Pulsed EPR Spectroscopy of ^{33}S-Labeled Molybdopterin in Sulfite Oxidase

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Supporting Information

Orbital Analysis for the Energy-Minimized Mo(V) DFT Model

The frontier orbital energy diagram for the optimized structure of the SO active site model is depicted in Figure S1, showing the canonical Kohn-Sham orbitals. The orbital scheme is typical for a Mo(V) center with d^1 configuration. Spin polarization effects strongly stabilize the majority spin orbitals such that the singly-occupied MO 168α is shifted below the highest occupied orbitals of mainly ligand character. As a result of strong intermixing between metal- and ligand-based orbitals, the d_{xy}-character (in the chosen coordinate system) is spread over orbitals 168α and 169α (~26% Mo character in each orbital, see Table S1). In the former, the d_{xy} orbital mixes with the out-of-plane p_z orbitals of the MPT S atoms, while the latter mixes d_{xy} orbital character with the S^V orbital of cysteine.[1,2] Similar interactions have been found for the DFT model $[MoO(SCH_3)(dithiolene)OH]^-$ (dithiolene = SCHCHS),[3] for example, which features the same inner-sphere coordination environment as SO. The empty β-spin d_{xy} orbital (172β) corresponds to the lowest unoccupied MO (LUMO) and is of predominantly Mo character (77%). Above the d_{xz} orbital lie the remaining unoccupied metal d-orbitals, having d_{yz} (173β), d_{xz} (174β), $d_{x^2-y^2}$ (176β), and d_{z^2} (177β) character, respectively.

Additionally, four corresponding empty α-spin d-orbitals can be readily identified within the vacant α-spin manifold.

A chemically more intuitive picture can be obtained by visualizing the electronic structure in terms of localized molecular orbitals (LMOs). The Pipek-Mezey population-localization protocol yields 10 molecular orbitals of mainly d-character localized on the Mo center, shown in Figure S2. Note that the MO diagram focuses entirely on the metal-centered orbital manifold, omitting ligand-orbitals. Furthermore, the energy splitting is represented in a schematic way since all information about orbital energies is lost in the process. All 10 orbitals of predominantly metal d-character can be identified in the diagram, and from this the d_{xy} character of the singly occupied orbital becomes much more recognizable.

