Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Rearrangement and Decomposition Pathways of Bare and Hydrogenated Molybdenum Oxysulfides in the Gas Phase

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Supporting Information

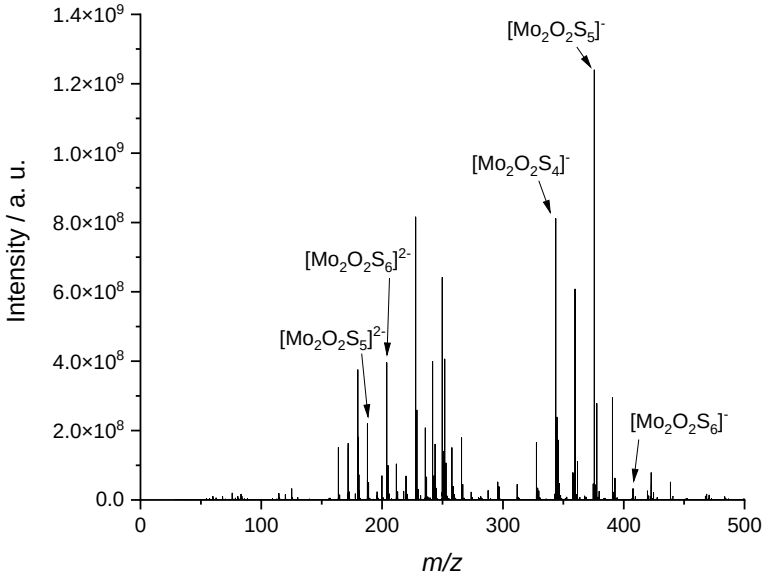

Figure S1: ESI mass spectrum of the $[(CH_3)_4N]_2[Mo_2O_2S_6]$ sample sprayed from pure acetonitrile. The peaks of interest are labelled.

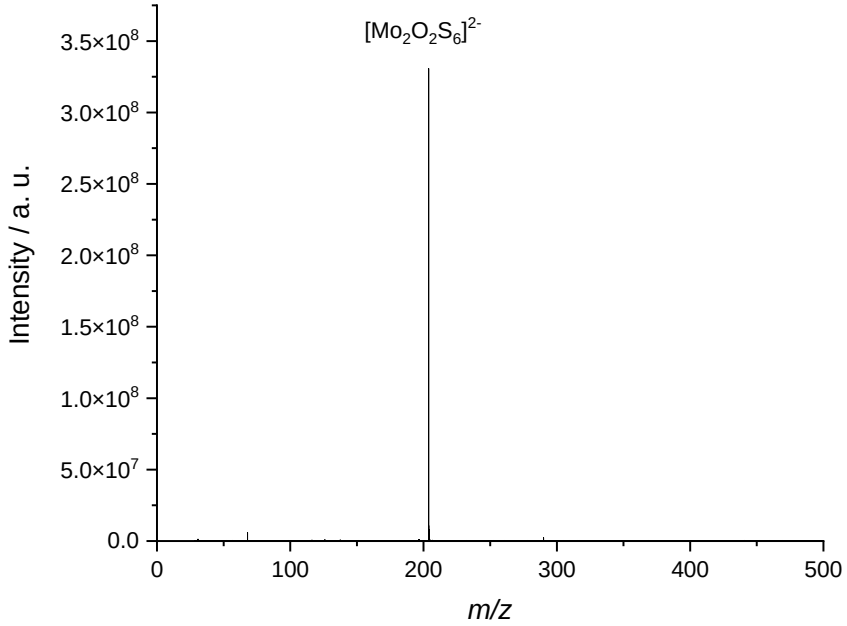

Figure S2: Isolated $[Mo_2O_2S_6]^{2-}$ used as precursor for a SORI-CID experiment. The peak at *m/z* 67.94 corresponds to the third harmonic of the isolated peak.

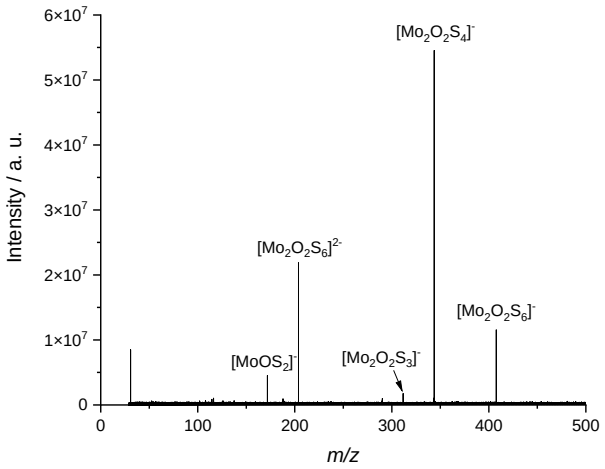

Figure S3 SORI-CID of $[Mo_2O_2S_6]^{2-}$ at 0.5% SORI power, frequency offset 500 Hz and pulse length of 1 s. Electron detachment followed by S_2 loss leads to the most intense fragment, $[Mo_2O_2S_4]^-$. The peak at m/z 31 is electronic noise, and is present in all mass spectra.

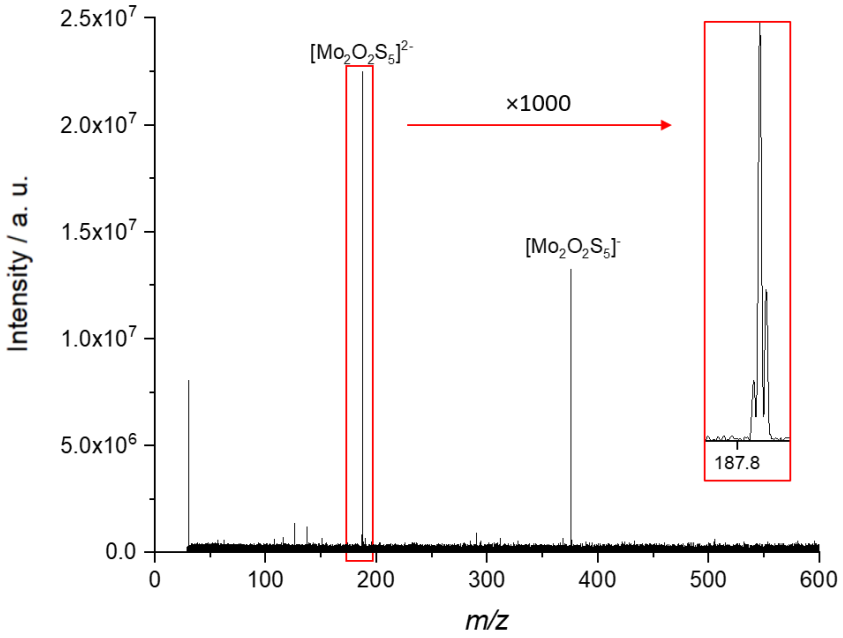

Figure S4: Mass spectrum of isolated $[Mo_2O_2S_5]^{2-}$ at 0% SORI power. A zoom on the *y*-axis of around 1000 shows that the peak of the precursor actually consists of 3 individual peaks, see text for assignment. Again, the peak at a *m/z* around 31 is noise.

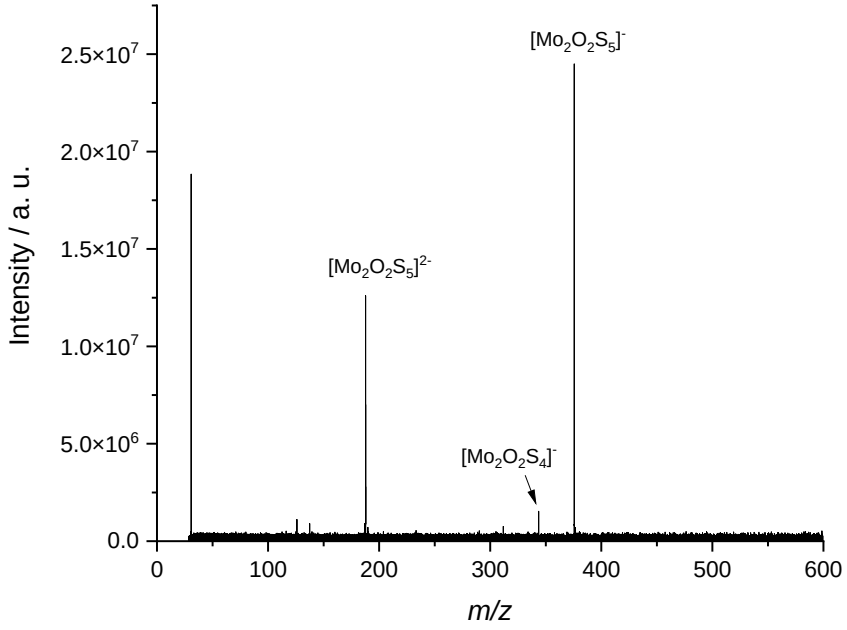

Figure S5: Mass spectrum obtained with the precursor $[Mo_2O_2S_5]^{2-}$ at 0.2% SORI power. The peak of the fragment $[Mo_2O_2S_5]^-$ is already higher than the one of the precursor. Also, $[Mo_2O_2S_4]^-$ can be seen.

