On the Performance of Ligand Field Molecular Mechanics for Peroxide-Bridged Fully-Oxidized Type 3 Copper Centres

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Supporting Information:
Optimized DFT and LFMM coordinates in XYZ format for compounds I, II, III and IV.

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90
Compound Ia (DFT)
C   -2.8500 -0.4040  2.9820
N   -3.1610 -0.1710  1.6740
C   -4.4190  0.1830  1.2930
C   -5.4230  0.3380  2.2680
C   -5.1250  0.1190  3.6180
C   -3.8310 -0.2600  3.9790
Cu  -1.8570 -0.3140  0.1940
N   -3.1940 -1.4790 -0.8660
C   -4.4160 -0.9100 -1.0170
C   -5.3800 -1.5120 -1.8470
C   -5.0740 -2.7150 -2.4990
C   -3.8300 -3.3120 -2.2840
C   -2.8960 -2.6750 -1.4460
C   -4.7230  0.4020 -0.2230
C   -6.2200  0.7420 -0.3870
C   -1.5760 -3.3140 -1.1210
C   -1.4500 -0.8210  3.3330
O    0.1360 -0.6820  0.7460
O   -0.1120 -0.5180 -0.6640
Cu   1.8750 -0.4510 -0.1380
N    3.1330 -0.2950 -1.6610
C    4.3640  0.1920 -1.3440
C    5.3140  0.3940 -2.3640
C    4.9930  0.0830 -3.6910
C    3.7310 -0.4390 -3.9830
C    2.8040 -0.6260 -2.9430
C    4.7010  0.5090  0.1470
C    4.4810 -0.7650  1.0240
N    3.2850 -1.4060  0.9500
C    3.0650 -2.5780  1.6110
C    4.0550 -3.1070  2.4610
C    5.2710 -2.4360  2.5980
C    5.4950 -1.2660  1.8600
C    1.7860 -3.3260  1.3620
C    1.4440 -1.2010 -3.2170
N    2.4590  1.5640  0.5340
C    1.6410  2.5760  0.9280
C    2.1630  3.7530  1.4980
C    3.5450  3.8810  1.6570
C    4.3760  2.8400  1.2260
C    3.8020  1.6840  0.6590
C    0.1510  2.4480  0.7100
C   -0.2420  2.5390 -0.7850
C   -1.7350  2.5770 -1.0240
N   -2.5190  1.5450 -0.6070
C   -3.8650  1.5880 -0.7730
C   -4.4740  2.6850 -1.4140
C   -3.6820  3.7450 -1.8700
C   -2.3020  3.6970 -1.6620
C    6.1840  0.9270  0.2440
H   -0.3590  3.2530  1.2750
H   -0.1890  1.4770  1.1210
H    0.1980  3.4540 -1.2260
H    0.1940  1.6710 -1.3170
H    1.4820  4.5570  1.8100
H    3.9790  4.7870  2.1060
H    5.4600  2.9460  1.3400
H    6.3820  1.8360 -0.3520
H    6.4720  1.1530  1.2850
H    6.8500  0.1230 -0.1190
H    6.4610 -0.7590  1.9480
H    6.0560 -2.8280  3.2620
H    3.8620 -4.0470  2.9970
H    1.5650 -4.0230  2.1910
H    0.9360 -2.6330  1.2150
H    1.8890 -3.9360  0.4380
H    6.3090  0.7900 -2.1390
H    5.7340  0.2400 -4.4890
H    3.4530 -0.7120 -5.0110
H    1.2330 -2.0530 -2.5410
H    0.6500 -0.4480 -3.0420
H    1.3680 -1.5500 -4.2620
H   -1.6530  4.5220 -1.9880
H   -4.1460  4.6070 -2.3740
H   -5.5570  2.7290 -1.5640
H   -6.8580 -0.0770 -0.0090
H   -6.4840  1.6660  0.1580
H   -6.4820  0.9010 -1.4480
H   -6.3660 -1.0620 -1.9970
H   -5.8180 -3.1890 -3.1560
H   -3.5740 -4.2730 -2.7510
H   -1.3550 -4.1500 -1.8100
H   -0.7610 -2.5660 -1.1580
H   -1.6030 -3.7270 -0.0900
H   -6.4420  0.6240  1.9890
H   -5.9080  0.2390  4.3820
H   -3.5670 -0.4500  5.0290
H   -1.1450 -1.7100  2.7460
H   -0.7240 -0.0180  3.0970
H   -1.3700 -1.0600  4.4080

90
Compound Ia (LFMM)
Cu   19.708  19.917  12.174
Cu   16.516  18.559  11.613
O    17.772  19.937  12.130
O    18.309  18.607  12.329
N    20.460  19.684  10.079
N    20.418  21.749  12.299
N    21.502  19.292  12.759
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N    16.310  16.840  10.620
N    15.246  17.902  13.238
N    14.822  19.213  10.777
C    18.520  18.395  9.2240
C    18.656  16.993  9.8200
C    19.858  19.059  9.0160
C    20.413  18.983  7.7390
C    21.640  19.573  7.5170
C    22.287  20.208  8.5660
C    21.689  20.243  9.8340
C    22.435  20.908  11.057
C    23.831  21.464  10.633
C    21.550  22.089  11.621
C    21.905  23.431  11.445
C    21.130  24.432  12.022
C    20.030  24.091  12.788
C    19.723  22.745  12.924
C    18.559  22.347  13.785
C    22.632  19.788  12.171
C    23.900  19.314  12.528
C    24.018  18.334  13.508
C    22.885  17.849  14.135
C    21.655  18.365  13.750
C    20.412  17.884  14.439
C    17.331  16.264  9.9110
C    17.217  15.035  9.2690
C    16.004  14.376  9.3210
C    14.936  14.957  9.9930
C    15.105  16.195  10.626
C    13.909  16.915  11.360
C    12.587  16.108  11.168
C    14.246  17.040  12.898
C    13.547  16.316  13.870
C    13.835  16.520  15.215
C    14.789  17.452  15.577
C    15.451  18.138  14.567
C    16.465  19.177  14.938
C    13.731  18.381  10.751
C    12.504  18.806  10.227
C    12.380  20.094  9.7190
C    13.469  20.944  9.7370
C    14.665  20.472  10.263
C    15.843  21.402  10.317
H    17.986  18.334  8.2650
H    17.905  19.048  9.8340
H    19.344  16.415  9.1880
H    19.129  17.004  10.806
H    19.903  18.473  6.9280
H    22.098  19.535  6.5340
H    23.254  20.648  8.3550
H    24.489  20.681  10.237
H    23.761  22.217  9.8390
H    24.352  21.933  11.478
H    22.775  23.744  10.880
H    21.402  25.475  11.893
H    19.438  24.861  13.271
H    18.483  23.002  14.659
H    17.629  22.415  13.215
H    18.688  21.329  14.161
H    24.817  19.673  12.077
H    24.998  17.959  13.787
H    22.969  17.097  14.912
H    19.722  18.719  14.581
H    19.934  17.100  13.846
H    20.637  17.481  15.432
H    18.048  14.593  8.7280
H    15.880  13.417  8.8270
H    13.997  14.417  9.9890
H    11.745  16.569  11.699
H    12.306  16.028  10.110
H    12.662  15.081  11.547
H    12.771  15.600  13.629
H    13.295  15.965  15.977
H    14.999  17.640  16.625
H    16.282  19.571  15.944
H    17.466  18.745  14.915
H    16.403  20.024  14.251
H    11.622  18.178  10.196
H    11.430  20.431  9.3140
H    13.376  21.953  9.3490
H    16.008  21.728  11.347
H    16.737  20.910  9.9310
H    15.680  22.293  9.7020

84
Compound Ib (DFT)
Cu  -1.8640  0.4100 -0.1430
Cu   1.8650  0.4120  0.1410
O   -0.1000  0.5560  0.7130
O    0.1010  0.5570 -0.7150
N   -3.1480  0.3090 -1.6680
N   -3.2360  1.3700  1.0420
N   -2.4700 -1.6260  0.5330
N    2.4690 -1.6270 -0.5300
N    3.1480  0.3130  1.6680
N    3.2370  1.3670 -1.0440
C   -1.5180  1.1570 -3.3120
C   -2.8820  0.6320 -2.9670
C   -3.8780  0.4770 -3.9490
C   -5.1440 -0.0020 -3.5940
C   -5.3990 -0.3150 -2.2530
C   -4.3760 -0.1470 -1.3070
C   -4.6250 -0.4760  0.1640
C   -1.7300  3.2350  1.6110
C   -3.0310  2.5020  1.7710
C   -4.0530  2.9970  2.6060
C   -5.2870  2.3410  2.6670
C   -5.4910  1.2020  1.8750
C   -4.4390  0.7440  1.0660
C   -3.8160 -1.6910  0.6340
C   -4.4800 -2.8180  1.1480
C   -3.7150 -3.9130  1.5680
C   -2.3220 -3.8490  1.4450
C   -1.7160 -2.6890  0.9200
C   -0.2170 -2.6230  0.7470
C    0.2160 -2.6230 -0.7430
C    1.7150 -2.6900 -0.9160
C    2.3210 -3.8510 -1.4380
C    3.7140 -3.9170 -1.5610
C    4.4790 -2.8210 -1.1430
C    3.8150 -1.6930 -0.6310
C    4.6250 -0.4780 -0.1630
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C    1.5180  1.1650  3.3090
C    2.8810  0.6380  2.9650
C    3.8770  0.4840  3.9480
C    5.1430  0.0030  3.5950
C    5.3980 -0.3130  2.2540
C    4.3750 -0.1450  1.3080
C    1.7320  3.2320 -1.6180
C    3.0330  2.4990 -1.7750
C    4.0550  2.9920 -2.6110
C    5.2890  2.3340 -2.6710
C    5.4920  1.1970 -1.8760
C    4.4400  0.7410 -1.0670
H   -0.7400  0.3890 -3.1260
H   -1.4670  1.4590 -4.3730
H   -1.2650  2.0320 -2.6810
H   -3.6500  0.7430 -4.9910
H   -5.9290 -0.1240 -4.3550
H   -6.3850 -0.6850 -1.9360
H   -5.6890 -0.7620  0.2430
H   -1.8010  3.9370  0.7520
H   -1.4990  3.8410  2.5070
H   -0.9010  2.5310  1.4060
H   -3.8720  3.9080  3.1950
H   -6.0900  2.7200  3.3160
H   -6.4550  0.6740  1.8810
H   -5.5770 -2.8340  1.2180
H   -4.2010 -4.8110  1.9790
H   -1.6930 -4.6960  1.7530
H    0.2390 -3.4880  1.2660
H    0.1630 -1.6990  1.2270
H   -0.2410 -3.4880 -1.2620
H   -0.1640 -1.6990 -1.2230
H    1.6920 -4.6990 -1.7460
H    4.1990 -4.8150 -1.9710
H    5.5760 -2.8380 -1.2120
H    5.6890 -0.7640 -0.2400
H    0.7390  0.3980  3.1250
H    1.4670  1.4700  4.3700
H    1.2660  2.0400  2.6770
H    3.6480  0.7520  4.9900
H    5.9270 -0.1190  4.3570
H    6.3830 -0.6840  1.9390
H    1.5010  3.8360 -2.5150
H    1.8040  3.9370 -0.7600
H    0.9030  2.5290 -1.4100
H    3.8750  3.9010 -3.2020
H    6.0930  2.7110 -3.3210
H    6.4560  0.6680 -1.8810