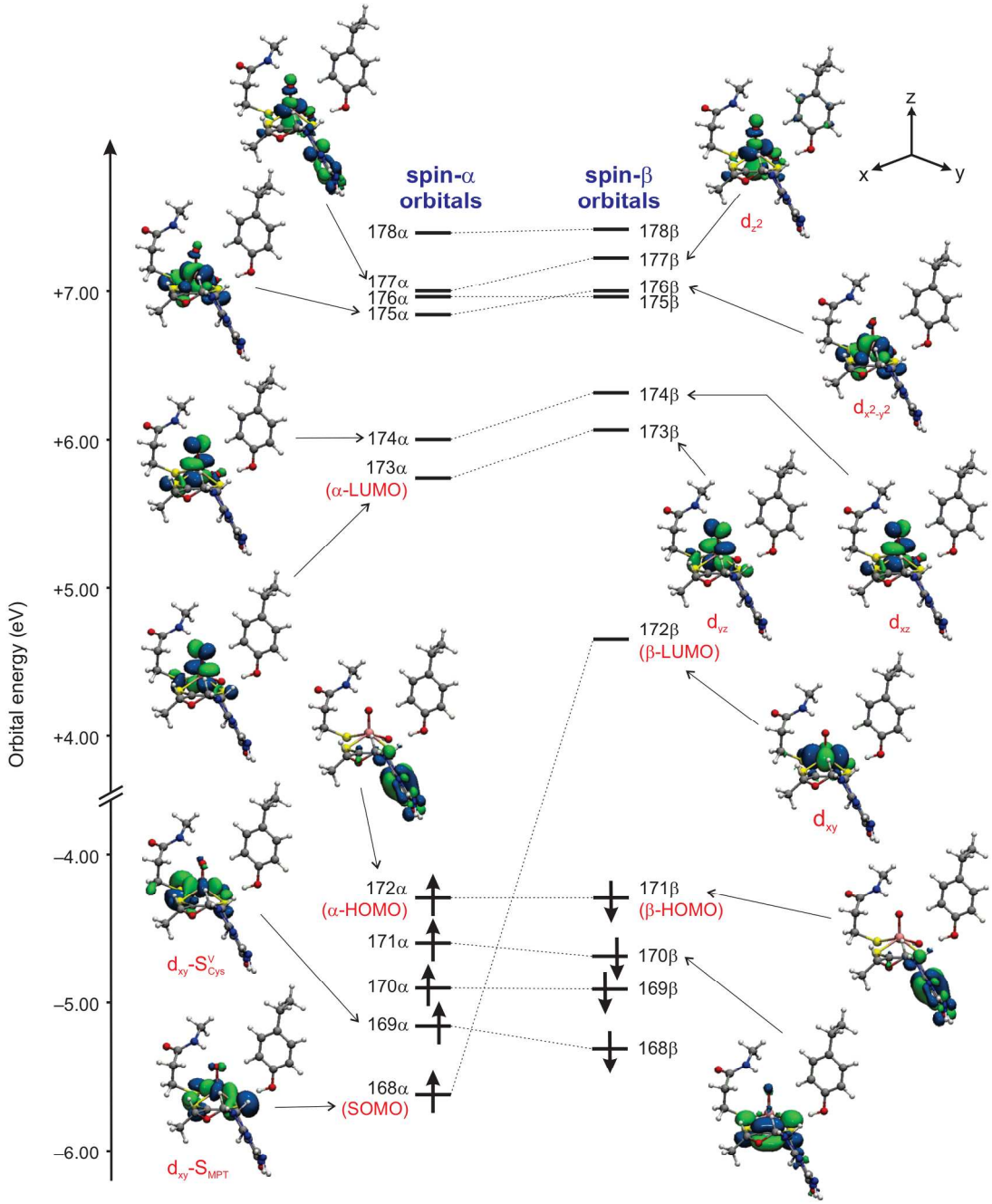

Figure S1. Canonical Kohn-Sham molecular orbital diagram (frontier orbital region) for the computational SO active site model (B3LYP/TZVP/ZORA). HOMO = Highest Molecular Orbital; LUMO = Lowest Unoccupied Molecular Orbital.

