88091984304911	7.96248527271239
C	-0.64759070867260	2.65362638137106	7.03889374924217
H	-1.46912533814209	3.31437741317882	7.34801772965169
C	-0.92724479459177	1.49131627288480	6.31058373483638
H	-1.96018662290643	1.23516970732624	6.04390470548769
C	0.89675482210779	-2.99052400848704	1.56413331225910
C	1.37767692716308	-3.52876121002635	0.35288919851479
H	1.01106513958122	-3.13973335079723	-0.60448615500438
C	2.32467447493656	-4.56221898068253	0.37468051683392
H	2.69615003653453	-4.97314531414839	-0.57378558306871
C	2.79145535013600	-5.07393944671498	1.59677378103751
H	3.53186322181947	-5.88452099170936	1.60886647578147
C	2.29465360020310	-4.55277204823140	2.80270542809384
H	2.64163422252583	-4.95711192972968	3.76327948804001
C	1.34901768311627	-3.51780143856032	2.79261622742833
H	0.96175164997889	-3.11224834671069	3.73573388697426
H	-0.68985571791399	5.82258439291383	-0.18562525797346
H	-0.63548034119734	5.74392742314644	3.88633364924736

[Fe₂(SPh)₃]⁺, S_{tot} = 7

G = -5676.22928608 E_h

Fe	-0.10707581374342	-0.16261112493571	-0.18910731149616
Fe	-0.23606475016787	0.11974293198904	2.93668866941666
S	0.02036469303468	-0.91250383414868	-2.32391179485884
S	-0.27359031927511	-0.77860681257126	4.99941012372016
S	-0.31224363675228	-1.70364756240525	1.58630177398549
N	-2.22898625402128	0.24842823446804	-0.10830363953337
N	-0.26767528387680	1.88053947907286	-0.09503139621378
N	1.92775360400827	0.57230461048698	0.10232222760791
N	1.70185064555701	0.57877799440446	2.99481211882543

N	-2.26883268504112	0.39856946073366	2.77425496843064
N	-0.34443383509232	1.95989396094812	3.18684881122777
C	-2.58556898122549	1.48124437595640	-0.32878085735191
C	-1.48658173295417	2.44908538149001	-0.25099397322209
C	-1.62234635133013	3.84576437351343	-0.32116375763763
H	-2.61129917187605	4.30199665010635	-0.43359048342821
C	-0.47617652727393	4.64635673716494	-0.24637246210602
C	0.78360420048737	4.03294182944321	-0.15961287923359
H	1.69501064317820	4.63951858069096	-0.14012016927607
C	0.85534920791159	2.63436067954404	-0.10481138265203
C	2.10077153681996	1.84780382162760	-0.05753444873543
C	3.03970740536318	-0.35523879775441	0.29487873165518
H	3.80418164292222	-0.22296363395169	-0.49786455333487
H	2.63928446864608	-1.37570723526729	0.18710871851233
C	3.70616386537374	-0.21437500195288	1.67502991164055
H	4.49490511323313	-0.99102696439864	1.73763740102445
H	4.21974765629743	0.76222541839116	1.74682619548669
C	2.77668334852430	-0.41214892245223	2.88378203248043
H	2.30810788148735	-1.40190657193115	2.82369637234988
H	3.38461284153715	-0.40795834116732	3.81080099623929
C	1.97349500414368	1.81982415713599	3.38038422506225
C	0.80646339786255	2.66754352268435	3.43377587794923
C	0.74344491842581	4.04461738153441	3.69731860013821
H	1.66400526220841	4.60650469390615	3.88906563609271
C	-0.49937188145999	4.69054198147746	3.70367196964614
C	-1.66921352501907	3.94266864790225	3.47649676687689
H	-2.65165655296961	4.42697745844391	3.50018711581277
C	-1.57065927696713	2.56948567714636	3.22910067021081
C	-2.66249798338950	1.62270628055915	3.05133604864695
C	-3.23559686939514	-0.70283849654211	2.64023101508705
H	-3.95052672383399	-0.67604719906056	3.48565883799556
H	-2.66662650987640	-1.64049177333436	2.73291128677045
C	-4.02919268693843	-0.71146248624023	1.31850133828373
H	-4.67244989057613	0.18647259999847	1.26465405130883
H	-4.71317240601248	-1.58327570551973	1.35899478294154
C	-3.20871261369142	-0.82673347908780	0.01949497137325
H	-2.65596926832450	-1.78032491170105	0.00597719653598
H	-3.90212118132370	-0.83946335872953	-0.84686571711023
C	-3.97441072048190	1.96949180342242	-0.65002090449472
H	-4.65724052642490	1.14583251952300	-0.91538125641562
H	-3.93570956365791	2.66504278462822	-1.50989396130952
H	-4.42044881757059	2.52164600103860	0.20123499504804
C	3.41928017489112	2.55932682421389	-0.21676551150095
H	3.63046385348089	3.21025128367456	0.65472015662884
H	3.38743955918801	3.21447155647396	-1.10932876632483
H	4.26488735644944	1.86310415418347	-0.33648971087632
C	3.32877413630905	2.35692754444912	3.75371931856581
H	4.03307336146324	1.55917157343382	4.04211082537088
H	3.23708711494825	3.04462945352799	4.61428677824111
H	3.79015915663323	2.92563681205374	2.92016032700310