84
Compound Ib (LFMM)
Cu  -0.2501 -1.2391  0.6430
Cu  -0.8675  1.3511 -1.7553
O   -1.1560  0.2471 -0.1920
O    0.0432 -0.1298 -0.9158
N    1.1230 -2.6902  0.7864
N   -1.4856 -2.3545  1.7810
N    0.5484 -0.2509  2.4871
N    0.5552  3.0201 -1.3035
N   -2.3635  2.6557 -2.0237
N   -0.4290  1.5149 -3.7168
C    1.5333 -2.7692 -1.6183
C    1.8603 -3.2230 -0.2279
C    2.8978 -4.1282 -0.0257
C    3.1710 -4.5432  1.2697
C    2.4070 -4.0572  2.3217
C    1.3895 -3.1452  2.0431
C    0.5221 -2.6153  3.1779
C   -3.3556 -2.1865  0.2114
C   -2.7870 -2.6530  1.5179
C   -3.6023 -3.3552  2.4012
C   -3.0518 -3.8117  3.5904
C   -1.7118 -3.5730  3.8625
C   -0.9605 -2.8566  2.9323
C    0.8104 -1.1540  3.4752
C    1.3218 -0.8068  4.7270
C    1.5849  0.5271  4.9908
C    1.3355  1.4746  4.0113
C    0.8191  1.0544  2.7839
C    0.5786  2.0909  1.7165
C    1.6886  2.0689  0.6686
C    1.5075  3.1768 -0.3370
C    2.2988  4.3205 -0.2130
C    2.1223  5.3562 -1.1161
C    1.1666  5.2334 -2.1110
C    0.4087  4.0625 -2.1711
C   -0.6431  3.9220 -3.2578
C   -4.0130  1.2510 -0.8996
C   -3.6425  2.5400 -1.5684
C   -4.5865  3.5572 -1.6726
C   -4.2225  4.7353 -2.3088
C   -2.9419  4.8680 -2.8274
C   -2.0470  3.8092 -2.6769
C   -0.4375 -0.9032 -4.0920
C   -0.2304  0.4940 -4.5945
C    0.1595  0.6894 -5.9164
C    0.3125  1.9896 -6.3767
C    0.0621  3.0541 -5.5218
C   -0.3183  2.7792 -4.2093
H    2.0538 -1.8326 -1.8371
H    1.8291 -3.5175 -2.3609
H    0.4540 -2.6239 -1.7192
H    3.4815 -4.5141 -0.8552
H    3.9709 -5.2527  1.4584
H    2.6078 -4.3919  3.3344
H    0.7889 -3.1952  4.0731
H   -3.9604 -2.9760 -0.2470
H   -3.9863 -1.3099  0.3771
H   -2.5630 -1.9351 -0.4976
H   -4.6432 -3.5565  2.1691
H   -3.6616 -4.3672  4.2965
H   -1.2711 -3.9485  4.7803
H    1.5163 -1.5555  5.4883
H    1.9858  0.8268  5.9540
H    1.5471  2.5212  4.2071
H    0.5241  3.0869  2.1772
H   -0.4079  1.9383  1.2737
H    2.6649  2.1759  1.1611
H    1.7455  1.1094  0.1501
H    3.0398  4.4125  0.5750
H    2.7247  6.2563 -1.0425
H    1.0208  6.0411 -2.8212
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H   -0.6255  4.8429 -3.8580
H   -3.7231  1.2808  0.1544
H   -5.0903  1.0654 -0.9627
H   -3.5122  0.4154 -1.3968
H   -5.5901  3.4402 -1.2766
H   -4.9389  5.5449 -2.4101
H   -2.6589  5.7821 -3.3395
H    0.5305 -1.3748 -3.9078
H   -0.9865 -1.4983 -4.8295
H   -1.0257 -0.9092 -3.1710
H    0.3312 -0.1491 -6.5836
H    0.6103  2.1734 -7.4045
H    0.1577  4.0726 -5.8839

84
Compound Ic (DFT)
Cu   0.1010 -1.9020  0.3860
Cu  -0.1010  1.9020  0.3860
O    0.7080  0.1150  0.3300
O   -0.7080 -0.1150  0.3300
N   -1.3510 -3.1120  1.1600
N    1.4790 -3.3480  0.6600
N   -0.0160 -2.6180 -1.7380
N    0.0160  2.6180 -1.7380
N   -1.4790  3.3480  0.6600
N    1.3510  3.1120  1.1600
C   -2.0140 -1.5310  2.9270
C   -2.2420 -2.7870  2.1380
C   -3.3030 -3.6620  2.4450
C   -3.4240 -4.8800  1.7680
C   -2.4550 -5.2250  0.8150
C   -1.4210 -4.3170  0.5410
C   -0.3030 -4.6860 -0.4310
C    3.0910 -1.8240  1.7150
C    2.7110 -3.1880  1.2200
C    3.5820 -4.2870  1.3400
C    3.1810 -5.5500  0.8890
C    1.9100 -5.6930  0.3180
C    1.0780 -4.5680  0.2150
C   -0.3400 -3.9290 -1.7640
C   -0.6260 -4.6120 -2.9580
C   -0.5420 -3.9080 -4.1680
C   -0.1440 -2.5680 -4.1400
C    0.1220 -1.9400 -2.9050
C    0.5870 -0.5060 -2.8550
C   -0.5870  0.5060 -2.8550
C   -0.1220  1.9400 -2.9050
C    0.1440  2.5680 -4.1400
C    0.5420  3.9080 -4.1680
C    0.6260  4.6120 -2.9580
C    0.3400  3.9290 -1.7640
C    0.3030  4.6860 -0.4310
C   -3.0910  1.8240  1.7150
C   -2.7110  3.1880  1.2200
C   -3.5820  4.2870  1.3400
C   -3.1810  5.5500  0.8890
C   -1.9100  5.6930  0.3180
C   -1.0780  4.5680  0.2150
C    2.0140  1.5310  2.9270
C    2.2420  2.7870  2.1380
C    3.3030  3.6620  2.4450
C    3.4240  4.8800  1.7680
C    2.4550  5.2250  0.8150
C    1.4210  4.3170  0.5410
H   -1.5800 -0.7370  2.2890
H   -2.9510 -1.1730  3.3920
H   -1.2960 -1.7380  3.7500
H   -4.0200 -3.3830  3.2300
H   -4.2510 -5.5690  1.9970
H   -2.4930 -6.1920  0.2930
H   -0.4470 -5.7540 -0.6750
H    2.4670 -1.5450  2.5890
H    4.1510 -1.7920  2.0260
H    2.9220 -1.0590  0.9320
H    4.5730 -4.1410  1.7930
H    3.8530 -6.4160  0.9800
H    1.5620 -6.6690 -0.0500
H   -0.8940 -5.6780 -2.9420
H   -0.7570 -4.4110 -5.1230
H   -0.0200 -2.0020 -5.0750
H    1.2370 -0.3150 -3.7330
H    1.1920 -0.3500 -1.9410
H   -1.1920  0.3500 -1.9410
H   -1.2370  0.3150 -3.7330
H    0.0200  2.0020 -5.0750
H    0.7570  4.4110 -5.1230
H    0.8940  5.6780 -2.9420
H    0.4470  5.7540 -0.6750
H   -2.4670  1.5450  2.5890
H   -4.1510  1.7920  2.0260
H   -2.9220  1.0590  0.9320
H   -4.5730  4.1410  1.7930
H   -3.8530  6.4160  0.9800
H   -1.5620  6.6690 -0.0500
H    1.2960  1.7380  3.7500
H    2.9510  1.1730  3.3920
H    1.5800  0.7370  2.2890
H    4.0200  3.3830  3.2300
H    4.2510  5.5690  1.9970
H    2.4930  6.1920  0.2930

84
Compound Ic (LFMM)
Cu  -0.0023  0.1466 -2.1534
Cu   0.4568 -0.5334  1.3605
O   -0.0712  0.4502 -0.2359
O    0.3949 -0.8844 -0.5490
N    0.7750 -0.7600 -3.7769
N   -0.2165  1.8039 -3.2955
N   -2.1265 -0.3349 -2.7210
N   -1.4062 -1.5024  2.1703
N    1.4764 -1.8983  2.4534
N    0.6409  0.7226  2.9259
C    2.8671 -1.3900 -2.6727
C    1.9428 -1.4552 -3.8490
C    2.3238 -2.2052 -4.9596
C    1.4973 -2.2077 -6.0727
C    0.3400 -1.4435 -6.0637
C    0.0271 -0.7180 -4.9137
C   -1.1732  0.2095 -4.9193
C    0.8102  3.2577 -1.6348
C    0.1542  3.0714 -2.9670
```

C	-0.0820	4.1756	-3.7809
C	-0.6953	3.9740	-5.0093
C	-1.0546	2.6900	-5.3944
C	-0.7951	1.6354	-4.5200
C	-2.3156	-0.3123	-4.0707
C	-3.5034	-0.6972	-4.6958
C	-4.5699	-1.0955	-3.9073
C	-4.4351	-1.0792	-2.5290
C	-3.2157	-0.6807	-1.9771
C	-3.0871	-0.6413	-0.4789
C	-2.5714	-1.9702	0.0570
C	-2.5351	-1.9641	1.5607
C	-3.6587	-2.4185	2.2545
C	-3.6248	-2.4388	3.6389
C	-2.4747	-2.0303	4.2932
C	-1.3916	-1.5886	3.5306
C	-0.0978	-1.2242	4.2314
C	3.0087	-2.4223	0.6360
C	2.5340	-2.6470	2.0374
C	3.1481	-3.6141	2.8281
C	2.6848	-3.8035	4.1224
C	1.6315	-3.0327	4.5939
C	1.0600	-2.0915	3.7386
C	1.7103	2.5028	1.6299
C	1.0912	2.0067	2.8999
C	1.0187	2.8693	3.9915
C	0.5074	2.3852	5.1858
C	0.1161	1.0573	5.2708
C	0.2203	0.2557	4.1336
H	2.5512	-0.6235	-1.9617
H	2.8955	-2.3624	-2.1773
H	3.8796	-1.1306	-2.9996
H	3.2529	-2.7662	-4.9686
H	1.7696	-2.7780	-6.9554
H	-0.2886	-1.4050	-6.9475
H	-1.5289	0.2642	-5.9581
H	1.4363	2.3928	-1.3990
H	1.4568	4.1410	-1.6270
H	0.0392	3.3749	-0.8687
H	0.2075	5.1757	-3.4747
H	-0.8880	4.8154	-5.6678
H	-1.5264	2.5266	-6.3578
H	-3.6093	-0.6756	-5.7757
H	-5.5072	-1.3977	-4.3636
H	-5.2710	-1.3682	-1.8995
H	-4.0660	-0.4062	-0.0390
H	-2.4442	0.1924	-0.1864
H	-1.5796	-2.2094	-0.3342
H	-3.2123	-2.7944	-0.2849
H	-4.5466	-2.7569	1.7293
H	-4.4824	-2.7899	4.2039
H	-2.4261	-2.0729	5.3766
H	-0.2223	-1.4537	5.2994
H	2.9086	-1.3667	0.3693
H	4.0645	-2.6890	0.5234
H	2.4130	-3.0337	-0.0468
H	3.9751	-4.2086	2.4535
H	3.1474	-4.5469	4.7644
H	1.2715	-3.1716	5.6082
H	2.6809	2.9660	1.8366
H	1.0557	3.2468	1.1719
H	1.8861	1.6847	0.9280
H	1.3668	3.8951	3.9229
H	0.4431	3.0315	6.0556
H	-0.2430	0.6595	6.2146

84

Compound IIa (DFT)

C	-4.4480	0.6980	-1.0780
N	-3.2570	1.3480	-1.0610
C	-3.0710	2.4710	-1.8100
C	-4.0990	2.9300	-2.6580
C	-5.3190	2.2480	-2.7120
C	-5.5040	1.1200	-1.8990
Cu	-1.8730	0.4470	0.1310
N	-3.1540	0.3360	1.6620
C	-2.8920	0.6840	2.9550
C	-3.8820	0.5200	3.9420
C	-5.1380	0.0070	3.5970
C	-5.3890	-0.3310	2.2610
C	-4.3710	-0.1520	1.3100
C	-1.5420	1.2500	3.2880
C	-4.6160	-0.5090	-0.1550
C	-3.7910	-1.7210	-0.6040
N	-2.4460	-1.6310	-0.5140
C	-1.6780	-2.6880	-0.8850
C	-2.2670	-3.8700	-1.3800
C	-3.6590	-3.9630	-1.4870
C	-4.4400	-2.8710	-1.0850
C	-0.1800	-2.5910	-0.7210
C	0.2590	-2.6530	0.7650
C	1.7590	-2.6930	0.9380
N	2.4980	-1.6190	0.5490
C	3.8450	-1.6610	0.6530
C	4.5260	-2.7760	1.1710
C	3.7780	-3.8830	1.5920
C	2.3840	-3.8410	1.4660
Cu	1.8560	0.3640	-0.1500
N	3.1480	0.2870	-1.6690
C	2.8800	0.5930	-2.9720
C	3.8890	0.4690	-3.9450
C	5.1690	0.0390	-3.5790
C	5.4240	-0.2590	-2.2340
C	4.3880	-0.1230	-1.2970
C	1.5010	1.0670	-3.3310
C	4.6370	-0.4380	0.1770
C	4.4250	0.7880	1.0680
N	3.2110	1.3880	1.0330
C	2.9820	2.5220	1.7510
C	3.9910	3.0470	2.5840
C	5.2380	2.4160	2.6550
C	5.4660	1.2730	1.8750
C	1.6630	3.2210	1.5830
C	-1.7880	3.2370	-1.6580
O	-0.1100	0.6140	-0.7250
O	0.0880	0.4990	0.6990
H	1.6950	3.8650	0.6780
H	0.8450	2.4880	1.4440
H	1.4440	3.8770	2.4450
H	3.7910	3.9600	3.1630
H	6.0320	2.8170	3.3010
H	6.4400	0.7630	1.8890

