

Supporting Information

Structures, Spectroscopic Properties, and Dioxygen reactivity of 5- and 6-coordinate Nonheme Iron(II) Complexes: A Combined Enzyme/Model Study of Thiol Dioxygenases

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S1. Optimized coordinates for **1** calculated using BP86.

	X	Y	Z
Fe	1.55025232467590	3.81832124656423	1.85515561631413
S	-0.38136228956202	4.84385007439815	0.85102500736694
N	3.38206412947050	2.86437433769840	2.80740991242341
N	2.34094257692502	2.66704470348407	0.10710709943851
N	3.18093900043017	5.23809014498616	1.14109647296172
N	0.76597304984783	4.95921250143381	3.60246403623916
O	0.48642956962921	2.03850621360958	2.60706589063529
C	-0.53981224355016	6.22997486191714	1.95848246465772
C	3.20721607835317	2.58852692248660	4.25267964650866
C	3.49279710313271	1.57850508922803	2.06150258985073
C	4.57691256130880	3.74204185650921	2.59857952952023
C	1.27495073793473	1.85535076775027	-0.52835485721584
C	3.47570456407587	1.78717939654037	0.54199054703408
C	2.78750892343976	3.73324768923827	-0.83220073876744
C	2.71335713711442	6.63654597241841	0.97526260614742
C	3.73788622930538	4.72989943876517	-0.15765427201162
C	4.17512281719336	5.17777338042872	2.24997236749348
C	0.06716106642618	6.17811151022568	3.24131721247094
H	1.36230928127663	5.13339548468965	4.42290136600255
H	0.06504936559872	4.25796743666112	3.92084463570868
S	-0.89522980391574	1.78064460216822	3.16606751233570
C	-1.22628003137420	7.41180017421343	1.59975708466786
H	2.28006471012319	2.01735984976357	4.40569287328219
H	3.13750239656316	3.54032698937931	4.80277597680191
H	4.06187321976751	2.01099098633224	4.66017096559958
H	2.62936303795312	0.96567770784915	2.36549337245374
H	4.41634910479117	1.02921793484296	2.34343208998277
H	5.21293199243083	3.31308413530116	1.80762670926705
H	5.20334647583398	3.76343260300039	3.50918343992572
H	0.43792313980510	2.51059872157447	-0.81763230270654
H	0.90442586821947	1.11338334778070	0.19410974199678
H	1.65425162231970	1.33547225685080	-1.43111718263245
H	4.42424725899142	2.23103568718827	0.20290133900502
H	3.40625945579408	0.80194673312135	0.04766973852522
H	1.87793094991335	4.25902669976008	-1.16969452977685
H	3.28116129983444	3.30031569374970	-1.72692390542265
H	2.23772968752563	6.98116888247024	1.90550694061004
H	1.96636338996942	6.67583160199436	0.16831026334582
H	3.55968979366886	7.30849786835303	0.72977887535481
H	4.72252950345184	4.27002691143267	0.02310298602215
H	3.92058326170792	5.57404058338560	-0.84586540438780
H	3.70230473951376	5.65837252166164	3.12384743521004

H	5.08286534072771	5.76658405409875	2.00325688226053
C	0.01195924024387	7.27962401209014	4.11084187101684
C	-0.60342585587664	0.22427936842379	4.21128776582483
O	-1.32158580013645	2.81136229844004	4.15876446587573
O	-1.90823242892562	1.36062624416622	2.17147150205887
H	-1.70017168236511	7.46612852055987	0.61382395086489
C	-1.28464802145039	8.51132642602695	2.47006802371829
C	-0.65781802032266	8.45378632646770	3.72721638388395
H	0.48806421148876	7.21165508802319	5.09639522326740
F	0.26518904786659	0.47720234767624	5.21249407248123
F	-1.76683489860676	-0.19016572717072	4.75128883749724
F	-0.10324281980466	-0.76775726034605	3.44966264009598
H	-1.81345297282668	9.41944254010975	2.16036222673933
H	-0.69553839592615	9.30966424022776	4.40926500217604

S2. Optimized coordinates for **2** calculated using BP86.

	X	Y	Z
Fe	3.21538099255514	3.63378423846588	11.16127968290790
S	5.18065659553849	2.26517368037541	11.45131372724795
N	1.71269122456055	2.02501090953640	10.74245433376164
N	2.18170843372223	3.32109173944490	13.17858215438898
N	1.42471823611427	4.92150470748729	10.83444640307862
N	4.20488484414789	3.93547288163452	9.17590534978315
O	4.15305776880752	5.49718034211556	11.85932594677096
C	5.55139834614876	1.96497582177687	9.74537974816008
C	2.01081625747071	1.26833659982783	9.50201537813779
C	1.84448240123595	1.12649362382971	11.92147756280123
C	0.34544512085610	2.62814817055869	10.65815050530203
C	3.14694470949321	3.64531031771967	14.26209377487038
C	1.75033821870149	1.88517392232953	13.27015251299912
C	1.00610263900672	4.25736062590142	13.25540904819043
C	1.64248130336366	6.13228038497008	10.00302395963196
C	1.05766264545920	5.37523107527831	12.20809464419346
C	0.39490240769294	4.07789584354742	10.16062554100931
C	5.01140423863922	2.81684890044579	8.73917226322112
H	4.84180586712894	4.70904004383199	9.45838593668288
H	3.66175991939533	4.30442715028012	8.38406349827361
S	5.54350523788290	6.08520707905182	11.74530129329766
C	6.35410081786993	0.87769035283800	9.32899553284973
H	1.31594749571972	0.41341712087417	9.38555639901459
H	2.83420215760584	0.65074502293130	11.83385033883859
H	1.07686989113911	0.32641458707605	11.88801569592940
H	-0.13482651744594	2.55953963307364	11.64224863252305
H	-0.28750014541255	2.03744665406010	9.96966213124388
H	2.69493976118432	3.48922546063850	15.26219966231620
H	3.46026482140147	4.69466369004128	14.16060023003739
H	4.03909244845546	3.00743898840022	14.16305665572960
H	0.72760329069497	1.83284527579497	13.68329244776334
H	2.40029660386223	1.36320660128050	13.99004719712928
H	0.96918928188441	4.72931661761683	14.25555703593585
H	0.07424620656414	3.68301447191043	13.16149391939147
H	0.71303370258435	6.73073074629173	9.91147596646948
H	1.96597012253715	5.83733175584695	8.99237156118103
H	2.42541306830582	6.75140631573973	10.46304720349777
H	0.07999971026481	5.90247349122090	12.19977715510415
H	1.82966926396571	6.10610978319747	12.49617759415600
H	0.65265885777155	4.07571205244133	9.08763989242899
H	-0.61217559392036	4.53662512825117	10.25014278198979
C	5.24167952941321	2.56276126151132	7.38382892913898

C	5.19631205107155	7.93691250941796	11.96924501116855
O	6.46132536976800	5.75317654470471	12.85832169916965
O	6.10231657898590	5.98027679318485	10.36438650864581
H	6.78234909433489	0.21556663114446	10.08814385073723
C	6.58993595613542	0.61976908519013	7.97380602025976
C	6.02578116438141	1.45809352712196	6.99456531832163
H	4.81925009507289	3.23370943026936	6.62770634267827
F	6.35567237000228	8.62358545368188	11.96484758649820
F	4.56681523252341	8.15865697282731	13.13904207066959
F	4.42038611653785	8.40214564642029	10.96831755505693
H	7.20417205130974	-0.23612562858985	7.68042942972961
C	6.23948150653723	1.20440268940944	5.53122212613521
F	5.06594598043336	0.93703632281606	4.86913309409027
F	6.77977679811458	2.28736555615898	4.88538046854251
F	7.06790717422025	0.15292405371628	5.28734678967731
H	1.90318870277163	1.93274471744969	8.63036336864910
H	3.04376157543306	0.89191662563064	9.53871253259158

S3. Optimized coordinates for **3** calculated using BP86.

	X	Y	Z
Fe	2.42363201726016	17.65442641480675	7.06908061108311
S	1.19111785777085	19.42197866182359	8.09622267180309
C	3.14897744385383	15.40561103428952	9.06441532938430
H	2.10148528592031	15.12777734259801	8.85257441316816
C	3.15131177087993	16.43428952178237	10.20216676880198
H	4.17535085017159	16.70895481166620	10.50883301987570
H	2.65010823472665	15.99843233506937	11.08183853448151
H	2.60637031439496	17.35393437147172	9.92847047630110
C	3.90131448262163	14.12497104640354	9.46827533790419
H	3.81734643154013	13.33129875122425	8.70847858514267
H	3.45837177834673	13.73573168690960	10.40042407331983
H	4.97097726452698	14.31212623165177	9.66615416769954
C	1.72765568311980	16.75882790619118	4.15191142944197
H	1.17834410144624	15.93615076264934	4.64581955115205
C	2.05157911763611	16.32503221009825	2.70930984671503
H	2.55904196285419	17.12887214819711	2.14893113863416
H	1.10549773834486	16.10227391289464	2.18750371434059
H	2.67584852975396	15.41732612507076	2.65887529064889
C	0.82880605255779	18.00772542487616	4.12821751347097
H	0.73031802321969	18.46839031197119	5.12840823435849
H	-0.17868113016211	17.72918238447106	3.77640094506085
H	1.21315620669467	18.78123969894698	3.44106732504945

