Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting information for "Subtle effects control the polymerisation mechanism in α-diimine iron catalysts"

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23 May 2011

Molecular structures of the studied complexes

The following pages list the molecular structures in standard XYZ format, with units in Ångström. All structures have been optimized at BP86-D/def2-TZVP level, using a simulated chloroform solution *via* the COSMO continuum model with ε=4.8 and solvent radius 3.17 Å, using TURBOMOLE V6-1.

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 63
# Fe(II)-Cl2, R"=PhF, S=2
Fe         -1.35528        1.33281       -1.07222
Cl         -1.02778        0.97436       -3.23989
Cl         -2.74824        2.90755       -0.42072
N          -1.33487       -0.50894       -0.27587
C          -0.10629       -0.92572       -0.05579
C          -2.52367       -1.33454       -0.09795
H          -2.25380       -2.32563        0.30379
C          -3.45390       -0.63176        0.90517
H          -3.67453        0.37898        0.52109
H          -2.92940       -0.51380        1.86575
C          -4.75493       -1.42494        1.08150
H          -4.52253       -2.41167        1.51985
H          -5.41236       -0.90069        1.79191
C          -5.46489       -1.62724       -0.26350
H          -5.76381       -0.64304       -0.66448
H          -6.38312       -2.21898       -0.12620
C          -4.53363       -2.31444       -1.27097
H          -5.03205       -2.42736       -2.24587
H          -4.29256       -3.32946       -0.90830
C          -3.23469       -1.52025       -1.44749
H          -2.55727       -2.01417       -2.16055
H          -3.45428       -0.51953       -1.85815
C           0.24945       -2.33793        0.19901
C           1.00665       -2.70353        1.32584
H           1.34021       -1.93663        2.02414
C           1.33305       -4.03795        1.56340
H           1.90965       -4.33776        2.43802
C           0.90529       -4.99687        0.64796
F           1.22994       -6.29796        0.86698
C           0.15931       -4.67499       -0.48322
H          -0.14779       -5.45757       -1.17647
C          -0.17110       -3.33695       -0.69672
H          -0.74884       -3.05630       -1.57777
N           0.47939        1.35506       -0.24933
C           0.92636        0.13337       -0.04579
C           1.31259        2.55016       -0.17569
H           2.38227        2.27972       -0.16203
C           0.97571        3.30587        1.12292
H          -0.10091        3.54526        1.10405
H           1.15330        2.65151        1.99101
C           1.80465        4.59217        1.22512
H           2.87535        4.32868        1.28959
H           1.54417        5.12633        2.15177
C           1.58074        5.49108        0.00171
H           0.52634        5.81728       -0.01564
H           2.20396        6.39586        0.07422
C           1.88878        4.73199       -1.29590
H           1.69223        5.36790       -2.17244
H           2.96146        4.46951       -1.31810
C           1.05350        3.44975       -1.39308
H           1.27240        2.89241       -2.31521
H          -0.02012        3.70842       -1.41095
C           2.34683       -0.21670        0.17493
C           3.08631        0.36475        1.21910
H           2.60675        1.08354        1.88353
C           4.41980        0.01320        1.43232
H           5.00197        0.44624        2.24527
C           5.00124       -0.91869        0.57654
F           6.30000       -1.26490        0.77495
C           4.30398       -1.51197       -0.47342
H           4.80175       -2.23312       -1.12108
C           2.96824       -1.16058       -0.66173
H           2.39900       -1.62117       -1.46897
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 63
# Fe(II)-Cl2, R"=PhF, S=1
Fe         -2.32745        2.33005       -0.62878
Cl         -3.27332        2.74029       -2.57064
Cl         -3.19568        3.73438        0.82318
N          -2.17766        0.46783       -0.55476
C          -0.97539       -0.02602       -0.20858
C          -3.37896       -0.37969       -0.60906
H          -3.15233       -1.32643       -0.08955
C          -4.54349        0.29444        0.13554
H          -4.80028        1.23549       -0.38053
H          -4.22933        0.55021        1.15832
C          -5.76588       -0.63358        0.14565
H          -5.51661       -1.54970        0.70993
H          -6.59717       -0.14171        0.67307
C          -6.18206       -1.01705       -1.28048
H          -6.50871       -0.10862       -1.81576
H          -7.03772       -1.70951       -1.25492
C          -5.00730       -1.64701       -2.04116
H          -5.29942       -1.88386       -3.07571
H          -4.72736       -2.59828       -1.55393
C          -3.79604       -0.70508       -2.05115
H          -2.95568       -1.14916       -2.60390
H          -4.05503        0.23580       -2.55838
C          -0.68532       -1.44576        0.07111
C          -0.03527       -1.78649        1.27256
H           0.22452       -1.00076        1.98162
C           0.27815       -3.11161        1.56976
H           0.77283       -3.38642        2.50101
C          -0.05994       -4.09415        0.64227
C          -0.69716       -3.80025       -0.56021
H          -0.93382       -4.59926       -1.26238
C          -1.00833       -2.46886       -0.83743
H          -1.48834       -2.22045       -1.78211
N          -0.51660        2.23037       -0.17348
C           0.00714        0.99713       -0.05519
C           0.32971        3.43313       -0.21275
H           1.37047        3.11252       -0.39048
C           0.28233        4.21944        1.10590
H          -0.74876        4.56733        1.26591
H           0.53761        3.56624        1.95280
C           1.23553        5.41927        1.02954
H           2.27062        5.05669        0.89608
H           1.20482        5.97651        1.97839
C           0.86626        6.33514       -0.14523
H          -0.13868        6.75601        0.03182
H           1.57007        7.17946       -0.20945
C           0.85442        5.55204       -1.46456
H           0.54605        6.20114       -2.29805
H           1.87708        5.19853       -1.68613
C          -0.08545        4.34154       -1.38199
H          -0.07568        3.76518       -2.31897
H          -1.11915        4.68949       -1.21423
C           1.43942        0.69276        0.12942
C           2.20212        1.27419        1.15742
H           1.73444        1.97461        1.84688
C           3.54725        0.94558        1.32769
H           4.14403        1.38242        2.12800
C           4.12010        0.02787        0.45133
C           3.40108       -0.57126       -0.58016
H           3.89032       -1.28141       -1.24636
C           2.05690       -0.23510       -0.73079
H           1.47386       -0.69556       -1.52804
F           5.43014       -0.29787        0.61000
F           0.24610       -5.38887        0.92059
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 71
# Fe(II)-Cl2, R"=PhOMe, S=2
Fe         -1.35636        1.33540       -1.05762
Cl         -1.05479        1.03019       -3.24248
Cl         -2.72996        2.91685       -0.35949
N          -1.33430       -0.52177       -0.29348
C          -0.10880       -0.94665       -0.06929
C          -2.52816       -1.34042       -0.11670
H          -2.26513       -2.33396        0.28337
C          -3.45352       -0.63418        0.88827
H          -3.66684        0.37956        0.50778
H          -2.92763       -0.52252        1.84892
C          -4.76059       -1.41766        1.06346
H          -4.53564       -2.40766        1.49857
H          -5.41427       -0.89077        1.77559
C          -5.47256       -1.61100       -0.28188
H          -5.76310       -0.62324       -0.68041
H          -6.39592       -2.19530       -0.14592
C          -4.54681       -2.30317       -1.29110
H          -5.04686       -2.41050       -2.26594
H          -4.31361       -3.32077       -0.93028
C          -3.24178       -1.51861       -1.46561
H          -2.56859       -2.01614       -2.18021
H          -3.45313       -0.51527       -1.87429
C           0.24020       -2.35697        0.18384
C           1.02569       -2.73069        1.28542
H           1.38837       -1.96528        1.97111
C           1.35107       -4.06560        1.52385
H           1.95177       -4.32348        2.39396
C           0.90414       -5.05821        0.63478
O           1.17971       -6.38500        0.76574
C           0.12068       -4.69810       -0.47790
H          -0.21216       -5.47727       -1.16453
C          -0.21019       -3.36722       -0.69051
H          -0.81019       -3.09183       -1.55853
N           0.48089        1.33763       -0.23705