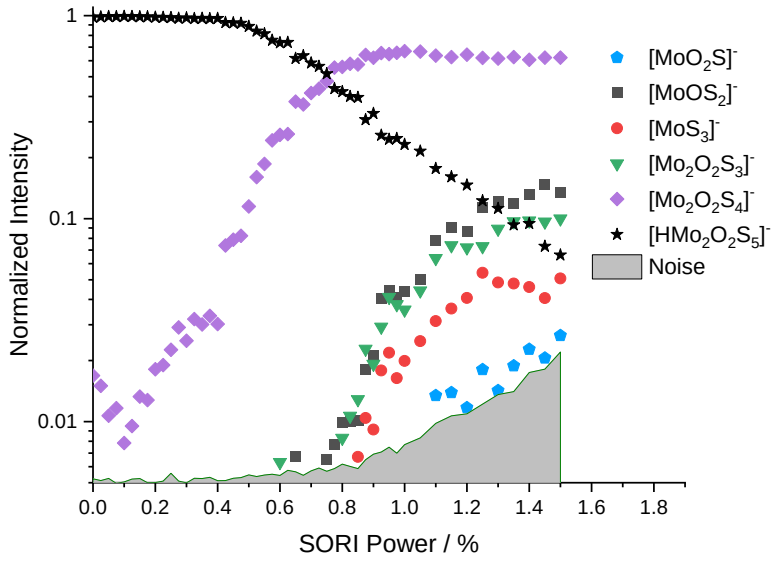

Figure S6: SORI-CID fragmentation curve of $[HMo_2O_2S_5]^-$. The only direct fragment observed is $[Mo_2O_2S_4]^-$. The other fragments correspond to fragmentation channels of $[Mo_2O_2S_4]^-$.

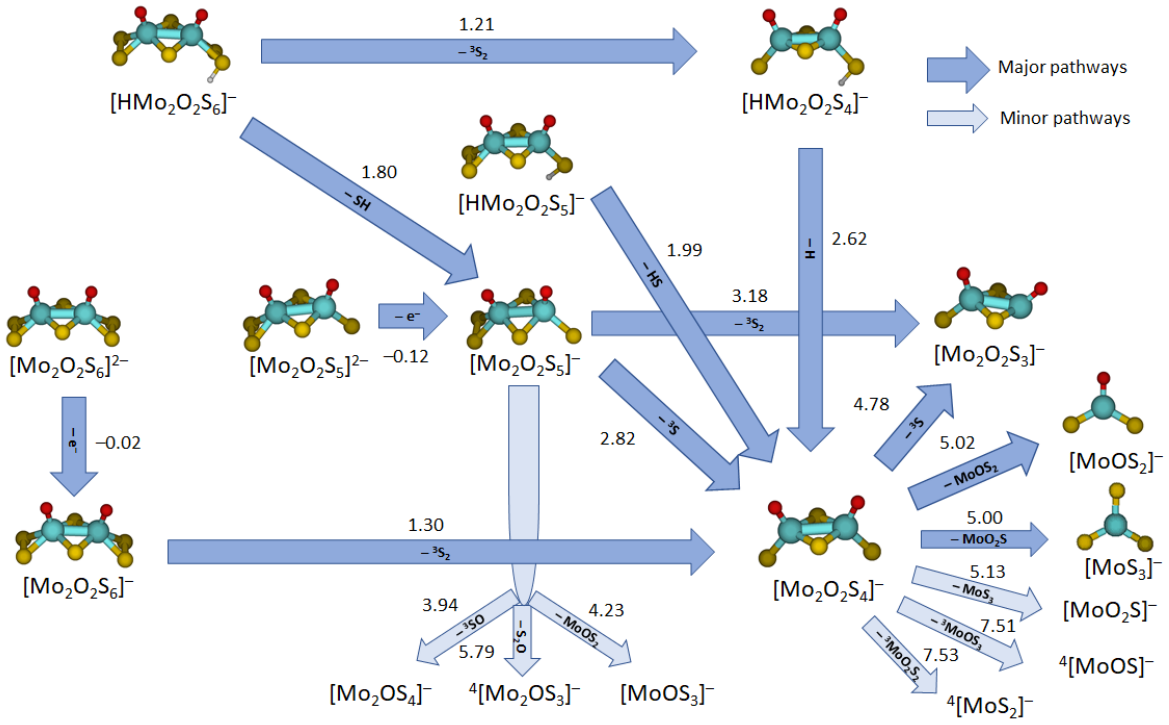

Figure S7: Important fragmentation pathways of the molybdenum oxysulfides studied by SORI-CID along with reaction energies at the B3LYP+D3/def2TZVP level. Reaction energies are given in eV. Color code: Mo – cyan, S – yellow, O – red, H – white. Other than singlet or doublet spin multiplicities are given explicitly.

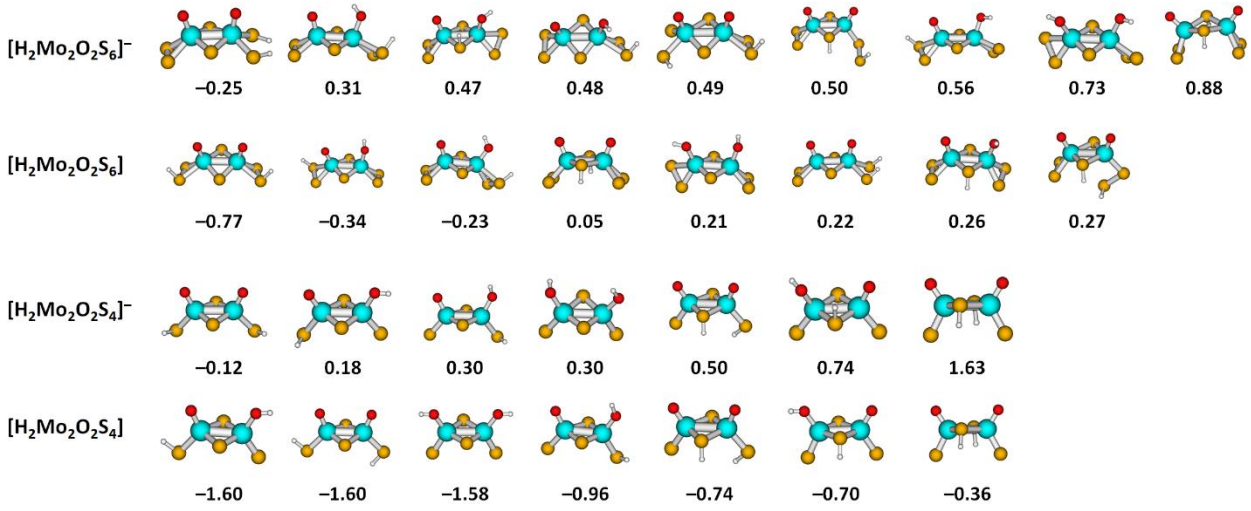

Figure S8: Selected isomers of $[H_2Mo_2O_2S_6]^-$, $[H_2Mo_2O_2S_6]$, $[H_2Mo_2O_2S_4]^-$, and $[H_2Mo_2O_2S_4]$ clusters. Calculated at the B3LYP+D3/def2TZVP level, relative energies are given in eV with respect to the limit of cluster + H_2 (i.e., positive energies denote clusters that are metastable with respect to H_2 dissociation). Color code: Mo – cyan, S – yellow, O – red, H – white.

Table S1. Predicted reactions for the observed fragment ions along with their reaction energy Δ*E* at the B3LYP+D3/def2TZVP level of theory. Other than singlet or doublet spin multiplicities are given explicitly.

Reaction	Reactant	Product	Δ*E* / eV
(1)	$[Mo_2O_2S_6]^{2-}$	$[Mo_2O_2S_6]^- + e^-$	-0.02
(2)	$[Mo_2O_2S_5]^{2-}$	$[Mo_2O_2S_5]^- + e^-$	-0.12
(3a)	$[HMo_2O_2S_6]^-$	$[HMo_2O_2S_4]^- + {}^3S_2$	1.21
(3b)	$[HMo_2O_2S_6]^-$	$[Mo_2O_2S_5]^- + HS$	1.80
(4)	$[HMo_2O_2S_5]^-$	$[Mo_2O_2S_4]^- + HS$	1.99
(5)	$[HMo_2O_2S_4]^-$	$[Mo_2O_2S_4]^- + H$	2.62
(6)	$[Mo_2O_2S_6]^-$	$[Mo_2O_2S_4]^- + {}^3S_2$	1.30
(7a)	$[Mo_2O_2S_5]^-$	$[Mo_2O_2S_3]^- + {}^3S_2$	3.18
(7b)	$[Mo_2O_2S_5]^-$	$[Mo_2O_2S_4]^- + {}^3S$	2.82
(7c)	$[Mo_2O_2S_5]^-$	$[Mo_2OS_4]^- + {}^3SO$	3.94
(7d)	$[Mo_2O_2S_5]^-$	$^4[Mo_2OS_3]^- + S_2O$	5.79
(7e)	$[Mo_2O_2S_5]^-$	$[MoOS_3]^- + MoOS_2$	4.23
(8a)	$[Mo_2O_2S_4]^-$	$[Mo_2O_2S_3]^- + {}^3S$	4.78
(8b)	$[Mo_2O_2S_4]^-$	$[MoOS_2]^- + MoOS_2$	5.02
(8c)	$[Mo_2O_2S_4]^-$	$[MoS_3]^- + MoO_2S$	5.00
(8d)	$[Mo_2O_2S_4]^-$	$[MoO_2S]^- + MoS_3$	5.13
(8e)	$[Mo_2O_2S_4]^-$	$^4[MoOS]^- + {}^3MoOS_3$	7.51
(8f)	$[Mo_2O_2S_4]^-$	$^4[MoS_2]^- + {}^3MoO_2S_2$	7.53

Table S2. Reaction profile of Figure 5 calculated using B3LYP+D3 and BLYP+D3 functionals along with the def2TZVP basis set in structures optimized at the B3LYP+D3/def2TZVP level with the respective zero-point correction. Energies are given in eV.

