Supporting Information

for

Heterodinuclear Ni(II) and Cu(II) Schiff base complexes and their activity in oxygen reduction

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Contents

HR-ESI/MS

Mass Spectrum Molecular Formula Report

Analysis Info **Electrospray (ESI)**

Analysis Name D:\Data\AUVIGO\MJCMJC1511471_000001.d
Sample Name PIU3
Comment

Acquisition Date 5/18/2015 3:21:58 PM
Instrument apex-Qe

Acquisition Parameter

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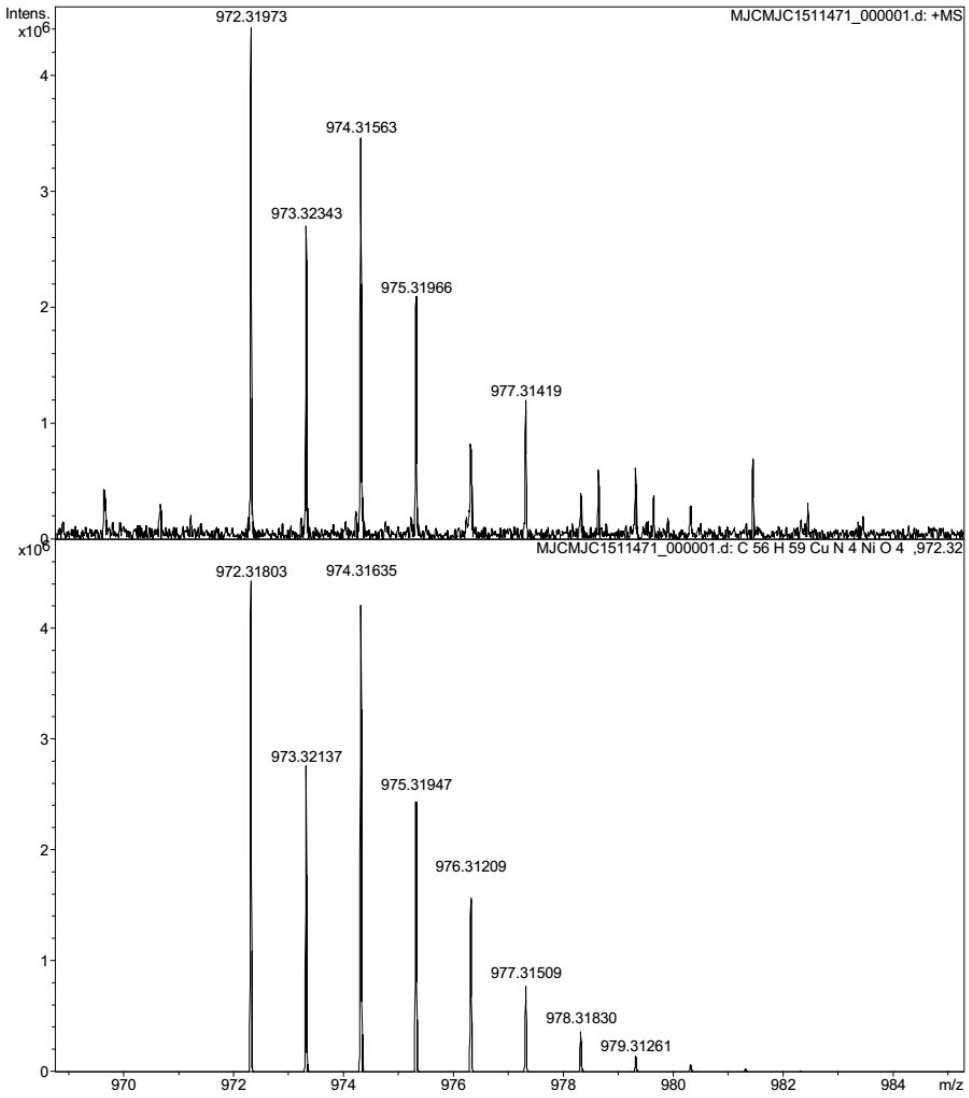
Skimmer 1 80.0 V



Mass Spectrum Molecular Formula Report

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
972.31973	1	C 56 H 59 Cu N 4 Ni O 4	79.51	972.31803	-1.70	-1.75	152.5	29.0	odd	ok
	2	C 59 H 57 Cu N 5 Ni O	100.00	972.32071	0.98	1.01	155.9	33.5	even	ok

Figure S1. HR-ESI/MS spectrum for complex **1** predicted (below) experimental (above).

Mass Spectrum Molecular Formula Report

Analysis Info **Electrospray (ESI)**

Analysis Name D:\Data\AUVIGO\MJCMJC1511472_000001.d
Sample Name PIU4
Comment

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Instrument apex-Qe

Acquisition Parameter

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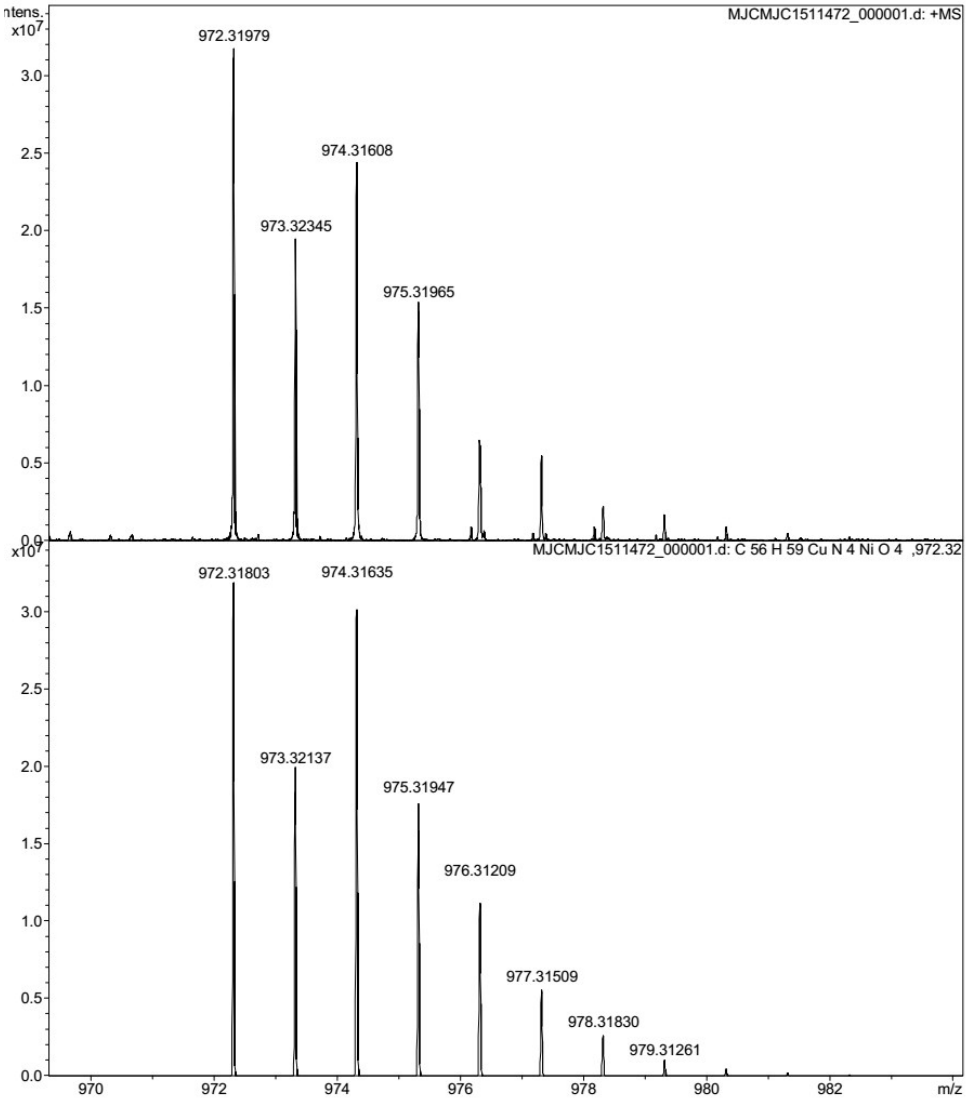

