Supporting information for "DFT Study of the Spin Crossover Dynamics in $Fe(dppen)_2X_2$ Complexes"

Huiwen Tan, Nadeem Natt, Benjamin J. Powell

Coordination structure along the reaction pathway

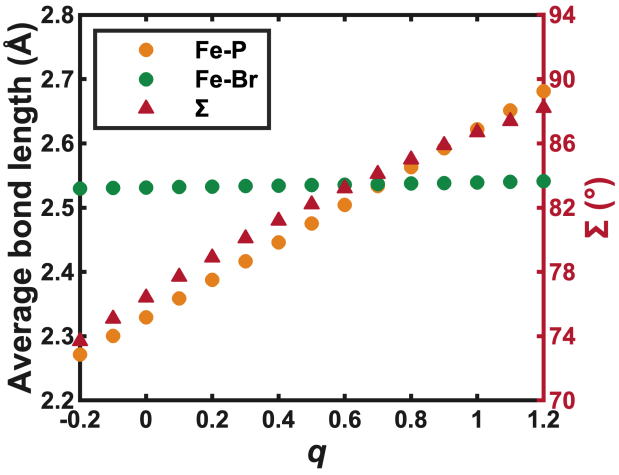

Figure S1: Variation of angular distortion and metal-ligand bond lengths with the reaction coordinate q, for $[Fe(dppen)_2Br_2]$.

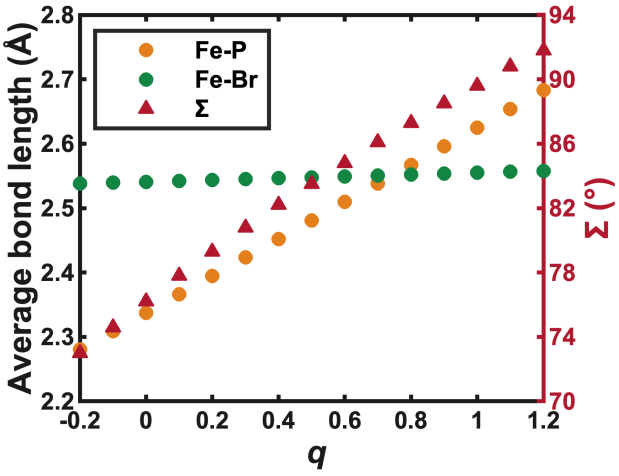

Figure S2: Variation of angular distortion and metal-ligand bond lengths with the reaction coordinate q, for $[Fe(dppen)_2Br_2] \cdot CHCl_3$.

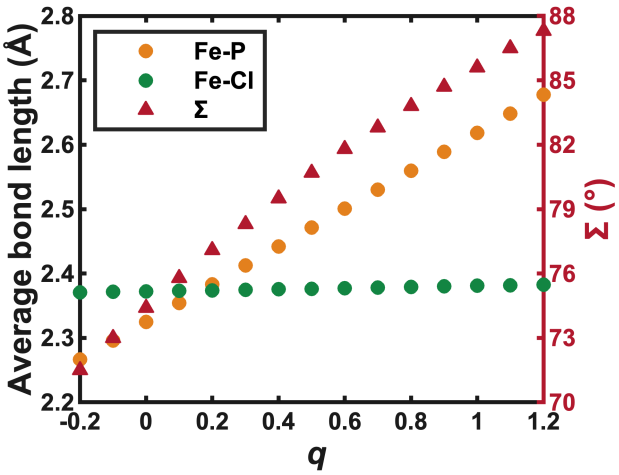

Figure S3: Variation of angular distortion and metal-ligand bond lengths with the reaction coordinate q, for $[Fe(dppen)_2Cl_2] \cdot CHCl_3$.

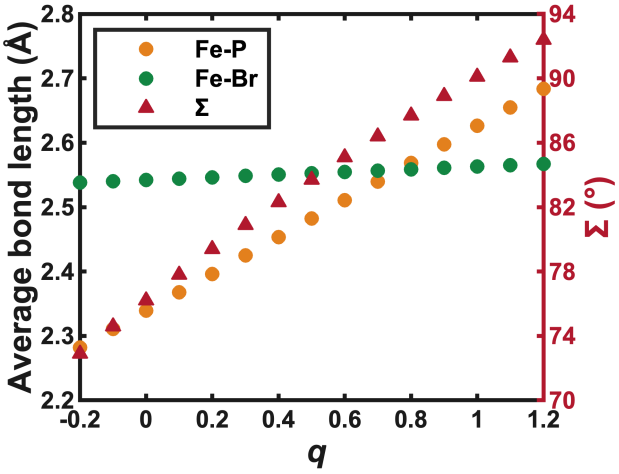

Figure S4: Variation of angular distortion and metal-ligand bond lengths with the reaction coordinate q, for $[Fe(dppen)_2Br_2] \cdot CH_2Cl_2$.

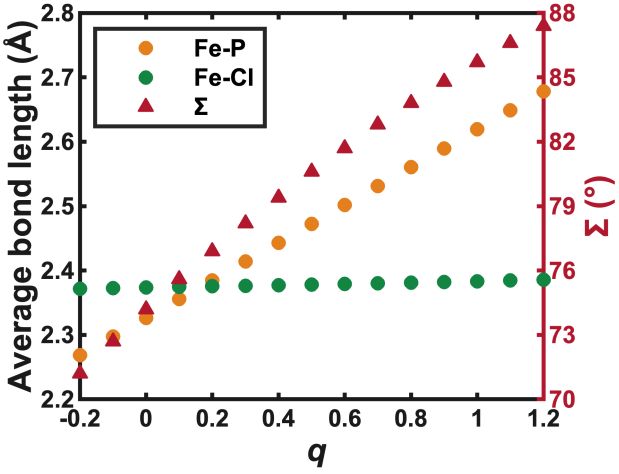

Figure S5: Variation of angular distortion and metal-ligand bond lengths with the reaction coordinate q, for $[Fe(dppen)_2Cl_2] \cdot CH_2Cl_2$.