```
H    5.7050 -0.7050  0.2630
H    1.2310  1.9660 -2.7410
H    1.4360  1.3170 -4.4050
H    0.7430  0.2910 -3.1010
H    3.6580  0.7190 -4.9910
H    5.9640 -0.0590 -4.3330
H    6.4200 -0.5920 -1.9080
H    5.6230 -2.7750  1.2430
H    4.2770 -4.7730  2.0040
H    1.7690 -4.6980  1.7740
H   -0.1460 -1.7640  1.2890
H   -0.1740 -3.5540  1.2430
H    0.1700 -1.6340 -1.1590
H    0.2970 -3.4180 -1.2830
H   -1.6250 -4.7120 -1.6790
H   -4.1330 -4.8780 -1.8740
H   -5.5370 -2.9090 -1.1450
H   -5.6760 -0.8100 -0.2290
H   -0.7420  0.5070  3.0950
H   -1.4900  1.5540  4.3490
H   -1.3230  2.1340  2.6570
H   -3.6580  0.8060  4.9790
H   -5.9180 -0.1230  4.3620
H   -6.3660 -0.7270  1.9520
H   -0.9480  2.5650 -1.3970
H   -1.8960  3.9840 -0.8410
H   -1.5470  3.8000 -2.5800
H   -3.9330  3.8320 -3.2630
H   -6.1270  2.5990 -3.3710
H   -6.4570  0.5730 -1.8990

84
Compound IIa (LFMM)
Cu   4.2990  4.9940  2.8200
Cu   4.0490  1.5660  2.1490
O    4.4030  3.4160  1.7160
O    3.4370  3.2680  2.7940
N    2.7260  6.3880  2.1930
N    5.6660  6.3900  2.3430
N    4.2520  5.6730  4.7080
N    5.4970  0.9620  3.7710
N    2.8780  0.0420  2.7200
N    4.9130  0.3790  0.8080
C    1.4840  4.8580  0.7450
C    1.6390  6.2010  1.3910
C    0.6670  7.1760  1.1840
C    0.8270  8.4130  1.7920
C    1.9420  8.6500  2.5830
C    2.8680  7.6210  2.7530
C    4.1140  7.8590  3.5940
C    7.1240  4.8380  1.1370
C    6.8120  6.2230  1.6230
C    7.6640  7.2730  1.2910
C    7.3490  8.5500  1.7340
C    6.2010  8.7530  2.4870
C    5.3890  7.6570  2.7730
C    4.1170  7.0170  4.8610
C    4.0120  7.6310  6.1070
C    4.0760  6.8360  7.2440
C    4.2600  5.4650  7.1190
C    4.3600  4.9210  5.8410
C    4.6000  3.4360  5.6770
C    5.8710  3.1400  4.8740
C    6.1390  1.6610  4.7560
C    7.0200  1.0760  5.6680
C    7.2690 -0.2840  5.5770
C    6.6310 -1.0280  4.5980
C    5.7550 -0.3780  3.7260
C    5.0020 -1.2030  2.6930
C    0.8490  1.3900  2.6220
C    1.5310  0.0870  2.9150
C    0.7940 -0.9950  3.3840
C    1.4570 -2.1900  3.6310
C    2.8250 -2.2790  3.4060
C    3.4980 -1.1490  2.9450
C    4.5920  1.9610 -1.0300
C    5.1590  0.6770 -0.4980
C    5.9200 -0.1360 -1.3330
C    6.4130 -1.3290 -0.8230
C    6.1290 -1.6870  0.4890
C    5.3670 -0.8180  1.2680
H    2.4530  4.4780  0.4150
H    1.0340  4.1610  1.4550
H    0.8430  4.9140 -0.1420
H   -0.1990  6.9870  0.5580
H    0.0880  9.1940  1.6430
H    2.0790  9.6200  3.0490
H    4.1020  8.9120  3.9080
H    6.5060  4.6040  0.2670
H    8.1770  4.7430  0.8490
H    6.9400  4.1050  1.9260
H    8.5590  7.1100  0.7000
H    7.9970  9.3870  1.4920
H    5.9520  9.7500  2.8350
H    3.8940  8.7050  6.2040
H    3.9990  7.2870  8.2290
H    4.3330  4.8460  8.0070
H    3.7160  2.9820  5.2180
H    4.6870  2.9660  6.6660
H    5.8270  3.5600  3.8700
H    6.7300  3.6340  5.3470
H    7.5070  1.6640  6.4390
H    7.9510 -0.7630  6.2720
H    6.8090 -2.0960  4.5310
H    5.3010 -2.2530  2.8210
H    0.9360  2.0600  3.4820
H   -0.2120  1.2430  2.3960
H    1.3070  1.8580  1.7460
H   -0.2760 -0.9220  3.5500
H    0.9080 -3.0530  3.9930
H    3.3440 -3.2130  3.5910
H    5.3160  2.7700 -0.9060
H    3.6650  2.2170 -0.5080
H    4.3460  1.8680 -2.0930
H    6.1210  0.1420 -2.3620
H    7.0060 -1.9870 -1.4510
H    6.4950 -2.6300  0.8820

90
Compound IIb (DFT)
Cu   1.8670 -0.1730  0.3890
Cu  -1.8670  0.1660  0.3970
```

```
O   -0.1310 -0.7150  0.6080
O    0.1300  0.7030  0.6040
N    2.4790  0.5870 -1.5490
N    3.2480  0.8890  1.4510
N    3.1410 -1.6740  0.2140
N   -2.4760 -0.5680 -1.5550
N   -3.2560 -0.9050  1.4380
N   -3.1370  1.6730  0.2330
C    0.1840  0.7640 -2.4860
C   -0.1790 -0.7400 -2.4880
C    1.6730  1.0210 -2.5560
C    2.2110  1.6810 -3.6770
C    3.5890  1.8930 -3.7530
C    4.4060  1.4160 -2.7220
C    3.8220  0.7540 -1.6240
C    4.7080  0.1850 -0.4660
C    6.1960  0.3140 -0.8590
C    4.4620  0.9890  0.8500
C    5.4690  1.7870  1.4250
C    5.2160  2.4590  2.6290
C    3.9780  2.2980  3.2540
C    2.9990  1.4890  2.6480
C    1.6890  1.2140  3.3310
C    4.3800 -1.3240 -0.2310
C    5.3450 -2.3240 -0.4560
C    5.0320 -3.6660 -0.2090
C    3.7630 -3.9930  0.2720
C    2.8190 -2.9720  0.4820
C    1.4470 -3.2860  1.0060
C   -1.6680 -0.9950 -2.5640
C   -2.2020 -1.6460 -3.6920
C   -3.5810 -1.8540 -3.7750
C   -4.4010 -1.3820 -2.7430
C   -3.8180 -0.7310 -1.6370
C   -4.7070 -0.1730 -0.4760
C   -6.1940 -0.2930 -0.8750
C   -4.4670 -0.9960  0.8310
C   -5.4780 -1.7990  1.3920
C   -5.2310 -2.4880  2.5870
C   -3.9950 -2.3380  3.2190
C   -3.0120 -1.5220  2.6280
C   -1.7050 -1.2610  3.3210
C   -4.3750  1.3310 -0.2190
C   -5.3370  2.3370 -0.4340
C   -5.0210  3.6750 -0.1700
C   -3.7530  3.9930  0.3200
C   -2.8130  2.9670  0.5190
C   -1.4420  3.2700  1.0520
H   -0.2210  1.2290 -1.5660
H   -0.2950  1.2620 -3.3520
H    0.2210 -1.2060 -1.5660
H    0.3030 -1.2370 -3.3520
H    1.5420  2.0220 -4.4800
H    4.0320  2.4160 -4.6140
H    5.4880  1.5670 -2.7900
H    6.8530 -0.0930 -0.0690
H    6.4090 -0.2250 -1.7990
H    6.4800  1.3690 -1.0160
H    6.4500  1.8950  0.9520
H    5.9940  3.0920  3.0810
H    3.7610  2.7830  4.2160
H    1.7260  0.2170  3.8200
H    0.8570  1.1970  2.6010
H    1.4860  1.9620  4.1200
H    6.3460 -2.0710 -0.8190
H    5.7850 -4.4490 -0.3830
H    3.4910 -5.0350  0.4940
H    0.6740 -3.0970  0.2350
H    1.3780 -4.3440  1.3160
H    1.1990 -2.6420  1.8730
H   -1.5310 -1.9830 -4.4950
H   -4.0220 -2.3680 -4.6420
H   -5.4830 -1.5290 -2.8160
H   -6.4020  0.2590 -1.8090
H   -6.4810 -1.3440 -1.0460
H   -6.8520  0.1060 -0.0820
H   -6.4570 -1.8990  0.9130
H   -6.0130 -3.1240  3.0270
H   -3.7830 -2.8370  4.1750
H   -1.7520 -0.2810  3.8450
H   -1.4970 -2.0330  4.0840
H   -0.8720 -1.2100  2.5940
H   -6.3370  2.0910 -0.8050
H   -5.7720  4.4620 -0.3370
H   -3.4790  5.0310  0.5560
H   -1.1990  2.6180  1.9130
H   -1.3700  4.3250  1.3720
H   -0.6660  3.0860  0.2820