Mass Spectrum Molecular Formula Report

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
972.31979	1	C 56 H 59 Cu N 4 Ni O 4	79.02	972.31803	-1.76	-1.81	162.0	29.0	odd	ok
	2	C 59 H 57 Cu N 5 Ni O	100.00	972.32071	0.92	0.95	166.1	33.5	even	ok

Figure S2. HR-ESI/MS spectrum for complex **2** predicted (below) experimental (above).

Electrochemical studies

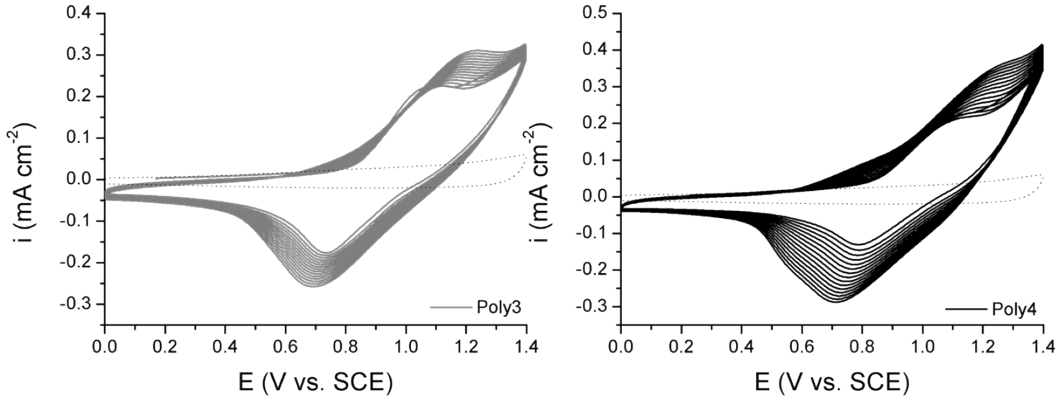

Figure S3. Cyclic voltammogram collected during the potentiodynamic growth of **Poly3** (grey) and **Poly4** (black) film on GCE from 1 mM dichloromethane solutions of the monomers. 0.1 M NBu_4PF_6 was used as supporting electrolyte (dotted line). 15 cycles, sweep rate = 200 mV s^{-1}.

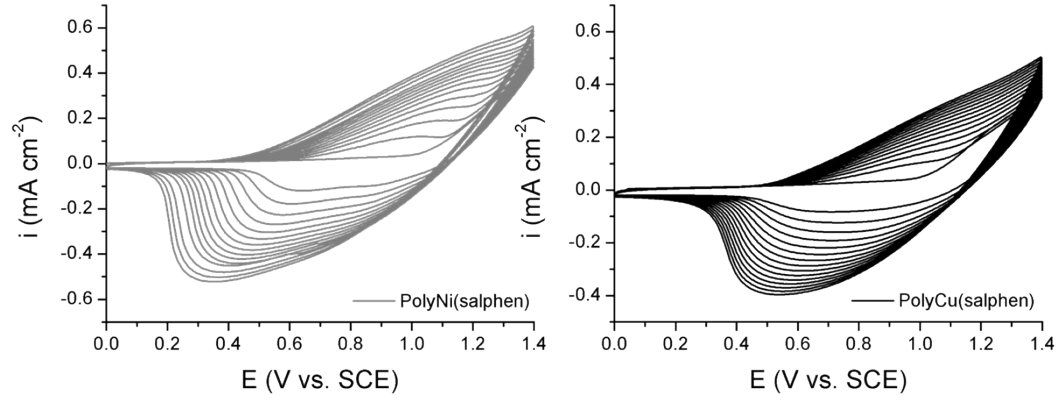

Figure S4. Cyclic voltammogram collected during the potentiodynamic growth of **PolyNi(salphen)** (grey) and **PolyCu(salphen)** (black) film on GCE from 1 mM dichloromethane solutions of the monomers. 0.1 M NBu_4PF_6 was used as supporting electrolyte (dotted line). 15 cycles, sweep rate = 200 mV s^{-1}.

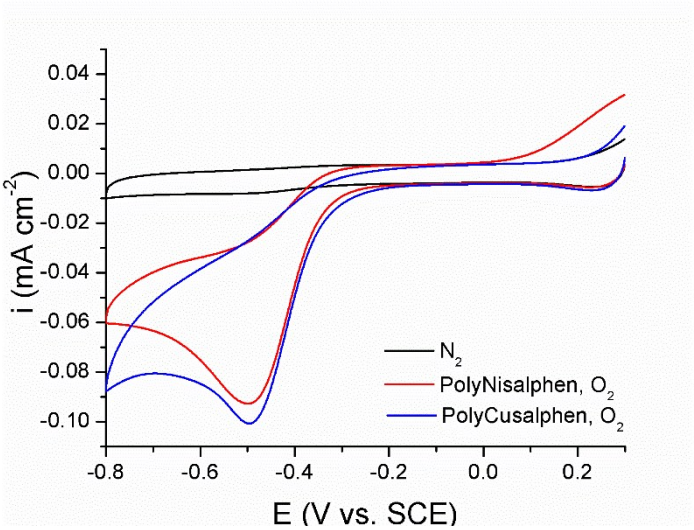

Figure S5. Cyclic voltammograms of **PolyNi(salphen)** (solid red line) and **PolyCu(salphen)** (solid blue line) at 50 mV s^{-1} in 0.1 M phospate buffer solution pH 7 in the presence of oxygen.