C           0.92992        0.11277       -0.05094
C           1.31900        2.52925       -0.16262
H           2.38776        2.25445       -0.16692
C           1.00464        3.27415        1.14756
H          -0.07030        3.52191        1.14402
H           1.18710        2.60965        2.00690
C           1.84439        4.55309        1.25343
H           2.91394        4.28075        1.30075
H           1.60078        5.07997        2.18896
C           1.61170        5.46673        0.04251
H           0.55958        5.80076        0.04269
H           2.24264        6.36625        0.11613
C           1.89603        4.71883       -1.26705
H           1.69343        5.36615       -2.13396
H           2.96631        4.44809       -1.30609
C           1.04905        3.44424       -1.36602
H           1.25009        2.89535       -2.29724
H          -0.02240        3.71178       -1.36649
C           2.34675       -0.24405        0.15665
C           3.11344        0.34477        1.17330
H           2.65434        1.08021        1.83438
C           4.44679       -0.01469        1.37868
H           5.00911        0.44946        2.18670
C           5.04116       -0.97383        0.54167
O           6.33195       -1.39180        0.65038
C           4.28561       -1.56754       -0.48745
H           4.76123       -2.30746       -1.13210
C           2.95651       -1.21413       -0.66555
H           2.37398       -1.68998       -1.45446
C           7.12700       -0.80325        1.69199
C           1.98592       -6.78063        1.88725
H           6.69163       -1.01590        2.68220
H           7.20566        0.28744        1.55298
H           8.11707       -1.26513        1.60912
H           1.49181       -6.51424        2.83582
H           2.97725       -6.30056        1.84228
H           2.09134       -7.86843        1.80994
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 71
# Fe(II)-Cl2, R"=PhOMe, S=1
Fe         -1.43004        1.43994       -0.65350
Cl         -2.28468        1.81844       -2.65202
Cl         -2.36815        2.88504        0.72399
N          -1.29802       -0.42292       -0.53741
C          -0.12947       -0.92088       -0.09332
C          -2.49961       -1.26196       -0.66293
H          -2.32232       -2.19764       -0.10565
C          -3.71262       -0.56354       -0.02637
H          -3.92209        0.36642       -0.58217
H          -3.47586       -0.28553        1.01145
C          -4.93913       -1.48430       -0.08815
H          -4.74046       -2.38802        0.51493
H          -5.80553       -0.97583        0.36164
C          -5.24747       -1.90043       -1.53260
H          -5.52502       -1.00335       -2.11292
H          -6.10793       -2.58722       -1.55646
C          -4.02240       -2.55503       -2.18582
H          -4.23693       -2.81601       -3.23360
H          -3.78684       -3.49532       -1.65551
C          -2.80812       -1.61925       -2.12478
H          -1.93044       -2.07896       -2.60177
H          -3.02214       -0.68901       -2.67094
C           0.12421       -2.33121        0.24636
C           0.72043       -2.64401        1.48003
H           0.96820       -1.83810        2.17096
C           1.00338       -3.96024        1.84202
H           1.45674       -4.16425        2.81025
C           0.69915       -5.00396        0.95160
O           0.94114       -6.32106        1.20067
C           0.10847       -4.70840       -0.29066
H          -0.11228       -5.52559       -0.97841
C          -0.17501       -3.39257       -0.63149
H          -0.61400       -3.17990       -1.60458
N           0.34738        1.33364       -0.07753
C           0.85348        0.10019        0.10283
C           1.20348        2.52966       -0.09565
H           2.25052        2.19798       -0.20054
C           1.08321        3.35345        1.19508
H           0.04825        3.71580        1.28024
H           1.27672        2.72179        2.07411
C           2.05296        4.54117        1.14543
H           3.09002        4.16449        1.08455
H           1.97213        5.12529        2.07513
C           1.76593        5.42804       -0.07389
H           0.75720        5.86369        0.03132
H           2.48217        6.26330       -0.11850
C           1.82307        4.60929       -1.37033
H           1.57183        5.23884       -2.23746
H           2.85332        4.24064       -1.52146
C           0.86764        3.40950       -1.31120
H           0.92753        2.80798       -2.23044
H          -0.17082        3.77090       -1.21551
C           2.26494       -0.20982        0.38577
C           2.98479        0.41189        1.41730
H           2.49443        1.15445        2.04455
C           4.31456        0.07993        1.68267
H           4.83711        0.57514        2.49899
C           4.95529       -0.89437        0.89971
O           6.24710       -1.29007        1.07125
C           4.24795       -1.52787       -0.13948
H           4.75724       -2.28016       -0.74290
C           2.92476       -1.19260       -0.38377
H           2.38231       -1.69442       -1.18503
C           6.99108       -0.65882        2.12518
C           1.55099       -6.64854        2.45941
H           6.51987       -0.84909        3.10351
H           7.05908        0.42860        1.95732
H           7.99053       -1.10692        2.09546
H           0.91069       -6.32897        3.29780
H           2.53953       -6.16892        2.54964
H           1.66055       -7.73872        2.46357
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 79
# Fe(II)-Cl2, R"=PhNMe2, S=2
Fe         -2.20412        2.21821       -1.36868
Cl         -1.79491        1.93892       -3.54756
Cl         -3.63779        3.79044       -0.74506
N          -2.19491        0.35776       -0.60833
C          -0.98016       -0.05294       -0.30283
C          -3.39086       -0.46745       -0.48457
H          -3.14494       -1.45288       -0.05450
C          -4.37588        0.24559        0.45657
H          -4.57480        1.25239        0.05057
H          -3.90425        0.37560        1.44285
C          -5.68564       -0.54439        0.57229
H          -5.47863       -1.52671        1.03339
H          -6.38152       -0.01263        1.23962
C          -6.32151       -0.76250       -0.80701
H          -6.59488        0.21760       -1.23562
H          -7.24803       -1.35051       -0.71359
C          -5.33724       -1.46288       -1.75336
H          -5.78295       -1.58851       -2.75229
H          -5.11842       -2.47343       -1.36430
C          -4.02913       -0.67220       -1.86670
H          -3.31498       -1.17574       -2.53601
H          -4.22263        0.32357       -2.30187
C          -0.63274       -1.45089       -0.01283
C           0.13740       -1.81021        1.11135
H           0.48943       -1.03262        1.78896
C           0.45860       -3.13197        1.38017
H           1.04909       -3.35952        2.26553
C           0.03649       -4.17776        0.51410
C          -0.72640       -3.81317       -0.62892
H          -1.05246       -4.57342       -1.33611
C          -1.05664       -2.48719       -0.86789
H          -1.63477       -2.23603       -1.75805
N          -0.41844        2.24382       -0.43834
C           0.04401        1.02445       -0.23176
C           0.40366        3.44454       -0.33613
H           1.47525        3.18177       -0.30565
C           0.04051        4.18898        0.96142
H          -1.03437        4.43370        0.91814
H           0.19221        3.52557        1.82757
C           0.87197        5.47038        1.09806
H           1.94001        5.20044        1.18180
H           0.59539        5.99710        2.02470
C           0.67900        6.38397       -0.12001
H          -0.37327        6.71596       -0.15506
H           1.30532        7.28493       -0.02512
C           1.00801        5.63697       -1.41981
H           0.83291        6.28493       -2.29244
H           2.07985        5.36917       -1.42287
C           0.16861        4.35952       -1.54680
H           0.40123        3.81191       -2.47146
H          -0.90315        4.62296       -1.58232
C           1.44985        0.68772        0.03697
C           2.19129        1.31562        1.05633
H           1.71099        2.06966        1.68045
C           3.50949        0.96845        1.31953
H           4.03118        1.46355        2.13631
C           4.17031       -0.02274        0.54407
C           3.42086       -0.65583       -0.48538
H           3.87897       -1.42747       -1.10103
C           2.09816       -0.31182       -0.71652
H           1.54575       -0.82762       -1.50205
N           5.47772       -0.35831        0.78178
N           0.35531       -5.48613        0.76911
C           6.09346       -1.45059        0.04191
C           6.18792        0.23704        1.90466