C	-4.07931829188327	2.07801984007392	3.28506880245646
H	-4.36188447433277	2.87334534639821	2.56685713095092
H	-4.17000842959079	2.51745151694373	4.29886900825082
H	-4.81901956603994	1.26745889518752	3.20148869052706
C	-0.31225664648251	0.68715433827041	-3.01745202945420
C	-1.63467536059091	1.07110543716781	-3.33564047437358
H	-2.44941935530062	0.35085927264619	-3.19195933217985
C	-1.89860335011680	2.35292873564771	-3.83880503428171
H	-2.93041416050928	2.63263554200081	-4.09432453788401
C	-0.85502086725859	3.27354240627050	-4.02594614176767
H	-1.06472312872747	4.27694101903414	-4.41913529366904
C	0.46411102405227	2.88991921155830	-3.73019126234867
H	1.29055950833243	3.59560596379774	-3.89381640679089
C	0.73740399257747	1.60804813693997	-3.23597107131748
H	1.76816750059687	1.30628738571821	-3.01102018725938
C	0.08600324787382	0.66288185599716	5.95646555436387
C	1.41391853622062	0.97680221321217	6.32034394792895
H	2.21909016885324	0.27892928174491	6.05846811729887
C	1.69873299331929	2.15876389295357	7.02177549417319
H	2.73544868328532	2.38239076517628	7.30991489506631
C	0.66834206773488	3.04922614539486	7.35808291556665
H	0.89250873155251	3.97440399069712	7.90528889738855
C	-0.65789503617889	2.73850867650533	7.00666775930332
H	-1.47220922799518	3.42388821013836	7.27925695960693
C	-0.94952209547749	1.55517718553107	6.31944741039681
H	-1.98411064747220	1.30887846588977	6.04885066139477
C	0.88768351818896	-3.00838206970641	1.58302280714991
C	1.37044779620398	-3.53095825636809	0.36458901656954
H	1.02493014671628	-3.10938592595914	-0.58809160826121
C	2.28133320369683	-4.59620193597653	0.37222386452756
H	2.65099359246417	-4.99821139280488	-0.58063887112470
C	2.71481941189538	-5.15013539623758	1.58837218318320
H	3.42846593412923	-5.98438507161338	1.59046138800155
C	2.21903636591246	-4.64235160713381	2.80074958693168
H	2.54065382368347	-5.08122183081502	3.75485188989211
C	1.30427637391954	-3.58018238510083	2.80425080759140
H	0.91264146446508	-3.18645835500055	3.75060185169614
H	-0.55899726032857	5.73928290686809	-0.28312627150295
H	-0.56211989723138	5.76745057066163	3.89988197491806

[Fe₂(SPh)₃]⁺, S_{tot} = 9

G = -5676.23453367 E_h

Fe	-0.28737983945174	-0.07333206320045	0.06820036919069
Fe	-0.21172003582023	-0.12559059809743	3.07810482451857
S	-0.31891215861342	-0.97480112580098	-2.03111854288704
S	-0.13728521572912	-1.12390666226238	5.12771105932317
S	-0.35575447139948	-1.92463881081790	1.53775749744564
N	-2.40736785810394	0.35941696688137	0.19907369548144
N	-0.43004667686919	1.98846748174387	0.03241703263779
N	1.73722774122173	0.63842086804031	0.10851451195249