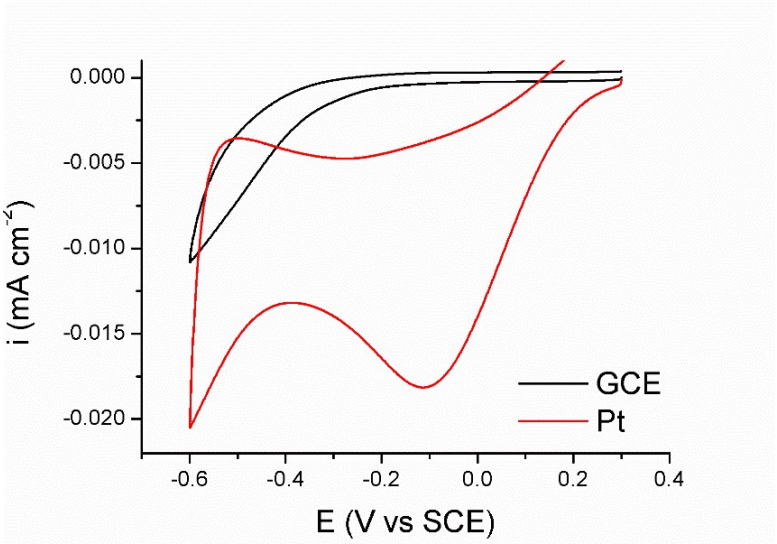

Figure S6. Cyclic voltammograms of GCE (black line) and Pt (red line at 50 mV s^{-1} in 0.1 M phosphate buffer solution pH 7 in the presence of oxygen.

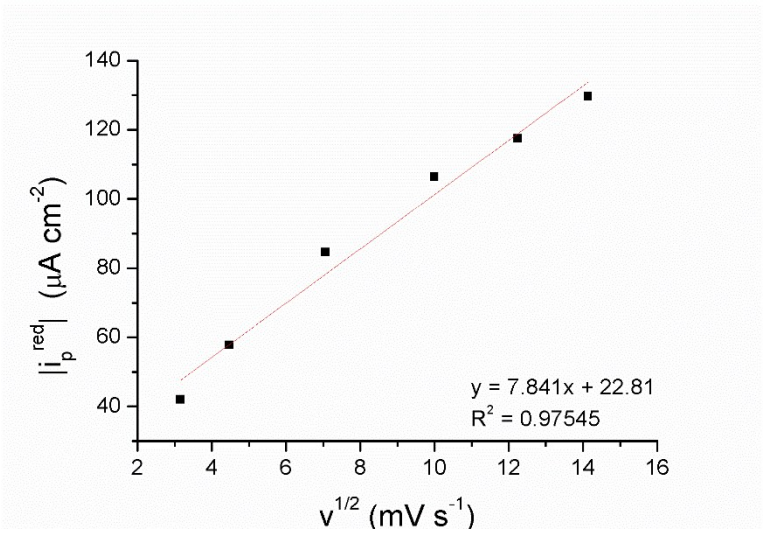

Figure S7. i_p^{red} versus $v^{1/2}$ plot for **PolyNi(salphen)** in PBS pH 7 solution in the presence of oxygen.

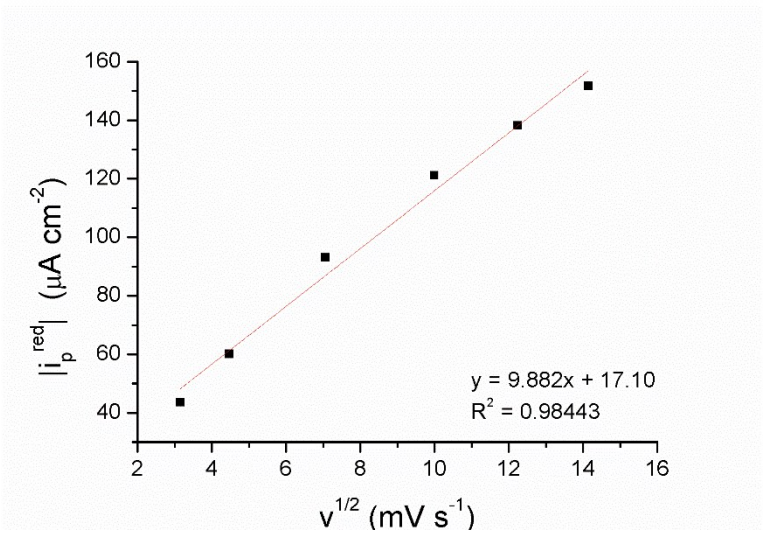

Figure S8. i_p^{red} versus $v^{1/2}$ plot for **PolyCu(salphen)** in PBS pH 7 solution in the presence of oxygen.

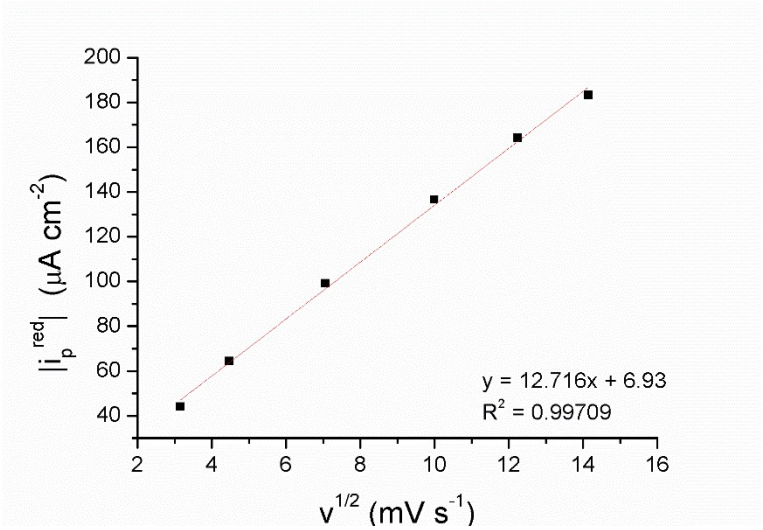

Figure S9. i_p^{red} versus $v^{1/2}$ plot for **Poly1** in PBS pH 7 solution in the presence of oxygen.