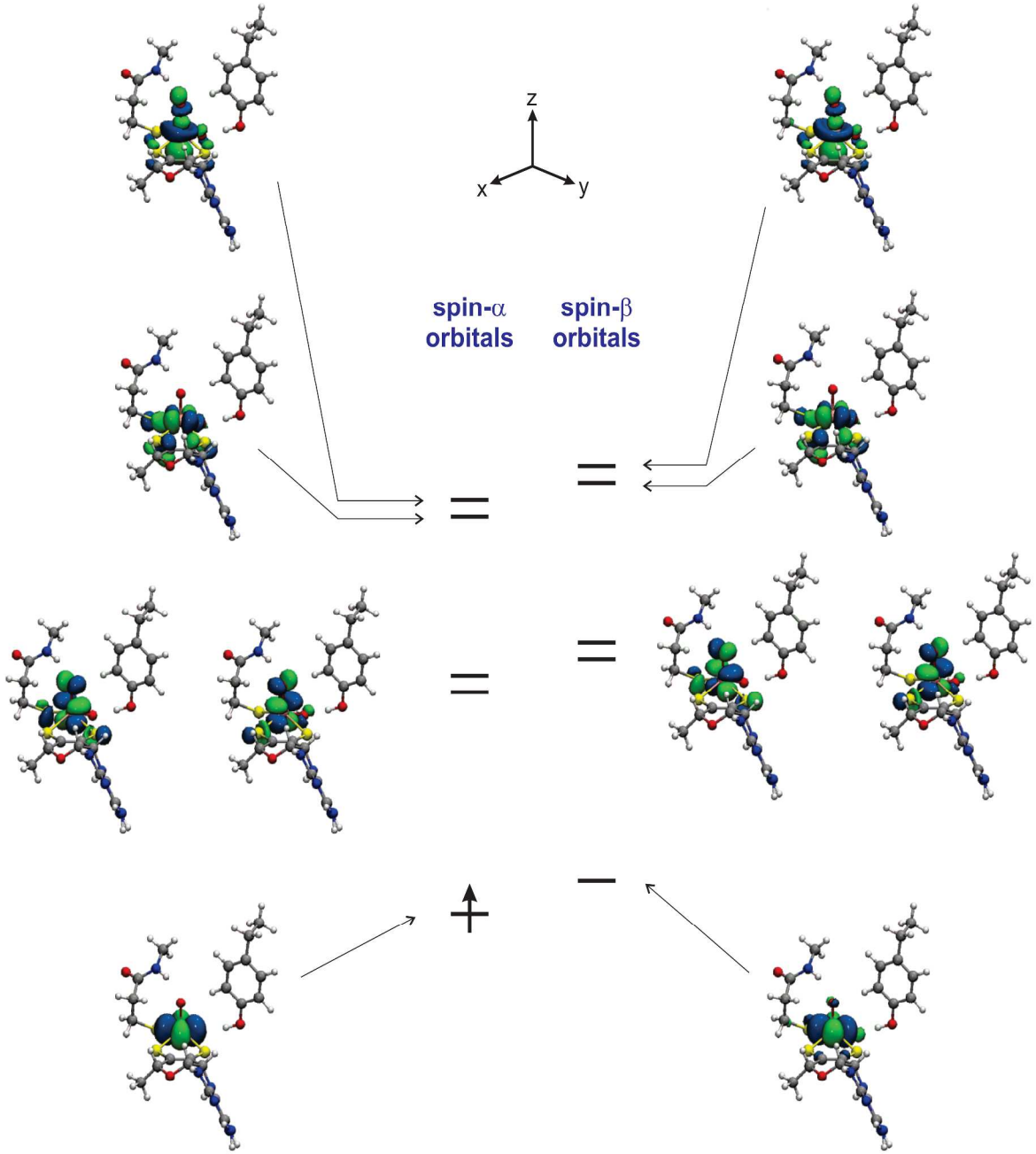

Figure S2. Pipek-Mezey localized molecular orbitals of the Mo *d*-orbital manifold of the computational SO active site model. Note that the diagram is a schematic representation of the ligand field splitting.

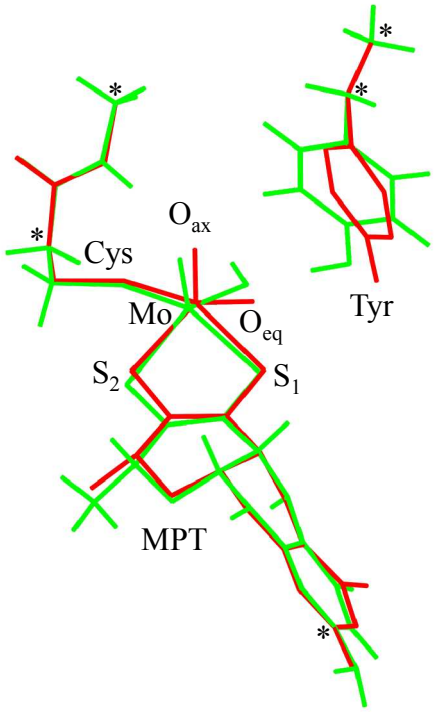

Figure S3. Overlay of the crystallographic atom coordinates (from pdb 1SOX) and the minimum-energy geometry optimized Mo(V) structure, including added H atoms (red and green structures, respectively). Atoms marked by asterisks were constrained to their relative crystallographic coordinate positions. S_1 and S_2 correspond to index numbers 30 and 32, respectively, in each of the DFT models (see below).

Table S1. Compositions of selected canonical KS orbitals in the frontier orbital region.[a]

Spin-α	Center					
	Mo(36)	S(4)	S(30)	S(32)	O(16)	O(37)
168α	26.4%	14.0%	28.0%	12.7%	4.3%	2.9%
169α	26.8%	38.6%	10.6%	4.3%	2.2%	2.1%
173α	59.0%	8.2%	8.6%	0.0%	0.0%	19.1%
174α	61.5%	0.6%	0.8%	9.7%	4.5%	18.5%
175α	41.5%	11.8%	8.6%	3.8%	4.2%	5.1%
177α	34.1%	0.8%	31.0%	5.6%	3.5%	8.9%

Spin-β	Center					
	Mo(36)	S(4)	S(30)	S(32)	O(16)	O(37)
172β	76.7%	6.4%	2.4%	2.6%	2.2%	0.5%
173β	62.1%	7.4%	7.5%	0.0%	0.0%	17.5%
174β	64.2%	0.6%	0.8%	9.0%	4.2%	16.4%
176β	36.9%	9.9%	7.5%	4.7%	4.1%	2.0%
177β	48.3%	1.8%	4.6%	5.9%	4.0%	13.0%

[a]The numbers in parentheses correspond to the atom coordinates of the DFT model (see below).

