Supplementary material for Low Temperature ^{65}Cu NMR Spectroscopy of the Cu^{+} Site in Azurin, by Andrew S. Lipton, Robert W. Heck, Wibe A. de Jong, Amy R. Gao, Xiongjian Wu, Adrienne Roehrich, Gerard S. Harbison and Paul D. Ellis

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Table 5: optimized coordinates of bis(imidazole) copper(I)methylsulfide

Cu	29.0	-0.1689029072	-0.5489970740	0.0000000000
H	1.0	-2.4915940951	-0.3844348329	-4.4682044451
H	1.0	-2.4915940951	-0.3844348329	4.4682044451
S	16.0	2.1258474413	-0.3813476530	0.0000000000
C	6.0	2.1464422778	1.4662955721	0.0000000000
H	1.0	3.1870522527	1.8270963879	0.0000000000
H	1.0	1.6436886554	1.8772710890	-0.8927627025
H	1.0	1.6436886554	1.8772710890	0.8927627025
N	7.0	-0.7045513895	-0.5077213523	-1.8287079781
N	7.0	-0.7045513895	-0.5077213523	1.8287079781
C	6.0	-1.9008252771	-0.5035030861	-2.4342152615
C	6.0	-1.9008252771	-0.5035030861	2.4342152615
C	6.0	0.2479689360	-0.4043287280	-2.8323071646
C	6.0	0.2479689360	-0.4043287280	2.8323071646
N	7.0	-1.7417059886	-0.4043872393	-3.7866021700
N	7.0	-1.7417059886	-0.4043872393	3.7866021700
C	6.0	-0.3885846422	-0.3408547007	-4.0625534917
C	6.0	-0.3885846422	-0.3408547007	4.0625534917
H	1.0	-0.0074032073	-0.2581965349	-5.0756380723
H	1.0	-0.0074032073	-0.2581965349	5.0756380723
H	1.0	1.3050156411	-0.3957464050	-2.5659833648
H	1.0	1.3050156411	-0.3957464050	2.5659833648
H	1.0	-2.8672281644	-0.5696218264	-1.9452355108
H	1.0	-2.8672281644	-0.5696218264	1.9452355108