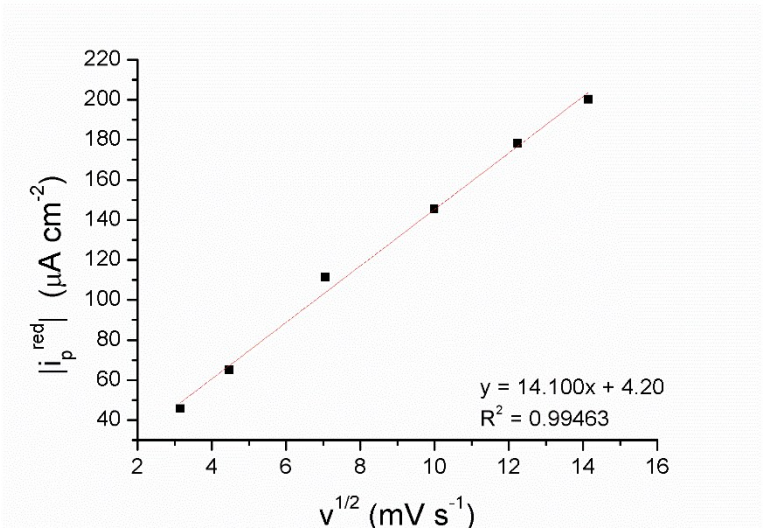

Figure S10. i_p^{red} versus $v^{1/2}$ plot for **Poly2** in PBS pH 7 solution in the presence of oxygen.

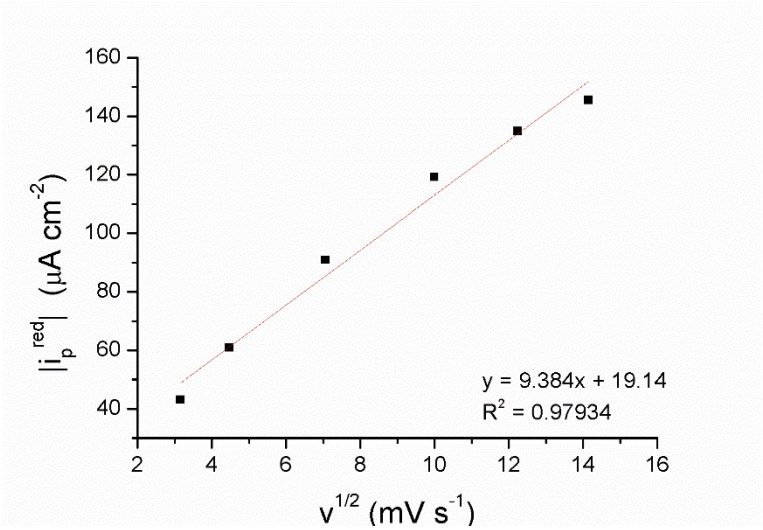

Figure S11. i_p^{red} versus $v^{1/2}$ plot for **Poly3** in PBS pH 7 solution in the presence of oxygen.

