Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information
for
Choosing the right precursor for thermal decomposition solution-phase synthesis of iron nanoparticles: Tunable dissociation energies of ferrocene derivatives

*Cameron H. W. Kelly and Matthias Lein**

Structural Data (Cartesian coordinates in Å) for all compounds considered.

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24
Energy: -1060191.0071752
Fe          0.04431         0.14356         0.00000
C           1.09035        -1.10567         1.21235
C           1.79893        -0.90900         0.00000
C          -0.23500        -1.56350         1.15395
H           1.51888        -0.74278         2.13978
C           1.09035        -1.10567        -1.21235
C          -0.23500        -1.56350        -1.15395
H           1.51888        -0.74278        -2.13978
C          -0.67149        -2.42303         0.00000
H          -1.75898        -2.51906         0.00000
H          -0.25286        -3.44336         0.00000
C          -1.48866         1.32762         0.70728
C          -0.23500         1.83744         1.14770
C          -1.48866         1.32762        -0.70728
H          -2.28998         0.97918         1.34068
C           0.53475         2.15516         0.00000
H           0.07881         1.94808         2.17471
C          -0.23500         1.83744        -1.14770
H          -2.28998         0.97918        -1.34068
H           1.54086         2.54716         0.00000
H           0.07881         1.94808        -2.17471
H          -0.82164        -1.54682        -2.06612
H          -0.82164        -1.54682         2.06612
H           2.79326        -0.48213         0.00000


21
Energy: -3342097.3309190
Fe          0.00000         0.00000         0.30759
C          -1.54646         0.89997         1.28989
C          -0.38839         1.71776         1.33169
C          -1.88414         0.71105        -0.07506
H          -2.06987         0.48996         2.13917
C           0.00000         2.02858        -0.00278
C          -0.92979         1.39626        -0.87945
C           0.38839        -1.71776         1.33169
C           0.00000        -2.02858        -0.00278
C           1.54646        -0.89997         1.28989
C           0.92979        -1.39626        -0.87945
C           1.88414        -0.71105        -0.07506
H           2.06987        -0.48996         2.13917
Cl         -3.25492        -0.11047        -0.65800
Cl         -0.96656         1.54937        -2.56752
Cl          1.25506         3.07001        -0.46596
Cl         -1.25506        -3.07001        -0.46596
Cl          0.96656        -1.54937        -2.56752
Cl          3.25492         0.11047        -0.65800
Cl         -0.36458        -2.31030         2.74304
Cl          0.36458         2.31030         2.74304


21
Energy: -3342097.2072996
Fe          0.00000         0.00000         0.12038
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C          0.00000       -2.01101        0.49423
C         -0.94080       -1.35858        1.33171
C         -0.38200       -1.76525       -0.84932
H          0.84839       -2.59198        0.81988
C         -1.88748       -0.68341        0.50988
C         -1.54479       -0.94306       -0.84926
C          1.88748        0.68341        0.50988
C          1.54479        0.94306       -0.84926
C          0.94080        1.35858        1.33171
C          0.38200        1.76525       -0.84932
C          0.00000        2.01101        0.49423
H         -0.84839        2.59198        0.81988
Cl        -3.25911        0.16412        1.04672
Cl        -2.44111       -0.47255       -2.20910
Cl         0.35743       -2.42443       -2.23223
Cl         0.99643        1.44939        3.02941
Cl         3.25911       -0.16412        1.04672
Cl         2.44111        0.47255       -2.20910
Cl        -0.35743        2.42443       -2.23223
Cl        -0.99643       -1.44939        3.02941


21
Energy: -2188832.4442279
Fe         0.73576       -0.14051        0.00000
C          0.06123        1.78313        0.00000
C         -0.40789        1.08564       -1.14370
C         -0.40789        1.08564        1.14370
H          0.65912        2.68025        0.00000
C         -1.16139       -0.04371       -0.71331
C         -1.16139       -0.04371        0.71331
C          2.78554       -0.07023        0.00000
C          2.31549       -0.75988        1.14906
C          2.31549       -0.75988       -1.14906
H          3.36825        0.83830        0.00000
C          1.55689       -1.87655        0.70990
H          2.46684       -0.46047        2.17520
C          1.55689       -1.87655       -0.70990
H          2.46684       -0.46047       -2.17520
H          1.02924       -2.57323        1.34379
H          1.02924       -2.57323       -1.34379
Cl        -2.01358       -1.12640       -1.71227
Cl        -2.01358       -1.12640        1.71227
Cl        -0.18839        1.56930       -2.76732
Cl        -0.18839        1.56930        2.76732


21
Energy: -3342096.9212244
Fe         0.00000        0.00000        0.40861
C          0.00000        1.63706        1.63502
C          1.14398        1.65649        0.79657
C         -1.14398        1.65649        0.79657
H          0.00000        1.63235        2.71325
C          0.71281        1.66484       -0.56000
C         -0.71281        1.66484       -0.56000
C          0.00000       -1.63706        1.63502
C         -1.14398       -1.65649        0.79657
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C          1.14398       -1.65649        0.79657
H          0.00000       -1.63235        2.71325
C         -0.71281       -1.66484       -0.56000
C          0.71281       -1.66484       -0.56000
Cl        -1.70682        1.79742       -1.92691
Cl        -2.75943        1.76719        1.31885
Cl         1.70682        1.79742       -1.92691
Cl         2.75943        1.76719        1.31885
Cl         2.75943       -1.76719        1.31885
Cl         1.70682       -1.79742       -1.92691
Cl        -1.70682       -1.79742       -1.92691
Cl        -2.75943       -1.76719        1.31885
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21
Energy: -3342097.3309190
Fe         0.00000        0.00000        0.30759
C          0.00000        2.02858       -0.00277
C         -0.92978        1.39627       -0.87945
C         -0.38839        1.71775        1.33169
C         -1.88414        0.71105       -0.07507
C         -1.54647        0.89996        1.28988
H         -2.06989        0.48995        2.13916
C          0.92978       -1.39627       -0.87945
C          1.88414       -0.71105       -0.07507
C          0.00000       -2.02858       -0.00277
C          1.54647       -0.89996        1.28988
C          0.38839       -1.71775        1.33169
H          2.06989       -0.48995        2.13916
Cl         3.25492        0.11046       -0.65804
Cl         1.25507        3.07000       -0.46594
Cl        -0.36454       -2.31029        2.74306
Cl        -1.25507       -3.07000       -0.46594
Cl        -3.25492       -0.11046       -0.65804
Cl         0.36454        2.31029        2.74306
Cl        -0.96654        1.54937       -2.56752
Cl         0.96654       -1.54937       -2.56752
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21
Energy: -3342097.2359204
Fe         0.00000        0.00000        0.00000
C          1.62905        1.01135        0.71313
C          1.62905        1.01135       -0.71313
C          0.42772        1.64170        1.14399
C          0.42772        1.64170       -1.14399
C         -0.32121        2.02060        0.00000
H         -1.28422        2.50611        0.00000
C         -0.42772       -1.64170       -1.14399
C          0.32121       -2.02060        0.00000
C         -1.62905       -1.01135       -0.71313
C         -0.42772       -1.64170        1.14399
H          1.28422       -2.50611        0.00000
C         -1.62905       -1.01135        0.71313
Cl         2.88663        0.45696        1.70977
Cl         0.00000        1.94820        2.76282
Cl         0.00000       -1.94820        2.76282
Cl        -2.88663       -0.45696        1.70977
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Cl        -2.88663       -0.45696       -1.70977
Cl         0.00000       -1.94820       -2.76282
Cl         2.88663        0.45696       -1.70977
Cl         0.00000        1.94820       -2.76282


21
Energy: -2188832.0719642
Fe         0.73115        0.13772        0.00000
C         -1.16641        0.03640        0.71319
C         -1.16641        0.03640       -0.71319
C         -0.41167       -1.09165        1.14336
C         -0.41167       -1.09165       -1.14336
C          0.05807       -1.78860        0.00000
H          0.65990       -2.68313        0.00000
C          1.88850        1.38184       -1.14864
C          1.41462        2.06881        0.00000
C          2.65311        0.26976       -0.71021
H          1.66367        1.63167       -2.17459
C          1.88850        1.38184        1.14864
H          0.76783        2.93319        0.00000
C          2.65311        0.26976        0.71021
H          3.11642       -0.46962       -1.34587
H          1.66367        1.63167        2.17459
H          3.11642       -0.46962        1.34587
Cl        -2.00823        1.12641        1.71240
Cl        -0.17989       -1.56736        2.76720
Cl        -0.17989       -1.56736       -2.76720
Cl        -2.00823        1.12641       -1.71240


21
Energy: -3342097.3309190
Fe         0.00000        0.00000       -0.30759
C         -0.92979        1.39626        0.87945
C          0.00000        2.02858        0.00277
C         -1.88414        0.71105        0.07506
C         -0.38839        1.71776       -1.33169
C         -1.54646        0.89996       -1.28988
H         -2.06988        0.48995       -2.13917
C          1.88414       -0.71105        0.07506
C          0.92979       -1.39626        0.87945
C          1.54646       -0.89996       -1.28988
C          0.00000       -2.02858        0.00277
C          0.38839       -1.71776       -1.33169
H          2.06988       -0.48995       -2.13917
Cl        -3.25492       -0.11047        0.65802
Cl        -0.96655        1.54938        2.56752
Cl         1.25506        3.07001        0.46595
Cl         0.96655       -1.54938        2.56752
Cl         3.25492        0.11047        0.65802
Cl        -1.25506       -3.07001        0.46595
Cl        -0.36456       -2.31029       -2.74305
Cl         0.36456        2.31029       -2.74305


21
Energy: -2477148.0901796
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Fe          0.00000         0.00000         0.78437
C           0.00000        -1.21212        -0.84048
C          -1.15280        -0.37457        -0.84048
C           1.15280        -0.37457        -0.84048
C          -0.71247         0.98063        -0.84048
C           0.71247         0.98063        -0.84048
C           0.00000        -1.20775         2.44051
C           1.14864        -0.37322         2.44051
C          -1.14864        -0.37322         2.44051
H           0.00000        -2.28641         2.39567
C           0.70990         0.97709         2.44051
H           2.17451        -0.70654         2.39567
C          -0.70990         0.97709         2.44051
H          -2.17451        -0.70654         2.39567
H           1.34392         1.84975         2.39567
H          -1.34392         1.84975         2.39567
Cl          1.71069         2.35456        -0.94556
Cl          2.76796        -0.89936        -0.94556
Cl         -1.71069         2.35456        -0.94556
Cl         -2.76796        -0.89936        -0.94556
Cl          0.00000        -2.91040        -0.94556


21
Energy: -3918726.9967006
Fe         -0.00003         0.00000         0.00000
C           0.97996         0.71199         1.65617
C          -0.37433         1.15203         1.65615
C           0.97996        -0.71199         1.65617
C          -1.21132         0.00000         1.65617
C          -0.37433        -1.15203         1.65615
C           0.97996         0.71199        -1.65617
C           0.97996        -0.71199        -1.65617
C          -0.37433         1.15203        -1.65615
C          -0.37433        -1.15203        -1.65615
C          -1.21132         0.00000        -1.65617
Cl         -2.90130         0.00000         1.78102
Cl         -0.89654        -2.75930         1.78099
Cl         -0.89654         2.75930         1.78099
Cl          2.34721         1.70535         1.78085
Cl          2.34721        -1.70535         1.78085
Cl         -0.89654        -2.75930        -1.78099
Cl          2.34721        -1.70535        -1.78085
Cl         -2.90130         0.00000        -1.78102
Cl         -0.89654         2.75930        -1.78099
Cl          2.34721         1.70535        -1.78085


21
Energy: -3918727.0422640
Fe          0.00000         0.00000         0.00000
C           0.36375         1.15569         1.64996
C          -0.98672         0.70307         1.64996
C           1.21153         0.01118         1.64996
C          -0.97357        -0.72116         1.64996
C           0.38502        -1.14878         1.64996
C          -1.21153         0.01118        -1.64996
C          -0.36375         1.15569        -1.64996
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C         -0.38502       -1.14878       -1.64996
C          0.98672        0.70307       -1.64996
C          0.97357       -0.72116       -1.64996
Cl         2.33426       -1.72896       -1.74064
Cl         2.90471        0.02671        1.74064
Cl         2.36566        1.68574       -1.74064
Cl         0.87220        2.77080        1.74064
Cl        -0.87220        2.77080       -1.74064
Cl        -2.36566        1.68574        1.74064
Cl        -2.90471        0.02671       -1.74064
Cl        -2.33426       -1.72896        1.74064
Cl        -0.92301       -2.75429       -1.74064
Cl         0.92301       -2.75429        1.74064


21
Energy: -2477147.7805727
Fe         0.00000        0.00000        0.77770
C          0.00000        1.21184       -0.84823
C          1.15253        0.37448       -0.84823
C         -1.15253        0.37448       -0.84823
C          0.71230       -0.98040       -0.84823
C         -0.71230       -0.98040       -0.84823
C          1.14848       -0.37316        2.43682
C          0.70980        0.97695        2.43682
C          0.00000       -1.20758        2.43682
H          2.17437       -0.70650        2.39281
C         -0.70980        0.97695        2.43682
H          1.34384        1.84963        2.39281
C         -1.14848       -0.37316        2.43682
H          0.00000       -2.28627        2.39281
H         -1.34384        1.84963        2.39281
H         -2.17437       -0.70650        2.39281
Cl         0.00000        2.91056       -0.93932
Cl         2.76811        0.89941       -0.93932
Cl        -2.76811        0.89941       -0.93932
Cl        -1.71079       -2.35469       -0.93932
Cl         1.71079       -2.35469       -0.93932


21
Energy: -3918727.0410090
Fe         0.00000        0.00000        0.00000
C          0.00000        1.21158        1.65004
C         -1.15228        0.37440        1.65004
C          1.15228        0.37440        1.65004
C         -0.71215       -0.98018        1.65004
C          0.71215       -0.98018        1.65004
C         -1.15228       -0.37440       -1.65004
C         -0.71215        0.98018       -1.65004
C          0.00000       -1.21158       -1.65004
C          0.71215        0.98018       -1.65004
C          1.15228       -0.37440       -1.65004
Cl         2.76261       -0.89763       -1.74134
Cl         2.76261        0.89763        1.74134
Cl         1.70739        2.35002       -1.74134
Cl         0.00000        2.90478        1.74134
Cl        -1.70739        2.35002       -1.74134
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Cl        -2.76261        0.89763        1.74134
Cl        -2.76261       -0.89763       -1.74134
Cl        -1.70739       -2.35002        1.74134
Cl         0.00000       -2.90478       -1.74134
Cl         1.70739       -2.35002        1.74134


21
Energy: -2188834.5938432
Fe         0.00000        0.00000        0.11152
C          0.39867       -1.71395        1.14658
C          0.00000       -2.02619       -0.17958
C          1.55787       -0.90012        1.06182
H         -0.09856       -2.00853        2.05770
C          0.92125       -1.40468       -1.06260
H         -0.84961       -2.62113       -0.47561
C          1.88554       -0.69184       -0.30371
C         -1.55787        0.90012        1.06182
C         -0.39867        1.71395        1.14658
C         -1.88554        0.69184       -0.30371
C          0.00000        2.02619       -0.17958
H          0.09856        2.00853        2.05770
C         -0.92125        1.40468       -1.06260
H         -2.71188        0.11678       -0.68880
H          0.84961        2.62113       -0.47561
H          2.71188       -0.11678       -0.68880
Cl         2.45941       -0.30705        2.39518
Cl         0.91797       -1.55374       -2.76683
Cl        -0.91797        1.55374       -2.76683
Cl        -2.45941        0.30705        2.39518


21
Energy: -2188834.9318010
Fe         0.00000        0.00000        0.28835
C          0.00000       -2.01816        0.61832
C         -0.91207       -1.37610        1.49662
C         -0.41039       -1.72772       -0.70888
H          0.86517       -2.59966        0.89641
C         -1.86963       -0.69791        0.69730
H         -0.88590       -1.38464        2.57485
C         -1.56460       -0.90204       -0.67367
C          1.86963        0.69791        0.69730
C          1.56460        0.90204       -0.67367
C          0.91207        1.37610        1.49662
C          0.41039        1.72772       -0.70888
H          2.09588        0.49933       -1.52111
C          0.00000        2.01816        0.61832
H          0.88590        1.38464        2.57485
H         -0.86517        2.59966        0.89641
H         -2.09588       -0.49933       -1.52111
Cl         3.21746       -0.17937        1.29324
Cl        -0.33455        2.32435       -2.13306
Cl        -3.21746        0.17937        1.29324
Cl         0.33455       -2.32435       -2.13306


21
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Energy: -1612199.7214273

Fe	0.46487	0.13697	0.00000
C	-0.94306	1.43634	0.71028
C	-0.94306	1.43634	-0.71028
C	-1.21950	0.11122	1.13665
H	-0.75957	2.27938	1.35753
C	-1.21950	0.11122	-1.13665
H	-0.75957	2.27938	-1.35753
C	-1.38834	-0.72257	0.00000
C	2.28664	0.74813	0.71036
C	2.00321	-0.57197	1.14929
C	2.28664	0.74813	-0.71036
H	2.44344	1.60690	1.34516
C	1.82986	-1.38779	0.00000
H	1.89272	-0.88944	2.17524
C	2.00321	-0.57197	-1.14929
H	2.44344	1.60690	-1.34516
H	1.57601	-2.43688	0.00000
H	1.89272	-0.88944	-2.17524
H	-1.60857	-1.77763	0.00000
Cl	-1.39364	-0.39303	2.76859
Cl	-1.39364	-0.39303	-2.76859

21

Energy: -2188833.9107866

Fe	0.00000	0.00000	0.35260
C	-0.70989	1.64105	1.34735
C	0.70989	1.64105	1.34735
C	-1.13752	1.66591	-0.00529
H	-1.35759	1.62336	2.20970
C	1.13752	1.66591	-0.00529
H	1.35759	1.62336	2.20970
C	0.00000	1.66180	-0.85352
C	-0.70989	-1.64105	1.34735
C	-1.13752	-1.66591	-0.00529
C	0.70989	-1.64105	1.34735
H	-1.35759	-1.62336	2.20970
C	0.00000	-1.66180	-0.85352
C	1.13752	-1.66591	-0.00529
H	1.35759	-1.62336	2.20970
H	0.00000	-1.67734	-1.93132
H	0.00000	1.67734	-1.93132
Cl	-2.76179	-1.77250	-0.53104
Cl	-2.76179	1.77250	-0.53104
Cl	2.76179	1.77250	-0.53104
Cl	2.76179	-1.77250	-0.53104

21

Energy: -2188834.9318010

Fe	0.00000	0.00000	0.28835
C	1.86963	0.69791	0.69730
C	1.56461	0.90205	-0.67367
C	0.91207	1.37609	1.49662
C	0.41039	1.72772	-0.70888
C	0.00000	2.01816	0.61832
H	0.88590	1.38463	2.57485

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H         -0.86517        2.59966        0.89642
C         -1.56461       -0.90205       -0.67367
C         -0.41039       -1.72772       -0.70888
C         -1.86963       -0.69791        0.69730
H         -2.09587       -0.49932       -1.52112
C          0.00000       -2.01816        0.61832
C         -0.91207       -1.37609        1.49662
H          0.86517       -2.59966        0.89642
H         -0.88590       -1.38463        2.57485
H          2.09587        0.49932       -1.52112
Cl        -0.33455        2.32436       -2.13305
Cl        -3.21746        0.17937        1.29324
Cl         0.33455       -2.32436       -2.13305
Cl         3.21746       -0.17937        1.29324


21
Energy: -2188834.1190319
Fe         0.00000        0.00000        0.00000
C         -0.44321        1.63899        1.13707
C          0.31272        2.02643        0.00000
C         -1.63675        1.00349        0.71053
C         -0.44321        1.63899       -1.13707
C         -1.63675        1.00349       -0.71053
H         -2.39000        0.58378        1.35881
H         -2.39000        0.58378       -1.35881
C          1.63675       -1.00349       -0.71053
C          1.63675       -1.00349        0.71053
C          0.44321       -1.63899       -1.13707
H          2.39000       -0.58378       -1.35881
C          0.44321       -1.63899        1.13707
H          2.39000       -0.58378        1.35881
C         -0.31272       -2.02643        0.00000
H         -1.26717       -2.52729        0.00000
H          1.26717        2.52729        0.00000
Cl         0.00000        1.93573        2.76486
Cl         0.00000       -1.93573        2.76486
Cl         0.00000       -1.93573       -2.76486
Cl         0.00000        1.93573       -2.76486


21
Energy: -1612199.2318382
Fe         0.46121       -0.13953        0.00000
C         -1.22558       -0.11118        1.13624
C         -1.39230        0.72300        0.00000
C         -0.95242       -1.43649        0.71017
C         -1.22558       -0.11118       -1.13624
C         -0.95242       -1.43649       -0.71017
H         -0.76737       -2.27924        1.35745
H         -0.76737       -2.27924       -1.35745
C          1.87676        1.16010       -0.71043
C          1.87676        1.16010        0.71043
C          2.16072       -0.15890       -1.14892
H          1.65865        2.00466       -1.34642
C          2.16072       -0.15890        1.14892
H          1.65865        2.00466        1.34642
C          2.33461       -0.97523        0.00000
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H          2.19506       -0.49043       -2.17572
H          2.19506       -0.49043        2.17572
H          2.53283       -2.03636        0.00000
H         -1.60582        1.77950        0.00000
Cl        -1.38408        0.39664        2.76822
Cl        -1.38408        0.39664       -2.76822


21
Energy: -2188834.9318010
Fe         0.00000        0.00000        0.28835
C         -1.86964       -0.69791        0.69729
C         -1.56460       -0.90205       -0.67368
C         -0.91208       -1.37608        1.49662
C         -0.41038       -1.72772       -0.70887
C          0.00000       -2.01815        0.61833
H         -0.88593       -1.38461        2.57485
H          0.86516       -2.59965        0.89645
C          0.41038        1.72772       -0.70887
C          0.00000        2.01815        0.61833
C          1.56460        0.90205       -0.67368
C          0.91208        1.37608        1.49662
H         -0.86516        2.59965        0.89645
C          1.86964        0.69791        0.69729
H          2.09586        0.49935       -1.52114
H          0.88593        1.38461        2.57485
H         -2.09586       -0.49935       -1.52114
Cl        -3.21746        0.17938        1.29323
Cl        -0.33458        2.32437       -2.13304
Cl         3.21746       -0.17938        1.29323
Cl         0.33458       -2.32437       -2.13304


21
Energy: -2765465.8079918
Fe         0.00000        0.00000        0.57987
C         -0.79105       -1.42284        1.80911
C         -1.76865       -0.97776        0.88266
C          0.29817       -1.95601        1.07178
H         -0.84447       -1.35985        2.88461
C         -1.28558       -1.24302       -0.42450
H         -2.70699       -0.49823        1.11438
C          0.00000       -1.84825       -0.31683
C          0.79105        1.42284        1.80911
C          1.76865        0.97776        0.88266
C         -0.29817        1.95601        1.07178
H          0.84447        1.35985        2.88461
C          1.28558        1.24302       -0.42450
H          2.70699        0.49823        1.11438
C          0.00000        1.84825       -0.31683
Cl         1.69245       -2.68933        1.73027
Cl         0.94073       -2.44571       -1.59604
Cl        -2.12902       -0.97794       -1.87956
Cl        -1.69245        2.68933        1.73027
Cl        -0.94073        2.44571       -1.59604
Cl         2.12902        0.97794       -1.87956
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21
Energy: -2765466.2087570
Fe 0.00000 0.00000 0.19775
C 1.55811 0.89532 1.16314
C 1.88163 0.69125 -0.20276
C 0.40219 1.71614 1.22009
H 2.06974 0.47963 2.01734
C 0.92980 1.39068 -0.98889
H 2.69089 0.09292 -0.59172
C 0.00000 2.02148 -0.11248
C -0.40219 -1.71614 1.22009
C -1.55811 -0.89532 1.16314
C 0.00000 -2.02148 -0.11248
C -1.88163 -0.69125 -0.20276
H -2.06974 -0.47963 2.01734
C -0.92980 -1.39068 -0.98889
H -2.69089 -0.09292 -0.59172
Cl 0.93910 1.53661 -2.68516
Cl -1.27522 3.05002 -0.56795
Cl -0.34051 2.31164 2.63717
Cl -0.93910 -1.53661 -2.68516
Cl 1.27522 -3.05002 -0.56795
Cl 0.34051 -2.31164 2.63717

21
Energy: -1900515.9437590
Fe -0.15570 -0.76629 0.00000
C -1.85065 0.12355 -0.70970
C -1.85065 0.12355 0.70970
C -0.69483 0.82142 -1.14668
H -2.58514 -0.33037 -1.35612
C -0.69483 0.82142 1.14668
H -2.58514 -0.33037 1.35612
C 0.03071 1.25698 0.00000
C -0.11517 -2.68932 -0.71038
C 1.03110 -1.97520 -1.14886
C -0.11517 -2.68932 0.71038
H -0.86991 -3.12791 -1.34522
C 1.73920 -1.53456 0.00000
H 1.29201 -1.76193 -2.17455
C 1.03110 -1.97520 1.14886
H -0.86991 -3.12791 1.34522
H 2.63122 -0.92631 0.00000
H 1.29201 -1.76193 2.17455
Cl -0.28405 1.16985 -2.76880
Cl 1.43151 2.22443 0.00000
Cl -0.28405 1.16985 2.76880

21
Energy: -2765465.2346176
Fe 0.00000 0.00000 0.77237
C 0.70943 1.63151 1.77618
C -0.70943 1.63151 1.77618
C 1.14674 1.66492 0.42711
H 1.35662 1.60686 2.63879
C -1.14674 1.66492 0.42711

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H         -1.35662        1.60686        2.63879
C          0.00000        1.67641       -0.41778
C          0.70943       -1.63151        1.77618
C          1.14674       -1.66492        0.42711
C         -0.70943       -1.63151        1.77618
H          1.35662       -1.60686        2.63879
C          0.00000       -1.67641       -0.41778
C         -1.14674       -1.66492        0.42711
H         -1.35662       -1.60686        2.63879
Cl         2.76129        1.78400       -0.10052
Cl         0.00000        1.82191       -2.10786
Cl        -2.76129        1.78400       -0.10052
Cl        -2.76129       -1.78400       -0.10052
Cl         0.00000       -1.82191       -2.10786
Cl         2.76129       -1.78400       -0.10052


21
Energy: -2765466.2087570
Fe         0.00000        0.00000        0.19777
C         -0.40215        1.71615        1.22009
C          0.00000        2.02147       -0.11249
C         -1.55808        0.89533        1.16319
C         -0.92983        1.39067       -0.98886
C         -1.88164        0.69126       -0.20271
H         -2.06970        0.47964        2.01739
H         -2.69092        0.09292       -0.59162
C          0.92983       -1.39067       -0.98886
C          1.88164       -0.69126       -0.20271
C          0.00000       -2.02147       -0.11249
C          1.55808       -0.89533        1.16319
H          2.69092       -0.09292       -0.59162
C          0.40215       -1.71615        1.22009
H          2.06970       -0.47964        2.01739
Cl         0.34061        2.31165        2.63715
Cl         1.27519        3.05003       -0.56801
Cl         0.93915       -1.53658       -2.68514
Cl        -1.27519       -3.05003       -0.56801
Cl        -0.34061       -2.31165        2.63715
Cl        -0.93915        1.53658       -2.68514


21
Energy: -2765466.1211943
Fe         0.00000        0.00000        0.00000
C         -0.44059        1.63304        1.14695
C          0.31075        2.02014        0.00000
C         -1.63384        1.00304        0.70952
C         -0.44059        1.63304       -1.14695
C         -1.63384        1.00304       -0.70952
H         -2.38643        0.57812        1.35536
H         -2.38643        0.57812       -1.35536
C          1.63384       -1.00304       -0.70952
C          1.63384       -1.00304        0.70952
C          0.44059       -1.63304       -1.14695
H          2.38643       -0.57812       -1.35536
C          0.44059       -1.63304        1.14695
H          2.38643       -0.57812        1.35536
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C         -0.31075       -2.02014        0.00000
Cl         0.00000       -1.94113       -2.76493
Cl        -1.77836       -2.87866        0.00000
Cl         0.00000       -1.94113        2.76493
Cl         1.77836        2.87866        0.00000
Cl         0.00000        1.94113        2.76493
Cl         0.00000        1.94113       -2.76493