Potential Eenrgy Surfaces

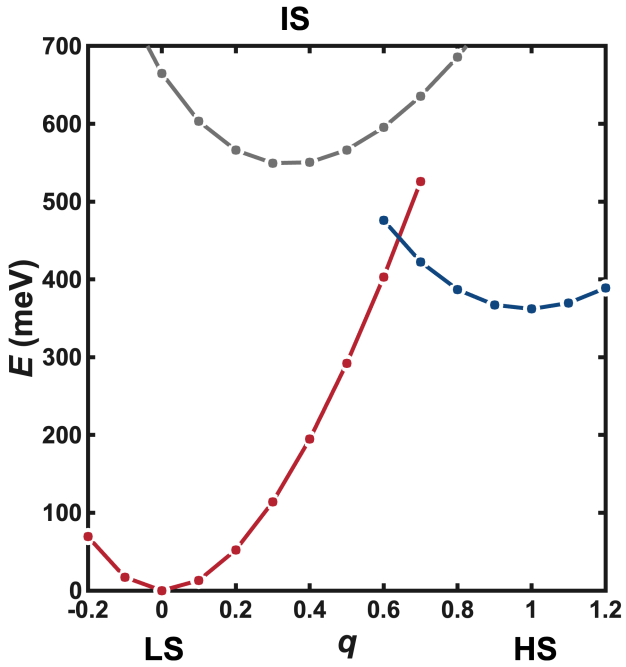

Figure S6: Potential energy surfaces of $[Fe(dppen)_2Br_2]$

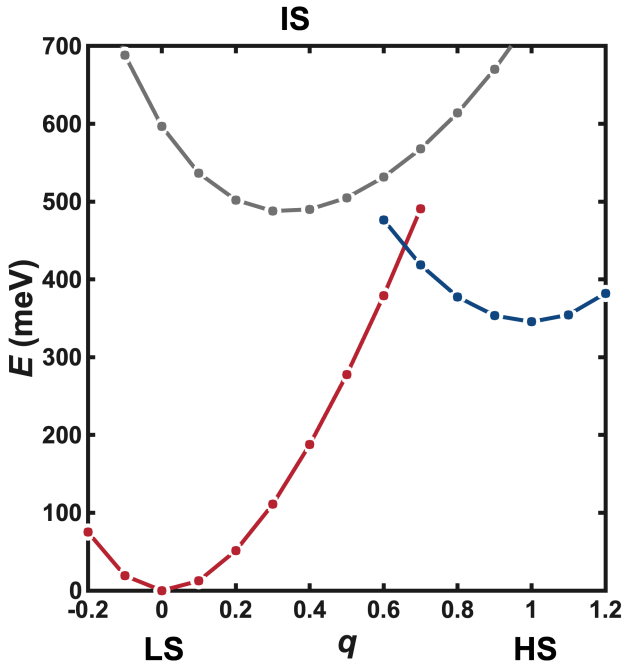

Figure S7: Potential energy surfaces of $[Fe(dppen)_2Br_2] \cdot CHCl_3$

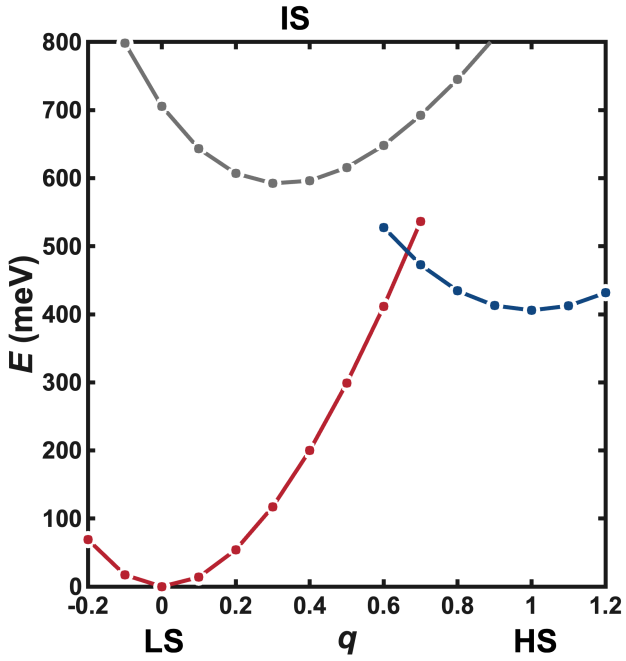

Figure S8: Potential energy surfaces of $[Fe(dppen)_2Cl_2] \cdot CHCl_3$

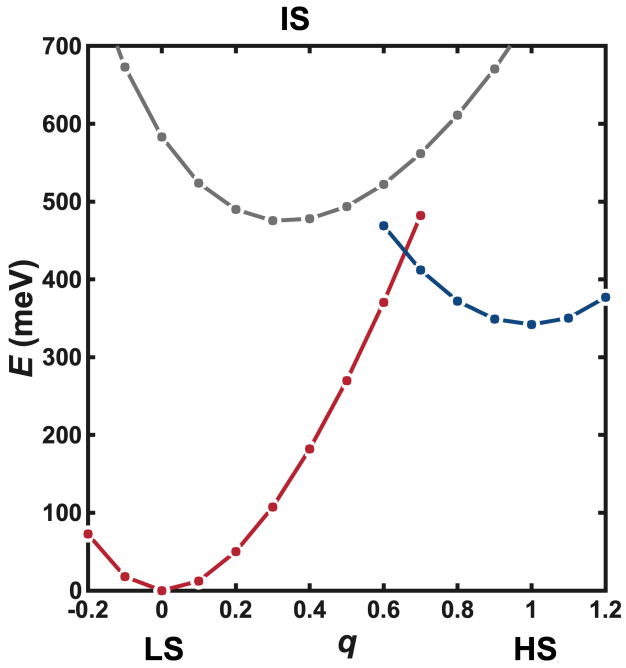

Figure S9: Potential energy surfaces of $[Fe(dppen)_2Br_2] \cdot CH_2Cl_2$

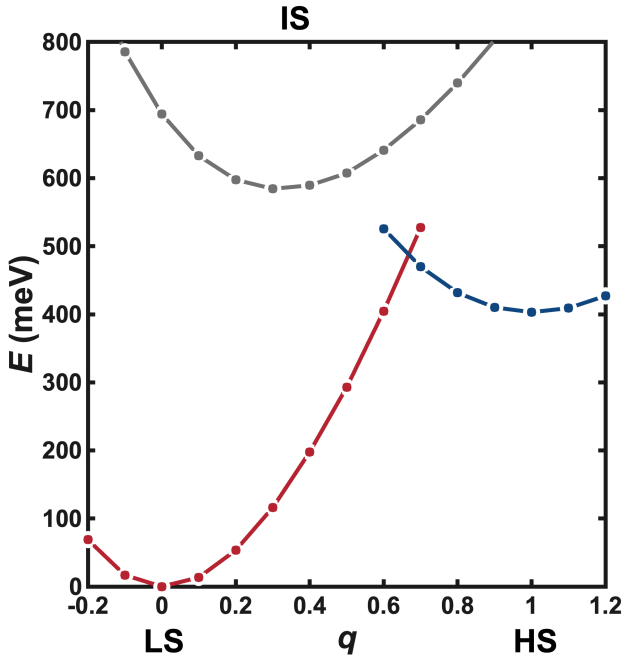

Figure S10: Potential energy surfaces of $[Fe(dppen)_2Cl_2] \cdot CH_2Cl_2$

Phonon Frequencies, Enthalpy and Entropy

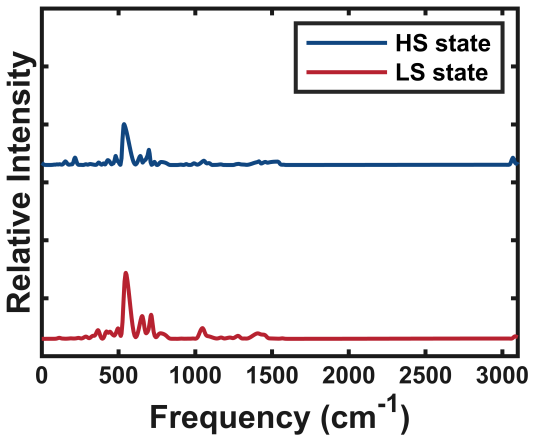

Figure S11: IR spectra of $[Fe(dppen)_2Br_2]$

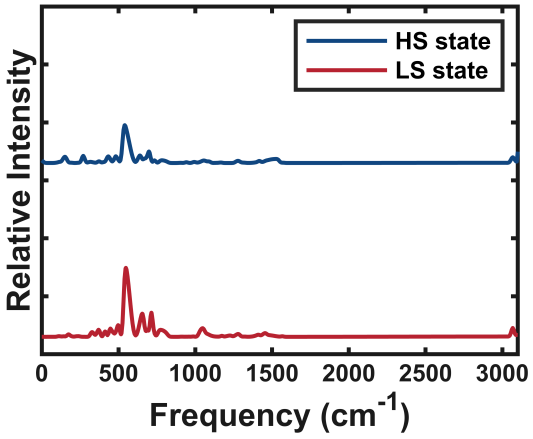

Figure S12: IR spectra of $[Fe(dppen)_2Cl_2]$

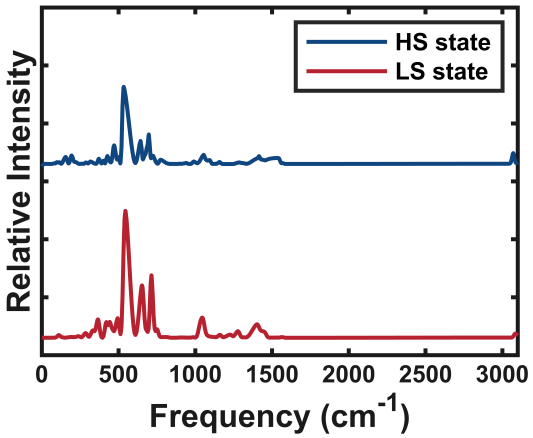

Figure S13: IR spectra of $[Fe(dppen)_2Br_2] \cdot CHCl_3$

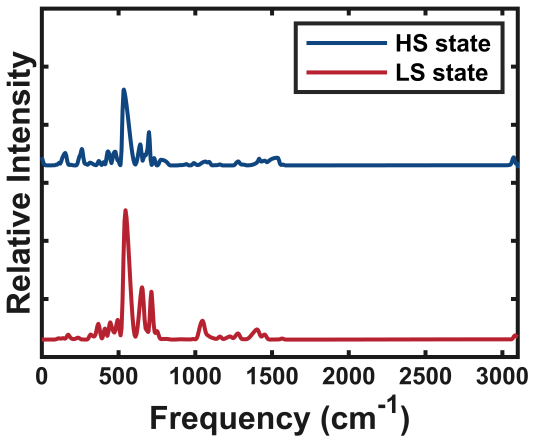

Figure S14: IR spectra of $[Fe(dppen)_2Cl_2] \cdot CHCl_3$

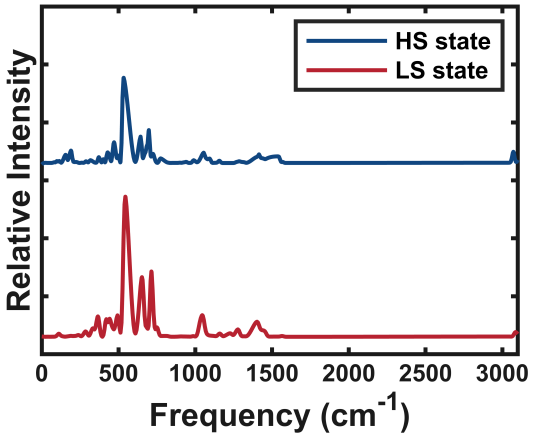

Figure S15: IR spectra of $[Fe(dppen)_2Br_2] \cdot CH_2Cl_2$

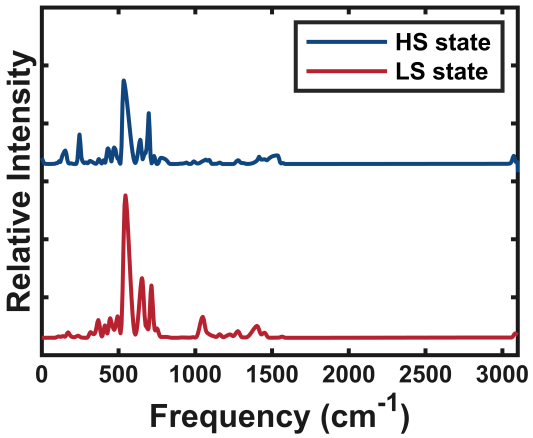

Figure S16: IR spectra of $[Fe(dppen)_2Cl_2] \cdot CH_2Cl_2$

$$H^{vib}_{\mathrm{HS/LS}}(T) = \sum_{i=1}^{303} \left(\frac{\hbar\omega_{i,\mathrm{HS/LS}}}{2} + \frac{\hbar\omega_{i,\mathrm{HS/LS}} \exp(-\frac{\hbar\omega_{i,\mathrm{HS/LS}}}{k_\mathrm{B}T})}{1 - \exp(-\frac{\hbar\omega_{i,\mathrm{HS/LS}}}{k_\mathrm{B}T})} \right) \tag{S1}$$

$$S^{vib}_{\mathrm{HS/LS}}(T) = \sum_{i=1}^{303} \left(\frac{\hbar\omega_{i,\mathrm{HS/LS}}}{2T \tanh\left(\frac{\hbar\omega_{i,\mathrm{HS/LS}}}{2k_\mathrm{B}T}\right)} - k_\mathrm{B} \ln\left[2 \sinh\left(\frac{\hbar\omega_{i,\mathrm{HS/LS}}}{2k_\mathrm{B}T}\right)\right] \right) \tag{S2}$$

Table S1: The $T_{1/2}$ (K) dependence of heating/cooling rates.

Compounds	Heating/Cooling rate		
	0.3 K/min	0.1 K/min	0.01 K/min
$[Fe(dppen)_2Br_2]$ (**Br.0**)	322.3	322.3	322.33
$[Fe(dppen)_2Cl_2]$ (**Cl.0**)	357.7	357.6	357.58
$[Fe(dppen)_2Br_2] \cdot nCHCl_3$ (**Br.1**)	303.7	303.7	303.72
$[Fe(dppen)_2Cl_2] \cdot nCHCl_3$ (**Cl.1**)	352.3	352.4	352.41
$[Fe(dppen)_2Br_2] \cdot nCH_2Cl_2$ (**Br.2**)	300.7	300.7	300.74
$[Fe(dppen)_2Cl_2] \cdot nCH_2Cl_2$ (**Cl.2**)	354.4	354.4	354.44

1 Optimized Geometries

The $Fe(dppen)_2X_2$ (X = Br^- or Cl^-) was optimized in the gas-phase by unrestricted PBE/TZP, as well in the implicit chloroform and dichloromethane solvents at the UPBE/TZP/COSMO level of theory. The Cartesian coordinates of the optimized low-spin and high-spin structures of all the materials involved in this paper are listed, followed by the single-point energy E (in Hartree) obtained using the same theoretical method and basis set.