90
Compound IIb (LFMM)
Cu  -0.9329  2.0310  0.1974
Cu   0.1944 -1.1875 -0.9026
O    0.3229  0.6259 -0.2572
O   -1.0363  0.2808 -0.6076
N   -2.0523  1.7074  2.0792
N   -2.3766  3.2679 -0.4196
N   -0.0809  3.6338  0.9971
N    0.7391 -2.3302  0.9127
N    1.8703 -1.8346 -1.7801
N   -0.6684 -2.8096 -1.6497
C   -1.5439 -0.7131  2.2558
C   -0.0443 -0.6187  2.5270
C   -2.2676  0.5221  2.7326
C   -3.1034  0.3879  3.8407
C   -3.7444  1.5098  4.3245
C   -3.5249  2.7336  3.7122
C   -2.6664  2.8131  2.6070
C   -2.3694  4.1982  1.9130
C   -3.0261  5.3743  2.7025
C   -2.9560  4.1515  0.4436
C   -4.0123  4.9743  0.0363
C   -4.4630  4.9151 -1.2779
C   -3.8462  4.0647 -2.1763
C   -2.7952  3.2818 -1.7185
C   -2.0785  2.3913 -2.6906
C   -0.7961  4.4158  1.8611
C   -0.1604  5.3681  2.6673
C    1.2108  5.5665  2.5493
C    1.9308  4.8380  1.6215
C    1.2491  3.9055  0.8516
C    2.0055  3.1261 -0.1817
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C    0.6533 -1.9204  2.2177
C    1.1536 -2.6514  3.2946
C    1.7588 -3.8659  3.0446
C    1.8329 -4.3314  1.7412
C    1.3042 -3.5599  0.6972
C    1.3409 -4.0814 -0.7909
C    1.8816 -5.5446 -0.8600
C    2.2854 -3.1254 -1.6273
C    3.4858 -3.5714 -2.1919
C    4.2587 -2.6951 -2.9460
C    3.8215 -1.4002 -3.1533
C    2.6163 -1.0181 -2.5800
C    2.0989  0.3668 -2.8364
C   -0.1328 -4.0389 -1.3832
C   -0.8607 -5.2107 -1.6236
C   -2.1245 -5.1315 -2.1982
C   -2.6418 -3.8986 -2.5479
C   -1.8776 -2.7705 -2.2825
C   -2.4069 -1.4256 -2.6810
H   -1.7756 -0.8969  1.2064
H   -1.9433 -1.5952  2.7760
H    0.4352  0.1969  1.9854
H    0.1088 -0.3634  3.5851
H   -3.2522 -0.5697  4.3293
H   -4.4029  1.4379  5.1846
H   -4.0339  3.5942  4.1289
H   -2.7952  6.3457  2.2465
H   -2.6909  5.4139  3.7462
H   -4.1188  5.2918  2.7474
H   -4.5062  5.6758  0.6975
H   -5.2830  5.5495 -1.6011
H   -4.1719  4.0307 -3.2106
H   -1.0476  2.2143 -2.3744
H   -2.6080  1.4403 -2.7754
H   -2.0311  2.8555 -3.6815
H   -0.6877  5.9801  3.3887
H    1.7091  6.3058  3.1693
H    2.9961  5.0049  1.5016
H    2.4094  2.2109  0.2594
H    2.8354  3.7139 -0.5884
H    1.3499  2.8796 -1.0216
H    1.0708 -2.2914  4.3152
H    2.1600 -4.4579  3.8613
H    2.3016 -5.2956  1.5856
H    1.2906 -6.2363 -0.2473
H    2.9107 -5.6300 -0.4908
H    1.8755 -5.9294 -1.8880
H    3.8535 -4.5840 -2.0796
H    5.1921 -3.0333 -3.3860
H    4.4036 -0.7163 -3.7620
H    1.0083  0.3956 -2.7744
H    2.3685  0.7032 -3.8433
H    2.5295  1.0588 -2.1100
H   -0.4848 -6.1995 -1.3910
H   -2.6927 -6.0367 -2.3904
H   -3.6146 -3.8277 -3.0229
H   -1.5801 -0.7519 -2.9223
H   -3.0297 -1.4987 -3.5790
H   -3.0094 -1.0043 -1.8716

90
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Compound IIc (DFT)
Cu   1.9080 -0.1730  0.3260
Cu  -1.9070  0.1740  0.3260
O    0.1670  0.6990  0.2650
O   -0.1660 -0.6980  0.2670
N    2.6670  0.1070 -1.6860
N    3.1140  1.1400  1.3060
N    3.3220 -1.5610  0.5100
N   -2.6670 -0.1090 -1.6860
N   -3.3220  1.5610  0.5080
N   -3.1130 -1.1380  1.3090
C    0.5690 -0.5250 -2.8190
C   -0.5700  0.5220 -2.8210
C    1.9490  0.0900 -2.8370
C    2.4930  0.5990 -4.0320
C    3.7890  1.1200 -4.0230
C    4.5410  1.0600 -2.8410
C    3.9560  0.5190 -1.6800
C    4.7800  0.3050 -0.3670
C    6.2770  0.5220 -0.6760
C    4.3430  1.2980  0.7520
C    5.2020  2.3080  1.2220
C    4.7930  3.1260  2.2830
C    3.5550  2.8920  2.8870
C    2.7250  1.8730  2.3860
C    1.4360  1.5150  3.0690
C    4.5670 -1.1620  0.1290
C    5.6340 -2.0780  0.1790
C    5.4090 -3.3900  0.6160
C    4.1220 -3.7710  1.0020
C    3.0800 -2.8290  0.9420
C    1.6810 -3.1820  1.3610
C   -1.9500 -0.0930 -2.8370
C   -2.4940 -0.6040 -4.0310
C   -3.7900 -1.1240 -4.0220
C   -4.5420 -1.0640 -2.8390
C   -3.9560 -0.5220 -1.6790
C   -4.7800 -0.3060 -0.3660
C   -6.2770 -0.5240 -0.6750
C   -4.5680  1.1610  0.1280
C   -5.6350  2.0770  0.1770
C   -5.4110  3.3900  0.6120
C   -4.1240  3.7720  0.9960
C   -3.0810  2.8310  0.9380
C   -1.6820  3.1850  1.3550
C   -4.3420 -1.2980  0.7540
C   -5.2000 -2.3080  1.2250
C   -4.7910 -3.1240  2.2880
C   -3.5530 -2.8890  2.8910
C   -2.7240 -1.8690  2.3900
C   -1.4350 -1.5080  3.0720
H    0.4660 -1.1630 -1.9220
H    0.4710 -1.1790 -3.7120
H   -0.4670  1.1610 -1.9240
H   -0.4720  1.1730 -3.7150
H    1.9030  0.5720 -4.9600
H    4.2330  1.5390 -4.9380
H    5.5740  1.4250 -2.8480
H    6.9000  0.3450  0.2190
H    6.4720  1.5530 -1.0160
H    6.6200 -0.1560 -1.4790
```

```
H    6.1890  2.4680  0.7750
H    5.4540  3.9250  2.6500
H    3.2270  3.4830  3.7540
H    1.5900  0.6150  3.7020
H    1.0950  2.3310  3.7320
H    0.6520  1.2760  2.3240
H    6.6450 -1.7850 -0.1230
H    6.2410 -4.1090  0.6540
H    3.9130 -4.7910  1.3530
H    0.9580 -2.9680  0.5490
H    1.3760 -2.5770  2.2390
H    1.6050 -4.2500  1.6340
H   -1.9040 -0.5780 -4.9600
H   -4.2340 -1.5450 -4.9360
H   -5.5740 -1.4280 -2.8450
H   -6.4720 -1.5560 -1.0130
H   -6.6200  0.1510 -1.4790
H   -6.9000 -0.3460  0.2200
H   -6.6460  1.7830 -0.1240
H   -6.2430  4.1080  0.6490
H   -3.9150  4.7930  1.3440
H   -0.9580  2.9630  0.5460
H   -1.3790  2.5870  2.2390
H   -1.6050  4.2550  1.6200
H   -6.1870 -2.4700  0.7790
H   -5.4510 -3.9240  2.6560
H   -3.2240 -3.4780  3.7590
H   -1.0940 -2.3230  3.7370
H   -0.6520 -1.2690  2.3280
H   -1.5910 -0.6080  3.7040