N	1.80843097090736	0.59318985197676	2.93630658135900
N	-2.32932328928827	0.30803389909068	3.04130088200681
N	-0.35375251216452	1.93927113119950	3.13173321330340
C	-2.76357626875370	1.58696431679233	-0.02942732915718
C	-1.65022336272753	2.55616604727735	-0.06378793225409
C	-1.78445830036712	3.94412741514291	-0.22150266389011
H	-2.77436996383840	4.40772456715544	-0.28436688549618
C	-0.62394750847198	4.72914048244734	-0.30965860364637
C	0.63203355499475	4.11000289575120	-0.28389840571580
H	1.54598167162958	4.70277627229638	-0.39357992109855
C	0.69845235783364	2.71504258403022	-0.12237129694588
C	1.92478091156245	1.90472249708990	-0.13494239389558
C	2.84699559336137	-0.30983902012865	0.18304132509414
H	3.51031678830865	-0.20393003154864	-0.69981359258814
H	2.41769907461777	-1.32191918732857	0.13800845543258
C	3.68796922813849	-0.17044957605668	1.46474802163855
H	4.47231508386262	-0.95318846732682	1.43205011907310
H	4.21072290749543	0.80491068978925	1.46564885002968
C	2.91477486632453	-0.34926856061930	2.78323727760038
H	2.48963517465884	-1.36331573501842	2.82186055663762
H	3.62064233860684	-0.26505091140125	3.63503977473443
C	2.00578856445064	1.85626053023391	3.18505735542572
C	0.77951682802769	2.66609176966902	3.23485240763165
C	0.72005959796173	4.06050047719298	3.40099009265980
H	1.63744549435328	4.65483157167257	3.46463302916248
C	-0.53465499934826	4.67790369603653	3.48990268632464
C	-1.69644368005526	3.89122380971566	3.46066477272752
H	-2.68270129144034	4.35300530137916	3.57462907825808
C	-1.56854843229014	2.50319172563188	3.29353047458820
C	-2.67777222249341	1.53157147838922	3.30744073701916
C	-3.30524222398499	-0.77708675651142	2.93513494021623
H	-3.97631468056582	-0.78823657149191	3.81788454094015
H	-2.74106621071824	-1.72423754178149	2.94821613423095
C	-4.15549564331866	-0.69488087853156	1.65331677936136
H	-4.79056213191597	0.21067931613617	1.68660878565128
H	-4.84423162371373	-1.56353651970013	1.65575214036529
C	-3.37603124038973	-0.73049792182922	0.32481086043337
H	-2.81251367197297	-1.67534152948382	0.24997556085289
H	-4.09499432005669	-0.71476317460304	-0.51898601083363
C	-4.16017592173397	2.08057111199282	-0.30700428626902
H	-4.89000044970804	1.26152317359272	-0.40730103221363
H	-4.17269100096814	2.66493710381576	-1.24830014830293
H	-4.51363649078496	2.75809579649595	0.49589011534753
C	3.23420432034026	2.57323001809213	-0.46196852491908
H	3.54011368257212	3.27796637963473	0.33727523855879
H	3.12942189365169	3.16308728823669	-1.39331056963834
H	4.05417707974008	1.85240982925067	-0.60968396230155
C	3.32915695941900	2.52088634695101	3.45997555923409
H	4.14901655605663	1.79566068020282	3.58598874842739
H	3.26036685230630	3.12031317213915	4.38848657205701

