Table S1 Selected bond distances (Å) and angles (degrees) for the reaction of $[MoO(mnt)_2]^{2-}$ and Me_3NO.

Parameter	$[MoO(mnt)_2]^{2-}$	$[MoO(ON(CH_3)_3)(mnt)_2]^{2-}$			$[MoO_2(mnt)_2]^{2-}$
		TS1	im	TS2	
$Mo=O_1$	1.734	1.739	1.749	1.747	1.765
$Mo\text{-}ON(CH_3)_3$	-	2.966	2.168	1.931	-
$Mo=O_2$	-				1.771
$O\text{-}N(CH_3)_3$	-	1.374	1.408	1.667	-
$Mo\text{-}S_1$	2.365	2.443	2.608	2.679	2.565
$Mo\text{-}S_2$	2.363	2.378	2.415	2.506	2.456
$Mo\text{-}S_3$	2.354	2.333	2.388	2.475	2.539
$Mo\text{-}S_4$	2.368	2.371	2.376	2.388	2.420
O-Mo-O	-	70.91	85.55	98.19	104.09
Mo-O-S	-	116.77	125.13	126.40	-
$S_1\text{-}Mo\text{-}S_2$	83.83	81.65	78.59	78.83	78.75
$S_3\text{-}Mo\text{-}S_4$	83.63	84.15	83.92	83.85	79.62
ADF reactionenergy (kJ/mol)	-13698.87	-20634.19	-20642.16	-20635.83	-14277.55
Me_3NO = -7007.81					
Me_3N = -6492.34					

Table S2 Selected bond distances (Å) and angles (degrees) for the reaction of $[Mo(OCH_3)(mnt)_2]^-$ and DMSO.

Parameter	$[Mo(OCH_3)(mnt)_2]^-$	$[Mo(OCH_3)(OS(CH_3)_2)(mnt)_2]^-$			$[MoO(OCH_3)(mnt)_2]^-$
		TS1	im	TS2	
Mo-OCH_3	1.851	1.868	1.979	2.025	1.918
O-CH_3	1.417	1.405	1.397	1.395	1.393
Mo-O_{DMSO}	-	2.994	2.169	1.854	-
Mo=O	-	-	-	-	1.743
O-S_{DMSO}	-	1.531	1.573	1.993	-
Mo-S_1	2.316	2.357	2.380	2.426	2.425
Mo-S_2	2.312	2.337	2.336	2.382	2.397
Mo-S_3	2.333	2.306	2.360	2.414	2.539
Mo-S_4	2.337	2.333	2.341	2.388	2.430
O-Mo-O	-	66.21	69.12	78.89	98.75
Mo-O-C	131.89	133.25	124.07	123.64	133.96
Mo-O-S	-	115.98	118.70	129.27	-
S_1-Mo-S_2	84.03	83.38	82.06	80.83	80.91
S_3-Mo-S_4	84.44	84.67	82.88	82.03	79.06
ADF reactionenergy (kJ/mol)	-15138.93	-19887.24	-19912.08	-19836.96	-15751.19
DMSO = -4790.27					
DMS = -4184.74					

Table S3 Selected bond distances (Å) and angles (degrees) for the TS found in the reaction of $[MoO(mnt)_2]^{2-}$ and DMSO.

Parameter	$[MoO(OS(CH_3)_2)(mnt)_2]^{2-}$
$Mo{=}O_1$	1.746
$Mo\text{-}O_{DMSO}$	1.871
$O\text{-}S_{DMSO}$	1.977
$Mo\text{-}S_1$	2.700
$Mo\text{-}S_2$	2.541
$Mo\text{-}S_3$	2.500
$Mo\text{-}S_4$	2.367
O-Mo-O	105.80
Mo-O-S	128.48
$S_1\text{-}Mo\text{-}S_2$	76.24
$S_3\text{-}Mo\text{-}S_4$	84.54
ADF reactionenergy	-18335.12 kJ/mol

Table S4 Selected bond distances (Å) and angles (degrees) for the rotated intermediate from the reaction of $[Mo(OCH_3)(mnt)_2]^-$ and DMSO depicted in figure 6c.

Parameter	$[Mo(OCH_3)(OS(CH_3)_2)(mnt)_2]^-$
Mo-OCH_3	1.974
O-CH_3	1.397
Mo-O_{DMSO}	2.124
O-S_{DMSO}	1.586
Mo-S_1	2.369
Mo-S_2	2.338
Mo-S_3	2.348
Mo-S_4	2.361
O-Mo-O	72.86
Mo-O-C	126.32
Mo-O-S	120.43
S_1-Mo-S_2	82.33
S_3-Mo-S_4	82.72
ADF reactionenergy	-19907.36 kJ/mol

Table S5. Coordinates (in pdb format) for the computed structures of all complexes depicted in Fig. 2-7 and other starting complexes and products.

