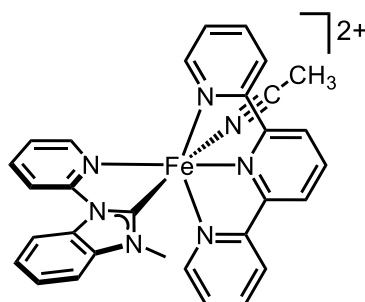


Coordinates for Optimized Geometries in MeCN

1. <i>C-trans</i> complexes	2
1.1 <i>C</i>-Fe-MeCN²⁺	2
1.2 <i>C</i>-Fe-MeCN⁺	3
1.3 <i>C</i>-Fe²⁺	5
1.4 <i>C</i>-Fe⁺	6
1.5 <i>C</i>-Fe⁰	8
1.6 <i>C</i>-Fe-CO₂⁰	9
1.7 <i>C</i>-Fe-CO²⁺	11
1.8 <i>C</i>-Fe-CO⁺	12
1.9 κ^1<i>C</i>-Fe-CO⁺	14
1.10 <i>C</i>-Fe-CO⁰	15
1.11 κ^1<i>C</i>-Fe-CO⁰	17
2. <i>N-trans</i> complexes	19
2.1 <i>N</i>-Fe-MeCN²⁺	19
2.2 <i>N</i>-Fe-MeCN⁺	20
2.3 <i>N</i>-Fe²⁺	22
2.4 <i>N</i>-Fe⁺	23
2.5 <i>N</i>-Fe-CO₂⁰	25
2.6 <i>N</i>-Fe-CO²⁺	26
2.7 <i>N</i>-Fe-CO⁺	28
2.8 κ^1<i>N</i>-Fe-CO⁺	29
2.9 κ^1<i>N</i>-Fe-CO⁰	31

1. C-trans complexes

1.1 C-Fe-MeCN²⁺

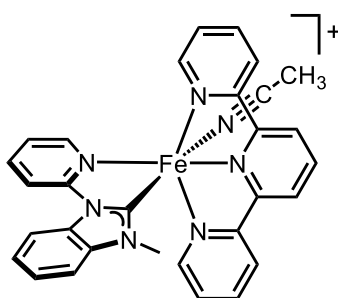


C-Fe-MeCN²⁺

Fe	-0.594111000000	0.353652000000	0.293664000000
N	-0.466132000000	-1.076036000000	1.698829000000
N	-1.769291000000	-0.929952000000	-0.479791000000
N	-1.147795000000	1.382359000000	-1.340151000000
N	2.196359000000	0.415830000000	-0.040820000000
N	0.677545000000	1.702307000000	1.089715000000
N	1.546374000000	-1.262069000000	-1.266098000000
C	-2.035784000000	0.715573000000	-2.128568000000
C	-2.407910000000	-0.617677000000	-1.621409000000
N	-2.162451000000	1.103410000000	1.258213000000
C	0.339006000000	2.748782000000	1.864684000000
H	-0.711524000000	2.846365000000	2.094249000000
C	0.272586000000	-2.099898000000	3.730157000000
H	0.869356000000	-2.023795000000	4.630035000000
C	1.979150000000	1.539464000000	0.769983000000
C	2.945621000000	-1.256326000000	-1.303258000000
C	-1.981211000000	-2.088594000000	0.167805000000
C	1.078711000000	-0.271386000000	-0.487107000000
C	2.971941000000	2.417915000000	1.194045000000
H	3.998833000000	2.288367000000	0.897271000000
C	0.250381000000	-1.041574000000	2.828536000000
H	0.817641000000	-0.138048000000	3.007460000000
C	-2.531800000000	1.276380000000	-3.302214000000
H	-3.233319000000	0.724584000000	-3.913689000000
C	-1.232835000000	-3.277259000000	2.280644000000
H	-1.831965000000	-4.145212000000	2.039946000000
C	-2.114183000000	2.550662000000	-3.672815000000
H	-2.488458000000	3.003893000000	-4.582739000000
C	3.378943000000	-0.180066000000	-0.514993000000
C	0.757241000000	-2.275339000000	-1.962450000000
H	1.192018000000	-2.445134000000	-2.947068000000
H	-0.258224000000	-1.923745000000	-2.087714000000
H	0.763345000000	-3.208376000000	-1.396880000000
C	3.833571000000	-2.114161000000	-1.942286000000
H	3.482470000000	-2.944519000000	-2.541205000000

C	-3.125510000000	1.459577000000	1.775341000000
C	-0.755905000000	2.610260000000	-1.700546000000
H	-0.056060000000	3.101761000000	-1.038158000000
C	-1.212140000000	-2.181298000000	1.422563000000
C	2.603786000000	3.490567000000	1.996305000000
H	3.358781000000	4.187855000000	2.338627000000
C	-3.295811000000	-1.524693000000	-2.197327000000
H	-3.809832000000	-1.287340000000	-3.118937000000
C	-3.506556000000	-2.745118000000	-1.558179000000
H	-4.188026000000	-3.467767000000	-1.989912000000
C	-2.853266000000	-3.037948000000	-0.362636000000
H	-3.023436000000	-3.978507000000	0.143603000000
C	1.266340000000	3.659521000000	2.344330000000
H	0.940011000000	4.482175000000	2.966893000000
C	4.740296000000	0.059656000000	-0.332923000000
H	5.118457000000	0.859419000000	0.284357000000
C	-1.214063000000	3.230379000000	-2.857905000000
H	-0.865794000000	4.224791000000	-3.106047000000
C	5.193157000000	-1.864946000000	-1.768090000000
H	5.918797000000	-2.511062000000	-2.247749000000
C	5.634403000000	-0.798221000000	-0.973969000000
H	6.697658000000	-0.632728000000	-0.846093000000
C	-0.478138000000	-3.236957000000	3.448822000000
H	-0.480614000000	-4.080366000000	4.128693000000
C	-4.330083000000	1.920629000000	2.432470000000
H	-4.784354000000	1.096912000000	2.987453000000
H	-5.037863000000	2.287252000000	1.685674000000
H	-4.082907000000	2.729916000000	3.123324000000

1.2 C-Fe-MeCN⁺



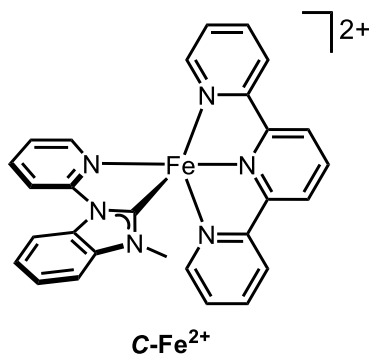
C-Fe-MeCN⁺

Fe	-0.568628000000	0.382022000000	0.254004000000
N	-0.650124000000	-0.893767000000	1.796346000000
N	-1.786332000000	-0.883023000000	-0.490464000000
N	-0.941448000000	1.274069000000	-1.510685000000
N	2.230377000000	0.287956000000	0.070701000000
N	0.726649000000	1.714083000000	1.039687000000
N	1.548529000000	-1.439906000000	-1.067109000000

C	-1.829560000000	0.599772000000	-2.297279000000
C	-2.344351000000	-0.642952000000	-1.693500000000
N	-2.173727000000	1.333890000000	1.008321000000
C	0.407589000000	2.810336000000	1.751465000000
H	-0.648318000000	2.989811000000	1.890548000000
C	-0.122853000000	-1.768649000000	3.972303000000
H	0.426004000000	-1.651572000000	4.897858000000
C	2.034745000000	1.446196000000	0.835833000000
C	2.945374000000	-1.459864000000	-1.106696000000
C	-2.152068000000	-1.957735000000	0.293043000000
C	1.093427000000	-0.390463000000	-0.355903000000
C	3.053668000000	2.251797000000	1.338806000000
H	4.090601000000	2.015314000000	1.171213000000
C	-0.000653000000	-0.823168000000	2.968185000000
H	0.643624000000	0.039314000000	3.094179000000
C	-2.192373000000	1.082707000000	-3.554643000000
H	-2.896402000000	0.530536000000	-4.163261000000
C	-1.654717000000	-2.976950000000	2.554251000000
H	-2.309894000000	-3.818337000000	2.362073000000
C	-1.643677000000	2.274289000000	-4.013493000000
H	-1.916017000000	2.661431000000	-4.988144000000
C	3.400451000000	-0.348816000000	-0.380389000000
C	0.744965000000	-2.467660000000	-1.721149000000
H	1.052931000000	-2.555179000000	-2.764016000000
H	-0.298302000000	-2.186593000000	-1.672813000000
H	0.891951000000	-3.425466000000	-1.218677000000
C	3.813291000000	-2.354818000000	-1.720364000000
H	3.441781000000	-3.207275000000	-2.274371000000
C	-3.157412000000	1.801586000000	1.377885000000
C	-0.420519000000	2.425941000000	-1.960581000000
H	0.270844000000	2.924520000000	-1.294168000000
C	-1.500335000000	-1.976877000000	1.560514000000
C	2.703675000000	3.377950000000	2.072870000000
H	3.479281000000	4.019082000000	2.474049000000
C	-3.276349000000	-1.511281000000	-2.240184000000
H	-3.720857000000	-1.323590000000	-3.207861000000
C	-3.637855000000	-2.656093000000	-1.482019000000
H	-4.359760000000	-3.356891000000	-1.884955000000
C	-3.091276000000	-2.875477000000	-0.232770000000
H	-3.386167000000	-3.740973000000	0.348307000000
C	1.357748000000	3.667350000000	2.283224000000
H	1.044181000000	4.535234000000	2.848477000000
C	4.766694000000	-0.101677000000	-0.256113000000
H	5.163599000000	0.741720000000	0.286276000000
C	-0.741572000000	2.960743000000	-3.200542000000
H	-0.292033000000	3.893876000000	-3.515764000000
C	5.178910000000	-2.106369000000	-1.590844000000
H	5.889953000000	-2.780234000000	-2.054012000000
C	5.642757000000	-0.997875000000	-0.871387000000
H	6.709131000000	-0.824483000000	-0.786899000000

C	-0.977565000000	-2.877456000000	3.747525000000
H	-1.095781000000	-3.641667000000	4.507606000000
C	-4.392530000000	2.399216000000	1.843294000000
H	-4.908681000000	1.705849000000	2.511034000000
H	-5.036424000000	2.624314000000	0.990164000000
H	-4.174168000000	3.323338000000	2.383433000000