ORCA Input Files and Optimized Model Coordinates

Input used for geometry optimization calculations:

```
! BP86 TZVP RI TZV/J OPT GRID4 NormalPrint VDW10
%geom
Constraints
{ C 0 C }
{ C 6 C }
{ C 7 C }
{ C 8 C }
{ C 18 C }
# additional angle constraints for the models with dihedral angles defined at
# 120, 150, 180, 210, and 240 degrees. Atoms 68 and 69 are dummy atoms located
# between the dithiolene sulfurs and adjacent carbon atoms, as described within
# the Materials and Methods section.
{ A 36 68 69 C }
{ A 30 68 32 C }
{ A 29 69 31 C }
end
end
* xyz -1 2
<atom coordinates>
*
%cosmo
epsilon 4
end
```

Input used for all properties calculations:

```
! B3LYP TZVP ZORA COSMO TightSCF NPA GRID4 LargePrint VDW10
* xyz -1 2
<atom coordinates>
*
%cosmo
epsilon 4
end
%rel
        SOCType 3
        SOCFlags 1,3,3,0
        method ZORA
        modelpot 1,1,1,1
        picturechange true
        modeldens rhoZORA
end
%eprnmr
        gtensor 1
        Nuclei = all Mo {aiso, adip, aorb, rho, fgrad}
        Nuclei = 38 {aiso, adip, aorb, rho, fgrad}
        Nuclei = 17 {aiso, adip, aorb, rho, fgrad}
        Nuclei = 68 {aiso, adip, aorb, rho, fgrad}
        Nuclei = 53 {aiso, adip, aorb, rho, fgrad}
        Nuclei = 31 {aiso, adip, aorb, rho, fgrad}
        Nuclei = 33 {aiso, adip, aorb, rho, fgrad}
        Nuclei = 5  {aiso, adip, aorb, rho, fgrad}
end
```

Optimized atom coordinates:

Dihedral Angle = "relaxed"

```
C -1.6330   2.8589  1.6059
C -0.5316   3.5803  2.3827
O -0.4775   4.8226  2.4282
C -1.5257   3.0956  0.0964
S -0.0422   2.3194 -0.7186
N  0.3581   2.7822  3.0276
C  1.5025   3.3233  3.7538
C  5.5613  -1.6784  5.8455
C  4.1389  -2.2351  5.5830
C  3.8534  -2.2162  4.0966
C  3.3564  -1.0577  3.4803
C  4.2123  -3.2897  3.2626
C  3.2330  -0.9571  2.0941
C  4.0886  -3.2111  1.8729
C  3.6029  -2.0363  1.2709
O  3.5176  -1.9897 -0.0886
O  1.8811   0.0000 -0.7847
N -4.1717  -7.7399 -1.1233
C -3.9495  -8.4585 -2.2020
N -4.5112  -9.7163 -2.3188
N -3.1297  -8.0373 -3.2105
C -2.3905  -6.8255 -3.1749
O -1.6836  -6.5077 -4.1504
N -1.8619  -4.8941 -1.7725
C -2.0087  -4.2296 -0.4701
C -3.4228  -4.4100  0.1244
N -3.7829  -5.7926  0.0959
C -2.5858  -6.0802 -1.9688
C -3.5109  -6.5438 -1.0346
C -1.7091  -2.7561 -0.5839
S  0.0039  -2.3053 -0.7575
C -2.7037  -1.8339 -0.5774
S -2.3268  -0.0932 -0.6646
C -4.1730  -2.2162 -0.4754
O -4.3677  -3.6378 -0.6458
C -5.0660  -1.5336 -1.5078
Mo 0.0000   0.0000  0.0000
O  0.0000   0.0000  1.7379
H -2.5885   3.2917  1.9463
H -1.6545   1.7849  1.8302
H -2.4215   2.7142 -0.4114
H -1.4396   4.1712 -0.1128
H  0.3276   1.7798  2.8221
H  1.1975   4.2360  4.2804
H  5.8044  -1.6767  6.9203
H  5.6463  -0.6467  5.4738
H  4.0656  -3.2618  5.9758
H  3.3971  -1.6253  6.1226
H  3.0657  -0.2051  4.1008
H  4.6004  -4.2102  3.7089
H  2.8392  -0.0480  1.6393
H  4.3600  -4.0566  1.2375
H  2.9515  -1.2034 -0.3755
H -5.2754  -9.8740 -1.6653
H -4.7140 -10.0448 -3.2603
H -2.9684  -8.6205 -4.0315
H -1.8823  -4.2570 -2.5695
H -1.2997  -4.6876  0.2425
H -3.4369  -4.0586  1.1720
H -4.5968  -6.0861  0.6316
H -4.5242  -1.9411  0.5424
H -5.0410  -0.4435 -1.3793
H -4.7282  -1.7761 -2.5251
H -6.1018  -1.8790 -1.3821
H  1.8484   2.5811  4.4835
H  2.3345   3.5772  3.0769
H  6.3158  -2.2864  5.3247
H  2.2653   0.8785 -0.9614
```