$[MoO(mnt)_2]^{2-}$

```
HEADER    [MoO(mnt)2]2-
AUTHOR    GENERATED BY BABEL 1.6
ATOM      1  O   UNK     1       2.257  -0.003  -0.005  1.00  0.00
ATOM      2  MO  UNK     1       1.690   1.635  -0.001  1.00  0.00
ATOM      3  S   UNK     1      -0.156   1.813   1.468  1.00  0.00
ATOM      4  C   UNK     1       0.470   2.447   2.983  1.00  0.00
ATOM      5  C   UNK     1      -0.402   2.509   4.073  1.00  0.00
ATOM      6  N   UNK     1      -1.139   2.554   4.970  1.00  0.00
ATOM      7  S   UNK     1       2.820   2.849   1.683  1.00  0.00
ATOM      8  C   UNK     1       1.751   2.904   3.072  1.00  0.00
ATOM      9  C   UNK     1       2.248   3.480   4.244  1.00  0.00
ATOM     10  N   UNK     1       2.678   3.976   5.203  1.00  0.00
ATOM     11  S   UNK     1       3.058   2.931  -1.411  1.00  0.00
ATOM     12  C   UNK     1       2.215   3.084  -2.946  1.00  0.00
ATOM     13  C   UNK     1       2.956   3.708  -3.951  1.00  0.00
ATOM     14  N   UNK     1       3.658   4.231  -4.714  1.00  0.00
ATOM     15  S   UNK     1       0.089   1.931  -1.721  1.00  0.00
ATOM     16  C   UNK     1       0.931   2.657  -3.087  1.00  0.00
ATOM     17  C   UNK     1       0.206   2.819  -4.271  1.00  0.00
ATOM     18  N   UNK     1      -0.422   2.958  -5.214  1.00  0.00
CONECT    1    2
CONECT    2    1    3    7   11   15
CONECT    3    2    4
CONECT    4    3    5    8
CONECT    5    4    6
CONECT    6    5
CONECT    7    2    8
CONECT    8    4    7    9
CONECT    9    8   10
CONECT   10    9
CONECT   11    2   12
CONECT   12   11   13   16
CONECT   13   12   14
CONECT   14   13
CONECT   15    2   16
CONECT   16   12   15   17
CONECT   17   16   18
CONECT   18   17
MASTER        0    0    0    0    0    0    0    0   18    0   18    0
END
```