1.1 $Fe(dppen)_2Br_2$ (Low-spin)

Fe	5.74680873	0.00015899	0.00067044
Br	3.56590921	0.85077223	0.96367524
P	5.89714786	1.41685218	-1.86880679
P	4.66450966	-1.36980185	-1.50976622
C	8.48592281	1.80409068	-2.99261319
C	9.63776614	2.54198176	-3.27880596
C	9.77239919	3.85014447	-2.80790668
C	8.74551817	4.42025951	-2.05015987
C	7.5898466	3.68812068	-1.76915068
C	7.44819808	2.37049625	-2.23622465
C	3.3497553	2.74275653	-1.94622925
C	2.40598489	3.62644547	-2.48024249
C	2.73385308	4.44468964	-3.56158819
C	4.01646265	4.37320975	-4.11354018
C	4.96388585	3.50114706	-3.57713318
C	4.64452823	2.67906585	-2.47882983
C	1.97643033	-1.86085224	-0.76183124
C	0.59064825	-1.75161579	-0.8730446
C	0.02227516	-1.0079976	-1.91155182
C	0.85171926	-0.37433072	-2.83749866
C	2.24150293	-0.48705375	-2.73123768
C	2.81903507	-1.23692812	-1.69648017
C	6.05497447	-3.81362472	-1.09679253
C	6.26472492	-5.18882913	-1.22596257
C	5.32832385	-5.98510872	-1.88907301
C	4.17990992	-5.39725006	-2.42591108
C	3.96688515	-4.02254063	-2.29764366
C	4.90169839	-3.21648634	-1.62584502
C	5.19745201	-0.87269997	-3.19865543
C	5.7686179	0.3235311	-3.34754068
H	8.40083489	0.77658599	-3.34558977
H	10.43375361	2.08693222	-3.87159156
H	10.6729032	4.42523761	-3.03347825
H	8.83964803	5.441799	-1.67693777
H	6.79243401	4.1530311	-1.18864537
H	3.07725533	2.10157969	-1.10636129
H	1.40605904	3.66704051	-2.04283573
H	1.99484778	5.13240446	-3.97819573
H	4.28516425	5.00169356	-4.965274
H	5.9617562	3.46879234	-4.01629948

```
H     2.40048353     -2.44201768     0.05601054
H     -0.04676346     -2.2445489     -0.13658338
H     -1.0628758     -0.92090492     -1.99563335
H     0.4210431     0.21339549     -3.65077697
H     2.87399966     0.02030046     -3.46009288
H     6.80166461     -3.1929165     -0.60108471
H     7.16831604     -5.6355019     -0.80561938
H     5.49249668     -7.0599687     -1.98945487
H     3.44142878     -6.01030778     -2.94679508
H     3.05997566     -3.58038778     -2.71238556
H     5.01631365     -1.55103228     -4.03821305
H     6.07702727     0.71325205     -4.32319407
Br     7.92700031     -0.85101451     -0.96329869
P     5.59681408     -1.41758515     1.86900012
C     4.04614407     -2.37228776     2.23493563
C     3.00678697     -1.80689982     2.98977387
C     1.85560901     -2.54625987     3.27492499
C     1.72347439     -3.85492396     2.8047324
C     2.75210112     -4.4240981     2.04861666
C     3.90669567     -3.69018311     1.76787607
H     4.70549448     -4.15421857     1.18853035
H     2.65985641     -5.44600771     1.67593254
H     0.82352618     -4.4311735     3.02958042
H     1.05818658     -2.09197326     3.8663662
H     3.08985159     -0.77894661     3.34192344
C     6.84926608     -2.68009564     2.47825903
C     8.144816     -2.74163914     1.9472603
C     9.08859217     -3.62563761     2.48069123
C     8.7601125     -4.44599378     3.56025739
C     7.47673927     -4.3766476     4.11066188
C     6.52914985     -3.50457212     3.5745148
H     5.53072292     -3.47384734     4.01251113
H     7.20752777     -5.00691269     4.96092328
H     9.49915545     -5.13387683     3.97652352
H     10.08903513     -3.66472099     2.04432622
H     8.41762051     -2.0992296     1.1084608
C     5.72497302     -0.32513077     3.34853003
C     6.29558757     0.87147678     3.20045267
P     6.82827469     1.36982594     1.51180986
C     8.67404119     1.23920288     1.69709857
C     9.51451524     1.86450889     0.76137882
C     10.90061014     1.75793211     0.871086
C     11.4715162     1.01606379     1.90946238
C     10.64429385     0.38118706     2.836543
C     9.2541457     0.49087474     2.73152567
H     8.62344074     -0.01731276     3.46132552
H     11.07697373     -0.20520504     3.6497243
H     12.55692529     0.93116074     1.99245323
H     11.53631954     2.25162395     0.13366907
H     9.08841354     2.44414227     -0.05652353
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C    6.59128591    3.21634591    1.62911536
C    5.43779985    3.81412545    1.1013066
C    5.22864808    5.18932992    1.2313761
C    6.16627201    5.98499879    1.89351896
C    7.31517699    5.39652849    2.42864718
C    7.52734816    4.02174172    2.29988875
H    8.43469464    3.57904129    2.71313473
H    8.05466122    6.00916353    2.94860645
H    6.00275477    7.05991794    1.9943348
H    4.32476084    5.63652357    0.81221905
H    4.69018444    3.193843    0.60651374
H    6.47591845    1.54954161    4.04039311
H    5.41672561    -0.71576707    4.32387735
E = -24.16314975
```

1.2 $Fe(dppen)_2Br_2$ (High-spin)

```
Fe    5.74664152    0.00011174    0.00012689
Br    3.52932167    0.83664038    0.91174445
P    5.83065848    1.52690293    -2.16466115
P    4.56230425    -1.48686995    -1.76412899
C    8.44390153    1.79088286    -3.26150113
C    9.65098426    2.46234811    -3.47410439
C    9.84108209    3.74810126    -2.96317705
C    8.81764696    4.36175205    -2.23345791
C    7.60853144    3.69643294    -2.02426517
C    7.40615293    2.4067987    -2.54671701
C    3.31859992    2.82569838    -2.15811416
C    2.34170193    3.70340592    -2.63846169
C    2.60877514    4.5238292    -3.73562789
C    3.86094724    4.46519009    -4.35630358
C    4.83942852    3.59199122    -3.8802694
C    4.57668912    2.76360791    -2.77436472
C    1.92556378    -1.96264793    -0.95680048
C    0.53805255    -1.83854159    -1.00353275
C    -0.06825941    -1.07739024    -2.00867119
C    0.72361028    -0.44275888    -2.96664974
C    2.11557348    -0.57338125    -2.9296282
C    2.7284009    -1.34024125    -1.92874792
C    5.97130722    -3.89274509    -1.39258469
C    6.20608535    -5.26443325    -1.51749974
C    5.29022861    -6.07636795    -2.19074864
C    4.13722785    -5.51045466    -2.74268702
C    3.89995787    -4.13940958    -2.62268025
C    4.81635964    -3.31750488    -1.94564707
C    5.14811758    -0.88533656    -3.39907726
C    5.69912323    0.3274421    -3.55460949
H    8.31889785    0.77414917    -3.63643239
H    10.44823441    1.97151986    -4.03584158
H    10.78556172    4.27077984    -3.12915564
```

```
H    8.96006608    5.36382258    -1.82428193
H    6.81687634    4.18579419    -1.4524848
H    3.10350977    2.18832162    -1.29723619
H    1.3679941    3.74297654    -2.14582329
H    1.84478666    5.20904619    -4.10899658
H    4.07782551    5.10324139    -5.21572466
H    5.81574241    3.56147299    -4.36732214
H    2.38582323    -2.54374224    -0.15542806
H    -0.07148576    -2.32803892    -0.24163595
H    -1.15479143    -0.97508512    -2.0397138
H    0.26046121    0.15948646    -3.75091122
H    2.72345615    -0.06760746    -3.68110186
H    6.69586508    -3.25748335    -0.87911591
H    7.11000425    -5.69739457    -1.0837472
H    5.47278415    -7.14874278    -2.28535069
H    3.41605998    -6.1389458    -3.2694217
H    2.99062273    -3.70995701    -3.04680811
H    5.0492291    -1.5625597    -4.25502297
H    6.03838288    0.6564533    -4.5443697
Br    7.96388083    -0.83687147    -0.91111813
P    5.66313116    -1.52654604    2.16491432
C    4.08831445    -2.40763287    2.54709118
C    3.05041653    -1.79316712    3.26288288
C    1.84415484    -2.46598571    3.47589312
C    1.65505717    -3.75165907    2.96439558
C    2.67869286    -4.36391398    2.2337851
C    3.88698077    -3.69722653    2.02414666
H    4.67882823    -4.18552636    1.45173049
H    2.537061    -5.36594646    1.82423544
H    0.71122842    -4.27541161    3.13069218
H    1.0467786    -1.9763023    4.03845138
H    3.17466277    -0.7765429    3.63836109
C    6.91783276    -2.76267189    2.77432844
C    8.17550773    -2.8246573    2.15724102
C    9.15289316    -3.701994    2.63728333
C    8.88666131    -4.52209197    3.73490721
C    7.63486437    -4.46353494    4.35636482
C    6.65585272    -3.59077923    3.8806091
H    5.679819    -3.56032651    4.36822389
H    7.41869225    -5.10133265    5.21615282
H    9.65102433    -5.20702794    4.10802307
H    10.1262762    -3.74158849    2.14400367
H    8.38981031    -2.18763341    1.29590181
C    5.7943124    -0.32701709    3.55483205
C    6.3449744    0.88590646    3.39922053
P    6.93092776    1.48729433    1.76426447
C    8.76482629    1.34076003    1.92892494
C    9.5676015    1.96226368    0.95634595
C    10.95510697    1.83808485    1.0030045
C    11.56148259    1.07779631    2.00875247
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C    10.76967652    0.44403809    2.9673662
C    9.37771566    0.57468451    2.93037291
H    8.76989246    0.06961065    3.68236276
H    11.23287118    -0.15757007    3.75208903
H    12.64801045    0.97543594    2.03975244
H    11.56458505    2.32687053    0.24060283
H    9.10728299    2.54267835    0.15450801
C    6.67676147    3.31795784    1.94532278
C    5.52135606    3.89266402    1.39264876
C    5.28633674    5.26435033    1.51712959
C    6.2023003    6.07673763    2.18969098
C    7.35567886    5.51130613    2.74133821
C    7.59328321    4.1402894    2.62165666
H    8.50291056    3.71119855    3.04551659
H    8.07690586    6.14016718    3.26754854
H    6.01951634    7.14909819    2.28400801
H    4.3821253    5.69695213    1.0836272
H    4.79676428    3.25704035    0.87967667
H    6.4436096    1.56325667    4.25509514
H    5.45514106    -0.65604416    4.54461504
E = -24.1498471
```