Cartesian coordinates of all the structures calculated

Complex 1

```
124
Complex 1
 Ni         5.73069        3.02175        5.29585
  C        15.14003        5.10615       15.07239
  N        13.28281        4.70663       12.71399
  O        15.27803        6.07613       14.21329
  C        15.93291        5.11373       16.28982
  N        13.41053        6.52824       10.80597
  O        15.56621        7.83644       12.12677
  C        15.77549        4.05575       17.17918
  H        16.37910        4.06523       18.09062
  N         7.36926        3.74460        4.74017
  O         4.98518        2.95112        3.59647
  C        14.88590        2.95329       16.99934
  N         6.43967        3.07390        7.03213
  O         4.08925        2.31314        5.79627
  C        14.12253        2.95592       15.84773
  H        13.41370        2.14657       15.64498
  C        14.21916        4.00062       14.87556
  C        13.36872        3.88086       13.74291
  H        12.71986        2.98990       13.74816
  C        12.39913        4.51980       11.63861
  C        11.46814        3.46706       11.51181
  H        11.38689        2.70601       12.29182
  C        10.65345        3.36397       10.38646
  H         9.97206        2.51328       10.29552
  C        10.73433        4.30938        9.33567
  C        11.65348        5.36676        9.46380
  H        11.70186        6.11270        8.66660
  C        12.47710        5.49600       10.59686
  C        13.55254        7.56024        9.99321
  H        12.87386        7.63621        9.12799
  C        14.50104        8.61396       10.09539
  C        14.44788        9.60787        9.06842
  H        13.67405        9.49517        8.30228
  C        15.33310       10.66771        9.02691
  C        16.31556       10.71893       10.06170
  H        17.02725       11.54801       10.03364
  C        16.43892        9.80035       11.09914
  C        15.49380        8.69783       11.15166
  C         5.51850        3.33758        2.47500
  C         4.75109        3.19702        1.27460
  C         5.26097        3.59658        0.05035
  H         4.64746        3.47712       -0.84867
  C         6.56211        4.15808       -0.06231
  C         7.33176        4.30469        1.07635
  H         8.33884        4.73245        1.01378
  C         6.84440        3.90523        2.35856
  C         7.67712        4.06819        3.49119
  H         8.66780        4.50357        3.30321
  H         3.75131        2.76576        1.36869
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H	6.94616	4.46723	-1.03757
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C	9.59052	4.43226	5.70881
H	10.01776	4.70957	4.74246
C	10.37788	4.55634	6.85218
H	11.40893	4.90720	6.75412
C	9.88614	4.18590	8.12756
C	8.57265	3.68627	8.21691
H	8.18138	3.42653	9.20318
C	7.76813	3.55661	7.07228
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C	4.47393	2.19932	8.19174
C	3.92402	1.85008	9.46334
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C	3.67980	2.02122	6.99559
Cu	14.42043	6.30928	12.48882
H	6.31746	2.80357	9.09107
H	2.23479	1.07691	10.55549
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H	17.49578	6.54702	14.47880
C	14.82105	1.84940	18.06780
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C	13.81332	0.74419	17.69729
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H	16.19333	0.41632	19.00065
H	16.98316	1.93695	18.51771
C	17.54478	9.93102	12.16509
C	18.45825	8.67953	12.11932
C	16.90965	10.07274	13.57143
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H	16.28826	9.20043	13.81408
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H	17.88143	7.76131	12.29686
H	19.23971	8.75556	12.89511
H	18.95839	8.59802	11.13928
C	15.31429	11.75785	7.94226
C	14.18694	11.53320	6.91626
C	16.66542	11.75716	7.18513
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H	16.83776	10.78771	6.68906
H	16.67312	12.54549	6.41269

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H	13.19196	11.54825	7.39208
C	14.38897	2.46525	19.42157
H	13.38842	2.92186	19.34440
H	14.35323	1.68719	20.20366
H	15.08917	3.24618	19.76006
C	16.11258	7.60129	16.67614
H	15.56372	7.80362	15.74602
H	15.39082	7.56413	17.50982
H	16.80433	8.44108	16.86213
C	18.43652	11.16799	11.92991
H	17.86409	12.11018	11.98010
H	19.20777	11.20929	12.71665
H	18.95933	11.12881	10.95880
C	15.09931	13.14147	8.60387
H	14.13419	13.17821	9.13559
H	15.89279	13.37627	9.33176
H	15.10153	13.93730	7.83903

Complex 1+ (S=0)

124
Complex 1 oxidized singlet

Ni	5.73922	3.07435	5.25968
C	15.05680	5.14265	15.05671
N	13.33179	4.61415	12.64320
O	15.00552	6.18737	14.28002
C	15.93031	5.14754	16.21895
N	13.37326	6.48812	10.79235
O	15.70207	7.58356	11.93439
C	15.85748	4.05771	17.08151
H	16.49519	4.07489	17.96819
N	7.46981	3.49403	4.67343
O	5.02126	2.90727	3.56726
C	15.02470	2.91124	16.90290
N	6.41624	3.23950	7.00054
O	4.01742	2.65160	5.78528
C	14.22602	2.89159	15.77109
H	13.58335	2.03241	15.55831
C	14.22596	3.96671	14.83591
C	13.39915	3.81213	13.69323
H	12.76850	2.91031	13.69376
C	12.40601	4.45936	11.60348
C	11.43329	3.43951	11.51250
H	11.31413	2.71100	12.31758
C	10.64500	3.31890	10.37298
H	9.93621	2.48954	10.29747
C	10.78577	4.21365	9.28055
C	11.72900	5.24882	9.37988
H	11.81507	5.95955	8.55445
C	12.50432	5.41606	10.54542
C	13.53486	7.51177	9.97082
H	12.85474	7.59085	9.10911
C	14.48468	8.55925	10.08632
C	14.37057	9.62821	9.15000

H	13.57245	9.56826	8.40450
C	15.22029	10.72110	9.18567
C	16.21537	10.72708	10.21017
H	16.88801	11.58674	10.24524
C	16.39179	9.73830	11.17333
C	15.51827	8.57774	11.11226
C	5.62334	3.04086	2.41937
C	4.85346	2.85198	1.23008
C	5.43905	2.97706	-0.02030
H	4.82654	2.82630	-0.91450
C	6.81591	3.29556	-0.16315
C	7.58859	3.48589	0.96911
H	8.65206	3.73226	0.87891
C	7.02469	3.36711	2.27485
C	7.85098	3.57126	3.40525
H	8.90207	3.81152	3.19829
H	3.79564	2.60620	1.34917
H	7.25760	3.38888	-1.15796
C	8.37002	3.71522	5.74016
C	9.72828	4.06702	5.62949
H	10.19884	4.19780	4.65278
C	10.50285	4.24061	6.77734
H	11.56510	4.47927	6.67414
C	9.94956	4.05973	8.06589
C	8.58923	3.71490	8.17422
H	8.15733	3.60328	9.17137
C	7.79563	3.55429	7.02641
C	5.70686	3.10039	8.11203
C	4.33037	2.77911	8.18747
C	3.71079	2.66488	9.46719
H	4.32066	2.83433	10.36115
C	2.36899	2.34704	9.58571
C	1.59617	2.13026	8.41246
H	0.53551	1.87835	8.50673
C	2.15895	2.23241	7.15099
C	3.54235	2.56216	6.99270
Cu	14.41030	6.24992	12.44839
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H	1.90472	2.26204	10.57104
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C	16.85552	6.34235	16.50977
C	17.83792	6.53245	15.32675
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C	14.10017	0.62999	17.57298
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H	14.15339	-0.15468	18.34436
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 H       16.26613        8.91047       13.81443
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 H       17.99421        7.69238       12.19192
 H       19.27642        8.73912       12.86102
 H       18.98984        8.69864       11.10187
 C       15.12998       11.90155        8.20747
 C       13.99161       11.72056        7.18540
 C       16.46733       12.02434        7.43399
 H       17.32269       12.19013        8.10847
 H       16.67115       11.11460        6.84582
 H       16.42244       12.87897        6.73851
 H       14.13318       10.81643        6.56945
 H       13.96861       12.58411        6.50172
 H       13.00460       11.66137        7.67458
 C       14.63926        2.34566       19.31965
 H       13.61693        2.75647       19.28614
 H       14.66237        1.54450       20.07708
 H       15.31503        3.14579       19.66221
 C       16.00827        7.62276       16.72726
 H       15.39093        7.85549       15.84822
 H       15.34392        7.50723       17.59999
 H       16.67407        8.48071       16.92056
 C       18.30406       11.15141       12.11148
 H       17.67085       12.04678       12.23242
 H       19.06548       11.17960       12.90729
 H       18.83600       11.22352       11.14773
 C       14.87220       13.20666        9.00216
 H       13.92300       13.15042        9.55975
 H       15.67692       13.41907        9.72422
 H       14.81312       14.06338        8.31040
```

