Supporting Information

Local hybrid QM/QM calculations of reaction pathways in metallobiosites

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The zero point and thermal corrections to the stationary points used in this work were collected from previous studies of the reaction profiles. In the case of SO free energies were taken from reference 1. The electronic energies were computed at the DFT/BP86 level of theory using the cc-pVTZ basis set which was similar to the standard triple-ζ STO basis set used in reference 1. The free energy correction was estimated as the difference between the free energies from reference 1 and our BP86/cc-PVTZ electronic energies. All results are shown in Table S1.

Table S1: Free energies and relative electronic energies (in kJ/mol) for the SO reaction. a) Values were taken from reference 1. b) Electronic energies were computed using the DFT/BP86 with the cc-pVTZ basis set.

	ΔG(298K)$^{a)}$	$\Delta E_{el}^{b)}$	ΔG(298K)-ΔE_{el}
RS	0.0	0.0	0.0
TS1	28.9	-12.3	41.1
IM1	-41.0	-72.47	31.5
TS2	19.7	32.4	-12.8
PS	-0.4	23.86	-24.3

In the case of DMSOR free energy correction were readily available from reference 2. In Table S2 we present the free energies based on DFT optimizations and frequency calculations (B3LYP-D2 and def2-TZVPP basis set) with the electronic energy computed at the local coupled cluster level (LCCSD(T0)). Further information is available in the aforementioned reference.

Table S2: Free energies and relative electronic energies (in kJ/mol) for the DMSOR reaction with CH_3O^-. a) Values were taken from the reference 2.

	ΔG(300K)$^{a)}$	$\Delta E_{el}^{a)}$	ΔG(300K)-ΔE_{el}
RS	0.0	0.0	0.0
TS1	60.5	20.9	39.6
IM1	48.2	16.3	31.9
TS2	125.9	75.4	50.5
PS	78.5	-136.2	57.7

References:
(1) Hernandez-Marin, E.; Ziegler, T. *Inorganic Chemistry* **2009**, *48*, 1323-1333
(2) Li, J.-L.; Mata, R. A.; Ryde, U. *J. Chem. Theory Comput.* **2013**, *9*, 1799-1807

Optimized structures for SO mechanism

RS

37

C -1.869030 1.124900 -3.835220
N -0.513390 1.597580 -3.647890
C -0.139170 2.777590 -4.183130
N 0.964310 3.403240 -3.770720
N -0.849110 3.329340 -5.191960
O 0.411220 5.926620 -3.665000
S -0.275270 6.230000 -2.234410
O -1.659070 6.850570 -2.591580
O 0.588920 7.365990 -1.614960
O -0.172420 1.496780 -0.894430
Mo 0.000000 -0.000000 -0.000000
S -2.277240 -0.746990 -0.376390
C -2.582800 -2.129580 0.796210
O -0.016060 0.220950 1.729420
S 2.469730 -0.108700 -0.197650
C 2.940530 -1.669900 -0.845860
C 2.023160 -2.589570 -1.187280
S 0.297790 -2.246960 -1.055300
C 4.366933 -1.878202 -1.002332
C 2.379115 -3.884049 -1.735112
H -1.935200 -2.980530 0.551910
H -2.403000 -1.797680 1.826110
H -3.634960 -2.416370 0.668970
H 1.402860 2.990530 -2.947850
H 0.756340 4.487300 -3.687100
H -0.632900 4.305360 -5.396040
H -1.819980 3.065700 -5.311430
H -0.176030 1.477440 -2.679530
H -2.047460 0.852540 -4.885770
H -2.006380 0.215910 -3.237570
H -2.625240 1.863170 -3.520580
H 4.546146 -2.872422 -1.408942
H 4.770639 -1.129657 -1.682497
H 4.855294 -1.788969 -0.033074
H 3.463500 -3.979038 -1.766868
H 1.964062 -4.670711 -1.106768
H 1.977118 -3.974598 -2.743140

TS1

37

C -0.338597 -3.102456 -1.837435
S -0.512850 -2.425177 -0.125620
Mo 0.008754 -0.006072 -0.009773
O -0.682340 -0.343175 1.726721
O 1.755863 -0.003713 -0.012829
S -0.598019 2.406840 -0.076733
C -0.884910 2.780993 -1.786348