C          -0.00588       -6.52166       -0.18871
C           1.23026       -5.81620        1.88477
H           6.06616       -1.25498       -1.04281
H           5.57787       -2.41060        0.22752
H           7.14044       -1.54705        0.35045
H           5.71272       -0.01711        2.86985
H           6.21065        1.33587        1.81640
H           7.21997       -0.13120        1.91212
H           0.47809       -6.35808       -1.16889
H          -1.09657       -6.54526       -0.34823
H           0.30825       -7.49621        0.20156
H           0.80313       -5.46188        2.83755
H           2.22968       -5.35825        1.76861
H           1.34541       -6.90449        1.94039
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 79
# Fe(II)-Cl2, R"=PhNMe2, S=1
Fe         -2.33143        2.33373       -0.62900
Cl         -3.32092        2.74120       -2.56876
Cl         -3.19438        3.77670        0.81358
N          -2.17398        0.46769       -0.56614
C          -0.97577       -0.03294       -0.20866
C          -3.37790       -0.37429       -0.63041
H          -3.16229       -1.31974       -0.10399
C          -4.54997        0.30522        0.09665
H          -4.80073        1.24369       -0.42719
H          -4.24670        0.56689        1.12148
C          -5.77344       -0.62183        0.10034
H          -5.53022       -1.53491        0.67256
H          -6.61128       -0.12758        0.61557
C          -6.17504       -1.01499       -1.32762
H          -6.49552       -0.10957       -1.87182
H          -7.03166       -1.70693       -1.30661
C          -4.99245       -1.64895       -2.07336
H          -5.27592       -1.89295       -3.10898
H          -4.71648       -2.59696       -1.57698
C          -3.78233       -0.70594       -2.07489
H          -2.93588       -1.14916       -2.61939
H          -4.03767        0.23374       -2.58631
C          -0.69283       -1.44356        0.08319
C           0.03388       -1.78341        1.24378
H           0.36391       -0.98900        1.91339
C           0.34515       -3.09785        1.55515
H           0.90585       -3.30363        2.46497
C          -0.05310       -4.16379        0.70315
C          -0.76900       -3.82215       -0.47536
H          -1.07372       -4.59735       -1.17593
C          -1.08065       -2.50004       -0.76303
H          -1.61419       -2.28045       -1.68619
N          -0.52052        2.22923       -0.15883
C           0.01263        0.99704       -0.05088
C           0.31826        3.43664       -0.19228
H           1.35984        3.12450       -0.37973
C           0.27667        4.21316        1.13249
H          -0.75407        4.56000        1.29744
H           0.53244        3.55270        1.97389
C           1.23006        5.41296        1.06287
H           2.26407        5.05035        0.91923
H           1.20653        5.96350        2.01617
C           0.85418        6.33912       -0.10211
H          -0.14974        6.75808        0.08542
H           1.55749        7.18447       -0.16373
C           0.83243        5.56773       -1.42853
H           0.51917        6.22558       -2.25361
H           1.85392        5.21646       -1.65994
C          -0.10617        4.35570       -1.34952
H          -0.10208        3.78794       -2.29209
H          -1.13914        4.70128       -1.17212
C           1.43953        0.69620        0.11750
C           2.25381        1.32684        1.07773
H           1.82156        2.07430        1.74084
C           3.59338        0.99674        1.23401
H           4.17080        1.49970        2.00742
C           4.20306        0.01102        0.41256
C           3.38077       -0.63164       -0.55263
H           3.79522       -1.40238       -1.19975
C           2.04247       -0.29546       -0.68482
H           1.43767       -0.81532       -1.42798
N           5.53019       -0.30957        0.54685
N           0.24431       -5.46853        1.00522
C           6.09058       -1.41219       -0.22076
C           6.31289        0.28090        1.62294
C          -0.07357       -6.52311        0.05345
C           1.08732       -5.77274        2.15230
H           5.97176       -1.23707       -1.30267
H           5.60066       -2.37274        0.02427
H           7.16068       -1.49521        0.00045
H           5.91628        0.00578        2.61775
H           6.31171        1.38086        1.54950
H           7.34856       -0.06930        1.54668
H           0.46287       -6.38728       -0.90382
H          -1.15435       -6.54216       -0.16316
H           0.21002       -7.49071        0.48277
H           0.63989       -5.38413        3.08191
H           2.09527       -5.32999        2.04894
H           1.18730       -6.86012        2.24515
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 64
# Fe(III)-Cl3, R"=PhF, S=5/2
Fe         -1.55400        1.67643       -0.96951
Cl         -1.44362        0.82874       -3.08810
Cl         -2.60800        1.89015        1.04382
Cl         -1.97016        3.80841       -1.61491
N          -1.41221       -0.47361       -0.40495
C          -0.21801       -0.84738       -0.09570
C          -2.55402       -1.39584       -0.36996
H          -2.27067       -2.35010       -0.84346
C          -2.91563       -1.69191        1.10326
H          -3.16027       -0.73528        1.58893
H          -2.03973       -2.11953        1.61264
C          -4.10983       -2.64967        1.17702
H          -3.82904       -3.61752        0.72504
H          -4.35733       -2.84143        2.23268
C          -5.32154       -2.07797        0.43066
H          -5.64230       -1.14529        0.92639
H          -6.16640       -2.78269        0.47547
C          -4.95665       -1.77206       -1.02675
H          -5.81438       -1.33470       -1.55961
H          -4.70298       -2.71676       -1.54044
C          -3.75901       -0.81730       -1.11766
H          -3.49055       -0.63176       -2.16550
H          -4.02055        0.15138       -0.65828
C           0.17448       -2.25070        0.18805
C           0.08771       -3.20958       -0.83279
H          -0.26024       -2.91412       -1.82327
C           0.46566       -4.53214       -0.59664
H           0.41686       -5.28840       -1.37953
C           0.91560       -4.87175        0.67681
F           1.28051       -6.15723        0.91721
C           1.01124       -3.94586        1.71358
H           1.36928       -4.25863        2.69390
C           0.64621       -2.62527        1.45575
H           0.72685       -1.87950        2.24654
N           0.46093        1.42766       -0.39689
C           0.81594        0.23587       -0.02285
C           1.40567        2.54496       -0.46137
H           2.40884        2.20123       -0.16283
C           0.97294        3.65051        0.51367
H          -0.05250        3.96370        0.26596
H           0.95801        3.24347        1.53709
C           1.92621        4.84747        0.41064
H           2.93552        4.54186        0.73942
H           1.58751        5.64203        1.09273
C           2.00450        5.36590       -1.03140
H           1.00673        5.72022       -1.34193
H           2.69452        6.22158       -1.09159
C           2.45758        4.24900       -1.98067
H           2.50388        4.61458       -3.01767
H           3.47693        3.92822       -1.70114
C           1.50598        3.04763       -1.91121
H           1.85889        2.22408       -2.55031
H           0.50764        3.34158       -2.26463
C           2.16062       -0.10184        0.49689
C           2.94411       -1.09009       -0.12193
H           2.57072       -1.60491       -1.00641
C           4.20182       -1.41429        0.38364
H           4.83103       -2.16629       -0.09119
C           4.64374       -0.75678        1.52982
F           5.85828       -1.08141        2.03769
C           3.88857        0.21889        2.17738
H           4.27330        0.70222        3.07475
C           2.64362        0.55001        1.64489
H           2.03121        1.31182        2.12874
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 64
# Fe(III)-Cl3, R"=PhF, S=3/2
Fe         -1.48076        1.41035       -1.10979
Cl         -1.97395        3.40699       -1.95437
Cl         -2.48215        1.91403        0.82529
Cl         -1.03820        0.55301       -3.11894
N          -1.34310       -0.45462       -0.45226
C          -0.15678       -0.84722       -0.09409
C          -2.51496       -1.35564       -0.42105
H          -2.22540       -2.31160       -0.88427
C          -2.91378       -1.63074        1.04205
H          -3.17593       -0.66911        1.50818
H          -2.05336       -2.04979        1.58375
C          -4.10633       -2.59366        1.08818
H          -3.80463       -3.56548        0.65877
H          -4.38852       -2.77377        2.13691