Complex 1+ (S=1)

```
124
Complex 1 oxidized triplet
 Ni       5.71976        3.07867        5.29480
  C      15.15134        5.08691       15.06505
  N      13.29068        4.67053       12.70954
  O      15.26892        6.05635       14.20561
  C      15.94397        5.11420       16.28619
  N      13.44440        6.46056       10.77143
  O      15.54103        7.82045       12.13176
  C      15.81175        4.04311       17.16880
  H      16.41214        4.06157       18.08101
  N       7.45342        3.52431        4.71035
  O       4.99548        2.92276        3.59484
  C      14.95397        2.92338       16.97626
  N       6.39602        3.26945        7.04168
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O	3.98864	2.66696	5.81869
C	14.18622	2.91440	15.81418
H	13.50068	2.08567	15.61333
C	14.25533	3.96138	14.85679
C	13.40233	3.83137	13.71909
H	12.78526	2.91903	13.70950
C	12.40210	4.47878	11.63100
C	11.43988	3.45458	11.53904
H	11.31818	2.73243	12.34979
C	10.63413	3.33656	10.40673
H	9.92053	2.51053	10.34089
C	10.76260	4.23384	9.32123
C	11.70730	5.27213	9.42108
H	11.78985	5.98091	8.59322
C	12.50877	5.42249	10.56629
C	13.57932	7.48830	9.95890
H	12.91134	7.55441	9.08551
C	14.51158	8.56360	10.07625
C	14.46133	9.54964	9.05598
H	13.71346	9.42767	8.26685
C	15.32758	10.63965	9.03825
C	16.28415	10.71778	10.09149
H	16.97315	11.56486	10.07873
C	16.40844	9.80014	11.13150
C	15.48120	8.67559	11.15659
C	5.60086	3.05610	2.45308
C	4.83591	2.85740	1.25829
C	5.42210	2.98777	0.00977
H	4.81440	2.82997	-0.88639
C	6.79644	3.31968	-0.12764
C	7.56492	3.51837	1.00829
H	8.62651	3.77305	0.91878
C	7.00155	3.39610	2.31210
C	7.82869	3.60996	3.44219
H	8.87517	3.86718	3.23114
H	3.78028	2.60174	1.37634
H	7.24156	3.41605	-1.12066
C	8.34842	3.74459	5.77601
C	9.70955	4.09439	5.66831
H	10.18140	4.22283	4.69177
C	10.48277	4.26345	6.81508
H	11.54583	4.49910	6.71396
C	9.92836	4.07928	8.10516
C	8.56896	3.73653	8.21216
H	8.13745	3.61955	9.20894
C	7.77255	3.58140	7.06338
C	5.67903	3.14955	8.14913
C	4.30210	2.82487	8.22083
C	3.67979	2.72652	9.50004
H	4.28796	2.90920	10.39266
C	2.33790	2.40591	9.62279
C	1.56839	2.16938	8.45198
H	0.50846	1.91472	8.54733
C	2.13400	2.25460	7.19038
C	3.51738	2.58866	7.02693
Cu	14.42016	6.27143	12.47779

H	6.18342	3.31937	9.10973
H	1.87346	2.33331	10.60897
H	1.55121	2.07659	6.28356
C	16.88379	6.29359	16.58831
C	17.95049	6.42289	15.46956
C	17.63138	6.11105	17.92551
H	16.94426	6.05268	18.78653
H	18.27338	5.21394	17.92545
H	18.28614	6.98174	18.08994
H	18.56453	5.50901	15.40592
H	18.62334	7.26587	15.70047
H	17.48646	6.60658	14.49146
C	14.90876	1.80822	18.02967
C	16.32374	1.19377	18.18217
C	13.92812	0.68361	17.64494
H	12.89222	1.05225	17.55555
H	14.21126	0.19754	16.69610
H	13.93367	-0.09302	18.42617
H	16.66638	0.74589	17.23511
H	16.30848	0.40263	18.95021
H	17.06956	1.94329	18.49230
C	17.48630	9.95489	12.21770
C	18.35251	11.21302	11.99861
C	18.42921	8.72330	12.18503
H	17.87848	7.78857	12.35903
H	18.94661	8.65220	11.21373
H	19.19693	8.82437	12.97048
H	18.89661	11.18634	11.03929
H	19.10686	11.27059	12.79949
H	17.75898	12.14202	12.04125
C	15.29885	11.72686	7.95568
C	14.20936	11.46677	6.89744
C	16.67388	11.77311	7.24109
H	17.49724	11.99592	7.93843
H	16.89744	10.81299	6.74800
H	16.66893	12.56175	6.47042
H	14.37311	10.51558	6.36322
H	14.22665	12.27221	6.14610
H	13.19930	11.45203	7.34052
C	14.45963	2.40698	19.38718
H	13.45106	2.84554	19.31334
H	14.43481	1.61660	20.15579
H	15.14606	3.19279	19.74115
C	16.05328	7.60012	16.68810
H	15.50905	7.80371	15.75550
H	15.32541	7.53988	17.51441
H	16.72523	8.45108	16.89054
C	16.81846	10.08202	13.61177
H	16.22321	9.19205	13.85518
H	17.59778	10.20165	14.38323
H	16.16424	10.96896	13.65304
C	15.01916	13.09882	8.62121
H	14.03901	13.10335	9.12542
H	15.78592	13.36072	9.36792
H	15.01517	13.89280	7.85591

Complex 2

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124
Complex 2
Cu        5.625135000      2.577565000      5.474120000
C        14.928642000      5.154128000     15.243277000
N        13.201348000      4.536750000     12.904254000
O        15.092717000      6.003542000     14.263955000
C        15.631695000      5.348521000     16.498711000
N        13.413859000      6.124833000     10.922139000
O        15.460925000      7.437604000     12.209219000
C        15.467384000      4.385244000     17.489600000
H        16.006504000      4.532479000     18.428659000
N         7.473349000      3.007127000      4.888929000
O         4.926142000      2.530591000      3.672350000
C        14.647457000      3.220661000     17.385830000
N         6.425063000      2.632915000      7.290237000
O         3.857553000      2.136158000      6.122610000
C        13.949983000      3.060694000     16.204525000
H        13.284023000      2.205166000     16.056111000
C        14.060129000      4.003753000     15.136714000
C        13.264253000      3.778998000     13.990250000
H        12.630948000      2.882035000     14.018587000
C        16.515593000      6.588611000     16.727450000
C        17.673030000      6.606082000     15.698807000
H        18.296221000      7.504425000     15.850377000
H        17.290499000      6.618120000     14.669981000
H        18.317620000      5.719600000     15.825611000
C        15.647841000      7.865599000     16.589832000
H        14.865903000      7.886389000     17.367942000
H        15.162343000      7.915435000     15.605437000
H        16.276037000      8.764362000     16.715015000
C        17.144169000      6.606541000     18.136357000
H        16.381361000      6.623036000     18.933656000
H        17.753534000      7.518873000     18.244823000
H        17.809855000      5.743267000     18.307669000
C        14.570707000      2.235230000     18.563889000
C        14.045470000      2.970240000     19.821923000
H        14.698562000      3.809335000     20.112299000
H        13.994108000      2.276197000     20.678571000
H        13.035220000      3.375945000     19.647709000
C        15.982228000      1.668050000     18.853725000
H        16.375395000      1.124837000     17.978561000
H        15.946692000      0.967371000     19.705856000
H        16.701569000      2.464282000     19.105494000
C        13.627248000      1.053777000     18.267632000
H        13.963852000      0.470257000     17.394079000
H        12.593982000      1.392204000     18.081118000
H        13.601983000      0.371342000     19.133128000
C        12.326561000      4.235118000     11.841562000
C        11.370955000      3.200889000     11.799472000
H        11.233148000      2.528186000     12.649169000
C        10.590920000      3.015185000     10.658554000
H         9.879615000      2.185172000     10.626296000
C        10.738989000      3.847908000      9.523034000
C        11.685815000      4.889129000      9.575209000
```