21
Energy: -1900515.5108151
Fe         0.16153        0.76237        0.00000
C          0.69924       -0.82749        1.14636
C         -0.02746       -1.26090        0.00000
C          1.85672       -0.13318        0.70953
C          0.69924       -0.82749       -1.14636
C          1.85672       -0.13318       -0.70953
H          2.59101        0.32122        1.35593
H          2.59101        0.32122       -1.35593
C         -1.54196        1.64860       -0.71005
C         -1.54196        1.64860        0.71005
C         -0.39974        2.36761       -1.14873
H         -2.25789        1.14774       -1.34416
C         -0.39974        2.36761        1.14873
H         -2.25789        1.14774        1.34416
C          0.30691        2.81164        0.00000
H         -0.09952        2.51317       -2.17542
H         -0.09952        2.51317        2.17542
H          1.23609        3.36115        0.00000
Cl        -1.43930       -2.21154        0.00000
Cl         0.27992       -1.16240        2.76874
Cl         0.27992       -1.16240       -2.76874


21
Energy: -2765465.8079918
Fe         0.00000        0.00000        0.57986
C         -0.29815       -1.95601        1.07179
C          0.00000       -1.84825       -0.31683
C          0.79107       -1.42284        1.80910
C          1.28558       -1.24302       -0.42451
C          1.76866       -0.97776        0.88265
H          0.84449       -1.35981        2.88461
H          2.70700       -0.49822        1.11435
C          0.00000        1.84825       -0.31683
C         -1.28558        1.24302       -0.42451
C          0.29815        1.95601        1.07179
C         -1.76866        0.97776        0.88265
C         -0.79107        1.42284        1.80910
H         -2.70700        0.49822        1.11435
H         -0.84449        1.35981        2.88461
Cl        -1.69243       -2.68933        1.73029
Cl        -2.12900        0.97795       -1.87957
Cl        -0.94074       -2.44572       -1.59603
Cl         2.12900       -0.97795       -1.87957
Cl         1.69243        2.68933        1.73029
Cl         0.94074        2.44572       -1.59603
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21
Energy: -1612199.8905097
Fe          0.00000         0.00000         0.58776
C          -0.71032        -1.49880         1.78663
C          -1.73176        -1.03605         0.91408
C           0.36953        -1.97277         0.99574
H          -0.73704        -1.47300         2.86529
C          -1.29270        -1.21866        -0.42362
H          -2.67000        -0.59408         1.21280
C           0.00000        -1.80046        -0.36375
H           1.30492        -2.38046         1.34516
H          -1.81753        -0.94382        -1.32530
C           0.71032         1.49880         1.78663
C           1.73176         1.03605         0.91408
C          -0.36953         1.97277         0.99574
H           0.73704         1.47300         2.86529
C           1.29270         1.21866        -0.42362
H           2.67000         0.59408         1.21280
C           0.00000         1.80046        -0.36375
H          -1.30492         2.38046         1.34516
H           1.81753         0.94382        -1.32530
Cl          0.94376        -2.27607        -1.71725
Cl         -0.94376         2.27607        -1.71725


21
Energy: -1612199.9998972
Fe          0.00000         0.00000         0.23263
C           0.36607        -1.75987         1.20721
C           0.00000        -2.00843        -0.14213
C           1.53008        -0.94584         1.21154
H          -0.16415        -2.10504         2.08162
C           0.93484        -1.35184        -0.98510
H          -0.86506        -2.56297        -0.47320
C           1.87512        -0.70240        -0.14323
H           2.05844        -0.56698         2.07210
H           0.93603        -1.32880        -2.06340
C          -1.53008         0.94584         1.21154
C          -0.36607         1.75987         1.20721
C          -1.87512         0.70240        -0.14323
H          -2.05844         0.56698         2.07210
C           0.00000         2.00843        -0.14213
H           0.16415         2.10504         2.08162
C          -0.93484         1.35184        -0.98510
H           0.86506         2.56297        -0.47320
H          -0.93603         1.32880        -2.06340
Cl          3.24686         0.18230        -0.67830
Cl         -3.24686        -0.18230        -0.67830


21
Energy: -1323881.7491475
Fe         -0.24014        -0.42642         0.00000
C           1.41781        -1.38955         0.71029
C           1.41781        -1.38955        -0.71029
C           1.40246        -0.04123         1.15613
H           1.40592        -2.26257         1.34479
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C          1.40246       -0.04123       -1.15613
H          1.40592       -2.26257       -1.34479
C          1.39609        0.78174        0.00000
H          1.38781        0.30881        2.17618
H          1.38781        0.30881       -2.17618
C         -1.89267       -1.40685        0.71012
C         -1.89267       -0.05568        1.14852
C         -1.89267       -1.40685       -0.71012
H         -1.86902       -2.27982        1.34454
C         -1.89147        0.77906        0.00000
H         -1.86652        0.27858        2.17452
C         -1.89267       -0.05568       -1.14852
H         -1.86902       -2.27982       -1.34454
H         -1.84929        1.85790        0.00000
H         -1.86652        0.27858       -2.17452
Cl         1.44292        2.49965        0.00000


21
Energy: -1612199.2180769
Fe         0.00000        0.00000        0.72166
C         -0.71030        1.63759        1.71481
C          0.71030        1.63759        1.71481
C         -1.15502        1.65545        0.36654
H         -1.34497        1.60247        2.58712
C          1.15502        1.65545        0.36654
H          1.34497        1.60247        2.58712
C          0.00000        1.67682       -0.45713
H         -2.17489        1.65043        0.01557
H          2.17489        1.65043        0.01557
C         -0.71030       -1.63759        1.71481
C         -1.15502       -1.65545        0.36654
C          0.71030       -1.63759        1.71481
H         -1.34497       -1.60247        2.58712
C          0.00000       -1.67682       -0.45713
H         -2.17489       -1.65043        0.01557
C          1.15502       -1.65545        0.36654
H          1.34497       -1.60247        2.58712
H          2.17489       -1.65043        0.01557
Cl         0.00000        1.79570       -2.16591
Cl         0.00000       -1.79570       -2.16591


21
Energy: -1612199.8905097
Fe         0.00000        0.00000        0.58777
C          0.00000       -1.80045       -0.36376
C          0.36955       -1.97278        0.99572
C         -1.29271       -1.21865       -0.42360
C         -0.71030       -1.49883        1.78663
H          1.30495       -2.38045        1.34512
C         -1.73175       -1.03607        0.91411
H         -1.81755       -0.94381       -1.32527
H         -0.73700       -1.47302        2.86529
H         -2.66999       -0.59411        1.21284
C          0.71030        1.49883        1.78663
C          1.73175        1.03607        0.91411
C         -0.36955        1.97278        0.99572
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H          0.73700        1.47302        2.86529
C          1.29271        1.21865       -0.42360
H          2.66999        0.59411        1.21284
C          0.00000        1.80045       -0.36376
H         -1.30495        2.38045        1.34512
H          1.81755        0.94381       -1.32527
Cl         0.94377       -2.27602       -1.71727
Cl        -0.94377        2.27602       -1.71727


21
Energy: -1612199.5029724
Fe         0.00000        0.00000        0.00000
C         -0.80184        1.87641        0.00000
C          0.00000        1.69195        1.15546
C          0.00000        1.69195       -1.15546
C          1.31595        1.39731        0.70951
H         -0.34514        1.75320        2.17554
C          1.31595        1.39731       -0.70951
H         -0.34514        1.75320       -2.17554
H          2.16132        1.17348        1.34226
H          2.16132        1.17348       -1.34226
C          0.00000       -1.69195        1.15546
C         -1.31595       -1.39731        0.70951
C          0.80184       -1.87641        0.00000
H          0.34514       -1.75320        2.17554
C         -1.31595       -1.39731       -0.70951
H         -2.16132       -1.17348        1.34226
C          0.00000       -1.69195       -1.15546
H         -2.16132       -1.17348       -1.34226
H          0.34514       -1.75320       -2.17554
Cl        -2.46676        2.29759        0.00000
Cl         2.46676       -2.29759        0.00000


21
Energy: -1323881.1856628
Fe        -0.23610       -0.42913        0.00000
C          1.39767        0.78530        0.00000
C          1.40798       -0.03728        1.15584
C          1.40798       -0.03728       -1.15584
C          1.43014       -1.38513        0.71000
H          1.38766        0.31258        2.17592
C          1.43014       -1.38513       -0.71000
H          1.38766        0.31258       -2.17592
H          1.41948       -2.25824        1.34452
H          1.41948       -2.25824       -1.34452
C         -1.89212       -0.80630        1.14842
C         -1.89212        0.54446        0.70948
C         -1.89308       -1.64086        0.00000
H         -1.86425       -1.13990        2.17470
C         -1.89212        0.54446       -0.70948
H         -1.85630        1.41872        1.34175
C         -1.89212       -0.80630       -1.14842
H         -1.86561       -2.72002        0.00000
H         -1.85630        1.41872       -1.34175
H         -1.86425       -1.13990       -2.17470
Cl         1.42100        2.50326        0.00000
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21
Energy: -1612199.8905097
Fe 0.00000 0.00000 0.58776
C 0.00000 -1.80047 -0.36376
C 0.36956 -1.97278 0.99572
C -1.29270 -1.21866 -0.42362
C -0.71029 -1.49882 1.78662
H 1.30495 -2.38049 1.34511
C -1.73174 -1.03607 0.91409
H -1.81755 -0.94385 -1.32529
H -0.73703 -1.47299 2.86528
H -2.66996 -0.59408 1.21284
C 1.73174 1.03607 0.91409
C 1.29270 1.21866 -0.42362
C 0.71029 1.49882 1.78662
H 2.66996 0.59408 1.21284
C 0.00000 1.80047 -0.36376
H 1.81755 0.94385 -1.32529
C -0.36956 1.97278 0.99572
H 0.73703 1.47299 2.86528
H -1.30495 2.38049 1.34511
Cl 0.94379 -2.27606 -1.71725
Cl -0.94379 2.27606 -1.71725

21
Energy: -2765467.0131865
Fe 0.00000 0.00000 0.22421
C 0.36893 1.72948 1.24663
C 1.53506 0.92307 1.18939
C 0.00000 2.01751 -0.09389
H -0.14910 2.05307 2.13539
C 1.88576 0.69433 -0.16589
C 0.93540 1.38623 -0.96297
C -1.53506 -0.92307 1.18939
C -1.88576 -0.69433 -0.16589
C -0.36893 -1.72948 1.24663
C -0.93540 -1.38623 -0.96297
H -2.71348 -0.10512 -0.52735
C 0.00000 -2.01751 -0.09389
H 0.14910 -2.05307 2.13539
H 2.71348 0.10512 -0.52735
Cl 1.28796 -3.02493 -0.58147
Cl -0.96286 -1.52119 -2.65965
Cl -2.41505 -0.35970 2.54686
Cl 0.96286 1.52119 -2.65965
Cl 2.41505 0.35970 2.54686
Cl -1.28796 3.02493 -0.58147

21
Energy: -2765466.6546401
Fe 0.00000 0.00000 0.13274
C -1.59271 0.87498 -0.80390
C -1.86115 0.72495 0.58070
C -0.43785 1.69306 -0.91591

```
H         -2.15175        0.44456       -1.61956
C         -0.87591        1.41929        1.32906
C          0.00000        2.03359        0.39601
C          0.43785       -1.69306       -0.91591
C          1.59271       -0.87498       -0.80390
C          0.00000       -2.03359        0.39601
C          1.86115       -0.72495        0.58070
H          2.15175       -0.44456       -1.61956
C          0.87591       -1.41929        1.32906
H          0.81328       -1.48834        2.40310
H         -0.81328        1.48834        2.40310
Cl         3.20233        0.09981        1.24483
Cl         1.28799        3.08135        0.77337
Cl        -0.25403       -2.25106       -2.37260
Cl        -1.28799       -3.08135        0.77337
Cl        -3.20233       -0.09981        1.24483
Cl         0.25403        2.25106       -2.37260


21
Energy: -1900516.5060514
Fe         0.48689        0.36200        0.00000
C         -1.18819        0.24225        1.15905
C         -1.43319        1.02326        0.00000
C         -0.79178       -1.04688        0.71201
H         -1.28945        0.55974        2.18420
C         -1.18819        0.24225       -1.15905
C         -0.79178       -1.04688       -0.71201
C          1.96081        1.20267        1.14837
C          2.35325       -0.08978        0.70972
C          1.71627        2.00130        0.00000
H          1.83611        1.51311        2.17457
C          2.35325       -0.08978       -0.70972
H          2.56638       -0.93747        1.34343
C          1.96081        1.20267       -1.14837
H          1.36238        3.02125        0.00000
H          2.56638       -0.93747       -1.34343
H          1.83611        1.51311       -2.17457
H         -1.28945        0.55974       -2.18420
Cl        -0.46631       -2.39526        1.71019
Cl        -2.00592        2.64046        0.00000
Cl        -0.46631       -2.39526       -1.71019


21
Energy: -2765466.2256433
Fe         0.00000        0.00000        0.29766
C         -1.15688        1.64743        0.67993
C          0.00000        1.65759        1.50023
C         -0.71176        1.66470       -0.66820
H         -2.18229        1.65077        1.01277
C          1.15688        1.64743        0.67993
C          0.71176        1.66470       -0.66820
C         -1.15688       -1.64743        0.67993
C         -0.71176       -1.66470       -0.66820
C          0.00000       -1.65759        1.50023
H         -2.18229       -1.65077        1.01277
C          0.71176       -1.66470       -0.66820
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C          1.15688       -1.64743        0.67993
H          2.18229       -1.65077        1.01277
H          2.18229        1.65077        1.01277
Cl         0.00000       -1.75678        3.20613
Cl        -1.70575       -1.78205       -2.04534
Cl         1.70575       -1.78205       -2.04534
Cl         1.70575        1.78205       -2.04534
Cl        -1.70575        1.78205       -2.04534
Cl         0.00000        1.75678        3.20613


21
Energy: -2765467.0131865
Fe         0.00000        0.00000        0.22421
C          0.36892       -1.72948        1.24663
C          0.00000       -2.01751       -0.09390
C          1.53505       -0.92308        1.18939
C          0.93541       -1.38624       -0.96297
C          1.88576       -0.69435       -0.16588
H          2.71349       -0.10514       -0.52734
C         -1.88576        0.69435       -0.16588
C         -1.53505        0.92308        1.18939
C         -0.93541        1.38624       -0.96297
H         -2.71349        0.10514       -0.52734
C         -0.36892        1.72948        1.24663
C          0.00000        2.01751       -0.09390
H          0.14912        2.05307        2.13539
H         -0.14912       -2.05307        2.13539
Cl        -2.41501        0.35968        2.54687
Cl        -0.96286        1.52120       -2.65965
Cl         1.28796        3.02493       -0.58148
Cl        -1.28796       -3.02493       -0.58148
Cl         2.41501       -0.35968        2.54687
Cl         0.96286       -1.52120       -2.65965


21
Energy: -2765466.4203846
Fe         0.00000        0.00000        0.00000
C          0.00000        1.68967        1.15748
C          1.31621        1.39422        0.71141
C         -0.79580        1.88414        0.00000
C          1.31621        1.39422       -0.71141
C          0.00000        1.68967       -1.15748
H         -0.32747        1.75815       -2.18246
C          0.79580       -1.88414        0.00000
C          0.00000       -1.68967        1.15748
C          0.00000       -1.68967       -1.15748
C         -1.31621       -1.39422        0.71141
H          0.32747       -1.75815        2.18246
C         -1.31621       -1.39422       -0.71141
H          0.32747       -1.75815       -2.18246
H         -0.32747        1.75815        2.18246
Cl         2.44660       -2.32797        0.00000
Cl         2.67863        1.15382        1.70770
Cl        -2.44660        2.32797        0.00000
Cl        -2.67863       -1.15382        1.70770
Cl        -2.67863       -1.15382       -1.70770
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Cl         2.67863        1.15382       -1.70770


21
Energy: -1900516.0829594
Fe        -0.48393        0.35847        0.00000
C          1.19398        0.24768        1.15883
C          0.80437       -1.04327        0.71176
C          1.43471        1.02956        0.00000
C          0.80437       -1.04327       -0.71176
C          1.19398        0.24768       -1.15883
H          1.28973        0.56686       -2.18404
C         -2.41618       -0.32706        0.00000
C         -2.17824        0.47243        1.14821
C         -2.17824        0.47243       -1.14821
H         -2.68077       -1.37373        0.00000
C         -1.79588        1.76830        0.70924
H         -2.23852        0.14060        2.17368
C         -1.79588        1.76830       -0.70924
H         -2.23852        0.14060       -2.17368
H         -1.51266        2.59605        1.34171
H         -1.51266        2.59605       -1.34171
H          1.28973        0.56686        2.18404
Cl         0.47187       -2.38916        1.71032
Cl         1.98474        2.65417        0.00000
Cl         0.47187       -2.38916       -1.71032


21
Energy: -2765467.0131865
Fe         0.00000        0.00000        0.22421
C          0.36893       -1.72948        1.24663
C          0.00000       -2.01751       -0.09390
C          1.53505       -0.92307        1.18939
C          0.93540       -1.38623       -0.96297
C          1.88576       -0.69433       -0.16589
H          2.71348       -0.10512       -0.52735
C         -0.93540        1.38623       -0.96297
C         -1.88576        0.69433       -0.16589
C          0.00000        2.01751       -0.09390
C         -1.53505        0.92307        1.18939
H         -2.71348        0.10512       -0.52735
C         -0.36893        1.72948        1.24663
H          0.14911        2.05307        2.13539
H         -0.14911       -2.05307        2.13539
Cl        -1.28795       -3.02494       -0.58148
Cl         2.41504       -0.35970        2.54687
Cl         0.96286       -1.52119       -2.65965
Cl        -0.96286        1.52119       -2.65965
Cl         1.28795        3.02494       -0.58148
Cl        -2.41504        0.35970        2.54687


21
Energy: -2188833.1490026
Fe         0.00000        0.00000        0.71740
C         -1.80360        0.19518        1.65333
C         -1.06104        1.40068        1.76150
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C         -1.99598       -0.09456        0.27781
H         -2.13948       -0.41482        2.47783
C         -0.79670        1.86134        0.44530
H         -0.73731        1.88802        2.66764
C         -1.37996        0.94166       -0.47189
H         -2.49703       -0.95245       -0.14296
C          1.06104       -1.40068        1.76150
C          0.79670       -1.86134        0.44530
C          1.80360       -0.19518        1.65333
H          0.73731       -1.88802        2.66764
C          1.37996       -0.94166       -0.47189
C          1.99598        0.09456        0.27781
H          2.13948        0.41482        2.47783
H          2.49703        0.95245       -0.14296
Cl         0.00000       -3.31456        0.02995
Cl         1.41307       -1.11566       -2.16672
Cl        -1.41307        1.11566       -2.16672
Cl         0.00000        3.31456        0.02995


21
Energy: -2188833.7933043
Fe         0.00000        0.00000        0.25991
C          0.00000        2.01594        0.58148
C          0.90719        1.37918        1.46803
C          0.39472        1.73044       -0.75121
H         -0.87107        2.58345        0.87199
C          1.87172        0.69691        0.68009
H          0.87861        1.38856        2.54618
C          1.55564        0.91536       -0.69123
H         -0.10224        2.04019       -1.65740
C         -1.87172       -0.69691        0.68009
C         -1.55564       -0.91536       -0.69123
C         -0.90719       -1.37918        1.46803
C         -0.39472       -1.73044       -0.75121
C          0.00000       -2.01594        0.58148
H         -0.87861       -1.38856        2.54618
H          0.10224       -2.04019       -1.65740
H          0.87107       -2.58345        0.87199
Cl        -2.46776       -0.35848       -2.02407
Cl        -3.22691        0.16246        1.26745
Cl         2.46776        0.35848       -2.02407
Cl         3.22691       -0.16246        1.26745


21
Energy: -1612198.9914518
Fe         0.21896        0.70421        0.00000
C          2.17711        0.12004        0.00000
C          1.51402       -0.37695        1.15272
C          1.51402       -0.37695       -1.15272
H          3.02744        0.78461        0.00000
C          0.43541       -1.18842        0.71201
H          1.76193       -0.17869        2.18352
C          0.43541       -1.18842       -0.71201
H          1.76193       -0.17869       -2.18352
C          0.16479        2.75373        0.00000
C         -0.49561        2.24215       -1.14889
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C         -0.49561        2.24215        1.14889
H          1.03225        3.39607        0.00000
C         -1.56213        1.41390       -0.70978
H         -0.21667        2.42519       -2.17541
C         -1.56213        1.41390        0.70978
H         -0.21667        2.42519        2.17541
H         -2.22547        0.84443       -1.34331
H         -2.22547        0.84443        1.34331
Cl        -0.62188       -2.08832       -1.71044
Cl        -0.62188       -2.08832        1.71044


21
Energy: -2188832.5883480
Fe         0.00000        0.00000        0.93170
C          0.00000        1.62732        2.16161
C          1.15187        1.64207        1.33235
C         -1.15187        1.64207        1.33235
H          0.00000        1.58461        3.24004
C          0.71182        1.67580       -0.01660
H          2.18305        1.62626        1.64835
C         -0.71182        1.67580       -0.01660
H         -2.18305        1.62626        1.64835
C          0.00000       -1.62732        2.16161
C         -1.15187       -1.64207        1.33235
C          1.15187       -1.64207        1.33235
H          0.00000       -1.58461        3.24004
C         -0.71182       -1.67580       -0.01660
H         -2.18305       -1.62626        1.64835
C          0.71182       -1.67580       -0.01660
H          2.18305       -1.62626        1.64835
Cl        -1.70643       -1.80635       -1.39434
Cl         1.70643       -1.80635       -1.39434
Cl         1.70643        1.80635       -1.39434
Cl        -1.70643        1.80635       -1.39434


21
Energy: -2188833.7933043
Fe         0.00000        0.00000       -0.25992
C         -1.55564       -0.91537        0.69123
C         -1.87172       -0.69691       -0.68009
C         -0.39472       -1.73044        0.75120
C         -0.90719       -1.37918       -1.46804
C          0.00000       -2.01594       -0.58149
H          0.10226       -2.04019        1.65739
H         -0.87862       -1.38855       -2.54619
H          0.87108       -2.58344       -0.87200
C          0.00000        2.01594       -0.58149
C          0.39472        1.73044        0.75120
C          0.90719        1.37918       -1.46804
H         -0.87108        2.58344       -0.87200
C          1.55564        0.91537        0.69123
H         -0.10226        2.04019        1.65739
C          1.87172        0.69691       -0.68009
H          0.87862        1.38855       -2.54619
Cl        -2.46775       -0.35849        2.02408
Cl        -3.22691        0.16246       -1.26744
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Cl         2.46775        0.35849        2.02408
Cl         3.22691       -0.16246       -1.26744


21
Energy: -2188833.5639182
Fe         0.00000        0.00000        0.00000
C          1.31588        1.38949        0.71166
C          1.31588        1.38949       -0.71166
C          0.00000        1.69042        1.15215
C          0.00000        1.69042       -1.15215
C         -0.80661        1.87773        0.00000
H         -0.31611        1.74049        2.18231
H         -0.31611        1.74049       -2.18231
H         -1.86646        2.08224        0.00000
C          0.00000       -1.69042       -1.15215
C          0.80661       -1.87773        0.00000
C         -1.31588       -1.38949       -0.71166
H          0.31611       -1.74049       -2.18231
C          0.00000       -1.69042        1.15215
H          1.86646       -2.08224        0.00000
C         -1.31588       -1.38949        0.71166
H          0.31611       -1.74049        2.18231
Cl         2.67979        1.13714        1.70884
Cl        -2.67979       -1.13714        1.70884
Cl        -2.67979       -1.13714       -1.70884
Cl         2.67979        1.13714       -1.70884


21
Energy: -1612198.4986561
Fe         0.22445        0.70184        0.00000
C          0.43948       -1.19206        0.71180
C          0.43948       -1.19206       -0.71180
C          1.52001       -0.38371        1.15242
C          1.52001       -0.38371       -1.15242
C          2.18415        0.11129        0.00000
H          1.76648       -0.18344        2.18324
H          1.76648       -0.18344       -2.18324
H          3.03460        0.77578        0.00000
C         -1.08589        1.77936       -1.14846
C         -1.74270        1.26501        0.00000
C         -0.02314        2.61281       -0.70974
H         -1.32781        1.54435       -2.17395
C         -1.08589        1.77936        1.14846
H         -2.56547        0.56604        0.00000
C         -0.02314        2.61281        0.70974
H          0.68177        3.12880       -1.34393
H         -1.32781        1.54435        2.17395
H          0.68177        3.12880        1.34393
Cl        -0.62941       -2.07716        1.71044
Cl        -0.62941       -2.07716       -1.71044


21
Energy: -2188833.1491909
Fe         0.00000        0.00000        0.72122
C         -0.90307       -1.40509       -0.46865
```

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C          0.00000       -2.02368        0.44188
C         -1.87386       -0.69816        0.28840
C         -0.41804       -1.70924        1.76128
C         -1.57617       -0.89371        1.66177
H         -2.67457       -0.10573       -0.12629
H          0.07586       -2.03308        2.66381
H         -2.12145       -0.46895        2.49061
C          1.87386        0.69816        0.28840
C          0.90307        1.40509       -0.46865
C          1.57617        0.89371        1.66177
H          2.67457        0.10573       -0.12629
C          0.00000        2.02368        0.44188
C          0.41804        1.70924        1.76128
H          2.12145        0.46895        2.49061
H         -0.07586        2.03308        2.66381
Cl        -0.87381       -1.57243       -2.16419
Cl         1.30250       -3.04426        0.01643
Cl         0.87381        1.57243       -2.16419
Cl        -1.30250        3.04426        0.01643


36
Energy: -1158812.4212752
Fe         0.00000        0.00000        0.49822
C          0.71403       -0.98277       -1.14420
C         -0.71403       -0.98277       -1.14420
C          1.15532        0.37539       -1.14420
C         -1.15532        0.37539       -1.14420
C          0.00000        1.21477       -1.14420
C          0.71025       -0.97758        2.15499
C          1.14922        0.37340        2.15499
C         -0.71025       -0.97758        2.15499
H          1.34485       -1.85102        2.13486
C          0.00000        1.20836        2.15499
H          2.17601        0.70703        2.13486
C         -1.14922        0.37340        2.15499
H         -1.34485       -1.85102        2.13486
H          0.00000        2.28799        2.13486
H         -2.17601        0.70703        2.13486
C          0.00000        2.70485       -1.19286
H          0.00000        3.06450       -2.22790
H         -0.88068        3.12367       -0.70262
H          0.88068        3.12367       -0.70262
C         -2.57246        0.83584       -1.19286
H         -3.24293        0.12769       -0.70262
H         -2.69864        1.80284       -0.70262
H         -2.91451        0.94698       -2.22790
C          2.57246        0.83584       -1.19286
H          2.91451        0.94698       -2.22790
H          2.69864        1.80284       -0.70262
H          3.24293        0.12769       -0.70262
C         -1.58987       -2.18827       -1.19286
H         -2.54853       -2.00945       -0.70262
H         -1.80127       -2.47923       -2.22790
H         -1.12356       -3.04475       -0.70262
C          1.58987       -2.18827       -1.19286
H          1.80127       -2.47923       -2.22790
H          2.54853       -2.00945       -0.70262
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H          1.12356       -3.04475       -0.70262