Structure	B3LYP+D3	BLYP+D3
LM1	0.00	0.00
TS1	0.74	0.76
LM2	0.68	0.63
TS2	1.48	1.31
LM3	1.37	1.17
TS3	1.45	1.24
LM4	0.70	0.65
TS4	1.21	0.95
LM5	1.07	0.98

Cartesian Coordinates of optimized ions and molecules (in Å, calculated at the B3LYP/def2TZVP level) along with the ZPE-corrected energies (in Hartree) and spin multiplicity *M*

[Mo2O2S6]2- (M = 1)
E = -2676.802849
Mo -1.431659 0.000013 0.355510
S -0.000001 1.821515 -0.030285
S 0.000001 -1.821499 -0.030227
Mo 1.431659 0.000014 0.355510
S 3.212144 -1.050943 -0.946558
S 3.212140 1.050876 -0.946633
S -3.212144 1.050875 -0.946628
S -3.212140 -1.050943 -0.946563
O -1.877398 0.000049 1.980466
O 1.877398 0.000052 1.980466

E = -2676.796733
S -0.000230 1.850496 0.000735
Mo -1.362427 0.000046 -0.481495
O -1.504580 0.000347 -2.163386
Mo 1.362469 -0.000078 0.481568
O 1.504743 -0.000454 2.163455
S 0.000238 -1.850539 -0.000573
S 3.328086 1.051610 -0.503385
S 3.328800 -1.050974 -0.503201
S -3.328079 -1.051520 0.503410
S -3.329006 1.051064 0.502787

E = -2676.742724
S -2.872379 -1.316053 -1.057663
S -2.874031 -1.314449 1.057814
Mo -1.290917 0.187733 -0.000192
Mo 1.290966 0.187769 0.000129
S 2.873601 -1.315093 -1.057402
S 2.872513 -1.315716 1.058070
O -0.000301 -0.149757 1.401666
O 0.000313 -0.149990 -1.401683
S -2.016923 2.212748 -0.001006
S 2.017085 2.212743 0.000361

E = -2676.788084
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S 0.633952 1.047382 -0.103431
S -0.597313 -0.409013 0.782391
S 3.480699 -0.302260 1.932359
Mo -2.744697 -0.085002 -0.210135
O -2.673797 -0.396326 -1.884773
S -3.970638 -1.569155 0.820000
S -3.432957 1.957867 0.133559

[Mo2O2S5]2- (M = 1)
E = -2278.559901
S -0.324782 1.820836 0.005462
Mo 1.140497 -0.000039 0.402959
O 1.502665 -0.000028 2.048775
Mo -1.750057 0.000066 0.138698
O -2.573751 0.000314 1.635908
S -0.325004 -1.820887 0.005908
S -3.124705 -0.000063 -1.592145
S 2.954819 -1.051678 -0.841907
S 2.955311 1.051580 -0.841509

E = -2278.463222
S -0.000001 -1.055991 1.658376
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O 1.785881 -1.727107 -1.190257
Mo -1.312898 -0.426440 -0.205104
O -1.785881 -1.727106 -1.190257
S -3.044836 0.827944 1.045574
S -2.291157 1.683010 -0.741235
S 2.291159 1.683009 -0.741236
S 3.044835 0.827943 1.045575

E = -2278.557368
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Mo -1.093457 -0.000023 0.464369
S -3.049580 1.051945 -0.537483
S -3.049861 -1.051833 -0.537317
Mo 1.696232 0.000025 -0.391367
S 3.415989 -0.000200 0.985938
O 2.160000 0.000226 -2.041608
S 0.317597 1.831041 -0.076829
O -1.227816 -0.000132 2.144331

[Mo2O2S4]- (M = 2)
E = -1880.266909
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Mo -0.785359 0.000024 0.422123
O -0.829074 0.000047 2.098268
Mo 1.922240 -0.000012 -0.357599
O 3.308566 -0.000020 0.634780
S 0.619111 1.830904 -0.253800
S -2.731148 1.044045 -0.514181
S -2.731100 -1.044099 -0.514173

E = -1880.328143 (M = 2)
S -0.000027 -0.048188 -1.765032
Mo -1.528526 -0.204352 -0.000116
O -2.315598 -1.705074 -0.001366
Mo 1.528551 -0.204372 -0.000157
O 2.315742 -1.705028 -0.001489
S 0.000025 -0.051391 1.765038
S 2.927910 1.438827 0.001105
S -2.928047 1.438704 0.001032

E = -1880.327594 (M = 2)
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S -3.108852 -1.085050 -0.000332
Mo 1.496513 -0.347143 -0.000079
S 3.108735 1.085186 0.000258
O 2.068715 -1.943046 -0.000510
S -0.000023 -0.000575 1.765615
O -2.068560 1.943079 0.000550

[HMo2O2S6]- (M = 1)
E = -2677.397162
S -0.101123 1.768501 0.073450
Mo 1.475685 0.035555 0.364812
O 1.946790 0.041403 1.974202
Mo -1.346876 -0.138101 0.381923
O -1.947018 -0.280762 1.952389
S 0.134215 -1.860988 -0.012774
S -3.550367 1.013596 -0.695792
S -2.867737 -0.862183 -1.322617
S 3.221475 -0.898037 -1.003200
S 3.103009 1.187896 -0.978371
H -4.439723 0.641237 0.253281

E = -2677.398379
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S -2.861095 -0.692172 -1.421439
S -3.521279 1.083889 -0.539103
Mo 1.463664 -0.012724 0.365609
S 3.066650 1.314301 -0.839792
S 3.201501 -0.751123 -1.125913
O 1.954359 -0.206066 1.957162
S 0.132882 -1.855552 -0.236020
O -1.931465 -0.557152 1.935071
H -2.850720 1.999065 -1.273103

E = -2677.386855
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Mo -1.389826 -0.056916 0.289705
O -1.797549 -0.229383 2.106586
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H -1.053025 -0.391771 2.703474

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Mo 1.437080 0.025309 0.386508
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Mo -1.437111 0.025288 0.386560
O -1.943972 0.252257 1.968979
S 0.000007 -1.804187 0.258055
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S 3.071642 -1.201096 -0.867328
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H -0.000135 2.146241 -1.273574

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E = -2279.168160
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S 2.897288 -1.043459 -0.897117
O 1.551490 -0.001818 2.027185
S -0.307131 -1.816573 0.020843
O -2.470921 -0.001433 1.694276
H -4.225920 0.000543 -0.857826

E = -2279.169462
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S 2.877673 -0.249300 1.359053

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O 1.556488 -1.271638 -1.587376
H -2.215499 1.615760 2.016480

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H -2.605115 2.239010 0.557432

E = -2279.156250
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Mo -1.065524 0.074957 0.431777
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Mo 1.788792 -0.078353 0.129827
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S 3.098065 0.028196 -1.602567
S -3.272259 -0.932025 -0.702166
S -2.683981 1.049585 -1.037311
O -1.535142 0.005864 2.047982
H -4.110899 -0.761692 0.346029

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S -0.322006 0.950065 1.555349
O -2.569792 1.368730 -0.842765
H 0.845264 2.672410 -0.861052

E = -2279.150543
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Mo -1.144610 -0.010248 -0.437642
S -2.765618 1.036826 0.971088
S -2.897552 -1.042276 0.820763
O -1.497958 0.062362 -2.075526
S 0.270131 -1.846346 -0.042774
O 2.677594 -0.125997 -1.541399
H 0.293460 2.240317 1.047732

E = -2279.164596
S -0.351180 0.102539 -1.825843
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S -0.351183 0.102390 1.825852
Mo -1.681683 0.060498 0.000002
O -2.816447 1.577770 0.000055
S -2.750772 -1.795255 -0.000073
S 2.856611 -0.852411 -1.044411
S 2.856609 -0.852504 1.044339
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H -2.380775 2.439809 0.000107

E = -2279.162697
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Mo 1.141421 0.000194 0.450090
O 1.516035 0.000901 2.085802
S -0.343318 -1.821104 0.099348
S 2.864184 1.043885 -0.850845
S 2.864068 -1.044657 -0.850029
O -2.829338 0.000759 1.582735
H -3.777569 0.000785 1.412206

[HMo2O2S4]- (M = 1)
E = -1880.925055
S -0.009976 -0.017467 -1.807024
Mo 1.381618 -0.283118 -0.000029
S 2.991394 1.478517 0.000212
Mo -1.483840 -0.182289 -0.000034
S -2.848380 1.509023 0.000195
O -2.246032 -1.699580 -0.000255
S -0.010001 -0.017981 1.807023
O 2.034561 -1.836751 -0.000244
H 4.016501 0.604288 0.000126

E = -1880.926540
S 0.000814 -0.043081 1.809036
Mo 1.473652 -0.186224 -0.000005
S 0.000804 -0.043009 -1.809031
Mo -1.390152 -0.302083 0.000001
O -2.059535 -1.849199 -0.000034
S -2.995170 1.451950 0.000013
S 2.805385 1.532103 0.000023
O 2.260694 -1.690948 -0.000038
H -2.105626 2.462644 0.000074

E = -1880.923058
S -0.033693 -0.151769 1.814574
Mo -1.415510 -0.138540 -0.000003

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S -2.547088 1.676102 0.000002
Mo 1.444599 -0.229058 0.000001
S 2.771699 1.487012 0.000010
O 2.226920 -1.741307 -0.000003
S -0.033687 -0.151756 -1.814575
O -2.447246 -1.726870 -0.000010
H -1.974814 -2.568890 -0.000010

E = -1880.920506
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Mo 1.458654 -0.241737 -0.000047
S -0.026207 -0.128165 -1.809173
Mo -1.411982 -0.146239 -0.000026
O -2.439908 -1.744496 -0.000328
S -2.554082 1.660974 0.000313
S 2.798166 1.466433 0.000275
O 2.236346 -1.754073 -0.000332
H -3.398487 -1.642759 -0.000307

E = -1880.903225
S 0.000024 -0.112732 1.913478
Mo 1.457032 -0.206574 -0.050725
S -0.000001 0.002376 -1.846040
Mo -1.457016 -0.206570 -0.050707
O -2.185419 -1.742701 -0.079119
S -2.770166 1.513848 0.072421
S 2.770043 1.513943 0.072466
O 2.185539 -1.742657 -0.079196
H -0.000036 -1.444086 2.129441