H	3.61227529331667	3.21565975415007	2.64392301123660
C	-4.06110688273692	2.01325777606585	3.66148943461508
H	-4.48242756594965	2.65588223242965	2.86252360734243
H	-4.02220444183932	2.62673815104492	4.58286584685110
H	-4.76548551591014	1.18421639664787	3.83663979504581
C	-0.15682137396540	0.60611839166902	-2.81669981633865
C	-1.30523142982998	1.37346716496338	-3.12072303213561
H	-2.29688817409865	0.95531366293901	-2.90673553197231
C	-1.17896699265648	2.64951539730035	-3.68423235330729
H	-2.08111065910111	3.23417778264718	-3.91244426055089
C	0.09105334388357	3.17920806377634	-3.96892637329618
H	0.18697943207914	4.17729705392884	-4.41625167085170
C	1.23512306966991	2.40957650820136	-3.70094839610511
H	2.23135931303730	2.80216986985677	-3.94908851261361
C	1.11662964440507	1.13653086429394	-3.12684801455855
H	2.00969541711541	0.53479663211686	-2.91848522360758
C	-0.02348095938153	0.45417699533131	5.92843283435352
C	1.23393729852724	1.04660544628534	6.19065561932252
H	2.14660996697819	0.49272806220880	5.93941298498536
C	1.31156043343649	2.32074040761487	6.76816811499824
H	2.29604859738694	2.76379521162206	6.97469553490468
C	0.14192254005123	3.02878273126248	7.09146279245868
H	0.20610675148128	4.02858013753811	7.54057630200218
C	-1.11038998801486	2.43484915115498	6.86065175206713
H	-2.03040510708916	2.96973807900147	7.13520818068782
C	-1.19576715041341	1.15780932123727	6.29172965785892
H	-2.17269836158039	0.68963660140416	6.11884986467465
C	0.97309856381895	-3.10140285470935	1.48451394134978
C	1.45032353243961	-3.57210524725220	0.24315117844237
H	1.01296388933392	-3.19238463739107	-0.68863430762855
C	2.48381204115080	-4.51855222085706	0.20473182508373
H	2.85091035726781	-4.87832647395983	-0.76600305010813
C	3.04225161225795	-5.00978122136067	1.39652978325635
H	3.85028242348997	-5.75233942018149	1.36229180396262
C	2.54918831517266	-4.55948344272517	2.63240390875380
H	2.96748644877188	-4.95153769857533	3.56932682792180
C	1.51593063759445	-3.61306860171883	2.68162060243300
H	1.12991619619479	-3.26652481219026	3.64827561162599
H	-0.70138884551136	5.81700758584474	-0.42777663677276
H	-0.60755406612830	5.76573429875790	3.61109780873284

[Fe₂(SPh)₂]⁰, S_{tot} = 1

G = -5360.72362658 E_h

Fe	-2.08434124760922	-0.54841561050919	-1.62503079331573
Fe	-0.00583533914341	0.01558783512217	-0.02448449064677
S	0.07104255907812	-0.55341739697165	-2.16533099042877
S	-2.16142425585519	0.01974572376407	0.51597091334987
N	-2.62225996058476	1.24732359748722	-2.16370469854674
N	-3.85305429930886	-0.86566782921282	-1.97804972794072
N	-2.09578412417977	-2.54037479507458	-1.62581369590565

C	-3.94289777994754	1.42786779568949	-2.28943238911662
C	-4.69455875214042	0.21508746849708	-2.13166152131356
C	-6.08829621916418	0.03581774717413	-2.11716700895015
H	-6.72727558857145	0.91892800295328	-2.19858495118868
C	-6.64953925735299	-1.25008411186158	-1.97048751881320
C	-5.75492907404066	-2.33855757355202	-1.86540409723554
H	-6.13920872333029	-3.35710245066326	-1.74915898368492
C	-4.36598244220434	-2.13813863845938	-1.85960089986058
C	-3.30778325298734	-3.09795888860617	-1.70416161688052
C	-0.93158641327735	-3.43937557498430	-1.67155565969304
H	-0.10425824598897	-2.86889717437796	-2.12449498407307
H	-1.13447332663692	-4.29537668925775	-2.34426568287850
C	-0.45623227543319	-3.97639232024884	-0.31508669548639
H	-1.15126901954217	-4.75206076641812	0.06725022791248
H	0.51598301399381	-4.48174574815900	-0.48125606185812
C	-0.35694513200555	-2.91280815649871	0.77950058866797
H	-1.36165589183941	-2.51114305203621	0.92751503070320
H	-0.07248564983505	-3.39602315772095	1.73660070827704
C	-4.62893745156787	2.73393460693458	-2.59512685768867
H	-4.94084057642633	3.25790287982572	-1.66599741161267
H	-5.54207670958430	2.56479723772083	-3.19736365263910
H	-3.98385057759840	3.42919293760561	-3.16152446520793
C	-8.16626453854174	-1.49632484260677	-1.88259764095141
C	-8.97519338236910	-0.18820141144279	-1.98948407317726
H	-8.80233894219249	0.32371556160256	-2.95682728861154
H	-8.71991132919366	0.51608649473482	-1.17347510439146
H	-10.05880596792872	-0.40865937257616	-1.91507637869221
C	-8.49115799752298	-2.15243732542344	-0.51660067926853
H	-9.58373421248552	-2.31667374479594	-0.41336733065878
H	-8.15544888429542	-1.50434700024874	0.31795764254892
H	-7.99119216734393	-3.13395339603549	-0.40306663673537
C	-8.60799435218128	-2.43700271295031	-3.03009707948013
H	-9.69966867894819	-2.62906175960719	-2.97640177250232
H	-8.09139065042500	-3.41563359188417	-2.98242646401185
H	-8.38335641680128	-1.98366174004393	-4.01637429990917
C	-3.56812151606629	-4.58166368464956	-1.72855014272330
H	-3.22901136464592	-5.04288845574990	-2.68093408696335
H	-4.64687231967140	-4.79613343004173	-1.63182962919775
H	-3.05249117927125	-5.11175552614695	-0.90557283580613
C	0.83476814430130	0.58979438550057	-3.29627163837324
C	0.21542469660620	0.90288291836441	-4.52681384810912
H	-0.79190892725247	0.51503490188966	-4.72872995489653
C	0.87179377279571	1.71213766196504	-5.46303579414475
H	0.37655454167876	1.95002634257612	-6.41533004329951
C	2.15337037622417	2.22246496434354	-5.18932260550599
H	2.66267995152223	2.86235564361430	-5.92289198105839
C	2.78010189931258	1.89642604877915	-3.97516983057551
H	3.78859746306801	2.27389280953779	-3.75205082637310
C	2.13313378351807	1.07858987355619	-3.03806403894497
H	2.64379808494432	0.80060002965745	-2.11216207206426