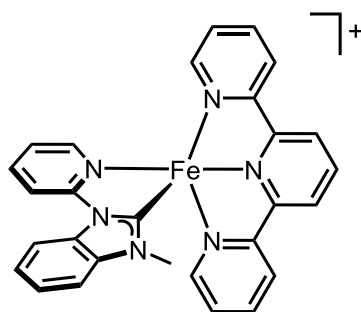
1.3 C-Fe²⁺



Fe	-0.600099000000	0.123480000000	0.804517000000
N	-0.804024000000	-1.875724000000	0.997964000000
N	-2.250515000000	-0.109484000000	-0.134062000000
N	-1.013333000000	2.046921000000	0.409666000000
N	2.029521000000	0.083289000000	-0.113333000000
N	1.039034000000	0.387343000000	1.910604000000
N	0.796935000000	-0.274070000000	-1.879536000000
C	-2.168465000000	2.231269000000	-0.292245000000
C	-2.902822000000	0.982294000000	-0.577914000000
C	1.029179000000	0.623022000000	3.232224000000
H	0.050339000000	0.646175000000	3.695791000000
C	-0.184711000000	-4.091972000000	1.652516000000
H	0.519843000000	-4.732282000000	2.167406000000
C	2.214211000000	0.342221000000	1.253587000000
C	2.130911000000	-0.338462000000	-2.297610000000
C	-2.766043000000	-1.348122000000	-0.247867000000
C	0.718306000000	-0.034485000000	-0.560708000000
C	3.430270000000	0.544151000000	1.898429000000
H	4.364674000000	0.518815000000	1.362723000000
C	0.030803000000	-2.718358000000	1.619153000000
H	0.891975000000	-2.270103000000	2.096220000000
C	-2.583356000000	3.498427000000	-0.686900000000
H	-3.499572000000	3.623102000000	-1.248369000000
C	-2.182903000000	-3.739816000000	0.369622000000
H	-3.063449000000	-4.117768000000	-0.132537000000
C	-1.802559000000	4.601865000000	-0.351998000000
H	-2.109189000000	5.596302000000	-0.652870000000
C	2.934656000000	-0.106076000000	-1.171003000000
C	-0.325362000000	-0.485426000000	-2.789108000000
H	-0.154153000000	0.083000000000	-3.703143000000

H	-1.234716000000	-0.136971000000	-2.316546000000
H	-0.414999000000	-1.546363000000	-3.028464000000
C	2.669201000000	-0.583793000000	-3.555130000000
H	2.034588000000	-0.767016000000	-4.412631000000
C	-0.269944000000	3.114338000000	0.729182000000
H	0.636621000000	2.915251000000	1.284868000000
C	-1.910954000000	-2.376279000000	0.378565000000
C	3.409612000000	0.786319000000	3.268098000000
H	4.342844000000	0.945895000000	3.794577000000
C	-4.128100000000	0.850550000000	-1.227379000000
H	-4.658111000000	1.718799000000	-1.594596000000
C	-4.659450000000	-0.428026000000	-1.388435000000
H	-5.608403000000	-0.555498000000	-1.894702000000
C	-3.986664000000	-1.542449000000	-0.890196000000
H	-4.407199000000	-2.533175000000	-0.994382000000
C	2.195646000000	0.825485000000	3.952334000000
H	2.150121000000	1.012327000000	5.016987000000
C	4.323560000000	-0.111682000000	-1.278057000000
H	4.973949000000	0.059298000000	-0.434295000000
C	-0.629326000000	4.408480000000	0.368805000000
H	0.005769000000	5.238542000000	0.650165000000
C	4.058840000000	-0.588209000000	-3.659602000000
H	4.520007000000	-0.776156000000	-4.621888000000
C	4.867897000000	-0.355728000000	-2.539214000000
H	5.945831000000	-0.366601000000	-2.648848000000
C	-1.306692000000	-4.609388000000	1.014459000000
H	-1.501949000000	-5.674889000000	1.016320000000

1.4 C-Fe⁺

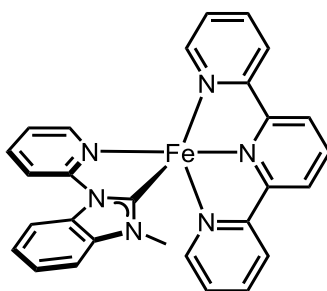


C-Fe⁺

Fe	-0.609227000000	-0.006559000000	0.738225000000
N	-0.962445000000	-1.974210000000	0.696781000000
N	-2.261888000000	-0.002203000000	-0.156109000000
N	-0.967922000000	1.959978000000	0.726747000000
N	2.071542000000	-0.002791000000	-0.074995000000
N	1.005722000000	-0.015272000000	1.937262000000
N	0.899444000000	0.020352000000	-1.916585000000
C	-2.093302000000	2.324323000000	0.020449000000
C	-2.863523000000	1.193242000000	-0.464006000000

C	0.964271000000	-0.024682000000	3.279669000000
H	-0.027666000000	-0.025515000000	3.714748000000
C	-0.457634000000	-4.300707000000	1.020514000000
H	0.203389000000	-5.044057000000	1.448060000000
C	2.206047000000	-0.013851000000	1.319704000000
C	2.244185000000	0.023945000000	-2.296464000000
C	-2.861016000000	-1.194489000000	-0.480793000000
C	0.770096000000	0.005107000000	-0.575764000000
C	3.405507000000	-0.021634000000	2.026326000000
H	4.355505000000	-0.020710000000	1.518764000000
C	-0.182372000000	-2.957801000000	1.195058000000
H	0.687373000000	-2.630618000000	1.749472000000
C	-2.418508000000	3.673090000000	-0.177552000000
H	-3.301555000000	3.932596000000	-0.747671000000
C	-2.409396000000	-3.677032000000	-0.232535000000
H	-3.292373000000	-3.929970000000	-0.805692000000
C	-1.608159000000	4.659573000000	0.356621000000
H	-1.849835000000	5.705762000000	0.211587000000
C	3.011514000000	0.009201000000	-1.119094000000
C	-0.204249000000	0.049357000000	-2.868363000000
H	-0.170045000000	0.974538000000	-3.446462000000
H	-1.134800000000	-0.001629000000	-2.313286000000
H	-0.130098000000	-0.803605000000	-3.544697000000
C	2.823471000000	0.038677000000	-3.558993000000
H	2.215486000000	0.050202000000	-4.454827000000
C	-0.191664000000	2.937637000000	1.242234000000
H	0.677636000000	2.603830000000	1.793451000000
C	-2.087535000000	-2.330662000000	-0.013893000000
C	3.347408000000	-0.031174000000	3.415445000000
H	4.266947000000	-0.037326000000	3.988198000000
C	-4.072720000000	1.214353000000	-1.148654000000
H	-4.546435000000	2.156789000000	-1.392803000000
C	-4.677897000000	0.004707000000	-1.507952000000
H	-5.621122000000	0.007467000000	-2.039913000000
C	-4.070316000000	-1.208588000000	-1.165501000000
H	-4.542195000000	-2.148515000000	-1.422512000000
C	2.110508000000	-0.032709000000	4.058992000000
H	2.032211000000	-0.039856000000	5.138183000000
C	4.402917000000	0.008867000000	-1.182543000000
H	5.028629000000	-0.001974000000	-0.303118000000
C	-0.470507000000	4.282354000000	1.088543000000
H	0.187459000000	5.020759000000	1.529171000000
C	4.217140000000	0.038295000000	-3.619071000000
H	4.708740000000	0.049673000000	-4.584707000000
C	4.988911000000	0.023793000000	-2.450439000000
H	6.070029000000	0.024077000000	-2.525106000000
C	-1.595525000000	-4.669584000000	0.284740000000
H	-1.834456000000	-5.714024000000	0.123516000000

1.5 C-Fe⁰

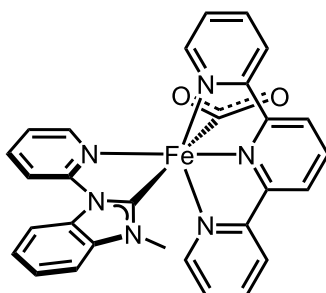


C-Fe⁰

Fe	0.604124000000	-0.003157000000	0.614887000000
N	0.956526000000	1.938980000000	0.660933000000
N	2.296855000000	0.027342000000	-0.176953000000
N	1.020444000000	-1.932065000000	0.648499000000
N	-2.119919000000	-0.022504000000	-0.023799000000
N	-0.950277000000	-0.025544000000	1.925797000000
N	-1.013579000000	-0.018514000000	-1.913047000000
C	2.180798000000	-2.298422000000	-0.041020000000
C	2.936176000000	-1.169216000000	-0.495330000000
C	-0.850852000000	-0.030380000000	3.265665000000
H	0.159941000000	-0.029250000000	3.654430000000
C	0.395158000000	4.261352000000	1.014516000000
H	-0.294713000000	4.981186000000	1.438416000000
C	-2.185828000000	-0.026850000000	1.372080000000
C	-2.368546000000	-0.020217000000	-2.240210000000
C	2.896082000000	1.246227000000	-0.487998000000
C	-0.826963000000	-0.017276000000	-0.568903000000
C	-3.350967000000	-0.031359000000	2.136390000000
H	-4.324176000000	-0.031226000000	1.673232000000
C	0.143102000000	2.916539000000	1.151062000000
H	-0.740505000000	2.565234000000	1.669166000000
C	2.515342000000	-3.654260000000	-0.226511000000
H	3.416063000000	-3.903055000000	-0.775693000000
C	2.395485000000	3.714429000000	-0.200784000000
H	3.287768000000	3.995695000000	-0.748041000000
C	1.706345000000	-4.648592000000	0.280552000000
H	1.959440000000	-5.693184000000	0.142389000000
C	-3.094696000000	-0.023918000000	-1.033105000000
C	0.065716000000	-0.005564000000	-2.890380000000
H	-0.031614000000	-0.857964000000	-3.565338000000
H	1.005798000000	-0.069994000000	-2.347467000000
H	0.037940000000	0.919401000000	-3.470463000000
C	-2.998062000000	-0.019730000000	-3.478457000000
H	-2.425132000000	-0.016395000000	-4.397266000000
C	0.239006000000	-2.938903000000	1.131299000000
H	-0.654203000000	-2.619574000000	1.653319000000
C	2.104305000000	2.347333000000	-0.025833000000
C	-3.226413000000	-0.035838000000	3.520858000000