C          -5.29554       -2.03970        0.29343
H          -5.64099       -1.10450        0.76717
H          -6.13556       -2.75102        0.31708
C          -4.88542       -1.74588       -1.15486
H          -5.72800       -1.31928       -1.71924
H          -4.60653       -2.69221       -1.65168
C          -3.69374       -0.78005       -1.21072
H          -3.38810       -0.59590       -2.24970
H          -3.98124        0.18501       -0.76137
C           0.18275       -2.25517        0.21106
C           0.63672       -2.62592        1.48651
H           0.72418       -1.87412        2.27057
C           0.97307       -3.95115        1.75886
H           1.31534       -4.26220        2.74529
C           0.86880       -4.88423        0.72946
F           1.20495       -6.17416        0.98476
C           0.43897       -4.54744       -0.55207
H           0.38607       -5.30912       -1.32935
C           0.08875       -3.22069       -0.80358
H          -0.23974       -2.92518       -1.80088
N           0.50630        1.39055       -0.40133
C           0.87989        0.21396       -0.00081
C           1.39028        2.54766       -0.40760
H           2.37810        2.28081        0.00372
C           0.78678        3.65690        0.46966
H          -0.21981        3.89141        0.09215
H           0.67583        3.28390        1.50008
C           1.67494        4.90588        0.42596
H           2.66021        4.67269        0.86821
H           1.22103        5.69784        1.04119
C           1.87459        5.38796       -1.01699
H           0.89604        5.67502       -1.43870
H           2.51914        6.28048       -1.03615
C           2.48243        4.27260       -1.87774
H           2.60995        4.61041       -2.91766
H           3.48618        4.02324       -1.48959
C           1.59955        3.01849       -1.85752
H           2.05671        2.20156       -2.43628
H           0.61950        3.23878       -2.30425
C           2.20533       -0.11405        0.57122
C           2.64896        0.55403        1.72522
H           2.01652        1.31668        2.18136
C           3.87967        0.23780        2.29970
H           4.23505        0.73592        3.20119
C           4.65802       -0.74385        1.69044
F           5.85859       -1.05576        2.24079
C           4.25384       -1.42079        0.54180
H           4.89960       -2.17842        0.09907
C           3.01201       -1.10674       -0.00865
H           2.66783       -1.63479       -0.89759
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 72
# Fe(III)-Cl3, R"=PhOMe, S=5/2
Fe         -1.53731        1.66249       -0.91743
Cl         -1.43497        0.90228       -3.07846
Cl         -2.55393        1.82606        1.13179
Cl         -2.00596        3.81229       -1.48986
N          -1.39686       -0.48533       -0.42474
C          -0.20562       -0.87109       -0.10891
C          -2.54992       -1.39617       -0.40348
H          -2.28587       -2.33445       -0.91707
C          -2.90414       -1.74500        1.05883
H          -3.13636       -0.80508        1.58188
H          -2.03076       -2.20152        1.54627
C          -4.10824       -2.69260        1.10368
H          -3.84064       -3.64417        0.61066
H          -4.35098       -2.92508        2.15239
C          -5.31954       -2.07943        0.39010
H          -5.62638       -1.16368        0.92493
H          -6.17201       -2.77627        0.41347
C          -4.96241       -1.71896       -1.05687
H          -5.81956       -1.25147       -1.56476
H          -4.72303       -2.64509       -1.60984
C          -3.75424       -0.77526       -1.11821
H          -3.49051       -0.55027       -2.15970
H          -4.00221        0.17696       -0.61811
C           0.17168       -2.27405        0.17297
C           0.02886       -3.25515       -0.82540
H          -0.34345       -2.97107       -1.81054
C           0.38683       -4.57382       -0.57914
H           0.29482       -5.33522       -1.35436
C           0.88130       -4.94406        0.68609
O           1.19803       -6.25801        0.83950
C           1.02532       -3.97336        1.69264
H           1.40622       -4.23898        2.67675
C           0.68334       -2.64887        1.42263
H           0.81301       -1.89535        2.19981
N           0.47158        1.40911       -0.37386
C           0.83347        0.20932       -0.01971
C           1.41321        2.52860       -0.44974
H           2.42480        2.18053       -0.18689
C           1.01106        3.62162        0.55191
H          -0.01933        3.94144        0.33420
H           1.01932        3.20132        1.56999
C           1.96546        4.81696        0.44193
H           2.98239        4.50221        0.73775
H           1.64994        5.60276        1.14517
C           2.00629        5.35761       -0.99360
H           1.00183        5.72157       -1.26964
H           2.69884        6.21098       -1.06026
C           2.42503        4.25343       -1.97322
H           2.44301        4.63569       -3.00521
H           3.45083        3.92376       -1.72908
C           1.47008        3.05531       -1.89298
H           1.79721        2.24116       -2.55720
H           0.46255        3.35969       -2.21005
C           2.17735       -0.13330        0.48068
C           2.93951       -1.16119       -0.11142
H           2.54026       -1.70715       -0.96544
C           4.19886       -1.47679        0.37395
H           4.80048       -2.25719       -0.09261
C           4.71669       -0.79371        1.49193
O           5.94768       -1.18467        1.90821
C           3.96056        0.22267        2.10399
H           4.33756        0.75491        2.97503
C           2.70923        0.55054        1.58600
H           2.12257        1.33905        2.05951
C           6.50728       -0.50706        3.04706
C           1.70896       -6.66617        2.11927
H           5.86823       -0.64603        3.93398
H           6.62205        0.56911        2.84022
H           7.48811       -0.96564        3.21305
H           0.97160       -6.46834        2.91420
H           2.64818       -6.13714        2.34975
H           1.89437       -7.74272        2.03668
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 72
# Fe(III)-Cl3, R"=PhOMe, S=3/2
Fe         -1.47713        1.41723       -1.07093
Cl         -1.98093        3.45012       -1.84003
Cl         -2.44211        1.86701        0.90170
Cl         -1.08576        0.62103       -3.11878
N          -1.33407       -0.46439       -0.46552
C          -0.14904       -0.86850       -0.11159
C          -2.51286       -1.35863       -0.44309
H          -2.23963       -2.30186       -0.93975
C          -2.89603       -1.67653        1.01530
H          -3.15018       -0.72820        1.51221
H          -2.03179       -2.11488        1.53455
C          -4.09126       -2.63692        1.04621
H          -3.79735       -3.59558        0.58290
H          -4.36203       -2.84955        2.09204
C          -5.28839       -2.05568        0.28344
H          -5.62553       -1.13489        0.79048
H          -6.13045       -2.76518        0.29428
C          -4.89390       -1.71657       -1.15933
H          -5.74188       -1.27012       -1.70000
H          -4.62362       -2.64754       -1.68904
C          -3.69963       -0.75303       -1.19801
H          -3.40681       -0.53569       -2.23415
H          -3.97789        0.19787       -0.71398
C           0.18120       -2.27684        0.18031
C           0.67619       -2.65774        1.43520
H           0.80812       -1.90580        2.21320
C           0.99683       -3.98690        1.70748
H           1.36433       -4.25802        2.69512
C           0.84936       -4.95535        0.69918
O           1.14629       -6.27288        0.85499
C           0.37296       -4.57825       -0.57145
H           0.28090       -5.33769       -1.34851
C           0.03530       -3.25547       -0.82090
H          -0.31947       -2.96437       -1.81064
N           0.51962        1.37193       -0.39797
C           0.89308        0.19132       -0.00397
C           1.41158        2.52327       -0.41423
H           2.41099        2.24142       -0.04275
C           0.84908        3.61929        0.50538
H          -0.16908        3.86699        0.16918
H           0.77249        3.22629        1.53170
C           1.74325        4.86365        0.45548
H           2.74153        4.61561        0.85921
H           1.31675        5.64738        1.10044
C           1.89801        5.37173       -0.98415
H           0.90765        5.67229       -1.36709
H           2.54761        6.26069       -1.00833
C           2.46812        4.26877       -1.88579
H           2.56544        4.62661       -2.92238
H           3.48195        4.00427       -1.53504