E = -1880.899516
S 0.017856 0.722088 -1.525793
Mo 1.580090 -0.161220 -0.123724
S 2.979515 1.331640 0.567672
Mo -1.636012 -0.223199 0.014274
S -3.014845 1.378055 0.413453
O -2.381896 -1.493300 -0.807735
S 0.268380 -0.903600 1.566310
O 2.411262 -1.447065 -0.859759
H -1.900716 -0.782378 1.590580

[Mo2O2S5]- (M = 2)
E = -2278.564204
S -0.321895 -1.403858 1.092570
Mo 1.233715 -0.284829 -0.322275
O 1.651887 -1.246213 -1.629562
Mo -1.807181 -0.095836 -0.093844
O -2.694965 -1.013489 -1.210114
S -0.351652 1.328394 -1.159257
S -3.130598 0.979724 1.231477
S 2.718533 1.519202 0.204402
S 3.112499 -0.294366 1.142956

S2 (M = 3)
E = -796.427415
S 0.000000 0.000000 0.951938
S 0.000000 0.000000 -0.951938

HS (M = 2)
E = -398.768116
H 0.000000 0.000000 -1.267962
S 0.000000 0.000000 0.079248

H (M = 2)
E = -0.502154
H 0.000000 0.000000 0.000000

[Mo2O2S3]- (M = 2)
E = -1482.019950
S -0.310332 1.821234 -0.227941
Mo -1.659039 -0.000010 -0.319750
S -0.310292 -1.821241 -0.227974
Mo 1.102003 0.000003 0.330950
S 2.848288 0.000036 -0.965887
O 1.422941 -0.000053 1.998143
O -2.953830 0.000033 0.786660

S (M = 3)
E = -398.132374
S 0.000000 0.000000 0.000000

SO (M = 3)
E = -473.426570
S 0.000000 0.000000 0.496640
O 0.000000 0.000000 -0.993281

[Mo2OS4]- (M = 2)
E = -1804.992945
S 0.142890 -1.827611 -0.348422
Mo -1.357439 -0.000359 -0.157980
S -2.360028 0.003384 1.764234
Mo 1.455388 -0.000667 -0.378061
S 2.997766 0.002082 1.112705
S 0.142797 1.826268 -0.354861
O -2.361081 -0.002860 -1.533098

OS2 (M = 1)
E = -871.673142
S 0.000000 0.673816 0.000000
O 1.455492 0.809236 0.000000
S -0.727746 -1.078434 0.000000
```

[Mo2OS3]- (M = 4)
E = -1406.678339
S 0.234967 -1.819745 -0.470506
Mo 1.574689 0.000053 0.040313
O 2.389478 0.000225 1.536436
Mo -1.166084 -0.000109 -0.387297
S -2.737052 0.000151 1.083906
S 0.234758 1.819628 -0.470785

MoOS2 (M = 1)
E = -940.007143
Mo -0.000003 0.304526 -0.272102
O 0.000034 1.730724 0.633647
S 1.749631 -0.832382 0.198719
S -1.749640 -0.832362 0.198725

[MoOS3]- (M = 2)
E = -1338.401602
Mo 0.000337 -0.000193 0.245223
S -0.705535 1.955594 -0.539021
O 0.000986 -0.000535 1.949884
S 2.046120 -0.367038 -0.540218
S -1.341964 -1.587782 -0.539414

[MoOS2]- (M = 2)
E = -940.136480
Mo -0.000000 0.246701 -0.044393
O -0.000008 1.955918 0.089185
S 1.912495 -0.812771 0.035970
S -1.912491 -0.812777 0.035970

[MoS3]- (M = 2)
E = -1263.112056
Mo 0.000000 0.000021 0.000000
S -0.776978 -2.023244 0.000000
S -1.363766 1.684538 0.000000
S 2.140744 0.338651 0.000000

MoO2S (M = 1)
E = -617.032160
Mo 0.304374 0.000000 -0.226960
O 1.012903 1.389471 0.446334
O 1.012915 -1.389465 0.446335
S -1.811891 -0.000003 0.149435

[MoO2S]- (M = 2)
E = -617.157940
Mo -0.289532 0.000003 -0.097526
O -1.150554 -1.473108 0.184001
O -1.150423 1.473161 0.183998
S 1.910509 -0.000034 0.072006

MoS3 (M = 1)
E = -1262.981702
Mo -0.000064 0.000000 0.383202
S 1.001069 1.732850 -0.335282
S 1.000480 -1.733190 -0.335282
S -2.001381 0.000340 -0.335342

[MoOS]- (M = 4)
E = -541.808426
Mo 0.000000 0.424240 0.000000
O 1.608869 1.053238 0.000000
S -0.804435 -1.640248 0.000000

MoOS3 (M = 3)
E = -1338.243636
Mo 0.000041 -0.070324 0.278694
S -0.000704 2.023539 -0.400136
O 0.000119 -0.262974 1.957443
S 1.879213 -0.853219 -0.655099
S -1.878677 -0.854233 -0.655058

[MoS2]- (M = 4)
E = -864.790468
Mo 0.000000 0.000000 0.347615
S 0.000000 2.034491 -0.456245
S -0.000000 -2.034491 -0.456245

MoO2S2 (M = 3)
E = -1015.260991
O -0.163676 1.253664 -1.397769
Mo -0.000003 0.308051 -0.000006
S 1.883537 -1.031190 -0.060721
S -1.883554 -1.031161 0.060759
O 0.163726 1.253768 1.397721

LM1 (M = 1)
E = -2676.802849
mo 1.431720 -0.000073 0.355029
o -1.877081 -0.000799 1.980020
s 0.000170 -1.821700 -0.030887
s -0.000181 1.821165 -0.031311
mo -1.431705 -0.000285 0.355003
s -3.212450 -1.050553 -0.946661
s -3.214336 1.051435 -0.944127
o 1.877163 -0.000174 1.980026
s 3.213643 1.051527 -0.944841
s 3.213075 -1.050446 -0.946028

TS1 (M = 1)
E = -2676.723163

```
mo -1.393745 -0.354524 0.347230
o 0.566600 0.057601 1.663644
s 0.222102 1.811538 -0.872774
s 0.176724 -1.631802 -1.016996
mo 1.276688 0.090939 0.060887
s 3.530117 1.073415 0.312394
s 3.445053 -0.932223 -0.335806
o -1.743976 -1.549150 1.479543
s -3.207165 -0.123867 -1.161728
s -3.270869 1.240626 0.432009

LM2 (M = 1)
E = -2676.769394
mo 1.329374 -0.532180 -0.044522
o 0.044862 0.000574 -1.412151
s -1.546402 2.466316 -0.013264
s 0.063085 -0.087450 1.888047
mo -1.224212 0.333876 -0.014696
s -2.959404 -0.801299 -1.293498
s -3.115720 -0.912854 0.803737
o 1.445868 -2.215008 -0.156253
s 3.385531 0.427833 0.824592
s 3.151495 0.535220 -1.269964

TS2 (M = 1)
E = -2676.721571
s 3.509604 -0.081845 -0.256524
s 2.211556 2.033529 -0.132543
s 2.365793 -2.199678 -0.074816
mo 1.243964 -0.104955 -0.015889
o -0.023551 -0.149504 -1.350562
s -0.075737 -0.140340 1.832039
mo -1.456124 0.435226 -0.043799
o -1.701892 2.094852 -0.145144
s -3.164800 -0.774154 -1.276843
s -3.426774 -0.677148 0.813220

LM3 (M = 1)
E = -2676.775538
o -0.049676 -0.247077 -1.344406
mo -1.409020 0.368988 -0.081554
s 2.074866 2.148939 -0.371688
mo 1.281529 0.177955 -0.040639
s -0.080869 0.187298 1.854618
s 2.795575 -1.457903 -1.082857
s 2.843954 -1.310770 1.018001
o -1.815444 1.977676 -0.386184
s -3.070430 -1.080631 -1.154780
s -3.295872 -0.787955 0.922759

TS3 (M = 1)
E = -2676.727594
o -0.145088 -0.075486 1.417371
mo 1.433696 0.201152 -0.312619
s -0.801556 2.099066 -0.688283
mo -1.246156 0.050721 0.057116
s -0.094114 -1.427828 -1.295590
s -3.486264 0.443654 1.038538
s -3.243126 -1.314414 -0.096462
o 1.997446 1.012524 -1.673174
s 3.163400 0.456464 1.420057
s 3.043191 -1.386627 0.420337

LM4 (M = 1)
E = -2676.796734
o -1.503200 -0.000902 -2.163987
mo 1.362650 -0.000050 0.481831
s -0.000616 -1.850571 0.001215
mo -1.362397 -0.000255 -0.481966
s -0.000170 1.850203 -0.000278
s -3.328979 -1.050509 0.503479
s -3.328147 1.051923 0.502956
o 1.504474 0.000117 2.163735
s 3.327820 -1.051298 -0.504072
s 3.328790 1.051445 -0.502823

LM5 (M = 2)
E = -1880.328144
mo -1.528819 -0.204650 0.000257
o 2.318809 -1.704029 0.004177
s -0.000179 -0.048050 1.764750
s 0.000261 -0.056489 -1.764762
mo 1.528918 -0.204723 0.000469
s 2.924125 1.441974 -0.003003
o -2.317967 -1.704328 0.003310
s -2.924888 1.441350 -0.002632

TS4 (M = 2)
E = -1880.269143
mo 1.501633 -0.295477 -0.209125
o -0.659876 -0.785635 -1.457290
s -0.562685 2.028554 -0.271560
s -0.018378 -0.903136 1.562792
mo -1.377426 0.007888 -0.085213
s -3.518728 -0.196289 0.167356
o 2.175944 -1.688328 -0.884648
s 3.015715 1.062774 0.485017