90
Compound IIc (LFMM)
Cu   1.6336  0.0912  1.9424
Cu  -0.9749  0.2858 -0.5370
O    0.6494  0.7782  0.4108
O    0.1374 -0.5007  0.8519
N    3.5063 -0.7014  1.0746
N    2.5352  1.5712  2.9254
N    2.1376 -1.0345  3.5154
N   -0.4242 -0.8250 -2.3679
N   -1.7370  1.6093 -1.8270
N   -2.8242 -0.4506 -0.4607
C    2.4551 -1.7852 -0.8692
C    2.0025 -0.8180 -1.9567
C    3.6768 -1.2798 -0.1493
C    4.9181 -1.4439 -0.7594
C    6.0461 -1.0390 -0.0729
C    5.9155 -0.5369  1.2139
C    4.6411 -0.4195  1.7808
C    4.4475 -0.0054  3.2864
C    5.8061 -0.0473  4.0519
C    3.8261  1.4398  3.3468
C    4.5451  2.5336  3.8422
C    3.9159  3.7658  3.9741
C    2.5783  3.8865  3.6485
C    1.9208  2.7667  3.1545
C    0.4474  2.8656  2.8945
C    3.4333 -1.0460  3.9635
C    3.8491 -1.9403  4.9560
C    2.9266 -2.8147  5.5210
C    1.6063 -2.7827  5.1097
C    1.2501 -1.8707  4.1262
C   -0.1750 -1.7954  3.6715
C    0.7975 -1.3368 -2.6949
C    0.9924 -2.2976 -3.6843
C   -0.1032 -2.7284 -4.4065
C   -1.3443 -2.1570 -4.1652
C   -1.4701 -1.1779 -3.1727
C   -2.8150 -0.3884 -2.9645
C   -3.7980 -0.6456 -4.1483
C   -2.4703  1.1759 -2.9012
C   -2.8824  2.0621 -3.9026
C   -2.5687  3.4129 -3.7940
C   -1.8675  3.8706 -2.6929
C   -1.4901  2.9469 -1.7283
C   -0.7473  3.4110 -0.5132
C   -3.4669 -0.8324 -1.6019
C   -4.6670 -1.5512 -1.5556
C   -5.2566 -1.8241 -0.3270
C   -4.6696 -1.3509  0.8309
C   -3.4744 -0.6510  0.7208
C   -2.8874 -0.0483  1.9619
H    1.6599 -1.9923 -0.1495
H    2.6915 -2.7653 -1.3060
H    1.7928  0.1769 -1.5576
H    2.8109 -0.6570 -2.6833
H    5.0098 -1.8857 -1.7465
H    7.0291 -1.1480 -0.5204
H    6.8231 -0.2745  1.7438
H    5.6794  0.1985  5.1141
H    6.5411  0.6605  3.6521
H    6.2815 -1.0344  3.9912
H    5.5805  2.4688  4.1535
H    4.4628  4.6182  4.3653
H    2.0609  4.8289  3.7950
H   -0.0679  3.2192  3.7940
H    0.2629  3.5750  2.0854
H    0.0139  1.8980  2.6371
H    4.8685 -1.9917  5.3186
H    3.2409 -3.5130  6.2912
H    0.8777 -3.4507  5.5567
H   -0.3177 -2.4083  2.7773
H   -0.4328 -0.7556  3.4547
H   -0.8618 -2.1435  4.4499
H    1.9779 -2.6991 -3.8973
H    0.0117 -3.4795 -5.1819
H   -2.1736 -2.4812 -4.7821
H   -4.0929 -1.6977 -4.2348
H   -3.3534 -0.3816 -5.1161
H   -4.7248 -0.0682 -4.0368
H   -3.4443  1.7514 -4.7749
H   -2.8835  4.1076 -4.5671
H   -1.6328  4.9251 -2.5935
H    0.3291  3.2896 -0.6611
H   -1.0712  2.8304  0.3543
H   -0.9559  4.4634 -0.2947
H   -5.1837 -1.8971 -2.4424
H   -6.1921 -2.3734 -0.2812
H   -5.1459 -1.5112  1.7926
H   -2.5976 -0.8404  2.6552
H   -2.0211  0.5768  1.7403
```

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H   -3.6285  0.5917  2.4525

164
Compound III (DFT)
C   -4.1850 -0.2140  3.6690
C   -2.9090 -0.1350  3.0650
N   -3.0640 -0.0980  1.7230
N   -4.4030 -0.1450  1.4510
C   -5.1130 -0.2220  2.6190
Cu  -1.8520 -0.2180  0.1270
N   -3.0430  1.4610 -0.8560
N   -4.3850  1.3020 -0.6430
C   -5.0800  2.4030 -1.0790
C   -4.1370  3.2970 -1.6000
C   -2.8790  2.6640 -1.4400
B   -4.8980 -0.0210 -0.0230
N   -4.3680 -1.2380 -0.8390
N   -3.0380 -1.5540 -0.8020
C   -2.8570 -2.6820 -1.5220
C   -4.1030 -3.0930 -2.0490
C   -5.0430 -2.1550 -1.6000
C   -1.5260 -3.3880 -1.6000
C   -1.4290 -4.4540 -0.4880
C   -1.5290  3.1410 -1.9200
C   -1.2640  2.6250 -3.3500
C   -1.5580 -0.0230  3.7260
C   -1.4870 -0.8490  5.0210
C   -6.5190 -2.0620 -1.9160
C   -7.1260 -3.4440 -2.2100
C   -6.5730  2.5850 -0.9170
C   -7.1730  3.4210 -2.0600
C   -6.6170 -0.3660  2.6830
C   -7.0410 -1.8350  2.4630
O    0.0040  0.3470  0.6330
O   -0.0040 -0.3470 -0.6330
Cu   1.8520  0.2180 -0.1270
N    3.0640  0.0980 -1.7230
N    4.4030  0.1450 -1.4510
C    5.1130  0.2220 -2.6190
C    4.1850  0.2140 -3.6690
C    2.9090  0.1350 -3.0650
B    4.8980  0.0210  0.0230
N    4.3850 -1.3020  0.6430
N    3.0430 -1.4610  0.8560
C    2.8790 -2.6640  1.4400
C    4.1370 -3.2970  1.6000
C    5.0800 -2.4030  1.0790
C    1.5290 -3.1410  1.9200
C    1.2640 -2.6250  3.3500
C    6.5730 -2.5850  0.9170
C    7.1730 -3.4210  2.0600
C    1.5580  0.0230 -3.7260
C    1.4870  0.8490 -5.0210
C    6.6170  0.3660 -2.6830
C    7.0410  1.8350 -2.4630
N    3.0380  1.5540  0.8020
N    4.3680  1.2380  0.8390
C    5.0430  2.1550  1.6000
C    4.1030  3.0930  2.0490
C    2.8570  2.6820  1.5220
C    1.5260  3.3880  1.6000
C    1.4290  4.4540  0.4880
C    6.5190  2.0620  1.9160
C    7.1260  3.4440  2.2100
C    1.2910  4.0170  2.9840
C    6.7710  1.0830  3.0850
C    1.4080 -4.6720  1.8610
C    6.9090 -3.2060 -0.4580
C    1.2140 -1.4570 -3.9940
C    7.1850 -0.1810 -4.0040
C   -1.2910 -4.0170 -2.9840
C   -1.4080  4.6720 -1.8610
C   -1.2140  1.4570  3.9940
C   -6.7710 -1.0830 -3.0850
C   -6.9090  3.2060  0.4580
C   -7.1850  0.1810  4.0040
H    6.1130  0.0380  0.0330
H    0.2760  4.4580  3.0450
H    2.0170  4.8330  3.1820
H    1.3910  3.2720  3.7970
H    2.2120  5.2300  0.6170
H    0.4420  4.9570  0.5090
H    1.5640  4.0000 -0.5140
H    0.7420  2.6230  1.4090
H    4.2990  3.9690  2.6730
H    7.0250  1.6480  1.0190
H    6.3550  0.0790  2.8700
H    6.2920  1.4520  4.0150
H    7.8580  0.9730  3.2790
H    6.6920  3.8890  3.1300
H    6.9540  4.1520  1.3760
H    8.2200  3.3590  2.3710
H    0.3890 -4.9990  2.1520
H    2.1190 -5.1570  2.5620
H    1.6200 -5.0630  0.8460
H    2.0120 -3.0370  4.0610
H    0.2570 -2.9270  3.7010
H    1.3330 -1.5210  3.3900
H    0.7680 -2.6900  1.2470
H    4.3380 -4.2780  2.0400
H    7.0380 -1.5780  0.9490
H    6.4920 -2.6020 -1.2880
H    6.4800 -4.2260 -0.5420
H    8.0070 -3.2820 -0.6010
H    6.7790 -4.4590  2.0530
H    6.9450 -2.9810  3.0520
H    8.2750 -3.4880  1.9580
H    1.9400 -1.9110 -4.7010
H    0.2020 -1.5480 -4.4380
H    1.2360 -2.0460 -3.0570
H    0.4650  0.8160 -5.4500
H    2.1790  0.4490 -5.7910
H    1.7520  1.9110 -4.8480
H    0.8110  0.4150 -3.0030
H    4.4050  0.2600 -4.7400
H    7.0460 -0.2330 -1.8530
H    6.8320  0.4110 -4.8740
H    6.8910 -1.2370 -4.1710
H    8.2930 -0.1290 -4.0000
H    6.6580  2.2250 -1.4990
H    6.6420  2.4840 -3.2700
H    8.1470  1.9310 -2.4610
```

H -6.1130 -0.0380 -0.0330
H -0.7420 -2.6230 -1.4090
H -4.2990 -3.9690 -2.6730
H -0.7680 2.6900 -1.2470
H -4.3380 4.2780 -2.0400
H -0.8110 -0.4150 3.0030
H -4.4050 -0.2600 4.7400
H -7.0250 -1.6480 -1.0190
H -1.3910 -3.2720 -3.7970
H -2.0170 -4.8330 -3.1820
H -0.2760 -4.4580 -3.0450
H -2.2120 -5.2300 -0.6170
H -1.5640 -4.0000 0.5140
H -0.4420 -4.9570 -0.5090
H -7.0380 1.5780 -0.9490
H -1.6200 5.0630 -0.8460
H -2.1190 5.1570 -2.5620
H -0.3890 4.9990 -2.1520
H -2.0120 3.0370 -4.0610
H -1.3330 1.5210 -3.3900
H -0.2570 2.9270 -3.7010
H -7.0460 0.2330 1.8530
H -1.9400 1.9110 4.7010
H -1.2360 2.0460 3.0570
H -0.2020 1.5480 4.4380
H -1.7520 -1.9110 4.8480
H -2.1790 -0.4490 5.7910
H -0.4650 -0.8160 5.4500
H -6.2920 -1.4520 -4.0150
H -6.3550 -0.0790 -2.8700
H -7.8580 -0.9730 -3.2790
H -6.9540 -4.1520 -1.3760
H -6.6920 -3.8890 -3.1300
H -8.2200 -3.3590 -2.3710
H -6.4800 4.2260 0.5420
H -6.4920 2.6020 1.2880
H -8.0070 3.2820 0.6010
H -6.9450 2.9810 -3.0520
H -6.7790 4.4590 -2.0530
H -8.2750 3.4880 -1.9580
H -6.8910 1.2370 4.1710
H -6.8320 -0.4110 4.8740
H -8.2930 0.1290 4.0000
H -6.6420 -2.4840 3.2700
H -6.6580 -2.2250 1.4990
H -8.1470 -1.9310 2.4610