C	4.36316758695779	20.25667733190631	7.09012079128915
H	3.84255384437259	20.34206723794507	8.06061770548868
C	3.53250594196274	21.00589252358745	6.03828414542399
H	4.03788139303410	21.04288945051395	5.05704629028533
H	3.38687185388671	22.04699214258853	6.37133999376898
H	2.53381034539799	20.55740587745561	5.90346342247595
C	5.75775985124280	20.89786188778017	7.22848090226720
H	6.34098027640795	20.46721126823815	8.05883818828292
H	5.63500075296244	21.97480336944792	7.43580010746120
H	6.34884513116063	20.80645468899652	6.29954624847518
C	3.48250006331556	15.04896174855680	6.63658269378266
H	2.47286036792629	14.61323066669219	6.71718834896222
H	4.20380656573828	14.21548774893533	6.73485953509512
C	3.68830142371845	15.67683010757613	5.24992572225282
H	4.76047383007907	15.85069606580349	5.06710123872045
H	3.37791967604147	14.92692184786713	4.50364991102331
C	3.85787535928646	18.01015473891056	4.47199995966265
H	3.23731105207712	18.87881305146014	4.20104068470765
H	4.34689980778588	17.65126323820334	3.54580500676010
C	4.94473621031692	18.44138172934450	5.46497176722936
H	5.71244550941324	17.65802334261317	5.56391605512658
H	5.47093558495070	19.31239384542608	5.03829562215474
C	5.14988864704732	18.07040567107285	7.90470964818030
H	4.75374601761494	18.45554699372391	8.85915421360026
H	6.22679486838642	18.32665184718805	7.86841799698971
C	5.04836774539529	16.53880941212844	7.86229025072972
H	5.63039204186424	16.13768437784473	7.01781110948325
H	5.53582054777250	16.14774126665458	8.77035792587959
C	0.10091288029653	18.36011164620896	9.03028895145976
C	-0.50679189561802	18.78416532063181	10.23166392854681
H	-0.31816784031787	19.80071594234557	10.59287905747303
C	-1.32430485280685	17.91334619026414	10.96757979144994
H	-1.77838897906079	18.25939417298788	11.90200646132065
C	-1.55059532574593	16.60140097039845	10.51558178126116
H	-2.18453517596353	15.91807523569429	11.09010156602901
C	-0.96925535263660	16.16878081073260	9.31284379107703
H	-1.15800871710921	15.15679959602990	8.93779652849912
C	-0.15438347784541	17.04234155033125	8.57482436094490
N	3.64158630644661	16.02395752825306	7.76441450511621
N	2.94652592564475	16.96998204259250	5.03702283600761
N	4.39033147109098	18.76152959241522	6.81819163422109
N	0.46835527199041	16.64041241784605	7.32942615897283
H	-0.05579783527863	17.06749310988213	6.54937022839693
H	0.36655946810878	15.61480422987258	7.18577367420985
C	0.54352474342992	11.70488864981567	8.25694861550216
F	1.75534413005943	11.38193369879746	7.75406432941361

F	-0.06479118839177	10.56826630267462	8.65694540879449
F	0.73060719859330	12.48913877375636	9.34064642995204
S	-0.50336130979330	12.59901381759159	6.95932221845469
O	0.32880425552187	13.80627635816347	6.63891380537393
O	-0.60328279971745	11.61755708381665	5.84548002850081
O	-1.77441921449208	12.89557838537303	7.67653944562561

S4. Optimized coordinates for **4** calculated using BP86.

	X	Y	Z
Fe	11.817595	13.568092	11.776051
S	13.206859	11.697466	11.306417
C	14.549778	14.006701	13.478973
H	14.932223	13.526522	12.560208
C	15.666368	14.897428	14.056943
H	16.073590	15.602485	13.314643
H	16.497690	14.252681	14.389635
H	15.325445	15.474172	14.934922
C	14.181786	12.897599	14.475083
H	13.901367	13.301826	15.463224
H	15.058528	12.245591	14.624990
H	13.354599	12.270602	14.101688
C	9.316233	13.347191	13.588502
H	8.724175	13.301524	12.658116
C	8.381192	13.810044	14.719946
H	8.892667	13.803288	15.697744
H	7.529024	13.113009	14.785194
H	7.967856	14.817502	14.545763
C	9.878865	11.948534	13.896463
H	10.703481	11.670360	13.212964
H	9.080522	11.195341	13.788633
H	10.263461	11.871167	14.927934
C	11.647439	15.377860	9.249053
H	10.933753	14.573564	8.994171
C	11.206172	16.652985	8.506281
H	10.170799	16.945098	8.744627
H	11.254367	16.463821	7.419919
H	11.869962	17.509037	8.721062
C	13.046275	14.938913	8.793528
H	13.797753	15.734819	8.938788
H	13.016169	14.705722	7.716112
H	13.386086	14.033780	9.325271
C	12.557778	15.372438	14.152176

H	12.327951	16.422267	13.915084
H	13.174769	15.408467	15.066469
C	11.271443	14.607021	14.478726
H	11.521637	13.636527	14.933108
H	10.697343	15.188569	15.224684
C	9.889536	15.606484	12.680376
H	10.301653	16.460038	13.240131
H	8.796153	15.645867	12.811608
C	10.154948	15.765761	11.174278
H	9.501805	15.082961	10.605857
H	9.861566	16.796459	10.896671
C	12.527895	16.477859	11.325824
H	11.986674	17.138223	12.021917
H	12.915433	17.138709	10.532490
C	13.723497	15.818165	12.024822
H	14.369707	15.319653	11.281868
H	14.322354	16.618501	12.500352
C	12.454963	11.322794	9.740130
C	13.167703	10.667005	8.710392
H	14.203069	10.362305	8.889646
C	12.578438	10.427886	7.465565
H	13.154023	9.931585	6.678501
C	11.255700	10.847856	7.222649
C	10.518589	11.479811	8.239150
H	9.485141	11.795155	8.068413
C	11.112337	11.708852	9.487499
C	10.615682	10.555385	5.894298
N	13.320641	14.771122	13.012487
N	10.435127	14.329594	13.268840
N	11.565595	15.478786	10.763218
N	10.386186	12.363635	10.557618
H	10.041943	11.638696	11.207024
H	9.535800	12.820094	10.166175
F	11.480671	10.731665	4.851287
F	10.179274	9.257260	5.799964
F	9.530098	11.340274	5.646440
C	6.049824	12.104729	10.419678
F	6.940274	11.450986	11.203182
F	5.837097	11.361598	9.314531
F	4.887466	12.206842	11.096238
S	6.714178	13.818185	9.963826
O	6.851911	14.500621	11.280027
O	8.018094	13.490437	9.292495
O	5.684330	14.379656	9.048295

S5. Optimized coordinates for **1-5coord** calculated using BP86.

	X	Y	Z
Fe	2.37991293602685	17.63234338139706	7.10183592136542
S	1.38512624367220	19.40650207475406	8.31668892520188
C	3.35435407692761	15.68771853558651	9.24062689179600
H	2.29841757977296	15.37692187537174	9.23902188110602
H	3.47334390282045	16.52774504184316	9.94339690584819
H	3.97993246218761	14.84031080537919	9.58384710223907
C	1.70036445908680	16.37993983664160	4.32277397245523
H	1.12469500658214	15.57301111347555	4.80182745293882
H	2.01880288523864	16.04330359780255	3.31710785323222
H	1.06082547009651	17.27098686277076	4.21131149845976
C	4.25338182599303	20.18647447041118	6.80529247439560
H	3.83922765569622	20.48121260366467	7.78177781195451
H	3.59325089015885	20.56845301871658	6.01069557389280
H	5.25824604673647	20.63736686911359	6.68738427295930
C	3.54892154672571	15.01458095191387	6.90259557189242
H	2.53238950068037	14.61637401881473	7.06424469420115
H	4.26563716863566	14.19175655437053	7.09612371793135
C	3.68910143603006	15.47921227963937	5.44575937716677
H	4.74315337921032	15.67306888676393	5.19202687506157
H	3.36283626337636	14.65877626617887	4.78342968718510
C	3.68143316417627	17.77427019800616	4.48264654133769
H	2.98486852019679	18.59221750501240	4.23070043249768
H	4.10063013278377	17.39028396871543	3.53067811916299
C	4.81545109457954	18.30114289793771	5.36514033559927
H	5.60690491874699	17.54373864507866	5.47557576937861
H	5.28960275640349	19.16146216866336	4.85991580981502
C	5.18028568606041	18.17993905126242	7.82199496689762
H	4.78350597968256	18.60424038668638	8.76143989475871
H	6.22701512694322	18.53068055584179	7.71510637800550
C	5.15350398206839	16.64921087147524	7.88616875802527
H	5.70759650557741	16.21061461235449	7.04201489281861
H	5.67712801622370	16.31629888181617	8.79989894046230
C	0.22151802024629	18.32990222054522	9.14489290399393
C	-0.31765115586267	18.65028375455058	10.40953179286994
H	-0.02606996432390	19.59149860473400	10.88744548144226
C	-1.19927317015141	17.77238408174385	11.05747122859950
H	-1.60031641242355	18.03817865414769	12.04093568096050
C	-1.557044464979343	16.55403399413978	10.45391739138359
H	-2.23964283644340	15.86337952126645	10.95982450527567
C	-1.04440495933652	16.22598511112386	9.18887966310949
H	-1.32844231005546	15.28731955359548	8.70036880220155
C	-0.16951429036064	17.11013787067501	8.53682959369290

N	3.74650973065676	16.12956991489772	7.87757398552325
N	2.87784555778082	16.71670867959493	5.16653683985238
N	4.31972179515005	18.70595922308595	6.72105492469888
N	0.38482252372972	16.80088296540690	7.22945440221849
H	-0.13639346348217	17.32903658815882	6.50929136031113
H	0.23773792358636	15.79536186522351	7.00603561586822
C	0.49355057507934	11.93718650147214	8.14399005848943
F	1.71818316327622	11.61174612369161	7.67672378339345
F	-0.11227911875967	10.80797921750589	8.56765161063393
F	0.65044925348245	12.75786284491783	9.20517044494506
S	-0.53473522076542	12.77667300638102	6.79519061737333
O	0.28168454413505	13.99237096295120	6.46646798499289
O	-0.58604544078933	11.76399633732047	5.70619575559751
O	-1.83139671367284	13.06682361541045	7.46909627253020

S6. Optimized coordinates for **1-MeCN** calculated using BP86.