LM6 (M = 2)
E = -1880.316805
mo 1.549551 -0.298063 -0.104393
o 0.111853 -0.031611 -1.341836
```

s -2.318964 1.964184 -0.116248
s 0.134956 -0.094012 1.753323
mo -1.312968 0.071334 -0.073911
s -2.642537 -1.604313 -0.204369
o 2.231587 -1.847696 -0.223951
s 3.033795 1.268960 -0.181763

TS5 (M = 2)
E = -1880.269771
mo 1.518250 0.207679 0.020242
o -0.393353 -0.848594 -1.355769
s -0.877115 2.014434 -0.420887
s -0.001549 -0.661745 1.687057
mo -1.350562 -0.106546 -0.113389
s -3.435738 -0.681753 -0.011522
s 2.910380 -1.289813 -0.652037
o 2.321034 1.555404 0.639567

LM7 (M = 2)
E = -1880.327595
mo -1.496689 -0.347707 -0.000059
o 2.070252 1.943084 -0.000653
s 0.000006 -0.000019 -1.765264
s 0.000023 0.000447 1.765139
mo 1.496679 0.347612 -0.000078
s 3.106763 -1.087130 0.000526
s -3.106776 1.087003 0.000314
o -2.070235 -1.943187 -0.000061

LM8 (M = 2)
E = -2676.803506
S 0.000047 1.825046 0.049726
Mo -1.413906 0.000033 0.406703
S -3.082612 -1.021043 -1.058175
S -3.082389 1.021050 -1.058414
Mo 1.413895 -0.000029 0.406688
S 3.082586 1.021025 -1.058207
S 3.082465 -1.021061 -1.058334
O 1.939618 -0.000092 1.998558
S -0.000062 -1.825033 0.049688
O -1.939631 0.000100 1.998574

TS6 (M = 2)
E = -2676.776241
s -0.149041 -0.234992 -1.780928
s -0.048999 -0.424721 1.848057
s 2.935101 1.143208 0.981902
s 2.810421 1.204770 -1.100170
s -3.312613 0.820607 -0.301880
s -2.199590 2.367676 0.321199
mo -1.438479 -0.648416 0.041701
mo 1.408404 -0.413108 -0.006693
o 2.086754 -1.943592 -0.096099
o -1.999415 -2.236506 -0.024055

LM9 (M = 2)
E = -2676.778413
s 0.092927 -0.382183 1.823130
s 0.092704 -0.382915 -1.823010
s -2.775418 1.281259 -1.036475
s -2.775293 1.281668 1.036290
s 3.162659 0.828532 -0.000359
s 2.342954 2.649889 -0.000572
mo 1.388828 -0.786911 0.000062
mo -1.408138 -0.409453 0.000157
o -2.166793 -1.903992 0.000502
o 1.987102 -2.367600 0.000343

TS7 (M = 2)
E = -2676.749130
mo -1.504601 -0.524339 -0.040219
mo 1.287617 -0.916711 0.028499
s -0.027211 -0.492633 -1.816852
s -0.164568 -0.903961 1.829109
o -2.480464 -1.889961 -0.240461
o 2.026933 -2.431639 -0.088629
s 2.737083 0.869119 0.053536
s 1.730230 2.628732 -0.221161
s -0.850324 2.338722 0.531899
s -2.628863 1.503578 -0.181222

LM10 (M = 2)
E = -2676.753009
mo -1.395719 -0.803426 -0.051927
mo 1.393065 -0.807047 0.051906
s 0.073577 -0.621672 -1.831296
s -0.075685 -0.620759 1.831178
o -2.262762 -2.254221 -0.094121
o 2.255826 -2.260355 0.094672
s 2.638621 1.131181 0.049609
s 1.407094 2.727318 -0.207318
s -1.397861 2.730146 0.207012
s -2.635311 1.138567 -0.049405

TS8 (M = 2)
E = -2676.750335
s -0.146341 2.625783 0.378915
s 2.127627 2.303214 -0.290396
s 2.799613 0.388908 0.104415
mo 1.066278 -1.135728 0.055433
s -0.377360 -0.756587 1.826482
mo -1.615172 -0.322752 -0.075016

s -0.110882 -0.526848 -1.827047
o 1.509006 -2.766144 0.000011
o -2.870573 -1.441612 -0.252653
s -2.171027 1.897918 -0.014642

LM11 (M = 2)
E = -2676.777664
mo -1.941903 0.525336 0.009606
mo 0.198314 -1.371480 0.038545
s -0.653114 -0.255410 -1.780422
s -0.714031 -0.269498 1.834234
o -3.485186 -0.178489 -0.011043
o -0.282268 -2.987417 0.021891
s 2.548622 -1.046822 -0.078987
s 2.798134 1.017339 -0.467494
s 4.434866 1.664966 0.371607
s -1.953828 2.693508 -0.010759

TS9 (M = 2)
E = -2676.758976
s -2.043954 2.740264 -0.427466
mo -2.015121 0.639235 0.065238
o -3.519833 0.087453 0.612770
s -0.320452 0.195165 1.619488
s -1.245151 -0.679330 -1.706305
mo 0.110104 -1.450920 0.027163
o -0.376511 -2.975670 0.573563
s 2.261901 -1.324880 -0.372848
s 3.213453 1.191980 0.199880
s 5.083041 1.451583 -0.148470

LM12 (M = 2)
E = -2676.764309
s -2.416208 -1.778408 -0.005950
mo -0.262443 -1.669466 -0.000312
o 0.440505 -3.209774 0.003724
s 0.555912 -0.364140 1.763153
s 0.566153 -0.368528 -1.762404
mo 1.733836 0.630111 0.002567
o 3.361364 0.164097 0.008046
s 1.513619 2.780370 -0.000734
s -2.046465 2.112739 -0.023265
s -3.936353 1.869114 0.017396

LM14 (M = 2)
E = -2677.982106
h -4.030034 -1.002352 -1.020456
o -1.905111 0.000285 1.873601
mo -1.454709 0.000057 0.262619
s -2.880518 1.677628 -0.836757
s -2.880819 -1.678250 -0.835657
h -4.029783 1.001816 -1.021567
s 0.061597 1.810868 -0.064503
mo 1.386172 0.000171 0.441502
s 0.061600 -1.810387 -0.065158
o 1.810869 0.000248 2.065993
s 3.184772 -1.000652 -0.943604
s 3.184138 0.999962 -0.944810

TS10 (M = 2)
E = -2677.927055
h -3.010920 -0.969009 1.064453
o -2.213654 -0.309800 1.747996
mo -1.404338 0.123172 0.223955
s -2.313830 1.823393 -1.193494
s -3.396963 -1.362761 -0.501553
h -3.387180 1.165229 -1.670154
s 0.153213 1.756434 0.667410
mo 1.403518 -0.211882 0.383898
s -0.168208 -1.572644 -0.704602
o 1.732589 -0.888100 1.882086
s 3.065097 -0.852863 -1.240157
s 3.303257 1.027990 -0.400402

LM15 (M = 2)
E = -2677.954548
h -2.707184 -0.960895 2.178036
o -1.979747 -0.352880 2.011086
mo -1.612541 -0.071759 0.156250
s -2.130113 1.941356 -1.042847
s -3.423501 -0.974199 -0.657346
h -3.272788 1.609972 -1.680025
s 0.127452 1.565867 0.887499
mo 1.471368 -0.204166 0.383433
s -0.143704 -1.518166 -0.796055
o 1.841510 -1.115771 1.746014
s 2.910246 -0.553704 -1.518043
s 3.473064 0.956908 -0.199550

TS11 (M = 2)
E = -2677.953750
s 3.716487 1.067445 -0.117961
s 2.481398 0.213179 1.761695
h 4.448037 -0.047623 -0.290325
mo 1.322933 -0.288733 -0.072872
s -0.236567 -1.819530 0.663585
mo -1.465966 -0.106499 -0.393469
s 0.199365 1.521266 -0.830288
o 2.124273 -1.381021 -1.421691
h 1.567824 -2.120936 -1.697984
o -1.896724 -0.706702 -1.902235
s -3.004313 1.570836 0.362596

```
s -3.270675 -0.336315 1.170753

LM16 (M = 2)
E = -2677.961862
s -3.739453 -0.860258 0.557360
s -2.849971 0.864728 1.348139
h -4.484868 -0.305450 -0.423853
mo -1.304171 0.072646 -0.263876
s 0.142626 1.860980 -0.008969
mo 1.481753 -0.053734 -0.351637
s -0.085444 -1.797091 0.104991
o -1.947078 0.209208 -2.052388
h -1.351826 0.709002 -2.628407
o 1.850451 -0.154294 -1.988037
s 3.162719 -1.125570 0.986971
s 3.316476 0.954887 0.838208

LM17 (M = 2)
E = -2677.955511
o 2.068879 -0.419634 2.055997
h 2.675424 0.271438 2.351214
h 4.614314 0.268980 0.143182
s 3.729984 0.937407 -0.628945
mo 1.304973 -0.168064 0.326108
s -0.182006 -1.872348 -0.116492
s 0.123609 1.756986 0.103360
mo -1.494507 0.029254 0.367732
o -1.923354 -0.004126 1.989250
s -3.307339 -0.831318 -0.963832
s -3.118933 1.250976 -0.910919
s 2.723842 -0.699225 -1.483028

TS12 (M = 2)
E = -2677.910165
o -2.163395 -0.002168 1.869661
h -3.249519 -0.319149 1.747076
h -4.136587 -0.613570 1.140156
s -3.471245 -0.830083 -0.673105
mo -1.333430 0.072787 0.273097
s 0.125890 1.843122 0.296301
s -0.081814 -1.748117 -0.227626
mo 1.486569 -0.083482 0.391112
o 1.908971 -0.352085 1.991366
s 3.255847 1.033931 -0.782155
s 3.120200 -1.025062 -1.098458
s -2.762024 0.989704 -1.369471