C           1.57551        3.02160       -1.85992
H           2.00584        2.21278       -2.46991
H           0.58345        3.25873       -2.26965
C           2.21332       -0.14136        0.56487
C           2.68753        0.55484        1.68730
H           2.07348        1.34335        2.12545
C           3.91760        0.24165        2.26488
H           4.25181        0.78640        3.14570
C           4.70633       -0.77641        1.70011
O           5.92055       -1.15620        2.17759
C           4.24432       -1.47475        0.56769
H           4.87023       -2.25819        0.13949
C           3.00791       -1.16905        0.01906
H           2.65068       -1.72602       -0.84687
C           6.42150       -0.46224        3.33276
C           1.64212       -6.68887        2.13858
H           5.74281       -0.59503        4.19094
H           6.53911        0.61263        3.11973
H           7.39658       -0.91170        3.55033
H           0.90103       -6.48234        2.92772
H           2.58620       -6.17208        2.37644
H           1.81424       -7.76757        2.05601
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 80
# Fe(III)-Cl3, R"=PhNMe2, S=5/2
Fe         -2.38953         2.49641        -1.14733
Cl         -2.36003         1.80240        -3.35318
Cl         -3.36023         2.63038         0.94355
Cl         -2.92433         4.65711        -1.66814
N          -2.22690         0.36276        -0.71534
C          -1.02438        -0.02417        -0.42512
C          -3.38079        -0.54800        -0.66883
H          -3.14618        -1.46945        -1.22431
C          -3.67936        -0.94420         0.79277
H          -3.89242        -0.02105         1.35289
H          -2.78921        -1.41526         1.23344
C          -4.88038        -1.89526         0.85278
H          -4.62962        -2.82975         0.31936
H          -5.08475        -2.16332         1.90138
C          -6.11855        -1.26329         0.20447
H          -6.40643        -0.36597         0.77966
H          -6.96894        -1.96272         0.23689
C          -5.81594        -0.85403        -1.24223
H          -6.69302        -0.37340        -1.70202
H          -5.59541        -1.76100        -1.83381
C          -4.61245         0.09473        -1.31524
H          -4.38663         0.35804        -2.35692
H          -4.84379         1.02737        -0.77255
C          -0.64280        -1.42320        -0.16047
C          -0.85934        -2.41740        -1.13080
H          -1.27651        -2.13850        -2.09957
C          -0.51429        -3.74100        -0.89907
H          -0.67366        -4.47379        -1.68772
C           0.04713        -4.13927         0.34601
N           0.36828        -5.44636         0.59248
C           0.26839        -3.12854         1.32186
H           0.70413        -3.38371         2.28571
C          -0.05817        -1.80700         1.06098
H           0.13385        -1.05109         1.82281
N          -0.38329         2.26735        -0.66927
C           0.00786         1.06176        -0.34220
C           0.54476         3.39623        -0.77708
H           1.57007         3.05627        -0.56031
C           0.17786         4.48247         0.24489
H          -0.86168         4.79768         0.06718
H           0.22504         4.05824         1.26030
C           1.12093         5.68365         0.10582
H           2.15072         5.37195         0.35797
H           0.83100         6.46422         0.82602
C           1.10125         6.23351        -1.32678
H           0.08421         6.59305        -1.55919
H           1.78591         7.09143        -1.41641
C           1.48470         5.13721        -2.32970
H           1.45979         5.52674        -3.35905
H           2.52133         4.81145        -2.12872
C           0.53938         3.93401        -2.21710
H           0.84074         3.12590        -2.90065
H          -0.48214         4.23540        -2.48934
C           1.36208         0.73146         0.11269
C           2.10352        -0.32266        -0.46152
H           1.67102        -0.90024        -1.27753
C           3.38125        -0.62800        -0.02462
H           3.92625        -1.43297        -0.51321
C           3.97695         0.09037         1.05003
N           5.22645        -0.22039         1.50305
C           3.22092         1.14407         1.63893
H           3.62799         1.71075         2.47390
C           1.95894         1.45807         1.16510
H           1.39847         2.26658         1.63643
C           5.81360         0.53056         2.60590
C           5.97415        -1.31250         0.89325
C           0.98304        -5.81904         1.85822
C           0.16533        -6.45473        -0.43832
H           5.19827         0.44436         3.51778
H           5.90339         1.60060         2.35345
H           6.81264         0.13480         2.81739
H           6.14052        -1.12787        -0.18158
H           5.43426        -2.26947         0.99600
H           6.94672        -1.40254         1.38884
H           0.33505        -5.54659         2.70860
H           1.95591        -5.31466         1.99757
H           1.14350        -6.90263         1.87465
H           0.45991        -7.43401        -0.04535
H           0.76780        -6.23832        -1.33831
H          -0.89413        -6.50202        -0.74208
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 80
# Fe(III)-Cl3, R"=PhNMe2, S=3/2
Fe         -2.28270        2.23498       -1.49186
Cl         -2.80422        4.29229       -2.21605
Cl         -3.34243        2.60433        0.46230
Cl         -1.83947        1.50690       -3.56733
N          -2.10916        0.34721       -0.93912
C          -0.93018       -0.03468       -0.52970
C          -3.26825       -0.57402       -0.98212
H          -2.96568       -1.49204       -1.50681
C          -3.68723       -0.95574        0.45072
H          -3.98368       -0.03254        0.97139
H          -2.82879       -1.38955        0.98281
C          -4.85452       -1.94966        0.41036
H          -4.51801       -2.88167       -0.07821
H          -5.15085       -2.20982        1.43858
C          -6.04493       -1.37548       -0.36797
H          -6.42477       -0.48471        0.16209
H          -6.86569       -2.10876       -0.41045
C          -5.61622       -0.96917       -1.78339
H          -6.46060       -0.52686       -2.33340
H          -5.30266       -1.87139       -2.33900
C          -4.45029        0.02875       -1.74757
H          -4.13428        0.29557       -2.76501
H          -4.77005        0.95147       -1.23613
C          -0.58242       -1.43318       -0.24438
C          -0.09246       -1.82457        1.01651
H           0.03095       -1.07521        1.79835
C           0.22271       -3.14611        1.28869
H           0.58134       -3.40834        2.28189
C           0.08996       -4.14798        0.28762
N           0.40270       -5.45397        0.54513
C          -0.37358       -3.74087       -0.99502
H          -0.45857       -4.46546       -1.80247
C          -0.71206       -2.41886       -1.23990
H          -1.04864       -2.13163       -2.23730
N          -0.32075        2.22962       -0.75432
C           0.07299        1.05374       -0.35156
C           0.54907        3.39876       -0.74303
H           1.54785        3.13225       -0.35806
C          -0.04601        4.47520        0.17834
H          -1.06356        4.70647       -0.17106
H          -0.13090        4.06983        1.19936
C           0.82415        5.73725        0.15648
H           1.82061        5.50403        0.57388
H           0.37284        6.50720        0.80154
C           0.99331        6.26217       -1.27561
H           0.00327        6.54453       -1.67310
H           1.62412        7.16516       -1.28070
C           1.60171        5.17928       -2.17680
H           1.71311        5.55030       -3.20754
H           2.61347        4.93101       -1.80790
C           0.73225        3.91556       -2.17937
H           1.18911        3.12058       -2.78846
H          -0.25558        4.13800       -2.60671
C           1.36889        0.75815        0.27338
C           1.80479        1.50198        1.38863
H           1.16567        2.29553        1.77961
C           3.00849        1.22758        2.01791
H           3.29222        1.80941        2.89260
C           3.86230        0.19621        1.53492
N           5.05668       -0.07578        2.14178
C           3.42573       -0.54329        0.40065
H           4.04778       -1.33765       -0.00688
C           2.20528       -0.27345       -0.19762
H           1.89290       -0.86728       -1.05625
C           5.89349       -1.16215        1.65119
C           5.46651        0.67840        3.31889
C           0.91768       -5.83588        1.85255
C           0.29173       -6.45338       -0.50883