Dihedral Angle = 120

```
C -1.6921  2.9107  1.4729
C -0.6236  3.5406  2.3737
O -0.5315  4.7702  2.4983
C -1.4101  3.1671 -0.0107
S  0.1136  2.3213 -0.6629
N  0.1915  2.6664  3.0308
C  1.3138  3.1384  3.8337
C  4.9720 -2.1356  5.9945
C  3.5441 -2.6083  5.6206
C  3.3589 -2.5089  4.1223
C  2.9682 -1.3000  3.5273
C  3.7334 -3.5596  3.2684
C  2.9690 -1.1284  2.1445
C  3.7277 -3.4116  1.8809
C  3.3569 -2.1854  1.2977
O  3.3982 -2.0744 -0.0522
O  1.9076  0.0000 -0.7338
N -4.0184 -7.1352  1.9856
C -4.3008 -8.0929  1.1401
N -4.9899 -9.2354  1.5703
N -3.8976 -8.0628 -0.1671
C -3.1189 -7.0149 -0.7371
O -2.8302 -7.0372 -1.9429
N -1.9434 -4.9640 -0.1781
C -1.6261 -3.8876  0.7643
C -2.7064 -3.7802  1.8611
N -2.9689 -5.0774  2.4234
C -2.7574 -6.0071  0.2209
C -3.2544 -6.0991  1.5173
C -1.4978 -2.5620  0.0505
S  0.0046 -2.2902 -0.8693
C -2.5052 -1.6421  0.1012
S -2.3398 -0.0541 -0.6996
C -3.8009 -1.8971  0.8490
O -3.9243 -3.2604  1.3032
C -5.0447 -1.6284  0.0050
Mo 0.0000  0.0000  0.0000
O  0.0000  0.0000  1.7335
H -2.6428  3.4051  1.7320
H -1.8099  1.8337  1.6547
H -2.2666  2.8442 -0.6181
H -1.2433  4.2417 -0.1750
H  0.1746  1.6837  2.7348
H  0.9950  4.0057  4.4265
H  5.1553 -2.1893  7.0807
H  5.1249 -1.0965  5.6680
H  3.3952 -3.6464  5.9609
H  2.7985 -1.9869  6.1430
H  2.6609 -0.4637  4.1625
H  4.0386 -4.5175  3.7015
H  2.6542 -0.1818  1.7067
H  4.0027 -4.2370  1.2222
```

```
H  2.8965 -1.2444 -0.3370
H -5.3330 -9.0951  2.5197
H -5.7429 -9.5326  0.9493
H -4.0773 -8.8451 -0.7944
H -1.9622 -4.7356 -1.1694
H -0.6687 -4.1062  1.2697
H -2.3394 -3.1086  2.6589
H -3.5848 -5.0839  3.2348
H -3.8099 -1.2277  1.7373
H -5.0863 -0.5745 -0.2989
H -5.0238 -2.2597 -0.8939
H -5.9413 -1.8713  0.5922
H  1.6407  2.3309  4.5018
H  2.1643  3.4507  3.2041
H  5.7233 -2.7567  5.4846
H  2.2812  0.8876 -0.8852
```