H	-4.116521000000	-0.039300000000	4.138638000000
C	4.162644000000	-1.153885000000	-1.146639000000
H	4.661028000000	-2.085713000000	-1.387864000000
C	4.762170000000	0.072000000000	-1.476854000000
H	5.721409000000	0.089537000000	-1.980009000000
C	4.122203000000	1.275407000000	-1.139305000000
H	4.589389000000	2.224657000000	-1.375053000000
C	-1.957952000000	-0.035851000000	4.101109000000
H	-1.825599000000	-0.039472000000	5.175190000000
C	-4.486381000000	-0.028159000000	-1.045752000000
H	-5.075656000000	-0.031321000000	-0.141041000000
C	0.533301000000	-4.273868000000	0.983894000000
H	-0.133331000000	-5.018444000000	1.402194000000
C	-4.394969000000	-0.023623000000	-3.486895000000
H	-4.921361000000	-0.023154000000	-4.434281000000
C	-5.122510000000	-0.027747000000	-2.291660000000
H	-6.205830000000	-0.030536000000	-2.325142000000
C	1.555704000000	4.678602000000	0.314623000000
H	1.775915000000	5.731724000000	0.185152000000

1.6 C-FeCO₂⁰

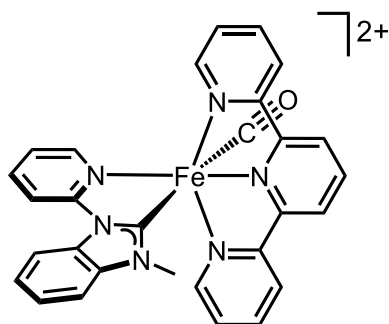


C-Fe-CO₂⁰

N	-2.199831000	0.285805000	-0.109056000
C	-3.293270000	-0.214614000	-0.838981000
C	-2.719144000	-1.019995000	-1.837120000
N	-1.334540000	-0.964964000	-1.666977000
C	-0.995534000	-0.189523000	-0.613108000
C	-3.486496000	-1.707808000	-2.769589000
C	-4.871773000	-1.570942000	-2.681673000
C	-5.453314000	-0.775064000	-1.687232000
C	-4.678492000	-0.086499000	-0.750692000
Fe	0.596005000	0.272413000	0.421620000
C	2.108537000	0.851870000	1.816978000
C	-0.406804000	-1.686889000	-2.529492000
C	-2.121713000	1.171521000	0.975677000
C	-3.214752000	1.841484000	1.521787000
C	-2.993282000	2.716926000	2.577267000
C	-1.696976000	2.893932000	3.051911000
C	-0.667139000	2.180240000	2.455983000

N	-0.858359000	1.325482000	1.432823000
N	1.947002000	-0.647817000	-0.459408000
C	2.705417000	0.020657000	-1.366196000
C	3.758827000	-0.624513000	-2.013660000
C	4.031397000	-1.956035000	-1.704710000
C	3.261718000	-2.621269000	-0.745933000
C	2.221674000	-1.936255000	-0.127151000
C	2.253990000	1.396171000	-1.546490000
C	2.815933000	2.310800000	-2.443895000
C	2.292476000	3.591300000	-2.530913000
C	1.202081000	3.929646000	-1.721736000
C	0.684157000	2.974767000	-0.861941000
N	1.187349000	1.731549000	-0.758754000
C	1.340981000	-2.411548000	0.938948000
C	1.359894000	-3.694469000	1.489373000
C	0.497573000	-3.999159000	2.534333000
C	-0.362638000	-3.005233000	3.007899000
C	-0.333953000	-1.751764000	2.415002000
N	0.487964000	-1.447423000	1.396799000
H	4.845451000	-2.471958000	-2.199002000
H	4.359126000	-0.097017000	-2.743626000
H	3.477763000	-3.648389000	-0.481409000
H	3.655197000	2.015540000	-3.060703000
H	2.718815000	4.313599000	-3.216952000
H	-0.160521000	3.196024000	-0.223102000
H	0.758080000	4.916768000	-1.756253000
H	2.045614000	-4.437636000	1.103343000
H	0.496844000	-4.989106000	2.974628000
H	-0.980302000	-0.953443000	2.752549000
H	-1.046628000	-3.195197000	3.825846000
H	-6.532440000	-0.689310000	-1.635091000
H	-5.505175000	-2.091619000	-3.390321000
H	-3.024516000	-2.327263000	-3.527849000
H	-5.164781000	0.507823000	0.007063000
H	-0.434549000	-2.755240000	-2.305236000
H	-0.689157000	-1.530615000	-3.571472000
H	0.594025000	-1.304017000	-2.369452000
H	-4.208123000	1.704270000	1.130280000
H	-3.826790000	3.253015000	3.015397000
H	0.350579000	2.251985000	2.806098000
H	-1.479138000	3.567117000	3.871194000
O	3.172540000	1.330178000	1.349732000
O	1.853855000	0.661958000	3.037278000

1.7 C-Fe-CO²⁺

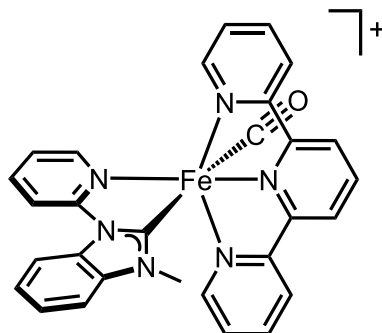


C-Fe-CO²⁺

Fe	-0.643457000000	0.385081000000	0.660374000000
N	-0.487498000000	-1.426772000000	1.523322000000
N	-2.060997000000	-0.511935000000	-0.261679000000
N	-1.238618000000	1.885031000000	-0.542055000000
N	2.061385000000	0.247167000000	-0.202225000000
N	0.949962000000	1.286926000000	1.517042000000
N	0.988731000000	-0.927581000000	-1.686208000000
C	-2.292607000000	1.558193000000	-1.341137000000
C	-2.774620000000	0.175637000000	-1.170510000000
C	-1.841734000000	0.902151000000	1.963947000000
C	0.911408000000	2.079643000000	2.605864000000
H	-0.057013000000	2.227588000000	3.060773000000
C	0.416119000000	-3.086319000000	2.983833000000
H	1.141760000000	-3.339838000000	3.745682000000
C	2.144614000000	1.087029000000	0.919017000000
C	2.351231000000	-1.044874000000	-1.991921000000
C	-2.307370000000	-1.799917000000	0.031913000000
C	0.807061000000	-0.166918000000	-0.598594000000
C	3.319263000000	1.673205000000	1.379931000000
H	4.255583000000	1.520973000000	0.872256000000
C	0.386133000000	-1.796118000000	2.466781000000
H	1.072965000000	-1.033216000000	2.807538000000
C	-2.833914000000	2.475331000000	-2.236630000000
H	-3.669891000000	2.196286000000	-2.863818000000
C	-1.410065000000	-3.641712000000	1.529069000000
H	-2.131335000000	-4.349549000000	1.143907000000
C	-2.285942000000	3.751947000000	-2.312600000000
H	-2.693412000000	4.478610000000	-3.004878000000
C	3.055464000000	-0.290217000000	-1.042277000000
C	-0.053538000000	-1.619786000000	-2.445697000000
H	0.291539000000	-1.756664000000	-3.468086000000
H	-0.952333000000	-1.015678000000	-2.468841000000
H	-0.260366000000	-2.592016000000	-1.998092000000
C	2.994167000000	-1.752108000000	-3.002678000000
H	2.440717000000	-2.337416000000	-3.724874000000
O	-2.626685000000	1.163373000000	2.744889000000
C	-0.721044000000	3.116708000000	-0.614817000000

H	0.107440000000	3.328392000000	0.047002000000
C	-1.389359000000	-2.333856000000	1.054997000000
C	3.258852000000	2.483595000000	2.505608000000
H	4.162008000000	2.949697000000	2.880104000000
C	-3.814386000000	-0.450279000000	-1.855015000000
H	-4.394774000000	0.086453000000	-2.592690000000
C	-4.084645000000	-1.787815000000	-1.572474000000
H	-4.885536000000	-2.295481000000	-2.095583000000
C	-3.332251000000	-2.478518000000	-0.625166000000
H	-3.538546000000	-3.517664000000	-0.408314000000
C	2.035251000000	2.690411000000	3.134859000000
H	1.943122000000	3.314627000000	4.013577000000
C	4.448649000000	-0.229767000000	-1.078578000000
H	5.033145000000	0.321889000000	-0.359547000000
C	-1.213815000000	4.078771000000	-1.489217000000
H	-0.759017000000	5.060560000000	-1.513837000000
C	4.383668000000	-1.682516000000	-3.040585000000
H	4.922276000000	-2.219827000000	-3.811986000000
C	5.095013000000	-0.935152000000	-2.091920000000
H	6.177095000000	-0.904750000000	-2.139318000000
C	-0.494409000000	-4.022622000000	2.505176000000
H	-0.495971000000	-5.036689000000	2.885759000000

1.8 C-Fe-CO⁺

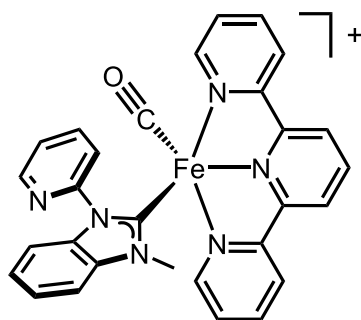


C-Fe-CO⁺

Fe	-0.634069000000	0.320336000000	0.707470000000
N	-0.633920000000	-1.584595000000	1.375784000000
N	-2.076615000000	-0.386246000000	-0.334238000000
N	-1.085866000000	1.973202000000	-0.341273000000
N	2.083468000000	0.142564000000	-0.127728000000
N	0.989466000000	1.020681000000	1.691291000000
N	0.990286000000	-0.783711000000	-1.763570000000
C	-2.154054000000	1.781808000000	-1.220005000000
C	-2.715658000000	0.473123000000	-1.204274000000
C	-1.855146000000	0.805472000000	1.979214000000
C	0.970346000000	1.680128000000	2.865640000000
H	0.001066000000	1.819091000000	3.321512000000