1.3 $Fe(dppen)_2Cl_2$ (Low-spin)

```
Fe    5.74733222    0.00053756    0.0000218
Cl    3.70138596    0.78981809    0.88954051
P    5.90204586    1.41071236    -1.8524826
P    4.66990302    -1.36201245    -1.51156234
C    8.52465566    1.75998998    -2.88277672
C    9.69209187    2.48234909    -3.14325048
C    9.81080287    3.8076798    -2.71781686
C    8.75350857    4.41048508    -2.03007078
C    7.58226744    3.69422019    -1.7745421
C    7.4554688    2.36086066    -2.19974655
C    3.35670029    2.70860953    -1.86206599
C    2.38886466    3.58291907    -2.36732156
C    2.67807823    4.40761191    -3.45503978
C    3.94553829    4.35349249    -4.04336718
C    4.91699313    3.48952976    -3.53773961
C    4.63543661    2.66093206    -2.4346336
C    1.97825244    -1.79737535    -0.75436146
C    0.59405488    -1.67127789    -0.8686602
C    0.03606574    -0.94990147    -1.92819407
C    0.87415337    -0.35475634    -2.87191387
C    2.26203274    -0.48434025    -2.76231608
C    2.82923053    -1.21329591    -1.70692455
C    6.10779642    -3.76949012    -1.135936
C    6.3293411    -5.14501586    -1.23675527
C    5.36292622    -5.97453607    -1.81083124
C    4.17333746    -5.41965312    -2.28964667
```

```
C    3.94686137    -4.04466265    -2.18921937
C    4.91082496    -3.2067296    -1.60445269
C    5.23007005    -0.87695018    -3.19473728
C    5.80010715    0.32101942    -3.33647053
H    8.45057525    0.7175741    -3.19244161
H    10.51347671    2.00188498    -3.67892308
H    10.72377229    4.37066933    -2.92295444
H    8.83712865    5.44481552    -1.69115347
H    6.76241826    4.18091007    -1.24459875
H    3.12022181    2.05939061    -1.01665663
H    1.40056303    3.6112787    -1.90334232
H    1.91981872    5.08784299    -3.84891491
H    4.1819933    4.98877044    -4.89970383
H    5.90330145    3.46789075    -4.00368577
H    2.39423716    -2.36024777    0.08000499
H    -0.04971856    -2.13421843    -0.1182838
H    -1.04778261    -0.84961242    -2.01469281
H    0.45173217    0.21652654    -3.70109917
H    2.90187101    -0.00560847    -3.50405269
H    6.87347711    -3.11922446    -0.71092252
H    7.26510229    -5.56694136    -0.86387997
H    5.53652969    -7.04989716    -1.88817903
H    3.4129806    -6.05890223    -2.74332102
H    3.00919145    -3.62715192    -2.55812981
H    5.06728418    -1.55964333    -4.03461954
H    6.12859233    0.70870384    -4.30653757
Cl    7.79255515    -0.79007111    -0.88998542
P    5.59202219    -1.41035357    1.85191942
C    4.03921434    -2.36194857    2.19769588
C    2.96833524    -1.76227317    2.87908054
C    1.80157901    -2.4862001    3.13830953
C    1.68559019    -3.81208259    2.71385105
C    2.7448413    -4.41387224    2.02819746
C    3.91497924    -3.69571652    1.7729867
H    4.73637272    -4.1815386    1.24462625
H    2.66335118    -5.44867136    1.690185
H    0.77327457    -4.37639307    2.91826832
H    0.97864944    -2.00657596    3.67236099
H    3.04026923    -0.71940784    3.18774804
C    6.85790538    -2.66123843    2.43383008
C    8.13650195    -2.71012207    1.86110367
C    9.10324048    -3.58591262    2.36588321
C    8.81306016    -4.41067599    3.45330257
C    7.54557658    -4.35555723    4.04152584
C    6.57508022    -3.49035977    3.53619309
H    5.58849713    -3.46834173    4.00156746
H    7.30826524    -4.99128375    4.89729419
H    9.57046233    -5.09209534    3.84676645
H    10.09141253    -3.61545993    1.90170522
H    8.37344353    -2.06135559    1.01548087
```

```
C    5.69282374    -0.32092443    3.33624806
C    6.26255786    0.87727913    3.19502986
P    6.82371864    1.36268197    1.51224906
C    8.66434905    1.2151361    1.70879596
C    9.51531964    1.80038798    0.75693218
C    10.89957607    1.67617606    0.87236338
C    11.45768947    0.95573089    1.93247832
C    10.61968705    0.35992545    2.8758362
C    9.23171715    0.48782415    2.76523753
H    8.59195053    0.00858414    3.50670514
H    11.04221355    -0.210486    3.70556959
H    12.54160154    0.85683643    2.01979958
H    11.54333515    2.13981163    0.12240251
H    9.09922389    2.36258916    -0.07781714
C    6.58335129    3.2072958    1.60551158
C    5.3857843    3.77057255    1.13911949
C    5.16490354    5.14612602    1.24085028
C    6.132969    5.97521105    1.81281796
C    7.32356263    5.41989654    2.28862973
C    7.54913225    4.04479434    2.18783351
H    8.48761725    3.62684026    2.55421515
H    8.08530185    6.05886214    2.74038258
H    5.96001828    7.05065053    1.89055998
H    4.22839565    5.56844066    0.87030054
H    4.61868077    3.1205694    0.71629717
H    6.4243813    1.55997036    4.03509161
H    5.36376502    -0.70885526    4.30602466
E = -24.20751169
```

1.4 $Fe(dppen)_2Cl_2$ (High-spin)

```
Fe    5.74707121    0.00027124    -0.00018594
Cl    3.68441517    0.80697111    0.83474758
P    5.84150473    1.51902982    -2.15153923
P    4.55887626    -1.48584563    -1.76896583
C    8.49274416    1.71299135    -3.13220229
C    9.71766079    2.35666611    -3.32295926
C    9.89523862    3.67482272    -2.89476617
C    8.84024377    4.34747022    -2.26959756
C    7.61318008    3.70887814    -2.08032911
C    7.42379547    2.38766102    -2.5221755
C    3.33580582    2.80342092    -2.07913268
C    2.33963718    3.6745312    -2.53084852
C    2.57061697    4.49903511    -3.63312589
C    3.80597563    4.45198018    -4.28814016
C    4.80357111    3.58461644    -3.84201989
C    4.57668407    2.75229227    -2.73139254
C    1.92819034    -1.94036473    -0.94209483
C    0.54081396    -1.81111545    -0.98188472
C    -0.06894256    -1.0654155    -1.99636386
```

```
C    0.71913637    -0.45059324    -2.97056627
C    2.11061198    -0.58612942    -2.94021367
C    2.72683356    -1.33891147    -1.93060351
C    6.01517697    -3.85722623    -1.42613262
C    6.27233616    -5.22535134    -1.54455462
C    5.3496562    -6.062631    -2.17653608
C    4.16683605    -5.52607397    -2.69370738
C    3.90601884    -4.15874595    -2.57984084
C    4.82938641    -3.31217648    -1.94449105
C    5.15818598    -0.88495917    -3.39915458
C    5.71770407    0.32533586    -3.54755717
H    8.37482215    0.67234143    -3.43756861
H    10.53909244    1.81984608    -3.80216584
H    10.85379447    4.17629147    -3.04535519
H    8.97147015    5.37521946    -1.92552119
H    6.79784059    4.24420566    -1.5887966
H    3.15180856    2.16195807    -1.21380485
H    1.37915616    3.7057506    -2.01222641
H    1.79117236    5.17905657    -3.98379178
H    3.99363678    5.09399499    -5.15165573
H    5.76631699    3.56107547    -4.35605212
H    2.39175803    -2.50878829    -0.13316033
H    -0.06563529    -2.28497822    -0.20755194
H    -1.15536244    -0.95903672    -2.02176025
H    0.25290113    0.14036635    -3.76182452
H    2.71652197    -0.09566918    -3.70365702
H    6.74226907    -3.20017987    -0.94395225
H    7.19891608    -5.63641892    -1.13778593
H    5.55031863    -7.13228577    -2.26611647
H    3.44103191    -6.17498568    -3.18853487
H    2.97464149    -3.75090416    -2.97704186
H    5.06829384    -1.56168406    -4.25683176
H    6.07548593    0.65160557    -4.53183927
Cl    7.80937545    -0.80720809    -0.8351284
P    5.65187957    -1.51823214    2.15120794
C    4.06930902    -2.38681663    2.52073779
C    2.99994647    -1.7122768    3.13016244
C    1.77478531    -2.3558758    3.31962822
C    1.59731345    -3.67374026    2.89050052
C    2.65265386    -4.34614853    2.26565781
C    3.88004174    -3.70772881    2.0779177
H    4.69561851    -4.242822    1.58653441
H    2.52145826    -5.37361224    1.92071187
H    0.63851048    -4.17508319    3.03993251
H    0.95301812    -1.81916145    3.79838743
H    3.11773639    -0.67174208    3.43598619
C    6.91649214    -2.75118017    2.73226907
C    8.1577108    -2.80262674    2.08070045
C    9.15371099    -3.67334784    2.53354972
C    8.92221343    -4.49710193    3.63627806
```

```
C    7.68651611    -4.44966903    4.29063521
C    6.68908965    -3.5826789    3.84340719
H    5.72610112    -3.55879083    4.35696659
H    7.49847787    -5.09106422    5.15452988
H    9.7015345    -5.17680342    3.98783882
H    10.11448555    -3.70482161    2.01548563
H    8.34213194    -2.16164722    1.21510998
C    5.77453293    -0.32422977    3.54705186
C    6.33449653    0.88587928    3.3987703
P    6.93539412    1.48596918    1.76888487
C    8.76713257    1.33723368    1.93213135
C    9.56730229    1.93652866    0.94355245
C    10.9544682    1.80538781    0.98443635
C    11.56248831    1.05991186    2.00012213
C    10.77288793    0.44727695    2.97446494
C    9.38162935    0.58476253    2.94302407
H    8.77449618    0.09583567    3.70648178
H    11.23774598    -0.14355569    3.76663003
H    12.64873421    0.95196457    2.02633504
H    11.56208834    2.27748531    0.20994298
H    9.10507853    2.50463018    0.1336236
C    6.66641746    3.31260583    1.94368859
C    5.48157755    3.85863415    1.42416659
C    5.22570488    5.22706339    1.54186335
C    6.14861476    6.06362425    2.17446268
C    7.33044665    5.52607001    2.692848
C    7.59012861    4.15848415    2.57944224
H    8.52075079    3.74984835    2.97759483
H    8.05641336    6.174413    3.18818222
H    5.94890289    7.13349757    2.2635699
H    4.29991925    5.6389294    1.13409605
H    4.75432605    3.20216551    0.94145557
H    6.42412349    1.56272404    4.25637878
H    5.41587166    -0.65017492    4.53112142
E = -24.19235719
```

1.5 $Fe(dppen)_2Br_2 \cdot CHCl_3$ (Low-spin)

```
Fe    5.74662362    0.00009171    -0.00005934
Br    3.55936402    0.86360287    0.9623368
P    5.89928128    1.42242354    -1.88121983
P    4.66218946    -1.37108511    -1.51246734
C    8.48090344    1.79919469    -3.02335194
C    9.63498308    2.5314362    -3.31708007
C    9.78109403    3.83749769    -2.84234564
C    8.76219037    4.41165994    -2.07594787
C    7.60590259    3.68342494    -1.78570816
C    7.45393997    2.36713742    -2.25364027
C    3.35997825    2.76928279    -1.95380237
C    2.42211651    3.65940147    -2.48841791
```