C -1.031390 1.827402 -2.726544
S -0.923023 0.097163 -2.337660
S -1.102069 0.890975 3.379741
O -2.627568 1.154591 3.478609
O -0.346344 2.200522 3.347091
O -0.682490 0.004525 4.530719
N -3.611116 1.489723 0.911468
C -3.852682 0.189679 0.651368
N -4.235177 -0.604426 1.679921
N -3.831551 -0.273573 -0.611827
C -3.965149 -1.696874 -0.913587
C -1.005696 4.188835 -2.111758
C -1.321547 2.157899 -4.108239
H -1.149130 -2.752716 -2.490517
H 0.623638 -2.813425 -2.279082
H -0.385552 -4.198438 -1.768611
H -3.000179 1.969024 0.238500
H -3.268164 1.625612 1.888983
H -3.889754 -0.264485 2.588234
H -4.108125 -1.605258 1.548030
H -3.200391 0.230184 -1.250099
H -4.907056 -2.082497 -0.498847
H -4.006784 -1.806426 -2.002778
H -3.103115 -2.269848 -0.529250
H -1.179082 4.300676 -3.181033
H -1.841719 4.618144 -1.561594
H -0.087001 4.705023 -1.837040
H -1.362579 3.240197 -4.221685
H -0.539239 1.755059 -4.749827
H -2.280740 1.726657 -4.390905

IM1

37
C -0.740660 -3.155600 -1.616040
S -0.715380 -2.312630 0.033360
Mo 0.010340 0.003520 -0.041190
O -0.708080 -0.286010 2.004080
S -0.794760 0.528950 3.336930
O -2.263490 0.495870 3.764231
O 1.746700 0.037010 0.000830
S -0.769680 2.297550 -0.055720
C -1.071010 2.719170 -1.769250
C -1.004440 1.788200 -2.736880
S -0.629580 0.083380 -2.335850
O -0.352130 1.939240 3.131340
O 0.037820 -0.194600 4.345970
N -3.568640 1.598950 1.504931
C -3.826300 0.381160 0.974711
N -4.025520 -0.658530 1.815091
N -3.986790 0.241970 -0.350319

C -4.164840 -1.056570 -0.996049
C -1.393370 4.106200 -2.042621
C -1.261512 2.088159 -4.132028
H -1.437860 -2.654510 -2.300640
H 0.259040 -3.156070 -2.068770
H -1.065550 -4.194230 -1.462870
H -2.971530 2.190840 0.903821
H -3.150500 1.505210 2.450451
H -3.494250 -0.539910 2.696091
H -3.928440 -1.585780 1.406481
H -3.633000 1.005950 -0.924429
H -5.081850 -1.539870 -0.628809
H -4.271410 -0.886440 -2.071849
H -3.291560 -1.706520 -0.818089
H -1.554015 4.237647 -3.111656
H -2.298244 4.381735 -1.502987
H -0.569956 4.740925 -1.718532
H -1.474842 3.150423 -4.241603
H -0.385866 1.830603 -4.726022
H -2.116898 1.508731 -4.476263

TS2

37
C -2.484789 -2.574435 -0.262296
S -1.029566 -1.965340 0.728564
Mo -0.000819 0.001034 -0.000419
S -0.694859 -0.007111 -2.212252
C -1.036258 1.697578 -2.672127
C -1.099088 2.650067 -1.732133
S -0.809786 2.236133 -0.003172
O 1.734291 0.002823 0.002966
N -3.275657 1.507723 2.043152
C -2.602045 1.708631 3.198538
N -1.791101 2.776419 3.321799
C -4.021633 0.276693 1.799583
N -2.804334 0.940833 4.280253
O -0.499878 1.751629 5.569354
S 0.715614 0.935989 5.052661
O 1.768770 1.917948 4.597729
O 0.263674 0.062694 3.907228
O 1.228562 0.097539 6.200658
C -1.261710 4.058243 -2.037249
C -1.222277 1.961428 -4.085732
H -3.320949 -1.879539 -0.135367
H -2.182855 -2.599068 -1.315630
H -2.743201 -3.573123 0.108777
H -1.451375 3.201238 2.459517
H -1.119116 2.684520 4.112955
H -2.038212 1.031179 4.985832
H -3.199061 0.015790 4.140487