N	0.53359969409551	-1.77992867579519	0.51344993075834
N	1.76405277433223	0.33299779388142	0.32284564386593
N	0.00541460108903	2.00757384357890	-0.02273409656294
C	1.85476679779884	-1.96075288151752	0.63299739004075
C	2.60600309224053	-0.74812751935598	0.47166407032777
C	3.99968501436307	-0.56932060757152	0.44852872063334
H	4.63898304067025	-1.45257049259118	0.52587436955531
C	4.56031464993872	0.71644356214006	0.29787111881730
C	3.66552554446595	1.80522784305139	0.19843260534840
H	4.04939992136835	2.82344430995725	0.07808084762046
C	2.27651230201438	1.60527953930647	0.20117598906433
C	1.21767402249744	2.56522032513497	0.05093553492698
C	-1.15877163634282	2.90630313584680	0.02646460753509
H	-1.98496346135851	2.33542858681985	0.48088260650721
H	-0.95456850839831	3.76211726999768	0.69903374214587
C	-1.63661524587592	3.44354734398575	-1.32917619365321
H	-0.94453128265638	4.22242067466479	-1.71036722260490
H	-2.61088987633890	3.94476130939383	-1.16260832693075
C	-1.73114148378847	2.38091796309095	-2.42511838204703
H	-0.72556338843040	1.98005251205757	-2.56934825069322
H	-2.01197026161786	2.86494156058173	-3.38284170945265
C	2.54186956664804	-3.26706427189541	0.93522608022441
H	2.84768341922131	-3.79171290959640	0.00445089578322
H	3.45872419858908	-3.09821020265555	1.53185169110537
H	1.89970732868577	-3.96158765032138	1.50588675231909
C	6.07633061951993	0.96198731201638	0.19655574084901
C	6.88641613366677	-0.34496768223625	0.30940382420240
H	6.71903920057702	-0.84910186762070	1.28180669257016
H	6.62690715719565	-1.05596641802115	-0.49940628594432
H	7.96950035114250	-0.12481451664994	0.22674813981310
C	6.38990036593057	1.60500344927696	-1.17832723658544
H	7.48100130412378	1.77358618208495	-1.29010367576060
H	6.05245853600293	0.94599840274045	-2.00358145065861
H	5.88350563189407	2.58231018289806	-1.29988280907764
C	6.52721971429544	1.91320377089911	1.33159889308863
H	7.61871538931092	2.10316135101325	1.26810590084959
H	6.01194577498696	2.89224294146020	1.27866275778530
H	6.30928757128948	1.46938561579301	2.32369290812674
C	1.47798776410246	4.04890449118714	0.07519101883845
H	1.13704678817095	4.51024585794632	1.02684580615103
H	2.55692710321351	4.26335744078893	-0.01934685662183
H	0.96381379690709	4.57893903754159	-0.74877970948149
C	-2.92363145708197	-1.12396333684664	1.64742743178601
C	-2.30625540402092	-1.42931941156302	2.88097181614144
H	-1.30114614536628	-1.03624377319745	3.08392969470733
C	-2.96129481303236	-2.23820056242072	3.81841322892340
H	-2.46749012053567	-2.47029542832921	4.77287978422917
C	-4.23992688305260	-2.75524124579657	3.54334600446764
H	-4.74838762777624	-3.39448907881842	4.27808321288265
C	-4.86487378963467	-2.43658024703635	2.32635454324949