51
Energy: -1282059.6721475
Fe         0.00000        0.00000        0.00000
C         -0.71348       -0.98202        1.66128
C          0.71348       -0.98202        1.66128
C         -1.15444        0.37510        1.66128
C          1.15444        0.37510        1.66128
C          0.00000        1.21385        1.66128
C         -0.71348       -0.98202       -1.66128
C         -1.15444        0.37510       -1.66128
C          0.71348       -0.98202       -1.66128
C          0.00000        1.21385       -1.66128
C          1.15444        0.37510       -1.66128
C          0.00000        2.70118        1.75319
H          0.00000        3.02775        2.79924
H          0.88023        3.13729        1.27746
H         -0.88023        3.13729        1.27746
C          2.56897        0.83471        1.75319
H          3.25575        0.13233        1.27746
H          2.71174        1.80662        1.27746
H          2.87956        0.93563        2.79924
C         -2.56897        0.83471        1.75319
H         -2.87956        0.93563        2.79924
H         -2.71174        1.80662        1.27746
H         -3.25575        0.13233        1.27746
C          1.58771       -2.18530        1.75319
H          2.55617       -2.02074        1.27746
H          1.77967       -2.44950        2.79924
H          1.13193       -3.05551        1.27746
C         -1.58771       -2.18530        1.75319
H         -1.77967       -2.44950        2.79924
H         -2.55617       -2.02074        1.27746
H         -1.13193       -3.05551        1.27746
C          0.00000        2.70118       -1.75319
H         -0.88023        3.13729       -1.27746
H          0.88023        3.13729       -1.27746
H          0.00000        3.02775       -2.79924
C         -2.56897        0.83471       -1.75319
H         -2.71174        1.80662       -1.27746
H         -2.87956        0.93563       -2.79924
H         -3.25575        0.13233       -1.27746
C         -1.58771       -2.18530       -1.75319
H         -2.55617       -2.02074       -1.27746
H         -1.77967       -2.44950       -2.79924
H         -1.13193       -3.05551       -1.27746
C          1.58771       -2.18530       -1.75319
H          1.13193       -3.05551       -1.27746
H          1.77967       -2.44950       -2.79924
H          2.55617       -2.02074       -1.27746
C          2.56897        0.83471       -1.75319
H          3.25575        0.13233       -1.27746
H          2.87956        0.93563       -2.79924
H          2.71174        1.80662       -1.27746
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51
Energy: -1282059.8828338
Fe 0.00000 0.00000 0.00000
C -1.04230 -0.62214 1.66006
C 0.26960 -1.18354 1.66006
C -0.91378 0.79904 1.66006
C 1.20893 -0.10933 1.66006
C 0.47756 1.11597 1.66006
C -1.20893 -0.10933 -1.66006
C -0.47756 1.11597 -1.66006
C -0.26960 -1.18354 -1.66006
C 0.91378 0.79904 -1.66006
C 1.04230 -0.62214 -1.66006
C 1.06220 2.48497 1.73670
H 1.17253 2.80667 2.77848
H 2.05124 2.52871 1.27762
H 0.43196 3.22259 1.23566
C 2.69159 -0.24232 1.73670
H 3.03881 -1.16943 1.27762
H 3.19835 0.58501 1.23566
H 3.03163 -0.24783 2.77848
C -2.03511 1.77811 1.73670
H -2.30697 1.98245 2.77848
H -1.77108 2.73226 1.27762
H -2.93138 1.40666 1.23566
C 0.60129 -2.63473 1.73670
H 1.54472 -2.86103 1.23566
H 0.70112 -2.95983 2.77848
H -0.17315 -3.25146 1.27762
C -2.31997 -1.38604 1.73670
H -2.59831 -1.58145 2.77848
H -3.14582 -0.84008 1.27762
H -2.24366 -2.35323 1.23566
C 2.03511 1.77811 -1.73670
H 1.77108 2.73226 -1.27762
H 2.93138 1.40666 -1.23566
H 2.30697 1.98245 -2.77848
C -1.06220 2.48497 -1.73670
H -0.43196 3.22259 -1.23566
H -1.17253 2.80667 -2.77848
H -2.05124 2.52871 -1.27762
C -2.69159 -0.24232 -1.73670
H -3.19835 0.58501 -1.23566
H -3.03163 -0.24783 -2.77848
H -3.03881 -1.16943 -1.27762
C -0.60129 -2.63473 -1.73670
H -1.54472 -2.86103 -1.23566
H -0.70112 -2.95983 -2.77848
H 0.17315 -3.25146 -1.27762
C 2.31997 -1.38604 -1.73670
H 2.24366 -2.35323 -1.23566
H 2.59831 -1.58145 -2.77848
H 3.14582 -0.84008 -1.27762

36
Energy: -1158811.9411677
Fe 0.00000 0.00000 0.49568

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C          0.00000        1.21444       -1.14954
C          1.15500        0.37528       -1.14954
C         -1.15500        0.37528       -1.14954
C          0.71383       -0.98250       -1.14954
C         -0.71383       -0.98250       -1.14954
C          1.14898       -0.37333        2.15605
C          0.71011        0.97738        2.15605
C          0.00000       -1.20810        2.15605
H          2.17576       -0.70695        2.13688
C         -0.71011        0.97738        2.15605
H          1.34470        1.85082        2.13688
C         -1.14898       -0.37333        2.15605
H          0.00000       -2.28773        2.13688
H         -1.34470        1.85082        2.13688
H         -2.17576       -0.70695        2.13688
C          0.00000        2.70452       -1.18968
H          0.00000        3.07074       -2.22234
H         -0.88051        3.12013       -0.69651
H          0.88051        3.12013       -0.69651
C          2.57215        0.83574       -1.18968
H          2.92045        0.94891       -2.22234
H          2.69533        1.80159       -0.69651
H          3.23951        0.12676       -0.69651
C          1.58968       -2.18800       -1.18968
H          1.80494       -2.48428       -2.22234
H          2.54631       -2.00669       -0.69651
H          1.12162       -3.04179       -0.69651
C         -2.57215        0.83574       -1.18968
H         -2.69533        1.80159       -0.69651
H         -2.92045        0.94891       -2.22234
H         -3.23951        0.12676       -0.69651
C         -1.58968       -2.18800       -1.18968
H         -1.12162       -3.04179       -0.69651
H         -2.54631       -2.00669       -0.69651
H         -1.80494       -2.48428       -2.22234


51
Energy: -1282059.8321059
Fe         0.00000        0.00000        0.00000
C          0.00000        1.21380        1.66107
C         -1.15439        0.37508        1.66107
C          1.15439        0.37508        1.66107
C         -0.71345       -0.98198        1.66107
C          0.71345       -0.98198        1.66107
C         -1.15439       -0.37508       -1.66107
C         -0.71345        0.98198       -1.66107
C          0.00000       -1.21380       -1.66107
C          0.71345        0.98198       -1.66107
C          1.15439       -0.37508       -1.66107
C          0.00000        2.70257        1.73534
H          0.00000        3.04380        2.77676
H          0.88135        3.13115        1.25458
H         -0.88135        3.13115        1.25458
C         -2.57029        0.83514        1.73534
H         -2.89482        0.94059        2.77676
H         -2.70555        1.80580        1.25458
H         -3.25025        0.12936        1.25458
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C         -1.58853       -2.18642        1.73534
H         -1.78910       -2.46248        2.77676
H         -2.55347       -2.01511        1.25458
H         -1.12741       -3.05120        1.25458
C          2.57029        0.83514        1.73534
H          2.70555        1.80580        1.25458
H          2.89482        0.94059        2.77676
H          3.25025        0.12936        1.25458
C          1.58853       -2.18642        1.73534
H          1.12741       -3.05120        1.25458
H          2.55347       -2.01511        1.25458
H          1.78910       -2.46248        2.77676
C          0.00000       -2.70257       -1.73534
H          0.00000       -3.04380       -2.77676
H          0.88135       -3.13115       -1.25458
H         -0.88135       -3.13115       -1.25458
C         -2.57029       -0.83514       -1.73534
H         -2.89482       -0.94059       -2.77676
H         -2.70555       -1.80580       -1.25458
H         -3.25025       -0.12936       -1.25458
C          2.57029       -0.83514       -1.73534
H          2.70555       -1.80580       -1.25458
H          2.89482       -0.94059       -2.77676
H          3.25025       -0.12936       -1.25458
C          1.58853        2.18642       -1.73534
H          2.55347        2.01511       -1.25458
H          1.78910        2.46248       -2.77676
H          1.12741        3.05120       -1.25458
C         -1.58853        2.18642       -1.73534
H         -1.78910        2.46248       -2.77676
H         -2.55347        2.01511       -1.25458
H         -1.12741        3.05120       -1.25458


33
Energy: -1134163.4519249
Fe         0.00000        0.00000        0.05581
C         -0.70786       -1.63497        1.04885
C         -1.14642       -1.65388       -0.30233
C          0.71487       -1.63898        1.06045
H         -1.34238       -1.59240        1.92270
C         -0.00248       -1.67301       -1.14742
H         -2.17338       -1.63314       -0.63766
C          1.13964       -1.66182       -0.29779
C         -0.71487        1.63898        1.06045
C          0.70786        1.63497        1.04885
C         -1.13964        1.66182       -0.29779
C          1.14642        1.65388       -0.30233
H          1.34238        1.59240        1.92270
C          0.00248        1.67301       -1.14742
H         -2.16791        1.64931       -0.63198
H          2.17338        1.63314       -0.63766
C          0.00000       -1.77042       -2.63392
H         -0.88537       -1.30081       -3.06689
H          0.88129       -1.29187       -3.06544
H          0.00561       -2.81813       -2.95179
H          2.16791       -1.64931       -0.63198
C          1.59289       -1.66816        2.26459
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H 2.54555 -1.16962 2.07465
H 1.11753 -1.17580 3.11545
H 1.81284 -2.69907 2.56084
C 0.00000 1.77042 -2.63392
H 0.88537 1.30081 -3.06689
H -0.88129 1.29187 -3.06544
H -0.00561 2.81813 -2.95179
C -1.59289 1.66816 2.26459
H -2.54555 1.16962 2.07465
H -1.11753 1.17580 3.11545
H -1.81284 2.69907 2.56084

33
Energy: -1134163.6728082
Fe 0.00000 0.00000 0.18353
C 1.70135 -1.06633 0.55376
C 0.64379 -1.51969 1.38758
C 1.30824 -1.23428 -0.80318
H 2.63557 -0.63786 0.88785
C -0.42006 -1.97394 0.55964
H 0.63176 -1.49742 2.46775
C 0.00000 -1.79585 -0.78905
C 0.42006 1.97394 0.55964
C 0.00000 1.79585 -0.78905
C -0.64379 1.51969 1.38758
C -1.30824 1.23428 -0.80318
H 0.59259 2.02369 -1.66467
C -1.70135 1.06633 0.55376
H -0.63176 1.49742 2.46775
H -2.63557 0.63786 0.88785
C -1.70641 -2.57239 1.01655
H -2.00871 -2.17122 1.98594
H -2.51098 -2.37760 0.30450
H -1.61496 -3.65840 1.12209
H -0.59259 -2.02369 -1.66467
C 2.12998 -0.93129 -2.00920
H 2.82105 -0.10680 -1.82242
H 2.72599 -1.80158 -2.30289
H 1.50251 -0.65974 -2.86058
C -2.12998 0.93129 -2.00920
H -2.72599 1.80158 -2.30289
H -1.50251 0.65974 -2.86058
H -2.82105 0.10680 -1.82242
C 1.70641 2.57239 1.01655
H 2.51098 2.37760 0.30450
H 1.61496 3.65840 1.12209
H 2.00871 2.17122 1.98594

27
Energy: -1084863.5274328
Fe -0.09498 0.25680 0.00000
C -1.28541 -1.23978 0.71042
C -1.28541 -1.23978 -0.71042
C 0.05094 -1.42674 1.16111
H -2.14672 -1.09156 1.34564
C 0.05094 -1.42674 -1.16111

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H         -2.14672       -1.09156       -1.34564
C          0.86653       -1.54319        0.00000
C         -0.83448        2.03095        0.71009
C          0.50326        1.84286        1.14927
C         -0.83448        2.03095       -0.71009
H         -1.70255        2.13053        1.34398
C          1.32995        1.72767        0.00000
H          0.83072        1.77457        2.17588
C          0.50326        1.84286       -1.14927
H         -1.70255        2.13053       -1.34398
H          2.39586        1.55679        0.00000
H          0.83072        1.77457       -2.17588
C          0.50368       -1.53247       -2.57715
H         -0.13739       -0.95176       -3.24332
H          1.52798       -1.17334       -2.69508
H          0.47731       -2.57293       -2.91706
H          1.94039       -1.66935        0.00000
C          0.50368       -1.53247        2.57715
H          1.52798       -1.17334        2.69508
H         -0.13739       -0.95176        3.24332
H          0.47731       -2.57293        2.91706


33
Energy: -1134163.1290211
Fe         0.00000        0.00000        0.21576
C         -0.71010        1.64321        1.20104
C          0.71010        1.64321        1.20104
C         -1.16071        1.66276       -0.14802
H         -1.34541        1.60903        2.07436
C          1.16071        1.66276       -0.14802
H          1.34541        1.60903        2.07436
C          0.00000        1.66897       -0.97142
C         -0.71010       -1.64321        1.20104
C         -1.16071       -1.66276       -0.14802
C          0.71010       -1.64321        1.20104
H         -1.34541       -1.60903        2.07436
C          0.00000       -1.66897       -0.97142
C          1.16071       -1.66276       -0.14802
H          1.34541       -1.60903        2.07436
H          0.00000       -1.66517       -2.05277
C          2.57418        1.75055       -0.60970
H          3.25685        1.27548        0.09735
H          2.70887        1.27340       -1.58231
H          2.88117        2.79659       -0.71112
H          0.00000        1.66517       -2.05277
C         -2.57418        1.75055       -0.60970
H         -2.88117        2.79659       -0.71112
H         -2.70887        1.27340       -1.58231
H         -3.25685        1.27548        0.09735
C          2.57418       -1.75055       -0.60970
H          2.70887       -1.27340       -1.58231
H          3.25685       -1.27548        0.09735
H          2.88117       -2.79659       -0.71112
C         -2.57418       -1.75055       -0.60970
H         -3.25685       -1.27548        0.09735
H         -2.70887       -1.27340       -1.58231
H         -2.88117       -2.79659       -0.71112
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33
Energy: -1134163.6619586
Fe 0.00000 0.00000 0.18378
C -0.74046 1.87751 0.55980
C -0.99151 1.49704 -0.78904
C -1.37665 0.91119 1.38744
C -1.77181 0.30622 -0.80351
C -2.00740 -0.05088 0.55332
H -1.35486 0.89931 2.46762
H -2.54983 -0.92394 0.88718
C 0.99151 -1.49704 -0.78904
C 1.77181 -0.30622 -0.80351
C 0.74046 -1.87751 0.55980
H 0.62279 -2.01421 -1.66446
C 2.00740 0.05088 0.55332
C 1.37665 -0.91119 1.38744
H 2.54983 0.92394 0.88718
H 1.35486 -0.89931 2.46762
C 0.00000 3.08758 1.01720
H -0.67745 3.94116 1.12404
H 0.47467 2.92022 1.98607
H 0.77721 3.37175 0.30483
H -0.62279 2.01421 -1.66446
C -2.28895 -0.40033 -2.00969
H -1.61258 -0.28545 -2.85919
H -2.41545 -1.46829 -1.82081
H -3.26364 -0.00003 -2.30741
C 2.28895 0.40033 -2.00969
H 1.61258 0.28545 -2.85919
H 2.41545 1.46829 -1.82081
H 3.26364 0.00003 -2.30741
C 0.00000 -3.08758 1.01720
H -0.77721 -3.37175 0.30483
H 0.67745 -3.94116 1.12404
H -0.47467 -2.92022 1.98607

33
Energy: -1134162.9601081
Fe 0.00000 0.00000 0.00000
C -0.39276 1.65417 1.16037
C 0.34691 2.01721 0.00000
C -1.60128 1.05571 0.71057
C -0.39276 1.65417 -1.16037
C -1.60128 1.05571 -0.71057
H -2.37284 0.64544 1.34624
H -2.37284 0.64544 -1.34624
C 1.60128 -1.05571 -0.71057
C 1.60128 -1.05571 0.71057
C 0.39276 -1.65417 -1.16037
H 2.37284 -0.64544 -1.34624
C 0.39276 -1.65417 1.16037
H 2.37284 -0.64544 1.34624
C -0.34691 -2.01721 0.00000
H -1.32697 -2.47409 0.00000
C 0.00000 1.90696 2.57557

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H         -0.32638        2.90154        2.89666
H         -0.45424        1.17917        3.25056
H          1.08343        1.85919        2.70380
H          1.32697        2.47409        0.00000
C          0.00000        1.90696       -2.57557
H          1.08343        1.85919       -2.70380
H         -0.45424        1.17917       -3.25056
H         -0.32638        2.90154       -2.89666
C          0.00000       -1.90696        2.57557
H          0.45424       -1.17917        3.25056
H         -1.08343       -1.85919        2.70380
H          0.32638       -2.90154        2.89666
C          0.00000       -1.90696       -2.57557
H         -1.08343       -1.85919       -2.70380
H          0.45424       -1.17917       -3.25056
H          0.32638       -2.90154       -2.89666


27
Energy: -1084862.9493272
Fe         0.09589        0.25575        0.00000
C         -0.05167       -1.43101        1.16070
C         -0.86725       -1.54618        0.00000
C          1.28448       -1.24594        0.71024
C         -0.05167       -1.43101       -1.16070
C          1.28448       -1.24594       -0.71024
H          2.14541       -1.09548        1.34557
H          2.14541       -1.09548       -1.34557
C         -1.09992        1.76272       -0.71038
C         -1.09992        1.76272        0.71038
C          0.23708        1.95009       -1.14873
H         -1.96163        1.61964       -1.34489
C          0.23708        1.95009        1.14873
H         -1.96163        1.61964        1.34489
C          1.06420        2.06427        0.00000
H          0.57068        1.97324       -2.17530
H          0.57068        1.97324        2.17530
H          2.13655        2.18826        0.00000
C         -0.50567       -1.52874        2.57675
H         -0.48288       -2.56753        2.92183
H          0.13660       -0.94661        3.24049
H         -1.52879       -1.16550        2.69220
H         -1.94177       -1.66730        0.00000
C         -0.50567       -1.52874       -2.57675
H         -1.52879       -1.16550       -2.69220
H          0.13660       -0.94661       -3.24049
H         -0.48288       -2.56753       -2.92183


33
Energy: -1134163.6619586
Fe         0.00000        0.00000        0.18378
C         -0.74046        1.87751        0.55979
C         -0.99151        1.49703       -0.78905
C         -1.37665        0.91119        1.38744
C         -1.77182        0.30621       -0.80351
C         -2.00740       -0.05087        0.55333
H         -1.35485        0.89932        2.46762
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H         -2.54982       -0.92395        0.88719
C          1.77182       -0.30621       -0.80351
C          2.00740        0.05087        0.55333
C          0.99151       -1.49703       -0.78905
C          1.37665       -0.91119        1.38744
H          2.54982        0.92395        0.88719
C          0.74046       -1.87751        0.55979
H          0.62279       -2.01419       -1.66447
H          1.35485       -0.89932        2.46762
C          0.00000        3.08758        1.01719
H         -0.67745        3.94116        1.12402
H          0.47465        2.92022        1.98607
H          0.77723        3.37174        0.30483
H         -0.62279        2.01419       -1.66447
C         -2.28895       -0.40036       -2.00968
H         -1.61258       -0.28547       -2.85918
H         -2.41544       -1.46831       -1.82079
H         -3.26365       -0.00007       -2.30739
C          2.28895        0.40036       -2.00968
H          3.26365        0.00007       -2.30739
H          1.61258        0.28547       -2.85918
H          2.41544        1.46831       -1.82079
C          0.00000       -3.08758        1.01719
H         -0.77723       -3.37174        0.30483
H          0.67745       -3.94116        1.12402
H         -0.47465       -2.92022        1.98607


27
Energy: -1084863.5236050
Fe         0.00000        0.00000        0.33746
C         -0.64289        1.52025        1.54505
C          0.41190        1.96748        0.70693
C         -1.70141        1.07221        0.71036
H         -0.63112        1.49724        2.62425
C          0.00000        1.79306       -0.64150
H          1.36825        2.34531        1.03569
C         -1.31052        1.23706       -0.64835
H         -2.63764        0.64969        1.04514
H          0.58940        2.01749       -1.51905
C          0.64289       -1.52025        1.54505
C         -0.41190       -1.96748        0.70693
C          1.70141       -1.07221        0.71036
H          0.63112       -1.49724        2.62425
C          0.00000       -1.79306       -0.64150
H         -1.36825       -2.34531        1.03569
C          1.31052       -1.23706       -0.64835
H          2.63764       -0.64969        1.04514
H         -0.58940       -2.01749       -1.51905
C         -2.13834        0.93488       -1.85041
H         -1.51427        0.67417       -2.70757
H         -2.82111        0.10364       -1.66383
H         -2.74306        1.80232       -2.13411
C          2.13834       -0.93488       -1.85041
H          2.82111       -0.10364       -1.66383
H          2.74306       -1.80232       -2.13411
H          1.51427       -0.67417       -2.70757
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27
Energy: -1084863.4957938

Fe	0.00000	0.00000	0.13067
C	-1.52660	-0.94324	1.10895
C	-1.88736	-0.68729	-0.24012
C	-0.36649	-1.76290	1.10109
H	-2.02694	-0.55921	1.98509
C	-0.94852	-1.35143	-1.07435
H	-2.71126	-0.07376	-0.57296
C	0.00000	-2.02001	-0.25017
H	0.16870	-2.11224	1.97209
H	-0.93492	-1.33233	-2.15449
C	0.36649	1.76290	1.10109
C	1.52660	0.94324	1.10895
C	0.00000	2.02001	-0.25017
H	-0.16870	2.11224	1.97209
C	1.88736	0.68729	-0.24012
H	2.02694	0.55921	1.98509
C	0.94852	1.35143	-1.07435
H	2.71126	0.07376	-0.57296
H	0.93492	1.33233	-2.15449
C	1.13136	-2.87212	-0.71465
H	0.81279	-3.91337	-0.82854
H	1.51070	-2.53582	-1.68161
H	1.95888	-2.85657	-0.00269
C	-1.13136	2.87212	-0.71465
H	-1.51070	2.53582	-1.68161
H	-1.95888	2.85657	-0.00269
H	-0.81279	3.91337	-0.82854

24
Energy: -1060213.3937010

Fe	0.16248	-0.20327	0.00000
C	1.67115	0.97753	0.70979
C	1.67115	0.97753	-0.70979
C	0.41201	1.47082	1.14466
H	2.47354	0.63521	1.34565
C	0.41201	1.47082	-1.14466
H	2.47354	0.63521	-1.34565
C	-0.37634	1.77840	0.00000
H	0.09044	1.57061	2.17120
H	0.09044	1.57061	-2.17120
C	0.47260	-2.09933	0.71018
C	-0.78538	-1.60742	1.14905
C	0.47260	-2.09933	-0.71018
H	1.29398	-2.39587	1.34466
C	-1.56296	-1.30274	0.00000
H	-1.08742	-1.46516	2.17560
C	-0.78538	-1.60742	-1.14905
H	1.29398	-2.39587	-1.34466
H	-2.56010	-0.88845	0.00000
H	-1.08742	-1.46516	-2.17560
C	-1.74804	2.36140	0.00000
H	-1.70524	3.45536	0.00000
H	-2.31046	2.05351	-0.88363
H	-2.31046	2.05351	0.88363

27
Energy: -1084863.2950159
Fe 0.00000 0.00000 0.40374
C -0.70985 1.63702 1.39850
C 0.70985 1.63702 1.39850
C -1.14451 1.65844 0.04656
H -1.34574 1.59608 2.26990
C 1.14451 1.65844 0.04656
H 1.34574 1.59608 2.26990
C 0.00000 1.67489 -0.79939
H -2.17108 1.64293 -0.28980
H 2.17108 1.64293 -0.28980
C -0.70985 -1.63702 1.39850
C -1.14451 -1.65844 0.04656
C 0.70985 -1.63702 1.39850
H -1.34574 -1.59608 2.26990
C 0.00000 -1.67489 -0.79939
H -2.17108 -1.64293 -0.28980
C 1.14451 -1.65844 0.04656
H 1.34574 -1.59608 2.26990
H 2.17108 -1.64293 -0.28980
C 0.00000 1.77469 -2.28577
H 0.00000 2.82302 -2.60119
H 0.88345 1.30160 -2.71868
H -0.88345 1.30160 -2.71868
C 0.00000 -1.77469 -2.28577
H 0.00000 -2.82302 -2.60119
H -0.88345 -1.30160 -2.71868
H 0.88345 -1.30160 -2.71868

27
Energy: -1084863.2950159
Fe -0.40374 -0.00001 0.00000
C -1.39850 0.70985 1.63702
C -1.39850 -0.70984 1.63703
C -0.04656 1.14451 1.65844
H -2.26990 1.34574 1.59608
C -0.04656 -1.14451 1.65845
H -2.26990 -1.34573 1.59610
C 0.79939 0.00000 1.67489
H 0.28980 2.17108 1.64293
H 0.28979 -2.17108 1.64296
C -1.39850 0.70985 -1.63702
C -0.04656 1.14451 -1.65844
C -1.39850 -0.70984 -1.63703
H -2.26990 1.34574 -1.59608
C 0.79939 0.00000 -1.67489
H 0.28980 2.17108 -1.64293
C -0.04656 -1.14451 -1.65845
H -2.26990 -1.34573 -1.59610
H 0.28979 -2.17108 -1.64296
C 2.28577 0.00000 1.77469
H 2.60119 0.00001 2.82302
H 2.71868 -0.88345 1.30160
H 2.71869 0.88345 1.30158

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C          2.28577        0.00000       -1.77469
H          2.60119        0.00001       -2.82302
H          2.71869        0.88345       -1.30158
H          2.71868       -0.88345       -1.30160


27
Energy: -1084863.5200659
Fe         0.00000        0.00000        0.33761
C          0.00000        1.80168       -0.64892
C         -0.39014        1.97307        0.70920
C          1.30438        1.23141       -0.64015
C          0.66155        1.51202        1.54545
H         -1.34079        2.36327        1.04253
C          1.71227        1.05247        0.70888
H          1.87370        0.95724       -1.51681
H          0.65155        1.48802        2.62464
H          2.64338        0.61718        1.03904
C         -0.66155       -1.51202        1.54545
C         -1.71227       -1.05247        0.70888
C          0.39014       -1.97307        0.70920
H         -0.65155       -1.48802        2.62464
C         -1.30438       -1.23141       -0.64015
H         -2.64338       -0.61718        1.03904
C          0.00000       -1.80168       -0.64892
H          1.34079       -2.36327        1.04253
H         -1.87370       -0.95724       -1.51681
C         -0.78663        2.19532       -1.85219
H         -0.56934        3.22976       -2.13742
H         -0.54817        1.56084       -2.70819
H         -1.86002        2.12304       -1.66626
C          0.78663       -2.19532       -1.85219
H          0.54817       -1.56084       -2.70819
H          1.86002       -2.12304       -1.66626
H          0.56934       -3.22976       -2.13742