H -2.795421 1.908322 1.221899
H -4.952491 0.268882 2.385604
H -4.296194 0.260651 0.738773
H -3.422983 -0.621950 2.019748
H -1.429453 4.181033 -3.106223
H -2.115585 4.452383 -1.488185
H -0.362226 4.598900 -1.746491
H -1.420975 3.021831 -4.234007
H -0.320862 1.681591 -4.628929
H -2.064702 1.379021 -4.455927

PS

37
C -3.882970 -0.146440 1.291070
N -3.236730 1.069140 1.759090
C -2.735550 1.172800 3.005130
N -1.970420 2.225570 3.349490
N -3.068530 0.295020 3.967410
O -1.154200 1.090250 5.776190
S 0.166940 0.279240 5.702550
O 1.305520 1.258590 5.548790
O 0.094330 -0.647680 4.512800
O 0.304080 -0.509110 6.983790
S -1.362660 2.002740 -0.748270
C -1.767920 2.339240 -2.476940
C -1.376660 1.486090 -3.431040
S -0.470680 -0.016220 -2.995210
Mo 0.031280 0.101370 -0.730020
S -0.571619 -1.993480 0.116810
C -1.939359 -2.838650 -0.803440
O 1.686760 0.592220 -0.563460
C -2.491354 3.568020 -2.740079
C -1.652727 1.681367 -4.841059
H -2.649629 -2.110330 -1.206900
H -1.493779 -3.412620 -1.625710
H -2.448319 -3.520460 -0.109630
H -1.537150 2.767730 2.607530
H -1.433010 2.080670 4.225960
H -2.426060 0.332210 4.793690
H -3.403150 -0.619480 3.679510
H -2.780720 1.630170 1.025190
H -4.809820 -0.339790 1.851760
H -4.151750 -0.000550 0.235730
H -3.217920 -1.020840 1.360360
H -2.676007 3.658651 -3.809476
H -3.441277 3.551091 -2.207837
H -1.900103 4.417175 -2.400551
H -2.199164 2.613296 -4.978301
H -0.714361 1.726283 -5.391853
H -2.251991 0.851181 -5.211997

Optimized structures for DMSOR mechanism

CH_3O^-

RS

30

Mo -2.919416 2.892386 1.407351
O -3.233962 2.411315 3.179769
C -4.333155 2.707439 4.029630
H -5.266505 2.378694 3.564734
H -4.191309 2.184310 4.979140
H -4.385926 3.784827 4.209425
S -0.676471 3.601306 1.175715
S -2.122311 1.018034 0.207704
S -3.502107 5.154637 1.224394
S -4.941029 2.576950 0.267287
C -0.345631 1.122781 0.127235
C 0.277278 2.234618 0.543961
C -5.785235 4.141198 0.179178
C -5.162562 5.255903 0.592360
C -5.713975 6.655392 0.537641
H -6.738702 6.684903 0.167350
H -5.699452 7.115493 1.530666
H -5.098882 7.285666 -0.112482
C -7.163701 4.061726 -0.419679
H -7.791747 3.368718 0.148583
H -7.663881 5.029952 -0.442441
H -7.116389 3.679196 -1.444232
C 1.759477 2.494314 0.499250
H 2.153980 2.661003 1.506838
H 2.313559 1.669312 0.051188
H 1.972247 3.400522 -0.076797
C 0.309115 -0.092676 -0.473576
H 1.392305 0.008588 -0.540959
H 0.088462 -0.984887 0.121160
H -0.078991 -0.279997 -1.479917

TS1

40

Mo -4.658265 1.719234 0.353907
O -6.064336 -0.458888 0.765457
S -5.815829 -1.190155 2.068281
O -4.944748 1.422405 2.250911
C -4.505183 2.216168 3.323618
H -4.824053 1.756658 4.267403
H -3.411723 2.307923 3.315475
H -4.927441 3.226072 3.254052
S -2.418407 2.414354 0.578361
S -3.630086 0.093285 -1.047582
S -5.062202 4.036896 0.433109
S -6.373448 1.835538 -1.281977