H	-5.87108916416060	-2.81945544006300	2.10208269964360
C	-4.21891939998665	-1.61978071057498	1.38758391802838
H	-4.72823309464378	-1.34773421874149	0.45921941309401

[Fe₂(SPh)₂]⁰, S_{tot} = 3

G = -5360.72813854 E_h

Fe	-2.03976439629764	-0.55734282751388	-1.89021072377948
Fe	-0.05139658126412	0.02336203755396	0.22072772690017
S	0.19866709452940	-0.54596627254884	-2.27205131839899
S	-2.28938495876317	0.01286208923203	0.60514206633830
N	-2.60497509095122	1.25997142236606	-2.29745315854414
N	-3.85656527874280	-0.86279232666021	-2.06276085432228
N	-2.06410466580181	-2.54139086810050	-1.73290477202398
C	-3.93286139324086	1.43192082134357	-2.39855446913403
C	-4.68770316660024	0.21665407281480	-2.23149081656297
C	-6.08515802599274	0.03751749818554	-2.17476481041776
H	-6.72861767646642	0.91415000400515	-2.28389246219373
C	-6.63637294267717	-1.23976743355532	-1.94214320601286
C	-5.74242238250168	-2.32545482196168	-1.78862701841676
H	-6.11971214476082	-3.33060565828026	-1.57718602157998
C	-4.35382635178234	-2.12140884170735	-1.84986469002402
C	-3.28662510236187	-3.07940866185073	-1.68007534952810
C	-0.88639771635673	-3.42368113394007	-1.73975749321801
H	-0.06058114275157	-2.84330876599761	-2.18014931619554
H	-1.06380609209228	-4.27991065741050	-2.42220053568353
C	-0.43025207298549	-3.96733616262606	-0.37642478630904
H	-1.11882647575054	-4.76735004660681	-0.03360980286878
H	0.55535430167120	-4.44967355889464	-0.53225257833277
C	-0.38186143371220	-2.94805284424295	0.76958275104405
H	-1.39452117864719	-2.55208605642311	0.88196166664048
H	-0.15250761890737	-3.48697290038066	1.71237872367430
C	-4.62747864476801	2.74412484953615	-2.64581224542535
H	-4.95075578514511	3.22175914690583	-1.69550941065983
H	-5.53685958189889	2.59262526275584	-3.25916365603728
H	-3.98537426006818	3.46900947502776	-3.17734956512071
C	-8.15037013608088	-1.47864986629178	-1.79987670770770
C	-8.96988089580562	-0.19547895999790	-2.04291669268636
H	-8.80123697278326	0.20893208753371	-3.06058237379734
H	-8.72058252174339	0.59525780105144	-1.30843082698487
H	-10.05138014083017	-0.41572566747539	-1.94235579394986
C	-8.44422765577669	-1.97709587321282	-0.36193541998208
H	-9.53342800185133	-2.13620215318218	-0.22078482361720
H	-8.09971059399235	-1.23661494332506	0.38769559200963
H	-7.93210860500029	-2.93567969613886	-0.14785664124891
C	-8.60870624454805	-2.54652594017305	-2.82324179867969
H	-9.69932386965163	-2.72832314297044	-2.73009589867078
H	-8.09212787295507	-3.51382401008273	-2.66908855651486
H	-8.39985472486594	-2.21165970026612	-3.85915747971258
C	-3.60044151991533	-4.53263324425626	-1.44684566980153
H	-2.76485093736831	-5.20211912532866	-1.71482509817543