Dihedral Angle = 150

```
C -1.5758  2.9381  1.5716
C -0.4472  3.5790  2.3847
O -0.3243  4.8096  2.4572
C -1.4111  3.1734  0.0680
S  0.0527  2.3239 -0.7017
N  0.3801  2.7130  3.0384
C  1.5298  3.1948  3.7964
C  5.3233 -2.0450  5.8012
C  3.8842 -2.5300  5.4918
C  3.6288 -2.4462  4.0040
C  3.1689 -1.2569  3.4203
C  3.9937 -3.4933  3.1413
C  3.0888 -1.1009  2.0379
C  3.9101 -3.3608  1.7554
C  3.4653 -2.1549  1.1823
O  3.4239 -2.0623 -0.1696
O  1.8892  0.0000 -0.7719
N -4.4523 -7.5467 -1.2104
C -4.3391 -8.1895 -2.3450
N -5.0484 -9.3797 -2.5591
N -3.4959 -7.7764 -3.3406
C -2.6458 -6.6360 -3.2460
O -1.9397 -6.3038 -4.2090
N -1.9134 -4.9012 -1.7076
C -1.9970 -4.2088 -0.4197
C -3.3964 -4.3892  0.2073
N -3.7792 -5.7750  0.1815
C -2.7323 -5.9815 -1.9688
C -3.6516 -6.4484 -1.0342
C -1.6985 -2.7338 -0.5638
S  0.0101 -2.2981 -0.7956
C -2.6930 -1.8096 -0.5397
S -2.3307 -0.0663 -0.6626
C -4.1549 -2.1937 -0.3872
O -4.3653 -3.6166 -0.5171
C -5.0690 -1.5460 -1.4240
Mo 0.0000  0.0000  0.0000
O  0.0000  0.0000  1.7343
H -2.5046  3.4370  1.8950
H -1.6806  1.8648  1.7809
H -2.3112  2.8405 -0.4677
H -1.2609  4.2457 -0.1244
H  0.3279  1.7213  2.7857
H  1.2391  4.0918  4.3586
H  5.5521 -2.0885  6.8792
H  5.4554 -1.0076  5.4602
H  3.7581 -3.5659  5.8480
H  3.1575 -1.9099  6.0415
H  2.8679 -0.4248  4.0640
H  4.3529 -4.4357  3.5668
H  2.7193 -0.1703  1.6084
H  4.1781 -4.1832  1.0900
H  2.9087 -1.2347 -0.4330
H -5.7177 -9.5232 -1.8039
H -5.5063 -9.4391 -3.4690
H -3.3748 -8.3227 -4.1919
H -1.5680 -4.3808 -2.5102
H -1.2672 -4.6483  0.2849
H -3.3606 -4.0494  1.2600
H -4.6446 -5.9975  0.6706
H -4.4819 -1.8854  0.6307
H -5.0489 -0.4525 -1.3296
H -4.7330 -1.8198 -2.4334
H -6.0980 -1.9036 -1.2780
H  1.8564  2.4097  4.4906
H  2.3717  3.4647  3.1367
H  6.0571 -2.6654  5.2655
H  2.2571  0.8768 -0.9818
```