C	2.75411707	4.46767695	-3.57675125
C	4.03377492	4.37841742	-4.1348194
C	4.97501364	3.49983659	-3.59664957
C	4.65180798	2.6887615	-2.49103799
C	1.98358976	-1.90964146	-0.76362232
C	0.595553	-1.81225564	-0.86567446
C	0.01449613	-1.04947028	-1.88448775
C	0.83370612	-0.3857119	-2.799684
C	2.22554905	-0.48569694	-2.70126513
C	2.81494469	-1.25269365	-1.68572258
C	6.02902774	-3.82617125	-1.05692452
C	6.24322017	-5.20020598	-1.19952698
C	5.3430466	-5.98028329	-1.92978029
C	4.22827502	-5.37767589	-2.5208016
C	4.01282003	-4.0044836	-2.37927624
C	4.91041493	-3.21460599	-1.64033642
C	5.18174711	-0.86726527	-3.20255817
C	5.7590589	0.32592364	-3.35494268
H	8.38407194	0.77769757	-3.39032233
H	10.42199988	2.0755928	-3.92111536
H	10.68254399	4.40838901	-3.07392668
H	8.86417662	5.43306085	-1.70424903
H	6.81557265	4.15168345	-1.19827356
H	3.0852618	2.13397992	-1.11074483
H	1.42414554	3.71482201	-2.04813766
H	2.02061277	5.16057637	-3.99425421
H	4.30471752	4.99713692	-4.99288995
H	5.96883924	3.4523123	-4.0433579
H	2.41821045	-2.5069398	0.03728992
H	-0.03531977	-2.33131986	-0.14122613
H	-1.07191144	-0.97334549	-1.96293286
H	0.39244882	0.21340845	-3.59882477
H	2.84913805	0.04116332	-3.42413077
H	6.74512262	-3.21912969	-0.50299425
H	7.11872833	-5.66022991	-0.73615699
H	5.50890356	-7.05379055	-2.03971238
H	3.5187041	-5.97786652	-3.09414156
H	3.13338435	-3.55178361	-2.83985763
H	4.9870826	-1.53900231	-4.044611
H	6.05981625	0.71263243	-4.334127
Br	7.93387215	-0.86322703	-0.96259707
P	5.59412684	-1.42192472	1.88113695
C	4.03990796	-2.36741682	2.253516
C	3.01282027	-1.80032194	3.02367221
C	1.85927007	-2.5333632	3.31749158
C	1.71380376	-3.83935551	2.84236595
C	2.73291852	-4.41272561	2.07565512
C	3.88876546	-3.68375942	1.78548355
H	4.67928914	-4.15141695	1.19784022
H	2.63148509	-5.43409992	1.70372409

```
H    0.81274609    -4.41084745    3.07398631
H    1.07214564    -2.07819292    3.92189611
H    3.10918276    -0.77891377    3.39101145
C    6.84202507    -2.68755759    2.49168811
C    8.13408436    -2.76774237    1.95498176
C    9.07219424    -3.65704781    2.49052908
C    8.74017347    -4.46482001    3.57923164
C    7.46029521    -4.37577005    4.13683489
C    6.5188547    -3.49791534    3.5978242
H    5.52487644    -3.45051186    4.04420148
H    7.18936405    -4.99405045    4.99522605
H    9.47386534    -5.15709313    3.99744247
H    10.07038747    -3.71218711    2.05071644
H    8.40887606    -2.13262018    1.1118153
C    5.73371336    -0.32515388    3.35471571
C    6.31120621    0.86794125    3.2022807
P    6.83130445    1.37123946    1.51220082
C    8.67848416    1.25208065    1.68566223
C    9.51026114    1.90793407    0.76317038
C    10.89823617    1.80961709    0.86520934
C    11.47879761    1.04694229    1.88438727
C    10.65916022    0.38418022    2.79992179
C    9.26738347    0.48503837    2.70145913
H    8.64344868    -0.04125773    3.42443512
H    11.10002371    -0.21497561    3.59925395
H    12.56515379    0.97004558    1.96278836
H    11.52945139    2.3278449    0.14046195
H    9.0760241    2.50504394    -0.03809456
C    6.5836846    3.2148971    1.6395023
C    5.46518117    3.82651344    1.0559412
C    5.25149769    5.20069831    1.19786397
C    6.1520007    5.98081253    1.92767788
C    7.2665801    5.37810475    2.51896499
C    7.48159692    4.00477865    2.37804455
H    8.36086426    3.55197781    2.83883926
H    7.97636166    5.97833113    3.09200761
H    5.98651839    7.05442826    2.03710997
H    4.37613404    5.660804    0.73429946
H    4.74887941    3.21945214    0.50230373
H    6.50591177    1.53973899    4.04427425
H    5.43283137    -0.71174729    4.33390695
E = -24.17419253
```

1.6 $Fe(dppen)_2Br_2{\cdot}CHCl_3$ (High-spin)

```
Fe    5.747244    0.00102163    0.00001914
Br    3.53667192    0.87908517    0.93298561
P    5.8526793    1.5456161    -2.18576069
P    4.56493906    -1.46531678    -1.75062009
C    8.44123757    1.74751657    -3.34964331
```

```
C    9.65642543    2.39154979    -3.60092622
C    9.88850982    3.67700203    -3.10441402
C    8.89809625    4.31818308    -2.35225187
C    7.68216869    3.67855881    -2.10321079
C    7.43864294    2.38870575    -2.6069916
C    3.35415202    2.86721411    -2.14673032
C    2.37900347    3.75752141    -2.60777793
C    2.64408826    4.58897607    -3.69784107
C    3.89114185    4.52697832    -4.3299952
C    4.86760835    3.64062461    -3.87224677
C    4.60766464    2.80269964    -2.77255124
C    1.95136339    -2.08164159    -0.95312275
C    0.56000979    -1.99157084    -0.97532818
C    -0.07915721    -1.18257919    -1.92241931
C    0.68417657    -0.46560633    -2.84629147
C    2.07996342    -0.55790738    -2.83046676
C    2.72474278    -1.37192011    -1.88805923
C    5.84104033    -3.90860837    -1.15315071
C    6.09423998    -5.27710879    -1.29047864
C    5.374053    -6.03318768    -2.21841005
C    4.39522355    -5.41840998    -3.00743786
C    4.13699853    -4.05338133    -2.86741018
C    4.8613225    -3.28584203    -1.9392275
C    5.10327596    -0.8578661    -3.39888795
C    5.66498988    0.3473668    -3.56917019
H    8.28110415    0.73618026    -3.72597852
H    10.42507915    1.88269923    -4.18615933
H    10.83823959    4.17808269    -3.30175369
H    9.07147615    5.32181845    -1.95906917
H    6.91680572    4.19224601    -1.51742902
H    3.14120939    2.21985983    -1.29283635
H    1.40894215    3.79993611    -2.10810469
H    1.88242525    5.28424567    -4.05702117
H    4.10521333    5.17168127    -5.18508602
H    5.83696806    3.60617613    -4.3724038
H    2.43674263    -2.70479614    -0.19923954
H    -0.02903354    -2.54965377    -0.24451708
H    -1.16852763    -1.1104491    -1.93663769
H    0.19463188    0.16941361    -3.58749005
H    2.66396657    0.01018317    -3.55641792
H    6.42057143    -3.31414939    -0.44451006
H    6.85905595    -5.75126421    -0.6721416
H    5.57292753    -7.10107916    -2.32809297
H    3.82794358    -6.0051213    -3.73296123
H    3.36078381    -3.58708933    -3.47778202
H    4.96243223    -1.52563231    -4.25657818
H    5.9735502    0.67467697    -4.56926514
Br    7.95754596    -0.87785107    -0.93250226
P    5.64026614    -1.54434827    2.18489658
C    4.053514    -2.38687173    2.60433978
```

```
C    3.0507255    -1.74529308    3.34639726
C    1.83431411    -2.38799272    3.5951386
C    1.60096847    -3.67225476    3.09614249
C    2.59138527    -4.31358788    2.34411066
C    3.8087028    -3.6754766    2.09800567
H    4.57396082    -4.18924952    1.51220618
H    2.41695454    -5.31621462    1.94882967
H    0.65016049    -4.17217677    3.2912152
H    1.06560651    -1.87892272    4.1801152
H    3.21175558    -0.73469203    3.72432389
C    6.88446882    -2.80218446    2.7717285
C    8.1377183    -2.86772516    2.14552909
C    9.11242768    -3.75844447    2.60673689
C    8.84710999    -4.5891834    3.69728703
C    7.60022855    -4.52620108    4.32970849
C    6.62415168    -3.63951881    3.87178265
H    5.65493136    -3.60426084    4.37214517
H    7.3860159    -5.17036623    5.18516854
H    9.60845642    -5.28471381    4.05663057
H    10.08231678    -3.80174087    2.10680296
H    8.35071764    -2.22099278    1.29116578
C    5.82768568    -0.34692141    3.56899695
C    6.39038667    0.8579801    3.39953076
P    6.93014641    1.46565997    1.75179912
C    8.77010186    1.36950799    1.89063926
C    9.54561984    2.0781909    0.9567397
C    10.93679721    1.9857965    0.9804381
C    11.57362338    1.17545658    1.92795089
C    10.80813466    0.4595354    2.85085221
C    9.41252619    0.55425316    2.83358962
H    8.82679581    -0.01292135    3.55887625
H    11.29582564    -0.1764349    3.59246195
H    12.6628532    1.10144885    1.94323019
H    11.52755001    2.54307308    0.25039466
H    9.062101    2.70236084    0.20252441
C    6.63599726    3.28651326    1.94110308
C    5.65775897    3.91106479    1.15459425
C    5.40652718    5.27989077    1.29230209
C    6.12712272    6.03451945    2.22109538
C    7.10454881    5.41797926    3.01048389
C    7.36091934    4.0526469    2.86999032
H    8.13597206    3.58494996    3.48075642
H    7.67210686    6.00351271    3.73674443
H    5.92977182    7.10266736    2.33105534
H    4.64289501    5.75544037    0.67357062
H    5.0778505    3.31778481    0.44528972
H    6.531629    1.52515655    4.25762069
H    5.51832593    -0.67448633    4.56875753
E = -24.16149613
```

1.7 $Fe(dppen)_2Cl_2 \cdot CHCl_3$ (Low-spin)