C	0.114566000000	-3.443725000000	2.680977000000
H	0.801961000000	-3.824626000000	3.425421000000
C	2.184131000000	0.830123000000	1.092094000000
C	2.349727000000	-0.901810000000	-2.074143000000
C	-2.432320000000	-1.677061000000	-0.187622000000
C	0.815729000000	-0.168961000000	-0.584712000000
C	3.378832000000	1.294333000000	1.636313000000
H	4.317555000000	1.143956000000	1.132281000000
C	0.188162000000	-2.112898000000	2.294173000000
H	0.920715000000	-1.440802000000	2.721241000000
C	-2.585431000000	2.858162000000	-2.037197000000
H	-3.409764000000	2.704353000000	-2.722941000000
C	-1.711303000000	-3.717407000000	1.147129000000
H	-2.472323000000	-4.327211000000	0.678480000000
C	-1.960849000000	4.080604000000	-1.957152000000
H	-2.289544000000	4.902405000000	-2.583246000000
C	3.068981000000	-0.305770000000	-1.028491000000
C	-0.050280000000	-1.308713000000	-2.645484000000
H	0.188942000000	-1.034904000000	-3.672971000000
H	-1.002775000000	-0.874084000000	-2.376030000000
H	-0.095211000000	-2.395572000000	-2.560386000000
C	2.973101000000	-1.483295000000	-3.172357000000
H	2.399735000000	-1.943336000000	-3.966753000000
O	-2.685142000000	1.086751000000	2.710387000000
C	-0.499555000000	3.178167000000	-0.275158000000
H	0.314413000000	3.265212000000	0.434543000000
C	-1.586497000000	-2.372782000000	0.799718000000
C	3.337005000000	1.971063000000	2.847793000000
H	4.254830000000	2.341786000000	3.287622000000
C	-3.784664000000	-0.044234000000	-1.975339000000
H	-4.308096000000	0.598769000000	-2.672089000000
C	-4.148729000000	-1.368144000000	-1.839129000000
H	-4.964103000000	-1.765466000000	-2.432082000000
C	-3.467297000000	-2.220940000000	-0.929408000000
H	-3.750174000000	-3.258742000000	-0.822349000000
C	2.112009000000	2.168042000000	3.478449000000
H	2.033371000000	2.690773000000	4.422446000000
C	4.463196000000	-0.279829000000	-1.059409000000
H	5.061690000000	0.157984000000	-0.276529000000
C	-0.886019000000	4.257340000000	-1.049899000000
H	-0.371979000000	5.204776000000	-0.953541000000
C	4.364972000000	-1.452889000000	-3.200649000000
H	4.891002000000	-1.896519000000	-4.037569000000
C	5.092935000000	-0.861250000000	-2.159617000000
H	6.175696000000	-0.854377000000	-2.203031000000
C	-0.852626000000	-4.259709000000	2.095591000000
H	-0.937391000000	-5.303178000000	2.374503000000

1.9 $\kappa^1\text{C-Fe-CO}^+$

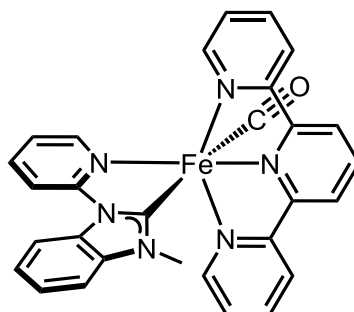


$^1\text{C-Fe-CO}^+$

Fe	0.797466000000	0.032486000000	0.112406000000
O	0.488026000000	0.825006000000	2.924403000000
N	0.976101000000	-1.927506000000	0.515206000000
N	2.686723000000	-0.171595000000	-0.071786000000
N	1.259216000000	1.821647000000	-0.663761000000
N	-2.120253000000	2.095090000000	1.261231000000
N	-2.301164000000	0.153410000000	-0.040183000000
N	-1.322141000000	-0.727528000000	-1.764476000000
C	-0.017096000000	-2.777406000000	0.836778000000
C	0.210732000000	-4.089839000000	1.217620000000
C	1.525817000000	-4.555601000000	1.281788000000
C	2.561155000000	-3.689604000000	0.959673000000
C	2.265312000000	-2.380204000000	0.574657000000
C	3.258045000000	-1.371798000000	0.200551000000
C	4.635945000000	-1.539059000000	0.089284000000
C	5.414404000000	-0.457550000000	-0.324253000000
C	4.809501000000	0.758986000000	-0.641324000000
C	3.427756000000	0.874880000000	-0.514610000000
C	2.599072000000	2.036857000000	-0.836998000000
C	3.089563000000	3.263107000000	-1.289334000000
C	2.199479000000	4.288676000000	-1.575166000000
C	0.832815000000	4.065618000000	-1.394482000000
C	0.407653000000	2.827931000000	-0.937575000000
C	-2.312557000000	2.746787000000	2.414886000000
C	-2.923031000000	2.167525000000	3.524542000000
C	-3.345362000000	0.843223000000	3.435868000000
C	-3.137149000000	0.149521000000	2.247658000000
C	-2.522388000000	0.829561000000	1.200424000000
C	-1.067142000000	-0.114580000000	-0.575541000000
C	-3.327196000000	-0.306587000000	-0.872879000000
C	-4.714619000000	-0.265752000000	-0.770127000000
C	-5.441419000000	-0.829002000000	-1.818392000000
C	-4.801712000000	-1.408030000000	-2.927582000000
C	-3.411809000000	-1.440288000000	-3.029590000000
C	-2.688904000000	-0.875467000000	-1.981507000000
C	-0.303167000000	-1.231504000000	-2.679913000000
C	0.564334000000	0.536929000000	1.807203000000

H	-1.019032000000	-2.373915000000	0.785262000000
H	-0.628397000000	-4.729498000000	1.459978000000
H	1.738165000000	-5.575229000000	1.579843000000
H	3.590217000000	-4.020698000000	1.004784000000
H	5.095136000000	-2.493245000000	0.311534000000
H	6.487919000000	-0.567953000000	-0.415282000000
H	5.402546000000	1.594817000000	-0.988538000000
H	4.155058000000	3.405562000000	-1.413275000000
H	2.562730000000	5.245612000000	-1.930119000000
H	0.102742000000	4.837594000000	-1.602460000000
H	-0.637422000000	2.617837000000	-0.758181000000
H	-1.967073000000	3.775048000000	2.447302000000
H	-3.060604000000	2.742335000000	4.432067000000
H	-3.819251000000	0.353688000000	4.278447000000
H	-3.431175000000	-0.885529000000	2.129725000000
H	-5.205649000000	0.179663000000	0.085575000000
H	-6.524319000000	-0.820123000000	-1.775034000000
H	-5.401261000000	-1.838718000000	-3.721159000000
H	-2.915273000000	-1.884516000000	-3.882953000000
H	-0.568280000000	-0.957665000000	-3.701861000000
H	-0.227782000000	-2.317874000000	-2.601623000000
H	0.655126000000	-0.780473000000	-2.425379000000

1.10 C-Fe-CO⁰

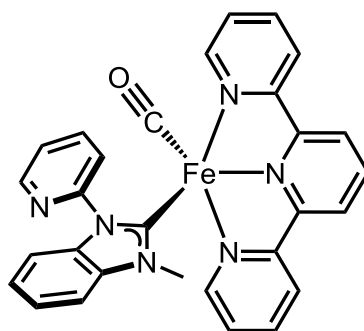


C-Fe-CO⁰

Fe	-0.622001000000	0.115247000000	0.769043000000
N	-0.904698000000	-1.883263000000	0.861525000000
N	-2.088385000000	-0.082270000000	-0.454969000000
N	-0.789616000000	2.041467000000	0.223804000000
N	2.107518000000	-0.031203000000	-0.058322000000
N	1.021005000000	0.288927000000	1.938955000000
N	0.997493000000	-0.340412000000	-1.902257000000
C	-1.873189000000	2.246572000000	-0.697310000000
C	-2.583340000000	1.108800000000	-1.043948000000
C	-1.852170000000	0.431401000000	2.062975000000
C	1.011623000000	0.515919000000	3.266520000000
H	0.039539000000	0.555425000000	3.736343000000
C	-0.451766000000	-4.125259000000	1.577336000000

H	0.157243000000	-4.792427000000	2.174506000000
C	2.218383000000	0.224051000000	1.317282000000
C	2.353182000000	-0.421172000000	-2.235891000000
C	-2.639283000000	-1.284463000000	-0.661929000000
C	0.831693000000	-0.121000000000	-0.589077000000
C	3.424068000000	0.415539000000	1.988511000000
H	4.365439000000	0.391128000000	1.467305000000
C	-0.187423000000	-2.764547000000	1.582914000000
H	0.617258000000	-2.347955000000	2.174974000000
C	-2.107755000000	3.591780000000	-1.165406000000
H	-2.920422000000	3.762996000000	-1.863949000000
C	-2.252025000000	-3.698385000000	0.046651000000
H	-3.072972000000	-4.036919000000	-0.571739000000
C	-1.326557000000	4.629545000000	-0.747156000000
H	-1.517460000000	5.633861000000	-1.112877000000
C	3.084022000000	-0.223199000000	-1.054317000000
C	-0.064103000000	-0.526026000000	-2.888284000000
H	0.170834000000	0.057198000000	-3.778864000000
H	-0.998302000000	-0.182446000000	-2.462740000000
H	-0.141109000000	-1.581911000000	-3.155556000000
C	2.966342000000	-0.661923000000	-3.459647000000
H	2.383921000000	-0.817297000000	-4.358685000000
O	-2.702395000000	0.668607000000	2.792481000000
C	-0.054294000000	3.091510000000	0.610792000000
H	0.742000000000	2.863731000000	1.313662000000
C	-1.936004000000	-2.340645000000	0.090974000000
C	3.391081000000	0.652988000000	3.356373000000
H	4.317162000000	0.804276000000	3.897691000000
C	-3.704790000000	0.947710000000	-1.927418000000
H	-4.124215000000	1.820071000000	-2.417665000000
C	-4.247794000000	-0.290957000000	-2.154063000000
H	-5.094043000000	-0.389306000000	-2.825972000000
C	-3.719374000000	-1.469951000000	-1.511732000000
H	-4.150101000000	-2.446064000000	-1.683989000000
C	2.164156000000	0.696804000000	4.012861000000
H	2.093033000000	0.876034000000	5.077632000000
C	4.477435000000	-0.271725000000	-1.073099000000
H	5.081438000000	-0.143226000000	-0.189129000000
C	-0.249707000000	4.392429000000	0.180649000000
H	0.386720000000	5.191406000000	0.538602000000
C	4.359116000000	-0.701166000000	-3.475566000000
H	4.877298000000	-0.886367000000	-4.409084000000
C	5.097410000000	-0.510670000000	-2.300139000000
H	6.179716000000	-0.552483000000	-2.337143000000
C	-1.506343000000	-4.603425000000	0.794920000000
H	-1.740581000000	-5.660934000000	0.767905000000