$\{[MoO(ON(CH_3)_3)(mnt)_2]^{2-}\}^{\ddagger}$, TS1

```
HEADER    [MoO(ONMe3)(mnt)2]2-, TS1
AUTHOR    GENERATED BY BABEL 1.6
ATOM      1  O   UNK     1       1.739    0.000    0.016  1.00  0.00
ATOM      2  MO  UNK     1       1.574    1.732   -0.004  1.00  0.00
ATOM      3  S   UNK     1       0.887    2.311    2.148  1.00  0.00
ATOM      4  C   UNK     1       2.340    2.704    3.076  1.00  0.00
ATOM      5  C   UNK     1       2.173    2.949    4.426  1.00  0.00
ATOM      6  N   UNK     1       1.993    3.132    5.559  1.00  0.00
ATOM      7  S   UNK     1       3.693    2.503    0.726  1.00  0.00
ATOM      8  C   UNK     1       3.550    2.787    2.454  1.00  0.00
ATOM      9  C   UNK     1       4.723    3.124    3.135  1.00  0.00
ATOM     10  N   UNK     1       5.727    3.382    3.660  1.00  0.00
ATOM     11  S   UNK     1       2.088    3.456   -1.656  1.00  0.00
ATOM     12  C   UNK     1       0.658    3.608   -2.627  1.00  0.00
ATOM     13  C   UNK     1       0.757    4.343   -3.812  1.00  0.00
ATOM     14  N   UNK     1       0.870    4.955   -4.795  1.00  0.00
ATOM     15  S   UNK     1      -0.648    2.217   -0.700  1.00  0.00
ATOM     16  C   UNK     1      -0.531    3.047   -2.236  1.00  0.00
ATOM     17  C   UNK     1      -1.693    3.193   -2.995  1.00  0.00
ATOM     18  N   UNK     1      -2.668    3.284   -3.624  1.00  0.00
ATOM     19  O   UNK     1       1.520    0.719   -2.791  1.00  0.00
ATOM     20  N   UNK     1       2.602   -0.022   -3.201  1.00  0.00
ATOM     21  C   UNK     1       2.463   -1.413   -2.728  1.00  0.00
ATOM     22  C   UNK     1       2.671   -0.008   -4.672  1.00  0.00
ATOM     23  C   UNK     1       3.847    0.551   -2.657  1.00  0.00
ATOM     24  H   UNK     1       1.551   -1.824   -3.182  1.00  0.00
ATOM     25  H   UNK     1       2.358   -1.361   -1.635  1.00  0.00
ATOM     26  H   UNK     1       3.344   -2.003   -3.024  1.00  0.00
ATOM     27  H   UNK     1       2.791    1.037   -4.987  1.00  0.00
ATOM     28  H   UNK     1       1.724   -0.414   -5.051  1.00  0.00
ATOM     29  H   UNK     1       3.520   -0.618   -5.016  1.00  0.00
ATOM     30  H   UNK     1       3.777    0.510   -1.560  1.00  0.00
ATOM     31  H   UNK     1       3.897    1.598   -2.987  1.00  0.00
ATOM     32  H   UNK     1       4.712   -0.024   -3.019  1.00  0.00
CONECT    1    2
CONECT    2    1    3    7   11   15
CONECT    3    2    4
CONECT    4    3    5    8
CONECT    5    4    6
CONECT    6    5
CONECT    7    2    8
CONECT    8    4    7    9
CONECT    9    8   10
CONECT   10    9
CONECT   11    2   12
CONECT   12   11   13   16
CONECT   13   12   14
CONECT   14   13
CONECT   15    2   16
CONECT   16   12   15   17
CONECT   17   16   18
CONECT   18   17
CONECT   19   20
CONECT   20   19   21   22   23
CONECT   21   20   24   25   26
CONECT   22   20   27   28   29
CONECT   23   20   30   31   32
CONECT   24   21
```

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CONECT   25   21
CONECT   26   21
CONECT   27   22
CONECT   28   22
CONECT   29   22
CONECT   30   23
CONECT   31   23
CONECT   32   23
MASTER        0    0    0    0    0    0    0    0   32    0   32    0
END
```

$[MoO(ON(CH_3)_3)(mnt)_2]^{2-}$, intermediate