	X	Y	Z
Fe	1.39736887719674	3.76474160360278	1.96381491103939
S	-0.36272123573789	4.97565947127788	0.75359455637634
N	3.06167238077494	2.61931302118691	3.03059638197137
N	2.36023636082496	2.74604055720945	0.20612033829161
N	3.18810161909000	5.14026896856408	1.62440553750029
N	0.46277323318000	4.87824827809960	3.65260502132843
O	3.81211017438244	7.01719465621081	5.73685282445734
C	-0.63308859197676	6.27233184339445	1.94427234113338
C	2.68684354657120	2.22450409784481	4.41153275202314
C	3.19728925786027	1.40619122378123	2.17414108345808
C	4.32128699471923	3.43121262162579	3.05710016073150
C	1.35586992660214	2.07457282928194	-0.65227024132300
C	3.37818080633333	1.75530673459362	0.68993567508797
C	2.98434667523304	3.87674043607977	-0.53847828249386
C	2.81382300291604	6.57342903204204	1.54925214913975
C	3.88487356627174	4.73199882787866	0.35998484081333
C	4.03761194597598	4.91783453468985	2.82892026969948
C	-0.18239828334439	6.12478474386538	3.28324211458532
H	1.03395183863114	5.01603419556494	4.50968478365424
H	-0.26415817977971	4.19507016636489	3.91411351414446
S	2.83854836801899	6.40965421065310	6.68632658937494
C	-1.28054248958950	7.47789945235339	1.58847734741604
H	1.71691408831073	1.70449906255423	4.39585322360630
H	2.60288026123318	3.12556371319726	5.03988863794940
H	3.44986795596356	1.55123626842387	4.85204620878774

H	2.27773400888412	0.81477257819407	2.31266222055556
H	4.05085529302512	0.77958504003778	2.50790076150643
H	5.01449074358409	3.04454554362419	2.29327531018861
H	4.83534180045025	3.30637644863657	4.02735971666485
H	0.58386336668214	2.80167495272965	-0.95130090605824
H	0.87467211458818	1.26333100603089	-0.08595068140703
H	1.82227179315849	1.65217544669185	-1.56488651029129
H	4.38716928522610	2.15855319406578	0.50833912847873
H	3.31328541386352	0.82487832400696	0.09912388179048
H	2.15649336083720	4.49364994860463	-0.92788599008493
H	3.57163432292012	3.50855177231391	-1.40551163065273
H	2.26728168272025	6.86206554378869	2.45995342993481
H	2.15596318940261	6.73404009390600	0.68147248623563
H	3.71310919778046	7.21393992259839	1.45110436671469
H	4.80837590071294	4.18726285268466	0.61247152187394
H	4.20517490402535	5.62538223133254	-0.20527840061951
H	3.49380688381685	5.33573904543012	3.69294790188956
H	4.99761662114912	5.46876049637924	2.74958035596209
C	-0.35505713549567	7.16266172172510	4.21542444798302
C	3.93262672514521	5.52521118416862	7.95443974505761
O	2.05476842775906	7.37735048690648	7.50393312230523
O	2.02970256429809	5.28008216097099	6.12346040386620
H	-1.63631450754020	7.60244188451586	0.56040629383009
C	-1.45503054926444	8.50963259537787	2.52239491653562
C	-0.98421360949329	8.36056035077600	3.83854593691893
H	0.00017109852972	7.02270604180917	5.24219305650063
F	4.73346797301710	6.41053484582844	8.58890203919060
F	3.17811970963018	4.89809174213722	8.88239268471414
F	4.71515098790309	4.60398344242574	7.35249772532867
H	-1.95344989961282	9.43611466740530	2.21700191454779
H	-1.11435281542564	9.16379200529405	4.57123156126489
N	0.10843044497907	2.17010273823943	2.42940600223816
C	-0.76039284155729	1.40858964449238	2.62338240867760
C	-1.84599340598473	0.46874714386759	2.85486949385239
H	-2.75199836967754	0.81019166478152	2.32695770976925
H	-2.06530903973250	0.39670236959691	3.93317083157324
H	-1.56850773996569	-0.52968168171528	2.47702000441128

S7. Optimized coordinates for 1-PrCN calculated using BP86.

	X	Y	Z
Fe	1.46172735584659	3.40734720770498	1.99409301527404
S	-0.47768283091086	4.43793203195962	0.91545610852616

C	-0.43957085247609	0.88365350065362	2.75929026011753
C	1.36873801001924	1.72349718246488	-0.63183382589875
H	0.49443698599402	2.36172409089689	-0.83692655236412
H	1.03904506421899	0.85814923792486	-0.03759899889371
H	1.78596987142921	1.36474080472573	-1.59408073200111
C	3.09262938625517	1.99278083645131	4.29172644110929
H	2.17965907563572	1.37954512522835	4.34570414692760
H	2.96453942459793	2.88481827305412	4.92567075591784
H	3.94932749494318	1.40004664044006	4.67181882301273
C	2.57952264705893	6.35142887328295	1.50647457112286
H	2.09286127652978	6.58066370580727	2.46603684998026
H	1.83580027959008	6.46748576136417	0.70329295591415
H	3.40957407221852	7.06825501555336	1.34474003405803
C	3.52320101294668	1.60639668798647	0.52058417877144
H	4.46845508013720	2.10937593587930	0.26015561476496
H	3.50255000492895	0.67773735052140	-0.07657659051450
C	3.50377057378467	1.23215232628866	2.01017448666152
H	2.66194853590776	0.55169848305478	2.21803442621123
H	4.43971282278078	0.69018128302064	2.26275580383635
C	4.49532090603619	3.34932710328277	2.82408132583451
H	5.16020112397740	3.03042458084893	2.00614634197548
H	5.09316561486365	3.27230030284418	3.75053551217504
C	4.05579656766928	4.80326406574920	2.63739834044429
H	3.56299783354239	5.16778338078476	3.55396786650824
H	4.95040572311058	5.44044375515298	2.47527419223714
C	3.69303585823726	4.62652740837209	0.18939549874509
H	4.69211824555212	4.18946579807071	0.34490097812777
H	3.85771094824164	5.55227311591029	-0.39078971935592
C	2.80865058323851	3.68480308380230	-0.63693611540522
H	1.88885383673559	4.21402479396122	-0.93960325987177
H	3.34941438480634	3.38759999517558	-1.56017372853343
N	2.37411875086507	2.49098900971641	0.14040800180107
N	3.32173022505361	2.42048406710837	2.88898849135438
N	3.08113400018593	4.95468949831761	1.51985333821277
C	-0.75435281323427	5.72715429503152	2.11295726356698
C	-1.49946317222493	6.88514902687600	1.79397415291728
H	-1.92897116488087	6.97653228410861	0.79098376120241
C	-1.67438662138801	7.91383120516904	2.73139318341185
H	-2.24852482834665	8.80493264086534	2.45466825683349
C	-1.10629559702396	7.80896022191163	4.01287699906495
H	-1.23510082260375	8.61123601826519	4.74689934335939
C	-0.37849803030736	6.65740051046916	4.35454268279808
H	0.05737898547227	6.55362246730130	5.35440369362380
C	-0.20511596478636	5.62296788834629	3.41871949251688
N	0.54924538903750	4.42726800170431	3.74784060924630
H	1.14784221837844	4.60516166801471	4.57996610149914

H	-0.11087552010535	3.69022850520246	4.03946292159649
N	0.37420292905692	1.69872765963756	2.53983462124166
O	3.91497188035116	6.50707443967489	5.75166375704683
S	2.93510976987535	5.92926417955380	6.71335297966565
O	2.12755473183189	6.91635470547236	7.48004174678333
C	4.02109550080165	5.10349722535364	8.02792741824977
F	4.80361037722642	6.01814582382589	8.64239326480365
F	3.26158798237439	4.49850842475580	8.96656581514520
F	4.82261745682739	4.17031532102431	7.46833344536003
O	2.14917242315834	4.76559564148839	6.18271725924519
C	-1.48811594499079	-0.10423749637827	2.99762444106878
C	-2.65543415317207	0.01044481195120	1.98099051903449
H	-1.86092364381808	0.02668889715088	4.03093321894414
H	-1.02814101794632	-1.10920451729453	2.94779436173568
C	-3.73910062769465	-1.03567532278047	2.26838967604104
H	-2.25708518988640	-0.11994191205894	0.95949497591795
H	-3.08008638742969	1.02819334127188	2.03510831138248
H	-3.33657568952366	-2.06155271960514	2.19163290031574
H	-4.56739362993697	-0.94068804083228	1.54613322372374
H	-4.15767871864360	-0.90964550883748	3.28273076587437

S8. Optimized coordinates for **1-MeOH** calculated using BP86.