C -1.873014 0.230007 -0.905620
C -1.341771 1.244180 -0.202486
C -7.034811 3.477278 -1.315957
C -6.464154 4.439408 -0.571925
C -6.873558 5.887333 -0.513062
H -7.704669 6.110149 -1.182340
H -7.173009 6.167639 0.502044
H -6.034695 6.536021 -0.785720
C -8.209116 3.653931 -2.242510
H -9.027971 2.985278 -1.957773
H -8.591318 4.674972 -2.240682
H -7.932464 3.395407 -3.269509
C 0.124405 1.537342 -0.020799
H 0.393449 1.539639 1.040419
H 0.758714 0.809056 -0.526587
H 0.369594 2.530762 -0.410164
C -1.103818 -0.835865 -1.641358
H -0.025365 -0.685169 -1.585698
H -1.329228 -1.826653 -1.233197
H -1.389878 -0.857795 -2.697506
C -6.415907 -2.867154 1.733341
H -7.495920 -2.802350 1.606995
H -5.945200 -3.227623 0.818484
H -6.171833 -3.507269 2.582707
C -4.052328 -1.610320 2.116221
H -3.511806 -0.671003 2.204555
H -3.883689 -2.247194 2.986019
H -3.787040 -2.112949 1.187577

IM1

40

Mo -4.710434 1.561635 0.398271
O -5.926334 -0.358406 0.803077
S -5.843482 -1.088955 2.148890
O -4.924556 1.333210 2.365233
C -4.446014 2.163394 3.385228
H -4.722005 1.737867 4.359920
H -3.353205 2.263982 3.337059
H -4.874052 3.171568 3.307959
S -2.472592 2.299089 0.647857
S -3.617769 0.005192 -1.050559
S -5.163325 3.879327 0.568380
S -6.382863 1.741627 -1.283518
C -1.871463 0.235902 -0.977651
C -1.370161 1.244067 -0.242215
C -7.003534 3.394048 -1.337963
C -6.470547 4.329041 -0.531765
C -6.859392 5.783259 -0.472255
H -7.649013 6.030457 -1.181901
H -7.209137 6.052157 0.529686

H -5.996886 6.422136 -0.687817
C -8.103993 3.613479 -2.343469
H -8.951835 2.952232 -2.137215
H -8.469599 4.640555 -2.343047
H -7.757092 3.376172 -3.354181
C 0.084590 1.611654 -0.104791
H 0.394599 1.590957 0.944869
H 0.736999 0.938322 -0.661038
H 0.260708 2.630395 -0.465389
C -1.073614 -0.743857 -1.798888
H -0.003960 -0.534611 -1.773582
H -1.227592 -1.766218 -1.437911
H -1.398093 -0.725926 -2.843902
C -6.512085 -2.709035 1.702365
H -7.565649 -2.566743 1.466557
H -5.972566 -3.085041 0.833246
H -6.403056 -3.378035 2.557417
C -4.119707 -1.610042 2.332944
H -3.542448 -0.707256 2.513365
H -4.063238 -2.295936 3.179109
H -3.807726 -2.085113 1.404109

TS2

40

Mo -4.908154 1.202310 0.253996
O -5.991814 -0.366463 0.299289
S -6.341572 -1.273111 1.922794
O -4.973145 0.827590 2.203026
C -4.519098 1.530583 3.322521
H -4.623155 0.894718 4.212389
H -3.465308 1.816943 3.208988
H -5.103175 2.445742 3.486027
S -2.692313 2.143770 0.468764
S -3.629753 -0.281464 -1.194446
S -5.673123 3.405474 0.899050
S -6.171808 1.823223 -1.722184
C -1.943907 0.195877 -1.233716
C -1.530401 1.247949 -0.499414
C -6.738603 3.479530 -1.571583
C -6.543948 4.163202 -0.426837
C -6.988460 5.577919 -0.151737
H -7.632050 5.969798 -0.939170
H -7.539348 5.631546 0.792478
H -6.127208 6.246968 -0.056804
C -7.442297 4.005441 -2.797529
H -8.235103 3.318951 -3.110523
H -7.889631 4.985323 -2.633004
H -6.745166 4.087667 -3.637568
C -0.119629 1.772490 -0.418034
H 0.236363 1.764499 0.616993