LM18 (M = 2)
E = -2677.973577
o -1.954850 -0.000220 1.912283
h -4.448498 -0.000516 2.131664
h -5.193308 -0.000453 2.174167
s -3.003749 -1.021014 -1.168040
mo -1.375406 -0.000036 0.337310
s 0.048280 1.824642 0.024849
s 0.048281 -1.824610 0.024440
mo 1.450381 -0.000020 0.427825
o 1.924457 -0.000149 2.035673
s 3.165890 1.020843 -0.982496
s 3.166031 -1.020714 -0.982487
s -3.003734 1.021246 -1.167837

LM19 (M = 2)
E = -2677.946368
s -0.107816 1.922692 0.035108
h -0.087119 2.083911 -1.300213
h -2.758924 1.709320 -1.773983
s -3.403523 1.204279 -0.709134
mo -1.445946 -0.122291 0.310235
mo 1.446899 0.066551 0.395840
s 0.159827 -1.837213 0.143347
s 2.986193 1.034769 -1.159927
o 1.862250 0.298004 2.005107
o -2.003361 -0.143053 1.891496
s -2.629101 -1.491707 -1.130961
s 3.240350 -1.001054 -0.788044

TS13 (M = 2)
E = -2677.915717
s -0.098087 1.787783 0.596742
h -0.735380 2.402884 -0.667442
h -1.699094 2.269467 -1.289815
s -2.923926 1.230050 -0.913999
mo -1.430589 -0.181591 0.437020
mo 1.444781 -0.058874 0.382645
s 0.057391 -1.832724 -0.240598
s 2.957268 1.231476 -0.946768
o 1.984712 -0.282784 1.955079
o -2.047687 -0.497060 1.968554
s -2.959304 -0.848596 -1.323692
s 3.113046 -0.838867 -1.162795