Fe	1.63462421842650	3.80855971122008	1.95926696290415
S	-0.19245650065474	4.92945629077938	0.83720327490369
C	-0.51460318445788	0.91501655070398	2.67541802025299
C	1.41614340376300	2.08766217437002	-0.65185687917034
H	0.68042863642230	2.84871154324001	-0.95556437662019
H	0.89743097123570	1.30846756680500	-0.07318547369542
H	1.85691455541702	1.62924373736698	-1.55963744654238
C	2.77767288436825	2.15008798584291	4.38549544618536
H	1.77451857950782	1.69539171187569	4.38071132229477
H	2.75834360405745	3.04202287388523	5.03116056807377
H	3.49832700238293	1.41838033763278	4.80356801349379
C	3.05383984397140	6.52505272294522	1.55324476671057
H	2.52761780672180	6.81022863719096	2.47696915402879
H	2.38792070708396	6.71078937633441	0.69652936193090
H	3.96612182265932	7.14385963526964	1.45205287281166
C	3.43976487510010	1.68399689217970	0.66068281971092
H	4.46309080769645	2.05372980231276	0.48939973750305
H	3.34392479652137	0.76382470937055	0.05795628625129
C	3.23666655613193	1.33004884358786	2.13932090484620
H	2.28933895597407	0.78037574211459	2.26708012241792
H	4.05537490028847	0.65894836275841	2.47264319261589

C	4.44998135086942	3.29919206519412	3.02234740364524
H	5.12010638657324	2.88150367318754	2.25449681910223
H	4.96378525845344	3.15020501234570	3.98890483422022
C	4.24763897638750	4.80186811555670	2.79873080361505
H	3.74714933346427	5.25866150209991	3.66805528433203
H	5.23635791418889	5.29385703555815	2.69702268892139
C	4.05639322885017	4.65219961578838	0.32235469781129
H	4.96755758493768	4.08181728199057	0.56242289771319
H	4.39017474710213	5.53894834829446	-0.24420568580232
C	3.11535853720492	3.82350191212091	-0.56177833004397
H	2.30631590241700	4.46598085622369	-0.94929012918347
H	3.68084598187496	3.43002848780886	-1.43149889051365
N	2.45791563704761	2.71786449488871	0.19461760027996
N	3.15253625648002	2.54358366405163	3.00426835117469
N	3.39706267540841	5.08053005035404	1.60252209914717
C	-0.58047341594837	6.12840141573056	2.10255997869472
C	-1.35496361809208	7.27567787252490	1.82322543586061
H	-1.74667155237999	7.41365708363205	0.80974519013030
C	-1.61108792433779	8.23551646124223	2.81396112650946
H	-2.20717909966385	9.12140915122613	2.56875405566821
C	-1.09931481312990	8.06427355465864	4.11200231932938
H	-1.29506678866714	8.80876576160946	4.89076158990491
C	-0.34218159683295	6.92000369989369	4.41142493766361
H	0.04162425216676	6.75859085388046	5.42481383404491
C	-0.08393468965055	5.95730776761882	3.42026921952526
N	0.70845766583956	4.77609858175683	3.70876014183125
H	1.23919011638961	4.91711578577400	4.59023097013552
H	0.07339458255170	3.97867942144028	3.88950447530879
O	-0.06603148070583	2.25689223063149	2.37725905435524
O	3.69575167438354	6.92205568146257	5.55450276551554
S	3.05638483793163	6.20099045666557	6.69050076354721
O	2.50345073408840	7.06339764670774	7.77111105712362
C	4.49955910952625	5.30315384434085	7.52528229227429
F	5.41994954314425	6.18829126799773	7.96527804937122
F	4.06715718367912	4.58126278453250	8.58092899758683
F	5.10599866547370	4.46106847605475	6.65783885204794
O	2.16211506026879	5.06625541432409	6.28615274373230
H	-1.47203366482839	0.94188375392757	3.22290785226071
H	0.25017805201359	0.44889157544508	3.31389271991234
H	-0.62963823276341	0.31791931916265	1.75378550960749
H	-0.75265961433350	2.73215281450983	1.85224697273195

S9. Optimized coordinates for **2-5coord** calculated using BP86.

	X	Y	Z
Fe	4.14426623559021	19.75922743157438	1.06487097470010
S	2.09994445166270	20.83140531276815	0.45667464739845
S	5.22747887937159	18.45702039749232	6.09743701579574
C	4.16087160213796	20.02304742671733	-2.09082079848070
H	3.40274150163157	20.80805291978499	-1.94594490137661
H	3.65558578412245	19.04399374212842	-2.10726373361402
H	4.66574318253523	20.18254949101237	-3.06396620547862
C	5.07235932455399	16.87952105091765	1.90432528883205
H	5.84887566359659	16.09059712639562	1.85737052307335
H	4.15647574844717	16.50145396617848	1.42268829110838
H	4.86395715535272	17.10634438481015	2.96058870736021
C	5.65608192568258	21.65201019881093	2.90283782162375
H	5.65316551942328	20.89282954042460	3.70147089872479
H	4.69597959310450	22.19260495300495	2.91258470871807
H	6.47548303882982	22.37207371286417	3.09803856558830
C	6.10700423681426	18.91644209889799	-1.13510254908689
H	7.12693890418511	19.27568556474892	-0.94786919975961
H	6.09646723551914	18.56364585769075	-2.18281373840298
C	5.78766682104396	17.73130998305628	-0.22673799650879
H	4.87476722192536	17.22207517947942	-0.57959952825811
H	6.61904267524690	16.99852974874713	-0.28143910717998
C	6.72766510010626	18.65813273586724	1.92683001479657
H	7.61505700393874	18.02203777843408	1.73729311437936
H	6.49227754558676	18.58452600560261	3.00270973498640
C	7.06292736834075	20.12484954080835	1.59889260274082
H	7.77806582496338	20.49273451077707	2.35770992453331
H	7.57211724465654	20.22036180417447	0.63200694950242
C	5.85167623860765	22.00371559877556	0.50013985750592
H	6.72410074894470	22.68001801762201	0.60310657660663
H	4.94303516184617	22.61397705099159	0.64232394402898
C	5.84432999958978	21.37966707793782	-0.91667740935757
H	5.33232969953242	22.08575232181536	-1.58930488256737
H	6.87013379960916	21.26677171253788	-1.30680078939928
N	5.13575981723034	20.05377784098022	-0.96882471259338
N	5.53147461008752	18.10990115917667	1.19772778050757
N	5.83690887557545	20.98621690771142	1.58774900619422
C	1.65020772501762	21.15758659627164	2.14671742155925
C	0.83719306809145	22.25376263416748	2.50730628103523
H	0.45477439102770	22.91486579017555	1.72401925240560
C	0.53433301427832	22.51821926761489	3.84852817090587
H	-0.08784264254526	23.37947496005270	4.10612633707598
C	1.04306606860488	21.68203056850123	4.85872568650838

C	1.83832684915474	20.56940531552757	4.52261601830173
H	2.22603020404175	19.90246197857575	5.29917600420413
C	2.13149041060980	20.30685317032951	3.18024731798058
C	0.76270417608607	21.95353915054795	6.31051985418379
C	6.04897568453330	16.79751034002601	6.49614031532176
N	2.95541099354005	19.18212413608365	2.79020255799490
H	2.34717080901979	18.44613098073496	2.39029434327014
H	3.40068801048121	18.75700459229737	3.62946310267395
O	6.29505846060088	19.21645333092629	5.38421761798742
O	4.07495030614922	18.04498244088859	5.22796759827469
O	4.83681714076769	18.99580643592611	7.42636477600748
F	1.90210779032882	22.25299949668299	7.01215258439237
F	0.21502040085218	20.87041690490058	6.94533591380846
F	-0.09409097989061	22.99323178448585	6.50024008913270
F	5.18774270905537	15.98265026794394	7.14067067200200
F	6.45141469789423	16.18010982757527	5.36444983722844
F	7.12934497290809	16.98329987904680	7.28446685110365

S10. Optimized coordinates for **2-MeCN** calculated using BP86.