H	11.786382000	5.547429000	8.709101000
C	12.461207000	5.099679000	10.727309000
C	13.578297000	7.097855000	10.039169000
H	12.911791000	7.107930000	9.166043000
C	14.539083000	8.135557000	10.089939000
C	14.555232000	9.066772000	9.011476000
H	13.793225000	8.952553000	8.231360000
C	15.498506000	10.077532000	8.932792000
C	16.467937000	10.120825000	9.975278000
H	17.236853000	10.891919000	9.916447000
C	16.518490000	9.252452000	11.066526000
C	15.496418000	8.231069000	11.170021000
C	5.596686000	2.641009000	2.565738000
C	4.884245000	2.517948000	1.327234000
C	5.530673000	2.610412000	0.106275000
H	4.949582000	2.507948000	-0.816244000
C	6.931427000	2.833617000	0.028234000
C	7.653810000	2.963079000	1.199244000
H	8.735230000	3.139091000	1.163035000
C	7.030241000	2.878442000	2.483263000
C	7.860364000	3.042787000	3.625471000
H	8.927858000	3.211917000	3.408765000
H	3.807367000	2.343317000	1.394713000
H	7.427124000	2.903159000	-0.943186000
C	8.341770000	3.220424000	5.972080000
C	9.686835000	3.634848000	5.873415000
H	10.139311000	3.809050000	4.893950000
C	10.461053000	3.829765000	7.014975000
H	11.510570000	4.118496000	6.908110000
C	9.920259000	3.630167000	8.307944000
C	8.575577000	3.229374000	8.410721000
H	8.137369000	3.132344000	9.407226000
C	7.780193000	3.014169000	7.270234000
C	5.780164000	2.293995000	8.392307000
C	4.408003000	1.936306000	8.492669000
C	3.904602000	1.621742000	9.793518000
H	4.601525000	1.663142000	10.638776000
C	2.581603000	1.280162000	10.000016000
C	1.700941000	1.240461000	8.886072000
H	0.650408000	0.972102000	9.039731000
C	2.144445000	1.533235000	7.607494000
C	3.509877000	1.887644000	7.348741000
Ni	14.289462000	6.020792000	12.570427000
C	17.630527000	9.367765000	12.125891000
C	15.485226000	11.081414000	7.762199000
C	18.423292000	8.036968000	12.182600000
H	19.200259000	8.092878000	12.964338000
H	17.763657000	7.187745000	12.408431000
H	18.924234000	7.844585000	11.218547000
C	17.005286000	9.683615000	13.506646000
H	16.290394000	8.905709000	13.804296000
H	17.796170000	9.743145000	14.274620000
H	16.481269000	10.654307000	13.482177000
C	18.636804000	10.491906000	11.801381000
H	19.413530000	10.513132000	12.583602000
H	19.145705000	10.332160000	10.835298000

H	18.160600000	11.487209000	11.784580000
C	14.141276000	11.850314000	7.763677000
H	14.106011000	12.568819000	6.926407000
H	13.281877000	11.168406000	7.657677000
H	14.009287000	12.411620000	8.703357000
C	15.635567000	10.318368000	6.423328000
H	15.619918000	11.023349000	5.574066000
H	16.587361000	9.762883000	6.390600000
H	14.818641000	9.594286000	6.271146000
C	16.628391000	12.110850000	7.857710000
H	16.563838000	12.712978000	8.779455000
H	17.620297000	11.629416000	7.828073000
H	16.572365000	12.805992000	7.003614000
H	6.338613000	2.276077000	9.342613000
H	2.215956000	1.045985000	11.002812000
H	1.472776000	1.501525000	6.745763000

Complex 2+ (S=0)

124
Complex 2 oxidized singlet

Cu	5.70280	2.40253	5.47218
C	14.91031	5.19189	15.26506
N	13.16225	4.57012	12.94515
O	15.07925	6.01518	14.26651
C	15.62204	5.40673	16.51330
N	13.40505	6.12101	10.93254
O	15.47677	7.39643	12.18842
C	15.45155	4.45748	17.51667
H	15.99504	4.61211	18.45112
N	7.45848	3.10378	4.92899
O	5.22134	1.90985	3.69147
C	14.62131	3.29795	17.43263
N	6.44600	2.50721	7.29111
O	3.90730	2.16464	6.07160
C	13.91309	3.12317	16.25550
H	13.23987	2.27068	16.12916
C	14.02654	4.04718	15.17684
C	13.22195	3.82049	14.03782
H	12.57880	2.93178	14.07733
C	16.51895	6.63895	16.72105
C	17.67951	6.62063	15.69506
H	18.31688	7.50910	15.84044
H	17.30642	6.62799	14.66275
H	18.30882	5.72596	15.83648
C	15.66494	7.92351	16.56148
H	14.87991	7.96579	17.33507
H	15.18461	7.97328	15.57441
H	16.30489	8.81394	16.68057
C	17.14422	6.67125	18.13134
H	16.38094	6.70917	18.92702
H	17.76138	7.57902	18.22668
H	17.80341	5.80630	18.31683
C	14.54102	2.33192	18.62351
C	14.02423	3.09462	19.86953
H	14.68550	3.93072	20.14927

H	13.97023	2.41154	20.73363
H	13.01620	3.50461	19.69370
C	15.95311	1.76468	18.91576
H	16.34332	1.20607	18.04928
H	15.91142	1.07648	19.77658
H	16.67687	2.55897	19.16009
C	13.59017	1.15144	18.34757
H	13.92066	0.54955	17.48412
H	12.55651	1.49016	18.16331
H	13.56600	0.48392	19.22378
C	12.27585	4.27165	11.89031
C	11.29142	3.26504	11.87431
H	11.13023	2.62022	12.74094
C	10.50931	3.07120	10.73595
H	9.77635	2.26018	10.72703
C	10.69040	3.86302	9.57726
C	11.67003	4.87860	9.60365
H	11.80004	5.50637	8.71927
C	12.43398	5.10562	10.75706
C	13.57567	7.08397	10.04120
H	12.89793	7.10150	9.17731
C	14.55780	8.10305	10.07397
C	14.58430	9.02537	8.99365
H	13.81590	8.92887	8.21852
C	15.55380	10.01663	8.90417
C	16.53281	10.04248	9.93613
H	17.31682	10.79656	9.86619
C	16.57613	9.17861	11.03329
C	15.52867	8.18387	11.14476
C	5.69318	2.45308	2.60862
C	4.93485	2.32340	1.40105
C	5.42280	2.80418	0.19737
H	4.83013	2.66736	-0.71237
C	6.67071	3.48051	0.12236
C	7.41534	3.65805	1.27345
H	8.37082	4.19214	1.23571
C	6.96219	3.16495	2.53546
C	7.76519	3.41267	3.67741
H	8.71734	3.93255	3.49096
H	3.97911	1.79840	1.46737
H	7.02866	3.86720	-0.83457
C	8.33296	3.23224	6.01002
C	9.69742	3.58769	5.91942
H	10.17601	3.69875	4.94370
C	10.44599	3.80099	7.07115
H	11.50384	4.06170	6.97835
C	9.87690	3.63999	8.36226
C	8.53310	3.23465	8.45385
H	8.08351	3.12806	9.44387
C	7.76447	2.98910	7.30124
C	5.77008	2.16407	8.37556
C	4.41097	1.76065	8.42454
C	3.88361	1.33413	9.68245
H	4.54437	1.35216	10.55593
C	2.57843	0.89670	9.80612
C	1.74549	0.86193	8.65528

```
  H        0.71301        0.51142        8.74909
  C        2.21581        1.25357        7.41296
  C        3.55102        1.74390        7.24942
 Ni       14.28132        6.02139       12.57939
  C       17.69696        9.27997       12.08193
  C       15.55307       11.01419        7.73097
  C       18.45856        7.93099       12.15135
  H       19.24341        7.98526       12.92424
  H       17.78716        7.09710       12.39851
  H       18.94778        7.71181       11.18743
  C       17.08523        9.63422       13.46026
  H       16.35575        8.87985       13.78205
  H       17.88406        9.69067       14.21913
  H       16.58425       10.61610       13.42233
  C       18.72726       10.37506       11.73333
  H       19.51047       10.38591       12.50836
  H       19.22514       10.19014       10.76634
  H       18.27761       11.38215       11.71034
  C       14.21961       11.80270        7.73766
  H       14.19710       12.51792        6.89828
  H       13.34749       11.13675        7.63298
  H       14.09956       12.37103        8.67442
  C       15.68333       10.23736        6.39702
  H       15.67641       10.94007        5.54685
  H       16.62544        9.66626        6.36080
  H       14.85181        9.52877        6.24961
  C       16.71373       12.02440        7.81704
  H       16.66418       12.63313        8.73522
  H       17.69804       11.52839        7.78030
  H       16.66273       12.71633        6.96094
  H        6.30017        2.16584        9.34076
  H        2.19221        0.56870       10.77389
  H        1.58078        1.23446        6.52423
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Complex 2+ (S=1)

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124
Complex 2 oxidized triplet
 Cu        5.63564        2.57985        5.46822
  C       14.92727        5.14992       15.23922
  N       13.19559        4.53089       12.90667
  O       15.07593        5.99374       14.25346
  C       15.63544        5.36034       16.49000
  N       13.40286        6.12521       10.92242
  O       15.44808        7.41506       12.19905
  C       15.48510        4.39067       17.47812
  H       16.02545        4.54145       18.41488
  N        7.49307        2.97027        4.88614
  O        4.94805        2.51658        3.66067
  C       14.67994        3.21662       17.37376
  N        6.41849        2.64826        7.28510
  O        3.86261        2.17170        6.09518
  C       13.97518        3.04581       16.19114
  H       13.32045        2.18120       16.05158
  C       14.06964        3.98824       15.13006
  C       13.27050        3.76409       13.98392
```