27
Energy: -1084860.2770907
Fe         0.00000        0.00000        0.00000
C         -0.82295        1.89535        0.00000
C          0.00000        1.70001        1.14368
C          0.00000        1.70001       -1.14368
C          1.31743        1.39186        0.70935
H         -0.33228        1.75711        2.17020
C          1.31743        1.39186       -0.70935
H         -0.33228        1.75711       -2.17020
H          2.16065        1.17200        1.34704
H          2.16065        1.17200       -1.34704
C          0.00000       -1.70001        1.14368
C         -1.31743       -1.39186        0.70935
C          0.82295       -1.89535        0.00000
H          0.33228       -1.75711        2.17020
C         -1.31743       -1.39186       -0.70935
H         -2.16065       -1.17200        1.34704
C          0.00000       -1.70001       -1.14368
H         -2.16065       -1.17200       -1.34704
H          0.33228       -1.75711       -2.17020
```

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C         -2.27356        2.26257        0.00000
H         -2.52179        2.85789       -0.88109
H         -2.92613        1.38696        0.00000
H         -2.52179        2.85789        0.88109
C          2.27356       -2.26257        0.00000
H          2.52179       -2.85789       -0.88109
H          2.92613       -1.38696        0.00000
H          2.52179       -2.85789        0.88109


24
Energy: -1060212.7781707
Fe         0.16356       -0.20248        0.00000
C         -0.38031        1.78075        0.00000
C          0.40872        1.47589        1.14430
C          0.40872        1.47589       -1.14430
C          1.66929        0.98740        0.70954
H          0.08539        1.57135        2.17076
C          1.66929        0.98740       -0.70954
H          0.08539        1.57135       -2.17076
H          2.47168        0.64472        1.34535
H          2.47168        0.64472       -1.34535
C         -0.08521       -1.88255        1.14873
C         -1.34511       -1.39553        0.70982
C          0.69249       -2.18436        0.00000
H          0.23539       -1.97847        2.17504
C         -1.34511       -1.39553       -0.70982
H         -2.15120       -1.05888        1.34427
C         -0.08521       -1.88255       -1.14873
H          1.70858       -2.54897        0.00000
H         -2.15120       -1.05888       -1.34427
H          0.23539       -1.97847       -2.17504
C         -1.75594        2.35391        0.00000
H         -1.72090        3.44810        0.00000
H         -2.31622        2.04192       -0.88353
H         -2.31622        2.04192        0.88353


27
Energy: -1084863.5200659
Fe         0.00000        0.00000        0.33761
C          0.00000        1.80168       -0.64893
C         -0.39017        1.97306        0.70918
C          1.30438        1.23142       -0.64013
C          0.66150        1.51203        1.54545
H         -1.34084        2.36327        1.04247
C          1.71225        1.05249        0.70891
H          1.87375        0.95729       -1.51677
H          0.65147        1.48803        2.62464
H          2.64335        0.61722        1.03911
C         -1.71225       -1.05249        0.70891
C         -1.30438       -1.23142       -0.64013
C         -0.66150       -1.51203        1.54545
H         -2.64335       -0.61722        1.03911
C          0.00000       -1.80168       -0.64893
H         -1.87375       -0.95729       -1.51677
C          0.39017       -1.97306        0.70918
H         -0.65147       -1.48803        2.62464
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H          1.34084       -2.36327        1.04247
C         -0.78661        2.19533       -1.85221
H         -1.86000        2.12305       -1.66630
H         -0.56931        3.22976       -2.13743
H         -0.54813        1.56084       -2.70821
C          0.78661       -2.19533       -1.85221
H          0.56931       -3.22976       -2.13743
H          0.54813       -1.56084       -2.70821
H          1.86000       -2.12305       -1.66630


39
Energy: -1183462.4630142
Fe         0.00000        0.00000        0.40284
C          0.65642       -1.48806        1.63108
C         -0.39855       -1.95852        0.80752
C          1.71903       -1.05179        0.79285
H          0.64811       -1.43542        2.71027
C          0.00000       -1.82383       -0.55088
H         -1.35419       -2.33264        1.14642
C          1.31422       -1.26213       -0.56142
C         -0.65642        1.48806        1.63108
C          0.39855        1.95852        0.80752
C         -1.71903        1.05179        0.79285
H         -0.64811        1.43542        2.71027
C          0.00000        1.82383       -0.55088
H          1.35419        2.33264        1.14642
C         -1.31422        1.26213       -0.56142
C          2.15171       -1.02315       -1.77041
H          2.75216       -1.90759       -2.01045
H          1.54118       -0.79846       -2.64706
H          2.84268       -0.19061       -1.62593
C         -0.78331       -2.27090       -1.73700
H         -1.85323       -2.28321       -1.51975
H         -0.62653       -1.62267       -2.60137
H         -0.49626       -3.28544       -2.03365
C          3.03616       -0.52847        1.25524
H          3.77927       -1.33118        1.31317
H          3.43159        0.23383        0.58079
H          2.95312       -0.08390        2.24888
C          0.78331        2.27090       -1.73700
H          0.62653        1.62267       -2.60137
H          0.49626        3.28544       -2.03365
H          1.85323        2.28321       -1.51975
C         -2.15171        1.02315       -1.77041
H         -2.75216        1.90759       -2.01045
H         -1.54118        0.79846       -2.64706
H         -2.84268        0.19061       -1.62593
C         -3.03616        0.52847        1.25524
H         -3.77927        1.33118        1.31317
H         -3.43159       -0.23383        0.58079
H         -2.95312        0.08390        2.24888


39
Energy: -1183462.6049505
Fe         0.00000        0.00000        0.16078
C         -1.29275       -1.20843        1.17037
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C         -1.73166       -1.02805       -0.16661
C          0.00000       -1.80112        1.14135
H         -1.82936       -0.91904        2.06277
C         -0.71800       -1.51019       -1.03994
H         -2.66495       -0.58010       -0.47720
C          0.35852       -1.98672       -0.22952
C          0.00000        1.80112        1.14135
C          1.29275        1.20843        1.17037
C         -0.35852        1.98672       -0.22952
C          1.73166        1.02805       -0.16661
H          1.82936        0.91904        2.06277
C          0.71800        1.51019       -1.03994
H          2.66495        0.58010       -0.47720
C          1.60960       -2.62597       -0.72800
H          1.48045       -3.70789       -0.84342
H          1.90378       -2.22726       -1.70085
H          2.44222       -2.46878       -0.03983
C         -0.80878       -1.57929       -2.52551
H         -1.50708       -0.83393       -2.91164
H          0.15733       -1.41171       -3.00533
H         -1.16736       -2.56276       -2.84784
C          0.80316       -2.20207        2.33158
H          0.64118       -3.25727        2.57679
H          1.87384       -2.06617        2.16603
H          0.52383       -1.61399        3.20805
C          0.80878        1.57929       -2.52551
H          1.50708        0.83393       -2.91164
H         -0.15733        1.41171       -3.00533
H          1.16736        2.56276       -2.84784
C         -1.60960        2.62597       -0.72800
H         -1.48045        3.70789       -0.84342
H         -1.90378        2.22726       -1.70085
H         -2.44222        2.46878       -0.03983
C         -0.80316        2.20207        2.33158
H         -0.64118        3.25727        2.57679
H         -1.87384        2.06617        2.16603
H         -0.52383        1.61399        3.20805


30
Energy: -1109513.2127087
Fe        -0.16599        0.43102        0.00000
C         -1.67542       -0.73868        0.70935
C         -1.67542       -0.73868       -0.70935
C         -0.42175       -1.23904        1.15769
H         -2.47469       -0.38916        1.34677
C         -0.42175       -1.23904       -1.15769
H         -2.47469       -0.38916       -1.34677
C          0.35674       -1.55115        0.00000
C         -0.46372        2.33167        0.71009
C          0.79082        1.83078        1.14928
C         -0.46372        2.33167       -0.71009
H         -1.28292        2.63518        1.34414
C          1.56644        1.52160        0.00000
H          1.09256        1.68751        2.17610
C          0.79082        1.83078       -1.14928
H         -1.28292        2.63518       -1.34414
H          2.56168        1.10250        0.00000
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H          1.09256        1.68751       -2.17610
C          1.72175       -2.14973        0.00000
H          1.67073       -3.24409        0.00000
H          2.29141       -1.85006       -0.88162
H          2.29141       -1.85006        0.88162
C         -0.02276       -1.44557       -2.57899
H         -0.57658       -0.77743       -3.24129
H          1.04240       -1.26272       -2.73416
H         -0.22837       -2.47290       -2.89824
C         -0.02276       -1.44557        2.57899
H         -0.22837       -2.47290        2.89824
H          1.04240       -1.26272        2.73416
H         -0.57658       -0.77743        3.24129


39
Energy: -1183462.2407378
Fe         0.00000        0.00000        0.49894
C          0.70906        1.63220        1.49676
C         -0.70906        1.63220        1.49676
C          1.15727        1.66641        0.14771
H          1.34650        1.58690        2.36802
C         -1.15727        1.66641        0.14771
H         -1.34650        1.58690        2.36802
C          0.00000        1.68509       -0.69032
C          0.70906       -1.63220        1.49676
C          1.15727       -1.66641        0.14771
C         -0.70906       -1.63220        1.49676
H          1.34650       -1.58690        2.36802
C          0.00000       -1.68509       -0.69032
C         -1.15727       -1.66641        0.14771
H         -1.34650       -1.58690        2.36802
C          0.00000        1.80031       -2.17594
H          0.00000        2.85086       -2.48701
H         -0.88107        1.33094       -2.61749
H          0.88107        1.33094       -2.61749
C         -2.57626        1.75983       -0.29667
H         -3.25059        1.32498        0.44353
H         -2.74501        1.24489       -1.24437
H         -2.87111        2.80530       -0.43727
C          2.57626        1.75983       -0.29667
H          2.87111        2.80530       -0.43727
H          2.74501        1.24489       -1.24437
H          3.25059        1.32498        0.44353
C          2.57626       -1.75983       -0.29667
H          2.74501       -1.24489       -1.24437
H          2.87111       -2.80530       -0.43727
H          3.25059       -1.32498        0.44353
C          0.00000       -1.80031       -2.17594
H          0.00000       -2.85086       -2.48701
H          0.88107       -1.33094       -2.61749
H         -0.88107       -1.33094       -2.61749
C         -2.57626       -1.75983       -0.29667
H         -2.87111       -2.80530       -0.43727
H         -2.74501       -1.24489       -1.24437
H         -3.25059       -1.32498        0.44353
```

39
Energy: -1183462.6049505
Fe 0.00000 0.00000 0.16078
C 0.00000 -1.80113 1.14135
C -0.35851 -1.98672 -0.22952
C 1.29275 -1.20843 1.17038
C 0.71801 -1.51018 -1.03994
C 1.73166 -1.02805 -0.16660
H 1.82935 -0.91904 2.06278
H 2.66495 -0.58010 -0.47719
C -0.71801 1.51018 -1.03994
C -1.73166 1.02805 -0.16660
C 0.35851 1.98672 -0.22952
C -1.29275 1.20843 1.17038
H -2.66495 0.58010 -0.47719
C 0.00000 1.80113 1.14135
H -1.82935 0.91904 2.06278
C -0.80317 -2.20208 2.33157
H -0.64119 -3.25728 2.57677
H -0.52383 -1.61400 3.20805
H -1.87385 -2.06616 2.16603
C -1.60960 -2.62596 -0.72801
H -1.48045 -3.70789 -0.84341
H -2.44222 -2.46877 -0.03984
H -1.90376 -2.22727 -1.70086
C 0.80879 -1.57928 -2.52550
H 1.16738 -2.56274 -2.84784
H -0.15732 -1.41170 -3.00533
H 1.50708 -0.83391 -2.91163
C -0.80879 1.57928 -2.52550
H 0.15732 1.41170 -3.00533
H -1.50708 0.83391 -2.91163
H -1.16738 2.56274 -2.84784
C 1.60960 2.62596 -0.72801
H 1.90376 2.22727 -1.70086
H 1.48045 3.70789 -0.84341
H 2.44222 2.46877 -0.03984
C 0.80317 2.20208 2.33157
H 1.87385 2.06616 2.16603
H 0.64119 3.25728 2.57677
H 0.52383 1.61400 3.20805

39
Energy: -1183462.2622300
Fe 0.00000 0.00000 0.00000
C -0.38018 1.65565 1.15706
C 0.37407 2.02141 0.00000
C -1.59264 1.06292 0.70944
C -0.38018 1.65565 -1.15706
C -1.59264 1.06292 -0.70944
H -2.36546 0.65829 1.34740
H -2.36546 0.65829 -1.34740
C 1.59264 -1.06292 -0.70944
C 1.59264 -1.06292 0.70944
C 0.38018 -1.65565 -1.15706
H 2.36546 -0.65829 -1.34740
C 0.38018 -1.65565 1.15706

H 2.36546 -0.65829 1.34740
C -0.37407 -2.02141 0.00000
C 0.00000 1.90000 2.57754
H -0.25912 2.91971 2.88213
H -0.52380 1.21462 3.24640
H 1.07238 1.77383 2.74151
C 1.69409 2.71381 0.00000
H 1.56892 3.80230 0.00000
H 2.28355 2.45345 0.88120
H 2.28355 2.45345 -0.88120
C 0.00000 1.90000 -2.57754
H -0.25912 2.91971 -2.88213
H 1.07238 1.77383 -2.74151
H -0.52380 1.21462 -3.24640
C 0.00000 -1.90000 -2.57754
H -1.07238 -1.77383 -2.74151
H 0.52380 -1.21462 -3.24640
H 0.25912 -2.91971 -2.88213
C -1.69409 -2.71381 0.00000
H -2.28355 -2.45345 -0.88120
H -1.56892 -3.80230 0.00000
H -2.28355 -2.45345 0.88120
C 0.00000 -1.90000 2.57754
H -1.07238 -1.77383 2.74151
H 0.25912 -2.91971 2.88213
H 0.52380 -1.21462 3.24640

30
Energy: -1109512.6685639
Fe 0.16837 0.42951 0.00000
C 0.42044 -1.24401 1.15731
C -0.35900 -1.55324 0.00000
C 1.67540 -0.74819 0.70913
C 0.42044 -1.24401 -1.15731
C 1.67540 -0.74819 -0.70913
H 2.47462 -0.39850 1.34665
H 2.47462 -0.39850 -1.34665
C -1.34951 1.61215 -0.71027
C -1.34951 1.61215 0.71027
C -0.09417 2.10990 -1.14883
H -2.15441 1.27225 -1.34474
C -0.09417 2.10990 1.14883
H -2.15441 1.27225 1.34474
C 0.68195 2.41690 0.00000
H 0.22435 2.21147 -2.17540
H 0.22435 2.21147 2.17540
H 1.69456 2.79101 0.00000
C 0.01867 -1.44263 2.57879
H 0.20955 -2.47215 2.89996
H 0.58224 -0.78121 3.23953
H -1.04363 -1.24382 2.73416
C -1.72816 -2.14179 0.00000
H -1.68520 -3.23646 0.00000
H -2.29565 -1.83786 0.88155
H -2.29565 -1.83786 -0.88155
C 0.01867 -1.44263 -2.57879
H 0.20955 -2.47215 -2.89996

```
H         -1.04363       -1.24382       -2.73416
H          0.58224       -0.78121       -3.23953


39
Energy: -1183462.2104228
Fe         0.00000        0.00000        0.49942
C          0.52014        1.97594        0.25086
C         -0.49354        1.61209       -0.68792
C          0.00000        1.74650        1.55412
C         -1.63681        1.16324        0.04264
C         -1.32174        1.24867        1.42665
H          0.53662        1.90135        2.47908
H         -1.97388        0.95648        2.23713
C          0.49354       -1.61209       -0.68792
C          1.63681       -1.16324        0.04264
C         -0.52014       -1.97594        0.25086
C          1.32174       -1.24867        1.42665
C          0.00000       -1.74650        1.55412
H          1.97388       -0.95648        2.23713
H         -0.53662       -1.90135        2.47908
C          1.84929        2.57192       -0.06225
H          1.76882        3.65712       -0.18701
H          2.56231        2.38620        0.74350
H          2.27447        2.16943       -0.98343
C         -0.40512        1.76061       -2.16802
H         -0.75261        2.75043       -2.48410
H          0.62133        1.64867       -2.52292
H         -1.01717        1.02016       -2.68619
C         -2.95325        0.76429       -0.53016
H         -3.58378        1.64299       -0.70356
H         -2.84543        0.24959       -1.48732
H         -3.49380        0.10039        0.14692
C          2.95325       -0.76429       -0.53016
H          3.58378       -1.64299       -0.70356
H          2.84543       -0.24959       -1.48732
H          3.49380       -0.10039        0.14692
C          0.40512       -1.76061       -2.16802
H          1.01717       -1.02016       -2.68619
H          0.75261       -2.75043       -2.48410
H         -0.62133       -1.64867       -2.52292
C         -1.84929       -2.57192       -0.06225
H         -2.27447       -2.16943       -0.98343
H         -1.76882       -3.65712       -0.18701
H         -2.56231       -2.38620        0.74350


39
Energy: -1183463.0885658
Fe         0.00000        0.00000        0.14701
C         -0.96951       -1.50022        1.13006
C         -1.75500       -0.31481        1.15555
C         -0.73910       -1.87983       -0.22301
H         -0.58042       -2.01413        1.99868
C         -2.01218        0.03437       -0.19861
C         -1.39484       -0.92227       -1.05416
C          1.75500        0.31481        1.15555
C          2.01218       -0.03437       -0.19861
```

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C          0.96951        1.50022        1.13006
C          1.39484        0.92227       -1.05416
H          2.56811       -0.90163       -0.52849
C          0.73910        1.87983       -0.22301
H          0.58042        2.01413        1.99868
C         -1.49259       -0.95491       -2.54046
H         -2.33210       -1.58106       -2.86110
H         -1.65579        0.04498       -2.94749
H         -0.58985       -1.36014       -3.00161
C          0.00000       -3.09210       -0.67732
H         -0.68368       -3.93388       -0.83182
H          0.52265       -2.91909       -1.62031
H          0.74041       -3.40126        0.06315
H         -2.56811        0.90163       -0.52849
C         -2.25900        0.39242        2.36692
H         -2.38781        1.46036        2.17909
H         -3.23050       -0.00769        2.67556
H         -1.57372        0.27812        3.20941
C          1.49259        0.95491       -2.54046
H          2.33210        1.58106       -2.86110
H          1.65579       -0.04498       -2.94749
H          0.58985        1.36014       -3.00161
C          0.00000        3.09210       -0.67732
H          0.68368        3.93388       -0.83182
H         -0.52265        2.91909       -1.62031
H         -0.74041        3.40126        0.06315
C          2.25900       -0.39242        2.36692
H          1.57372       -0.27812        3.20941
H          2.38781       -1.46036        2.17909
H          3.23050        0.00769        2.67556