Fe	4.02526284722328	19.38671733255928	0.79079377018606
S	2.15602574188341	20.97421566692667	0.49325075910326
C	4.27524540186418	19.74330015502403	-2.29447621522869
H	3.42137691510618	20.42544168868578	-2.15606251809822
H	3.89296862979865	18.71409136865271	-2.36441072727770
H	4.79304308020137	20.00061511818833	-3.23992752193948
C	5.36627719451908	16.68806422570678	1.76969207455510
H	6.23898277643988	16.00595846945956	1.81311411971278
H	4.55037075276356	16.18867166104686	1.22617393649798
H	5.03655701146569	16.90668276608972	2.79688015017228
C	5.34041851457338	21.46550659029924	2.77016712711520
H	5.38084205383873	20.70661972616520	3.56792793180694
H	4.33410494616823	21.91045187461143	2.74275251766615
H	6.07901837647298	22.26057379434781	2.99817798160322
C	6.28841589311020	18.82621732015521	-1.25429679742534
H	7.25893154568577	19.30884506989319	-1.07321710183447
H	6.32927261044993	18.44923407465661	-2.29295335536170
C	6.11218503491625	17.61810810216992	-0.32485734249106
H	5.30991649833557	16.97004043926384	-0.71537956786168
H	7.05009782596569	17.02466100871350	-0.33079830935807
C	6.78324569914961	18.64002338792000	1.87393243264077
H	7.75417068235615	18.11547936915559	1.75807052299135
H	6.48757150008489	18.54996870830519	2.93368183859981
C	6.95422608188372	20.12412398479498	1.53114614078124

H	7.60038863722963	20.59261431754132	2.29758241577553
H	7.47609822384582	20.25529420851709	0.57527041636551
C	5.62003783345602	21.85412236216458	0.38974090972751
H	6.42733697282184	22.60102518659112	0.53958951858223
H	4.65535519825721	22.37857416489792	0.48414382188012
C	5.74434830180078	21.24431462461628	-1.02755253784118
H	5.19053138460922	21.89708144989671	-1.72080271492134
H	6.79312254381972	21.24881661389045	-1.37189938235961
N	5.19073120065640	19.84977639435438	-1.12889769971170
N	5.72100401375150	17.95518846960638	1.07691506743067
N	5.63792619773932	20.82903894405468	1.46437039136542
C	1.71557898459561	21.16600393586548	2.19755399860835
C	0.95028058716639	22.26970390584154	2.64504857935032
H	0.60532439588335	23.00704393410344	1.91372513771353
C	0.64406577343776	22.44170087043648	3.99805251125636
H	0.05694553472356	23.30762947489184	4.31721853663375
C	1.09781741239956	21.50181971719905	4.94401990968924
C	1.84437747616308	20.38571934088215	4.52199056421712
H	2.18570646408134	19.64112558970459	5.24776526025074
C	2.14434088116567	20.21266531689403	3.16447705389885
C	0.83524409249466	21.71380085262864	6.40704567545075
N	2.90217161960076	19.07093501896086	2.70211273735457
H	2.24498062041063	18.34828840801993	2.37096844822226
H	3.41156315930662	18.63866994477564	3.49874530857279
N	2.90681111851158	17.80120836755309	-0.01356928709695
F	1.83640540696157	22.42447828973514	7.02443156603759
F	0.72948093905409	20.54238869687901	7.09954002026559
F	-0.31425173708865	22.41439833984948	6.63692215593450
O	6.15410718727970	19.14404828487739	5.39289893699720
S	5.13635808168268	18.22364784223960	5.97773998739647
O	4.55800472555076	18.65024546006919	7.27983007411430
C	6.12964642580541	16.66842301035582	6.40571077296071
F	7.09600559347384	16.95745495474047	7.30414997330679
F	5.32658653313468	15.72179681283863	6.93731960643283
F	6.71671135941064	16.15578786835758	5.30324549534077
O	4.13244845503639	17.70176648093039	4.99175936921870
C	2.11581050313059	17.05498345244743	-0.44837385453399
C	1.12157015460845	16.14238832418829	-0.98949885807847
H	0.16304650671805	16.28044270775372	-0.46196470198799
H	1.45536470972358	15.09967539126973	-0.85359278008725
H	0.97089891333385	16.33445076678933	-2.06532425028833

S11. Optimized coordinates for **2-PrCN** calculated using BP86.

	X	Y	Z
Fe	3.97163144977133	19.23977673823040	0.74849530113204
S	2.06948277151637	20.76106116643309	0.39922957405605
C	4.19618600735772	19.54949138234358	-2.34501891652106
H	3.32498738905559	20.21075124512641	-2.21429649139549
H	3.84028076185626	18.50925722823315	-2.38941423324926
H	4.69958299567787	19.79903508993936	-3.30065070611807
C	5.40437323574504	16.59816483673015	1.76171469972840
H	6.29841111287445	15.94494928949556	1.81750845834637
H	4.60463302282906	16.06223322331208	1.22899555356753
H	5.06892642720424	16.82664729169013	2.78485758121541
C	5.24951449561031	21.38758614597210	2.68594445522696
H	5.32538424587810	20.64598358102597	3.49710470403540
H	4.22903616126291	21.79876055490053	2.66143508988611
H	5.96414842047819	22.21067044326704	2.88994935684134
C	6.24281363526600	18.71280331632156	-1.30370250809484
H	7.19913400132444	19.22683518800196	-1.13302706500890
H	6.29192703076159	18.32121052491355	-2.33701876933556
C	6.10622247215615	17.51446189750287	-0.35462113225866
H	5.31842759622910	16.83969501554106	-0.72900081044051
H	7.05958649251792	16.94534478259047	-0.36071641720785
C	6.76581181847687	18.58957781434182	1.82081336944237
H	7.75058356217585	18.09072436532016	1.70420014056857
H	6.48295001747544	18.50881995116480	2.88463568574324
C	6.89059992957218	20.07281170701597	1.45464938825623
H	7.52760813291036	20.57069820283428	2.21010089900762
H	7.40153267399632	20.20594794308004	0.49263516751026
C	5.49767534831560	21.74319808810510	0.29754667926816
H	6.28588316811213	22.51410990085504	0.42842033183301
H	4.52049262234839	22.24355119928126	0.39250866548794
C	5.62566905774960	21.11628902241503	-1.11264488811409
H	5.04245463532555	21.74113606408519	-1.80739515380154
H	6.66989933710493	21.15034619073811	-1.46996868862106
N	5.11602785149774	19.70413499882659	-1.18905964952080
N	5.71743282991991	17.86217671330689	1.04371332926895
N	5.55370428186092	20.73695873533903	1.38799348066164
C	1.63108580759770	20.99677936081052	2.09958405437645
C	0.84124673009652	22.09607485487906	2.51277193754418
H	0.47731750133287	22.80020597245720	1.75843835167196
C	0.53478242375120	22.30400229084759	3.86053560902338
H	-0.07228905241932	23.16527297854077	4.15427338462403
C	1.01282962345484	21.40645224246463	4.83514472771137
C	1.78465097605512	20.29546920295359	4.44766727787528

H	2.14522801201359	19.58340941921686	5.19651897175442
C	2.08497024174655	20.08624289567947	3.09503071773065
C	0.74555559624701	21.66217772292585	6.29137615228389
N	2.86788044259140	18.94743793276838	2.66592215773858
H	2.22395853596750	18.19949566732092	2.36692219033264
H	3.39255441032647	18.55196152283508	3.47332446909696
N	2.90327936920389	17.59958160387779	-0.00280671699038
F	1.71134350238554	22.44613706818767	6.87229469776971
F	0.69918137462569	20.51574932694490	7.02815531308096
F	-0.43719801795773	22.31429669543454	6.49751500838349
O	6.17092476917513	19.13068472078945	5.26365189379000
S	5.17565947047928	18.21271852646433	5.89110629126584
O	4.60658573421883	18.66627897251179	7.18608770097008
C	6.19920194275633	16.68493554592732	6.34623010460281
F	7.17309472154932	17.01102012653798	7.22276767998369
F	5.41915979963713	15.73904347662761	6.91161661721099
F	6.78035006770153	16.15283755949129	5.24811326047783
O	4.16917039208369	17.64659429963129	4.93023183196556
C	2.11433481736179	16.82158104733087	-0.38605952891045
C	1.12702168464562	15.87462987296099	-0.89562492541187
C	1.27365394526047	15.60235007410042	-2.41658694752918
H	0.12463817849238	16.28496234879622	-0.66988193372332
H	1.22210598102135	14.93421758718870	-0.32154982213300
C	0.21568060083378	14.60330163490375	-2.90189198439593
H	2.28732923558816	15.21211397550956	-2.61571142926837
H	1.17966255996710	16.55675645822175	-2.96290894910254
H	0.30913267895109	13.63542871410818	-2.37928362507740
H	0.32936337495744	14.41734639311849	-3.98306978947730
H	-0.80577242391372	14.98645206935491	-2.72792123064090

S12. Optimized coordinates for **2-MeOH** calculated using BP86.