164
Compound III (LFMM)
C -4.1980 -0.1550 3.7510
C -2.9280 -0.2830 3.1490
N -2.9750 -0.2730 1.8090
N -4.3140 -0.1590 1.5190
C -5.1160 -0.0640 2.6360
Cu -1.7440 -0.3840 0.2170
N -2.8530 1.2570 -0.7610
N -4.2170 1.0770 -0.6890
C -4.9390 2.0830 -1.2920
C -3.9370 3.0030 -1.7870
C -2.7070 2.4140 -1.4210
B -4.7990 -0.1650 0.0410
N -4.2840 -1.4550 -0.6580
N -2.9380 -1.7310 -0.6760
C -2.8450 -2.8920 -1.3400
C -4.0930 -3.3750 -1.7870
C -5.0490 -2.3980 -1.3090
C -1.4890 -3.5310 -1.5740
C -1.5180 -5.0230 -1.2310
C -1.3290 2.9780 -1.7030
C -1.1060 3.1020 -3.2120
C -1.5980 -0.4110 3.8720
C -1.6390 -1.5710 4.8720
C -6.5390 -2.3480 -1.4860
C -7.1470 -3.7500 -1.4320
C -6.4350 2.1780 -1.3610
C -6.8860 2.6690 -2.7380
C -6.6120 0.0670 2.6260
C -7.2520 -1.3220 2.6670
O -0.0060 0.3670 0.6310
O 0.0010 -0.3690 -0.6270
Cu 1.7380 0.3830 -0.2140
N 2.9670 0.2720 -1.8070
N 4.3070 0.1600 -1.5190
C 5.1070 0.0640 -2.6370
C 4.1870 0.1530 -3.7510
C 2.9180 0.2810 -3.1470
B 4.7940 0.1660 -0.0410
N 4.2130 -1.0760 0.6890
N 2.8490 -1.2560 0.7640
C 2.7050 -2.4130 1.4250
C 3.9350 -3.0010 1.7900
C 4.9360 -2.0820 1.2920
C 1.3270 -2.9760 1.7110
C 1.1070 -3.0960 3.2210
C 6.4330 -2.1770 1.3580
C 6.8860 -2.6680 2.7340
C 1.5870 0.4070 -3.8680
C 1.6260 1.5630 -4.8720
C 6.6020 -0.0670 -2.6290
C 7.2420 1.3220 -2.6740
N 2.9320 1.7310 0.6790
N 4.2790 1.4560 0.6580
C 5.0440 2.3990 1.3080
C 4.0870 3.3740 1.7900
C 2.8390 2.8900 1.3450
C 1.4820 3.5260 1.5840
C 1.5090 5.0190 1.2500
C 6.5340 2.3510 1.4810
C 7.1400 3.7540 1.4250
C 1.0530 3.3010 3.0350
C 6.8750 1.6670 2.8060
C 1.1610 -4.3390 1.0330
C 6.9370 -3.1130 0.2570
C 1.2500 -0.9100 -4.5730
C 7.0880 -0.9230 -3.8000
C -1.0570 -3.3160 -3.0260
C -1.1640 4.3390 -1.0210
C -1.2630 0.9030 4.5820
C -6.8760 -1.6630 -2.8120
C -6.9410 3.1130 -0.2600
C -7.0990 0.9220 3.7970
H 5.9560 0.1430 -0.0140

```
H    0.0450  3.6940  3.2030
H    1.7290  3.7980  3.7400
H    1.0520  2.2330  3.2780
H    2.1820  5.5750  1.9130
H    0.5100  5.4560  1.3570
H    1.8450  5.1860  0.2210
H    0.7630  3.0300  0.9190
H    4.2970  4.2650  2.3640
H    6.9870  1.7860  0.6620
H    6.4490  0.6600  2.8550
H    6.4860  2.2310  3.6620
H    7.9600  1.5780  2.9270
H    6.7980  4.3830  2.2550
H    6.8770  4.2600  0.4890
H    8.2330  3.7010  1.4800
H    0.1520 -4.7270  1.2010
H    1.8690 -5.0780  1.4240
H    1.3260 -4.2610 -0.0470
H    1.8200 -3.7890  3.6840
H    0.1010 -3.4700  3.4310
H    1.2260 -2.1240  3.7110
H    0.5810 -2.2840  1.3010
H    4.1060 -3.9290  2.3170
H    6.8830 -1.1920  1.2160
H    6.6130 -2.7720 -0.7330
H    6.5620 -4.1340  0.3920
H    8.0310 -3.1540  0.2560
H    6.5430 -3.6870  2.9420
H    6.5050 -2.0170  3.5300
H    7.9800 -2.6680  2.7990
H    1.9580 -1.1290 -5.3800
H    0.2470 -0.8680 -5.0090
H    1.2870 -1.7480 -3.8690
H    0.6470  1.6970 -5.3440
H    2.3540  1.3850 -5.6710
H    1.9000  2.5030 -4.3790
H    0.8170  0.6170 -3.1130
H    4.4300  0.1290 -4.8030
H    6.9220 -0.5790 -1.7170
H    6.8700 -0.4570 -4.7670
H    6.6140 -1.9110 -3.7890
H    8.1720 -1.0720 -3.7420
H    6.9120  1.9390 -1.8310
H    6.9800  1.8560 -3.5950
H    8.3330  1.2470 -2.6260
H   -5.9610 -0.1410  0.0120
H   -0.7700 -3.0330 -0.9100
H   -4.3020 -4.2660 -2.3610
H   -0.5840  2.2860 -1.2930
H   -4.1070  3.9310 -2.3130
H   -0.8270 -0.6180  3.1180
H   -4.4430 -0.1310  4.8030
H   -6.9930 -1.7820 -0.6680
H   -1.0570 -2.2500 -3.2750
H   -1.7320 -3.8180 -3.7280
H   -0.0490 -3.7080 -3.1900
H   -2.1920 -5.5810 -1.8900
H   -1.8540 -5.1830 -0.2000
H   -0.5210 -5.4620 -1.3350
H   -6.8860  1.1930 -1.2210
H   -1.3320  4.2590  0.0580
H   -1.8720  5.0790 -1.4110
H   -0.1550  4.7290 -1.1860
H   -1.8160  3.7980 -3.6740
H   -1.2260  2.1320 -3.7050
H   -0.0990  3.4750 -3.4190
H   -6.9290  0.5810  1.7130
H   -1.9720  1.1200  5.3890
H   -1.2990  1.7440  3.8810
H   -0.2600  0.8600  5.0190
H   -1.9110 -2.5080  4.3750
H   -2.3700 -1.3960  5.6700
H   -0.6610 -1.7060  5.3460
H   -6.4850 -2.2270 -3.6670
H   -6.4470 -0.6570 -2.8590
H   -7.9600 -1.5730 -2.9350
H   -6.8870 -4.2560 -0.4950
H   -6.8040 -4.3790 -2.2600
H   -8.2400 -3.6960 -1.4890
H   -6.5660  4.1340 -0.3950
H   -6.6190  2.7720  0.7290
H   -8.0360  3.1540 -0.2620
H   -6.5030  2.0190 -3.5330
H   -6.5420  3.6890 -2.9440
H   -7.9790  2.6700 -2.8050
H   -6.6250  1.9100  3.7880
H   -6.8830  0.4540  4.7640
H   -8.1830  1.0710  3.7370
H   -6.9920 -1.8570  3.5880
H   -6.9210 -1.9370  1.8240
H   -8.3430 -1.2460  2.6180

112
Compound IVa (DFT)
C   -1.4200  3.1360  1.4230
C   -1.9090  3.0630 -0.0250
C   -2.4250  4.4330 -0.5020
N   -2.8880  1.9240 -0.2280
C   -4.1080  2.0460  0.6320
C   -4.1330  1.1740  1.8960
C   -4.3190 -0.3400  1.7070
N   -3.1070 -1.1280  1.2850
C   -2.3260 -1.7010  2.4750
C   -1.8130 -0.6150  3.4220
Cu  -1.8760 -0.0600  0.0430
O    0.0360 -0.1080  0.7590
Cu   1.8600  0.1580  0.0130
N    2.9640  0.8890 -1.5780
C    2.1220  1.9250 -2.3290
C    1.8300  3.1530 -1.4660
O   -0.0380  0.2950 -0.6390
N   -3.1490 -0.7360 -1.6380
C   -2.3510 -1.2360 -2.8280
C   -3.2160 -1.7510 -3.9930
C   -3.2330  1.7960 -1.6650
C   -3.9350  0.4810 -1.9970
C   -3.9910 -1.7960 -1.0010
C   -3.4750 -2.2530  0.3630
C   -1.3240 -2.2870 -2.4050
C   -3.0860 -2.7870  3.2560
N    3.1250  0.1360  1.6710
C    2.3910  0.7550  2.8650
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C    3.1010  0.5510  4.2140
N    2.9520 -1.9590 -0.4970
C    2.0640 -3.1420 -0.7910
C    2.8270 -4.4380 -1.1220
C    3.3210 -1.3250  1.9250
C    3.7920 -2.1310  0.7110
C    4.4310  0.8200  1.3790
C    4.4020  1.9120  0.3010
C    4.2980  1.4360 -1.1530
C    3.7130 -1.5380 -1.6970
C    3.1150 -0.3360 -2.4270
C    2.0700  2.2330  2.6430
C    1.0500 -3.3770  0.3340
C    2.7010  2.3350 -3.6930
H   -3.8940  2.6240 -2.0100
H   -2.2890  1.8810 -2.2410
H   -4.1900  0.4860 -3.0770
H   -4.9050  0.4380 -1.4670
H   -4.0620 -2.6920 -1.6500
H   -5.0300 -1.4220 -0.9120
H   -2.5610 -2.8670  0.2380
H   -4.2470 -2.9070  0.8270
H   -5.1170 -0.5120  0.9580
H   -4.7020 -0.7790  2.6510
H   -3.2480  1.3830  2.5230
H   -5.0050  1.5170  2.4940
H   -4.2370  3.1060  0.9370
H   -5.0030  1.8150  0.0210
H   -1.0430  2.7760 -0.6580
H   -1.0140  2.1620  1.7590
H   -2.2160  3.4590  2.1230
H   -0.6100  3.8880  1.5000
H   -2.7000  4.4450 -1.5740
H   -1.6290  5.1910 -0.3640
H   -3.2990  4.7860  0.0820
H   -1.7960 -0.3390 -3.1760
H   -0.6820 -2.5440 -3.2700
H   -1.8060 -3.2310 -2.0770
H   -0.6770 -1.9030 -1.5930
H   -2.5630 -1.9700 -4.8610
H   -3.9720 -1.0200 -4.3390
H   -3.7410 -2.6950 -3.7420
H   -1.4450 -2.1740  1.9930
H   -2.4290 -3.1620  4.0650
H   -3.3640 -3.6620  2.6400
H   -4.0010 -2.3990  3.7480
H   -2.6240 -0.1600  4.0240
H   -1.2720  0.1840  2.8770
H   -1.1050 -1.0740  4.1390
H    4.0590 -1.4780  2.7420
H    2.3490 -1.7150  2.2860
H    4.8410 -1.8670  0.4690
H    3.8370 -3.1950  1.0280
H    4.7600 -1.3190 -1.4070
H    3.7930 -2.3610 -2.4390
H    3.7540 -0.1170 -3.3100
H    2.1040 -0.5890 -2.8080
H    4.5660  2.2760 -1.8260
H    5.0690  0.6610 -1.3320
H    3.6200  2.6600  0.5230
H    5.3660  2.4580  0.3820
H    5.1680  0.0490  1.0840
H    4.8200  1.2540  2.3230
H    1.4320  0.1980  2.8900
H    1.5530  2.4010  1.6780
H    2.9710  2.8760  2.6870
H    1.3910  2.5790  3.4460
H    2.4820  1.0070  5.0110
H    4.0900  1.0510  4.2580
H    3.2360 -0.5140  4.4830
H    1.4940 -2.8390 -1.6960
H    0.5080 -2.4430  0.5850
H    1.5360 -3.7670  1.2510
H    0.3160 -4.1450  0.0200
H    2.1120 -5.2200 -1.4440
H    3.3670 -4.8430 -0.2410
H    3.5590 -4.3140 -1.9440
H    1.1610  1.3980 -2.5040
H    2.8120  1.4880 -4.3950
H    3.6800  2.8490 -3.6080
H    2.0070  3.0570 -4.1680
H    1.0860  3.7910 -1.9810
H    2.7270  3.7830 -1.3020
H    1.4060  2.8680 -0.4830

112
Compound IVa (LFMM)
Cu  -1.4400  2.2120  11.694
O   -2.8120  2.1460  10.277
N   -2.4210  3.5660  13.177
C   -3.2330  2.5840  13.930
C   -2.3980  1.3460  14.320
N   -1.7680  0.6920  13.143
C   -0.4180  0.2010  13.519
C    0.6820  0.7490  12.567
N    0.5280  2.1820  12.207
C    0.8010  3.0480  13.376
C   -0.0150  4.3510  13.466
C   -1.4260  4.2170  14.060
C   -3.3150  4.5550  12.505
C   -2.5570  5.6150  11.697
C   -4.3360  5.2680  13.413
C   -2.6430 -0.3600  12.559
C   -2.0290 -0.9600  11.289
C   -3.0590 -1.5160  13.488
C    1.4030  2.4920  11.028
C    2.8870  2.0950  11.170
C    1.3500  3.9480  10.544
Cu  -2.8980  2.6070  8.3640
O   -1.6380  2.8530  9.8480
N   -2.1110  3.7040  6.7870
C   -1.1940  2.7440  6.1120
C   -1.8170  1.3660  5.7780
N   -2.5490  0.8110  6.9380
C   -3.9160  0.4150  6.5300
C   -4.9620  0.8540  7.5780
N   -4.9110  2.3050  7.9000
C   -5.3580  3.1150  6.7430
C   -4.5470  4.3900  6.4780
C   -3.1660  4.1540  5.8520
C   -1.2950  4.8430  7.3250
C   -2.1190  5.8620  8.1160
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C   -0.4120  5.6040  6.3160
C   -1.8250 -0.2980  7.6180
C   -0.4400  0.1250  8.1270
C   -1.6460 -1.6020  6.8120
C   -5.7470  2.5640  9.1190
C   -7.2190  2.1070  9.0600
C   -5.7020  4.0270  9.5760
H   -3.6590  3.0270  14.839
H   -4.0710  2.2390  13.312
H   -3.0180  0.6610  14.904
H   -1.6420  1.6810  15.037
H   -0.3560 -0.8930  13.521
H   -0.1400  0.4800  14.542
H    0.6310  0.1480  11.650
H    1.6590  0.5540  13.026
H    0.6180  2.5110  14.313
H    1.8670  3.3000  13.422
H   -0.0500  4.8780  12.513
H    0.5420  5.0210  14.136
H   -1.7640  5.2140  14.366
H   -1.3180  3.6920  15.016
H   -3.9040  3.9830  11.782
H   -1.8250  5.1570  11.029
H   -2.0340  6.3310  12.339
H   -3.2530  6.1890  11.077
H   -5.0330  4.5620  13.875
H   -4.9450  5.9650  12.825
H   -3.8550  5.8450  14.208
H   -3.5670  0.1390  12.240
H   -2.7810 -1.5310  10.734
H   -1.1980 -1.6380  11.508
H   -1.6580 -0.1750  10.630
H   -3.6280 -2.2670  12.927
H   -3.7120 -1.1810  14.298
H   -2.1980 -2.0250  13.931
H    1.0100  1.8930  10.198
H    3.4380  2.3510  10.257
H    3.0110  1.0170  11.310
H    3.3770  2.6100  12.001
H    1.8620  4.6260  11.233
H    0.3250  4.2970  10.408
H    1.8450  4.0420  9.5700
H   -0.8010  3.1670  5.1790
H   -0.3310  2.5620  6.7630
H   -2.4580  1.4960  4.8990
H   -1.0230  0.7000  5.4240
H   -4.2040  0.8600  5.5720
H   -4.0220 -0.6590  6.3580
H   -5.9540  0.5660  7.2090
H   -4.7750  0.2730  8.4910
H   -6.4110  3.3990  6.8430
H   -5.3450  2.5390  5.8120
H   -4.4890  5.0120  7.3710
H   -5.1230  4.9860  5.7570
H   -3.3170  3.4290  5.0460
H   -2.8610  5.0660  5.3280
H   -0.6010  4.4020  8.0510
H   -2.7700  5.3620  8.8350
H   -2.7320  6.4910  7.4630
H   -1.4590  6.5280  8.6850
H    0.1590  6.3860  6.8300
H   -0.9960  6.0930  5.5320
H    0.3240  4.9490  5.8400
H   -2.4210 -0.5550  8.4990
H   -0.4920  1.0550  8.6910
H    0.2780  0.2610  7.3120
H   -0.0270 -0.6370  8.7970
H   -1.0570 -2.3250  7.3890
H   -1.1210 -1.4380  5.8660
H   -2.5970 -2.0930  6.5920
H   -5.2950  1.9850  9.9340
H   -7.3050  1.0270  8.9070
H   -7.7860  2.6120  8.2720
H   -7.7200  2.3270  10.010
H   -6.1410  4.1280  10.575
H   -6.2650  4.6860  8.9070
H   -4.6740  4.3890  9.6360

112
Compound IVb (DFT)
Cu  -0.0720  0.0820  1.8190
O    0.4930  0.6180 -0.0260
N   -1.7010 -0.7920  2.8600
C   -1.1670 -1.3680  4.1300
C    0.2670 -1.9260  4.0560
N    1.2410 -1.1180  3.2830
C    1.8470 -0.0170  4.0720
C    0.9560  1.2240  4.2600
N    0.3150  1.7520  3.0130
C   -1.0150  2.3890  3.2970
C   -2.1120  1.5260  3.9200
C   -2.6540  0.3330  3.1330
C   -2.4020 -1.8190  1.9670
C   -3.7440 -2.3300  2.5230
C   -1.5010 -3.0030  1.6050
C    2.2920 -2.0370  2.6840
C    3.2030 -2.7000  3.7310
C    3.1110 -1.3600  1.5830
C    1.1710  2.7940  2.2750
C    1.3430  4.1220  3.0370
C    2.5370  2.2590  1.8460
Cu   0.1200 -0.0410 -1.9110
O   -0.2760 -0.6140 -0.0440
N   -1.8870  0.8410 -2.5000
C   -1.5510  1.5150 -3.7790
C   -0.1050  2.0500 -3.8580
N    0.9790  1.1220 -3.3920
C    1.3920  0.1440 -4.4430
C    0.4250 -1.0280 -4.5660
N    0.1540 -1.6780 -3.2480
C   -1.1880 -2.3450 -3.2190
C   -2.4000 -1.4760 -3.5790
C   -2.8180 -0.3170 -2.6650
C   -2.4610  1.7730 -1.4490
C   -1.5450  2.9610 -1.1390
C   -3.8860  2.2780 -1.7500
C    2.1710  1.9280 -2.8750
C    2.8420  2.7840 -3.9600
C    3.1860  1.0410 -2.1500
C    1.2810 -2.6590 -2.9060
C    1.4000 -3.8520 -3.8730