H	-4.48367776023295	-4.84503361967633	-2.03697275576303
H	-3.84187976088184	-4.70745600217811	-0.37583859694256
C	0.95495507247130	0.66148678065896	-3.31963376147930
C	0.33068150793150	1.11985343351910	-4.50341659708234
H	-0.67600622249594	0.75541432496620	-4.74677019711905
C	0.97831604480276	2.03588534495279	-5.34149325856359
H	0.47550746714538	2.38381521948766	-6.25535459661230
C	2.26396589894433	2.50912269823472	-5.02230096172885
H	2.76732853713556	3.23161955586805	-5.67944058229963
C	2.90491197436599	2.03233649421327	-3.86676473566146
H	3.91985366784652	2.37222840724911	-3.61476338489551
C	2.26306866162933	1.11041546744258	-3.02747983580070
H	2.78292986930263	0.71838622070285	-2.14813005378831
N	0.51378085859565	-1.79404314536003	0.63068529034518
N	1.76547167320743	0.32906027746414	0.39795732891280
N	-0.02637406742760	2.00758473496548	0.06512389621826
C	1.84173087007342	-1.96571897565875	0.73473288884178
C	2.59657827256710	-0.75037502910406	0.56892999682890
C	3.99409192144771	-0.57097168183425	0.51495407857680
H	4.63740888130525	-1.44755437531639	0.62538090257356
C	4.54567187140507	0.70632238699787	0.28346048847893
C	3.65203883255090	1.79193944059251	0.12835488488025
H	4.02970618587843	2.79719069881628	-0.08196511907412
C	2.26327218556625	1.58794876741947	0.18670213635866
C	1.19636413920524	2.54594529988965	0.01500053521109
C	-1.20370564138161	2.89046591877330	0.07111603148565
H	-2.03003259027918	2.31048515958287	0.51123310306754
H	-1.02657237422946	3.74688974469474	0.75329291238311
C	-1.65894671140114	3.43369545952832	-1.29271565400606
H	-0.96905838587557	4.23234756527895	-1.63611254277581
H	-2.64374823451513	3.91776990247018	-1.13728429796783
C	-1.70880635768919	2.41340267035972	-2.43775098178543
H	-0.69646058791049	2.01684774153698	-2.55043129635984
H	-1.93880044182426	2.95147501834035	-3.38092497541679
C	2.53600894825014	-3.27800866176197	0.98237075529734
H	2.86309803907190	-3.75412522316330	0.03261091576613
H	3.44296552366526	-3.12709487388712	1.59945595693553
H	1.89203926579622	-4.00385119776027	1.51035790686328
C	6.06006760030529	0.94546589066501	0.14514104016910
C	6.87920229070391	-0.33761620245107	0.38995662062839
H	6.70776455853416	-0.74241720160244	1.40699931126404
H	6.63216437075465	-1.12815825862759	-0.34550364153575
H	7.96092579004046	-0.11711215806949	0.29250611922936
C	6.35778343087071	1.44457455783567	-1.29174833087608
H	7.44737016657435	1.60361230806795	-1.42999311684753
H	6.01511209573891	0.70456567770692	-2.04268599226487
H	5.84631579405312	2.40332526844274	-1.50658376997335
C	6.51539715366927	2.01301329883079	1.17013347065077
H	7.60611809152940	2.19546783098568	1.07953908145121
H	5.99862018882787	2.98012269392223	1.01541886547930

H	6.30445422501863	1.67738958503946	2.20538403565155
C	1.51092710449944	3.99906399761723	-0.21764820174946
H	0.67424969748402	4.66884693110419	0.04614084923634
H	2.39163221883710	4.31173016694749	0.37613393997013
H	1.75716849745745	4.17317784442942	-1.28770148030518
C	-3.04275640071570	-1.19447958498888	1.65491283367907
C	-2.41555185820797	-1.65193118232609	2.83752988779330
H	-1.40848284638733	-1.28683007681631	3.07826916351924
C	-3.06072568873478	-2.56821450958697	3.67722100624212
H	-2.55564947367705	-2.91568974012817	4.59000570799771
C	-4.34667672184978	-3.04260446879973	3.36083811814242
H	-4.84795080861013	-3.76553058014156	4.01910097756775
C	-4.99042936504458	-2.56678891917946	2.20647575621223
H	-6.00553729961730	-2.90785527855852	1.95660963847878
C	-4.35103152316741	-1.64469369532402	1.36550892347602
H	-4.87297686464739	-1.25341055020943	0.48703767852326