	X	Y	Z
Fe	4.16387564846446	19.50346988935880	0.89181986160417
S	2.27616042444249	20.98825598264176	0.53186045648511
C	4.34953855775015	19.76281728360936	-2.21046104758702
H	3.54409587668961	20.50415142469500	-2.09036645256482
H	3.90004579336630	18.75849838832237	-2.23112483345074
H	4.86764219385381	19.94257479285818	-3.17353046228327
C	5.32064569559680	16.71831086752361	1.84752233038855
H	6.16555600026063	16.00123379183496	1.88147078075580
H	4.47715956315080	16.24123561382902	1.32620271637103
H	5.01730463752048	16.95787154990564	2.87756898437308

C	5.46948759838484	21.52983012914590	2.80351360055966
H	5.49744066188484	20.78020030379396	3.61020347559158
H	4.46919837379762	21.98892054460340	2.76550209478152
H	6.22083383977346	22.31479615349383	3.01794471142458
C	6.34215229403293	18.78976626827428	-1.18605985563143
H	7.33102897419916	19.22457240558967	-0.98562647453431
H	6.38169794242079	18.41680038896346	-2.22634616850253
C	6.08993184010655	17.59482965316152	-0.26100186783519
H	5.25389452684428	16.99283633410058	-0.65645631236154
H	6.98961720935368	16.94469251155324	-0.26174047451878
C	6.80242056329048	18.61777592271427	1.92446457903834
H	7.75189084566786	18.05621122263631	1.80732318724433
H	6.50699109582013	18.54194357109439	2.98472152111748
C	7.04250432781696	20.09646489576908	1.58651098885247
H	7.69611251200896	20.53199305639873	2.36471780031320
H	7.58094969227496	20.21105229546854	0.63822407500550
C	5.78668368521093	21.87688207426179	0.41093342822730
H	6.62119390644836	22.59205386838970	0.55774834315660
H	4.84202572357793	22.43911103452671	0.49246495703164
C	5.89504746845785	21.23223028311471	-0.99331652751853
H	5.37211945115268	21.89078057091658	-1.70457026673697
H	6.94530099782247	21.18706352924898	-1.32864646504380
N	5.28935270520544	19.85781172151895	-1.06388643437434
N	5.70882251631836	17.96482072364739	1.13457775467769
N	5.76188549469709	20.86900392071484	1.50601906182261
C	1.73569023638434	21.13861864377624	2.21735754759963
C	0.88007774895423	22.18505712611525	2.63086377005209
H	0.51476922605992	22.89711845922597	1.88414191936097
C	0.50959289703906	22.33512073513518	3.97121024393097
H	-0.14695744828554	23.15863751140589	4.26670448891901
C	0.98708805656084	21.42456948615046	4.93348234614890
C	1.82245941400818	20.36148093969431	4.54238210247838
H	2.17992498339736	19.63630094364813	5.28025092038909
C	2.18794089543493	20.21315257605367	3.19781841975802
C	0.65507962428284	21.61312473807789	6.38625475893349
N	3.05442369762534	19.13722704993760	2.77248589913315
H	2.48252501504386	18.37916636432944	2.36076397896678
H	3.52868607943917	18.71772704822492	3.59607142200019
O	2.63719023091488	17.97205697206867	0.06028794848495
F	1.59480819290625	22.36813656422327	7.04541083526476
F	0.58197568319002	20.43264423811127	7.06750799316743
F	-0.53622849505503	22.25297528982493	6.57377568799846
O	6.23943545786515	19.31571889571891	5.44913844651087
S	5.29703662183924	18.32796082418833	6.05080589168792
O	4.78496796310402	18.67226420907449	7.40382810087089
C	6.37769290236784	16.80100644783780	6.34717371354574

F	7.37598911758819	17.08879500995719	7.21015220923410
F	5.64539320649521	15.79294743130598	6.86725482604697
F	6.92876339434867	16.37219044720146	5.19122779217199
O	4.25572848951561	17.80854649763365	5.10321737505294
C	2.36643831997246	16.73008238359405	-0.63093981822967
H	3.11420853063840	15.99737795005906	-0.29651085719418
H	2.44305646032504	16.85826705282629	-1.72556196589368
H	1.36079593395712	16.35963917654795	-0.36991792342831
H	1.90952892641832	18.61211602037219	-0.11723913884081

Coordinates for DFT-calculated models for calibration curve

S13. Optimized coordinates for Fe^{II}(TMCS)(PF₆) calculated using TPSSh.

	X	Y	Z
Fe	-0.15614768178075	0.25370250858757	-0.19725937477747
S	0.16043033274416	-0.00706947297176	2.10493482579404
N	-0.14197748571966	2.44563746136890	0.20970925757447
N	1.79208952063562	0.64682214382153	-1.12609071182146
N	-0.22070772971904	-1.84816242984641	-0.94303644773210
N	-2.30064652076428	0.22454064250397	-0.64269683391295
C	2.91041770411751	0.29626892743057	-0.20675341155696
C	-0.41017609819510	2.70015091326272	1.65736158113051
C	0.35217667929761	1.76317593074994	2.59339348922267
C	1.77857997386770	2.12596654805166	-1.35061112441949
C	1.24980736322371	2.87332389398252	-0.12949075174520
C	-1.08652754452342	3.24955987090815	-0.62713034282113
C	-2.54153126287928	2.77073684115341	-0.64441796500620
C	-2.79273918728762	1.44278225430813	-1.36362340753311
C	-3.11329134207538	0.02340323375472	0.58910234820042
C	0.40276156175687	-2.80764592489126	0.00461222973418
C	-2.47501690711247	-0.95865930229566	-1.54212679293081
C	-1.68077761128022	-2.15789996994634	-1.03379504553906
C	0.38675482908355	-2.02486253662867	-2.30058198474297
C	1.83463418569801	-1.54517543811213	-2.43842540539240
C	2.01993177196203	-0.02557563812185	-2.44587761144709
H	3.86877781275988	0.59255826634876	-0.65572807347914
H	2.91462551216153	-0.77802901785196	-0.02192639012761
H	2.78288022831558	0.79661568077950	0.75230416429428
H	-1.48197291018737	2.55942423202284	1.81676516220125
H	-0.17070213669297	3.75020180793175	1.89088616310872
H	-0.04404525101877	1.89875976657869	3.60394886216515
H	1.41763256412312	2.01446795926936	2.63284733457145
H	1.14591860120963	2.31852516897400	-2.22246929718057
H	2.79095629403617	2.47905190665383	-1.59220804722643
H	1.27722777618116	3.95507365918698	-0.32156476316363
H	1.88857866012977	2.68522669446821	0.73526823382409
H	-1.05389056051361	4.29341996583805	-0.27881139892216
H	-0.70837080398480	3.23714044499530	-1.65276589166064
H	-2.98107249624966	2.77377330684686	0.35875806581296
H	-3.09924777599760	3.52884702157614	-1.20740775315255
H	-2.30441326215205	1.46463037112012	-2.33988273972349
H	-3.87315898245707	1.32225526954574	-1.53320046299533
H	-4.17858609467963	-0.04107469292548	0.32471296943654
H	-2.95685406318516	0.85163323558862	1.27957662393879

H	-2.80561667436492	-0.89049084421218	1.09819394354260
H	0.28335533241237	-3.84078328542875	-0.35403407899087
H	-0.06908503175852	-2.70541998364106	0.98388822023277
H	1.46668057312399	-2.59032213791305	0.11229369484713
H	-2.13785729478439	-0.66537720612399	-2.53965109240147
H	-3.53943863971018	-1.22210109907837	-1.61521846627377
H	-1.84684632061090	-3.01990776327280	-1.69500839914225
H	-2.01987784400862	-2.44552484564642	-0.03517077576013
H	0.33050124721513	-3.09286375179490	-2.56072447758759
H	-0.23155596896838	-1.47863117985535	-3.01749027660163
H	2.48987230504120	-2.02985871886334	-1.70737078117052
H	2.18032642659753	-1.89733293255827	-3.41806126598598
H	1.32357705001535	0.41601827598460	-3.16217685263549
H	3.04020180201789	0.21663443833714	-2.77901577564760
P	-0.94836137306013	1.88754549302849	-5.25058517444933
F	-2.55666578410669	1.61009119461254	-5.25298495037579
F	-1.14702155509479	3.00682158864359	-4.06902345965605
F	-1.12873400824082	3.04191906823192	-6.38351655028947
F	0.66544028388513	2.15193630878634	-5.21339139784315
F	-0.76675311846411	0.72277795355481	-4.09348531451586
F	-0.74178906998386	0.75820792319205	-6.40706605129513

S14. Optimized coordinates for $[\text{Fe}^{\text{III}}(\text{N3PyO}^{\text{Ph}_2})(\text{OMe})]\text{ClO}_4$ calculated using TPSSh

	X	Y	Z
Fe	-2.72350948258538	0.51425494600968	10.03225821054583
C	-6.23739813067322	3.32635828894970	11.93663306016410
H	-7.14147871987854	2.72715824116703	12.00964641847414
C	-6.32551717747332	4.67980285412300	11.60415665508324
H	-7.29880626934815	5.12760656211959	11.42421031351680
C	-5.16493874161605	5.45475438536019	11.50400029062029
H	-5.23318812455005	6.50939401055229	11.25238633062941
C	-3.91573910119904	4.86763447821836	11.73560090424658
H	-3.01242280742481	5.46842428373206	11.67572744012022
C	-3.82570132596193	3.51150741550717	12.05620327905169
H	-2.86202253726520	3.06310767654759	12.26634388712502
C	-4.98424186693722	2.72661769598602	12.15430822967411
C	-4.91809773639709	1.30989439650595	12.59649120729021
C	-5.74241105397855	0.91529523117991	13.66570950981513
H	-6.40696800338525	1.64505658817171	14.11503395990355
C	-5.66567411856773	-0.37837523014533	14.16886769421984
H	-6.27885993022495	-0.68264608355707	15.01124440756390
C	-4.76979705780799	-1.27001437080004	13.57937839620714