39
Energy: -1183462.7923813
Fe         0.00000        0.00000        0.06627
C          0.98742        1.47529       -0.93864
C          0.72473        1.89729        0.39369
C          1.78191        0.29421       -0.90729
H          0.62110        1.95902       -1.83415
C          1.36318        0.96118        1.25212
C          2.02094       -0.02478        0.46342
C         -1.78191       -0.29421       -0.90729
C         -0.98742       -1.47529       -0.93864
C         -2.02094        0.02478        0.46342
C         -0.72473       -1.89729        0.39369
H         -0.62110       -1.95902       -1.83415
C         -1.36318       -0.96118        1.25212
H         -1.34164       -0.98448        2.33308
C          2.87372       -1.13017        0.98338
H          3.92143       -0.81626        1.04191
H          2.56461       -1.42943        1.98683
H          2.83485       -2.01400        0.34396
C          2.31275       -0.43357       -2.09498
H          3.31533       -0.07873       -2.35716
H          2.38416       -1.50812       -1.91447
H          1.67199       -0.28287       -2.96611
H          1.34164        0.98448        2.33308
C          0.00000        3.13113        0.80742
```

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H         -0.49545        3.00209        1.77160
H          0.69524        3.97152        0.90423
H         -0.75710        3.41655        0.07413
C         -2.31275        0.43357       -2.09498
H         -3.31533        0.07873       -2.35716
H         -2.38416        1.50812       -1.91447
H         -1.67199        0.28287       -2.96611
C         -2.87372        1.13017        0.98338
H         -2.83485        2.01400        0.34396
H         -3.92143        0.81626        1.04191
H         -2.56461        1.42943        1.98683
C          0.00000       -3.13113        0.80742
H          0.75710       -3.41655        0.07413
H          0.49545       -3.00209        1.77160
H         -0.69524       -3.97152        0.90423


30
Energy: -1109513.4384427
Fe        -0.05785       -0.35338        0.00000
C          1.05904        0.91220        1.14091
C          1.80220        0.50163        0.00000
C         -0.13281        1.56468        0.71397
H          1.33687        0.72939        2.16984
C          1.05904        0.91220       -1.14091
C         -0.13281        1.56468       -0.71397
C         -0.52655       -1.98483        1.14900
C         -1.71017       -1.33367        0.71032
C          0.20567       -2.38633        0.00000
H         -0.22450       -2.12718        2.17557
C         -1.71017       -1.33367       -0.71032
H         -2.46476       -0.89433        1.34553
C         -0.52655       -1.98483       -1.14900
H          1.16253       -2.88662        0.00000
H         -2.46476       -0.89433       -1.34553
H         -0.22450       -2.12718       -2.17557
C         -1.15943        2.17800       -1.60367
H         -0.94867        3.23975       -1.77062
H         -1.17617        1.68817       -2.57920
H         -2.16163        2.10778       -1.17612
C         -1.15943        2.17800        1.60367
H         -0.94867        3.23975        1.77062
H         -2.16163        2.10778        1.17612
H         -1.17617        1.68817        2.57920
H          1.33687        0.72939       -2.16984
C          3.12783       -0.17943        0.00000
H          3.25129       -0.80878       -0.88362
H          3.94159        0.55323        0.00000
H          3.25129       -0.80878        0.88362


39
Energy: -1183462.5341110
Fe         0.00000        0.00000        0.19184
C         -1.14046        1.65394        0.57027
C          0.00000        1.65247        1.41889
C         -0.71371        1.66574       -0.78763
H         -2.16954        1.63287        0.90204
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C          1.14046        1.65394        0.57027
C          0.71371        1.66574       -0.78763
C         -1.14046       -1.65394        0.57027
C         -0.71371       -1.66574       -0.78763
C          0.00000       -1.65247        1.41889
H         -2.16954       -1.63287        0.90204
C          0.71371       -1.66574       -0.78763
C          1.14046       -1.65394        0.57027
H          2.16954       -1.63287        0.90204
C          1.60192        1.75757       -1.98014
H          1.76343        2.80309       -2.26382
H          2.58036        1.31692       -1.77957
H          1.17745        1.24808       -2.84740
C         -1.60192        1.75757       -1.98014
H         -1.76343        2.80309       -2.26382
H         -1.17745        1.24808       -2.84740
H         -2.58036        1.31692       -1.77957
H          2.16954        1.63287        0.90204
C          0.00000        1.73259        2.90622
H          0.88337        1.25504        3.33446
H          0.00000        2.77738        3.23396
H         -0.88337        1.25504        3.33446
C         -1.60192       -1.75757       -1.98014
H         -2.58036       -1.31692       -1.77957
H         -1.17745       -1.24808       -2.84740
H         -1.76343       -2.80309       -2.26382
C          1.60192       -1.75757       -1.98014
H          1.76343       -2.80309       -2.26382
H          1.17745       -1.24808       -2.84740
H          2.58036       -1.31692       -1.77957
C          0.00000       -1.73259        2.90622
H          0.88337       -1.25504        3.33446
H         -0.88337       -1.25504        3.33446
H          0.00000       -2.77738        3.23396


39
Energy: -1183462.7923813
Fe         0.00000        0.00000        0.06627
C          1.36318        0.96118        1.25212
C          2.02094       -0.02478        0.46342
C          0.72473        1.89729        0.39368
C          1.78191        0.29421       -0.90729
C          0.98742        1.47529       -0.93864
H          0.62110        1.95902       -1.83415
C         -0.98742       -1.47529       -0.93864
C         -0.72473       -1.89729        0.39368
C         -1.78191       -0.29421       -0.90729
H         -0.62110       -1.95902       -1.83415
C         -1.36318       -0.96118        1.25212
C         -2.02094        0.02478        0.46342
H         -1.34164       -0.98448        2.33307
C          2.87372       -1.13016        0.98339
H          3.92143       -0.81625        1.04192
H          2.56461       -1.42943        1.98683
H          2.83486       -2.01399        0.34397
C          2.31275       -0.43358       -2.09498
H          3.31533       -0.07874       -2.35715
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H          2.38416       -1.50813       -1.91446
H          1.67200       -0.28288       -2.96611
H          1.34164        0.98448        2.33307
C         -2.31275        0.43358       -2.09498
H         -2.38416        1.50813       -1.91446
H         -1.67200        0.28288       -2.96611
H         -3.31533        0.07874       -2.35715
C         -2.87372        1.13016        0.98339
H         -2.83486        2.01399        0.34397
H         -3.92143        0.81625        1.04192
H         -2.56461        1.42943        1.98683
C          0.00000        3.13114        0.80741
H         -0.75710        3.41655        0.07412
H         -0.49545        3.00210        1.77159
H          0.69524        3.97153        0.90422
C          0.00000       -3.13114        0.80741
H          0.75710       -3.41655        0.07412
H          0.49545       -3.00210        1.77159
H         -0.69524       -3.97153        0.90422


39
Energy: -1183462.4965294
Fe         0.00000        0.00000        0.00000
C          0.00000        1.69766        1.14060
C          1.32583        1.40265        0.71340
C         -0.82701        1.88536        0.00000
C          1.32583        1.40265       -0.71340
C          0.00000        1.69766       -1.14060
H         -0.32848        1.74851       -2.16980
C          0.82701       -1.88536        0.00000
C          0.00000       -1.69766        1.14060
C          0.00000       -1.69766       -1.14060
C         -1.32583       -1.40265        0.71340
H          0.32848       -1.74851        2.16980
C         -1.32583       -1.40265       -0.71340
H          0.32848       -1.74851       -2.16980
C          2.50245        1.19659        1.60459
H          3.01705        2.14404        1.79755
H          2.19807        0.78506        2.56912
H          3.23245        0.51494        1.16407
C          2.50245        1.19659       -1.60459
H          3.01705        2.14404       -1.79755
H          3.23245        0.51494       -1.16407
H          2.19807        0.78506       -2.56912
H         -0.32848        1.74851        2.16980
C         -2.26391        2.27936        0.00000
H         -2.78168        1.90325        0.88463
H         -2.36553        3.36964        0.00000
H         -2.78168        1.90325       -0.88463
C         -2.50245       -1.19659       -1.60459
H         -3.01705       -2.14404       -1.79755
H         -3.23245       -0.51494       -1.16407
H         -2.19807       -0.78506       -2.56912
C         -2.50245       -1.19659        1.60459
H         -3.23245       -0.51494        1.16407
H         -3.01705       -2.14404        1.79755
H         -2.19807       -0.78506        2.56912
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C          2.26391       -2.27936        0.00000
H          2.78168       -1.90325        0.88463
H          2.36553       -3.36964        0.00000
H          2.78168       -1.90325       -0.88463


30
Energy: -1109512.9048589
Fe         0.05443       -0.35276        0.00000
C         -1.05554        0.92312        1.14057
C          0.14036        1.56735        0.71372
C         -1.80127        0.51793        0.00000
C          0.14036        1.56735       -0.71372
C         -1.05554        0.92312       -1.14057
H         -1.33303        0.73933       -2.16951
C          1.90587       -1.23666        0.00000
C          1.17182       -1.63324        1.14895
C          1.17182       -1.63324       -1.14895
H          2.84522       -0.70411        0.00000
C         -0.01569       -2.27732        0.70968
H          1.45438       -1.45463        2.17554
C         -0.01569       -2.27732       -0.70968
H          1.45438       -1.45463       -2.17554
H         -0.79439       -2.67330        1.34411
H         -0.79439       -2.67330       -1.34411
C          1.17509        2.16629        1.60349
H          0.97916        3.23069        1.77127
H          1.18550        1.67532        2.57851
H          2.17613        2.08229        1.17570
C          1.17509        2.16629       -1.60349
H          0.97916        3.23069       -1.77127
H          2.17613        2.08229       -1.17570
H          1.18550        1.67532       -2.57851
H         -1.33303        0.73933        2.16951
C         -3.12827       -0.16010        0.00000
H         -3.25292       -0.78939        0.88347
H         -3.94057        0.57410        0.00000
H         -3.25292       -0.78939       -0.88347


39
Energy: -1183463.0885658
Fe         0.00000        0.00000        0.14701
C          0.96951       -1.50022        1.13006
C          0.73910       -1.87983       -0.22300
C          1.75500       -0.31481        1.15555
C          1.39483       -0.92227       -1.05416
C          2.01218        0.03437       -0.19861
H          2.56811        0.90163       -0.52850
C         -1.39483        0.92227       -1.05416
C         -2.01218       -0.03437       -0.19861
C         -0.73910        1.87983       -0.22300
C         -1.75500        0.31481        1.15555
H         -2.56811       -0.90163       -0.52850
C         -0.96951        1.50022        1.13006
H         -0.58042        2.01412        1.99868
C          0.00000       -3.09209       -0.67732
H          0.68368       -3.93388       -0.83184
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H         -0.74040       -3.40127        0.06316
H         -0.52267       -2.91908       -1.62030
C          1.49259       -0.95491       -2.54046
H          2.33209       -1.58108       -2.86111
H          0.58983       -1.36013       -3.00161
H          1.65580        0.04497       -2.94749
H          0.58042       -2.01412        1.99868
C          2.25900        0.39242        2.36691
H          1.57372        0.27813        3.20940
H          3.23050       -0.00769        2.67556
H          2.38782        1.46036        2.17908
C         -1.49259        0.95491       -2.54046
H         -2.33209        1.58108       -2.86111
H         -0.58983        1.36013       -3.00161
H         -1.65580       -0.04497       -2.94749
C          0.00000        3.09209       -0.67732
H          0.52267        2.91908       -1.62030
H         -0.68368        3.93388       -0.83184
H          0.74040        3.40127        0.06316
C         -2.25900       -0.39242        2.36691
H         -2.38782       -1.46036        2.17908
H         -1.57372       -0.27813        3.20940
H         -3.23050        0.00769        2.67556


45
Energy: -1232761.6628143
Fe         0.00000        0.00000       -0.22541
C         -0.43773        1.69329       -1.27029
C         -1.59442        0.87308       -1.17189
C          0.00000        2.03898        0.03700
H          0.04822        1.98466       -2.19173
C         -1.88257        0.70778        0.21621
C         -0.89582        1.42455        0.96267
C          1.59442       -0.87308       -1.17189
C          1.88257       -0.70778        0.21621
C          0.43773       -1.69329       -1.27029
C          0.89582       -1.42455        0.96267
C          0.00000       -2.03898        0.03700
H         -0.04822       -1.98466       -2.19173
C         -0.86019        1.58080        2.44424
H         -1.45980        2.44080        2.76296
H         -1.25551        0.70130        2.95570
H          0.15719        1.74311        2.80583
C         -3.05870       -0.00830        0.78547
H         -3.38634       -0.82475        0.13956
H         -2.83971       -0.43107        1.76801
H         -3.90862        0.67248        0.90721
C          1.13303        2.94980        0.36416
H          0.77983        3.97816        0.49706
H          1.64302        2.65955        1.28465
H          1.87373        2.95998       -0.43826
C         -2.38716        0.33934       -2.31614
H         -2.80751       -0.64466       -2.09806
H         -3.22247        1.00476       -2.56021
H         -1.76835        0.24611       -3.21088
C         -1.13303       -2.94980        0.36416
H         -1.64302       -2.65955        1.28465
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H         -1.87373       -2.95998       -0.43826
H         -0.77983       -3.97816        0.49706
C          0.86019       -1.58080        2.44424
H         -0.15719       -1.74311        2.80583
H          1.45980       -2.44080        2.76296
H          1.25551       -0.70130        2.95570
C          3.05870        0.00830        0.78547
H          2.83971        0.43107        1.76801
H          3.90862       -0.67248        0.90721
H          3.38634        0.82475        0.13956
C          2.38716       -0.33934       -2.31614
H          2.80751        0.64466       -2.09806
H          3.22247       -1.00476       -2.56021
H          1.76835       -0.24611       -3.21088


45
Energy: -1232761.5465808
Fe         0.00000        0.00000       -0.11119
C         -1.59484       -1.17441       -0.60383
C         -0.44643       -1.59527       -1.32781
C         -1.33210       -1.28174        0.78871
H         -2.51502       -0.81179       -1.04194
C          0.54823       -1.96263       -0.37235
C          0.00000       -1.77369        0.93412
C         -0.54823        1.96263       -0.37235
C          0.00000        1.77369        0.93412
C          0.44643        1.59527       -1.32781
C          1.33210        1.28174        0.78871
C          1.59484        1.17441       -0.60383
H          2.51502        0.81179       -1.04194
C          0.66587       -2.11785        2.22198
H          0.47268       -3.16142        2.49454
H          1.74846       -1.99148        2.16718
H          0.30092       -1.49669        3.04257
C          1.89785       -2.51433       -0.68373
H          2.26884       -2.14736       -1.64255
H          2.63049       -2.24345        0.07903
H          1.87404       -3.60848       -0.73950
C         -2.30733       -1.01362        1.88290
H         -2.82394       -1.93326        2.17846
H         -1.82507       -0.61006        2.77518
H         -3.06904       -0.29924        1.56326
C         -0.34161       -1.71442       -2.80929
H          0.66665       -1.49907       -3.16886
H         -0.59361       -2.72938       -3.13530
H         -1.02776       -1.02949       -3.31077
C          2.30733        1.01362        1.88290
H          2.82394        1.93326        2.17846
H          1.82507        0.61006        2.77518
H          3.06904        0.29924        1.56326
C         -0.66587        2.11785        2.22198
H         -0.30092        1.49669        3.04257
H         -0.47268        3.16142        2.49454
H         -1.74846        1.99148        2.16718
C         -1.89785        2.51433       -0.68373
H         -2.63049        2.24345        0.07903
H         -1.87404        3.60848       -0.73950
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H         -2.26884        2.14736       -1.64255
C          0.34161        1.71442       -2.80929
H         -0.66665        1.49907       -3.16886
H          0.59361        2.72938       -3.13530
H          1.02776        1.02949       -3.31077


33
Energy: -1134163.0191755
Fe         0.05599        0.45623        0.00000
C          1.66299       -0.79161        0.00000
C          0.87070       -1.01896        1.15849
C          0.87070       -1.01896       -1.15849
H          2.69385       -0.46497        0.00000
C         -0.43295       -1.39733        0.71532
C         -0.43295       -1.39733       -0.71532
C          0.75661        2.38443        0.00000
C         -0.04482        2.15117       -1.14921
C         -0.04482        2.15117        1.14921
H          1.79872        2.66605        0.00000
C         -1.34232        1.77463       -0.71026
H          0.28188        2.22418       -2.17577
C         -1.34232        1.77463        0.71026
H          0.28188        2.22418        2.17577
H         -2.17553        1.51126       -1.34467
H         -2.17553        1.51126        1.34467
C         -1.57741       -1.77779       -1.59133
H         -1.57914       -2.85520       -1.79036
H         -2.53639       -1.52958       -1.13281
H         -1.52972       -1.26834       -2.55554
C         -1.57741       -1.77779        1.59133
H         -1.52972       -1.26834        2.55554
H         -2.53639       -1.52958        1.13281
H         -1.57914       -2.85520        1.79036
C          1.34201       -0.92708       -2.56968
H          1.67035       -1.90509       -2.93777
H          0.55654       -0.57308       -3.24030
H          2.18777       -0.24204       -2.65504
C          1.34201       -0.92708        2.56968
H          0.55654       -0.57308        3.24030
H          1.67035       -1.90509        2.93777
H          2.18777       -0.24204        2.65504


45
Energy: -1232761.3003461
Fe         0.00000        0.00000        0.27585
C          0.00000        1.64314        1.48734
C          1.15775        1.65637        0.66354
C         -1.15775        1.65637        0.66354
H          0.00000        1.61094        2.56835
C          0.71479        1.67128       -0.69305
C         -0.71479        1.67128       -0.69305
C          0.00000       -1.64314        1.48734
C         -1.15775       -1.65637        0.66354
C          1.15775       -1.65637        0.66354
H          0.00000       -1.61094        2.56835
C         -0.71479       -1.67128       -0.69305
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C          0.71479       -1.67128       -0.69305
C         -1.58913        1.77085       -1.89555
H         -1.77366        2.81824       -2.15932
H         -1.13814        1.29158       -2.76642
H         -2.56069        1.30231       -1.72789
C          1.58913        1.77085       -1.89555
H          2.56069        1.30231       -1.72789
H          1.13814        1.29158       -2.76642
H          1.77366        2.81824       -2.15932
C         -2.56617        1.74203        1.14156
H         -2.88995        2.78644        1.20728
H         -3.26036        1.22922        0.47320
H         -2.67350        1.30211        2.13490
C          2.56617        1.74203        1.14156
H          3.26036        1.22922        0.47320
H          2.88995        2.78644        1.20728
H          2.67350        1.30211        2.13490
C          2.56617       -1.74203        1.14156
H          2.88995       -2.78644        1.20728
H          3.26036       -1.22922        0.47320
H          2.67350       -1.30211        2.13490
C          1.58913       -1.77085       -1.89555
H          2.56069       -1.30231       -1.72789
H          1.77366       -2.81824       -2.15932
H          1.13814       -1.29158       -2.76642
C         -1.58913       -1.77085       -1.89555
H         -1.13814       -1.29158       -2.76642
H         -1.77366       -2.81824       -2.15932
H         -2.56069       -1.30231       -1.72789
C         -2.56617       -1.74203        1.14156
H         -3.26036       -1.22922        0.47320
H         -2.88995       -2.78644        1.20728
H         -2.67350       -1.30211        2.13490


45
Energy: -1232761.6189954
Fe         0.00000        0.00000        0.19747
C          0.00000        2.04401       -0.04308
C         -0.87916        1.43409       -0.99120
C         -0.44658        1.69108        1.26584
C         -1.87335        0.70695       -0.27016
C         -1.59814        0.87203        1.11486
H         -2.15913        0.42418        1.92410
C          0.87916       -1.43409       -0.99120
C          1.87335       -0.70695       -0.27016
C          0.00000       -2.04401       -0.04308
C          1.59814       -0.87203        1.11486
C          0.44658       -1.69108        1.26584
H          2.15913       -0.42418        1.92410
C          1.13009        2.96209       -0.35993
H          0.78425        3.99993       -0.42255
H          1.90612        2.92459        0.40706
H          1.59814        2.71781       -1.31508
C         -0.82075        1.60176       -2.47084
H         -1.39123        2.48156       -2.78891
H          0.20413        1.73546       -2.82281
H         -1.23815        0.73797       -2.99146
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C         -3.03831       -0.01885       -0.85000
H         -3.87239        0.66702       -1.03394
H         -2.79287       -0.49353       -1.80239
H         -3.39607       -0.79663       -0.17276
C          0.13816        2.14496        2.55988
H          1.22341        2.25026        2.50320
H         -0.26971        3.11785        2.85521
H         -0.08691        1.43796        3.36102
C          3.03831        0.01885       -0.85000
H          2.79287        0.49353       -1.80239
H          3.39607        0.79663       -0.17276
H          3.87239       -0.66702       -1.03394
C          0.82075       -1.60176       -2.47084
H          1.23815       -0.73797       -2.99146
H          1.39123       -2.48156       -2.78891
H         -0.20413       -1.73546       -2.82281
C         -1.13009       -2.96209       -0.35993
H         -1.59814       -2.71781       -1.31508
H         -0.78425       -3.99993       -0.42255
H         -1.90612       -2.92459        0.40706
C         -0.13816       -2.14496        2.55988
H         -1.22341       -2.25026        2.50320
H          0.26971       -3.11785        2.85521
H          0.08691       -1.43796        3.36102


45
Energy: -1232761.3861391
Fe         0.00000        0.00000        0.00000
C          0.12737        1.92439        0.71476
C          0.12737        1.92439       -0.71476
C         -1.08256        1.31118        1.15771
C         -1.08256        1.31118       -1.15771
C         -1.81629        0.93532        0.00000
H         -2.77137        0.42757        0.00000
C          1.08256       -1.31118       -1.15771
C          1.81629       -0.93532        0.00000
C         -0.12737       -1.92439       -0.71476
C          1.08256       -1.31118        1.15771
H          2.77137       -0.42757        0.00000
C         -0.12737       -1.92439        0.71476
C          1.17575        2.52484        1.58790
H          0.98748        3.59180        1.75191
H          1.20395        2.04598        2.56829
H          2.17014        2.43434        1.14607
C          1.17575        2.52484       -1.58790
H          0.98748        3.59180       -1.75191
H          2.17014        2.43434       -1.14607
H          1.20395        2.04598       -2.56829
C         -1.54103        1.15782       -2.56746
H         -2.05356        2.06279       -2.91139
H         -0.71003        0.97709       -3.25218
H         -2.24319        0.32735       -2.66395
C         -1.54103        1.15782        2.56746
H         -0.71003        0.97709        3.25218
H         -2.05356        2.06279        2.91139
H         -2.24319        0.32735        2.66395
C          1.54103       -1.15782       -2.56746
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H          0.71003       -0.97709       -3.25218
H          2.24319       -0.32735       -2.66395
H          2.05356       -2.06279       -2.91139
C         -1.17575       -2.52484       -1.58790
H         -1.20395       -2.04598       -2.56829
H         -0.98748       -3.59180       -1.75191
H         -2.17014       -2.43434       -1.14607
C         -1.17575       -2.52484        1.58790
H         -2.17014       -2.43434        1.14607
H         -0.98748       -3.59180        1.75191
H         -1.20395       -2.04598        2.56829
C          1.54103       -1.15782        2.56746
H          0.71003       -0.97709        3.25218
H          2.05356       -2.06279        2.91139
H          2.24319       -0.32735        2.66395


33
Energy: -1134162.5091735
Fe         0.05803        0.45422        0.00000
C         -0.43432       -1.40034        0.71514
C         -0.43432       -1.40034       -0.71514
C          0.86997       -1.02568        1.15812
C          0.86997       -1.02568       -1.15812
C          1.66262       -0.80055        0.00000
H          2.69334       -0.47325        0.00000
C         -0.75885        1.94630       -1.14890
C         -1.56111        1.71439        0.00000
C          0.53873        2.31983       -0.71022
H         -1.07397        1.83460       -2.17564
C         -0.75885        1.94630        1.14890
H         -2.59325        1.39719        0.00000
C          0.53873        2.31983        0.71022
H          1.38398        2.54046       -1.34466
H         -1.07397        1.83460        2.17564
H          1.38398        2.54046        1.34466
C         -1.58192       -1.77066        1.59108
H         -1.59549       -2.84843        1.78745
H         -1.52769       -1.26417        2.55649
H         -2.53850       -1.51046        1.13415
C         -1.58192       -1.77066       -1.59108
H         -1.59549       -2.84843       -1.78745
H         -2.53850       -1.51046       -1.13415
H         -1.52769       -1.26417       -2.55649
C          1.33934       -0.92716       -2.56934
H          1.65385       -1.90573       -2.94769
H          0.55730       -0.55581       -3.23463
H          2.19379       -0.25244       -2.64993
C          1.33934       -0.92716        2.56934
H          0.55730       -0.55581        3.23463
H          1.65385       -1.90573        2.94769
H          2.19379       -0.25244        2.64993


45
Energy: -1232761.6628143
Fe         0.00000        0.00000        0.22542
C         -0.89580        1.42456       -0.96267
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C         -1.88257        0.70778       -0.21622
C          0.00000        2.03899       -0.03698
C         -1.59442        0.87308        1.17188
C         -0.43774        1.69329        1.27030
H          0.04821        1.98464        2.19175
C          0.00000       -2.03899       -0.03698
C          0.89580       -1.42456       -0.96267
C          0.43774       -1.69329        1.27030
C          1.88257       -0.70778       -0.21622
C          1.59442       -0.87308        1.17188
H         -0.04821       -1.98464        2.19175
C         -0.86016        1.58081       -2.44423
H         -1.45976        2.44081       -2.76296
H          0.15722        1.74312       -2.80582
H         -1.25549        0.70131       -2.95570
C         -3.05870       -0.00829       -0.78549
H         -3.90861        0.67250       -0.90724
H         -2.83970       -0.43107       -1.76803
H         -3.38634       -0.82474       -0.13958
C         -2.38718        0.33932        2.31612
H         -3.22250        1.00472        2.56017
H         -2.80751       -0.64469        2.09805
H         -1.76838        0.24612        3.21087
C          1.13304        2.94980       -0.36413
H          1.64303        2.65955       -1.28461
H          0.77984        3.97817       -0.49703
H          1.87373        2.95998        0.43830
C          2.38718       -0.33932        2.31612
H          3.22250       -1.00472        2.56017
H          2.80751        0.64469        2.09805
H          1.76838       -0.24612        3.21087
C          3.05870        0.00829       -0.78549
H          3.38634        0.82474       -0.13958
H          3.90861       -0.67250       -0.90724
H          2.83970        0.43107       -1.76803
C          0.86016       -1.58081       -2.44423
H          1.25549       -0.70131       -2.95570
H          1.45976       -2.44081       -2.76296
H         -0.15722       -1.74312       -2.80582
C         -1.13304       -2.94980       -0.36413
H         -1.64303       -2.65955       -1.28461
H         -0.77984       -3.97817       -0.49703
H         -1.87373       -2.95998        0.43830


33
Energy: -1134163.0740261
Fe         0.00000        0.00000        0.46275
C         -1.30043        1.21843        1.45721
C          0.00000        1.78656        1.45139
C         -1.70743        1.06330        0.10671
H         -1.86473        0.92767        2.33041
C          0.40283        1.98337        0.10017
H          0.60191        2.00632        2.32131
C         -0.66383        1.53675       -0.73847
H         -2.64140        0.63760       -0.23177
C          0.00000       -1.78656        1.45139
C         -0.40283       -1.98337        0.10017
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C          1.30043       -1.21843        1.45721
H         -0.60191       -2.00632        2.32131
C          0.66383       -1.53675       -0.73847
C          1.70743       -1.06330        0.10671
H          1.86473       -0.92767        2.33041
H          2.64140       -0.63760       -0.23177
C         -0.71763        1.62413       -2.22478
H          0.26014        1.45646       -2.68043
H         -1.41026        0.88871       -2.63866
H         -1.06094        2.61416       -2.54314
C          1.68222        2.60307       -0.34824
H          2.46928        2.45969        0.39450
H          2.03025        2.17705       -1.29144
H          1.56342        3.68120       -0.50046
C          0.71763       -1.62413       -2.22478
H          1.06094       -2.61416       -2.54314
H         -0.26014       -1.45646       -2.68043
H          1.41026       -0.88871       -2.63866
C         -1.68222       -2.60307       -0.34824
H         -2.03025       -2.17705       -1.29144
H         -1.56342       -3.68120       -0.50046
H         -2.46928       -2.45969        0.39450


33
Energy: -1134163.2476392
Fe         0.00000        0.00000        0.17842
C          1.88557       -0.68789        0.54383
C          0.95059       -1.34975        1.38172
C          1.51668       -0.94933       -0.80167
H          2.71054       -0.07276        0.87110
C          0.00000       -2.01969        0.56027
H          0.93833       -1.32904        2.46190
C          0.35315       -1.77039       -0.80139
H          2.01253       -0.56879       -1.68338
C          0.00000        2.01969        0.56027
C         -0.35315        1.77039       -0.80139
C         -0.95059        1.34975        1.38172
C         -1.51668        0.94933       -0.80167
C         -1.88557        0.68789        0.54383
H         -0.93833        1.32904        2.46190
H         -2.01253        0.56879       -1.68338
H         -2.71054        0.07276        0.87110
C         -0.33251       -2.31259       -2.00882
H         -1.41037       -2.40043       -1.85854
H         -0.16651       -1.67020       -2.87587
H          0.04527       -3.30964       -2.25927
C         -1.12482       -2.87036        1.04335
H         -1.44724       -2.56491        2.04061
H         -1.99012       -2.81406        0.37988
H         -0.82424       -3.92202        1.10042
C          0.33251        2.31259       -2.00882
H          1.41037        2.40043       -1.85854
H          0.16651        1.67020       -2.87587
H         -0.04527        3.30964       -2.25927
C          1.12482        2.87036        1.04335
H          1.99012        2.81406        0.37988
H          0.82424        3.92202        1.10042
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H          1.44724        2.56491        2.04061


27
Energy: -1084863.3386278
Fe         0.19645        0.36591        0.00000
C          2.00188       -0.58397        0.00000
C          1.24980       -0.95352        1.14530
C          1.24980       -0.95352       -1.14530
H          2.95847       -0.08370        0.00000
C          0.03089       -1.55030        0.71440
H          1.53370       -0.78541        2.17411
C          0.03089       -1.55030       -0.71440
H          1.53370       -0.78541       -2.17411
C          0.55747        2.38399        0.00000
C         -0.19235        2.01709       -1.14905
C         -0.19235        2.01709        1.14905
H          1.53662        2.83832        0.00000
C         -1.40555        1.42271       -0.71032
H          0.11705        2.14402       -2.17540
C         -1.40555        1.42271        0.71032
H          0.11705        2.14402        2.17540
H         -2.18015        1.01931       -1.34533
H         -2.18015        1.01931        1.34533
C         -1.02396       -2.11802       -1.60129
H         -0.86666       -3.19026       -1.75930
H         -2.02183       -1.99400       -1.17593
H         -1.01443       -1.63564       -2.58054
C         -1.02396       -2.11802        1.60129
H         -1.01443       -1.63564        2.58054
H         -2.02183       -1.99400        1.17593
H         -0.86666       -3.19026        1.75930


33
Energy: -1134162.9018062
Fe         0.00000        0.00000        0.56728
C          0.00000        1.62520        1.80032
C          1.14513        1.64469        0.96271
C         -1.14513        1.64469        0.96271
H          0.00000        1.57138        2.87853
C          0.71425        1.67857       -0.39368
H          2.17399        1.61400        1.29123
C         -0.71425        1.67857       -0.39368
H         -2.17399        1.61400        1.29123
C          0.00000       -1.62520        1.80032
C         -1.14513       -1.64469        0.96271
C          1.14513       -1.64469        0.96271
H          0.00000       -1.57138        2.87853
C         -0.71425       -1.67857       -0.39368
H         -2.17399       -1.61400        1.29123
C          0.71425       -1.67857       -0.39368
H          2.17399       -1.61400        1.29123
C         -1.60009        1.78407       -1.58698
H         -1.17838        1.27456       -2.45560
H         -2.58216        1.35043       -1.38916
H         -1.75251        2.83201       -1.86631
C          1.60009        1.78407       -1.58698
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H          2.58216        1.35043       -1.38916
H          1.17838        1.27456       -2.45560
H          1.75251        2.83201       -1.86631
C          1.60009       -1.78407       -1.58698
H          2.58216       -1.35043       -1.38916
H          1.75251       -2.83201       -1.86631
H          1.17838       -1.27456       -2.45560
C         -1.60009       -1.78407       -1.58698
H         -1.17838       -1.27456       -2.45560
H         -1.75251       -2.83201       -1.86631
H         -2.58216       -1.35043       -1.38916


33
Energy: -1134163.2476392
Fe         0.00000        0.00000        0.17841
C          0.35314        1.77039       -0.80139
C          0.00000        2.01969        0.56027
C          1.51667        0.94933       -0.80168
C          0.95060        1.34975        1.38171
C          1.88557        0.68789        0.54382
H          2.01251        0.56882       -1.68341
H          0.93835        1.32904        2.46190
H          2.71056        0.07278        0.87109
C         -1.88557       -0.68789        0.54382
C         -1.51667       -0.94933       -0.80168
C         -0.95060       -1.34975        1.38171
H         -2.71056       -0.07278        0.87109
C         -0.35314       -1.77039       -0.80139
H         -2.01251       -0.56882       -1.68341
C          0.00000       -2.01969        0.56027
H         -0.93835       -1.32904        2.46190
C         -0.33253        2.31259       -2.00881
H          0.04523        3.30965       -2.25926
H         -0.16652        1.67022       -2.87586
H         -1.41040        2.40041       -1.85852
C         -1.12482        2.87036        1.04336
H         -0.82425        3.92202        1.10041
H         -1.99013        2.81404        0.37989
H         -1.44723        2.56492        2.04062
C          0.33253       -2.31259       -2.00881
H          1.41040       -2.40041       -1.85852
H         -0.04523       -3.30965       -2.25926
H          0.16652       -1.67022       -2.87586
C          1.12482       -2.87036        1.04336
H          0.82425       -3.92202        1.10041
H          1.99013       -2.81404        0.37989
H          1.44723       -2.56492        2.04062


33
Energy: -1134162.7734177
Fe         0.00000        0.00000        0.00000
C          1.32499        1.40049        0.71398
C          1.32499        1.40049       -0.71398
C          0.00000        1.69303        1.14518
C          0.00000        1.69303       -1.14518
C         -0.81831        1.87274        0.00000
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H -0.32653 1.73876 2.17428
H -0.32653 1.73876 -2.17428
H -1.87810 2.07988 0.00000
C 0.00000 -1.69303 -1.14518
C 0.81831 -1.87274 0.00000
C -1.32499 -1.40049 -0.71398
H 0.32653 -1.73876 -2.17428
C 0.00000 -1.69303 1.14518
H 1.87810 -2.07988 0.00000
C -1.32499 -1.40049 0.71398
H 0.32653 -1.73876 2.17428
C 2.50228 1.17973 1.60101
H 3.05411 2.11230 1.75987
H 2.19143 0.80945 2.57980
H 3.20026 0.45570 1.17579
C 2.50228 1.17973 -1.60101
H 3.05411 2.11230 -1.75987
H 3.20026 0.45570 -1.17579
H 2.19143 0.80945 -2.57980
C -2.50228 -1.17973 1.60101
H -2.19143 -0.80945 2.57980
H -3.20026 -0.45570 1.17579
H -3.05411 -2.11230 1.75987
C -2.50228 -1.17973 -1.60101
H -3.05411 -2.11230 -1.75987
H -3.20026 -0.45570 -1.17579
H -2.19143 -0.80945 -2.57980

27
Energy: -1084862.7713467
Fe 0.19935 0.36451 0.00000
C 0.02870 -1.55360 0.71418
C 0.02870 -1.55360 -0.71418
C 1.24963 -0.96191 1.14493
C 1.24963 -0.96191 -1.14493
C 2.00292 -0.59548 0.00000
H 1.53266 -0.79194 2.17375
H 1.53266 -0.79194 -2.17375
H 2.95998 -0.09596 0.00000
C -0.86009 1.69196 -1.14894
C -1.61058 1.32667 0.00000
C 0.35388 2.28364 -0.70980
H -1.14971 1.52515 -2.17554
C -0.86009 1.69196 1.14894
H -2.57208 0.83528 0.00000
C 0.35388 2.28364 0.70980
H 1.15028 2.64258 -1.34406
H -1.14971 1.52515 2.17554
H 1.15028 2.64258 1.34406
C -1.03241 -2.10923 1.60105
H -0.89032 -3.18398 1.75597
H -1.01459 -1.62940 2.58141
H -2.02915 -1.96942 1.17781
C -1.03241 -2.10923 -1.60105
H -0.89032 -3.18398 -1.75597
H -2.02915 -1.96942 -1.17781
H -1.01459 -1.62940 -2.58141

33
Energy: -1134163.0735681
Fe 0.00000 0.00000 0.46624
C 0.68259 1.52852 -0.73494
C -0.38945 1.98386 0.09209
C 1.71597 1.05320 0.12160
C 0.00000 1.79049 1.44772
C 1.29742 1.21579 1.46769
H 2.65084 0.62139 -0.20648
H -0.60853 2.01686 2.31132
H 1.85219 0.92575 2.34721
C -1.71597 -1.05320 0.12160
C -0.68259 -1.52852 -0.73494
C -1.29742 -1.21579 1.46769
H -2.65084 -0.62139 -0.20648
C 0.38945 -1.98386 0.09209
C 0.00000 -1.79049 1.44772
H -1.85219 -0.92575 2.34721
H 0.60853 -2.01686 2.31132
C 0.75074 1.60990 -2.22101
H 1.10303 2.59664 -2.53980
H 1.44289 0.86881 -2.62556
H -0.22367 1.44641 -2.68523
C -1.66157 2.60791 -0.37079
H -1.53543 3.68434 -0.52901
H -2.00429 2.17769 -1.31406
H -2.45548 2.47376 0.36637
C -0.75074 -1.60990 -2.22101
H -1.44289 -0.86881 -2.62556
H 0.22367 -1.44641 -2.68523
H -1.10303 -2.59664 -2.53980
C 1.66157 -2.60791 -0.37079
H 1.53543 -3.68434 -0.52901
H 2.00429 -2.17769 -1.31406
H 2.45548 -2.47376 0.36637

1
Energy: -792267.6421416
Fe 0.00000 0.00000 0.00000

27
Energy: -1458355.5934345
Fe 0.00000 0.00000 0.94376
C -0.77868 -1.46119 2.15885
C -1.76638 -1.00210 1.24713
C 0.31491 -1.96503 1.41287
H -0.83418 -1.40471 3.23522
C -1.29047 -1.21930 -0.06949
H -2.70308 -0.53367 1.50734
C 0.00000 -1.80925 0.03385
H 1.23400 -2.36923 1.80762
H -1.79122 -0.95476 -0.98791
C 0.77868 1.46119 2.15885
C 1.76638 1.00210 1.24713

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C         -0.31491        1.96503        1.41287
H          0.83418        1.40471        3.23522
C          1.29047        1.21930       -0.06949
H          2.70308        0.53367        1.50734
C          0.00000        1.80925        0.03385
H         -1.23400        2.36923        1.80762
H          1.79122        0.95476       -0.98791
C          0.84809       -2.25920       -1.10047
F          0.59723       -3.53881       -1.42288
F          0.64091       -1.53445       -2.20569
F          2.15551       -2.18746       -0.80781
C         -0.84809        2.25920       -1.10047
F         -0.64091        1.53445       -2.20569
F         -2.15551        2.18746       -0.80781
F         -0.59723        3.53881       -1.42288


27
Energy: -1458356.0826723
Fe         0.00000        0.00000        0.37156
C         -0.34979        1.77512        1.34389
C          0.00000        2.01744       -0.01084
C         -1.50725        0.95815        1.36463
H          0.19343        2.12243        2.20925
C         -0.93833        1.35352       -0.83843
H          0.85836        2.57467       -0.35361
C         -1.86658        0.69144        0.01368
H         -2.01422        0.57863        2.23805
H         -0.93816        1.32331       -1.91680
C          1.50725       -0.95815        1.36463
C          0.34979       -1.77512        1.34389
C          1.86658       -0.69144        0.01368
H          2.01422       -0.57863        2.23805
C          0.00000       -2.01744       -0.01084
H         -0.19343       -2.12243        2.20925
C          0.93833       -1.35352       -0.83843
H         -0.85836       -2.57467       -0.35361
H          0.93816       -1.32331       -1.91680
C         -3.05070       -0.08760       -0.43070
F         -4.13182        0.69574       -0.57325
F         -2.84787       -0.68172       -1.61519
F         -3.38277       -1.04415        0.44838
C          3.05070        0.08760       -0.43070
F          2.84787        0.68172       -1.61519
F          3.38277        1.04415        0.44838
F          4.13182       -0.69574       -0.57325


24
Energy: -1246960.0212389
Fe         0.20840       -0.85762        0.00000
C          2.09548       -0.47122        0.71025
C          2.09548       -0.47122       -0.71025
C          1.18220        0.51643        1.15500
H          2.66722       -1.13167        1.34404
C          1.18220        0.51643       -1.15500
H          2.66722       -1.13167       -1.34404
C          0.61193        1.12254        0.00000
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H          0.93666        0.75470        2.17810
H          0.93666        0.75470       -2.17810
C         -0.35277       -2.69374        0.71004
C         -1.26408       -1.69662        1.14881
C         -0.35277       -2.69374       -0.71004
H          0.25417       -3.32195        1.34417
C         -1.82643       -1.08048        0.00000
H         -1.47079       -1.43147        2.17443
C         -1.26408       -1.69662       -1.14881
H          0.25417       -3.32195       -1.34417
H         -2.52967       -0.26162        0.00000
H         -1.47079       -1.43147       -2.17443
C         -0.35366        2.24955        0.00000
F          0.27300        3.43907        0.00000
F         -1.14673        2.23673       -1.08130
F         -1.14673        2.23673        1.08130


27
Energy: -1458352.8414478
Fe         0.00000        0.00000        1.17341
C         -0.71019        1.61019        2.21984
C          0.71019        1.61019        2.21984
C         -1.15372        1.67265        0.87609
H         -1.34374        1.53660        3.09051
C          1.15372        1.67265        0.87609
H          1.34374        1.53660        3.09051
C          0.00000        1.71116        0.04662
H         -2.17612        1.67692        0.53173
H          2.17612        1.67692        0.53173
C         -0.71019       -1.61019        2.21984
C         -1.15372       -1.67265        0.87609
C          0.71019       -1.61019        2.21984
H         -1.34374       -1.53660        3.09051
C          0.00000       -1.71116        0.04662
H         -2.17612       -1.67692        0.53173
C          1.15372       -1.67265        0.87609
H          1.34374       -1.53660        3.09051
H          2.17612       -1.67692        0.53173
C          0.00000        1.96025       -1.41967
F          0.00000        3.28322       -1.67076
F          1.08205        1.45757       -2.02082
F         -1.08205        1.45757       -2.02082
C          0.00000       -1.96025       -1.41967
F          0.00000       -3.28322       -1.67076
F         -1.08205       -1.45757       -2.02082
F          1.08205       -1.45757       -2.02082


27
Energy: -1458356.0819444
Fe         0.00000        0.00000        0.36961
C          0.00000       -1.99089        0.01353
C         -0.37627       -1.74522        1.36385
C         -0.94230       -1.35108       -0.84016
C         -1.54426       -0.94344        1.34115
H          0.15475       -2.08806        2.23816
C         -1.89156       -0.70086       -0.01418
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H         -0.91295       -1.34156       -1.91850
H         -2.05950       -0.55384        2.20561
H         -2.71191       -0.08984       -0.35837
C          1.54426        0.94344        1.34115
C          1.89156        0.70086       -0.01418
C          0.37627        1.74522        1.36385
H          2.05950        0.55384        2.20561
C          0.94230        1.35108       -0.84016
H          2.71191        0.08984       -0.35837
C          0.00000        1.99089        0.01353
H         -0.15475        2.08806        2.23816
H          0.91295        1.34156       -1.91850
C          1.14143       -2.83236       -0.42867
F          2.15409       -2.80922        0.44999
F          0.78183       -4.11856       -0.56709
F          1.62776       -2.43966       -1.61455
C         -1.14143        2.83236       -0.42867
F         -0.78183        4.11856       -0.56709
F         -1.62776        2.43966       -1.61455
F         -2.15409        2.80922        0.44999


27
Energy: -1458355.4816751
Fe         0.00000        0.00000        0.00000
C          0.10289        2.02444        0.00000
C          0.75829        1.51150        1.15412
C          0.75829        1.51150       -1.15412
C          1.80830        0.67202        0.71016
H          0.47633        1.70568        2.17730
C          1.80830        0.67202       -0.71016
H          0.47633        1.70568       -2.17730
H          2.46546        0.09457        1.34216
H          2.46546        0.09457       -1.34216
C         -0.75829       -1.51150        1.15412
C         -1.80830       -0.67202        0.71016
C         -0.10289       -2.02444        0.00000
H         -0.47633       -1.70568        2.17730
C         -1.80830       -0.67202       -0.71016
H         -2.46546       -0.09457        1.34216
C         -0.75829       -1.51150       -1.15412
H         -2.46546       -0.09457       -1.34216
H         -0.47633       -1.70568       -2.17730
C         -1.02768        2.98780        0.00000
F         -1.80830        2.84908        1.08124
F         -0.59353        4.25840        0.00000
F         -1.80830        2.84908       -1.08124
C          1.02768       -2.98780        0.00000
F          1.80830       -2.84908        1.08124
F          0.59353       -4.25840        0.00000
F          1.80830       -2.84908       -1.08124


24
Energy: -1246959.3687545
Fe         0.20983       -0.85720        0.00000
C          0.61200        1.12630        0.00000
C          1.18344        0.52153        1.15462
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C          1.18344        0.52153       -1.15462
C          2.09861       -0.46383        0.71003
H          0.93513        0.75722        2.17774
C          2.09861       -0.46383       -0.71003
H          0.93513        0.75722       -2.17774
H          2.66897       -1.12554        1.34383
H          2.66897       -1.12554       -1.34383
C         -0.75941       -2.25391        1.14826
C         -1.67023       -1.25787        0.71004
C         -0.19520       -2.86929        0.00000
H         -0.51297       -2.48036        2.17458
C         -1.67023       -1.25787       -0.71004
H         -2.23433       -0.58949        1.34259
C         -0.75941       -2.25391       -1.14826
H          0.55312       -3.64730        0.00000
H         -2.23433       -0.58949       -1.34259
H         -0.51297       -2.48036       -2.17458
C         -0.35726        2.25034        0.00000
F          0.26608        3.44164        0.00000
F         -1.15017        2.23560       -1.08131
F         -1.15017        2.23560        1.08131


27
Energy: -1458355.5934345
Fe         0.00000        0.00000        0.94376
C          0.00000        1.80925        0.03385
C         -0.31491        1.96503        1.41288
C          1.29046        1.21930       -0.06950
C          0.77869        1.46120        2.15884
H         -1.23400        2.36923        1.80762
C          1.76638        1.00211        1.24712
H          1.79122        0.95476       -0.98791
H          0.83418        1.40471        3.23521
H          2.70308        0.53368        1.50734
C         -1.76638       -1.00211        1.24712
C         -1.29046       -1.21930       -0.06950
C         -0.77869       -1.46120        2.15884
H         -2.70308       -0.53368        1.50734
C          0.00000       -1.80925        0.03385
H         -1.79122       -0.95476       -0.98791
C          0.31491       -1.96503        1.41288
H         -0.83418       -1.40471        3.23521
H          1.23400       -2.36923        1.80762
C         -0.84810        2.25919       -1.10047
F         -2.15552        2.18746       -0.80780
F         -0.59724        3.53880       -1.42289
F         -0.64092        1.53443       -2.20569
C          0.84810       -2.25919       -1.10047
F          0.59724       -3.53880       -1.42289
F          0.64092       -1.53443       -2.20569
F          2.15552       -2.18746       -0.80780


33
Energy: -1881137.8374073
Fe         0.00000        0.00000        0.27274
C          0.00000        2.04391        0.53324
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C          0.83873        1.41959        1.48649
C          0.47472        1.71597       -0.75773
H         -0.87908        2.63049        0.75083
C          1.83448        0.68571        0.78678
H          0.72998        1.45215        2.55927
C          1.60835        0.87175       -0.61505
H          0.03692        2.01334       -1.69721
C         -0.83873       -1.41959        1.48649
C         -1.83448       -0.68571        0.78678
C          0.00000       -2.04391        0.53324
H         -0.72998       -1.45215        2.55927
C         -1.60835       -0.87175       -0.61505
C         -0.47472       -1.71597       -0.75773
H          0.87908       -2.63049        0.75083
H         -0.03692       -2.01334       -1.69721
C          2.43472        0.37960       -1.76310
F          2.52473       -0.95322       -1.82919
F          1.91567        0.79483       -2.92379
F          3.68408        0.85266       -1.68893
C          2.95011       -0.03719        1.46702
F          2.59325       -0.40380        2.70613
F          3.33384       -1.13915        0.81857
F          4.02832        0.74681        1.58561
C         -2.43472       -0.37960       -1.76310
F         -3.68408       -0.85266       -1.68893
F         -2.52473        0.95322       -1.82919
F         -1.91567       -0.79483       -2.92379
C         -2.95011        0.03719        1.46702
F         -3.33384        1.13915        0.81857
F         -4.02832       -0.74681        1.58561
F         -2.59325        0.40380        2.70613


33
Energy: -1881137.8374073
Fe         0.00000        0.00000        0.27274
C          0.00000       -2.04390        0.53325
C         -0.83873       -1.41958        1.48650
C         -0.47472       -1.71598       -0.75772
H          0.87908       -2.63048        0.75086
C         -1.83448       -0.68570        0.78678
H         -0.72998       -1.45212        2.55927
C         -1.60834       -0.87175       -0.61505
H         -0.03692       -2.01335       -1.69720
C          1.83448        0.68570        0.78678
C          1.60834        0.87175       -0.61505
C          0.83873        1.41958        1.48650
C          0.47472        1.71598       -0.75772
C          0.00000        2.04390        0.53325
H          0.72998        1.45212        2.55927
H          0.03692        2.01335       -1.69720
H         -0.87908        2.63048        0.75086
C         -2.43471       -0.37960       -1.76310
F         -2.52473        0.95321       -1.82918
F         -1.91565       -0.79483       -2.92379
F         -3.68407       -0.85268       -1.68894
C         -2.95012        0.03719        1.46702
F         -2.59328        0.40379        2.70614
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F         -3.33384        1.13916        0.81858
F         -4.02833       -0.74681        1.58558
C          2.43471        0.37960       -1.76310
F          2.52473       -0.95321       -1.82918
F          1.91565        0.79483       -2.92379
F          3.68407        0.85268       -1.68894
C          2.95012       -0.03719        1.46702
F          3.33384       -1.13916        0.81858
F          4.02833        0.74681        1.58558
F          2.59328       -0.40379        2.70614


27
Energy: -1458351.9641959
Fe        -1.17192        0.01030        0.24408
C         -0.77705        0.00545        2.26502
C         -0.23155       -1.14434        1.64763
C         -0.21243        1.14915        1.65307
H         -1.52300        0.01014        3.04458
C          0.67148       -0.71848        0.63493
H         -0.47097       -2.17198        1.87123
C          0.68468        0.71507        0.63845
H         -0.43233        2.17910        1.88437
C         -3.20853       -0.03002        0.03840
C         -2.67914        1.14697       -0.55402
C         -2.62522       -1.14933       -0.61218
H         -3.90875       -0.06737        0.85911
C         -1.76919        0.75458       -1.57051
H         -2.90575        2.16146       -0.26329
C         -1.73508       -0.66351       -1.60625
H         -2.80221       -2.18683       -0.37294
H         -1.17441        1.41622       -2.18079
H         -1.11188       -1.26549       -2.24979
C          1.54171        1.64371       -0.16007
F          2.83744        1.48521        0.14424
F          1.43354        1.48577       -1.48306
F          1.22580        2.91924        0.10669
C          1.50853       -1.66145       -0.16093
F          0.93328       -2.87168       -0.22725
F          1.72280       -1.25319       -1.41369
F          2.71270       -1.83532        0.40419


33
Energy: -1881131.5209660
Fe         0.00000        0.00000        1.27247
C          0.00000        1.57401        2.58753
C          1.14534        1.63162        1.76063
C         -1.14534        1.63162        1.76063
H          0.00000        1.46053        3.66067
C          0.71533        1.72349        0.40986
H          2.17514        1.58908        2.07857
C         -0.71533        1.72349        0.40986
H         -2.17514        1.58908        2.07857
C          0.00000       -1.57401        2.58753
C         -1.14534       -1.63162        1.76063
C          1.14534       -1.63162        1.76063
H          0.00000       -1.46053        3.66067
```

```
C         -0.71533       -1.72349        0.40986
H         -2.17514       -1.58908        2.07857
C          0.71533       -1.72349        0.40986
H          2.17514       -1.58908        2.07857
C         -1.66761        1.99778       -0.71296
F         -1.34491        1.41071       -1.85758
F         -2.90413        1.60177       -0.38388
F         -1.72823        3.31871       -0.94606
C          1.66761        1.99778       -0.71296
F          2.90413        1.60177       -0.38388
F          1.34491        1.41071       -1.85758
F          1.72823        3.31871       -0.94606
C          1.66761       -1.99778       -0.71296
F          2.90413       -1.60177       -0.38388
F          1.72823       -3.31871       -0.94606
F          1.34491       -1.41071       -1.85758
C         -1.66761       -1.99778       -0.71296
F         -1.34491       -1.41071       -1.85758
F         -1.72823       -3.31871       -0.94606
F         -2.90413       -1.60177       -0.38388


33
Energy: -1881137.8374073
Fe         0.00000        0.00000        0.27273
C         -1.60835        0.87175       -0.61505
C         -1.83448        0.68570        0.78678
C         -0.47473        1.71597       -0.75774
C         -0.83873        1.41959        1.48649
C          0.00000        2.04390        0.53324
H         -0.03693        2.01334       -1.69722
H         -0.72997        1.45213        2.55926
H          0.87908        2.63048        0.75084
C          0.00000       -2.04390        0.53324
C          0.47473       -1.71597       -0.75774
C          0.83873       -1.41959        1.48649
H         -0.87908       -2.63048        0.75084
C          1.60835       -0.87175       -0.61505
H          0.03693       -2.01334       -1.69722
C          1.83448       -0.68570        0.78678
H          0.72997       -1.45213        2.55926
C         -2.43473        0.37960       -1.76310
F         -3.68409        0.85266       -1.68892
F         -1.91568        0.79483       -2.92379
F         -2.52474       -0.95322       -1.82919
C         -2.95012       -0.03718        1.46702
F         -4.02832        0.74682        1.58559
F         -3.33385       -1.13915        0.81858
F         -2.59327       -0.40378        2.70614
C          2.43473       -0.37960       -1.76310
F          2.52474        0.95322       -1.82919
F          3.68409       -0.85266       -1.68892
F          1.91568       -0.79483       -2.92379
C          2.95012        0.03718        1.46702
F          4.02832       -0.74682        1.58559
F          3.33385        1.13915        0.81858
F          2.59327        0.40378        2.70614
```