H 0.576253 1.186626 -1.017896
H -0.071436 2.811190 -0.760730
C -1.073717 -0.656391 -2.123740
H -0.033145 -0.333178 -2.122130
H -1.103959 -1.703669 -1.805536
H -1.435139 -0.628424 -3.156250
C -7.090446 -2.620008 0.984543
H -8.037174 -2.251574 0.592209
H -6.429118 -2.888001 0.161142
H -7.261237 -3.469596 1.646900
C -4.731684 -2.014129 2.237709
H -4.289471 -1.502726 3.087891
H -4.852739 -3.079515 2.433825
H -4.126221 -1.843013 1.343564

PS

31

Mo -3.446248 2.507518 2.276397
O -2.850039 3.147511 4.009839
O -4.514615 1.318643 2.874416
C -2.078812 4.212961 4.486479
H -2.441749 5.172942 4.099141
H -2.131756 4.229310 5.580360
H -1.032837 4.096836 4.168872
S -1.167557 3.496107 1.483755
S -2.350949 0.575174 1.306975
S -4.580574 4.651300 2.348547
S -4.241417 2.662972 -0.040576
C -1.015028 1.063017 0.322419
C -0.486743 2.314425 0.429024
C -5.223396 4.113839 -0.213286
C -5.371592 4.973552 0.808077
C -6.185360 6.241638 0.799652
H -6.630183 6.437039 -0.175128
H -6.992045 6.187503 1.537354
H -5.564367 7.101911 1.067780
C -5.839299 4.257769 -1.581466
H -6.506517 3.416208 -1.791849
H -6.412377 5.178440 -1.683450
H -5.064006 4.251353 -2.353271
C 0.721336 2.703885 -0.389695
H 1.512831 1.953862 -0.302431
H 0.458231 2.769343 -1.451131
H 1.115525 3.670187 -0.077923
C -0.435818 0.039614 -0.627870
H -0.477733 0.398927 -1.661196
H 0.616716 -0.157061 -0.398756
H -0.977006 -0.904797 -0.575065

DMS

9

S -0.519580 -1.004559 -0.072955
C -1.029473 0.735724 0.049964
H -2.108382 0.828501 -0.084889
H -0.759364 1.084975 1.046347
H -0.511531 1.340088 -0.696546
C -1.063585 -1.341603 -1.774124
H -0.816811 -2.379518 -1.996750
H -2.141620 -1.199214 -1.865680
H -0.544861 -0.688778 -2.477824

DMSO

10

S -0.567087 -1.034501 -0.032911
O 0.934749 -1.076417 -0.012995
C -1.038223 0.716785 0.026042
H -2.118481 0.798576 -0.103384
H -0.744801 1.094113 1.004676
H -0.505785 1.245647 -0.766020
C -1.069815 -1.314134 -1.754681
H -0.796358 -2.337709 -2.007108
H -2.149448 -1.179363 -1.836089
H -0.536164 -0.605756 -2.389987

Optimized structures for DMSOR mechanism

PhO^-

RS

37

Mo -2.992105 2.967908 1.368604
O -3.282556 2.627724 3.203286
S -0.790945 3.751849 1.057059
S -2.096868 1.031093 0.367140
S -3.679490 5.160856 0.945602
S -4.969870 2.461943 0.237240
C -0.321511 1.201667 0.268425
C 0.244682 2.379801 0.567340
C -5.921459 3.955986 0.036595
C -5.358145 5.134199 0.346529
C -5.990822 6.492101 0.219262
H -7.005297 6.440228 -0.171816
H -6.031467 6.992546 1.190357
H -5.404752 7.132694 -0.444443
C -7.307293 3.738014 -0.504661
H -7.891374 3.107275 0.170229
H -7.849346 4.672189 -0.641838
H -7.270624 3.224234 -1.468626
C 1.710030 2.712650 0.501240
H 2.081051 3.029614 1.479392
H 2.312648 1.867328 0.172636
H 1.887563 3.541442 -0.189202
C 0.386251 -0.040174 -0.201219
H 1.464208 0.097362 -0.266753
H 0.195456 -0.876343 0.476703
H 0.024604 -0.342366 -1.187517
C -6.121685 3.122893 6.185126
C -4.908809 2.490680 6.450481
C -3.963239 2.330014 5.443734
C -4.230061 2.804952 4.157490
C -5.444951 3.441265 3.883550
C -6.381361 3.594520 4.900174
H -6.855545 3.246955 6.970415
H -4.695441 2.120142 7.445002
H -3.018061 1.839801 5.636205
H -5.643024 3.806184 2.885438
H -7.320957 4.087475 4.684641