H	-4.66317598231611	-2.28807983305175	13.93789333034513
C	-4.00847875884170	-0.82250461463106	12.50289353621948
C	-3.13347006349747	-1.79129710102456	11.72337850319477
H	-2.91886042479175	-2.67602009196789	12.33482110311607
C	-3.94533012195126	-2.19685027882549	10.49910725612741
C	-4.65213843990113	-3.39421538512783	10.47481357909871
H	-4.55702301161785	-4.10169161415171	11.29206689119565
C	-5.47750740114708	-3.65079766812288	9.37868147640414
H	-6.04355211035733	-4.57467762535448	9.31604056794728
C	-5.54534597565943	-2.70913182219414	8.35871421831653
H	-6.15165050344460	-2.89255896983287	7.47881977634593
C	-4.78817989460275	-1.52488359198453	8.43252108295474
C	-4.84515882547133	-0.57690587660232	7.29107831374215
C	-6.09180164681111	-0.28582532738547	6.70548870267500
H	-7.00149990310162	-0.68713551139939	7.14451730640591
C	-6.17065116148084	0.53556777347320	5.57988130101216
H	-7.14010759840459	0.76269667152907	5.14582698069065
C	-5.00408018355498	1.06139287332042	5.01426187124869
H	-5.06289616036815	1.69081884799626	4.13054151312391
C	-3.76205123382366	0.77069954205981	5.58893628825419
H	-2.85300070094195	1.17145243266491	5.14906665411601
C	-3.67775180278651	-0.03805982751136	6.72468178321798
H	-2.70995339554079	-0.25886528353881	7.16300190984363
C	-1.10946875996593	-0.54608929702350	12.41815725309037
H	-0.33990128100467	-1.25391706435730	12.74483878516969
H	-1.78634031690388	-0.38771409432773	13.26381506504641
C	-0.49026338304430	0.78097555182193	12.04056308378871
C	0.69209908099570	1.24665280417849	12.62246968237961
H	1.22333098506538	0.62813470646046	13.33881322925215
C	1.17352544780186	2.50331084986448	12.26010075340434
H	2.09121460498237	2.88406405138763	12.69663749568916
C	0.46792307601103	3.25853837518863	11.31707609688220
H	0.81585531606899	4.23420142232098	10.99801411464182
C	-0.69822536169681	2.72652620863479	10.77984009578221
H	-1.28580222792254	3.25666654271783	10.03791201184174
C	-1.04006853179970	-2.05324803483018	10.47409964193312
H	-1.68969331271311	-2.46390107891039	9.69510347132332
H	-0.71787175976532	-2.87898817296041	11.12237960702682
C	0.14444542092853	-1.37560539700065	9.84300447790677
C	1.44849854754748	-1.84006603564203	10.04896369636914
H	1.61129015153257	-2.67474545166982	10.72833266842020
C	2.53264970069406	-1.25501258832160	9.38772778127464
H	3.54003234726290	-1.62518841048359	9.55606812954002
C	2.30442102643850	-0.18772793101630	8.50863723812256
H	3.13591413563267	0.28245502202626	7.99064798196892
C	1.01249570992804	0.29040289046647	8.29078527947349

H	0.83381789082720	1.12211778565923	7.61539469475139
C	-0.08844837352776	-0.29402933609578	8.95233025823055
C	-4.72118319113198	2.56634572234728	8.78177938462934
H	-4.70302763930262	2.62624080730425	7.68450351677812
H	-4.69658120785883	3.58277930564796	9.19690684539893
H	-5.66292410184192	2.09023293615340	9.08870697178827
N	-4.06415345490548	0.43352815869786	12.00893557153887
N	-4.00335469872853	-1.27357997078455	9.51180441714690
N	-1.89078305435904	-1.11256333880413	11.28219837904653
N	-1.17571119288937	1.52092582889438	11.14781044767702
O	-1.32018597281597	0.16751290793445	8.74842285292241
O	-3.61846817275060	1.83889496236680	9.23362446409433
O	4.72601399126252	4.42819783932915	6.09472469864190
O	3.01059531874443	2.75701245819305	6.57438942416078
Cl	3.85922107897769	3.36138783290395	5.50235785283323
O	4.72158576795311	2.30607737141907	4.88725259053796
O	2.98054388196179	3.96145477234424	4.44970584964817

S15. Optimized coordinates for $[\text{Fe}^{\text{II}}(\text{N3PyO}^{\text{Ph}_2})(\text{MeCN})]\text{ClO}_4$ calculated using BP86.

	X	Y	Z
Fe	0.52284883266456	2.59213614345854	12.89790268683380
C	-2.40492045590997	-1.08854445481096	14.11211822579040
H	-3.31394123489055	-0.73932512058738	14.61327943321811
C	-2.44893581987447	-2.24154332257374	13.31597376952796
H	-3.39041845205053	-2.79009657942170	13.20710676179819
C	-1.28810390560124	-2.69060376373602	12.66211148682614
H	-1.31759684092764	-3.59963733457074	12.05229564765088
C	-0.08938280346394	-1.97025657673572	12.80054598161952
H	0.82010945611674	-2.31963018388523	12.30020295842839
C	-0.04367204958624	-0.80577909080330	13.58331872455289
H	0.89496831375089	-0.25011202491760	13.68376054542605
C	-1.20358057637961	-0.35484831757299	14.25006276922954
C	-1.17222314224854	0.82214209607082	15.16141266695299
C	-1.75809871128188	0.69577920656455	16.44177705626231
H	-2.21289010306391	-0.25577312355930	16.72761469735316
C	-1.71665159611616	1.76293263272415	17.34238441105902
H	-2.14960755331548	1.66744183086021	18.34224368539043
C	-1.09115858692565	2.95149523087113	16.94212577522889
H	-1.02168481094530	3.81298050388658	17.61278492009591
C	-0.54549779140837	3.01834039096677	15.65504210662067
C	0.02870549147738	4.33659052277100	15.12827571808093
H	0.23304581787669	5.00845829919351	15.98487246613687

C	-1.06845301624087	4.94990373462818	14.26107248218602
C	-1.92496201769569	5.92143075351349	14.79774427773976
H	-1.73844256650298	6.33146621901182	15.79355121066452
C	-3.01996860833798	6.33722005226805	14.03001891875447
H	-3.71481665897589	7.09254279953200	14.41000549071545
C	-3.19736584701753	5.78071979110236	12.76078482922729
H	-4.02575647711787	6.10066675526905	12.12285866757816
C	-2.26917516155283	4.83451326630149	12.26954134342036
C	-2.43590111610956	4.32311060491150	10.88229206241511
C	-1.35393385374975	4.32260069185401	9.97836117612946
H	-0.37762509584618	4.67175645742504	10.32047803689021
C	-1.53084295814868	3.89175261388997	8.65605836551511
H	-0.68226097633257	3.88432046024696	7.96486498576285
C	-2.79367937707436	3.45447008876623	8.22016333202931
H	-2.92436638300360	3.10894440365182	7.18979421493795
C	-3.88093657688082	3.45867390120164	9.11143484170137
H	-4.86681248452703	3.11668055088360	8.77946822105377
C	-3.70585129206327	3.89662438455619	10.43297006003591
H	-4.55254716770607	3.88525203051089	11.12799298889474
C	1.78034746392662	5.27040983303831	13.62612360440526
H	2.56175464048516	5.77103914504539	14.22623704698097
H	0.95638245944827	5.99497991073715	13.50604207392408
C	2.31176995731401	4.92097811974836	12.24762856263357
C	3.33845182622702	5.66474061791330	11.64429171472906
H	3.81379822472365	6.48325337353350	12.19317234136102
C	3.74282655978582	5.33812925808283	10.34369824079097
H	4.54235281243634	5.90324348890206	9.85476768976627
C	3.11164593030954	4.27141173855185	9.68382276194683
H	3.39220274498554	3.97913307232482	8.66900280507933
C	2.09781227869058	3.57896584956404	10.35386795072041
H	1.56938342694197	2.74870381869641	9.87527549801814
C	2.31955211472244	3.45362849475352	15.19907756985966
H	1.83326562489817	2.62449143466362	15.74116147157942
H	2.64456608898081	4.20116782131792	15.95100965070712
C	3.51162939928444	2.92737424472740	14.43809187777036
C	4.81404941662015	3.35777650386306	14.74790033915303
H	4.94517840443456	4.14636801701246	15.50013119632763
C	5.93757933962605	2.78824899256329	14.12773692058329
H	6.94429271607020	3.13390294583598	14.38345831643033
C	5.75047349467957	1.76532393580373	13.17893058705350
H	6.61803734879450	1.30682047702771	12.69054319236870
C	4.46251107203483	1.32512161740072	12.84838334051071
H	4.30871760963252	0.52982263428511	12.11045412278796
C	3.31711014766889	1.89527655823521	13.46477746556113
N	-0.57887856456542	1.98737120564011	14.76726943159153
N	-1.21835289504645	4.41261575386055	13.02667934419142

N	1.25646503802822	4.06921295090409	14.33302523254633
N	1.69474567882473	3.89735880971502	11.60607595907189
N	-0.49312639053885	1.58043789878217	11.48610466238178
C	-0.98062646121655	0.92062470665121	10.65288255818244
C	-1.58705174351015	0.08505679916115	9.63102309126431
H	-1.52839995866415	-0.97386955966230	9.93733744539500
H	-1.06638238812321	0.21344436173461	8.66433790472712
H	-2.64806130074875	0.35967382663840	9.50912333277756
O	2.09392989530578	1.47300236379895	13.14968288686307
O	1.65253810492143	1.10774280736038	4.91453165916807
O	0.22169501164968	0.26620515798984	6.74378099505859
O	-0.37235110487193	2.36046219037471	5.57035806725307
Cl	0.77119507700431	1.51269282724712	6.07743933410011
O	1.58844505581651	2.29941947245920	7.07682375464401

S16. Optimized coordinates for [Et₄N]₂[Fe^{III}(N₂S₂)(Cl)] calculated using BP86.