33
Energy: -1881137.4601799

Fe	0.00000	0.00000	0.00000
C	-0.66017	1.78012	0.71643
C	-0.66017	1.78012	-0.71643
C	-1.53334	0.74464	1.14565
C	-1.53334	0.74464	-1.14565
C	-2.06051	0.10541	0.00000
H	-1.71675	0.47572	2.17413
H	-1.71675	0.47572	-2.17413
H	-2.70809	-0.75726	0.00000
C	1.53334	-0.74464	-1.14565
C	2.06051	-0.10541	0.00000
C	0.66017	-1.78012	-0.71643
H	1.71675	-0.47572	-2.17413
C	1.53334	-0.74464	1.14565
H	2.70809	0.75726	0.00000
C	0.66017	-1.78012	0.71643
H	1.71675	-0.47572	2.17413
C	0.02550	2.72140	1.65483
F	-0.55067	3.92887	1.62973
F	-0.05240	2.26941	2.91296
F	1.32081	2.89974	1.37927
C	0.02550	2.72140	-1.65483
F	-0.55067	3.92887	-1.62973
F	1.32081	2.89974	-1.37927
F	-0.05240	2.26941	-2.91296
C	-0.02550	-2.72140	1.65483
F	0.05240	-2.26941	2.91296
F	-1.32081	-2.89974	1.37927
F	0.55067	-3.92887	1.62973
C	-0.02550	-2.72140	-1.65483
F	0.55067	-3.92887	-1.62973
F	-1.32081	-2.89974	-1.37927
F	0.05240	-2.26941	-2.91296

27
Energy: -1458351.9584981

Fe	-0.24404	1.17608	0.00000
C	-0.64464	-0.67129	-0.71706
C	-0.64464	-0.67129	0.71706
C	-1.65517	0.23278	-1.14654
C	-1.65517	0.23278	1.14654
C	-2.26737	0.79053	0.00000
H	-1.88120	0.46361	-2.17536
H	-1.88120	0.46361	2.17536
H	-3.04357	1.53999	0.00000
C	1.59174	1.74586	0.70948
C	1.59174	1.74586	-0.70948
C	0.59079	2.65204	1.14884
H	2.21598	1.13318	1.34151
C	0.59079	2.65204	-1.14884
H	2.21598	1.13318	-1.34151
C	-0.02802	3.21210	0.00000
H	0.32681	2.85561	2.17544
H	0.32681	2.85561	-2.17544

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H         -0.84534        3.91726        0.00000
C          0.14615       -1.52043       -1.65651
F         -0.30012       -2.78508       -1.65714
F          0.03371       -1.06486       -2.91291
F          1.45024       -1.57080       -1.37200
C          0.14615       -1.52043        1.65651
F         -0.30012       -2.78508        1.65714
F          1.45024       -1.57080        1.37200
F          0.03371       -1.06486        2.91291
```

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33
Energy: -1881132.3492785
Fe         0.00000        0.00000        1.24925
C          0.00000        1.93443        0.58343
C         -1.22652        1.29027        0.22307
C          0.10159        1.90769        1.99921
C         -1.85728        0.86970        1.42432
C         -1.03875        1.24790        2.51226
H          0.93282        2.29600        2.56660
H         -2.78889        0.32819        1.47407
H         -1.22797        1.02826        3.55183
C         -0.10159       -1.90769        1.99921
C          0.00000       -1.93443        0.58343
C          1.03875       -1.24790        2.51226
H         -0.93282       -2.29600        2.56660
C          1.22652       -1.29027        0.22307
C          1.85728       -0.86970        1.42432
H          1.22797       -1.02826        3.55183
H          2.78889       -0.32819        1.47407
C          0.97482        2.67447       -0.27729
F          0.52815        3.91313       -0.53011
F          2.15095        2.80428        0.35467
F          1.20846        2.09153       -1.44720
C         -1.91018        1.23579       -1.10943
F         -2.39425        2.44959       -1.41986
F         -1.12787        0.85752       -2.11148
F         -2.95244        0.39757       -1.06448
C         -0.97482       -2.67447       -0.27729
F         -2.15095       -2.80428        0.35467
F         -1.20846       -2.09153       -1.44720
F         -0.52815       -3.91313       -0.53011
C          1.91018       -1.23579       -1.10943
F          2.39425       -2.44959       -1.41986
F          1.12787       -0.85752       -2.11148
F          2.95244       -0.39757       -1.06448
```

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39
Energy: -2303910.0976541
Fe         0.00000        0.00000        0.60988
C         -0.98103       -1.28094        1.87390
C         -1.84477       -0.90736        0.82598
C          0.15969       -1.90276        1.30580
H         -1.12758       -1.08649        2.92478
C         -1.25669       -1.30153       -0.40194
H         -2.77988       -0.37904        0.92213
C          0.00000       -1.92244       -0.11592
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C          0.98103        1.28094        1.87390
C          1.84477        0.90736        0.82598
C         -0.15969        1.90276        1.30580
H          1.12758        1.08649        2.92478
C          1.25669        1.30153       -0.40194
H          2.77988        0.37904        0.92213
C          0.00000        1.92244       -0.11592
C          0.92579       -2.62133       -1.07859
F          1.05527       -3.90583       -0.72337
F          0.46113       -2.59171       -2.32216
F          2.14848       -2.09010       -1.09391
C         -1.99164       -1.19473       -1.71268
F         -3.15206       -0.55657       -1.53086
F         -1.31880       -0.54456       -2.65539
F         -2.28519       -2.41263       -2.18016
C          1.25167       -2.49574        2.14410
F          1.03006       -3.79402        2.36166
F          2.46123       -2.37939        1.59897
F          1.29287       -1.89530        3.34308
C          1.99164        1.19473       -1.71268
F          1.31880        0.54456       -2.65539
F          2.28519        2.41263       -2.18016
F          3.15206        0.55657       -1.53086
C         -0.92579        2.62133       -1.07859
F         -1.05527        3.90583       -0.72337
F         -0.46113        2.59171       -2.32216
F         -2.14848        2.09010       -1.09391
C         -1.25167        2.49574        2.14410
F         -1.03006        3.79402        2.36166
F         -2.46123        2.37939        1.59897
F         -1.29287        1.89530        3.34308


39
Energy: -2303911.7937558
Fe         0.00000        0.00000        0.33271
C          1.46546        0.97241        1.39831
C          1.91712        0.73304        0.08583
C          0.28207        1.75397        1.32836
H          1.90607        0.59309        2.30618
C          1.02482        1.36925       -0.81229
H          2.76997        0.13916       -0.20219
C          0.00000        2.01286       -0.05059
C         -0.28207       -1.75397        1.32836
C         -1.46546       -0.97241        1.39831
C          0.00000       -2.01286       -0.05059
C         -1.91712       -0.73304        0.08583
H         -1.90607       -0.59309        2.30618
C         -1.02482       -1.36925       -0.81229
H         -2.76997       -0.13916       -0.20219
C         -1.07397        2.90768       -0.61784
F         -0.53919        3.78217       -1.47296
F         -2.01881        2.23111       -1.27568
F         -1.68017        3.60824        0.33885
C          1.28785        1.47236       -2.28603
F          2.05388        0.46201       -2.69992
F          0.17614        1.47774       -3.01580
F          1.95118        2.60488       -2.55202
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C         -0.44105        2.23429        2.55481
F         -0.23475        3.53643        2.75659
F         -1.76146        2.03472        2.50504
F          0.01318        1.58803        3.63450
C         -1.28785       -1.47236       -2.28603
F         -2.05388       -0.46201       -2.69992
F         -0.17614       -1.47774       -3.01580
F         -1.95118       -2.60488       -2.55202
C          1.07397       -2.90768       -0.61784
F          0.53919       -3.78217       -1.47296
F          2.01881       -2.23111       -1.27568
F          1.68017       -3.60824        0.33885
C          0.44105       -2.23429        2.55481
F          0.23475       -3.53643        2.75659
F          1.76146       -2.03472        2.50504
F         -0.01318       -1.58803        3.63450


30
Energy: -1669742.0558807
Fe        -1.18780       -0.05486        0.00000
C         -0.52395       -1.86905        0.70447
C         -0.52395       -1.86905       -0.70447
C          0.30641       -0.80827        1.15209
H         -1.07555       -2.53724        1.34586
C          0.30641       -0.80827       -1.15209
H         -1.07555       -2.53724       -1.34586
C          0.83099       -0.13655        0.00000
C         -3.09363        0.19649        0.71000
C         -2.26385        1.26132        1.14809
C         -3.09363        0.19649       -0.71000
H         -3.60885       -0.50773        1.34544
C         -1.74960        1.91803        0.00000
H         -2.02985        1.50331        2.17293
C         -2.26385        1.26132       -1.14809
H         -3.60885       -0.50773       -1.34544
H         -1.05908        2.74762        0.00000
H         -2.02985        1.50331       -2.17293
C          1.86107        0.94972        0.00000
F          3.09584        0.43167        0.00000
F          1.76282        1.73456       -1.07564
F          1.76282        1.73456        1.07564
C          0.62509       -0.57606       -2.59927
F         -0.01080       -1.47902       -3.35942
F          0.27108        0.62824       -3.05567
F          1.93535       -0.71508       -2.82933
C          0.62509       -0.57606        2.59927
F          1.93535       -0.71508        2.82933
F          0.27108        0.62824        3.05567
F         -0.01080       -1.47902        3.35942


39
Energy: -2303902.4581091
Fe         0.00000        0.00000        0.90435
C          0.70320        1.59222        1.99853
C         -0.70320        1.59222        1.99853
C          1.15056        1.69677        0.65726
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H          1.34728        1.50492        2.85889
C         -1.15056        1.69677        0.65726
H         -1.34728        1.50492        2.85889
C          0.00000        1.75429       -0.19288
C          0.70320       -1.59222        1.99853
C          1.15056       -1.69677        0.65726
C         -0.70320       -1.59222        1.99853
H          1.34728       -1.50492        2.85889
C          0.00000       -1.75429       -0.19288
C         -1.15056       -1.69677        0.65726
H         -1.34728       -1.50492        2.85889
C          0.00000        2.06815       -1.66602
F          0.00000        3.39801       -1.83443
F         -1.07205        1.58663       -2.28547
F          1.07205        1.58663       -2.28547
C         -2.59905        1.97177        0.34974
F         -3.35306        1.65128        1.41062
F         -3.09311        1.33323       -0.69651
F         -2.75674        3.28506        0.13373
C          2.59905        1.97177        0.34974
F          2.75674        3.28506        0.13373
F          3.09311        1.33323       -0.69651
F          3.35306        1.65128        1.41062
C          2.59905       -1.97177        0.34974
F          3.09311       -1.33323       -0.69651
F          2.75674       -3.28506        0.13373
F          3.35306       -1.65128        1.41062
C          0.00000       -2.06815       -1.66602
F          0.00000       -3.39801       -1.83443
F          1.07205       -1.58663       -2.28547
F         -1.07205       -1.58663       -2.28547
C         -2.59905       -1.97177        0.34974
F         -2.75674       -3.28506        0.13373
F         -3.09311       -1.33323       -0.69651
F         -3.35306       -1.65128        1.41062


39
Energy: -2303909.9446360
Fe         0.00000        0.00000        0.55309
C          0.07114        1.88472        1.32478
C          0.00000        1.94339       -0.10263
C         -1.08806        1.21885        1.79757
C         -1.22262        1.30930       -0.48818
C         -1.87635        0.86281        0.68604
H         -1.29902        0.99250        2.83081
H         -2.80383        0.31415        0.70884
C          1.22262       -1.30930       -0.48818
C          1.87635       -0.86281        0.68604
C          0.00000       -1.94339       -0.10263
C          1.08806       -1.21885        1.79757
H          2.80383       -0.31415        0.70884
C         -0.07114       -1.88472        1.32478
H          1.29902       -0.99250        2.83081
C          1.10832        2.47406        2.24009
F          1.22593        3.78762        2.04607
F          0.74830        2.28345        3.51563
F          2.32354        1.93716        2.09730
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C          0.93899        2.70846       -0.99080
F          0.61167        4.00525       -0.99322
F          2.20209        2.61704       -0.56715
F          0.90055        2.28225       -2.24819
C         -1.88320        1.26720       -1.84141
F         -2.10579        2.51448       -2.27360
F         -1.19162        0.63330       -2.77671
F         -3.07171        0.66004       -1.74261
C          1.88320       -1.26720       -1.84141
F          1.19162       -0.63330       -2.77671
F          3.07171       -0.66004       -1.74261
F          2.10579       -2.51448       -2.27360
C         -0.93899       -2.70846       -0.99080
F         -0.90055       -2.28225       -2.24819
F         -0.61167       -4.00525       -0.99322
F         -2.20209       -2.61704       -0.56715
C         -1.10832       -2.47406        2.24009
F         -2.32354       -1.93716        2.09730
F         -1.22593       -3.78762        2.04607
F         -0.74830       -2.28345        3.51563