TS1

47

Mo -4.397113 1.782751 0.097723
O -6.313271 -0.447776 0.333490
S -6.126202 -1.208406 1.654269
O -4.622267 1.166716 1.904235
S -2.180597 2.524872 0.154997
S -3.483680 0.095601 -1.288049

S -4.911646 4.048077 0.501275
S -6.015197 2.062348 -1.607559
C -1.699147 0.220476 -1.225297
C -1.131849 1.284834 -0.611099
C -6.810487 3.648083 -1.390061
C -6.341111 4.513828 -0.457187
C -6.872531 5.895611 -0.161114
H -7.698733 6.179160 -0.822930
H -7.234939 5.964627 0.875212
H -6.079508 6.650228 -0.268118
C -7.973785 3.885773 -2.322553
H -8.773180 3.150137 -2.148951
H -8.406812 4.885482 -2.206591
H -7.663765 3.771001 -3.371670
C 0.342808 1.585729 -0.501230
H 0.656680 1.639468 0.551625
H 0.962158 0.829941 -0.997100
H 0.578221 2.562501 -0.949666
C -0.972256 -0.900921 -1.926895
H 0.116203 -0.774884 -1.907541
H -1.207826 -1.869847 -1.462262
H -1.285461 -0.972376 -2.978838
C -7.120668 -2.727147 1.426982
H -8.166376 -2.407850 1.372299
H -6.819375 -3.201057 0.486257
H -6.972541 -3.398643 2.280481
C -4.477867 -2.001544 1.570298
H -3.746896 -1.193887 1.652998
H -4.381054 -2.710914 2.399687
H -4.382987 -2.492249 0.596607
C -4.244291 2.705241 5.745628
C -3.151060 2.090405 5.118904
C -3.268327 1.583798 3.820748
C -4.493257 1.683079 3.136378
C -5.589198 2.308100 3.759405
C -5.461029 2.812183 5.056724
H -4.148055 3.099685 6.756745
H -2.198398 2.007629 5.642986
H -2.424553 1.122118 3.310404
H -6.520779 2.392161 3.202898
H -6.316205 3.293456 5.532268

IM1

47

Mo -4.578146 1.369627 0.174754
O -5.799108 -0.490932 0.341553
S -6.345429 -1.087142 1.655155
O -4.702533 0.888289 2.148484
S -2.402235 2.256895 0.475495
S -3.375348 0.005786 -1.357970

S -5.231436 3.590917 0.664904
S -6.085064 1.760289 -1.626959
C -1.650355 0.388256 -1.319327
C -1.228682 1.389163 -0.524614
C -6.812176 3.367854 -1.498199
C -6.442494 4.172705 -0.484163
C -6.937958 5.570654 -0.222061
H -7.666460 5.897804 -0.962469
H -7.409622 5.639720 0.761892
H -6.110506 6.284673 -0.227470
C -7.806748 3.696128 -2.579689
H -8.651601 3.002659 -2.556254
H -8.201826 4.706444 -2.486352
H -7.350667 3.604382 -3.569030
C 0.186465 1.885918 -0.390290
H 0.537521 1.793008 0.640718
H 0.879396 1.339767 -1.028287
H 0.253087 2.945498 -0.652763
C -0.795532 -0.451226 -2.231827
H 0.251634 -0.153619 -2.209799
H -0.848815 -1.507177 -1.952169
H -1.142212 -0.379953 -3.266115
C -7.452908 -2.356100 1.020839
H -8.287386 -1.843016 0.547820
H -6.921460 -2.973598 0.299043
H -7.809541 -2.950443 1.861284
C -5.042740 -2.166668 2.279355
H -4.244076 -1.516424 2.622940
H -5.447185 -2.753439 3.102787
H -4.702058 -2.808543 1.468433
C -3.737433 2.802288 5.695315
C -2.794038 2.011201 5.040199
C -3.104816 1.386791 3.837830
C -4.377608 1.537959 3.267595
C -5.323108 2.334861 3.930018
C -5.002631 2.957594 5.130681
H -3.490071 3.289945 6.629470
H -1.806814 1.882402 5.467767
H -2.374782 0.787390 3.311664
H -6.297269 2.459511 3.477920
H -5.745428 3.569497 5.628707