Dihedral Angle = 180

```
C -1.6844  2.8868  1.6207
C -0.6005  3.5537  2.4739
O -0.5518  4.7845  2.6067
C -1.4663  3.1430  0.1249
S  0.0589  2.3568 -0.5859
N  0.2860  2.7115  3.0786
C  1.4190  3.2345  3.8361
C  5.3443 -1.8972  5.8668
C  3.9168 -2.4194  5.5641
C  3.6560 -2.3685  4.0759
C  3.1854 -1.1951  3.4694
C  4.0135 -3.4346  3.2340
C  3.0862 -1.0728  2.0847
C  3.9110 -3.3359  1.8466
C  3.4526 -2.1467  1.2494
O  3.3924 -2.0938 -0.1040
O  1.8957  0.0000 -0.7402
N -3.6754 -6.7564 -4.5861
C -3.0410 -7.0798 -5.6845
N -3.5345 -8.0906 -6.5232
N -1.8487 -6.5056 -6.0375
C -1.1825 -5.5094 -5.2683
O -0.1181 -5.0151 -5.6686
N -1.3500 -4.2534 -3.1919
C -1.9276 -4.0403 -1.8717
C -3.4527 -4.2819 -1.9314
N -3.7444 -5.5318 -2.5791
C -1.8743 -5.1926 -4.0475
C -3.0812 -5.8291 -3.7709
C -1.6703 -2.6403 -1.3654
S -0.0350 -2.3189 -0.7682
C -2.6315 -1.6881 -1.3898
S -2.3166 -0.0636 -0.7401
C -4.0225 -1.9520 -1.9439
O -4.0973 -3.2151 -2.6412
C -4.4973 -0.9012 -2.9436
```

```
Mo 0.0000  0.0000  0.0000
O  0.0000  0.0000  1.7351
H -2.6383  3.3540  1.9148
H -1.7592  1.8084  1.8182
H -2.3274  2.7790 -0.4544
H -1.3524  4.2223 -0.0524
H  0.2876  1.7286  2.7882
H  1.0749  4.0443  4.4930
H  5.5723 -1.9188  6.9454
H  5.4540 -0.8626  5.5096
H  3.8143 -3.4516  5.9378
H  3.1761 -1.8077  6.1045
H  2.8891 -0.3488  4.0965
H  4.3817 -4.3654  3.6769
H  2.7058 -0.1537  1.6408
H  4.1750 -4.1730  1.1982
H  2.8855 -1.2711 -0.3942
H -4.4571 -8.3818 -6.2024
H -3.5577 -7.8389 -7.5121
H -1.3311 -6.8291 -6.8531
H -0.5069 -3.7569 -3.4637
H -1.5123 -4.7612 -1.1386
H -3.8397 -4.3225 -0.8946
H -4.7275 -5.7977 -2.5876
H -4.7321 -1.9872 -1.0866
H -4.5708  0.0830 -2.4636
H -3.7812 -0.8343 -3.7738
H -5.4820 -1.1898 -3.3381
H  1.8494  2.4245  4.4387
H  2.1986  3.6448  3.1724
H  6.0923 -2.5092  5.3411
H  2.3046  0.8847 -0.7607
```

Dihedral Angle = 210

```
C -1.6302  2.9796  1.4550
C -0.5407  3.6350  2.3111
O -0.4553  4.8666  2.4111
C -1.3627  3.1713 -0.0436
S  0.1681  2.3238 -0.6594
N  0.3106  2.7809  2.9507
C  1.4660  3.2844  3.6868
C  5.1528 -1.9228  5.9581
C  3.7071 -2.3963  5.6616
C  3.4625 -2.3618  4.1700
C  3.0801 -1.1709  3.5354
C  3.7688 -3.4622  3.3525
C  3.0192 -1.0645  2.1475
C  3.7010 -3.3799  1.9617
C  3.3334 -2.1733  1.3361
O  3.3051 -2.1381 -0.0179
O  1.9219  0.0000 -0.6925
N -2.0696 -5.0380 -6.7831
C -1.0667 -5.1430 -7.6175
N -1.2034 -5.8893 -8.7948
N  0.1629 -4.6007 -7.3641
C  0.4769 -3.8501 -6.1912
O  1.6133 -3.3808 -6.0392
N -0.5164 -2.9776 -4.1347
C -1.4305 -3.2979 -3.0384
C -2.8616 -3.4196 -3.5996
N -2.8920 -4.3301 -4.7089
C -0.6349 -3.7389 -5.2893
C -1.8368 -4.3623 -5.6120
C -1.4060 -2.2251 -1.9798
S -0.0518 -2.2984 -0.8455
C -2.3648 -1.2626 -1.9332
S -2.3646 -0.0355 -0.6487
C -3.4971 -1.1903 -2.9458
O -3.3425 -2.1397 -4.0259
C -3.6153  0.1736 -3.6229
Mo 0.0000  0.0000  0.0000
O  0.0000  0.0000  1.7285
H -2.5738  3.4889  1.7091
H -1.7463  1.9118  1.6894
H -2.2117  2.7930 -0.6315
H -1.2227  4.2407 -0.2588
H  0.2855  1.7914  2.6859
H  1.1627  4.1522  4.2868
H  5.3783 -1.9309  7.0376
H  5.3022 -0.9006  5.5805
H  3.5625 -3.4165  6.0536
H  2.9887 -1.7446  6.1854
H  2.8276 -0.2968  4.1432
H  4.0694 -4.4063  3.8177
H  2.7095 -0.1309  1.6797
H  3.9248 -4.2421  1.3313
H  2.8504 -1.2905 -0.3324
H -2.1788 -6.1507 -8.9307
H -0.8218 -5.4403 -9.6274
H  0.9557 -4.7754 -7.9797
H  0.4373 -2.7408 -3.8605
H -1.1763 -4.2704 -2.5658
H -3.5179 -3.8133 -2.7982
H -3.8038 -4.5320 -5.1119
H -4.4474 -1.4190 -2.4127
H -3.8456  0.9507 -2.8834
H -2.6631  0.4220 -4.1105
H -4.4117  0.1394 -4.3803
H  1.8445  2.4915  4.3448
H  2.2736  3.6059  3.0075
H  5.8777 -2.5735  5.4469
H  2.3214  0.8878 -0.7572
```