C    1.2030 -3.1550 -1.4610
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H   -1.2180 -0.5810  4.9020
H   -1.8330 -2.1780  4.4980
H    0.2430 -2.9280  3.5930
H    0.6080 -2.0790  5.1060
H    2.1370 -0.3610  5.0920
H    2.7820  0.2750  3.5650
H    0.1520  0.9970  4.9810
H    1.5670  2.0170  4.7430
H   -0.8630  3.2560  3.9740
H   -1.3700  2.8020  2.3300
H   -1.8430  1.2300  4.9550
H   -2.9760  2.2090  4.0660
H   -3.5310 -0.0560  3.6930
H   -3.0320  0.6720  2.1460
H   -2.6000 -1.2500  1.0340
H   -4.1520 -3.0850  1.8230
H   -4.5130 -1.5420  2.6260
H   -3.6320 -2.8380  3.5030
H   -0.5040 -2.6760  1.2530
H   -1.3810 -3.7130  2.4470
H   -1.9770 -3.5720  0.7820
H    1.6920 -2.8330  2.1960
H    2.6350 -3.2270  4.5220
H    3.8470 -3.4560  3.2390
H    3.8790 -1.9690  4.2170
H    3.8280 -0.6130  1.9780
H    3.7150 -2.1270  1.0600
H    2.4570 -0.8680  0.8360
H    0.5820  2.9930  1.3560
H    0.3960  4.6640  3.2130
H    1.9830  4.7910  2.4310
H    1.8580  3.9910  4.0110
H    2.9940  2.9840  1.1440
H    3.2400  2.1630  2.6970
H    2.4560  1.2910  1.3200
H   -1.7400  0.8090 -4.6070
H   -2.2270  2.3760 -3.9840
H    0.0880  2.3630 -4.9080
H   -0.0200  2.9580 -3.2370
H    2.4000 -0.2280 -4.1800
H    1.4850  0.6430 -5.4320
H    0.8330 -1.7590 -5.2960
H   -0.5310 -0.6870 -4.9920
H   -1.3170 -2.7550 -2.1980
H   -1.1800 -3.2120 -3.9140
H   -3.2660 -2.1710 -3.5760
H   -2.3490 -1.1440 -4.6370
H   -2.9940 -0.7110 -1.6420
H   -3.8050  0.0340 -3.0390
H   -2.4980  1.1380 -0.5370
H   -1.5460  3.7200 -1.9470
H   -1.9230  3.4790 -0.2350
H   -0.5100  2.6320 -0.9310
H   -4.6410  1.4700 -1.8040
H   -3.9330  2.8560 -2.6950
H   -4.2080  2.9640 -0.9430
H    1.7170  2.6060 -2.1220
H    2.1390  3.4750 -4.4630
H    3.6300  3.4060 -3.4940
H    3.3380  2.1640 -4.7330
H    3.9060  1.6850 -1.6080
H    3.7860  0.4150 -2.8410
H    2.6930  0.3880 -1.4010
H    2.2010 -2.0460 -3.0010
H    2.3250 -4.4090 -3.6300
H    1.4770 -3.5640 -4.9390
H    0.5590 -4.5650 -3.7650
H    1.0740 -2.3210 -0.7450
H    0.3750 -3.8780 -1.3120
H    2.1400 -3.6910 -1.2150

112
Compound IVb (LFMM)
Cu   2.2873  1.0665  1.3463
O    0.8776  2.0453  0.4097
N    2.1306 -1.1802  1.2823
C    3.3823 -1.6593  1.9041
C    4.5849 -0.7239  1.6490
N    4.3209  0.7378  1.7849
C    4.4392  1.1971  3.1875
C    3.1620  0.9489  4.0306
N    1.9092  1.3397  3.3411
C    0.7803  0.4600  3.7472
C    0.8645 -1.0582  3.5370
C    0.9627 -1.5807  2.0974
C    1.9434 -1.6711 -0.1264
C    1.5899 -3.1652 -0.2852
C    3.0876 -1.3603 -1.1014
C    5.2648  1.4726  0.8781
C    6.7530  1.3212  1.2423
C    4.9480  2.9619  0.7110
C    1.4851  2.7610  3.6067
C    1.2474  3.1585  5.0783
C    2.3774  3.8277  2.9717
Cu   0.4714  2.5647 -1.4256
O    1.8225  1.4721 -0.5102
N   -1.3140  1.2304 -1.7293
C   -2.3760  2.1575 -2.1695
C   -2.2206  3.5814 -1.5602
N   -0.8414  4.1486 -1.5639
C   -0.5198  4.7982 -2.8554
C   -0.0786  3.7835 -3.9334
N    0.9708  2.8674 -3.4121
C    0.9367  1.5636 -4.1065
C   -0.3816  0.7654 -4.1201
C   -0.9565  0.2589 -2.7869
C   -1.6793  0.4853 -0.4730
C   -2.1581  1.3380  0.7118
C   -2.6937 -0.6664 -0.6457
C   -0.6671  5.0820 -0.4131
C   -1.5415  6.3438 -0.4671
C    0.8004  5.4822 -0.1870
C    2.3111  3.5377 -3.5575
C    2.8921  3.5985 -4.9843
C    3.3768  2.9517 -2.6308
H    3.2940 -1.7474  2.9871
H    3.6336 -2.6750  1.5765
H    4.9456 -0.9422  0.6399
H    5.4108 -1.0306  2.3048
H    5.2989  0.7333  3.6883
H    4.6345  2.2690  3.2265
H    3.1685 -0.1128  4.2766
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H     3.2690   1.4403   5.0027
H     0.5781   0.5900   4.8164
H    -0.1213   0.7920   3.2163
H     1.6367  -1.4997   4.1732
H    -0.0687  -1.4737   3.9458
H     0.9136  -2.6743   2.1725
H     0.0483  -1.2586   1.5857
H     1.0819  -1.1198  -0.5153
H     1.5140  -3.4307  -1.3463
H     0.6183  -3.4046   0.1576
H     2.3462  -3.8172   0.1616
H     3.4334  -0.3291  -1.0214
H     3.9395  -2.0318  -0.9545
H     2.7481  -1.4963  -2.1353
H     5.1351   1.0523  -0.1280
H     7.0659   0.2729   1.2608
H     7.3796   1.8258   0.4980
H     6.9811   1.7647   2.2170
H     5.1612   3.5464   1.6101
H     5.5520   3.3888  -0.0981
H     3.9041   3.1074   0.4364
H     0.5178   2.8871   3.0990
H     0.5103   2.5221   5.5738
H     0.8518   4.1801   5.1309
H     2.1696   3.1446   5.6663
H     1.9009   4.8128   3.0440
H     3.3472   3.9104   3.4667
H     2.5194   3.6341   1.9108
H    -2.3924   2.2710  -3.2537
H    -3.3744   1.7698  -1.9336
H    -2.9192   4.2582  -2.0702
H    -2.5920   3.5348  -0.5331
H     0.3025   5.5096  -2.7426
H    -1.3650   5.3902  -3.2291
H     0.2517   4.3251  -4.8269
H    -0.9717   3.2594  -4.2625
H     1.6976   0.9093  -3.6655
H     1.2062   1.6936  -5.1615
H    -0.1816  -0.1337  -4.7221
H    -1.1514   1.2881  -4.6956
H    -0.2101  -0.4343  -2.3795
H    -1.8353  -0.3416  -3.0535
H    -0.7510   0.0177  -0.1345
H    -3.1795   1.7031   0.5627
H    -2.1659   0.7369   1.6289
H    -1.5051   2.1896   0.9060
H    -2.2894  -1.4778  -1.2589
H    -3.6303  -0.3231  -1.0954
H    -2.9387  -1.1137   0.3248
H    -0.9478   4.5303   0.4940
H    -2.6057   6.0975  -0.5323
H    -1.4048   6.9394   0.4426
H    -1.2851   6.9825  -1.3186
H     0.9128   5.9530   0.7963
H     1.1601   6.2015  -0.9288
H     1.4637   4.6135  -0.2068
H     2.2034   4.5779  -3.2261
H     3.7628   4.2645  -5.0065
H     2.1767   3.9908  -5.7120
H     3.2316   2.6158  -5.3288
H     3.1160   3.1630  -1.5950
H     3.5070   1.8739  -2.7606
H     4.3506   3.4234  -2.8061

112
Compound IVc (DFT)
Cu   -0.0470  -0.0110  -1.8870
O    -0.3070  -0.6490  -0.0630
N    -1.4350  -1.1400  -2.9880
C    -1.3690  -0.5190  -4.3480
C    -1.0390   0.9800  -4.3300
N     0.1360   1.3380  -3.4740
C     1.4480   1.0690  -4.1530
C     2.0020  -0.3600  -4.0260
N     1.8830  -0.9470  -2.6700
C     1.6480  -2.4190  -2.7160
C     0.4230  -2.9050  -3.4950
C    -0.9790  -2.5740  -2.9830
C    -2.8290  -1.1030  -2.3570
C    -3.3450   0.3190  -2.1350
C    -3.8870  -1.9390  -3.1010
C     0.1040   2.8130  -3.0590
C    -1.0010   3.1270  -2.0500
C     0.0630   3.7770  -4.2550
C     3.0700  -0.6660  -1.7700
C     3.3140   0.8330  -1.5670
C     4.3790  -1.3610  -2.1930
Cu    0.0500   0.0150   1.8860
O     0.3070   0.6550   0.0620
N    -1.8980   0.9160   2.6710
C    -2.0070   0.3260   4.0260
C    -1.4300  -1.0930   4.1520
N    -0.1140  -1.3400   3.4730
C     1.0550  -0.9630   4.3290
C     1.3610   0.5400   4.3490
N     1.4170   1.1640   2.9890
C     0.9380   2.5900   2.9850
C    -0.4700   2.8980   3.4980
C    -1.6870   2.3920   2.7190
C    -3.0800   0.6170   1.7710
C    -4.3990   1.2920   2.1930
C    -3.3010  -0.8860   1.5680
C    -0.0570  -2.8130   3.0550
C     0.0030  -3.7780   4.2490
C     1.0510  -3.1060   2.0430
C     2.8120   1.1500   2.3590
C     3.3530  -0.2620   2.1390
C     3.8540   2.0060   3.1030
H    -2.3260  -0.6610  -4.8950
H    -0.6100  -1.0630  -4.9370
H    -0.8710   1.3100  -5.3780
H    -1.9040   1.5510  -3.9510
H     2.1730   1.7820  -3.7240
H     1.3710   1.3130  -5.2350
H     3.0580  -0.3370  -4.3770
H     1.4810  -1.0220  -4.7390
H     1.5700  -2.7580  -1.6610
H     2.5310  -2.9390  -3.1490
H     0.4780  -4.0150  -3.4740
H     0.5160  -2.6700  -4.5760
H    -1.0800  -2.9190  -1.9330
H    -1.6930  -3.1750  -3.5850
```

```
H   -2.6610 -1.5560 -1.3580
H   -2.5940  0.9530 -1.6280
H   -4.2440  0.2790 -1.4890
H   -3.6630  0.8090 -3.0770
H   -3.6460 -3.0170 -3.1580
H   -4.8470 -1.8570 -2.5560
H   -4.0760 -1.5680 -4.1290
H    1.0720  2.9500 -2.5350
H   -0.9490  2.4510 -1.1710
H   -0.8640  4.1650 -1.6870
H   -2.0160  3.0820 -2.4920
H    0.1930  4.8140 -3.8900
H   -0.9090  3.7420 -4.7860
H    0.8700  3.5900 -4.9880
H    2.7560 -1.0860 -0.7910
H    3.7690  1.3110 -2.4580
H    4.0390  0.9740 -0.7410
H    2.3830  1.3650 -1.2920
H    5.1800 -1.0980 -1.4750
H    4.3100 -2.4650 -2.2030
H    4.7280 -1.0270 -3.1920
H   -1.4980  0.9960  4.7400
H   -3.0630  0.2850  4.3780
H   -2.1420 -1.8180  3.7230
H   -1.3490 -1.3370  5.2340
H    1.9290 -1.5200  3.9490
H    0.8930 -1.2980  5.3770
H    0.5930  1.0720  4.9380
H    2.3160  0.6970  4.8950
H    1.0320  2.9380  1.9360
H    1.6410  3.2020  3.5880
H   -0.5430  4.0060  3.4780
H   -0.5590  2.6600  4.5790
H   -2.5790  2.8970  3.1540
H   -1.6160  2.7340  1.6650
H   -2.7720  1.0410  0.7920
H   -4.3480  2.3970  2.2010
H   -4.7430  0.9550  3.1930
H   -5.1970  1.0150  1.4760
H   -4.0230 -1.0380  0.7420
H   -2.3620 -1.4040  1.2940
H   -3.7490 -1.3700  2.4590
H   -1.0240 -2.9660  2.5320
H    0.9750 -3.7280  4.7790
H   -0.1100 -4.8170  3.8820
H   -0.8070 -3.6070  4.9840
H    0.9300 -4.1440  1.6760
H    0.9870 -2.4270  1.1670
H    2.0660 -3.0460  2.4840
H    2.6370  1.5990  1.3590
H    4.2530 -0.2070  1.4960
H    2.6150 -0.9100  1.6310
H    3.6760 -0.7460  3.0830
H    4.8170  1.9390  2.5600
H    4.0480  1.6410  4.1320
H    3.5950  3.0800  3.1560

112
Compound IVc (LFMM)
Cu  -0.1475 -1.4257 -1.9632
O   -0.0963 -0.6268 -0.1789
N   -0.5994 -3.4259 -1.7352
C   -0.8010 -3.9271 -3.1152
C   -1.3301 -2.8408 -4.0926
N   -0.6182 -1.5474 -3.9834
C    0.6641 -1.5589 -4.7507
C    1.9037 -2.1155 -4.0094
N    1.9967 -1.6562 -2.6091
C    2.6196 -2.6890 -1.7542
C    1.9414 -4.0610 -1.6595
C    0.5297 -4.1213 -1.0654
C   -1.8131 -3.5876 -0.8589
C   -3.0632 -2.8536 -1.3430
C   -2.2283 -5.0304 -0.4994
C   -1.4509 -0.4004 -4.4783
C   -2.6550 -0.0564 -3.5936
C   -1.9264 -0.5390 -5.9360
C    2.7493 -0.3659 -2.4538
C    2.2687  0.7921 -3.3379
C    4.2832 -0.4531 -2.6072
Cu  -0.1273  1.1771  0.5690
O   -0.1802  0.3785 -1.2155
N   -2.2706  1.4076  1.2186
C   -2.1752  1.8659  2.6191
C   -0.9344  1.3083  3.3579
N    0.3465  1.2973  2.5885
C    1.0590  2.5903  2.6974
C    0.5287  3.6776  1.7217
N    0.3244  3.1775  0.3416
C   -0.8058  3.8735 -0.3255
C   -2.2163  3.8131  0.2709
C   -2.8947  2.4412  0.3656
C   -3.0240  0.1177  1.0636
C   -4.5576  0.2055  1.2201
C   -2.5422 -1.0414  1.9457
C    1.1798  0.1495  3.0808
C    1.6577  0.2864  4.5379
C    2.3823 -0.1938  2.1938
C    1.5366  3.3397 -0.5366
C    2.7889  2.6092 -0.0529
C    1.9484  4.7827 -0.8992
H   -1.4702 -4.7938 -3.1419
H    0.1301 -4.2967 -3.5461
H   -1.2940 -3.2326 -5.1174
H   -2.3913 -2.7056 -3.8818
H    0.9142 -0.5429 -5.0674
H    0.5454 -2.1105 -5.6932
H    2.8107 -1.8718 -4.5754
H    1.8324 -3.2005 -4.0823
H    2.6898 -2.2981 -0.7305
H    3.6441 -2.8894 -2.0913
H    2.5768 -4.6677 -0.9970
H    1.9865 -4.5961 -2.6121
H    0.6105 -3.7365 -0.0398
H    0.3042 -5.1914 -0.9842
H   -1.5505 -3.1046  0.0907
H   -2.8318 -1.8202 -1.5883
H   -3.8232 -2.8270 -0.5537
H   -3.5234 -3.3436 -2.2052
H   -1.4672 -5.5431  0.0956
H   -3.1368 -5.0239  0.1147
H   -2.4417 -5.6341 -1.3860
```

```
H   -0.8216  0.4982 -4.4311
H   -2.3555  0.0986 -2.5554
H   -3.1140  0.8809 -3.9296
H   -3.4346 -0.8223 -3.6295
H   -2.4496  0.3703 -6.2532
H   -2.6211 -1.3761 -6.0603
H   -1.0904 -0.6813 -6.6274
H    2.5666 -0.0484 -1.4210
H    2.5560  0.6514 -4.3846
H    2.7301  1.7327 -3.0184
H    1.1887  0.9343 -3.2777
H    4.7354  0.5429 -2.5336
H    4.7397 -1.0516 -1.8129
H    4.5753 -0.8755 -3.5734
H   -2.1033  2.9508  2.6928
H   -3.0812  1.6220  3.1865
H   -1.1843  0.2920  3.6740
H   -0.8141  1.8590  4.3007
H    2.1198  2.4549  2.4849
H    1.0246  2.9814  3.7226
H   -0.4015  4.0474  2.1545
H    1.1984  4.5440  1.7476
H   -0.8884  3.4896 -1.3512
H   -0.5803  4.9437 -0.4061
H   -2.8528  4.4206 -0.3898
H   -2.2596  4.3475  1.2241
H   -3.9186  2.6416  0.7046
H   -2.9666  2.0511 -0.6582
H   -2.8434 -0.1989  0.0301
H   -5.0154  0.8048  0.4271
H   -4.8476  0.6272  2.1871
H   -5.0104 -0.7902  1.1465
H   -3.0045 -1.9815  1.6261
H   -1.4624 -1.1838  1.8836
H   -2.8276 -0.9015  2.9930
H    0.5501 -0.7489  3.0337
H    2.3525  1.1235  4.6620
H    2.1816 -0.6232  4.8530
H    0.8229  0.4278  5.2309
H    2.8407 -1.1324  2.5273
H    2.0813 -0.3464  1.1557
H    3.1627  0.5712  2.2303
H    1.2734  2.8545 -1.4851
H    3.5483  2.5833 -0.8430
H    2.5603  1.5757  0.1940
H    3.2490  3.1015  0.8081
H    2.8574  4.7772 -1.5127
H    2.1594  5.3892 -0.0139
H    1.1864  5.2918 -1.4962
```