1.11 $\kappa^1\text{C-Fe-CO}^0$



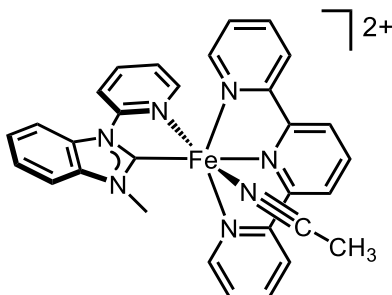
$^1\text{C-Fe-CO}^0$

Fe	-0.799720000000	-0.206607000000	0.467115000000
O	0.105958000000	-1.267095000000	3.015018000000
N	-0.939873000000	1.682578000000	1.027771000000
N	-2.577185000000	0.119926000000	0.037059000000
N	-1.265593000000	-1.931398000000	-0.391727000000
N	2.575045000000	-2.110923000000	0.792728000000
N	2.173840000000	-0.064394000000	-0.290665000000
N	0.845475000000	0.899750000000	-1.710199000000
C	0.055870000000	2.444997000000	1.547281000000
C	-0.117246000000	3.755229000000	1.932675000000
C	-1.392090000000	4.345828000000	1.793343000000
C	-2.420184000000	3.591858000000	1.269176000000
C	-2.188199000000	2.257671000000	0.880225000000
C	-3.150152000000	1.360562000000	0.307683000000
C	-4.486456000000	1.604982000000	0.018194000000
C	-5.270295000000	0.601509000000	-0.565027000000
C	-4.689207000000	-0.639403000000	-0.861307000000
C	-3.353186000000	-0.867708000000	-0.563320000000
C	-2.579950000000	-2.054014000000	-0.801159000000
C	-3.051320000000	-3.248440000000	-1.380115000000
C	-2.193338000000	-4.312946000000	-1.557955000000
C	-0.850309000000	-4.177630000000	-1.147762000000
C	-0.439469000000	-2.992329000000	-0.577859000000
C	3.051301000000	-2.802159000000	1.836143000000
C	3.662117000000	-2.200521000000	2.933527000000
C	3.777421000000	-0.812835000000	2.952549000000
C	3.273517000000	-0.082962000000	1.880528000000
C	2.682500000000	-0.786972000000	0.835804000000
C	0.842250000000	0.159411000000	-0.560227000000
C	3.000070000000	0.541975000000	-1.240045000000
C	4.382980000000	0.601319000000	-1.383607000000
C	4.874505000000	1.315322000000	-2.476682000000
C	4.010722000000	1.943603000000	-3.389515000000
C	2.625093000000	1.878522000000	-3.242269000000
C	2.137882000000	1.163159000000	-2.150792000000
C	-0.336384000000	1.435692000000	-2.375024000000
C	-0.162324000000	-0.845140000000	1.961282000000

H	1.013675000000	1.949616000000	1.643934000000
H	0.719971000000	4.310777000000	2.336689000000
H	-1.559546000000	5.374084000000	2.091727000000
H	-3.409482000000	4.015141000000	1.146500000000
H	-4.918262000000	2.573803000000	0.239981000000
H	-6.312110000000	0.786126000000	-0.795761000000
H	-5.278993000000	-1.419476000000	-1.328023000000
H	-4.088967000000	-3.317548000000	-1.682620000000
H	-2.545400000000	-5.235831000000	-2.003853000000
H	-0.140431000000	-4.986613000000	-1.269544000000
H	0.579396000000	-2.846202000000	-0.241549000000
H	2.940604000000	-3.880689000000	1.786847000000
H	4.034372000000	-2.807841000000	3.749447000000
H	4.242310000000	-0.305557000000	3.789712000000
H	3.323532000000	0.997718000000	1.849498000000
H	5.045184000000	0.119562000000	-0.675158000000
H	5.946008000000	1.387019000000	-2.623158000000
H	4.429493000000	2.491274000000	-4.225894000000
H	1.956919000000	2.363362000000	-3.942976000000
H	-0.269832000000	1.238758000000	-3.446203000000
H	-0.404559000000	2.512779000000	-2.208204000000
H	-1.217486000000	0.948028000000	-1.965760000000

2. *N-trans* complexes

2.1 *N*-Fe-MeCN²⁺

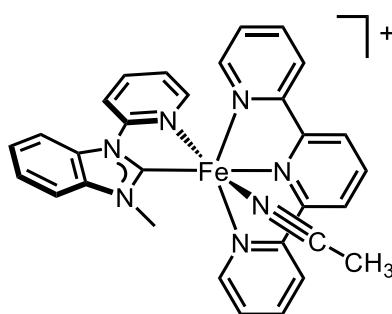


***N*-Fe-MeCN²⁺**

Fe	0.443331000000	-0.060740000000	0.273488000000
C	1.361060000000	-0.122858000000	3.225393000000
N	0.906469000000	-2.005992000000	0.056547000000
N	2.324933000000	0.103482000000	-0.138015000000
N	0.628576000000	1.949709000000	0.332581000000
N	-0.152195000000	0.071672000000	-1.642688000000
N	-2.215268000000	-0.018524000000	-0.651327000000
N	-2.388966000000	-0.352814000000	1.494008000000
C	0.075859000000	-3.050255000000	0.166398000000
C	0.495313000000	-4.363306000000	-0.018530000000
C	1.829291000000	-4.603520000000	-0.330021000000
C	2.701685000000	-3.525267000000	-0.442149000000
C	2.215795000000	-2.236263000000	-0.242326000000
C	3.041305000000	-1.015410000000	-0.330632000000
C	4.409627000000	-0.935713000000	-0.586203000000
C	5.001355000000	0.325209000000	-0.631731000000
C	4.240137000000	1.473411000000	-0.420428000000
C	2.876735000000	1.326429000000	-0.167997000000
C	1.891952000000	2.396656000000	0.086337000000
C	2.197118000000	3.754621000000	0.085863000000
C	1.187264000000	4.676926000000	0.342736000000
C	-0.099945000000	4.215303000000	0.595480000000
C	-0.335359000000	2.844641000000	0.581699000000
C	0.657742000000	0.164320000000	-2.711147000000
C	0.181876000000	0.310434000000	-4.004204000000
C	-1.194902000000	0.364605000000	-4.200743000000
C	-2.046665000000	0.264460000000	-3.108125000000
C	-1.486832000000	0.113580000000	-1.842392000000
C	-1.483158000000	-0.190524000000	0.513580000000
C	-3.596771000000	-0.047281000000	-0.387440000000
C	-4.746575000000	0.090949000000	-1.164040000000
C	-5.977364000000	0.015070000000	-0.512143000000
C	-6.066269000000	-0.191218000000	0.870625000000
C	-4.920246000000	-0.329808000000	1.650236000000
C	-3.693982000000	-0.257090000000	0.998325000000
C	-2.066526000000	-0.575041000000	2.902411000000

N	0.947425000000	-0.129661000000	2.153183000000
H	-0.952222000000	-2.818379000000	0.409630000000
H	-0.217999000000	-5.171464000000	0.080766000000
H	2.188705000000	-5.613863000000	-0.483483000000
H	3.744592000000	-3.682750000000	-0.683296000000
H	4.998850000000	-1.828502000000	-0.744651000000
H	6.062455000000	0.413482000000	-0.830587000000
H	4.698876000000	2.452188000000	-0.451280000000
H	3.207981000000	4.085490000000	-0.111380000000
H	1.406183000000	5.737863000000	0.345666000000
H	-0.915764000000	4.895870000000	0.802430000000
H	-1.321557000000	2.444910000000	0.776072000000
H	1.718150000000	0.121956000000	-2.511578000000
H	0.878852000000	0.380433000000	-4.828837000000
H	-1.609698000000	0.481337000000	-5.194590000000
H	-3.113388000000	0.298497000000	-3.246902000000
H	-4.718801000000	0.258012000000	-2.229384000000
H	-6.884281000000	0.123034000000	-1.095259000000
H	-7.039985000000	-0.240325000000	1.343437000000
H	-4.983085000000	-0.483124000000	2.719518000000
H	-2.912958000000	-1.054102000000	3.389892000000
H	-1.852212000000	0.373952000000	3.395961000000
H	-1.204931000000	-1.231706000000	2.970862000000
C	1.852137000000	-0.116893000000	4.587197000000
H	1.335825000000	0.657278000000	5.159393000000
H	1.667805000000	-1.089800000000	5.048587000000
H	2.925224000000	0.086869000000	4.592116000000

2.2 *N*-Fe-MeCN⁺



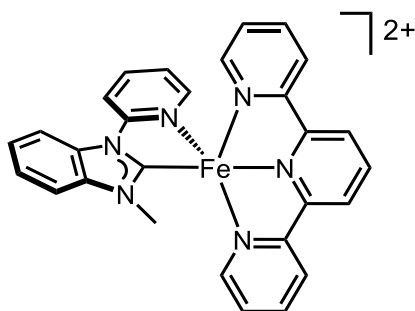
***N*-Fe-MeCN⁺**

Fe	0.443331000000	-0.060740000000	0.273488000000
C	1.361060000000	-0.122858000000	3.225393000000
N	0.906469000000	-2.005992000000	0.056547000000
N	2.324933000000	0.103482000000	-0.138015000000
N	0.628576000000	1.949709000000	0.332581000000
N	-0.152195000000	0.071672000000	-1.642688000000
N	-2.215268000000	-0.018524000000	-0.651327000000
N	-2.388966000000	-0.352814000000	1.494008000000
C	0.075859000000	-3.050255000000	0.166398000000