Fe	5.74676811	-0.00000907	-0.00013772
Cl	3.69814001	0.79963347	0.8896646
P	5.90250683	1.41336121	-1.86215456
P	4.66224459	-1.36474608	-1.51112318
C	8.51466695	1.75585572	-2.92142054
C	9.68519494	2.4717384	-3.18790343
C	9.82009305	3.79088854	-2.74646539
C	8.7752197	4.39355699	-2.03887431
C	7.60218889	3.68199577	-1.7759913
C	7.4601581	2.35432711	-2.21429053
C	3.3618141	2.72606136	-1.87865339
C	2.40125173	3.60770896	-2.38570276
C	2.70056997	4.43082219	-3.47273544
C	3.96982919	4.36645197	-4.05778018
C	4.93389243	3.49529723	-3.54860914
C	4.6425703	2.66947943	-2.44573599
C	1.97620442	-1.84495738	-0.75587672
C	0.58989286	-1.72972481	-0.86439686
C	0.02252373	-0.98757086	-1.90582778
C	0.8535812	-0.36206609	-2.83717903
C	2.24339141	-0.4807303	-2.73267725
C	2.81937428	-1.22840496	-1.69502554
C	6.08749907	-3.77553597	-1.09413743
C	6.32138203	-5.1484777	-1.20954351
C	5.38799021	-5.9700866	-1.84735957
C	4.22013343	-5.4099379	-2.3737449
C	3.98409189	-4.03717878	-2.26039086
C	4.9147313	-3.20689143	-1.61299187
C	5.20911606	-0.87382013	-3.19612921
C	5.78657497	0.32064829	-3.34143003
H	8.42544861	0.72255657	-3.25628904
H	10.49416243	1.99350448	-3.74391791
H	10.73477903	4.34915673	-2.95630763
H	8.87067301	5.42415811	-1.69171234
H	6.79297341	4.16903843	-1.23039027
H	3.1185539	2.07651658	-1.0361687
H	1.41126808	3.6449836	-1.92595964
H	1.94876435	5.11665909	-3.86899197
H	4.21348634	4.99836989	-4.91450446
H	5.91957462	3.46442018	-4.01503634
H	2.39983131	-2.42577205	0.06257411
H	-0.04997782	-2.21878864	-0.12708988
H	-1.06244739	-0.89709364	-1.98874235
H	0.42332774	0.22224508	-3.653121
H	2.87652599	0.01769032	-3.46725405
H	6.82533921	-3.13273531	-0.6136377
H	7.23837386	-5.57570197	-0.79775205
H	5.56921443	-7.04316991	-1.93551156
H	3.48545743	-6.04336193	-2.87505163

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H    3.06474163    -3.61683339    -2.6706592
H    5.03061063    -1.54924014    -4.03888478
H    6.10563493    0.70561481    -4.31567313
Cl    7.79518709    -0.80022791    -0.88978044
P    5.59059287    -1.41282588    1.8622172
C    4.03296829    -2.35379342    2.21451965
C    2.9782338    -1.75520538    2.92119657
C    1.80803241    -2.47139819    3.18829844
C    1.67379508    -3.79102932    2.74810494
C    2.71903614    -4.39391165    2.04123544
C    3.89170627    -3.68201277    1.77765291
H    4.70136559    -4.16934597    1.23298935
H    2.62413945    -5.42493118    1.69515728
H    0.75936876    -4.34953881    2.95843607
H    0.99880645    -1.99302988    3.74382183
H    3.06699284    -0.72156899    3.25515559
C    6.85050213    -2.66864672    2.44665902
C    8.13112855    -2.72614165    1.87942617
C    9.09142648    -3.60772391    2.38710988
C    8.79198237    -4.42968039    3.47498127
C    7.52286606    -4.3642452    4.06023878
C    6.5590117    -3.49325867    3.55037582
H    5.57340738    -3.46157898    4.01691165
H    7.27915029    -4.99523365    4.91763216
H    9.54360511    -5.11540923    3.87176713
H    10.08130291    -3.64584936    1.92720404
H    8.37443093    -2.07751521    1.03624708
C    5.70603992    -0.31955231    3.3411154
C    6.28395778    0.87467158    3.19560429
P    6.83167757    1.36463768    1.51059971
C    8.67441845    1.22726277    1.69502897
C    9.51817038    1.84222206    0.75536248
C    10.90439229    1.72628098    0.8643357
C    11.47107936    0.98498337    1.90674349
C    10.63943294    0.36100036    2.83859102
C    9.24971833    0.48036451    2.73362371
H    8.61612226    -0.01691957    3.46857061
H    11.06913898    -0.22265258    3.65529319
H    12.55597735    0.89394653    1.98999771
H    11.54472824    2.21410115    0.12660821
H    9.09508093    2.42221588    -0.06395219
C    6.58050694    3.20704903    1.61135571
C    5.40833333    3.77618591    1.09172172
C    5.17555971    5.14941548    1.20592522
C    6.10948349    5.9707874    1.84327217
C    7.27681859    5.4101499    2.37029715
C    7.51180004    4.03711379    2.25807894
H    8.43078575    3.61636162    2.66875021
H    8.01192062    6.04340663    2.8711915
H    5.92913752    7.04409902    1.93044187
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H     4.25903013     5.57705123     0.79353424
H     4.67010579     3.13359987     0.61154663
H     6.46224583     1.55041745     4.03814233
H     5.38638305    -0.70399995     4.3153665
E = -24.21888352
```

1.8 $Fe(dppen)_2Cl_2 \cdot CHCl_3$ (High-spin)

```
Fe     5.74698721     0.00001553    -0.00008732
Cl     3.66834386     0.80115629     0.84025019
P     5.84718187     1.51630496    -2.15922883
P     4.55919456    -1.48840292     -1.7657503
C     8.47050961     1.73356817    -3.22589123
C     9.69226558     2.38165128    -3.42974222
C     9.89564314     3.67295781    -2.93576166
C     8.87045078     4.31494271    -2.23216908
C     7.64787603     3.67143508    -2.03004266
C     7.43274495     2.37668915    -2.53487464
C     3.34838899     2.81897444    -2.09077678
C     2.36263127     3.70399827    -2.53897991
C     2.6083135     4.53620451    -3.63309132
C     3.84681861     4.48157131    -4.28280712
C     4.8339471     3.60017317    -3.83880312
C     4.59268364     2.76121678    -2.73596226
C     1.9276784    -1.98216491    -0.95203879
C     0.53906016     -1.86021461     -0.99221883
C     -0.0728819     -1.09297534     -1.99061915
C     0.71485767     -0.45018599     -2.94778801
C     2.10756907     -0.57834147     -2.9163448
C     2.72569496     -1.35139974     -1.92291777
C     5.99625212     -3.86365086     -1.35733553
C     6.25932289     -5.23181849     -1.46919525
C     5.36797395     -6.06494087     -2.15079677
C     4.21237766     -5.5241907     -2.72414818
C     3.94760403     -4.15663766     -2.61695815
C     4.83895773     -3.31383702     -1.93193016
C     5.14602706     -0.88743892     -3.39945265
C     5.70665657     0.32194087     -3.55233309
H     8.33137443     0.71717458     -3.59720488
H     10.4888428     1.87117807     -3.97507655
H     10.85082281     4.17730876     -3.09521716
H     9.02264912     5.32227086     -1.83971501
H     6.85582969     4.18275546     -1.47811478
H     3.15444424     2.17024285     -1.23354095
H     1.39919488     3.74188494     -2.02633426
H     1.83790948     5.22728224     -3.98168299
H     4.04514894     5.12795796     -5.14047074
H     5.79724413     3.57014858     -4.35120673
H     2.39222004     -2.56972951     -0.15757934
H     -0.0687096     -2.35899677     -0.23453213
```

```
H    -1.15991236    -0.99433323    -2.01788239
H    0.24702029    0.15423124    -3.72762615
H    2.71112806    -0.06935583    -3.66936707
H    6.69591363    -3.211031    -0.83098983
H    7.16341428    -5.64717608    -1.01872891
H    5.57119871    -7.13445476    -2.23458127
H    3.51107926    -6.17008714    -3.25660957
H    3.03883761    -3.74736445    -3.06213682
H    5.03818099    -1.55819932    -4.2595939
H    6.04742744    0.64922343    -4.54207216
Cl    7.825476    -0.80140868    -0.84039807
P    5.6469469    -1.51612684    2.15906135
C    4.06195887    -2.37771535    2.53444795
C    3.02379444    -1.73607423    3.22619702
C    1.80263882    -2.38539232    3.42975171
C    1.60038788    -3.67656648    2.93496547
C    2.62608138    -4.31716671    2.2308345
C    3.84805051    -3.67242368    2.02899217
H    4.64050116    -4.18266644    1.47665175
H    2.47470709    -5.32435148    1.83768385
H    0.64568552    -4.18189182    3.09419873
H    1.00566425    -1.87600457    3.97551994
H    3.16209832    -0.71985033    3.59829372
C    6.90192174    -2.76032732    2.73641639
C    8.14638368    -2.81779064    2.09155788
C    9.13228327    -3.70242187    2.54022937
C    8.88656282    -4.53444547    3.63447445
C    7.64788441    -4.4800329    4.28388907
C    6.66055333    -3.59913228    3.83935082
H    5.69708578    -3.56931484    4.35144536
H    7.44955595    -5.12626715    5.14166954
H    9.65708968    -5.22520217    3.98343149
H    10.09584912    -3.74017116    2.02781422
H    8.34026844    -2.16931335    1.23412272
C    5.78665186    -0.32155451    3.55205583
C    6.34710378    0.88791404    3.3992065
P    6.93437629    1.48871692    1.76561274
C    8.76785576    1.35192087    1.92309278
C    9.56592745    1.98199041    0.95180825
C    10.95456374    1.86042598    0.99240695
C    11.56644841    1.0939404    1.99141673
C    10.7786585    0.45174333    2.94892427
C    9.38594486    0.57973391    2.9172149
H    8.78234507    0.07123662    3.67052957
H    11.24645901    -0.1520213    3.72929035
H    12.65349361    0.99553656    2.01897181
H    11.56238226    2.35892288    0.23457147
H    9.10142979    2.56892737    0.15685209
C    6.65418065    3.31411365    1.93142691
C    5.49629335    3.86325689    1.35738358
```

```
C     5.23267155     5.23132378     1.46913463
C     6.12421953     6.06503215     2.1497698
C     7.28049316     5.52496034     2.72239445
C     7.54563011     4.15743878     2.6156675
H     8.45493148     3.7486747     3.06021762
H     7.98194525     6.17133205     3.25407717
H     5.92061775     7.13448955     2.23335407
H     4.32805684     5.64617548     1.01925308
H     4.79647113     3.21018197     0.83181984
H     6.45438895     1.55886715     4.25926486
H     5.44563857     -0.64875458     4.54173785
E = -24.20396822
```

1.9 $Fe(dppen)_2Br_2{\cdot}CH_2Cl_2$ (Low-spin)