Table 6: optimized coordinates of the quantum region of azurin, in pdb notation.

```
ATOM      1 C                    3.007  -6.959 -10.675  6.00
ATOM      2 O                    2.722  -5.790 -10.927  8.00
ATOM      3 N                    3.418  -7.815 -11.647  7.00
ATOM      4 H                    3.627  -8.809 -11.432  1.00
ATOM      5 C                    3.488  -7.353 -12.996  6.00
ATOM      6 H                    3.889  -6.326 -13.036  1.00
ATOM      7 C                    6.392  -0.911 -11.588  6.00
ATOM      8 O                    6.385  -1.776 -10.714  8.00
ATOM      9 N                    6.729   0.366 -11.324  7.00
ATOM     10 H                    6.636   1.106 -12.036  1.00
ATOM     11 C                    6.967   0.716  -9.963  6.00
ATOM     12 H                    7.362   1.753  -9.921  1.00
ATOM     13 H                    7.710   0.020  -9.517  1.00
ATOM     14 C                    5.678   0.645  -9.169  6.00
ATOM     15 O                    4.629   1.090  -9.644  8.00
ATOM     16 N                    5.801   0.117  -7.945  7.00
ATOM     17 H                    6.703  -0.302  -7.644  1.00
ATOM     18 C                    4.704   0.122  -7.034  6.00
ATOM     19 H                    3.890   0.750  -7.482  1.00
ATOM     20 C                    4.114  -1.262  -6.769  6.00
ATOM     21 H                    3.261  -1.103  -6.064  1.00
ATOM     22 H                    4.863  -1.890  -6.237  1.00
ATOM     23 C                    3.640  -1.950  -7.993  6.00
ATOM     24 N                    2.848  -1.322  -8.925  7.00
ATOM     25 C                    2.562  -2.232  -9.847  6.00
ATOM     26 H                    1.940  -2.049 -10.735  1.00
ATOM     27 N                    3.125  -3.419  -9.550  7.00
ATOM     28 H                    2.999  -4.316 -10.084  1.00
ATOM     29 C                    3.822  -3.261  -8.383  6.00
ATOM     30 H                    4.413  -4.071  -7.932  1.00
ATOM     31 C                    5.147   0.687  -5.712  6.00
ATOM     32 O                    6.198   0.311  -5.188  8.00
ATOM     33 N                    4.287   1.545  -5.145  7.00
ATOM     34 H                    3.446   1.881  -5.691  1.00
ATOM     35 C                    4.459   1.904  -3.783  6.00
ATOM     36 H                    5.275   1.269  -3.371  1.00
ATOM     37 C                    0.355   1.740  -6.479  6.00
ATOM     38 H                   -0.477   1.473  -7.169  1.00
ATOM     39 H                    0.550   0.881  -5.803  1.00
ATOM     40 S                    1.865   2.131  -7.434 16.00
ATOM     41 C                    1.592   6.304  -8.524  6.00
ATOM     42 O                    1.796   7.324  -9.180  8.00
ATOM     43 N                    2.025   5.091  -8.945  7.00
ATOM     44 H                    1.839   4.196  -8.398  1.00
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ATOM     45 C                2.726   5.024 -10.172  6.00
ATOM     46 H                3.475   5.842 -10.201  1.00
ATOM     47 C                3.337   3.653 -10.366  6.00
ATOM     48 H                2.554   2.862 -10.267  1.00
ATOM     49 H                3.997   3.477  -9.488  1.00
ATOM     50 C                4.122   3.459 -11.623  6.00
ATOM     51 C                3.475   3.238 -12.847  6.00
ATOM     52 H                2.371   3.165 -12.868  1.00
ATOM     53 C                4.200   3.134 -14.032  6.00
ATOM     54 H                3.660   3.045 -14.995  1.00
ATOM     55 C                5.592   3.208 -14.021  6.00
ATOM     56 H                6.161   3.145 -14.965  1.00
ATOM     57 C                6.254   3.397 -12.805  6.00
ATOM     58 H                7.353   3.479 -12.779  1.00
ATOM     59 C                5.521   3.527 -11.624  6.00
ATOM     60 H                6.042   3.696 -10.665  1.00
ATOM     61 C               -0.590   1.846 -10.605  6.00
ATOM     62 H               -0.785   1.077  -9.816  1.00
ATOM     63 H               -0.285   2.758 -10.044  1.00
ATOM     64 C                0.534   1.333 -11.437  6.00
ATOM     65 N                1.662   0.822 -10.841  7.00
ATOM     66 C                2.480   0.438 -11.811  6.00
ATOM     67 H                3.501   0.060 -11.638  1.00
ATOM     68 N                1.921   0.649 -13.017  7.00
ATOM     69 H                2.380   0.505 -13.955  1.00
ATOM     70 C                0.701   1.232 -12.809  6.00
ATOM     71 H                0.048   1.533 -13.640  1.00
ATOM     72 C               -2.609  -0.343  -7.728  6.00
ATOM     73 H               -2.016  -0.346  -6.786  1.00
ATOM     74 H               -2.558   0.696  -8.117  1.00
ATOM     75 C               -2.011  -1.327  -8.705  6.00
ATOM     76 H               -2.403  -1.197  -9.736  1.00
ATOM     77 H               -2.231  -2.383  -8.425  1.00
ATOM     78 S               -0.209  -1.182  -8.841 16.00
ATOM     79 C                0.209  -1.830  -7.217  6.00
ATOM     80 H                1.307  -1.991  -7.202  1.00
ATOM     81 H               -0.314  -2.796  -7.034  1.00
ATOM     82 H               -0.048  -1.115  -6.406  1.00
ATOM     83 Cu               2.110   0.510  -8.934 29.00
ATOM     84 H                3.903   0.145 -15.548  1.00
ATOM     85 O                2.968   0.472 -15.521  8.00
ATOM     86 H                3.061   1.430 -15.704  1.00
ATOM     87 H_L              2.948  -7.361  -9.645  1.00
ATOM     88 H_L              4.078  -8.015 -13.634  1.00
ATOM     89 H_L              2.409  -7.295 -13.476  1.00
ATOM     90 H_L              6.152  -1.131 -12.634  1.00
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ATOM     91 H_L                  4.709   2.925  -3.637  1.00
ATOM     92 H_L                  3.468   1.611  -3.200  1.00
ATOM     93 H_L                  0.046   2.593  -5.850  1.00
ATOM     94 H_L                  1.030   6.344  -7.587  1.00
ATOM     95 H_L                  1.963   5.265 -11.068  1.00
ATOM     96 H_L                 -1.496   2.043 -11.173  1.00
ATOM     97 H_L                 -3.646  -0.593  -7.492  1.00
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