LM20 (M = 2)
E = -2677.974123
s 0.000009 1.438214 -1.113668
h 0.041849 2.309066 1.832292
h 0.052339 2.520300 2.546781
s 3.080195 1.420353 0.253992
mo 1.414132 -0.261187 -0.356711
mo -1.414848 -0.259960 -0.355699
s -0.000365 -1.549645 0.982806
s -3.084947 1.419101 0.254669
```

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o -1.945172 -1.175277 -1.656077
o 1.944356 -1.176685 -1.657101
s 3.073019 -0.244017 1.436250
s -3.071512 -0.241850 1.438924

LM21 (M = 1)
E = -2677.852906
o -2.210472 1.802306 0.882314
h -1.770783 2.626743 1.129725
h -4.449042 -0.193906 0.149259
s -3.517898 -1.160047 0.310271
mo -1.293900 0.395902 0.054078
s 0.150510 1.297399 -1.390571
s -0.172218 -0.913146 1.488152
mo 1.476226 0.288836 0.293516
o 2.006129 1.522283 1.292110
s 3.087782 -0.345002 -1.330611
s 2.929256 -1.590830 0.316237
s -2.465127 -0.900159 -1.473060

TS14 (M = 1)
E = -2677.782104
o -2.123866 -0.260323 1.786878
h -3.309839 -0.584991 1.625879
h -4.037219 -0.786493 0.927014
s -3.426858 -0.782288 -0.776982
mo -1.333423 0.003911 0.229240
s 0.122980 1.797643 0.335949
s -0.005996 -1.727217 -0.457841
mo 1.459067 -0.115438 0.416925
o 1.846271 -0.492758 1.991986
s 3.300687 1.104770 -0.686803
s 3.247468 -0.831261 -1.128930
s -2.970107 1.193368 -1.030564

LM22 (M = 1)
E = -2677.844804
o -1.883769 -0.002573 1.927970
h -4.485367 -0.005182 2.064714
h -5.174807 -0.007359 1.782831
s -3.082822 -0.990661 -1.121070
mo -1.358666 -0.000454 0.345693
s 0.050094 1.811007 -0.039032
s 0.049955 -1.811035 -0.043632
mo 1.436957 -0.000642 0.421489
o 1.872388 -0.002756 2.029565
s 3.234907 0.994146 -0.954291
s 3.234732 -0.991551 -0.957289
s -3.082928 0.994420 -1.117778

LM23 (M = 1)
E = -2677.834833
s -0.170469 -0.636032 1.960801
h -0.227552 0.652563 2.342102
h -1.280378 2.690229 1.354073
s -1.212822 2.439992 0.030850
s -2.954234 1.282931 -0.114123
mo -1.534353 -0.583819 -0.049830
o -2.227327 -2.103380 0.017111
s -0.170754 -0.521972 -1.860182
mo 1.303207 -0.524309 -0.021455
o 1.973771 -2.050395 0.040032
s 2.691941 1.069022 -1.081999
s 2.644123 1.142856 0.992194

TS15 (M = 1)
E = -2677.778706
s -0.219951 -0.210617 1.868413
h -0.715161 1.551435 1.881099
h -1.055873 2.227604 1.380203
s -1.729374 2.645929 -0.127038
s -2.969922 1.042337 -0.267070
mo -1.472116 -0.745074 -0.021787
o -2.149686 -2.268197 0.134370
s -0.043501 -0.643308 -1.790582
mo 1.342011 -0.509816 0.093592
o 2.066796 -1.982194 0.384802
s 2.860390 0.920365 -1.136532
s 2.596017 1.428386 0.800904

LM24 (M = 1)
E = -2677.812870
s -0.138081 -0.185715 1.815596
h -1.604307 2.284105 2.890206
h -2.072733 2.789841 3.171783
s -2.019277 2.470592 -0.394340
s -3.181807 0.862435 -0.172747
mo -1.419249 -0.744419 0.017085
o -1.964546 -2.317704 0.189095
s -0.051331 -0.605655 -1.801185
mo 1.380814 -0.478334 0.050984
o 2.114233 -1.959748 0.240822
s 2.851791 1.128002 -1.094438
s 2.794569 1.361672 0.874598

LM25 (M = 2)
E = -1881.479345
s -0.075887 0.812295 1.678851
h -0.025032 2.117874 1.339615
h -2.647666 2.322549 0.446966
s -2.785298 1.493959 -0.608132
mo -1.407575 -0.365991 0.018612
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mo 1.480132 -0.184668 0.098896
s 0.105094 -1.003659 -1.603271
s 2.713360 1.417305 -0.700187
o 2.281163 -1.434605 0.921742
o -2.242538 -1.669288 0.703499

TS16 (M = 2)
E = -1881.447846
s -0.225708 0.730928 1.540410
h -0.720153 2.290130 1.121570
h -1.448140 2.550273 0.439384
s -2.321547 1.659594 -0.597070
mo -1.495182 -0.353145 -0.045203
mo 1.488408 -0.205794 0.151818
s 0.123058 -1.198414 -1.490279
s 2.719533 1.357944 -0.684799
o 2.345241 -1.374327 1.034550
o -2.629311 -1.396393 0.674080

LM26 (M = 2)
E = -1881.498010
s -0.000015 -0.082074 1.764364
h 0.372679 3.339375 0.000259
h -0.372734 3.338945 0.000917
s -2.936180 1.391554 -0.000392
mo -1.527547 -0.245005 0.000051
mo 1.527555 -0.245003 0.000044
s -0.000015 -0.082916 -1.764341
s 2.936199 1.391543 -0.000332
o 2.307213 -1.749235 0.000321
o -2.307228 -1.749226 0.000434

LM27 (M = 2)
E = -1881.486826
O -2.277942 -1.870113 -0.351615
Mo -1.378524 -0.262490 0.086852
Mo 1.459163 -0.196427 -0.070060
S 2.842138 1.460911 0.201325
S -2.682316 1.691194 0.061683
S 0.095871 -0.438129 1.819928
S -0.098637 0.314621 -1.740288
O 2.219075 -1.676658 -0.425086
H -2.089861 -2.289280 -1.199609
H -3.338944 1.480409 1.225581

TS17 (M = 2)
E = -1881.432959
o -2.586661 -1.500180 -0.000000
h -3.667267 -1.049555 -0.000000
h -4.240695 -0.117739 -0.000000
s -3.040296 1.282207 0.000000
mo -1.408195 -0.124371 -0.000000
s 0.048442 -0.027526 1.780693
s 0.048442 -0.027525 -1.780693
mo 1.609322 -0.225986 -0.000000
o 2.332995 -1.757733 -0.000000
s 3.036536 1.394445 0.000000

LM28 (M = 2)
E = -1881.498137
o -1.899744 2.078942 0.000000
h -2.274496 4.489755 0.000000
h -2.388190 5.227975 0.000000
s 1.164836 2.996131 0.000000
mo -0.327676 1.440134 0.000000
s -0.021799 -0.063380 1.764582
s -0.021799 -0.063380 -1.764582
mo -0.021799 -1.601155 0.000000
o -1.435256 -2.535637 0.000000
s 1.755050 -2.825700 0.000000

LM29 (M = 1)
E = -1881.366672
s 0.062406 -0.394984 1.891019
h -0.004185 0.878472 2.324982
h -1.943696 2.455824 -0.034108
s -2.883792 1.497507 0.105405
mo -1.413203 -0.303732 -0.046657
mo 1.481667 -0.182561 -0.064571
s -0.016570 0.055173 -1.824135
s 2.606456 1.629360 0.138755
o 2.392297 -1.593926 -0.208786
o -2.045245 -1.843936 -0.115713

TS18 (M = 1)
E = -1881.308330
s -0.189780 0.462520 1.654446
h -0.569394 2.164357 1.297368
h -1.134763 2.521198 0.650040
s -2.068364 1.743523 -0.551655
mo -1.533148 -0.336656 -0.076518
mo 1.510097 -0.223273 0.130214
s 0.154397 -1.390941 -1.347321
s 2.322602 1.540579 -0.724721
o 2.710253 -1.158610 0.840182
o -2.813928 -1.198819 0.572991

LM30 (M = 1)
E = -1881.340115
s -0.000106 -0.221701 1.803298
h 0.003848 3.236952 2.265980
h 0.002940 2.937631 1.583907

s -2.121890 1.726654 -0.477194
mo -1.538616 -0.246461 0.028266
mo 1.538496 -0.246657 0.028212
s -0.000077 -1.104729 -1.526872
s 2.122101 1.726406 -0.477109
o 2.882805 -1.218357 0.288805
o -2.883079 -1.217857 0.289203

LM31 (M = 1)
E = -1881.374694
o 2.317308 -1.799279 0.279092
h 1.980374 -2.701806 0.358067
h 3.405936 1.222861 -1.065307
s 2.548472 1.735631 -0.152167
mo 1.358952 -0.239190 0.011050
s 0.017728 -0.496864 -1.768436
s 0.070590 0.238599 1.769365
mo -1.462411 -0.206669 0.035643
o -2.289486 -1.651403 0.326836
s -2.715766 1.510790 -0.230094

TS19 (M = 1)
E = -1881.284306
o 2.426491 -0.000000 -1.592371
h 3.626320 -0.000000 -1.098951
h 4.109721 -0.000000 -0.232676
s 3.019083 -0.000000 1.225882
mo 1.387095 0.000000 -0.163815
s -0.046231 1.780620 0.225188
s -0.046231 -1.780620 0.225187
mo -1.535834 0.000000 -0.202070
o -1.995255 0.000000 -1.819820
s -3.235303 -0.000000 1.073512

LM32 (M = 1)
E = -1881.338115
O -1.146805 2.403910 -0.000000
H -0.643648 4.910897 -0.000000
H -0.149319 5.468078 -0.000000
S 1.976243 2.671189 -0.000000
Mo 0.239275 1.452481 -0.000000
S 0.239275 -0.130150 1.729675
S 0.239275 -0.130150 -1.729675
Mo -0.595668 -1.475626 0.000000
O -2.274110 -1.546064 0.000000
S 0.240756 -3.427744 0.000000

H2Mo2O2S6-, iso1 (M = 2)
E = -2677.982106
S -0.061584 -1.810483 -0.065136
Mo 1.454976 -0.000000 0.262799
S 2.880984 1.677508 -0.836253
S 2.880620 -1.677995 -0.836102
Mo -1.386033 0.000226 0.440987
S -3.185678 -1.000596 -0.942800
S -3.185518 1.000099 -0.943513
O -1.810381 0.000618 2.065556
S -0.061275 1.810592 -0.065641
O 1.905777 0.000029 1.873660
H 4.030043 -1.002509 -1.021145
H 4.030403 1.001849 -1.020482

H2Mo2O2S6-, iso2 (M = 2)
E = -2677.961862
s -3.739453 -0.860258 0.557360
s -2.849971 0.864728 1.348139
h -4.484868 -0.305450 -0.423853
mo -1.304171 0.072646 -0.263876
s 0.142626 1.860980 -0.008969
mo 1.481753 -0.053734 -0.351637
s -0.085444 -1.797091 0.104991
o -1.947078 0.209208 -2.052388
h -1.351826 0.709002 -2.628407
o 1.850451 -0.154294 -1.988037
s 3.162719 -1.125570 0.986971
s 3.316476 0.954887 0.838208

H2Mo2O2S6-, iso3 (M = 2)
E = -2677.955782
S -0.103999 -1.635982 0.775242
Mo -1.365201 0.147138 0.203632
S 0.121564 1.970857 -0.557534
Mo 1.450936 0.103984 0.388398
O 1.911126 0.710942 1.884138
S 3.055723 0.388264 -1.347382
S 3.009999 -1.503304 -0.471969
S -3.435120 -1.147281 -0.164607
S -2.661284 0.059191 -1.709580
O -1.992705 1.260036 1.629652
H -2.776801 0.886590 2.054320
H 0.038469 2.690521 0.583392

H2Mo2O2S6-, iso4 (M = 2)
E = -2677.955505
S -0.123645 1.756422 0.111488
Mo -1.305222 -0.169610 0.324773
S -2.723724 -0.691337 -1.487239
S -3.728008 0.940963 -0.623295
Mo 1.494173 0.027338 0.367947
S 3.118465 1.255549 -0.904901
S 3.307021 -0.826483 -0.967815
O 1.923182 -0.013376 1.989260

S 0.181981 -1.872360 -0.124173
O -2.068325 -0.431075 2.053620
H -4.613213 0.268828 0.144676
H -2.675023 0.258121 2.352996

H2Mo2O2S6-, iso5 (M = 2)
E = -2677.955022
S -0.067750 1.720751 -0.040748
Mo 1.553044 -0.015229 0.258401
S 0.037695 -1.888392 -0.013986
Mo -1.331085 -0.123020 0.387420
O -1.883228 -0.190439 1.982448
S -2.961240 -0.829888 -1.214449
S -3.567143 1.075226 -0.600127
S 3.117692 1.612732 -0.782064
S 2.921709 -1.437443 -0.959939
O 2.000517 -0.029142 1.874636
H -4.409789 0.744837 0.405217
H 2.453839 2.770500 -0.605338

H2Mo2O2S6-, iso6 (M = 2)
E = -2677.954583
S -0.396476 0.848914 1.486706
Mo -1.240456 -0.910725 0.071936
S -2.818433 0.350292 -1.156554
S -3.520557 2.080421 -0.129073
Mo 1.520531 -0.160125 0.312282
S 2.536923 1.984463 0.038395
S 3.155549 0.510013 -1.303797
O 2.199572 -1.090248 1.531604
S 0.479830 -1.548239 -1.297187
O -1.927071 -2.174411 0.966809
H -4.271570 1.469243 0.806240
H -0.660989 2.009921 0.853454