```
Fe     5.74648428     0.00031348     -0.00012569
Br     3.5583952     0.866182     0.96199255
P     5.89932685     1.42399207     -1.88354176
P     4.66168247     -1.37103285     -1.51320948
C     8.47925855     1.79747575     -3.02986936
C     9.63396943     2.52803416     -3.32567538
C     9.78366194     3.83324304     -2.8494702
C     8.76742078     4.40836116     -2.08012723
C     7.61041245     3.68183249     -1.78822887
C     7.45508116     2.36622968     -2.25704015
C     3.36017365     2.7713409     -1.9566709
C     2.42265068     3.661858     -2.49130302
C     2.75546938     4.47041534     -3.57930156
C     4.03531061     4.38062654     -4.13702361
C     4.97621097     3.50169441     -3.59857109
C     4.65246014     2.69093149     -2.49284796
C     1.98481154     -1.91758052     -0.76465566
C     0.59641594     -1.82234758     -0.86534445
C     0.01332749     -1.05640154     -1.88085984
C     0.83081161     -0.38758485     -2.79410238
C     2.22297244     -0.48525989     -2.69683275
C     2.8142567     -1.25513738     -1.6845497
C     6.02198266     -3.8287293     -1.04634332
C     6.2368155     -5.20263487     -1.19067559
C     5.34608689     -5.97904871     -1.93635607
C     4.2403161     -5.37303264     -2.54097061
C     4.02423739     -4.00014142     -2.39734271
C     4.91226558     -3.2138899     -1.6429662
C     5.178778     -0.86572148     -3.20343194
C     5.75671696     0.32713587     -3.35645067
H     8.37890816     0.77762021     -3.40045028
H     10.41809299     2.07211171     -3.93340078
H     10.68531861     4.40299167     -3.08288264
H     8.87195956     5.42937461     -1.70808683
H     6.82220945     4.15111412     -1.1987823
```

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H    3.08474781    2.13501303    -1.11475459
H    1.42425113    3.71733626    -2.05199477
H    2.02221791    5.16326274    -3.99727078
H    4.30656356    4.99881972    -4.9953433
H    5.96952368    3.45297165    -4.04619944
H    2.42120877    -2.51771301    0.03323956
H    -0.03336697    -2.34615824    -0.14330485
H    -1.0732694    -0.98250064    -1.95876536
H    0.3878217    0.21314497    -3.59106364
H    2.84502536    0.04490212    -3.41863226
H    6.7303518    -3.22485574    -0.47921012
H    7.10469512    -5.66574259    -0.71614275
H    5.51218563    -7.052345    -2.04760807
H    3.53827288    -5.97033942    -3.12643255
H    3.15195725    -3.54500393    -2.86912402
H    4.98154109    -1.53613721    -4.04598314
H    6.05558038    0.71372888    -4.33625662
Br    7.9341074    -0.86646594    -0.96235277
P    5.59356485    -1.42286723    1.88360169
C    4.03833611    -2.36591972    2.2574589
C    3.01404447    -1.79794426    3.030673
C    1.86004831    -2.52942432    3.32699757
C    1.7113292    -3.83488727    2.85118842
C    2.72790022    -4.4093928    2.0818197
C    3.88405063    -3.68181572    1.78912673
H    4.6726918    -4.15075525    1.20000035
H    2.62423316    -5.43067458    1.71026561
H    0.81027645    -4.40537587    3.08511609
H    1.07574306    -2.07403902    3.93489296
H    3.11369817    -0.77796321    3.40109416
C    6.84090896    -2.68916363    2.4934938
C    8.13312916    -2.76953562    1.95718326
C    9.0708402    -3.65969826    2.49208459
C    8.73827136    -4.46776214    3.58052875
C    7.45847583    -4.3779288    4.13837653
C    6.51735148    -3.49942055    3.59961785
H    5.52403277    -3.45071843    4.04723798
H    7.18743554    -4.99579038    4.99700138
H    9.47167638    -5.16031317    3.99871476
H    10.06917507    -3.71528021    2.05264395
H    8.40824682    -2.13370092    1.11478611
C    5.73566362    -0.32547772    3.35616839
C    6.31390732    0.86722476    3.20301274
P    6.83191137    1.37158007    1.51281452
C    8.67920679    1.25399966    1.68425928
C    9.50943364    1.91401331    0.76332122
C    10.89771896    1.81724809    0.86409593
C    11.47993196    1.05212254    1.88072591
C    10.66167713    0.3855493    2.79491068
C    9.26962851    0.48468036    2.69747606
```

```
H    8.64696861    -0.04387173    3.41992414
H    11.103966    -0.21466395    3.59265048
H    12.56644168    0.97698931    1.9586613
H    11.5281012    2.33920824    0.14124368
H    9.07374192    2.51335278    -0.03554724
C    6.58265943    3.2146821    1.6417408
C    5.47125438    3.8291442    1.04780532
C    5.25698314    5.20317457    1.191689
C    6.14998085    5.98010187    1.93414088
C    7.25741565    5.37445528    2.53604609
C    7.47298971    4.00142386    2.39285686
H    8.34641888    3.54652673    2.86270178
H    7.96112346    5.97214901    3.11910408
H    5.98435348    7.05351412    2.0449762
H    4.387741    5.66599325    0.71936994
H    4.76120228    3.22483084    0.48324963
H    6.51101222    1.53788655    4.0453895
H    5.43643967    -0.71171947    4.33600663
E = -24.17637417
```

1.10 $Fe(dppen)_2Br_2{\cdot}CH_2Cl_2$ (High-spin)

```
Fe    5.74664084    0.00007598    -0.00001092
Br    3.53043366    0.88120284    0.93839479
P    5.85417991    1.54172844    -2.1841939
P    4.5605549    -1.4681736    -1.75383675
C    8.44002759    1.74809891    -3.35406849
C    9.65472665    2.39299756    -3.60583609
C    9.8891103    3.67562864    -3.10274904
C    8.90128464    4.31330163    -2.34416493
C    7.6859143    3.67262976    -2.09445751
C    7.44028198    2.38549825    -2.60407556
C    3.35575436    2.86481799    -2.14417998
C    2.38141082    3.75646471    -2.60457232
C    2.64774132    4.58885791    -3.69377683
C    3.89508422    4.52630363    -4.32551798
C    4.8708401    3.63893186    -3.8679604
C    4.60970414    2.80024515    -2.76900708
C    1.9473766    -2.08170027    -0.95561205
C    0.55573113    -1.9925094    -0.9788902
C    -0.08315181    -1.1852309    -1.92780082
C    0.68051616    -0.46925708    -2.85243094
C    2.07646418    -0.56085613    -2.83558249
C    2.72083013    -1.37295049    -1.89126061
C    5.83267529    -3.91159187    -1.15126368
C    6.08587685    -5.28037277    -1.28760608
C    5.36971353    -6.03559868    -2.2194568
C    4.39536653    -5.419891    -3.0135597
C    4.1372164    -4.0546781    -2.87465731
C    4.85732522    -3.28805112    -1.94233457
```

```
C     5.10013123     -0.8587627     -3.40059228
C     5.66501281     0.34527866     -3.5687416
H     8.27752305     0.73973538     -3.73719265
H     10.42097462     1.88737204     -4.19703571
H     10.83842034     4.17738811     -3.30024078
H     9.07605057     5.3149482     -1.94662885
H     6.92244397     4.18376287     -1.50400139
H     3.14204633     2.21688042     -1.29108546
H     1.41115525     3.79916293     -2.10526643
H     1.88683496     5.28502643     -4.05272289
H     4.11001225     5.17136534     -5.18008637
H     5.84008069     3.60381189     -4.36827237
H     2.43266799     -2.70358901     -0.20052101
H     -0.03355401     -2.55037985     -0.24807106
H     -1.17256124     -1.11406681     -1.94331995
H     0.19104541     0.16378695     -3.59535877
H     2.66073836     0.00546812     -3.56268895
H     6.40832251     -3.31794064     -0.43883833
H     6.84691548     -5.75546809     -0.66534742
H     5.56803733     -7.10365982     -2.32806232
H     3.8317025     -6.00604061     -3.74226385
H     3.3654945     -3.58737172     -3.48991543
H     4.95685276     -1.52410381     -4.25975302
H     5.97419935     0.67387882     -4.56815993
Br     7.96283857     -0.88165349     -0.93765954
P     5.63889462     -1.54085368     2.18460458
C     4.05295673     -2.38497469     2.60440342
C     3.05324222     -1.74874655     3.35540095
C     1.83862024     -2.39411746     3.60635798
C     1.60423131     -3.67596668     3.10128182
C     2.59201297     -4.31243663     2.34161353
C     3.80733348     -3.67133603     2.09282938
H     4.5707333     -4.18143177     1.50136073
H     2.4172006     -5.31342674     1.94243229
H     0.65494697     -4.17805122     3.298058
H     1.07234418     -1.8893839     4.19827747
H     3.2155776     -0.74081492     3.73975169
C     6.88351331     -2.79908002     2.76981885
C     8.13704613     -2.8646467     2.14428203
C     9.11145183     -3.75598014     2.60515799
C     8.84552911     -4.58708314     3.6954517
C     7.59852519     -4.52360748     4.32779114
C     6.62272615     -3.63650319     3.86981781
H     5.65375838     -3.60059177     4.37060546
H     7.38392919     -5.16769866     5.18317744
H     9.60648943     -5.28299497     4.05477982
H     10.08144539     -3.79942044     2.10540182
H     8.35043123     -2.21759212     1.29043162
C     5.82783004     -0.343847     3.56872251
C     6.39295139     0.86003305     3.40025316
```

```
P     6.93336713     1.46834645     1.7533805
C     8.77297073     1.37138653     1.89129028
C     9.54729656     2.07964766     0.95597314
C     10.93887245     1.98938814     0.97970224
C     11.57681626     1.18157904     1.92878736
C     10.81227707     0.46607615     2.8530656
C     9.41639688     0.55871795     2.8357552
H     8.83145689     -0.00740316     3.56247155
H     11.30102151     -0.16746261     3.59605089
H     12.66616638     1.10962809     1.94472927
H     11.52881203     2.54680727     0.24906662
H     9.06273208     2.70193466     0.20074092
C     6.63808283     3.28850446     1.9413393
C     5.66254001     3.91242428     1.1508177
C     5.41016604     5.28136957     1.28707922
C     6.12737007     6.03638257     2.21830653
C     7.10189433     5.42028296     3.01187905
C     7.35920024     4.05490156     2.87306408
H     8.13099565     3.58725959     3.48796548
H     7.66629451     6.00624755     3.74016366
H     5.92972528     7.10457904     2.32685046
H     4.64892941     5.75674715     0.66528553
H     5.08598145     3.31891476     0.43901916
H     6.5362729     1.52564036     4.25919461
H     5.51862476     -0.67209861     4.56825308
E = -24.16380394
```