C	0.495313000000	-4.363306000000	-0.018530000000
C	1.829291000000	-4.603520000000	-0.330021000000
C	2.701685000000	-3.525267000000	-0.442149000000
C	2.215795000000	-2.236263000000	-0.242326000000
C	3.041305000000	-1.015410000000	-0.330632000000
C	4.409627000000	-0.935713000000	-0.586203000000
C	5.001355000000	0.325209000000	-0.631731000000
C	4.240137000000	1.473411000000	-0.420428000000
C	2.876735000000	1.326429000000	-0.167997000000
C	1.891952000000	2.396656000000	0.086337000000
C	2.197118000000	3.754621000000	0.085863000000
C	1.187264000000	4.676926000000	0.342736000000
C	-0.099945000000	4.215303000000	0.595480000000
C	-0.335359000000	2.844641000000	0.581699000000
C	0.657742000000	0.164320000000	-2.711147000000
C	0.181876000000	0.310434000000	-4.004204000000
C	-1.194902000000	0.364605000000	-4.200743000000
C	-2.046665000000	0.264460000000	-3.108125000000
C	-1.486832000000	0.113580000000	-1.842392000000
C	-1.483158000000	-0.190524000000	0.513580000000
C	-3.596771000000	-0.047281000000	-0.387440000000
C	-4.746575000000	0.090949000000	-1.164040000000
C	-5.977364000000	0.015070000000	-0.512143000000
C	-6.066269000000	-0.191218000000	0.870625000000
C	-4.920246000000	-0.329808000000	1.650236000000
C	-3.693982000000	-0.257090000000	0.998325000000
C	-2.066526000000	-0.575041000000	2.902411000000
N	0.947425000000	-0.129661000000	2.153183000000
H	-0.952222000000	-2.818379000000	0.409630000000
H	-0.217999000000	-5.171464000000	0.080766000000
H	2.188705000000	-5.613863000000	-0.483483000000
H	3.744592000000	-3.682750000000	-0.683296000000
H	4.998850000000	-1.828502000000	-0.744651000000
H	6.062455000000	0.413482000000	-0.830587000000
H	4.698876000000	2.452188000000	-0.451280000000
H	3.207981000000	4.085490000000	-0.111380000000
H	1.406183000000	5.737863000000	0.345666000000
H	-0.915764000000	4.895870000000	0.802430000000
H	-1.321557000000	2.444910000000	0.776072000000
H	1.718150000000	0.121956000000	-2.511578000000
H	0.878852000000	0.380433000000	-4.828837000000
H	-1.609698000000	0.481337000000	-5.194590000000
H	-3.113388000000	0.298497000000	-3.246902000000
H	-4.718801000000	0.258012000000	-2.229384000000
H	-6.884281000000	0.123034000000	-1.095259000000
H	-7.039985000000	-0.240325000000	1.343437000000
H	-4.983085000000	-0.483124000000	2.719518000000
H	-2.912958000000	-1.054102000000	3.389892000000
H	-1.852212000000	0.373952000000	3.395961000000
H	-1.204931000000	-1.231706000000	2.970862000000

C	1.852137000000	-0.116893000000	4.587197000000
H	1.335825000000	0.657278000000	5.159393000000
H	1.667805000000	-1.089800000000	5.048587000000
H	2.925224000000	0.086869000000	4.592116000000

2.3 $N\text{-Fe}^{2+}$

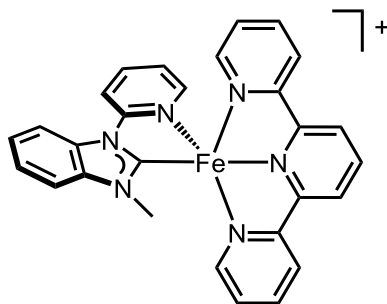


$N\text{-Fe}^{2+}$

Fe	0.500061000000	0.000011000000	-0.541547000000
N	0.840462000000	1.987098000000	-0.532121000000
N	2.432437000000	-0.000050000000	-0.364728000000
N	0.840343000000	-1.987109000000	-0.532073000000
N	0.057004000000	0.000037000000	1.379764000000
N	-2.075553000000	0.000070000000	0.545430000000
N	-2.360625000000	0.000040000000	-1.615493000000
C	-0.075821000000	2.961527000000	-0.610078000000
C	0.260581000000	4.310309000000	-0.566674000000
C	1.599039000000	4.663134000000	-0.437006000000
C	2.559636000000	3.658548000000	-0.353562000000
C	2.155272000000	2.328962000000	-0.404959000000
C	3.077788000000	1.177298000000	-0.331220000000
C	4.467685000000	1.211015000000	-0.237017000000
C	5.156121000000	-0.000127000000	-0.187017000000
C	4.467614000000	-1.211230000000	-0.236988000000
C	3.077718000000	-1.177434000000	-0.331195000000
C	2.155135000000	-2.329046000000	-0.404920000000
C	2.559423000000	-3.658655000000	-0.353532000000
C	1.598770000000	-4.663188000000	-0.436978000000
C	0.260331000000	-4.310288000000	-0.566638000000
C	-0.075995000000	-2.961486000000	-0.610032000000
C	0.951289000000	0.000022000000	2.383049000000
C	0.575915000000	0.000024000000	3.716597000000
C	-0.781773000000	0.000044000000	4.025154000000
C	-1.719369000000	0.000063000000	2.999488000000
C	-1.262173000000	0.000057000000	1.686072000000
C	-1.414103000000	0.000056000000	-0.668272000000
C	-3.468845000000	0.000058000000	0.350681000000
C	-4.575205000000	0.000063000000	1.196374000000
C	-5.837740000000	0.000049000000	0.600777000000
C	-5.997699000000	0.000032000000	-0.791304000000

C	-4.892649000000	0.000029000000	-1.641282000000
C	-3.637753000000	0.000041000000	-1.045998000000
C	-2.078662000000	0.000005000000	-3.046020000000
H	-1.104748000000	2.642004000000	-0.707644000000
H	-0.518804000000	5.058400000000	-0.633966000000
H	1.895722000000	5.704274000000	-0.399196000000
H	3.607742000000	3.906209000000	-0.251133000000
H	5.001396000000	2.150903000000	-0.207089000000
H	6.236793000000	-0.000158000000	-0.113723000000
H	5.001271000000	-2.151147000000	-0.207035000000
H	3.607516000000	-3.906379000000	-0.251113000000
H	1.895395000000	-5.704344000000	-0.399179000000
H	-0.519096000000	-5.058334000000	-0.633934000000
H	-1.104904000000	-2.641904000000	-0.707592000000
H	1.991068000000	0.000005000000	2.092046000000
H	1.335086000000	0.000010000000	4.487576000000
H	-1.115050000000	0.000047000000	5.055773000000
H	-2.773666000000	0.000080000000	3.221285000000
H	-4.485855000000	0.000077000000	2.272257000000
H	-6.714446000000	0.000051000000	1.237618000000
H	-6.995103000000	0.000022000000	-1.214473000000
H	-5.000816000000	0.000016000000	-2.718581000000
H	-2.504672000000	0.891532000000	-3.508725000000
H	-2.504680000000	-0.891540000000	-3.508682000000
H	-0.997381000000	-0.000004000000	-3.174714000000

2.4 $N\text{-Fe}^+$

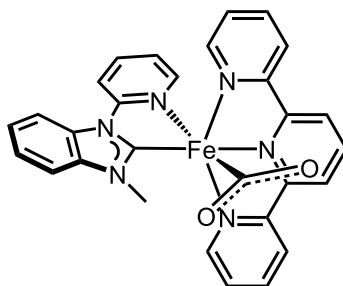


$N\text{-Fe}^+$

Fe	0.537754000000	0.000026000000	-0.441638000000
N	0.874990000000	1.964649000000	-0.530683000000
N	2.430162000000	0.000399000000	-0.380292000000
N	0.875741000000	-1.964425000000	-0.531126000000
N	-0.022066000000	-0.000470000000	1.489001000000
N	-2.104731000000	-0.000073000000	0.540387000000
N	-2.297275000000	-0.000299000000	-1.632089000000
C	-0.046749000000	2.949435000000	-0.611522000000
C	0.276624000000	4.293247000000	-0.582864000000
C	1.624176000000	4.663613000000	-0.460021000000
C	2.584852000000	3.671150000000	-0.369134000000

C	2.198698000000	2.325196000000	-0.406620000000
C	3.105022000000	1.191757000000	-0.331468000000
C	4.491804000000	1.212301000000	-0.236807000000
C	5.191130000000	0.000882000000	-0.189934000000
C	4.492230000000	-1.210789000000	-0.236885000000
C	3.105449000000	-1.190700000000	-0.331559000000
C	2.199537000000	-2.324488000000	-0.406866000000
C	2.586189000000	-3.670295000000	-0.369316000000
C	1.625880000000	-4.663105000000	-0.460362000000
C	0.278217000000	-4.293224000000	-0.583441000000
C	-0.045643000000	-2.949531000000	-0.612143000000
C	0.822604000000	-0.000827000000	2.532490000000
C	0.383537000000	-0.000939000000	3.847552000000
C	-0.989149000000	-0.000667000000	4.087155000000
C	-1.876296000000	-0.000343000000	3.016183000000
C	-1.352068000000	-0.000296000000	1.726368000000
C	-1.384079000000	-0.000226000000	-0.646667000000
C	-3.487518000000	-0.000148000000	0.283775000000
C	-4.632282000000	-0.000026000000	1.077498000000
C	-5.868345000000	-0.000050000000	0.427018000000
C	-5.966655000000	-0.000178000000	-0.970149000000
C	-4.823647000000	-0.000274000000	-1.769383000000
C	-3.596084000000	-0.000264000000	-1.119389000000
C	-1.961285000000	-0.000723000000	-3.049866000000
H	-1.074884000000	2.623875000000	-0.702581000000
H	-0.508516000000	5.035237000000	-0.656308000000
H	1.910404000000	5.708277000000	-0.434313000000
H	3.632390000000	3.925609000000	-0.269290000000
H	5.024844000000	2.153946000000	-0.203086000000
H	6.271754000000	0.001074000000	-0.118868000000
H	5.025580000000	-2.152258000000	-0.203226000000
H	3.633804000000	-3.924361000000	-0.269272000000
H	1.912473000000	-5.707667000000	-0.434591000000
H	-0.506643000000	-5.035497000000	-0.657014000000
H	-1.073874000000	-2.624311000000	-0.703361000000
H	1.875332000000	-0.001003000000	2.281599000000
H	1.101776000000	-0.001215000000	4.657134000000
H	-1.373490000000	-0.000709000000	5.099969000000
H	-2.939355000000	-0.000130000000	3.190464000000
H	-4.594007000000	0.000074000000	2.156107000000
H	-6.772115000000	0.000037000000	1.025032000000
H	-6.944125000000	-0.000189000000	-1.437861000000
H	-4.884513000000	-0.000370000000	-2.850426000000
H	-2.368817000000	0.890434000000	-3.530365000000
H	-2.368498000000	-0.892359000000	-3.529754000000
H	-0.875754000000	-0.000565000000	-3.135658000000