H           6.17875       -0.99833        0.59817
H           5.36916       -2.13189        1.71508
H           6.80496       -1.21474        2.25643
H           4.74707        0.55197        4.14688
H           5.54038        1.75562        3.09304
H           6.44856        0.32260        3.64904
H           0.20032       -5.57998        2.65065
H           1.87058       -5.32356        2.07465
H           1.08796       -6.91788        1.86956
H           0.96109       -6.22113       -1.35585
H          -0.74003       -6.50738       -0.89521
H           0.56474       -7.43387       -0.10362
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 77
# Fe(III)-Bn, R"=PhF, S=5/2
Fe         -1.38819        0.39250       -0.42419
Cl         -1.56899        1.07304        1.84402
Cl         -1.05225       -0.26596       -2.64758
N          -0.74431       -1.50223        0.20834
C           0.52003       -1.56252        0.47536
C          -1.68440       -2.59342        0.42917
H          -1.23335       -3.37004        1.07062
C          -2.94466       -2.04749        1.11749
H          -3.37877       -1.25945        0.47370
H          -2.67130       -1.56738        2.06656
C          -3.97021       -3.16830        1.32315
H          -3.54480       -3.92314        2.00783
H          -4.86791       -2.75873        1.81065
C          -4.33452       -3.84128       -0.00602
H          -4.83571       -3.10424       -0.65747
H          -5.04402       -4.66595        0.16322
C          -3.07520       -4.35694       -0.71463
H          -3.33268       -4.80192       -1.68799
H          -2.61416       -5.15247       -0.10278
C          -2.06162       -3.22663       -0.92422
H          -1.15783       -3.59130       -1.43415
H          -2.48828       -2.43961       -1.56549
C           1.19232       -2.74376        1.06892
N           0.71137        0.73230       -0.20319
C           1.33946       -0.32658        0.20113
C           1.39355        1.97979       -0.51514
H           2.48202        1.81092       -0.58960
C           1.14137        3.00996        0.60245
H           0.06277        3.23033        0.63058
H           1.40843        2.58503        1.58111
C           1.94801        4.27946        0.30405
H           3.02453        4.03040        0.30534
H           1.78424        5.01741        1.10481
C           1.55981        4.87259       -1.05713
H           0.51437        5.21466       -1.00793
H           2.18678        5.74927       -1.28426
C           1.67675        3.83113       -2.17812
H           1.30182        4.24979       -3.12475
H           2.74045        3.57543       -2.33205
C           0.89622        2.55169       -1.84823
H           1.00515        1.80039       -2.64251
H          -0.17727        2.77911       -1.75869
C           2.81070       -0.41704        0.37998
H          -3.79827        1.28932        0.07752
C          -3.28443        1.31104       -0.88790
C          -2.81474        2.60139       -1.33516
C          -2.54484        3.64915       -0.41017
C          -2.07304        4.88309       -0.84486
C          -1.84264        5.11857       -2.20944
C          -2.09070        4.09423       -3.13697
C          -2.56433        2.85793       -2.71205
H          -2.70665        3.45799        0.65179
H          -1.87441        5.67198       -0.11676
H          -1.46521        6.08540       -2.54484
H          -1.90725        4.26683       -4.19915
H          -2.73514        2.05381       -3.42877
C           3.53269       -1.39839       -0.32025
C           4.91373       -1.51016       -0.16944
C           5.55363       -0.64127        0.71186
C           4.87118        0.33594        1.43133
C           3.49195        0.44698        1.25176
C           1.13474       -4.00215        0.44964
C           1.77837       -5.10411        1.01396
C           2.46226       -4.92564        2.21334
C           2.53326       -3.69458        2.86232
C           1.90277       -2.60040        2.27346
H           3.00935       -2.07883       -0.99189
H           5.48960       -2.25677       -0.71539
F           6.89666       -0.75446        0.87744
H           5.41253        0.98989        2.11432
H           2.93573        1.20056        1.80786
H           0.60072       -4.11624       -0.49271
H           1.75570       -6.08404        0.53817
F           3.08795       -5.99305        2.77213
H           3.07608       -3.60310        3.80256
H           1.95797       -1.62479        2.75580
H          -3.70691        0.65994       -1.66013
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 77
# Fe(III)-Bn, R"=PhF, S=3/2
Fe         -1.28266        0.42093       -0.35294
Cl         -1.46420        1.07558        1.81577
Cl         -1.26052       -0.13286       -2.55682
N          -0.71418       -1.47398        0.19730
C           0.55950       -1.58182        0.46458
C          -1.67422       -2.55065        0.41509
H          -1.23917       -3.32606        1.06992
C          -2.93665       -1.99055        1.08784
H          -3.36252       -1.20941        0.43110
H          -2.66736       -1.50161        2.03355
C          -3.96953       -3.10300        1.30345
H          -3.55122       -3.84892        2.00230
H          -4.86960       -2.68377        1.77860
C          -4.32742       -3.79631       -0.01712
H          -4.82191       -3.06810       -0.68367
H          -5.04117       -4.61567        0.16090
C          -3.06522       -4.32679       -0.70971
H          -3.31892       -4.78837       -1.67648
H          -2.60967       -5.11275       -0.08135
C          -2.04847       -3.20106       -0.93049
H          -1.14463       -3.57532       -1.43298
H          -2.47350       -2.42237       -1.58244
C           1.19355       -2.78589        1.05669
N           0.73872        0.66934       -0.25367
C           1.37890       -0.38037        0.19503
C           1.42075        1.90994       -0.61120
H           2.51218        1.74954       -0.61950
C           1.10212        3.00835        0.41705
H           0.01688        3.19653        0.39856
H           1.35021        2.66090        1.43084
C           1.86764        4.28827        0.06108
H           2.95297        4.09040        0.12327
H           1.63776        5.07277        0.79890
C           1.51653        4.76399       -1.35478
H           0.45061        5.04322       -1.37995
H           2.10249        5.66000       -1.61407
C           1.75552        3.65329       -2.38526
H           1.44158        3.98586       -3.38681
H           2.83641        3.43119       -2.43996
C           0.99756        2.37309       -2.01166
H           1.18238        1.57084       -2.73983
H          -0.08686        2.56662       -2.01032
C           2.84294       -0.43342        0.42749
H          -3.61873        1.28426        0.24479
C          -3.09453        1.34610       -0.71493
C          -2.72566        2.70640       -1.11149
C          -2.52959        3.71994       -0.14373
C          -2.20116        5.01916       -0.52563
C          -2.04984        5.33956       -1.88174
C          -2.22502        4.34443       -2.85336
C          -2.55633        3.04503       -2.47487
H          -2.63629        3.46116        0.91028
H          -2.05866        5.78839        0.23535
H          -1.79029        6.35668       -2.17911
H          -2.10336        4.58689       -3.91043
H          -2.68079        2.26289       -3.22440
C           3.62054       -1.41728       -0.20587
C           4.99487       -1.49479        0.01739
C           5.57317       -0.58300        0.89719
C           4.83598        0.40175        1.54932
C           3.46432        0.47227        1.30290
C           1.12520       -4.03724        0.42458
C           1.73526       -5.15854        0.98965
C           2.40339       -5.00595        2.20102
C           2.48784       -3.78292        2.86234
C           1.88422       -2.67162        2.27567
H           3.14416       -2.12950       -0.87946
H           5.61218       -2.24647       -0.47381
F           6.91059       -0.65900        1.13001
H           5.32973        1.09042        2.23445
H           2.86350        1.22883        1.80718
H           0.60681       -4.13265       -0.52842
H           1.69984       -6.13341        0.50404
F           2.99890       -6.09287        2.76002
H           3.01772       -3.71061        3.81175
H           1.94738       -1.70181        2.76887
H          -3.56475        0.75970       -1.51118
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 85
# Fe(III)-Bn, R"=PhOMe, S=5/2
Fe         -1.40536        0.35415       -0.48630
Cl         -1.59087        0.97158        1.80988
Cl         -1.09869       -0.21737       -2.74372
N          -0.77186       -1.55529        0.07400
C           0.49400       -1.63124        0.34351