H2Mo2O2S6-, iso7 (M = 2)
E = -2677.952568
S -0.205153 1.733998 0.459823
Mo 1.419991 0.036981 0.260219
S 0.208084 -1.764908 -0.452864
Mo -1.379955 -0.238786 0.353581
O -1.935943 -0.791615 1.848337
S -2.900706 -0.618284 -1.457928
S -3.659614 1.022054 -0.400872
S 2.816834 1.255631 -1.131883
S 3.642704 -0.628359 -0.715929
O 2.110101 -0.135071 2.024280
H -4.515721 0.390322 0.434630
H 3.006558 -0.503119 1.999286

H2Mo2O2S6-, iso8 (M = 2)
E = -2677.946213
S -0.261525 -0.149939 1.809229
Mo 1.372605 -0.310220 0.155616
S 0.261972 -0.154998 -1.809549
Mo -1.372332 -0.310133 -0.155400
O -2.151899 -2.001021 -0.532519
S -2.557468 1.546180 -0.785947
S -3.574197 0.549091 0.755318
S 2.555791 1.548387 0.782802
S 3.573954 0.548788 -0.755577
O 2.153237 -1.999525 0.538077
H 3.046249 -2.070467 0.170550
H -3.044859 -2.070475 -0.164481

H2Mo2O2S6-, iso9 (M = 2)
E = -2677.940824
S 0.000156 -0.898006 1.721089
Mo 1.715383 -0.470412 -0.000209
S -0.000453 -0.898616 -1.720664
Mo -1.715463 -0.470393 0.000300
O -2.785367 -1.760595 0.000982
S -2.524738 1.501838 -1.049049
S -2.523956 1.502723 1.048599
S 2.525854 1.501581 1.048748
S 2.523588 1.502447 -1.048875
O 2.784944 -1.760901 -0.001143
H -0.000848 0.146688 -2.575552
H 0.000361 0.147627 2.575438

H2Mo2O2S4-, iso1 (M = 2)
E = -1881.502195
S 0.000417 -0.630903 1.744362
Mo 1.414286 -0.281170 -0.050908
S 2.919163 1.564439 0.290006
Mo -1.414440 -0.281586 -0.050338
O -2.161893 -1.713066 -0.544845
S -2.918648 1.565095 0.289244
S -0.000236 0.574189 -1.659697
O 2.161183 -1.712815 -0.545836
H -3.717619 0.941192 1.178837
H 3.718648 0.936501 1.176280

H2Mo2O2S4-, iso2 (M = 2)
E = -1881.491108
S -0.052693 -0.154759 1.809711
Mo 1.408346 -0.353999 -0.001082
S 2.897093 1.526400 -0.050342
Mo -1.433348 -0.130019 -0.008188
O -2.482028 -1.713714 -0.084691
S -2.594611 1.678622 0.066641
S -0.036347 0.004591 -1.804917

O 2.206108 -1.847885 -0.052605
H 3.280249 1.534421 1.242645
H -3.437896 -1.590529 -0.092433

H2Mo2O2S4-, iso3 (M = 2)
E = -1881.486828
S -0.096136 -0.437968 -1.819913
Mo 1.378388 -0.262402 -0.086939
S 2.684084 1.690272 -0.061824
Mo -1.459230 -0.196154 0.070233
O -2.218544 -1.676620 0.425436
S 0.098882 0.315271 1.740168
S -2.842993 1.460466 -0.201594
O 2.276538 -1.870572 0.351741
H 3.340365 1.477172 -1.225484
H 2.089641 -2.288967 1.200340

H2Mo2O2S4-, iso4 (M = 2)
E = -1881.486697
S -0.065463 -0.121785 1.842606
Mo 1.399669 -0.143991 0.060956
S 2.608848 1.630664 -0.054327
Mo -1.410561 -0.144011 -0.010407
O -2.512352 -1.699532 0.183431
S -2.495755 1.692805 -0.187066
S 0.003029 -0.406522 -1.782150
O 2.417861 -1.790329 -0.028124
H -2.080544 -2.523750 0.435286
H 2.483384 -2.183887 -0.905812

H2Mo2O2S4-, iso5 (M = 2)
E = -1881.479338
S -0.077013 0.815941 1.676675
Mo -1.406961 -0.366306 0.018108
S -2.786635 1.492225 -0.608922
Mo 1.479830 -0.184213 0.099530
O 2.280704 -1.431758 0.926238
S 0.106380 -1.007419 -1.601941
S 2.712337 1.416811 -0.702569
O -2.239487 -1.668773 0.707561
H -2.644847 2.324426 0.442768
H -0.026504 2.120692 1.334152

H2Mo2O2S4-, iso6 (M = 2)
E = -1881.470454
S 0.006890 0.540617 1.805140
Mo 1.455627 -0.178934 0.112306
S 2.727363 1.422867 -0.607006
Mo -1.400987 -0.079810 0.116442
O -2.225808 -1.831473 0.273613
S -2.680662 1.532396 -0.513586
S -0.012323 -0.842051 -1.722007
O 2.206573 -1.605122 0.663404
H -2.839343 -1.922132 1.012032
H 0.038057 -2.179117 -1.516218

H2Mo2O2S4-, iso7 (M = 2)
E = -1881.437712
S -0.039215 -0.256375 1.924749
Mo 1.475274 -0.266949 -0.000467
S 2.594043 1.587743 0.002942
Mo -1.494081 -0.262415 -0.000592
O -2.667247 -1.499497 -0.003766
S -2.294991 1.804127 0.004092
S -0.039364 -0.247232 -1.925701
O 2.294516 -1.750786 -0.003568
H 0.122272 1.017548 -2.371452
H 0.121930 1.005797 2.377276

H2Mo2O2S6, iso1 (M = 1)
E = -2677.872756
S -0.000235 1.746755 -0.120636
Mo 1.395706 -0.040908 0.374476
S 0.000046 -1.873220 0.090316
Mo -1.396048 -0.040803 0.374938
O -1.921464 -0.006190 1.963024
S -2.988474 -0.944307 -1.149471
S -3.432999 1.057904 -0.813581
S 3.433014 1.058235 -0.813316
S 2.989921 -0.944237 -1.148249
O 1.920737 -0.005839 1.962634
H -4.327969 0.954045 0.198812
H 4.327757 0.955988 0.199540

H2Mo2O2S6, iso2 (M = 1)
E = -2677.857064
S -0.069222 1.765257 -0.188458
Mo 1.445591 0.078201 0.297936
S 0.160828 -1.822702 0.203993
Mo -1.353293 -0.068185 0.391691
O -1.889573 -0.003869 1.977038
S -2.867015 -1.092940 -1.129134
S -3.469961 0.875918 -0.825163
S 2.916670 0.948638 -1.286474
S 3.230979 -1.034806 -0.760559
O 1.928414 0.426718 2.040128
H -4.369182 0.708545 0.174163
H 1.745475 1.258135 2.496908

H2Mo2O2S6, iso3 (M = 1)
E = -2677.852906
S -0.171249 0.913882 1.486815

Mo -1.293702 -0.395694 0.053933
S -2.466249 0.899007 -1.473178
S -3.518220 1.159958 0.310783
Mo 1.476488 -0.289566 0.292993
S 2.927181 1.591892 0.316734
S 3.087632 0.347005 -1.330258
O 2.007904 -1.522660 1.291299
S 0.149968 -1.299029 -1.390345
O -2.208683 -1.801174 0.885474
H -4.448250 0.192519 0.151411
H -1.767566 -2.624337 1.134686

H2Mo2O2S6, iso4 (M = 1)
E = -2677.842612
S -0.000560 1.968674 0.409931
Mo 1.451595 0.000320 0.406391
S 0.000089 -1.968067 0.410916
Mo -1.451660 -0.000101 0.406523
O -2.075344 -0.000518 1.949148
S -2.832322 -1.037392 -1.199084
S -2.833441 1.036448 -1.198630
S 2.832448 1.036589 -1.199513
S 2.834106 -1.037336 -1.197493
O 2.075100 0.001767 1.949067
H 0.001057 -2.375534 -0.872180
H -0.001486 2.373727 -0.873961

H2Mo2O2S6, iso5 (M = 1)
E = -2677.836918
S -0.169505 -0.104548 -1.742998
Mo 1.420779 0.362234 -0.093275
S 0.146128 0.393561 1.840943
Mo -1.364258 0.330265 0.119496
O -2.179640 2.008419 0.084991
S -2.359383 -1.572322 0.826633
S -3.472572 -0.726125 -0.717686
S 2.753814 -1.319774 -0.980187
S 3.140915 -0.817693 0.988394
O 1.965663 2.073161 -0.489710
H 1.849624 2.516595 -1.340143
H -3.141999 2.096239 0.035035

H2Mo2O2S6, iso6 (M = 1)
E = -2677.836707
S 0.038034 1.802009 -0.058704
Mo -1.383288 0.000000 0.353667
S -3.049569 -1.394309 -0.958913
S -3.049597 1.394279 -0.958922
Mo 1.420931 0.000003 0.409787
S 3.217174 0.992739 -0.967664
S 3.217194 -0.992739 -0.967639
O 1.859839 0.000012 2.017625
S 0.038038 -1.802010 -0.058688
O -1.855444 0.000010 1.949601
H -4.098235 1.207976 -0.137107
H -4.098314 -1.207789 -0.137281

H2Mo2O2S6, iso7 (M = 1)
E = -2677.835203
S -0.089570 -1.401329 1.156362
Mo -1.432977 0.209413 0.300406
S 0.014091 1.849954 -0.820309
Mo 1.407620 0.207771 0.346053
O 1.957106 1.117073 1.636157
S 2.946678 0.105165 -1.443514
S 2.878290 -1.564713 -0.218770
S -2.989097 -1.481750 -0.245437
S -2.538138 -0.101287 -1.702513
O -2.002655 1.400553 1.588851
H -2.166334 2.351169 1.550950
H 0.039668 1.489428 -2.115377

H2Mo2O2S6, iso8 (M = 1)
E = -2677.834832
S 0.170411 -0.636247 -1.960624
Mo 1.534515 -0.583746 0.049686
S 2.953346 1.283821 0.114170
S 1.211720 2.440263 -0.030636
Mo -1.303078 -0.524533 0.021713
S -2.643388 1.142753 -0.992480
S -2.692053 1.068989 1.081686
O -1.973595 -2.050648 -0.039876
S 0.171187 -0.522367 1.860295
O 2.227901 -2.103111 -0.017726
H 1.278673 2.690232 -1.353942
H 0.226982 0.652210 -2.342573

H2Mo2O2S4, iso1 (M = 1)
E = -1881.398381
S -0.036260 -0.062170 1.798834
Mo 1.384070 -0.310328 -0.000241
S 2.955020 1.424105 -0.000163
Mo -1.446147 -0.122167 0.000419
O -2.456594 -1.690431 0.000956
S -2.534442 1.684026 -0.000650
S -0.037129 -0.063199 -1.798766
O 2.016058 -1.857119 0.000215
H 3.996121 0.566599 -0.000776
H -3.419653 -1.745622 -0.004168

H2Mo2O2S4, iso2 (M = 1)
E = -1881.398087

S -0.005463 0.026211 1.804472
Mo 1.399108 -0.250648 -0.000547
S 2.969145 1.481859 0.002856
Mo -1.408899 -0.259185 -0.000211
O -2.036253 -1.806873 -0.004585
S -3.043255 1.403990 0.002516
S -0.005931 0.035817 -1.803644
O 2.031658 -1.796345 -0.004563
H -2.192937 2.449716 0.004973
H 4.009010 0.622968 0.000839

H2Mo2O2S4, iso3 (M = 1)
E = -1881.397372
S -0.000081 -0.201538 1.803582
Mo 1.415495 -0.183659 0.000165
S 2.436762 1.659817 -0.000831
Mo -1.415363 -0.183728 0.000054
O -2.465677 -1.731717 0.000531
S -2.438065 1.659024 -0.000425
S 0.000201 -0.203241 -1.803390
O 2.467162 -1.730767 0.000808
H -3.430319 -1.748223 -0.003165
H 3.431815 -1.746638 0.000283

H2Mo2O2S4, iso4 (M = 1)
E = -1881.374693
S -0.017792 -0.496913 1.768377
Mo -1.358838 -0.239110 -0.011153
S -2.549657 1.734889 0.152375
Mo 1.462543 -0.206593 -0.035626
O 2.289591 -1.651288 -0.327113
S -0.070396 0.239102 -1.769302
S 2.715841 1.510869 0.230403
O -2.316670 -1.799495 -0.279330
H -3.407568 1.220598 1.064250
H -1.979370 -2.701951 -0.357651

H2Mo2O2S4, iso5 (M = 1)
E = -1881.366671
S 0.062145 -0.394584 1.890118
Mo -1.413646 -0.303706 -0.046887
S -2.882189 1.498479 0.105427
Mo 1.481674 -0.182704 -0.064443
O 2.391386 -1.594813 -0.207298
S -0.016075 0.054623 -1.824317
S 2.606580 1.629250 0.138523
O -2.046164 -1.843805 -0.114565
H -1.941467 2.456339 -0.033155
H -0.004874 0.877534 2.327912

H2Mo2O2S4, iso6 (M = 1)
E = -1881.364976
S -0.042313 -0.228069 1.826076
Mo 1.444224 -0.262880 0.034603
S 2.643959 1.508738 0.039521
Mo -1.444469 -0.144607 0.034130
O -2.538978 -1.655135 0.021172
S -2.252131 1.797205 0.010869
S -0.003604 -0.274015 -1.912620
O 2.286211 -1.726969 -0.004935
H -3.497015 -1.690146 -0.093128
H -0.005148 0.999687 -2.345070

H2Mo2O2S4, iso7 (M = 1)
E = -1881.352577
S 0.000272 -0.308303 1.917250
Mo 1.483418 -0.226950 -0.000646
S 2.491487 1.656236 0.004051
Mo -1.483283 -0.227005 -0.000315
O -2.406179 -1.636076 -0.003545
S -2.492435 1.655628 0.003600
S -0.000174 -0.298567 -1.918980
O 2.407086 -1.635531 -0.004151
H 0.000163 0.985792 -2.321668
H 0.000486 0.973235 2.328838