39
Energy: -2303912.4343927
Fe         0.00000        0.00000        0.00000
C         -0.87389        1.45775        1.14972
C         -0.24055        2.02278        0.00000
C         -1.86294        0.54433        0.70500
C         -0.87389        1.45775       -1.14972
C         -1.86294        0.54433       -0.70500
H         -2.47841       -0.06492        1.34791
H         -2.47841       -0.06492       -1.34791
C          1.86294       -0.54433       -0.70500
C          1.86294       -0.54433        0.70500
C          0.87389       -1.45775       -1.14972
H          2.47841        0.06492       -1.34791
C          0.87389       -1.45775        1.14972
H          2.47841        0.06492        1.34791
C          0.24055       -2.02278        0.00000
C         -0.66872        1.83224        2.59267
F         -0.76669        3.15601        2.74762
F         -1.61119        1.26935        3.35152
F          0.51457        1.45827        3.08184
C          0.81154        3.09382        0.00000
F          0.25520        4.30632        0.00000
F          1.59865        3.01161        1.07514
F          1.59865        3.01161       -1.07514
C         -0.66872        1.83224       -2.59267
F         -0.76669        3.15601       -2.74762
F          0.51457        1.45827       -3.08184
F         -1.61119        1.26935       -3.35152
C          0.66872       -1.83224       -2.59267
F         -0.51457       -1.45827       -3.08184
F          1.61119       -1.26935       -3.35152
F          0.76669       -3.15601       -2.74762
C         -0.81154       -3.09382        0.00000
F         -1.59865       -3.01161       -1.07514
F         -0.25520       -4.30632        0.00000
```

F -1.59865 -3.01161 1.07514
C 0.66872 -1.83224 2.59267
F -0.51457 -1.45827 3.08184
F 0.76669 -3.15601 2.74762
F 1.61119 -1.26935 3.35152

30
Energy: -1669742.0558807
Fe 1.18780 -0.05485 0.00000
C -0.30642 -0.80827 1.15209
C -0.83099 -0.13655 0.00000
C 0.52396 -1.86905 0.70447
C -0.30642 -0.80827 -1.15209
C 0.52396 -1.86905 -0.70447
H 1.07556 -2.53723 1.34586
H 1.07556 -2.53723 -1.34586
C 1.74960 1.91804 0.00000
C 2.26385 1.26132 1.14810
C 2.26385 1.26132 -1.14810
H 1.05907 2.74763 0.00000
C 3.09363 0.19650 0.70999
H 2.02986 1.50329 2.17294
C 3.09363 0.19650 -0.70999
H 2.02986 1.50329 -2.17294
H 3.60885 -0.50773 1.34542
H 3.60885 -0.50773 -1.34542
C -0.62509 -0.57606 2.59928
F -1.93535 -0.71508 2.82933
F 0.01081 -1.47902 3.35942
F -0.27108 0.62824 3.05568
C -1.86108 0.94972 0.00000
F -3.09585 0.43166 0.00000
F -1.76283 1.73455 1.07564
F -1.76283 1.73455 -1.07564
C -0.62509 -0.57606 -2.59928
F -1.93535 -0.71508 -2.82933
F -0.27108 0.62824 -3.05568
F 0.01081 -1.47902 -3.35942

39
Energy: -2303910.0976541
Fe 0.00000 0.00000 0.60989
C 0.15972 1.90276 1.30579
C 0.00000 1.92243 -0.11592
C -0.98100 1.28095 1.87392
C -1.25670 1.30154 -0.40191
C -1.84476 0.90737 0.82602
H -1.12753 1.08652 2.92481
H -2.77987 0.37906 0.92218
C 0.00000 -1.92243 -0.11592
C 1.25670 -1.30154 -0.40191
C -0.15972 -1.90276 1.30579
C 1.84476 -0.90737 0.82602
C 0.98100 -1.28095 1.87392
H 2.77987 -0.37906 0.92218
H 1.12753 -1.08652 2.92481

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C          1.25172        2.49574        2.14407
F          1.03013        3.79402        2.36162
F          1.29293        1.89531        3.34306
F          2.46127        2.37936        1.59892
C          0.92578        2.62133       -1.07861
F          1.05526        3.90582       -0.72339
F          2.14847        2.09009       -1.09394
F          0.46110        2.59170       -2.32217
C         -1.99166        1.19471       -1.71265
F         -2.28521        2.41260       -2.18015
F         -1.31882        0.54452       -2.65535
F         -3.15209        0.55655       -1.53080
C          1.99166       -1.19471       -1.71265
F          2.28521       -2.41260       -2.18015
F          1.31882       -0.54452       -2.65535
F          3.15209       -0.55655       -1.53080
C         -0.92578       -2.62133       -1.07861
F         -0.46110       -2.59170       -2.32217
F         -1.05526       -3.90582       -0.72339
F         -2.14847       -2.09009       -1.09394
C         -1.25172       -2.49574        2.14407
F         -2.46127       -2.37936        1.59892
F         -1.03013       -3.79402        2.36162
F         -1.29293       -1.89531        3.34306


36
Energy: -2092508.9304774
Fe         0.00000        0.00000        1.07389
C          0.37668       -1.15932       -0.55259
C         -0.98617       -0.71650       -0.55259
C          1.21898        0.00000       -0.55259
C         -0.98617        0.71650       -0.55259
C          0.37668        1.15932       -0.55259
C          0.03611       -1.20652        2.73354
C          1.15862       -0.33849        2.73354
C         -1.13631       -0.40718        2.73354
H          0.06896       -2.28445        2.69298
C          0.67996        0.99732        2.73354
H          2.19396       -0.64035        2.69298
C         -0.73838        0.95487        2.73354
H         -2.15133       -0.77152        2.69298
H          1.28698        1.88870        2.69298
H         -1.39856        1.80763        2.69298
C          0.82574        2.60652       -0.62216
F          0.40397        3.16650       -1.75856
F          0.36157        3.33299        0.39908
F          2.14831        2.73143       -0.59939
C         -2.22378        1.59078       -0.62216
F         -3.05813        1.37382        0.39908
F         -1.93388        2.88722       -0.59939
F         -2.88668        1.36270       -1.75856
C          2.73412        0.02013       -0.62216
F          3.13635        0.59430       -1.75856
F          3.28159        0.68608        0.39908
F          3.26161       -1.19911       -0.59939
C         -2.20011       -1.62336       -0.62216
F         -3.34351       -0.94703       -0.59939
```

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F         -2.18804       -2.32430       -1.75856
F         -2.25159       -2.48392        0.39908
C          0.86403       -2.59408       -0.62216
F          1.53440       -2.79920       -1.75856
F          1.66657       -2.90897        0.39908
F         -0.13253       -3.47252       -0.59939


36
Energy: -2092509.4861370
Fe         0.01604        0.01417        1.07492
C          1.15005        0.41210       -0.54383
C          0.73647       -0.95842       -0.57988
C         -0.02766        1.22979       -0.56122
C         -0.69113       -0.98797       -0.53243
C         -1.16648        0.36155       -0.54902
C          1.24007        0.09427        2.72024
C          0.33151        1.18375        2.73240
C          0.48410       -1.10703        2.72939
H          2.31560        0.16588        2.66908
C         -0.98554        0.65580        2.74774
H          0.59480        2.22962        2.68984
C         -0.89126       -0.76018        2.74645
H          0.88545       -2.10761        2.67996
H         -1.89901        1.22919        2.71870
H         -1.72057       -1.45030        2.71758
C         -2.62918        0.75059       -0.65429
F         -3.22316        0.01886       -1.60170
F         -3.29984        0.56547        0.48638
F         -2.79277        2.02457       -0.99216
C         -1.54342       -2.23385       -0.45142
F         -0.97810       -3.16348        0.32557
F         -2.73916       -1.98047        0.08159
F         -1.74770       -2.76817       -1.65458
C         -0.09150        2.73456       -0.71158
F         -0.59769        3.05402       -1.90581
F         -0.85177        3.30192        0.22957
F          1.10426        3.30927       -0.64446
C          1.64240       -2.14798       -0.83725
F          0.95830       -3.18051       -1.32598
F          2.55309       -1.83733       -1.76332
F          2.28490       -2.57334        0.25175
C          2.58569        0.88747       -0.46157
F          3.00237        1.37180       -1.63189
F          2.75873        1.83743        0.46102
F          3.40653       -0.10470       -0.11434


36
Energy: -2092487.5042607
Fe         0.00000        0.00000        1.18822
C          0.72159       -0.99319       -0.43110
C         -0.72159       -0.99319       -0.43110
C          1.16756        0.37936       -0.43110
C         -1.16756        0.37936       -0.43110
C          0.00000        1.22765       -0.43110
C          0.70992       -0.97712        2.84361
C          1.14867        0.37323        2.84361
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C         -0.70992       -0.97712        2.84361
H          1.34414       -1.85005        2.81039
C          0.00000        1.20779        2.84361
H          2.17487        0.70666        2.81039
C         -1.14867        0.37323        2.84361
H         -1.34414       -1.85005        2.81039
H          0.00000        2.28679        2.81039
H         -2.17487        0.70666        2.81039
C          0.00000        2.74797       -0.63346
F          0.00000        2.97839       -1.95464
F         -1.04562        3.37604       -0.11509
F          1.04562        3.37604       -0.11509
C         -2.61347        0.84917       -0.63346
F         -3.53392        0.04881       -0.11509
F         -2.88769        2.03770       -0.11509
F         -2.83262        0.92037       -1.95464
C          2.61347        0.84917       -0.63346
F          2.83262        0.92037       -1.95464
F          2.88769        2.03770       -0.11509
F          3.53392        0.04881       -0.11509
C         -1.61521       -2.22315       -0.63346
F         -2.83031       -2.11667       -0.11509
F         -1.75065       -2.40957       -1.95464
F         -1.13846       -3.34587       -0.11509
C          1.61521       -2.22315       -0.63346
F          1.75065       -2.40957       -1.95464
F          2.83031       -2.11667       -0.11509
F          1.13846       -3.34587       -0.11509


51
Energy: -3149386.9508965
Fe         0.00000        0.00000        0.00000
C         -0.71947       -0.99027        1.67257
C          0.71947       -0.99027        1.67257
C         -1.16413        0.37825        1.67257
C          1.16413        0.37825        1.67257
C          0.00000        1.22404        1.67257
C         -0.71947       -0.99027       -1.67257
C         -1.16413        0.37825       -1.67257
C          0.71947       -0.99027       -1.67257
C          0.00000        1.22404       -1.67257
C          1.16413        0.37825       -1.67257
C          0.00000        2.74104        1.94803
F          0.00000        2.87755        3.28130
F          1.04733        3.38588        1.46952
F         -1.04733        3.38588        1.46952
C          2.60688        0.84703        1.94803
F          3.54381        0.05022        1.46952
F          2.89652        2.04237        1.46952
F          2.73671        0.88921        3.28130
C         -2.60688        0.84703        1.94803
F         -2.73671        0.88921        3.28130
F         -2.89652        2.04237        1.46952
F         -3.54381        0.05022        1.46952
C          1.61114       -2.21754        1.94803
F          2.83748       -2.12363        1.46952
F          1.69138       -2.32798        3.28130
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F 1.14286 -3.35484 1.46952
C -1.61114 -2.21754 1.94803
F -1.69138 -2.32798 3.28130
F -2.83748 -2.12363 1.46952
F -1.14286 -3.35484 1.46952
C 0.00000 2.74104 -1.94803
F -1.04733 3.38588 -1.46952
F 1.04733 3.38588 -1.46952
F 0.00000 2.87755 -3.28130
C -2.60688 0.84703 -1.94803
F -2.89652 2.04237 -1.46952
F -2.73671 0.88921 -3.28130
F -3.54381 0.05022 -1.46952
C -1.61114 -2.21754 -1.94803
F -2.83748 -2.12363 -1.46952
F -1.69138 -2.32798 -3.28130
F -1.14286 -3.35484 -1.46952
C 1.61114 -2.21754 -1.94803
F 1.14286 -3.35484 -1.46952
F 1.69138 -2.32798 -3.28130
F 2.83748 -2.12363 -1.46952
C 2.60688 0.84703 -1.94803
F 3.54381 0.05022 -1.46952
F 2.73671 0.88921 -3.28130
F 2.89652 2.04237 -1.46952

51
Energy: -3149424.2420272
Fe 0.00000 0.00000 0.00000
C -1.11171 -0.49063 1.69835
C 0.12308 -1.20891 1.69835
C -0.81016 0.90568 1.69835
C 1.18778 -0.25651 1.69835
C 0.61100 1.05038 1.69835
C -1.18778 -0.25651 -1.69835
C -0.61100 1.05038 -1.69835
C -0.12308 -1.20891 -1.69835
C 0.81016 0.90568 -1.69835
C 1.11171 -0.49063 -1.69835
C 1.34815 2.37025 1.90642
F 1.01347 2.85709 3.10450
F 2.66424 2.22793 1.89980
F 1.04837 3.27288 0.98079
C 2.67085 -0.54972 1.90642
F 2.94219 -1.84538 1.89980
F 3.43666 0.01431 0.98079
F 3.03043 -0.08098 3.10450
C -1.83764 2.01462 1.90642
F -2.40407 1.84676 3.10450
F -1.29560 3.22232 1.89980
F -2.78873 2.00843 0.98079
C 0.30252 -2.71000 1.90642
F 1.07560 -3.26403 0.98079
F 0.85944 -2.90714 3.10450
F -0.84587 -3.36844 1.89980
C -2.48388 -1.12515 1.90642
F -2.49927 -1.71573 3.10450

F -3.46496 -0.23643 1.89980
F -2.77190 -2.03160 0.98079
C 1.83764 2.01462 -1.90642
F 1.29560 3.22232 -1.89980
F 2.78873 2.00843 -0.98079
F 2.40407 1.84676 -3.10450
C -1.34815 2.37025 -1.90642
F -1.04837 3.27288 -0.98079
F -1.01347 2.85709 -3.10450
F -2.66424 2.22793 -1.89980
C -2.67085 -0.54972 -1.90642
F -3.43666 0.01431 -0.98079
F -3.03043 -0.08098 -3.10450
F -2.94219 -1.84538 -1.89980
C -0.30252 -2.71000 -1.90642
F -1.07560 -3.26403 -0.98079
F -0.85944 -2.90714 -3.10450
F 0.84587 -3.36844 -1.89980
C 2.48388 -1.12515 -1.90642
F 2.77190 -2.03160 -0.98079
F 2.49927 -1.71573 -3.10450
F 3.46496 -0.23643 -1.89980

36
Energy: -2092486.6956708
Fe 0.00000 0.00000 1.18748
C 0.00000 1.22725 -0.43557
C 1.16719 0.37924 -0.43557
C -1.16719 0.37924 -0.43557
C 0.72136 -0.99287 -0.43557
C -0.72136 -0.99287 -0.43557
C 1.14823 -0.37308 2.84818
C 0.70964 0.97674 2.84818
C 0.00000 -1.20732 2.84818
H 2.17428 -0.70647 2.80792
C -0.70964 0.97674 2.84818
H 1.34378 1.84955 2.80792
C -1.14823 -0.37308 2.84818
H 0.00000 -2.28617 2.80792
H -1.34378 1.84955 2.80792
H -2.17428 -0.70647 2.80792
C 0.00000 2.74829 -0.63419
F 0.00000 2.98173 -1.95483
F -1.04558 3.37530 -0.11444
F 1.04558 3.37530 -0.11444
C 2.61378 0.84927 -0.63419
F 2.83580 0.92141 -1.95483
F 2.88700 2.03743 -0.11444
F 3.53321 0.04862 -0.11444
C 1.61540 -2.22341 -0.63419
F 1.75262 -2.41227 -1.95483
F 2.82985 -2.11610 -0.11444
F 1.13807 -3.34525 -0.11444
C -2.61378 0.84927 -0.63419
F -2.88700 2.03743 -0.11444
F -2.83580 0.92141 -1.95483
F -3.53321 0.04862 -0.11444

C -1.61540 -2.22341 -0.63419
F -1.13807 -3.34525 -0.11444
F -2.82985 -2.11610 -0.11444
F -1.75262 -2.41227 -1.95483

51
Energy: -3149423.9103132
Fe 0.00000 0.00000 0.00000
C -0.00367 1.21621 1.69980
C -1.15689 0.37351 1.70063
C 1.15419 0.37986 1.70031
C -0.71179 -0.98374 1.70123
C 0.71660 -0.97980 1.70104
C -1.15419 -0.37986 -1.70031
C -0.71660 0.97980 -1.70104
C 0.00367 -1.21621 -1.69980
C 0.71179 0.98374 -1.70123
C 1.15689 -0.37351 -1.70063
C 0.01587 2.72872 1.90298
F 0.54653 2.98743 3.10132
F 0.72669 3.36010 0.97714
F -1.19614 3.26108 1.89261
C -2.58884 0.85991 1.90601
F -2.66781 1.44748 3.10314
F -2.97202 1.72876 0.97905
F -3.46971 -0.12828 1.90043
C -1.61677 -2.19513 1.90745
F -2.19742 -2.08963 3.10592
F -2.56353 -2.28963 0.98240
F -0.94955 -3.33846 1.89934
C 2.59819 0.82848 1.90588
F 2.72968 2.14575 1.89912
F 3.00717 0.40073 3.10353
F 3.41913 0.35000 0.97973
C 1.58944 -2.21491 1.90498
F 1.38520 -3.14358 0.97927
F 2.88301 -1.93363 1.89481
F 1.31172 -2.73575 3.10334
C -0.01587 -2.72872 -1.90298
F -0.54653 -2.98743 -3.10132
F 1.19614 -3.26108 -1.89261
F -0.72669 -3.36010 -0.97714
C -2.59819 -0.82848 -1.90588
F -3.00717 -0.40073 -3.10353
F -2.72968 -2.14575 -1.89912
F -3.41913 -0.35000 -0.97973
C 2.58884 -0.85991 -1.90601
F 2.97202 -1.72876 -0.97905
F 2.66781 -1.44748 -3.10314
F 3.46971 0.12828 -1.90043
C 1.61677 2.19513 -1.90745
F 2.56353 2.28963 -0.98240
F 2.19742 2.08963 -3.10592
F 0.94955 3.33846 -1.89934
C -1.58944 2.21491 -1.90498
F -1.31172 2.73575 -3.10334
F -2.88301 1.93363 -1.89481

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F         -1.38520        3.14358       -0.97927


33
Energy: -1881143.4064973
Fe         0.00000        0.00000        0.40707
C          0.73096        1.46838        1.63602
C          1.74489        1.02244        0.75862
C         -0.34658        1.95374        0.84318
H          0.74887        1.41648        2.71343
C          1.29272        1.23508       -0.57294
H          2.67982        0.56355        1.04110
C          0.00000        1.81990       -0.52669
C          0.34658       -1.95374        0.84318
C         -0.73096       -1.46838        1.63602
C          0.00000       -1.81990       -0.52669
C         -1.74489       -1.02244        0.75862
H         -0.74887       -1.41648        2.71343
C         -1.29272       -1.23508       -0.57294
H          0.61630       -2.08115       -1.37285
H         -2.67982       -0.56355        1.04110
C          2.08434        0.97087       -1.80809
F          2.88314       -0.09323       -1.67013
F          1.29989        0.76045       -2.86803
F          2.87225        2.01573       -2.10135
H         -0.61630        2.08115       -1.37285
C         -1.60029        2.56041        1.37148
F         -2.62447        2.41115        0.52689
F         -1.95592        2.01796        2.54473
F         -1.44971        3.87521        1.58087
C         -2.08434       -0.97087       -1.80809
F         -2.88314        0.09323       -1.67013
F         -1.29989       -0.76045       -2.86803
F         -2.87225       -2.01573       -2.10135
C          1.60029       -2.56041        1.37148
F          2.62447       -2.41115        0.52689
F          1.95592       -2.01796        2.54473
F          1.44971       -3.87521        1.58087


33
Energy: -1881143.4064973
Fe         0.00000        0.00000        0.40707
C          1.74490       -1.02242        0.75860
C          0.73098       -1.46837        1.63602
C          1.29272       -1.23507       -0.57295
H          2.67983       -0.56353        1.04107
C         -0.34656       -1.95374        0.84319
H          0.74892       -1.41647        2.71342
C          0.00000       -1.81990       -0.52668
C          0.34656        1.95374        0.84319
C          0.00000        1.81990       -0.52668
C         -0.73098        1.46837        1.63602
C         -1.29272        1.23507       -0.57295
H          0.61631        2.08116       -1.37283
C         -1.74490        1.02242        0.75860
H         -0.74892        1.41647        2.71342
H         -2.67983        0.56353        1.04107
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C         -1.60026       -2.56042        1.37151
F         -1.95591       -2.01793        2.54474
F         -2.62444       -2.41121        0.52691
F         -1.44966       -3.87520        1.58095
H         -0.61631       -2.08116       -1.37283
C          2.08432       -0.97086       -1.80811
F          2.88307        0.09328       -1.67019
F          2.87228       -2.01569       -2.10135
F          1.29985       -0.76050       -2.86805
C         -2.08432        0.97086       -1.80811
F         -2.87228        2.01569       -2.10135
F         -1.29985        0.76050       -2.86805
F         -2.88307       -0.09328       -1.67019
C          1.60026        2.56042        1.37151
F          2.62444        2.41121        0.52691
F          1.44966        3.87520        1.58095
F          1.95591        2.01793        2.54474


27
Energy: -1458355.4999544
Fe        -0.75484       -0.18116        0.00000
C          0.55940       -1.58512        0.70684
C          0.55940       -1.58512       -0.70684
C          0.91798       -0.27776        1.14142
H          0.30223       -2.41361        1.34802
C          0.91798       -0.27776       -1.14142
H          0.30223       -2.41361       -1.34802
C          1.15286        0.53394        0.00000
C         -2.61400       -0.66519        0.71014
C         -2.24192        0.63271        1.14852
C         -2.61400       -0.66519       -0.71014
H         -2.82833       -1.51063        1.34594
C         -2.01250        1.43525        0.00000
H         -2.11764        0.94366        2.17468
C         -2.24192        0.63271       -1.14852
H         -2.82833       -1.51063       -1.34594
H         -1.68718        2.46429        0.00000
H         -2.11764        0.94366       -2.17468
C          1.08260        0.15094       -2.55524
F          0.26611       -0.51842       -3.38050
F          0.83813        1.45822       -2.71545
F          2.33352       -0.06486       -2.99162
H          1.42982        1.57620        0.00000
C          1.08260        0.15094        2.55524
F          0.83813        1.45822        2.71545
F          0.26611       -0.51842        3.38050
F          2.33352       -0.06486        2.99162


33
Energy: -1881137.3375395
Fe         0.00000        0.00000        0.49096
C         -0.70664        1.62840        1.52756
C          0.70664        1.62840        1.52756
C         -1.13960        1.68548        0.17534
H         -1.35091        1.57475        2.39132
C          1.13960        1.68548        0.17534
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H          1.35091        1.57475        2.39132
C          0.00000        1.71468       -0.66636
C         -0.70664       -1.62840        1.52756
C         -1.13960       -1.68548        0.17534
C          0.70664       -1.62840        1.52756
H         -1.35091       -1.57475        2.39132
C          0.00000       -1.71468       -0.66636
C          1.13960       -1.68548        0.17534
H          1.35091       -1.57475        2.39132
H          0.00000       -1.76369       -1.74400
C          2.54222        1.91856       -0.27341
F          3.43597        1.40282        0.57272
F          2.77577        1.42185       -1.48885
F          2.78454        3.23862       -0.33815
H          0.00000        1.76369       -1.74400
C         -2.54222        1.91856       -0.27341
F         -2.78454        3.23862       -0.33815
F         -2.77577        1.42185       -1.48885
F         -3.43597        1.40282        0.57272
C          2.54222       -1.91856       -0.27341
F          2.77577       -1.42185       -1.48885
F          3.43597       -1.40282        0.57272
F          2.78454       -3.23862       -0.33815
C         -2.54222       -1.91856       -0.27341
F         -3.43597       -1.40282        0.57272
F         -2.77577       -1.42185       -1.48885
F         -2.78454       -3.23862       -0.33815


33
Energy: -1881143.4064785
Fe         0.00000        0.00000        0.40709
C          0.34668        1.95374        0.84311
C          0.00000        1.81987       -0.52673
C         -0.73082        1.46845        1.63605
C         -1.29275        1.23511       -0.57286
C         -1.74483        1.02253        0.75874
H         -0.74866        1.41659        2.71346
H         -2.67977        0.56369        1.04129
C          0.00000       -1.81987       -0.52673
C          1.29275       -1.23511       -0.57286
C         -0.34668       -1.95374        0.84311
H         -0.61624       -2.08109       -1.37295
C          1.74483       -1.02253        0.75874
C          0.73082       -1.46845        1.63605
H          2.67977       -0.56369        1.04129
H          0.74866       -1.41659        2.71346
C          1.60044        2.56040        1.37132
F          1.44996        3.87524        1.58051
F          1.95602        2.01809        2.54465
F          2.62461        2.41093        0.52675
H          0.61624        2.08109       -1.37295
C         -2.08448        0.97093       -1.80794
F         -1.30014        0.76009       -2.86788
F         -2.88360       -0.09290       -1.66977
F         -2.87209        2.01598       -2.10136
C          2.08448       -0.97093       -1.80794
F          1.30014       -0.76009       -2.86788
```

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F          2.88360        0.09290       -1.66977
F          2.87209       -2.01598       -2.10136
C         -1.60044       -2.56040        1.37132
F         -2.62461       -2.41093        0.52675
F         -1.44996       -3.87524        1.58051
F         -1.95602       -2.01809        2.54465


33
Energy: -1881140.3447092
Fe         0.00000        0.00000        0.00000
C          1.67220        0.31225        1.14012
C          2.00114       -0.46243        0.00000
C          1.14511        1.56005        0.70624
C          1.67220        0.31225       -1.14012
C          1.14511        1.56005       -0.70624
H          0.77814        2.34403        1.35017
H          0.77814        2.34403       -1.35017
C         -1.14511       -1.56005       -0.70624
C         -1.14511       -1.56005        0.70624
C         -1.67220       -0.31225       -1.14012
H         -0.77814       -2.34403       -1.35017
C         -1.67220       -0.31225        1.14012
H         -0.77814       -2.34403        1.35017
C         -2.00114        0.46243        0.00000
H         -2.41593        1.45860        0.00000
C          1.97335       -0.07513        2.54775
F          3.27654        0.10341        2.81366
F          1.28985        0.65992        3.42507
F          1.70561       -1.36530        2.78489
H          2.41593       -1.45860        0.00000
C          1.97335       -0.07513       -2.54775
F          1.70561       -1.36530       -2.78489
F          1.28985        0.65992       -3.42507
F          3.27654        0.10341       -2.81366
C         -1.97335        0.07513        2.54775
F         -1.28985       -0.65992        3.42507
F         -1.70561        1.36530        2.78489
F         -3.27654       -0.10341        2.81366
C         -1.97335        0.07513       -2.54775
F         -1.70561        1.36530       -2.78489
F         -1.28985       -0.65992       -3.42507
F         -3.27654       -0.10341       -2.81366


27
Energy: -1458355.4999544
Fe         0.75483       -0.18118        0.00000
C         -0.91799       -0.27776        1.14142
C         -1.15286        0.53394        0.00000
C         -0.55941       -1.58512        0.70684
C         -0.91799       -0.27776       -1.14142
C         -0.55941       -1.58512       -0.70684
H         -0.30224       -2.41361        1.34801
H         -0.30224       -2.41361       -1.34801
C          2.24190        0.63271       -1.14853
C          2.01250        1.43524        0.00000
C          2.61399       -0.66519       -0.71017
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H          2.11761        0.94368       -2.17468
C          2.24190        0.63271        1.14853
H          1.68718        2.46429        0.00000
C          2.61399       -0.66519        0.71017
H          2.82831       -1.51063       -1.34598
H          2.11761        0.94368        2.17468
H          2.82831       -1.51063        1.34598
C         -1.08258        0.15094        2.55525
F         -2.33351       -0.06485        2.99163
F         -0.26610       -0.51842        3.38050
F         -0.83811        1.45822        2.71546
H         -1.42981        1.57621        0.00000
C         -1.08258        0.15094       -2.55525
F         -0.83811        1.45822       -2.71546
F         -0.26610       -0.51842       -3.38050
F         -2.33351       -0.06485       -2.99163


33
Energy: -1881143.4064911
Fe         0.00000        0.00000        0.40707
C          0.34659        1.95374        0.84317
C          0.00000        1.81989       -0.52670
C         -0.73094        1.46839        1.63603
C         -1.29272        1.23508       -0.57293
C         -1.74488        1.02245        0.75864
H         -0.74884        1.41650        2.71343
H         -2.67981        0.56358        1.04113
C          1.29272       -1.23508       -0.57293
C          1.74488       -1.02245        0.75864
C          0.00000       -1.81989       -0.52670
C          0.73094       -1.46839        1.63603
H          2.67981       -0.56358        1.04113
C         -0.34659       -1.95374        0.84317
H         -0.61629       -2.08114       -1.37287
H          0.74884       -1.41650        2.71343
C          1.60032        2.56041        1.37145
F          1.44975        3.87521        1.58082
F          1.95594        2.01797        2.54471
F          2.62449        2.41113        0.52686
H          0.61629        2.08114       -1.37287
C         -2.08436        0.97088       -1.80806
F         -1.29994        0.76038       -2.86800
F         -2.88323       -0.09316       -1.67006
F         -2.87222        2.01578       -2.10136
C          2.08436       -0.97088       -1.80806
F          2.87222       -2.01578       -2.10136
F          1.29994       -0.76038       -2.86800
F          2.88323        0.09316       -1.67006
C         -1.60032       -2.56041        1.37145
F         -2.62449       -2.41113        0.52686
F         -1.44975       -3.87521        1.58082
F         -1.95594       -2.01797        2.54471


39
Energy: -2303919.2758022
Fe         0.00000        0.00000        0.27210
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```
C          0.36021        1.72476        1.31794
C          1.52227        0.91405        1.27908
C          0.00000        2.02711       -0.01943
H         -0.17945        2.02997        2.20072
C          1.89861        0.72585       -0.07370
C          0.96067        1.41107       -0.88208
C         -1.52227       -0.91405        1.27908
C         -1.89861       -0.72585       -0.07370
C         -0.36021       -1.72476        1.31794
C         -0.96067       -1.41107       -0.88208
H         -2.73147       -0.14272       -0.43386
C          0.00000       -2.02711       -0.01943
H          0.17945       -2.02997        2.20072
C          1.13065        1.59423       -2.36024
F          1.71954        2.77247       -2.60372
F          1.91767        0.64573       -2.86894
F         -0.02191        1.58149       -3.02372
C         -1.13804        2.93194       -0.39481
F         -0.68531        4.02086       -1.02190
F         -2.03109        2.35218       -1.19960
F         -1.78909        3.33548        0.69948
H          2.73147        0.14272       -0.43386
C          2.28150        0.41196        2.46278
F          2.90457       -0.73920        2.19429
F          3.21723        1.29419        2.83129
F          1.48603        0.21349        3.51709
C         -1.13065       -1.59423       -2.36024
F         -1.71954       -2.77247       -2.60372
F         -1.91767       -0.64573       -2.86894
F          0.02191       -1.58149       -3.02372
C          1.13804       -2.93194       -0.39481
F          0.68531       -4.02086       -1.02190
F          2.03109       -2.35218       -1.19960
F          1.78909       -3.33548        0.69948
C         -2.28150       -0.41196        2.46278
F         -1.48603       -0.21349        3.51709
F         -2.90457        0.73920        2.19429
F         -3.21723       -1.29419        2.83129


39
Energy: -2303916.1797646
Fe         0.00000        0.00000        0.12008
C          1.26605        1.24624       -0.92719
C          1.08965        1.73653        0.38810
C          1.80889       -0.05938       -0.83459
H          1.00974        1.76157       -1.83916
C          1.52411        0.74675        1.30238
C          1.97785       -0.36485        0.55281
C         -1.80889        0.05938       -0.83459
C         -1.26605       -1.24624       -0.92719
C         -1.97785        0.36485        0.55281
C         -1.08965       -1.73653        0.38810
H         -1.00974       -1.76157       -1.83916
C         -1.52411       -0.74675        1.30238
H         -1.51764       -0.82050        2.37869
C          2.71895       -1.50823        1.17667
F          4.03144       -1.23906        1.17918
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```
F          2.34903       -1.67652        2.44884
F          2.55230       -2.65982        0.53629
C          2.22268       -0.87093       -2.02764
F          3.54916       -1.02615       -2.05118
F          1.67814       -2.08766       -2.05925
F          1.86726       -0.24640       -3.15523
H          1.51764        0.82050        2.37869
C          0.72605        3.14027        0.75086
F          0.05971        3.20384        1.90433
F          1.84519        3.86456        0.90343
F          0.00000        3.73175       -0.19406
C         -2.22268        0.87093       -2.02764
F         -3.54916        1.02615       -2.05118
F         -1.67814        2.08766       -2.05925
F         -1.86726        0.24640       -3.15523
C         -2.71895        1.50823        1.17667
F         -2.55230        2.65982        0.53629
F         -4.03144        1.23906        1.17918
F         -2.34903        1.67652        2.44884
C         -0.72605       -3.14027        0.75086
F          0.00000       -3.73175       -0.19406
F         -0.05971       -3.20384        1.90433
F         -1.84519       -3.86456        0.90343


30
Energy: -1669746.3088512
Fe        -0.41686        0.81342       -0.02003
C         -0.55762       -0.84135        1.16846
C         -1.37367       -0.98130        0.01782
C          0.77702       -0.64389        0.72930
H         -0.88895       -0.84956        2.19455
C         -0.55388       -0.89583       -1.13571
C          0.78009       -0.67883       -0.70384
C         -0.99697        2.41650        1.11466
C          0.31853        2.61658        0.61846
C         -1.86547        2.26039        0.00274
H         -1.28096        2.35861        2.15431
C          0.26198        2.58537       -0.79889
H          1.21151        2.73277        1.21352
C         -1.08756        2.36458       -1.18023
H         -2.92471        2.05785        0.04930
H          1.10527        2.67179       -1.46643
H         -1.45335        2.26093       -2.19036
C          1.94869       -0.61619       -1.63734
F          2.75977       -1.66599       -1.45793
F          1.53103       -0.64683       -2.90960
F          2.69571        0.48216       -1.49717
C          1.93542       -0.53888        1.66614
F          2.52712       -1.72904        1.83298
F          2.87548        0.31109        1.24906
F          1.53081       -0.12920        2.87629
H         -0.88160       -0.95652       -2.16094
C         -2.84018       -1.23640        0.02070
F         -3.43599       -0.73450       -1.06810
F         -3.10578       -2.55009        0.03962
F         -3.43674       -0.70309        1.09409
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39
Energy: -2303911.4531248
Fe          0.00000         0.00000         0.35074
C          -1.14835         1.66963         0.75905
C           0.00000         1.66392         1.58379
C          -0.71491         1.69525        -0.58979
H          -2.17488         1.66144         1.09032
C           1.14835         1.66963         0.75905
C           0.71491         1.69525        -0.58979
C          -1.14835        -1.66963         0.75905
C          -0.71491        -1.69525        -0.58979
C           0.00000        -1.66392         1.58379
H          -2.17488        -1.66144         1.09032
C           0.71491        -1.69525        -0.58979
C           1.14835        -1.66963         0.75905
H           2.17488        -1.66144         1.09032
C           1.67302         1.94588        -1.71793
F           1.75274         3.26549        -1.94167
F           2.89917         1.52596        -1.38834
F           1.33506         1.36968        -2.86148
C          -1.67302         1.94588        -1.71793
F          -1.75274         3.26549        -1.94167
F          -1.33506         1.36968        -2.86148
F          -2.89917         1.52596        -1.38834
H           2.17488         1.66144         1.09032
C           0.00000         1.88951         3.06072
F           1.08269         1.38358         3.64947
F           0.00000         3.20873         3.30368
F          -1.08269         1.38358         3.64947
C          -1.67302        -1.94588        -1.71793
F          -2.89917        -1.52596        -1.38834
F          -1.33506        -1.36968        -2.86148
F          -1.75274        -3.26549        -1.94167
C           1.67302        -1.94588        -1.71793
F           1.75274        -3.26549        -1.94167
F           1.33506        -1.36968        -2.86148
F           2.89917        -1.52596        -1.38834
C           0.00000        -1.88951         3.06072
F           1.08269        -1.38358         3.64947
F          -1.08269        -1.38358         3.64947
F           0.00000        -3.20873         3.30368


39
Energy: -2303916.1797646
Fe          0.00000         0.00000         0.12008
C           1.52411         0.74675         1.30238
C           1.97785        -0.36485         0.55281
C           1.08965         1.73653         0.38810
C           1.80889        -0.05938        -0.83459
C           1.26605         1.24624        -0.92719
H           1.00974         1.76157        -1.83916
C          -1.26605        -1.24624        -0.92719
C          -1.08965        -1.73653         0.38810
C          -1.80889         0.05938        -0.83459
H          -1.00974        -1.76157        -1.83916
C          -1.52411        -0.74675         1.30238
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C -1.97785 0.36485 0.55281
H -1.51764 -0.82050 2.37869
C 2.71895 -1.50823 1.17667
F 4.03144 -1.23906 1.17918
F 2.34903 -1.67652 2.44884
F 2.55230 -2.65982 0.53629
C 2.22268 -0.87093 -2.02764
F 3.54916 -1.02615 -2.05118
F 1.67814 -2.08766 -2.05925
F 1.86727 -0.24639 -3.15523
H 1.51764 0.82050 2.37869
C -2.22268 0.87093 -2.02764
F -1.67814 2.08766 -2.05925
F -1.86727 0.24639 -3.15523
F -3.54916 1.02615 -2.05118
C -2.71895 1.50823 1.17667
F -2.55230 2.65982 0.53629
F -4.03144 1.23906 1.17918
F -2.34903 1.67652 2.44884
C 0.72605 3.14027 0.75086
F 0.00000 3.73175 -0.19406
F 0.05971 3.20384 1.90433
F 1.84519 3.86456 0.90343
C -0.72605 -3.14027 0.75086
F 0.00000 -3.73175 -0.19406
F -0.05971 -3.20384 1.90433
F -1.84519 -3.86456 0.90343

39
Energy: -2303912.6241077
Fe 0.00000 0.00000 0.00000
C -1.70377 0.23182 1.14739
C -1.22032 1.49161 0.71659
C -2.00589 -0.53650 0.00000
C -1.22032 1.49161 -0.71659
C -1.70377 0.23182 -1.14739
H -1.80808 -0.08465 -2.17369
C 2.00589 0.53650 0.00000
C 1.70377 -0.23182 1.14739
C 1.70377 -0.23182 -1.14739
C 1.22032 -1.49161 0.71659
H 1.80808 0.08465 2.17369
C 1.22032 -1.49161 -0.71659
H 1.80808 0.08465 -2.17369
C -0.98403 2.60267 1.69738
F -2.13040 3.26442 1.90638
F -0.59628 2.10220 2.87820
F -0.07795 3.48971 1.31541
C -0.98403 2.60267 -1.69738
F -2.13040 3.26442 -1.90638
F -0.07795 3.48971 -1.31541
F -0.59628 2.10220 -2.87820
H -1.80808 -0.08465 2.17369
C -2.75964 -1.82719 0.00000
F -2.50663 -2.55987 1.08233
F -4.07622 -1.56570 0.00000
F -2.50663 -2.55987 -1.08233