C          -1.72033       -2.64565        0.26300
H          -1.27401       -3.44402        0.88052
C          -2.97559       -2.11368        0.97107
H          -3.40793       -1.30424        0.35315
H          -2.69669       -1.66338        1.93303
C          -4.00719       -3.23420        1.14683
H          -3.58348       -4.01189        1.80671
H          -4.90130       -2.83507        1.64966
C          -4.37996       -3.86524       -0.20056
H          -4.87908       -3.10595       -0.82765
H          -5.09384       -4.69060       -0.05360
C          -3.12602       -4.36605       -0.92925
H          -3.38992       -4.78032       -1.91449
H          -2.66741       -5.18232       -0.34327
C          -2.10674       -3.23539       -1.10687
H          -1.20767       -3.58864       -1.63282
H          -2.53141       -2.42614       -1.72156
C           1.15892       -2.82986        0.89714
N           0.68190        0.68658       -0.25949
C           1.31655       -0.38437        0.11021
C           1.35588        1.94626       -0.54000
H           2.44456        1.78370       -0.62449
C           1.10534        2.94576        0.60491
H           0.02635        3.16340        0.64114
H           1.37356        2.49566        1.57193
C           1.90772        4.22516        0.33949
H           2.98498        3.97853        0.32981
H           1.74573        4.94143        1.16025
C           1.51303        4.85383       -1.00390
H           0.46643        5.19051       -0.94176
H           2.13616        5.73865       -1.20975
C           1.62860        3.84321       -2.15297
H           1.25040        4.28706       -3.08685
H           2.69252        3.59391       -2.31662
C           0.85212        2.55339       -1.85481
H           0.95957        1.82447       -2.66983
H          -0.22166        2.77657       -1.75678
C           2.78360       -0.47738        0.28311
H          -3.81312        1.23213        0.05886
C          -3.30411        1.29073       -0.90761
C          -2.85198        2.60178       -1.31305
C          -2.58398        3.61856       -0.35413
C          -2.12524        4.87119       -0.74810
C          -1.90671        5.15703       -2.10495
C          -2.15353        4.16379       -3.06588
C          -2.61451        2.90932       -2.68137
H          -2.73447        3.38774        0.70164
H          -1.92683        5.63508        0.00638
H          -1.53911        6.13807       -2.40868
H          -1.97911        4.37487       -4.12272
H          -2.78278        2.12911       -3.42473
C           3.50934       -1.47548       -0.39864
C           4.88364       -1.58384       -0.25128
C           5.57052       -0.70876        0.61214
C           4.86059        0.28293        1.30956
C           3.48101        0.39464        1.13055
C           1.05657       -4.08764        0.27244
C           1.69899       -5.19985        0.79895
C           2.44744       -5.08449        1.98511
C           2.54793       -3.83834        2.62867
C           1.91917       -2.72604        2.07285
H           2.98424       -2.16999       -1.05441
H           5.44798       -2.34573       -0.78986
O           6.91363       -0.90090        0.70898
H           5.36985        0.96474        1.98796
H           2.93490        1.16068        1.67986
H           0.48962       -4.18444       -0.65259
H           1.63751       -6.17003        0.30490
O           3.03966       -6.22515        2.42945
H           3.11605       -3.72805        3.55021
H           2.01796       -1.75899        2.56555
H          -3.72924        0.66559       -1.69970
C           7.64163       -0.02377        1.58398
C           3.81755       -6.13644        3.63495
H           7.27960       -0.11921        2.62077
H           7.54199        1.02372        1.25600
H           8.68856       -0.34022        1.51998
H           3.18978       -5.81120        4.48029
H           4.65480       -5.43127        3.50588
H           4.20127       -7.14633        3.81678
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 85
# Fe(III)-Bn, R"=PhOMe, S=3/2
Fe         -1.31119        0.39245       -0.41476
Cl         -1.47887        0.99132        1.77562
Cl         -1.29673       -0.09920       -2.63504
N          -0.74132       -1.51852        0.07673
C           0.53463       -1.64168        0.32933
C          -1.70613       -2.59467        0.27429
H          -1.26498       -3.39652        0.89200
C          -2.95027       -2.05074        0.99303
H          -3.38421       -1.24294        0.37522
H          -2.65759       -1.59817        1.94985
C          -3.98677       -3.16336        1.19025
H          -3.55942       -3.93739        1.85223
H          -4.87384       -2.75606        1.69934
C          -4.37770       -3.80589       -0.14665
H          -4.88033       -3.05028       -0.77559
H          -5.09407       -4.62622        0.01662
C          -3.13435       -4.31915       -0.88486
H          -3.41207       -4.74379       -1.86202
H          -2.67150       -5.13044       -0.29515
C          -2.11419       -3.19279       -1.08527
H          -1.22421       -3.55363       -1.62118
H          -2.54726       -2.38768       -1.69891
C           1.17033       -2.86573        0.86744
N           0.71063        0.63412       -0.31550
C           1.35675       -0.42953        0.09175
C           1.38682        1.88605       -0.64391
H           2.47811        1.72690       -0.66832
C           1.07842        2.95430        0.41838
H          -0.00693        3.14323        0.41521
H           1.33506        2.57731        1.41943
C           1.84047        4.24438        0.09326
H           2.92646        4.04464        0.13821
H           1.61867        5.00719        0.85609
C           1.47521        4.76143       -1.30446
H           0.40893        5.04057       -1.31090
H           2.05836        5.66510       -1.54333
C           1.70358        3.68122       -2.36926
H           1.37976        4.04337       -3.35744
H           2.78395        3.46098       -2.44118
C           0.94911        2.39061       -2.02541
H           1.12585        1.61009       -2.77873
H          -0.13510        2.58480       -2.00835
C           2.81979       -0.49090        0.30625
H          -3.64625        1.23534        0.22322
C          -3.12629        1.32195       -0.73710
C          -2.76571        2.69445       -1.10098
C          -2.56349        3.68289       -0.10896
C          -2.23780        4.99200       -0.45881
C          -2.09562        5.34854       -1.80682
C          -2.27744        4.37880       -2.80248
C          -2.60603        3.06963       -2.45579
H          -2.66166        3.39607        0.93865
H          -2.08969        5.74073        0.32144
H          -1.83772        6.37311       -2.07913
H          -2.16255        4.64847       -3.85380
H          -2.73376        2.30709       -3.22476
C           3.59389       -1.47899       -0.33341
C           4.96338       -1.55850       -0.12530
C           5.59609       -0.65814        0.75237
C           4.83797        0.32729        1.40595
C           3.46366        0.40436        1.17154
C           1.05890       -4.10833        0.21607
C           1.67760       -5.24231        0.72732
C           2.41735       -5.16258        1.92094
C           2.53040       -3.93164        2.58949
C           1.91804       -2.79946        2.05283
H           3.10924       -2.19222       -1.00034
H           5.56498       -2.31637       -0.62835
O           6.94016       -0.81995        0.90621
H           5.30496        1.02935        2.09421
H           2.87686        1.16490        1.68691
H           0.49953       -4.17849       -0.71608
H           1.60430       -6.20169        0.21380
O           2.98916       -6.32318        2.34853
H           3.09392       -3.84751        3.51677
H           2.02463       -1.84354        2.56569
H          -3.60233        0.75694       -1.54566
C           7.60984        0.08121        1.80128
C           3.75750       -6.26696        3.56068
H           7.20584       -0.01123        2.82296
H           7.50201        1.12355        1.45888
H           8.66557       -0.21182        1.78631
H           3.12788       -5.94855        4.40761
H           4.60538       -5.57063        3.45253
H           4.12671       -7.28495        3.72790
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 93
# Fe(III)-Bn, R"=PhNMe2, S=5/2
Fe         -1.40247        0.37173       -0.50857
Cl         -1.62762        0.92690        1.81854
Cl         -1.11905       -0.11258       -2.80064
N          -0.76918       -1.53938       -0.01370
C           0.49598       -1.61418        0.28430
C          -1.71771       -2.63538        0.13767
H          -1.28612       -3.43613        0.76300