1.11 $Fe(dppen)_2Cl_2 \cdot CH_2Cl_2$ (Low-spin)

```
Fe     5.74777739     -0.00022502     -0.00062649
Cl     3.69687077     0.80102304     0.88611414
P     5.90425408     1.41380653     -1.86493593
P     4.6631718     -1.36580063     -1.51207847
C     8.51330217     1.75498989     -2.93229222
C     9.68470382     2.46915969     -3.19990703
C     9.82436502     3.78609301     -2.75319609
C     8.78309305     4.3883846     -2.03987852
C     7.60955904     3.67815778     -1.77528731
C     7.46294882     2.35250223     -2.21825604
C     3.36470441     2.72849953     -1.87753476
C     2.40410074     3.61135246     -2.3824783
C     2.70241822     4.43410246     -3.47019801
C     3.97045327     4.36799879     -4.05788761
C     4.93469492     3.49593036     -3.55038227
C     4.64448725     2.67071412     -2.44672718
C     1.97902867     -1.85166454     -0.75443242
C     0.5922899     -1.73857633     -0.86112982
C     0.02250504     -0.99588526     -1.90108243
C     0.8515447     -0.36781084     -2.83268066
C     2.24176311     -0.48400795     -2.72973112
```

```
C    2.82003067    -1.23191534    -1.6934848
C    6.08395962    -3.77908727    -1.08780809
C    6.31765864    -5.15201965    -1.20500145
C    5.38822797    -5.97107777    -1.85196761
C    4.22473044    -5.40842873    -2.38554742
C    3.9894257    -4.03560651    -2.27095539
C    4.91614521    -3.20774753    -1.61473605
C    5.20729593    -0.87358787    -3.19746344
C    5.78520939    0.32064103    -3.3434402
H    8.41964384    0.72440559    -3.27425593
H    10.49020761    1.99177456    -3.76162931
H    10.73957215    4.34309253    -2.9639367
H    8.88197485    5.41759042    -1.68955351
H    6.80305593    4.16531722    -1.22582612
H    3.12248305    2.07917307    -1.03469359
H    1.41506526    3.65029647    -1.92083054
H    1.95072166    5.12085896    -3.86498278
H    4.21307627    4.99920662    -4.91539549
H    5.91897835    3.46334727    -4.01955049
H    2.40473048    -2.4328294    0.06277531
H    -0.04620687    -2.23018179    -0.12428482
H    -1.06270647    -0.90748335    -1.98294165
H    0.41927918    0.21616021    -3.64779282
H    2.87310954    0.0155409    -3.46509197
H    6.81805217    -3.13870326    -0.59860297
H    7.23082633    -5.58147683    -0.78703001
H    5.56887919    -7.04413064    -1.94121388
H    3.49308625    -6.03989987    -2.89366102
H    3.07387902    -3.61349466    -2.68795904
H    5.02663184    -1.54804993    -4.04056486
H    6.10264567    0.70526694    -4.3183451
Cl    7.79841272    -0.80099333    -0.88827526
P    5.59026393    -1.41378171    1.86391739
C    4.03128086    -2.35259009    2.21570549
C    2.97994189    -1.75503926    2.92823709
C    1.808363    -2.46937121    3.19465065
C    1.66940346    -3.78637754    2.74793666
C    2.71145452    -4.38851554    2.03562676
C    3.88536696    -3.67830466    1.7726778
H    4.69230542    -4.16520883    1.22364734
H    2.61303644    -5.41771319    1.68513627
H    0.75401519    -4.34346466    2.9576522
H    1.00216755    -1.99205345    3.75543706
H    3.07301476    -0.72433877    3.27002218
C    6.84927343    -2.67021076    2.44862376
C    8.1302248    -2.72845673    1.88216792
C    9.08990504    -3.61058082    2.3901605
C    8.78940759    -4.43224177    3.47809259
C    7.52020283    -4.36551254    4.06318154
C    6.55697439    -3.49400689    3.55279003
```

```
H     5.57179558     -3.46084647     4.02003356
H     7.27591733     -4.99571387     4.92095929
H     9.54033732     -5.11853151     3.87514486
H     10.07996287     -3.64977858     1.93073068
H     8.37430631     -2.07964468     1.03948574
C     5.70749386     -0.31993799     3.34204926
C     6.2859872     0.87403405     3.19619392
P     6.83184024     1.36543693     1.51112519
C     8.67477194     1.23110551     1.69433106
C     9.51693186     1.84965868     0.75554535
C     10.90352251     1.73623293     0.86380048
C     11.47199177     0.99412578     1.90488446
C     10.64179554     0.36718585     2.83620132
C     9.25173813     0.48401825     2.73189338
H     8.61946942     -0.01461418     3.46708333
H     11.07301302     -0.21632228     3.65220033
H     12.55708961     0.90539543     1.98789911
H     11.54294076     2.22707072     0.12724173
H     9.09228859     2.43047008     -0.06245237
C     6.57896503     3.20746326     1.61281049
C     5.41124254     3.77843478     1.08527743
C     5.17751961     5.15144027     1.20161499
C     6.10678916     5.97086992     1.84835144
C     7.27011772     5.40853268     2.38263538
C     7.50544163     4.03563498     2.26895088
H     8.42088271     3.61374177     2.68640916
H     8.0016175     6.04031306     2.89057296
H     5.92609615     7.04396925     1.93695101
H     4.2645123     5.58067934     0.78307156
H     4.67737826     3.13777354     0.59607731
H     6.46586172     1.54883947     4.03918658
H     5.38865799     -0.70396758     4.31673143
E = -24.22113127
```

1.12 $Fe(dppen)_2Cl_2 \cdot CH_2Cl_2$ (High-spin)

```
Fe     5.74658106     -0.00061598     0.00019709
Cl     3.66608027     0.80271584     0.84075725
P     5.84751319     1.515125     -2.16003943
P     4.55868795     -1.4888188     -1.7664829
C     8.46569725     1.74066984     -3.2420124
C     9.68586483     2.39160583     -3.44729039
C     9.89177791     3.67800555     -2.94152643
C     8.87072473     4.31231823     -2.2250919
C     7.65051021     3.66528754     -2.02015528
C     7.43320646     2.375246     -2.53572634
C     3.34940867     2.82044305     -2.09326591
C     2.36567517     3.70742014     -2.54202334
C     2.61433641     4.54016388     -3.635158
C     3.85340817     4.4836319     -4.28365435
```

```
C    4.83843346    3.6001272    -3.83911633
C    4.59436863    2.76123064    -2.73673659
C    1.92638837    -1.99063577    -0.95950106
C    0.53768099    -1.87011812    -1.00115372
C    -0.07351793    -1.09761907    -1.99609761
C    0.71504585    -0.44854268    -2.94833852
C    2.10794607    -0.57488311    -2.91501491
C    2.72527624    -1.35292248    -1.92505696
C    5.98233675    -3.86986571    -1.33932253
C    6.24166526    -5.23896467    -1.4495132
C    5.35702099    -6.06715037    -2.14582239
C    4.21269781    -5.52063071    -2.73626925
C    3.95360004    -4.15167364    -2.63340325
C    4.83732588    -3.3141854    -1.93225889
C    5.14464498    -0.88789804    -3.40021101
C    5.70563271    0.32132667    -3.55320374
H    8.32390039    0.72963695    -3.62685905
H    10.47851505    1.88813441    -4.00465545
H    10.84497209    4.18521365    -3.10351607
H    9.02531176    5.31555846    -1.82326929
H    6.86189361    4.17072848    -1.45792583
H    3.15369246    2.17109364    -1.23693457
H    1.40168982    3.74740434    -2.03060323
H    1.84567579    5.23292375    -3.98414578
H    4.05386456    5.13020435    -5.14064418
H    5.80161649    3.56818295    -4.35157245
H    2.39038112    -2.5829003    -0.16822147
H    -0.07134371    -2.37464991    -0.24826371
H    -1.16063922    -1.00073421    -2.02501769
H    0.2475943    0.15923638    -3.72575721
H    2.71176392    -0.06165234    -3.66490699
H    6.67583072    -3.22131625    -0.79992119
H    7.13596393    -5.65962053    -0.98476257
H    5.55647101    -7.13749091    -2.22749533
H    3.51714264    -6.16270021    -3.28073556
H    3.05375035    -3.7381074    -3.09265845
H    5.03354373    -1.55698049    -4.26124769
H    6.04461799    0.64859069    -4.543519
Cl    7.82698777    -0.80437441    -0.84000321
P    5.64689969    -1.51561856    2.16091165
C    4.06244933    -2.3776401    2.53757105
C    3.02941193    -1.74490087    3.24466511
C    1.81093881    -2.39841159    3.45179593
C    1.60754222    -3.68586609    2.94770886
C    2.62933072    -4.31857621    2.23090229
C    3.84750502    -3.66857709    2.02326571
H    4.63685164    -4.17292034    1.46107546
H    2.47685158    -5.32283522    1.8308069
H    0.65580876    -4.19524239    3.11147279
H    1.01781219    -1.89632262    4.00972599
```

```
H    3.16942099    -0.7333159    3.6287174
C    6.90131623    -2.76043736    2.73770864
C    8.14580455    -2.81939084    2.09336794
C    9.13030827    -3.70557323    2.54201434
C    8.8827657    -4.53785572    3.63575853
C    7.64402256    -4.48174881    4.28493276
C    6.65827644    -3.59893123    3.84061609
H    5.6953196    -3.56733671    4.35352182
H    7.44441177    -5.12808148    5.14230154
H    9.65200767    -5.23003393    3.98461812
H    10.09398042    -3.74535121    2.02998506
H    8.34054097    -2.17048116    1.23648717
C    5.78840701    -0.32116736    3.55355997
C    6.34871355    0.8883212    3.40004192
P    6.93393771    1.4890381    1.76598376
C    8.7676182    1.35528041    1.92327657
C    9.56478545    1.9922293    0.95577658
C    10.95367622    1.87339196    0.99613223
C    11.56682605    1.10353538    1.99191774
C    10.78001304    0.45526933    2.94616466
C    9.38690796    0.5798062    2.91403026
H    8.78450409    0.0672646    3.6655177
H    11.24900894    -0.15044904    3.72426193
H    12.65409317    1.00805621    2.01992786
H    11.56130505    2.37729097    0.24169527
H    9.09924805    2.5825882    0.16395448
C    6.65354571    3.31421982    1.93075601
C    5.50687851    3.8678923    1.33914093
C    5.24590856    5.23672285    1.44869374
C    6.13046994    6.06658868    2.14311918
C    7.27637184    5.52203215    2.73231678
C    7.53726879    4.15338211    2.6298856
H    8.43820621    3.74130083    3.0883314
H    7.97177347    6.16540125    3.27544058
H    5.92969045    7.13671565    2.22433152
H    4.35035796    5.65585506    0.98497539
H    4.81354085    3.21803848    0.80110578
H    6.45918435    1.55793303    4.26074413
H    5.44996481    -0.64826386    4.54411319
E = -24.20631742
```