```
C          0.98403       -2.60267       -1.69738
F          2.13040       -3.26442       -1.90638
F          0.07795       -3.48971       -1.31541
F          0.59628       -2.10220       -2.87820
C          0.98403       -2.60267        1.69738
F          0.07795       -3.48971        1.31541
F          2.13040       -3.26442        1.90638
F          0.59628       -2.10220        2.87820
C          2.75964        1.82719        0.00000
F          2.50663        2.55987        1.08233
F          4.07622        1.56570        0.00000
F          2.50663        2.55987       -1.08233


30
Energy: -1669746.2920403
Fe        -0.81385        0.41425        0.00000
C          0.86840        0.55647        1.15217
C          0.66205       -0.77834        0.71705
C          0.98003        1.37453        0.00000
C          0.66205       -0.77834       -0.71705
C          0.86840        0.55647       -1.15217
H          0.90179        0.88590       -2.17817
C         -2.59952       -0.29972        0.70942
C         -2.39296        1.03470        1.14864
C         -2.59952       -0.29972       -0.70942
H         -2.69798       -1.16912        1.34117
C         -2.26508        1.85901        0.00000
H         -2.31336        1.36021        2.17462
C         -2.39296        1.03470       -1.14864
H         -2.69798       -1.16912       -1.34117
H         -2.06558        2.91985        0.00000
H         -2.31336        1.36021       -2.17462
C          0.57988       -1.93877        1.65654
F          1.71934       -2.64250        1.64889
F          0.38618       -1.51283        2.91196
F         -0.40710       -2.79083        1.37106
C          0.57988       -1.93877       -1.65654
F          1.71934       -2.64250       -1.64889
F         -0.40710       -2.79083       -1.37106
F          0.38618       -1.51283       -2.91196
H          0.90179        0.88590        2.17817
C          1.23282        2.84146        0.00000
F          0.71422        3.43680        1.08119
F          2.54625        3.10909        0.00000
F          0.71422        3.43680       -1.08119


39
Energy: -2303919.2758022
Fe         0.00000        0.00000        0.27213
C         -0.36022        1.72478        1.31794
C          0.00000        2.02710       -0.01945
C         -1.52227        0.91407        1.27909
C         -0.96067        1.41104       -0.88208
C         -1.89861        0.72584       -0.07369
H         -2.73146        0.14270       -0.43384
C          0.96067       -1.41104       -0.88208
```

```
C          1.89861       -0.72584       -0.07369
C          0.00000       -2.02710       -0.01945
C          1.52227       -0.91407        1.27909
H          2.73146       -0.14270       -0.43384
C          0.36022       -1.72478        1.31794
H         -0.17944       -2.03001        2.20071
C          1.13803        2.93193       -0.39483
F          0.68528        4.02091       -1.02180
F          1.78916        3.33538        0.69946
F          2.03102        2.35222       -1.19971
C         -1.13068        1.59418       -2.36025
F         -1.71954        2.77243       -2.60373
F          0.02187        1.58141       -3.02375
F         -1.91772        0.64570       -2.86891
H          0.17944        2.03001        2.20071
C         -2.28150        0.41198        2.46280
F         -1.48603        0.21348        3.51709
F         -3.21720        1.29424        2.83133
F         -2.90461       -0.73915        2.19429
C          1.13068       -1.59418       -2.36025
F          1.71954       -2.77243       -2.60373
F         -0.02187       -1.58141       -3.02375
F          1.91772       -0.64570       -2.86891
C         -1.13803       -2.93193       -0.39483
F         -2.03102       -2.35222       -1.19971
F         -0.68528       -4.02091       -1.02180
F         -1.78916       -3.33538        0.69946
C          2.28150       -0.41198        2.46280
F          2.90461        0.73915        2.19429
F          1.48603       -0.21348        3.51709
F          3.21720       -1.29424        2.83133


45
Energy: -2726679.7581607
Fe         0.00000        0.00000        0.26260
C          1.08394        1.52047        1.14684
C          1.67471        0.26949        1.42672
C          1.06827        1.70712       -0.25339
H          0.68906        2.20814        1.87634
C          2.03387       -0.33728        0.18712
C          1.66214        0.56052       -0.86164
C         -1.67471       -0.26949        1.42672
C         -2.03387        0.33728        0.18712
C         -1.08394       -1.52047        1.14684
C         -1.66214       -0.56052       -0.86164
C         -1.06827       -1.70712       -0.25339
H         -0.68906       -2.20814        1.87634
C          2.03232        0.39254       -2.32061
F          3.33866        0.12716       -2.41819
F          1.36911       -0.59375       -2.91453
F          1.80390        1.50643       -3.00747
C          2.85845       -1.59367        0.05718
F          2.57712       -2.45795        1.03234
F          2.67005       -2.21290       -1.10035
F          4.15451       -1.28639        0.15153
C          0.66051        3.02725       -0.86046
F          1.75362        3.71787       -1.19964
```

F -0.11115 2.92602 -1.93039
F 0.00000 3.75132 0.04954
C 1.97693 -0.19919 2.82855
F 1.34032 -1.31889 3.17306
F 3.28451 -0.41557 2.97131
F 1.62361 0.74304 3.70478
C -0.66051 -3.02725 -0.86046
F 0.11115 -2.92602 -1.93039
F 0.00000 -3.75132 0.04954
F -1.75362 -3.71787 -1.19964
C -2.03232 -0.39254 -2.32061
F -1.80390 -1.50643 -3.00747
F -3.33866 -0.12716 -2.41819
F -1.36911 0.59375 -2.91453
C -2.85845 1.59367 0.05718
F -2.67005 2.21290 -1.10035
F -4.15451 1.28639 0.15153
F -2.57712 2.45795 1.03234
C -1.97693 0.19919 2.82855
F -1.34032 1.31889 3.17306
F -3.28451 0.41557 2.97131
F -1.62361 -0.74304 3.70478

45
Energy: -1220.6449577
Fe 0.00000 0.00000 0.09486
C 0.13126 1.66593 1.29718
C 1.31944 0.84703 1.42897
C 0.00000 2.03772 -0.07637
H -0.42490 2.11192 2.12899
C 1.92263 0.69691 0.12437
C 1.07987 1.40281 -0.81716
C -1.92263 -0.69691 0.12437
C -1.07987 -1.40281 -0.81716
C -1.31944 -0.84703 1.42897
C 0.00000 -2.03772 -0.07637
C -0.13126 -1.66593 1.29718
H 0.42490 -2.11192 2.12899
C 1.38094 1.70934 -2.25808
F 1.73401 2.97483 -2.46409
F 2.36819 1.01285 -2.79982
F 0.34956 1.50456 -3.06769
C 3.30789 0.16941 -0.13568
F 3.65194 -0.87760 0.60743
F 3.56012 -0.21712 -1.37756
F 4.24350 1.08523 0.12132
C -0.95214 3.07911 -0.58393
F -1.59068 3.73250 0.39898
F -0.37442 4.05442 -1.29559
F -1.92604 2.61501 -1.37006
C 1.97870 0.58767 2.75232
F 2.37882 -0.66928 2.97312
F 3.07646 1.33345 2.93746
F 1.20299 0.87452 3.80853
C 0.95214 -3.07911 -0.58393
F 1.59068 -3.73250 0.39898
F 0.37442 -4.05442 -1.29559

```
F          1.92604       -2.61501       -1.37006
C         -1.38094       -1.70934       -2.25808
F         -0.34956       -1.50456       -3.06769
F         -1.73401       -2.97483       -2.46409
F         -2.36819       -1.01285       -2.79982
C         -3.30789       -0.16941       -0.13568
F         -3.56012        0.21712       -1.37756
F         -4.24350       -1.08523        0.12132
F         -3.65194        0.87760        0.60743
C         -1.97870       -0.58767        2.75232
F         -2.37882        0.66928        2.97312
F         -3.07646       -1.33345        2.93746
F         -1.20299       -0.87452        3.80853


33
Energy: -1881131.1947677
Fe         0.02860       -0.75775        0.75693
C          0.00511       -1.22281       -1.24180
C         -1.15000       -0.48926       -0.88886
C          1.14520       -0.45180       -0.91413
H          0.01608       -2.21498       -1.66150
C         -0.73099        0.76350       -0.34008
C          0.70135        0.79525       -0.36961
C         -0.21379       -2.50175        1.80988
C          1.09962       -1.99724        1.99412
C         -1.12920       -1.51901        2.27035
H         -0.47282       -3.45108        1.36613
C          0.99632       -0.70307        2.56589
H          2.01605       -2.49163        1.70991
C         -0.38138       -0.40730        2.73624
H         -2.20499       -1.58595        2.22955
H          1.81858       -0.04125        2.78896
H         -0.78842        0.51822        3.11402
C          1.55785        1.98618       -0.01963
F          1.05958        3.09561       -0.57343
F          1.65080        2.20476        1.29558
F          2.79882        1.84013       -0.48282
C         -1.63743        1.88146        0.08639
F         -2.81736        1.41973        0.50739
F         -1.11547        2.59890        1.08384
F         -1.87702        2.71719       -0.92799
C          2.53972       -0.94173       -1.17130
F          3.08265       -0.34539       -2.23527
F          3.36512       -0.75787       -0.13835
F          2.51964       -2.25814       -1.42696
C         -2.54025       -0.97755       -1.18402
F         -3.29244       -1.18233       -0.10046
F         -3.19281       -0.11272       -1.96528
F         -2.48162       -2.14442       -1.83934


45
Energy: -2726667.5611211
Fe         0.00000        0.00000        0.40017
C          0.00000        1.62788        1.67046
C          1.14775        1.67522        0.85197
C         -1.14775        1.67522        0.85197
```

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H          0.00000        1.57750        2.74679
C          0.71672        1.73240       -0.50847
C         -0.71672        1.73240       -0.50847
C          0.00000       -1.62788        1.67046
C         -1.14775       -1.67522        0.85197
C          1.14775       -1.67522        0.85197
H          0.00000       -1.57750        2.74679
C         -0.71672       -1.73240       -0.50847
C          0.71672       -1.73240       -0.50847
C         -1.60450        2.04180       -1.69511
F         -1.51375        3.34980       -1.96439
F         -1.27366        1.37878       -2.79263
F         -2.87945        1.77367       -1.43511
C          1.60450        2.04180       -1.69511
F          2.87945        1.77367       -1.43511
F          1.27366        1.37878       -2.79263
F          1.51375        3.34980       -1.96439
C         -2.49803        1.94653        1.47544
F         -2.75605        3.25508        1.36149
F         -3.52118        1.28809        0.96678
F         -2.44654        1.66046        2.78287
C          2.49803        1.94653        1.47544
F          3.52118        1.28809        0.96678
F          2.75605        3.25508        1.36149
F          2.44654        1.66046        2.78287
C          2.49803       -1.94653        1.47544
F          2.75605       -3.25508        1.36149
F          3.52118       -1.28809        0.96678
F          2.44654       -1.66046        2.78287
C          1.60450       -2.04180       -1.69511
F          2.87945       -1.77367       -1.43511
F          1.51375       -3.34980       -1.96439
F          1.27366       -1.37878       -2.79263
C         -1.60450       -2.04180       -1.69511
F         -1.27366       -1.37878       -2.79263
F         -1.51375       -3.34980       -1.96439
F         -2.87945       -1.77367       -1.43511
C         -2.49803       -1.94653        1.47544
F         -3.52118       -1.28809        0.96678
F         -2.75605       -3.25508        1.36149
F         -2.44654       -1.66046        2.78287


45
Energy: -2726679.7581607
Fe         0.00000        0.00000        0.26260
C         -2.03387        0.33729        0.18712
C         -1.66213       -0.56051       -0.86164
C         -1.67471       -0.26948        1.42672
C         -1.06827       -1.70711       -0.25339
C         -1.08395       -1.52047        1.14684
H         -0.68907       -2.20814        1.87634
C          1.66213        0.56051       -0.86164
C          1.06827        1.70711       -0.25339
C          2.03387       -0.33729        0.18712
C          1.08395        1.52047        1.14684
C          1.67471        0.26948        1.42672
H          0.68907        2.20814        1.87634
```

C -2.85844 1.59368 0.05718
F -4.15451 1.28641 0.15152
F -2.57711 2.45795 1.03234
F -2.67003 2.21292 -1.10034
C -2.03231 -0.39253 -2.32061
F -3.33865 -0.12716 -2.41819
F -1.36911 0.59377 -2.91452
F -1.80388 -1.50641 -3.00748
C -0.66051 -3.02725 -0.86045
F -1.75363 -3.71786 -1.19963
F 0.11115 -2.92603 -1.93039
F 0.00000 -3.75131 0.04955
C -1.97694 0.19920 2.82855
F -1.34032 1.31889 3.17306
F -3.28452 0.41557 2.97130
F -1.62361 -0.74304 3.70478
C 0.66051 3.02725 -0.86045
F -0.11115 2.92603 -1.93039
F 0.00000 3.75131 0.04955
F 1.75363 3.71786 -1.19963
C 2.03231 0.39253 -2.32061
F 1.80388 1.50641 -3.00748
F 3.33865 0.12716 -2.41819
F 1.36911 -0.59377 -2.91452
C 2.85844 -1.59368 0.05718
F 2.67003 -2.21292 -1.10034
F 4.15451 -1.28641 0.15152
F 2.57711 -2.45795 1.03234
C 1.97694 -0.19920 2.82855
F 1.34032 -1.31889 3.17306
F 3.28452 -0.41557 2.97130
F 1.62361 0.74304 3.70478

45
Energy: -2726675.4915732
Fe 0.00000 0.00000 0.00000
C 1.91618 0.19056 0.71609
C 1.91618 0.19056 -0.71609
C 1.14316 1.31266 1.14726
C 1.14316 1.31266 -1.14726
C 0.66533 1.97629 0.00000
H 0.03889 2.85286 0.00000
C -1.14316 -1.31266 -1.14726
C -0.66533 -1.97629 0.00000
C -1.91618 -0.19056 -0.71609
C -1.14316 -1.31266 1.14726
H -0.03889 -2.85286 0.00000
C -1.91618 -0.19056 0.71609
C 2.71677 -0.73032 1.60585
F 4.02101 -0.49820 1.44704
F 2.42419 -0.53566 2.88704
F 2.49946 -2.01757 1.33569
C 2.71677 -0.73032 -1.60585
F 4.02101 -0.49820 -1.44704
F 2.49946 -2.01757 -1.33569
F 2.42419 -0.53566 -2.88704
C 1.02414 1.95425 -2.51215

```
F          2.24193        2.30622       -2.93636
F          0.46422        1.20494       -3.44610
F          0.29781        3.07273       -2.41173
C          1.02414        1.95425        2.51215
F          0.46422        1.20494        3.44610
F          2.24193        2.30622        2.93636
F          0.29781        3.07273        2.41173
C         -1.02414       -1.95425       -2.51215
F         -0.46422       -1.20494       -3.44610
F         -0.29781       -3.07273       -2.41173
F         -2.24193       -2.30622       -2.93636
C         -2.71677        0.73032       -1.60585
F         -2.42419        0.53566       -2.88704
F         -4.02101        0.49820       -1.44704
F         -2.49946        2.01757       -1.33569
C         -2.71677        0.73032        1.60585
F         -2.49946        2.01757        1.33569
F         -4.02101        0.49820        1.44704
F         -2.42419        0.53566        2.88704
C         -1.02414       -1.95425        2.51215
F         -0.46422       -1.20494        3.44610
F         -2.24193       -2.30622        2.93636
F         -0.29781       -3.07273        2.41173


33
Energy: -1881130.0955657
Fe         0.73917        0.76650        0.00000
C         -0.78246       -0.35997        0.71804
C         -0.78246       -0.35997       -0.71804
C          0.47274       -0.89810        1.14798
C          0.47274       -0.89810       -1.14798
C          1.22586       -1.23081        0.00000
H          2.22330       -1.63717        0.00000
C          1.04494        2.44040       -1.14783
C          0.27778        2.76649        0.00000
C          2.28833        1.91431       -0.70925
H          0.72363        2.53281       -2.17399
C          1.04494        2.44040        1.14783
H         -0.73297        3.14423        0.00000
C          2.28833        1.91431        0.70925
H          3.07724        1.54162       -1.34501
H          0.72363        2.53281        2.17399
H          3.07724        1.54162        1.34501
C         -1.94104        0.01073        1.60423
F         -2.93696       -0.87059        1.46474
F         -1.59112        0.01429        2.89006
F         -2.43989        1.21857        1.33133
C         -1.94104        0.01073       -1.60423
F         -2.93696       -0.87059       -1.46474
F         -2.43989        1.21857       -1.33133
F         -1.59112        0.01429       -2.89006
C          0.98634       -1.16574       -2.53499
F          0.24536       -2.08347       -3.16002
F          1.03292       -0.08273       -3.31357
F          2.23643       -1.64599       -2.46797
C          0.98634       -1.16574        2.53499
F          1.03292       -0.08273        3.31357
```

```
F          0.24536       -2.08347        3.16002
F          2.23643       -1.64599        2.46797


45
Energy: -2726679.7581607
Fe         0.00000        0.00000        0.26260
C          1.66214       -0.56051       -0.86164
C          2.03387        0.33729        0.18713
C          1.06828       -1.70711       -0.25339
C          1.67471       -0.26949        1.42672
C          1.08394       -1.52047        1.14684
H          0.68906       -2.20815        1.87633
C         -1.06828        1.70711       -0.25339
C         -1.66214        0.56051       -0.86164
C         -1.08394        1.52047        1.14684
C         -2.03387       -0.33729        0.18713
C         -1.67471        0.26949        1.42672
H         -0.68906        2.20815        1.87633
C          2.03234       -0.39253       -2.32061
F          3.33867       -0.12713       -2.41818
F          1.80394       -1.50643       -3.00747
F          1.36912        0.59374       -2.91454
C          2.85844        1.59368        0.05719
F          4.15451        1.28641        0.15152
F          2.67003        2.21292       -1.10033
F          2.57711        2.45795        1.03235
C          1.97693        0.19918        2.82856
F          3.28450        0.41555        2.97132
F          1.34032        1.31888        3.17307
F          1.62359       -0.74306        3.70478
C          0.66051       -3.02725       -0.86047
F         -0.11113       -2.92601       -1.93041
F          1.75364       -3.71786       -1.19965
F          0.00000       -3.75132        0.04952
C         -1.97693       -0.19918        2.82856
F         -3.28450       -0.41555        2.97132
F         -1.34032       -1.31888        3.17307
F         -1.62359        0.74306        3.70478
C         -2.85844       -1.59368        0.05719
F         -2.57711       -2.45795        1.03235
F         -4.15451       -1.28641        0.15152
F         -2.67003       -2.21292       -1.10033
C         -2.03234        0.39253       -2.32061
F         -1.36912       -0.59374       -2.91454
F         -3.33867        0.12713       -2.41818
F         -1.80394        1.50643       -3.00747
C         -0.66051        3.02725       -0.86047
F          0.11113        2.92601       -1.93041
F         -1.75364        3.71786       -1.19965
F          0.00000        3.75132        0.04952


51
Energy: -1282013.9427275
Fe         0.00000        0.00000        0.00000
C         -1.16678        1.18055       -1.20107
C         -0.85137        1.87102       -0.00000
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C	-1.78998	-0.07180	-1.17429
H	-0.76709	1.56642	-2.13443
C	-1.16678	1.18055	1.20107
C	-1.78998	-0.07179	1.17429
H	-0.76709	1.56643	2.13443
C	-2.67395	-0.40999	0.00000
H	-2.82438	-1.49714	0.00000
C	0.85137	-1.87102	-0.00000
C	1.16678	-1.18055	-1.20107
C	1.16678	-1.18055	1.20106
C	1.78998	0.07180	-1.17429
H	0.76709	-1.56642	-2.13444
C	1.78998	0.07179	1.17429
H	0.76709	-1.56643	2.13443
C	2.67395	0.40999	0.00000
H	2.82438	1.49714	0.00000
C	4.04857	-0.26244	0.00000
H	4.62876	0.02230	0.88249
H	3.94025	-1.34956	0.00000
H	4.62876	0.02230	-0.88249
C	-4.04857	0.26244	0.00000
H	-4.62876	-0.02231	-0.88249
H	-4.62876	-0.02230	0.88249
H	-3.94025	1.34956	-0.00000
C	-0.21025	3.22046	-0.00000
H	0.41427	3.36401	0.88466
H	0.41428	3.36401	-0.88466
H	-0.96372	4.01559	-0.00001
C	-1.98031	-0.84465	2.44237
H	-1.28218	-0.53107	3.22186
H	-2.99587	-0.70940	2.83484
H	-1.84735	-1.91863	2.28148
C	-1.98031	-0.84465	-2.44237
H	-2.99586	-0.70939	-2.83485
H	-1.28216	-0.53108	-3.22185
H	-1.84737	-1.91863	-2.28147
C	1.98031	0.84465	-2.44237
H	2.99587	0.70940	-2.83483
H	1.28218	0.53107	-3.22186
H	1.84735	1.91863	-2.28147
C	1.98031	0.84464	2.44237
H	1.28216	0.53108	3.22186
H	2.99586	0.70938	2.83485
H	1.84737	1.91863	2.28148
C	0.21025	-3.22046	-0.00001
H	-0.41427	-3.36401	-0.88467
H	0.96372	-4.01559	0.00000
H	-0.41428	-3.36401	0.88465