LFMM parameters

```
# LFMM parameters for MMFF94
#
#
# Developed by the Inorganic Computational Chemistry Group (ICCG),
# Robert J. Deeth (rjd), Natalie Fey (nf), David L. Foulis (dlf),
# Benjamin J. Williams-Hubbard (bjwh),
# Chemistry Department, University of Warwick, UK-CV4 7AL
#

[Morse]
#T1   T2    dist        D           a
Cu+2  N     2.02         58.0       1.60        0.0   0.0
Cu+2  NPYD  2.00         70.0       1.3         0.0   0.0
Cu+2  N5A   2.00         70.0       1.3         0.0   0.0
Cu+2  N5B   2.000        70.0       1.20        0.0   0.0
Cu+2  Omu2  2.02         60.0       1.50        0.0   0.0
%

[ll]
#M    L     A     n
Cu+2  N     8000    6
Cu+2  NPYD  3000    6
Cu+2  N5A   2500    6
Cu+2  N5B   2500    6
Cu+2  Omu2  2000  6
%

[esig]
#M    L     esig0 esig1 esig2 esig3 esig4 esig5 esig6
Cu+2  N     0     0     0     0     122000      0     0
Cu+2  NPYD  0     0     0     0     105000      0     0
```

```
Cu+2  N5A   0     0     0     0     102000      0     0
Cu+2  N5B   0     0     0     0     102000      0     0
Cu+2  Omu2  0     0     0     0     0     333000      0
%

[epix]
#M    L     epix0 epix1 epix2 epix3 epix4 epix5 epix6
Cu+2  N     0     0     0     0     0     0     0
Cu+2  NPYD  0     0     0     0     0     0     0
Cu+2  N5A   0     0     0     0     0     0     0
Cu+2  N5B   0     0     0     0     0     0     0
Cu+2  Omu2  0     0     0     0     85000 0     0
%

[epiy]
#M    L     epiy0 epiy1 epiy2 epiy3 epiy4 epiy5 epiy6
Cu+2  Omu2  0     0     0     0     24500 0     0
Cu+2  N     0     0     0     0     0     0     0
Cu+2  NPYD  0     0     0     0     20000 0     0
Cu+2  N5A   0     0     0     0     20000 0     0
Cu+2  N5B   0     0     0     0     16000 0     0
%

[exds]
#M    L     exds0 exds1 exds2 exds3 exds4 exds5 exds6
Cu+2  Omu2  0     0     0     0     0     0     330000
Cu+2  N     0     0     0     0     0     0     167000
Cu+2  NPYD  0     0     0     0     0     0     147000
Cu+2  N5A   0     0     0     0     0     0     137000
Cu+2  N5B   0     0     0     0     0     0     137000
%
```