2.5 $N\text{-Fe-CO}_2^0$

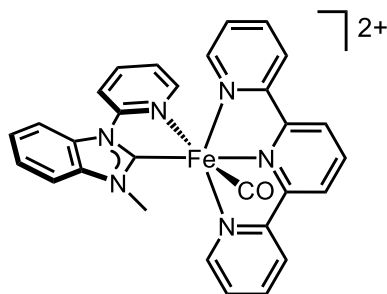


$N\text{-Fe-CO}_2^0$

N	-0.103579000	0.467380000	1.554889000
C	-1.415157000	0.731415000	1.699164000
C	-1.939920000	1.304494000	2.857765000
C	-1.072500000	1.572331000	3.910453000
C	0.282290000	1.273147000	3.778911000
C	0.721681000	0.732735000	2.579464000
N	-2.159907000	0.380776000	0.564219000
C	-1.451409000	-0.038227000	-0.572417000
N	-2.416319000	-0.384979000	-1.459868000
C	-3.695859000	-0.225278000	-0.926971000
C	-3.546814000	0.266855000	0.379102000
C	-4.942918000	-0.487639000	-1.483378000
C	-6.062306000	-0.241189000	-0.688666000
C	-5.922637000	0.241811000	0.618096000
C	-4.667952000	0.501708000	1.174236000
Fe	0.486043000	-0.092292000	-0.347196000
N	0.626969000	-2.008839000	0.154806000
C	1.899415000	-2.418250000	0.430703000
C	2.184306000	-3.733661000	0.802329000
C	1.151839000	-4.658432000	0.883000000
C	-0.147970000	-4.238062000	0.599004000
C	-0.361750000	-2.912460000	0.246139000
C	2.900712000	-1.354208000	0.321415000
N	2.343615000	-0.166001000	-0.004278000
C	3.095755000	0.952602000	-0.117543000
C	4.472788000	0.908501000	0.083323000
C	5.064105000	-0.314932000	0.404644000
C	4.276363000	-1.458123000	0.528825000
C	2.279795000	2.118136000	-0.478909000
N	0.963552000	1.820502000	-0.669336000
C	0.131614000	2.812589000	-1.018989000
C	0.551351000	4.125411000	-1.188686000
C	1.897124000	4.433958000	-0.992158000
C	2.771038000	3.415023000	-0.633265000
C	-2.203601000	-0.948807000	-2.788431000
C	0.959516000	-0.512853000	-2.302159000
H	6.134448000	-0.374845000	0.559885000
H	4.725537000	-2.409508000	0.781892000

H	5.073946000	1.802906000	-0.014318000
H	3.202826000	-4.024770000	1.024279000
H	1.354850000	-5.684804000	1.164888000
H	-1.356062000	-2.552630000	0.018104000
H	-0.986741000	-4.921269000	0.647797000
H	3.821799000	3.619047000	-0.474073000
H	2.257934000	5.448109000	-1.115915000
H	-0.902470000	2.532689000	-1.165943000
H	-0.166496000	4.885417000	-1.471214000
H	-6.806604000	0.418440000	1.219803000
H	-7.051993000	-0.431942000	-1.086895000
H	-5.038501000	-0.872008000	-2.490722000
H	-4.600190000	0.861672000	2.188932000
H	-2.406455000	-2.022491000	-2.772976000
H	-2.883930000	-0.468104000	-3.493589000
H	-1.180493000	-0.754950000	-3.091156000
H	-2.983852000	1.557741000	2.938796000
H	-1.456553000	2.016573000	4.820985000
H	1.766172000	0.502048000	2.415074000
H	0.986499000	1.462564000	4.578769000
O	0.730048000	0.375134000	-3.177383000
O	1.498141000	-1.630600000	-2.543662000

2.6 $N\text{-Fe-CO}^{2+}$

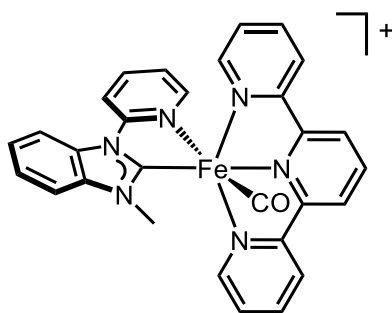


$N\text{-Fe-CO}^{2+}$

Fe	-0.477415000000	-0.032966000000	-0.517611000000
O	-1.019537000000	-0.062066000000	-3.403118000000
N	-0.881236000000	-1.999474000000	-0.366504000000
N	-2.384907000000	0.055777000000	-0.191933000000
N	-0.720245000000	1.968523000000	-0.481823000000
N	-0.037960000000	0.031830000000	1.481077000000
N	2.097617000000	-0.013085000000	0.649895000000
N	2.446735000000	-0.189848000000	-1.493369000000
C	-0.006506000000	-3.007374000000	-0.470277000000
C	-0.386498000000	-4.338185000000	-0.336912000000
C	-1.722449000000	-4.633540000000	-0.089463000000
C	-2.638892000000	-3.591385000000	0.013579000000
C	-2.193812000000	-2.281254000000	-0.132111000000

C	-3.064209000000	-1.092951000000	-0.043416000000
C	-4.437879000000	-1.063348000000	0.190093000000
C	-5.068605000000	0.176626000000	0.269978000000
C	-4.340314000000	1.355737000000	0.123105000000
C	-2.970079000000	1.261737000000	-0.114918000000
C	-2.007849000000	2.368242000000	-0.280419000000
C	-2.348328000000	3.716037000000	-0.233757000000
C	-1.351151000000	4.673712000000	-0.391747000000
C	-0.040016000000	4.258005000000	-0.593789000000
C	0.233350000000	2.895302000000	-0.635432000000
C	-0.929123000000	0.077522000000	2.484982000000
C	-0.556269000000	0.141228000000	3.817621000000
C	0.800402000000	0.161589000000	4.124010000000
C	1.735492000000	0.115301000000	3.097792000000
C	1.275884000000	0.048958000000	1.786053000000
C	1.470343000000	-0.104905000000	-0.577181000000
C	3.496478000000	-0.024292000000	0.496636000000
C	4.577886000000	0.050963000000	1.374161000000
C	5.856995000000	0.018134000000	0.822086000000
C	6.060266000000	-0.085971000000	-0.560686000000
C	4.984239000000	-0.163347000000	-1.440000000000
C	3.707827000000	-0.133449000000	-0.887511000000
C	2.229432000000	-0.320427000000	-2.934549000000
C	-0.758780000000	-0.060763000000	-2.293336000000
H	1.021068000000	-2.732131000000	-0.665106000000
H	0.359171000000	-5.117435000000	-0.427676000000
H	-2.050651000000	-5.659933000000	0.020646000000
H	-3.684471000000	-3.792493000000	0.204914000000
H	-5.000288000000	-1.978779000000	0.311034000000
H	-6.134817000000	0.224662000000	0.454170000000
H	-4.828605000000	2.317877000000	0.195362000000
H	-3.376737000000	4.011850000000	-0.077097000000
H	-1.598678000000	5.727681000000	-0.357308000000
H	0.766737000000	4.968150000000	-0.720916000000
H	1.238585000000	2.529948000000	-0.795629000000
H	-1.971306000000	0.062010000000	2.205860000000
H	-1.316081000000	0.174209000000	4.587141000000
H	1.136551000000	0.212088000000	5.152482000000
H	2.787299000000	0.130335000000	3.324222000000
H	4.460925000000	0.134073000000	2.442983000000
H	6.712426000000	0.076869000000	1.484453000000
H	7.069788000000	-0.104694000000	-0.953476000000
H	5.137714000000	-0.239378000000	-2.508271000000
H	3.178759000000	-0.530428000000	-3.420049000000
H	1.821699000000	0.606598000000	-3.337245000000
H	1.552958000000	-1.150903000000	-3.126600000000

2.7 $N\text{-Fe-CO}^+$

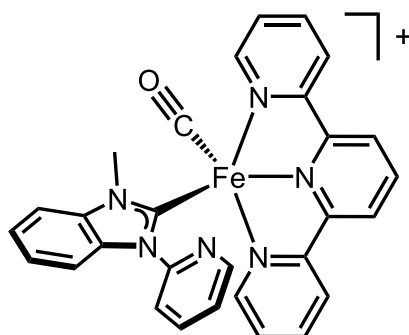


$N\text{-Fe-CO}^+$

Fe	-0.476415000000	-0.053690000000	-0.533317000000
O	-1.048149000000	-0.060147000000	-3.394352000000
N	-0.922959000000	-2.012481000000	-0.337862000000
N	-2.367903000000	0.066658000000	-0.180772000000
N	-0.675215000000	1.944742000000	-0.516809000000
N	-0.032060000000	0.047774000000	1.488851000000
N	2.098858000000	-0.025728000000	0.654047000000
N	2.447846000000	-0.269140000000	-1.482806000000
C	-0.066623000000	-3.042708000000	-0.435712000000
C	-0.465171000000	-4.362614000000	-0.288078000000
C	-1.810605000000	-4.633517000000	-0.032178000000
C	-2.705271000000	-3.576206000000	0.062695000000
C	-2.243271000000	-2.268736000000	-0.095047000000
C	-3.087287000000	-1.066970000000	-0.015656000000
C	-4.448259000000	-1.015511000000	0.221481000000
C	-5.066682000000	0.259700000000	0.282603000000
C	-4.321820000000	1.413048000000	0.113239000000
C	-2.935612000000	1.319334000000	-0.125497000000
C	-1.986517000000	2.371673000000	-0.307548000000
C	-2.280179000000	3.755512000000	-0.289201000000
C	-1.276212000000	4.678789000000	-0.469906000000
C	0.050247000000	4.228451000000	-0.679592000000
C	0.287439000000	2.867647000000	-0.698566000000
C	-0.925234000000	0.133473000000	2.485479000000
C	-0.553747000000	0.245003000000	3.816722000000
C	0.803371000000	0.270075000000	4.123132000000
C	1.740772000000	0.183550000000	3.100722000000
C	1.279637000000	0.072747000000	1.791482000000
C	1.467067000000	-0.151530000000	-0.571204000000
C	3.497140000000	-0.043718000000	0.500327000000
C	4.579417000000	0.058781000000	1.373845000000
C	5.859249000000	0.007423000000	0.822835000000
C	6.061851000000	-0.141248000000	-0.555593000000
C	4.984445000000	-0.245005000000	-1.431628000000
C	3.708341000000	-0.196118000000	-0.880399000000
C	2.228772000000	-0.430228000000	-2.919266000000
C	-0.770147000000	-0.079697000000	-2.284263000000