TS2
47
Mo -4.805752 1.223553 0.267030
O -5.880481 -0.332242 0.364383
S -6.354656 -1.183969 2.022596
O -4.837602 0.914239 2.263111
S -2.598379 2.183551 0.403967
S -3.551296 -0.260916 -1.181854

S -5.631035 3.420220 0.870558
S -6.034555 1.820841 -1.740900
C -1.877641 0.251242 -1.325110
C -1.455087 1.321056 -0.619356
C -6.663271 3.462859 -1.615762
C -6.503225 4.157445 -0.471946
C -6.993046 5.557462 -0.203478
H -7.599441 5.946816 -1.019337
H -7.597159 5.589819 0.707035
H -6.155416 6.243935 -0.054622
C -7.365410 3.952776 -2.856144
H -8.145019 3.251546 -3.164943
H -7.831623 4.925568 -2.711380
H -6.665969 4.036711 -3.692277
C -0.057736 1.883178 -0.609250
H 0.332002 1.933550 0.410460
H 0.632870 1.285985 -1.201841
H -0.042818 2.902614 -1.004574
C -1.039111 -0.586070 -2.257059
H 0.004334 -0.276642 -2.267235
H -1.073353 -1.640424 -1.970407
H -1.416061 -0.523113 -3.281263
C -7.205690 -2.480880 1.114026
H -8.122588 -2.049181 0.718915
H -6.572727 -2.823457 0.297749
H -7.442746 -3.298057 1.793856
C -4.819038 -2.038800 2.401509
H -4.284477 -1.443703 3.134721
H -5.042402 -3.030370 2.790728
H -4.239370 -2.102892 1.480300
C -3.737127 2.786009 5.789775
C -2.791939 2.087895 5.038521
C -3.149263 1.476132 3.842837
C -4.470740 1.549991 3.378601
C -5.419685 2.248224 4.138798
C -5.051465 2.859897 5.331711
H -3.453073 3.264384 6.718159
H -1.767934 2.021357 5.385716
H -2.422127 0.947225 3.242860
H -6.434566 2.304519 3.770475
H -5.795308 3.397704 5.907157

PS

38

Mo -5.028784 1.010235 0.520288
O -5.974350 -0.414653 0.461533
S -2.809449 2.308193 0.799315
S -3.385075 -0.475921 -0.480720
S -6.566556 2.871880 0.683707
S -5.125405 1.720609 -1.812334

C -1.915665 0.358602 -0.833679
C -1.648459 1.555622 -0.229789
C -6.343061 2.988143 -1.997452
C -6.972607 3.487279 -0.921566
C -8.033066 4.556029 -0.914502
H -8.214686 4.957561 -1.909173
H -8.978703 4.162155 -0.532961
H -7.745640 5.385613 -0.263512
C -6.562277 3.407416 -3.426964
H -6.962806 2.579245 -4.017491
H -7.254752 4.242571 -3.507496
H -5.619294 3.705680 -3.891757
C -0.329099 2.254296 -0.437312
H -0.233274 3.124237 0.208953
H 0.509775 1.582432 -0.243014
H -0.235352 2.592803 -1.473185
C -0.934929 -0.301765 -1.772340
H -0.640820 0.379148 -2.574723
H -0.021663 -0.593949 -1.246340
H -1.358718 -1.195096 -2.226377
C -4.952213 1.950877 3.570132
C -4.569321 3.299780 3.527113
C -5.195629 1.351092 4.818238
C -4.432065 4.021126 4.708540
H -4.401211 3.775092 2.573469
C -5.047424 2.081048 5.988227
H -5.493213 0.310752 4.842346
C -4.664647 3.422094 5.943309
H -4.138319 5.062317 4.659331
H -5.231835 1.601466 6.941452
H -4.551141 3.989568 6.857465
O -5.088916 1.194294 2.482635