Dihedral Angle = 240

```
C -1.6237  3.0005  1.4545
C -0.5544  3.6764  2.3183
O -0.4983  4.9091  2.4251
C -1.3355  3.1805 -0.0428
S  0.2057  2.3341 -0.6311
N  0.3166  2.8389  2.9547
C  1.4643  3.3624  3.6892
C  5.3092 -1.7672  5.8730
C  3.8783 -2.2793  5.5694
C  3.6283 -2.2543  4.0792
C  3.1911 -1.0820  3.4452
C  3.9679 -3.3453  3.2621
C  3.1042 -0.9858  2.0579
C  3.8758 -3.2734  1.8723
C  3.4474 -2.0867  1.2467
O  3.3891 -2.0597 -0.1048
O  1.8932  0.0000 -0.7813
N  0.5941 -2.4700 -7.6904
C  1.8430 -2.3317 -8.0573
N  2.2229 -2.5865 -9.3819
```

```
N  2.8364 -2.0020 -7.1771
C  2.6238 -1.7556 -5.7868
O  3.5749 -1.4414 -5.0595
N  0.8609 -1.6614 -4.0943
C -0.3783 -2.2815 -3.6361
C -1.4697 -2.0592 -4.7008
N -1.0099 -2.5053 -5.9845
C  1.2498 -1.9202 -5.3984
C  0.3122 -2.2876 -6.3602
C -0.8191 -1.6807 -2.3254
S -0.0018 -2.3071 -0.8852
C -1.7720 -0.7023 -2.2959
S -2.3481 -0.0129 -0.7531
C -2.4149 -0.1568 -3.5617
O -1.8164 -0.6712 -4.7731
C -2.3116  1.3639 -3.6739
Mo 0.0000  0.0000  0.0000
O  0.0000  0.0000  1.7219
H -2.5770  3.5005  1.6896
H -1.7288  1.9329  1.6944
H -2.1749  2.7883 -0.6350
H -1.1991  4.2486 -0.2673
H  0.3111  1.8512  2.6869
H  1.1551  4.2580  4.2430
H  5.5290 -1.7704  6.9536
H  5.4333 -0.7410  5.4970
H  3.7612 -3.3029  5.9624
H  3.1412 -1.6485  6.0929
H  2.9136 -0.2154  4.0530
H  4.3120 -4.2746  3.7272
H  2.7553 -0.0665  1.5886
H  4.1250 -4.1293  1.2427
H  2.8819 -1.2373 -0.4082
H  1.3951 -2.7170 -9.9617
H  2.8461 -1.8858 -9.7836
H  3.8137 -1.9877 -7.4645
H  1.6029 -1.5558 -3.4012
H -0.2639 -3.3775 -3.4963
H -2.3637 -2.6500 -4.4172
H -1.6788 -2.4658 -6.7498
H -3.4878 -0.4558 -3.5445
H -2.8922  1.8456 -2.8775
H -1.2622  1.6708 -3.5706
H -2.6955  1.6842 -4.6530
H  1.8240  2.5971  4.3894
H  2.2869  3.6459  3.0111
H  6.0541 -2.3976  5.3650
H  2.2722  0.8854 -0.9393
```

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