C          -2.99815       -2.12127        0.81285
H          -3.42137       -1.31076        0.18980
H          -2.75118       -1.67647        1.78596
C          -4.02448       -3.25230        0.94976
H          -3.61233       -4.03183        1.61507
H          -4.93693       -2.86661        1.42991
C          -4.35267       -3.87618       -0.41266
H          -4.84062       -3.11622       -1.04774
H          -5.06300       -4.70919       -0.29284
C          -3.07378       -4.35893       -1.10985
H          -3.30639       -4.76800       -2.10530
H          -2.62441       -5.17601       -0.51734
C          -2.06092       -3.21691       -1.24703
H          -1.14500       -3.55535       -1.75362
H          -2.47619       -2.40472       -1.86451
C           1.15460       -2.80761        0.83820
N           0.65788        0.72176       -0.26008
C           1.30987       -0.35289        0.08565
C           1.31331        1.99687       -0.51497
H           2.40365        1.85081       -0.60827
C           1.05354        2.96762        0.65186
H          -0.02838        3.16991        0.69420
H           1.32704        2.49921        1.60881
C           1.83751        4.26402        0.41606
H           2.91818        4.03232        0.39826
H           1.66797        4.95969        1.25308
C           1.43130        4.91758       -0.91204
H           0.37945        5.23606       -0.84124
H           2.04039        5.81662       -1.09853
C           1.56009        3.93506       -2.08386
H           1.17663        4.39570       -3.00758
H           2.62747        3.70340       -2.25214
C           0.80087        2.62861       -1.81458
H           0.91622        1.92019       -2.64639
H          -0.27570        2.83653       -1.71231
C           2.77161       -0.43306        0.25243
H          -3.82034        1.20482        0.06333
C          -3.31144        1.30580       -0.89974
C          -2.89354        2.64199       -1.26077
C          -2.64548        3.63062       -0.26827
C          -2.21563        4.90645       -0.61907
C          -2.00733        5.24488       -1.96537
C          -2.23482        4.28001       -2.95925
C          -2.66749        3.00285       -2.61749
H          -2.78515        3.35863        0.77924
H          -2.03112        5.64726        0.16167
H          -1.66190        6.24375       -2.23542
H          -2.06767        4.53099       -4.00865
H          -2.81846        2.24467       -3.38700
C           3.50554       -1.45084       -0.39049
C           4.88035       -1.55414       -0.25446
C           5.60127       -0.64724        0.57066
C           4.85795        0.36597        1.23563
C           3.48563        0.47060        1.06226
C           1.01904       -4.08167        0.25419
C           1.65663       -5.19591        0.77951
C           2.44980       -5.09453        1.95513
C           2.57805       -3.80878        2.55034
C           1.95875       -2.70282        1.99258
H           2.98176       -2.17429       -1.01525
H           5.40334       -2.34911       -0.78235
N           6.95764       -0.74922        0.72256
H           5.36031        1.07124        1.89484
H           2.94607        1.25230        1.59561
H           0.43158       -4.19383       -0.65604
H           1.54601       -6.15299        0.27352
N           3.07022       -6.19011        2.49038
H           3.17493       -3.67895        3.45087
H           2.09151       -1.72969        2.46457
H          -3.72842        0.70255       -1.71303
C           7.65834        0.14954        1.62916
C           7.68096       -1.84315        0.08993
C           3.93624       -6.04232        3.65184
C           2.97491       -7.48049        1.82174
H           7.30210        0.03545        2.66883
H           7.51052        1.20151        1.33314
H           8.73060       -0.07323        1.59760
H           7.54482       -1.82531       -1.00435
H           7.33459       -2.82506        0.45974
H           8.74957       -1.74119        0.30931
H           3.38239       -5.61632        4.50503
H           4.79250       -5.37844        3.43595
H           4.31862       -7.02719        3.94187
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 93
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Cl         -1.29814       -0.02514       -2.66736
N          -0.75396       -1.48714        0.02215
C           0.52243       -1.60906        0.28416
C          -1.71748       -2.56772        0.19694
H          -1.27900       -3.37757        0.80627
C          -2.96967       -2.04125        0.91472
H          -3.40512       -1.22696        0.30672
H          -2.68589       -1.60075        1.87977
C          -4.00062       -3.16296        1.08980
H          -3.57201       -3.94402        1.74287
H          -4.89365       -2.76938        1.59953
C          -4.38006       -3.78913       -0.25827
H          -4.88386       -3.02762       -0.87915
H          -5.09233       -4.61620       -0.11088
C          -3.12937       -4.28321       -0.99738
H          -3.39956       -4.69541       -1.98214
H          -2.66443       -5.10027       -0.41701
C          -2.11571       -3.14711       -1.17356
H          -1.22142       -3.49182       -1.71306
H          -2.55141       -2.33444       -1.77552
C           1.16024       -2.83333        0.80516
N           0.67787        0.68546       -0.30879
C           1.33796       -0.38144        0.07287
C           1.33905        1.95111       -0.61440
H           2.43165        1.80326       -0.65037
C           1.02786        2.99365        0.47234
H          -0.05899        3.17448        0.47677
H           1.28940        2.59642        1.46428
C           1.77906        4.29643        0.17405
H           2.86668        4.10285        0.20781
H           1.55688        5.04041        0.95536
C           1.40175        4.84282       -1.20933
H           0.33328        5.11367       -1.20344
H           1.97674        5.75623       -1.43116
C           1.63129        3.78875       -2.29983
H           1.29864        4.17145       -3.27743
H           2.71300        3.57860       -2.38296
C           0.88916        2.48449       -1.98098
H           1.06717        1.72315       -2.75332
H          -0.19643        2.67002       -1.95451
C           2.79792       -0.43447        0.27647
H          -3.69069        1.23153        0.20358
C          -3.16394        1.33567       -0.75144
C          -2.82225        2.71878       -1.09630
C          -2.63013        3.69541       -0.09078
C          -2.31451        5.01215       -0.42151
C          -2.17276        5.38952       -1.76384
C          -2.34571        4.43217       -2.77284
C          -2.66444        3.11545       -2.44506
H          -2.72594        3.39262        0.95261
H          -2.17287        5.75046        0.36993
H          -1.92171        6.41971       -2.02115
H          -2.23095        4.71711       -3.82027
H          -2.78271        2.36250       -3.22495
C           3.57530       -1.43477       -0.33725
C           4.94593       -1.51549       -0.13970
C           5.61612       -0.59457        0.71063
C           4.82699        0.40152        1.34606
C           3.45923        0.47775        1.11862
C           1.01573       -4.08248        0.17594
C           1.63789       -5.22383        0.66577
C           2.42746       -5.17357        1.84539
C           2.57212       -3.91021        2.48073
C           1.96063       -2.77839        1.96307
H           3.08913       -2.16971       -0.97921
H           5.50295       -2.30559       -0.63946
N           6.97207       -0.66679        0.91262
H           5.28726        1.11506        2.02684
H           2.88006        1.24729        1.62940
H           0.42816       -4.15645       -0.73852
H           1.51617       -6.16101        0.12601
N           3.02936       -6.29917        2.35034
H           3.17625       -3.81503        3.38089
H           2.10674       -1.82187        2.46493
H          -3.62986        0.77664       -1.57046
C           7.60473        0.20468        1.89215
C           7.72731       -1.78239        0.36147
C           3.94466       -6.18719        3.47669
C           2.97165       -7.54712        1.60304
H           7.21512        0.02862        2.91218
H           7.43260        1.26424        1.64177
H           8.68514        0.02082        1.89020
H           7.62309       -1.82226       -0.73514
H           7.38669       -2.75161        0.77117
H           8.78831       -1.65062        0.60257
H           3.43842       -5.74512        4.35032
H           4.81933       -5.55526        3.23426
H           4.29751       -7.18759        3.75210
H           3.45792       -7.45743        0.61377
H           1.92649       -7.85725        1.44019
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