H	0.964479000000	-2.785935000000	-0.638788000000
H	0.266674000000	-5.155747000000	-0.372988000000
H	-2.155386000000	-5.653366000000	0.089587000000
H	-3.754191000000	-3.756274000000	0.258668000000
H	-5.026174000000	-1.918661000000	0.361538000000
H	-6.131968000000	0.328016000000	0.467659000000
H	-4.799182000000	2.383857000000	0.165634000000
H	-3.302316000000	4.076760000000	-0.130466000000
H	-1.499794000000	5.739297000000	-0.453342000000
H	0.868875000000	4.921156000000	-0.825452000000
H	1.286000000000	2.480850000000	-0.861733000000
H	-1.964381000000	0.110801000000	2.192722000000
H	-1.312617000000	0.310278000000	4.585320000000
H	1.138559000000	0.356280000000	5.149714000000
H	2.792520000000	0.201760000000	3.328173000000
H	4.462946000000	0.177526000000	2.439443000000
H	6.714902000000	0.087302000000	1.482793000000
H	7.071172000000	-0.173535000000	-0.948255000000
H	5.136586000000	-0.355077000000	-2.497260000000
H	3.167722000000	-0.702816000000	-3.394615000000
H	1.866389000000	0.503033000000	-3.351089000000
H	1.510501000000	-1.229554000000	-3.090132000000

2.8 $\kappa^1N\text{-Fe-CO}^+$

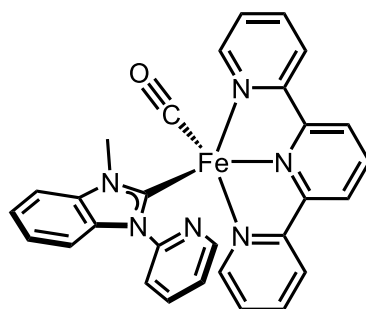


$^1N\text{-Fe-CO}^+$

Fe	0.589805000000	0.471913000000	-0.724674000000
O	0.849783000000	1.287230000000	-3.538771000000
N	1.166722000000	2.167523000000	0.196071000000
N	2.362390000000	-0.024601000000	-0.193932000000
N	0.550130000000	-1.486601000000	-1.173045000000
N	-0.263826000000	-0.576257000000	2.149068000000
N	-1.974250000000	-0.185629000000	0.592229000000
N	-2.377617000000	1.302177000000	-0.938377000000
C	0.441710000000	3.287406000000	0.368279000000
C	0.962895000000	4.444306000000	0.926659000000
C	2.298729000000	4.456742000000	1.330480000000
C	3.057585000000	3.305957000000	1.169672000000

C	2.470557000000	2.170964000000	0.607624000000
C	3.152263000000	0.888221000000	0.420482000000
C	4.435903000000	0.545652000000	0.838307000000
C	4.882445000000	-0.760102000000	0.636041000000
C	4.042245000000	-1.702408000000	0.043560000000
C	2.770201000000	-1.305958000000	-0.361372000000
C	1.729325000000	-2.143558000000	-0.960500000000
C	1.885441000000	-3.489463000000	-1.295017000000
C	0.821595000000	-4.178279000000	-1.860950000000
C	-0.376550000000	-3.499908000000	-2.089427000000
C	-0.467372000000	-2.163100000000	-1.736422000000
C	0.461035000000	-1.416320000000	2.899696000000
C	0.194555000000	-2.779753000000	2.988150000000
C	-0.876908000000	-3.295264000000	2.261579000000
C	-1.627472000000	-2.436497000000	1.465342000000
C	-1.268268000000	-1.090724000000	1.444768000000
C	-1.365856000000	0.601155000000	-0.365148000000
C	-3.359518000000	0.003554000000	0.599033000000
C	-4.385378000000	-0.539281000000	1.368143000000
C	-5.679497000000	-0.096435000000	1.098062000000
C	-5.935720000000	0.857407000000	0.098834000000
C	-4.904567000000	1.406265000000	-0.661759000000
C	-3.613081000000	0.962201000000	-0.388718000000
C	-2.241332000000	2.247100000000	-2.041304000000
C	0.732892000000	1.004950000000	-2.422236000000
H	-0.588804000000	3.238498000000	0.047622000000
H	0.328951000000	5.314163000000	1.042753000000
H	2.737955000000	5.345774000000	1.766704000000
H	4.094541000000	3.282220000000	1.477475000000
H	5.070178000000	1.274268000000	1.325315000000
H	5.875820000000	-1.047647000000	0.957707000000
H	4.368603000000	-2.725394000000	-0.088818000000
H	2.830625000000	-3.984667000000	-1.115087000000
H	0.924649000000	-5.224180000000	-2.123717000000
H	-1.231610000000	-3.995134000000	-2.531583000000
H	-1.376696000000	-1.600139000000	-1.897684000000
H	1.284286000000	-0.974429000000	3.451335000000
H	0.811903000000	-3.416367000000	3.609757000000
H	-1.115152000000	-4.351702000000	2.297584000000
H	-2.447781000000	-2.794338000000	0.857538000000
H	-4.189268000000	-1.273717000000	2.138245000000
H	-6.505641000000	-0.498901000000	1.672610000000
H	-6.955849000000	1.174234000000	-0.084228000000
H	-5.097557000000	2.144013000000	-1.430216000000
H	-2.867969000000	3.117660000000	-1.845653000000
H	-2.550384000000	1.779688000000	-2.978517000000
H	-1.205990000000	2.563245000000	-2.112705000000

2.9 $\kappa^1N\text{-Fe-CO}^0$



$^1N\text{-Fe-CO}^0$

Fe	0.435669000000	0.329773000000	-1.219293000000
O	0.158284000000	0.835798000000	-4.069781000000
N	0.701818000000	2.188591000000	-0.594421000000
N	2.013311000000	0.117101000000	-0.260048000000
N	0.677445000000	-1.622008000000	-1.394638000000
N	-0.093146000000	0.428130000000	2.438578000000
N	-1.599301000000	-0.272418000000	0.779758000000
N	-2.649504000000	0.431339000000	-0.981553000000
C	-0.113327000000	3.244887000000	-0.836316000000
C	0.138125000000	4.516092000000	-0.368939000000
C	1.300578000000	4.744157000000	0.396428000000
C	2.143231000000	3.684259000000	0.658714000000
C	1.835334000000	2.402399000000	0.164498000000
C	2.606090000000	1.206209000000	0.368571000000
C	3.782399000000	1.056489000000	1.089292000000
C	4.383582000000	-0.205160000000	1.190445000000
C	3.785478000000	-1.304501000000	0.562863000000
C	2.606484000000	-1.136156000000	-0.149600000000
C	1.820680000000	-2.136657000000	-0.814341000000
C	2.108898000000	-3.513206000000	-0.881739000000
C	1.235927000000	-4.369335000000	-1.518473000000
C	0.063251000000	-3.838991000000	-2.097950000000
C	-0.165798000000	-2.483606000000	-2.017082000000
C	0.892603000000	0.163791000000	3.304807000000
C	1.447593000000	-1.104191000000	3.466379000000
C	0.950295000000	-2.151036000000	2.693360000000
C	-0.072922000000	-1.890574000000	1.788170000000
C	-0.538777000000	-0.583430000000	1.695695000000
C	-1.396355000000	0.187108000000	-0.499119000000
C	-2.953664000000	-0.326383000000	1.102930000000
C	-3.632518000000	-0.711918000000	2.254597000000
C	-5.025141000000	-0.639673000000	2.219752000000
C	-5.706566000000	-0.197407000000	1.073325000000
C	-5.019926000000	0.191152000000	-0.077484000000
C	-3.629215000000	0.120681000000	-0.039248000000
C	-2.975829000000	0.923031000000	-2.313269000000
C	0.185782000000	0.651219000000	-2.916542000000

H	-0.991047000000	3.024203000000	-1.430328000000
H	-0.553738000000	5.317943000000	-0.595131000000
H	1.527519000000	5.734407000000	0.773639000000
H	3.042512000000	3.825588000000	1.245564000000
H	4.228781000000	1.913758000000	1.578954000000
H	5.299708000000	-0.329704000000	1.754364000000
H	4.231387000000	-2.288593000000	0.644340000000
H	3.014753000000	-3.888069000000	-0.421506000000
H	1.445199000000	-5.431350000000	-1.570134000000
H	-0.652975000000	-4.475230000000	-2.602973000000
H	-1.048556000000	-2.030438000000	-2.450860000000
H	1.253382000000	1.002685000000	3.891199000000
H	2.249596000000	-1.260075000000	4.177058000000
H	1.356962000000	-3.151252000000	2.784253000000
H	-0.485119000000	-2.660830000000	1.150310000000
H	-3.100714000000	-1.051708000000	3.134652000000
H	-5.592865000000	-0.931121000000	3.095927000000
H	-6.789703000000	-0.157120000000	1.082150000000
H	-5.545252000000	0.531316000000	-0.961096000000
H	-3.763726000000	1.673338000000	-2.235866000000
H	-3.318958000000	0.103815000000	-2.949285000000
H	-2.092924000000	1.377318000000	-2.747444000000