Fe	4.13534344197520	4.02717561690294	4.91207984752432
S	6.15661332490676	3.83291883924948	5.80043545347079
S	4.81427857405838	3.56865366072502	2.84647620427740
N	3.43057045298286	3.70210721153982	6.67815627724389
N	2.36425301718895	3.52268423297225	4.33565139772422
Cl	3.71971896032289	6.55334016105551	4.89271529248558
C	5.70133912391228	4.01649802638134	7.59694367874385
C	4.21140999783301	3.65823451185010	7.80644036629549
C	2.02943695617810	3.49534614555175	6.70033417969754
C	1.20510480203851	3.40121921431203	7.84510872937654
C	-0.18058124871014	3.21110716924335	7.71179365098254
C	-0.76006110612999	3.10945175055800	6.43839173469513
C	0.04073186765987	3.19944986716981	5.28734304291947
C	1.43683719237184	3.39486535114347	5.39830207409034
C	2.03248713332264	3.30581768633161	3.02184564753666
C	3.15712951602583	3.58787641332689	1.99741418211808
C	6.58859942702812	3.09384858603952	8.44850018302814
C	5.89183608555108	5.48698225919732	8.03565563603922
C	3.13310823613657	2.52595903341713	0.88673116989023
C	2.90185199766144	4.98987181668260	1.39808848824601
O	3.81305382009714	3.40471364044689	8.96414277769244
O	0.91064849791408	2.95357910543729	2.59715523985982
H	1.66625243943231	3.47537873092139	8.82906852132530
H	-0.80187262226338	3.14161532839293	8.61203418169554
H	-1.84055306229353	2.95863418132884	6.33013158795844
H	-0.39986179198960	3.11757094606518	4.29433497297131

H	6.29247026889398	3.16362616234929	9.51077685604342
H	7.64837930233751	3.39037682131816	8.35413449257650
H	6.49473058760393	2.04106692270822	8.13063243115127
H	5.57961106648193	5.61050805550397	9.09051809784479
H	6.95557383681015	5.77169570047508	7.95227523980986
H	5.29481558328762	6.16240935050776	7.40111062032840
H	2.13872881989751	2.50948874684224	0.40631899493748
H	3.89525859000236	2.75621089794825	0.12208986129812
H	3.33718546976120	1.51983338711230	1.29121734087278
H	1.90504771121556	5.01928780054277	0.91800581918846
H	2.94798373413788	5.76053396773347	2.18609846240617
H	3.66774532123869	5.22053698023358	0.63744685937770
N	7.86213075011722	7.34269258039366	2.82321905516930
C	7.30385881886226	7.26145783495656	4.25095631956226
C	7.36296695028179	8.55221765561315	5.06128025328286
C	9.30350700958123	7.86348593550483	2.82134235252818
C	10.29549901639351	7.06288549594108	3.65846196276254
C	7.78598200946593	5.92330012504081	2.24845211384042
C	8.25464023383174	5.77635707365952	0.80375352273149
C	7.04543956945489	8.32270244376639	1.97253878485117
C	5.59163058996224	7.93385112821989	1.73051470910882
H	7.86960732727094	6.45934565260549	4.74767482243195
H	6.26580144063583	6.90348860955052	4.16369631688243
H	6.91520960584823	8.32771788543774	6.04355837451336
H	8.39011982806022	8.90856171866777	5.24012558610844
H	6.77143083971682	9.36886339544497	4.61681443346981
H	9.24422442675601	8.90419234338093	3.17168905404419
H	9.61193981656437	7.89080644132998	1.76568979171114
H	11.28106117080530	7.54498064097823	3.54325427692256
H	10.05029873118183	7.06766035390567	4.73256225215140
H	10.39827363137776	6.01949394449658	3.32033230179112
H	8.39160687393760	5.29941230963336	2.92207853168434
H	6.73845062045452	5.59874823964941	2.36449600769995
H	8.13700104678406	4.71528198424229	0.52560989512594
H	9.31786668919372	6.03076260739892	0.66452442586907
H	7.65302548369739	6.36631161099734	0.09410731234328
H	7.11522585919037	9.29148916327071	2.48831782791775
H	7.59185801170703	8.41947674915684	1.02214477421884
H	5.11945791481334	8.76775935396329	1.18317248728116
H	5.02212060266403	7.77527260800419	2.66108982534864
H	5.49192416774508	7.03029090589989	1.10851448366141
N	7.27278572637093	-0.33384819442208	3.09531287609365
C	8.59888673221347	-1.02364161060032	3.44539833093701
C	9.76172099172317	-0.09910639880177	3.79082214101022
C	6.75032500344082	0.49353313859049	4.27929573878712
C	6.38963803734466	-0.29327434911374	5.53277852491887

C	7.45053105381236	0.65113751563281	1.93518586043714
C	7.94055154845714	0.04738947692476	0.62321280720398
C	6.29228343290755	-1.45223590663338	2.73052541163811
C	4.89810053073725	-0.99787649835893	2.31553336250610
H	8.36809939202730	-1.69577111090304	4.28475818277807
H	8.84590743188995	-1.65460154288782	2.57904856029521
H	10.62269055785635	-0.74440230751778	4.03318020126404
H	9.56603585523889	0.53158847071741	4.67245077857611
H	10.06221746710024	0.54539989935737	2.94918744873424
H	7.53031986835584	1.23786267159791	4.49461420283722
H	5.88546375535735	1.05941659137506	3.89767570110289
H	6.09239375864415	0.45360126093467	6.28830837836855
H	7.23567024358959	-0.86447974518864	5.94805933221044
H	5.53520895090852	-0.97277968196353	5.38386390760311
H	8.15238667659441	1.41344955519067	2.30579497113144
H	6.47594487975536	1.14977147690834	1.81477514184857
H	8.01676633675813	0.87196844087590	-0.10559050074089
H	8.94002206929475	-0.40897924346806	0.70609532754100
H	7.24171038500317	-0.69572466617166	0.20596857752792
H	6.77577190948372	-2.02378161205068	1.92441417653199
H	6.24880085326252	-2.10331464648250	3.61588804741371
H	4.29262687134854	-1.90520803659902	2.15428441699861
H	4.90028539376503	-0.43165588229893	1.37031847406150
H	4.39402992552402	-0.39499813527102	3.08750817164706

S17. Optimized coordinates for Fe^{II}(tsalen)(py)(CO) calculated using TPSSh.

	X	Y	Z
Fe	0.27933228897034	2.60697940126843	1.38229641543002
S	0.67628857156521	0.93318411125602	-0.15117658873182
S	1.89477844787799	1.59835567099715	2.66855149151887
N	-1.13289746853890	3.39989503237261	0.31042685957087
N	-0.09857290372258	4.01454410648962	2.67383758695884
C	0.15639860960007	1.47063701131681	-1.74704036374439
C	0.64210604615128	0.74870849239318	-2.86859654427493
C	0.25368546907473	1.06354304920807	-4.17285841634923
C	-0.64948184824479	2.12099767535633	-4.41330445803633
C	-1.15024122389558	2.83687975128188	-3.32813825561885
C	-0.76585344940198	2.54182262468599	-1.98913528677166
C	-1.40243964590160	3.35008497774319	-0.96517950318695
C	2.11185537695536	2.42464144415953	4.20550689810548
C	3.08281281630959	1.88827213077766	5.09450886290862
C	3.33376327658194	2.45831933035108	6.34306184840238

C	2.62021973223997	3.60214730828502	6.76356054991302
C	1.66408976750715	4.14628545177946	5.91146863933113
C	1.38416589263859	3.58508841107493	4.63080144257705
C	0.37276799049719	4.28542297736897	3.86104885294656
C	-1.97240758927758	4.27900529236658	1.14772831868112
C	-1.04142022772042	5.00867700940943	2.10695262279547
N	-1.20571768677124	1.38919011617823	2.29067112614346
C	-2.14452888030474	0.76091532473960	1.54102060733931
C	-3.14906728689097	-0.04369366145553	2.09142246003603
C	-3.19575618982453	-0.21920462160072	3.48200249082443
C	-2.23190305414334	0.43135457647705	4.26493564065802
C	-1.26191392396695	1.21954002577963	3.63401464022191
C	1.52984344895363	3.51201420018597	0.62433409475264
O	2.38538150929123	4.12119937214421	0.10343758848243
H	-0.03452058020461	5.17995781990874	4.35834178363588
H	-2.21647382340111	3.99922914595709	-1.32777188440440
H	-0.49989943432414	1.73570547759414	4.22096228036299
H	1.34588561565918	-0.07315117538850	-2.69449667862934
H	0.65961342441876	0.48530631344961	-5.00948047106856
H	-0.95661616187749	2.37311391556411	-5.43249666840180
H	-1.86165438356680	3.65443720412467	-3.49428312710020
H	3.64416723318376	1.00179695721182	4.77918260258164
H	4.09269910186606	2.01244923190498	6.99529458574010
H	2.81555310774306	4.05487356750407	7.73987644278322
H	1.10399574872246	5.03751881430342	6.21757106777346
H	-2.67676615360115	3.64479146898402	1.71569240412828
H	-2.55300586551486	4.98895282343794	0.53324744502819
H	-1.60732165893209	5.52023986234002	2.90466169776353
H	-0.45327163889273	5.76358541908662	1.55245207207950
H	-2.07659900640053	0.91211326919339	0.46140461641854
H	-3.87592675019067	-0.52341562752817	1.43012247456668
H	-3.96551559601236	-0.84514422686959	3.94418239361426
H	-2.21876104428381	0.33346314683124	5.35431734224452