H	12.64601	2.86177	14.00677
C	16.50794	6.60594	16.71805
C	17.67034	6.62338	15.69376
H	18.29180	7.52019	15.85512
H	17.29955	6.64142	14.66071
H	18.31502	5.73775	15.82181
C	15.63072	7.87689	16.57637
H	14.84427	7.89340	17.34937
H	15.15074	7.93370	15.58955
H	16.25471	8.77636	16.71032
C	17.13006	6.62846	18.13002
H	16.36461	6.64024	18.92437
H	17.72949	7.54628	18.24012
H	17.80557	5.77389	18.30412
C	14.61927	2.22769	18.54636
C	14.09704	2.95968	19.80880
H	14.74751	3.79922	20.10294
H	14.05693	2.25869	20.65907
H	13.08232	3.35810	19.64565
C	16.04210	1.67814	18.82094
H	16.43704	1.14213	17.94247
H	16.01484	0.97318	19.66854
H	16.75393	2.47927	19.07745
C	13.68511	1.03824	18.25289
H	14.02206	0.45522	17.37913
H	12.64595	1.36451	18.07758
H	13.67364	0.35628	19.11799
C	12.31266	4.23390	11.84429
C	11.35030	3.20747	11.81167
H	11.20307	2.54316	12.66605
C	10.57304	3.01818	10.66896
H	9.85667	2.19282	10.64310
C	10.73325	3.83646	9.52562
C	11.68769	4.87494	9.57286
H	11.79923	5.52218	8.70006
C	12.45080	5.09106	10.72856
C	13.55009	7.10773	10.05111
H	12.87017	7.12714	9.18925
C	14.51367	8.14641	10.10122
C	14.52104	9.08794	9.04051
H	13.75294	8.99438	8.26504
C	15.47558	10.09846	8.96764
C	16.45709	10.12074	9.99552
H	17.22862	10.88846	9.93752
C	16.51807	9.23600	11.07636
C	15.48619	8.22348	11.16998
C	5.62083	2.59320	2.55671
C	4.90462	2.45873	1.31946
C	5.55725	2.51492	0.10029
H	4.98152	2.40578	-0.82384
C	6.96263	2.70973	0.02984
C	7.68943	2.84912	1.20148
H	8.77338	3.00266	1.15890
C	7.06277	2.80247	2.48113
C	7.89086	2.97331	3.62594
H	8.96211	3.11568	3.41185

H	3.82494	2.30579	1.38931
H	7.46412	2.75030	-0.93996
C	8.35608	3.18913	5.97246
C	9.70513	3.58966	5.87509
H	10.16584	3.74528	4.89664
C	10.47382	3.79535	7.01838
H	11.52672	4.07099	6.91230
C	9.92184	3.61401	8.30854
C	8.57121	3.22571	8.41061
H	8.12649	3.14344	9.40544
C	7.78113	3.00820	7.26926
C	5.75591	2.34018	8.38540
C	4.37601	2.00696	8.47444
C	3.84832	1.72641	9.77070
H	4.52922	1.77063	10.62817
C	2.51345	1.41096	9.96036
C	1.64791	1.36384	8.83663
H	0.59165	1.11583	8.97993
C	2.11613	1.62475	7.55880
C	3.49117	1.95108	7.32029
Ni	14.28191	6.01251	12.56709
C	17.64005	9.33592	12.12314
C	15.45309	11.11766	7.81462
C	18.42188	7.99722	12.16745
H	19.20908	8.05185	12.93781
H	17.76493	7.14894	12.40449
H	18.91044	7.80077	11.19841
C	17.02634	9.65724	13.50882
H	16.31109	8.88524	13.82060
H	17.82690	9.71484	14.26561
H	16.50861	10.63085	13.48908
C	18.65277	10.45214	11.79023
H	19.43862	10.46065	12.56247
H	19.14980	10.29152	10.81855
H	18.18850	11.45276	11.78712
C	14.10769	11.88577	7.84639
H	14.06925	12.61552	7.02041
H	13.24440	11.20954	7.73493
H	13.98645	12.43534	8.79408
C	15.58453	10.36777	6.46512
H	15.56298	11.08777	5.62999
H	16.53382	9.81019	6.41123
H	14.76108	9.65213	6.30760
C	16.59992	12.14225	7.91279
H	16.54720	12.73363	8.84205
H	17.59090	11.66117	7.86053
H	16.53371	12.84890	7.07002
H	6.30122	2.33086	9.34292
H	2.12917	1.20198	10.96142
H	1.45843	1.58782	6.68698