```
HEADER    [MoO(ONMe3)(mnt2)]2-, im
AUTHOR    GENERATED BY BABEL 1.6
ATOM      1  O   UNK     1       1.409  -0.005   0.008  1.00  0.00
ATOM      2  MO  UNK     1       1.171   1.728   0.008  1.00  0.00
ATOM      3  S   UNK     1       0.905   2.107   2.351  1.00  0.00
ATOM      4  C   UNK     1       2.485   2.566   2.963  1.00  0.00
ATOM      5  C   UNK     1       2.596   2.790   4.323  1.00  0.00
ATOM      6  N   UNK     1       2.676   2.965   5.469  1.00  0.00
ATOM      7  S   UNK     1       3.368   2.552   0.380  1.00  0.00
ATOM      8  C   UNK     1       3.550   2.742   2.122  1.00  0.00
ATOM      9  C   UNK     1       4.806   3.118   2.602  1.00  0.00
ATOM     10  N   UNK     1       5.865   3.420   2.974  1.00  0.00
ATOM     11  S   UNK     1       1.016   4.211  -0.775  1.00  0.00
ATOM     12  C   UNK     1      -0.554   4.313  -1.483  1.00  0.00
ATOM     13  C   UNK     1      -0.857   5.440  -2.255  1.00  0.00
ATOM     14  N   UNK     1      -1.085   6.382  -2.898  1.00  0.00
ATOM     15  S   UNK     1      -1.219   2.023  -0.172  1.00  0.00
ATOM     16  C   UNK     1      -1.517   3.347  -1.257  1.00  0.00
ATOM     17  C   UNK     1      -2.810   3.477  -1.768  1.00  0.00
ATOM     18  N   UNK     1      -3.886   3.565  -2.201  1.00  0.00
ATOM     19  O   UNK     1       1.004   1.535  -2.144  1.00  0.00
ATOM     20  N   UNK     1       2.089   1.406  -3.032  1.00  0.00
ATOM     21  C   UNK     1       2.990   0.326  -2.603  1.00  0.00
ATOM     22  C   UNK     1       1.507   1.076  -4.341  1.00  0.00
ATOM     23  C   UNK     1       2.832   2.670  -3.134  1.00  0.00
ATOM     24  H   UNK     1       2.396  -0.592  -2.509  1.00  0.00
ATOM     25  H   UNK     1       3.416   0.604  -1.628  1.00  0.00
ATOM     26  H   UNK     1       3.782   0.209  -3.356  1.00  0.00
ATOM     27  H   UNK     1       0.823   1.889  -4.617  1.00  0.00
ATOM     28  H   UNK     1       0.964   0.128  -4.239  1.00  0.00
ATOM     29  H   UNK     1       2.317   0.978  -5.079  1.00  0.00
ATOM     30  H   UNK     1       3.235   2.915  -2.141  1.00  0.00
ATOM     31  H   UNK     1       2.129   3.450  -3.454  1.00  0.00
ATOM     32  H   UNK     1       3.645   2.544  -3.863  1.00  0.00
CONECT    1    2
CONECT    2    1    3    7   11   15   19
CONECT    3    2    4
CONECT    4    3    5    8
CONECT    5    4    6
CONECT    6    5
CONECT    7    2    8
CONECT    8    4    7    9
CONECT    9    8   10
CONECT   10    9
CONECT   11    2   12
CONECT   12   11   13   16
CONECT   13   12   14
CONECT   14   13
CONECT   15    2   16
CONECT   16   12   15   17
CONECT   17   16   18
CONECT   18   17
CONECT   19    2   20
CONECT   20   19   21   22   23
CONECT   21   20   24   25   26
CONECT   22   20   27   28   29
CONECT   23   20   30   31   32
CONECT   24   21
CONECT   25   21
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CONECT   26   21
CONECT   27   22
CONECT   28   22
CONECT   29   22
CONECT   30   23
CONECT   31   23
CONECT   32   23
MASTER        0    0    0    0    0    0    0    0   32    0   32    0
END
```

$\{[MoO(ON(CH_3)_3)(mnt)_2]^{2-}\}^{\ddagger}$, TS2

```
HEADER    [MoO(ONMe3)(mnt)2]2-, TS2
AUTHOR    GENERATED BY BABEL 1.6
ATOM      1  H   UNK     1       2.649   3.724  -3.675  1.00  0.00
ATOM      2  O   UNK     1       1.078  -0.030   0.165  1.00  0.00
ATOM      3  MO  UNK     1       0.868   1.703   0.128  1.00  0.00
ATOM      4  S   UNK     1       0.816   1.979   2.587  1.00  0.00
ATOM      5  C   UNK     1       2.391   2.580   2.992  1.00  0.00
ATOM      6  C   UNK     1       2.684   2.766   4.350  1.00  0.00
ATOM      7  N   UNK     1       2.902   2.911   5.481  1.00  0.00
ATOM      8  C   UNK     1       3.343   2.870   2.050  1.00  0.00
ATOM      9  S   UNK     1       3.044   2.666   0.324  1.00  0.00
ATOM     10  C   UNK     1       4.603   3.331   2.432  1.00  0.00
ATOM     11  N   UNK     1       5.669   3.705   2.719  1.00  0.00
ATOM     12  S   UNK     1      -1.624   1.607   0.372  1.00  0.00
ATOM     13  C   UNK     1      -2.250   3.178   0.022  1.00  0.00
ATOM     14  C   UNK     1      -3.644   3.286  -0.051  1.00  0.00
ATOM     15  N   UNK     1      -4.804   3.368  -0.104  1.00  0.00
ATOM     16  C   UNK     1      -1.467   4.315  -0.084  1.00  0.00
ATOM     17  S   UNK     1       0.244   4.309   0.111  1.00  0.00
ATOM     18  C   UNK     1      -2.084   5.553  -0.304  1.00  0.00
ATOM     19  N   UNK     1      -2.565   6.597  -0.486  1.00  0.00
ATOM     20  O   UNK     1       0.402   1.884  -1.737  1.00  0.00
ATOM     21  N   UNK     1       1.458   2.152  -2.999  1.00  0.00
ATOM     22  C   UNK     1       2.505   1.175  -2.851  1.00  0.00
ATOM     23  C   UNK     1       0.625   1.935  -4.161  1.00  0.00
ATOM     24  C   UNK     1       1.919   3.513  -2.875  1.00  0.00
ATOM     25  H   UNK     1       2.083   0.170  -2.987  1.00  0.00
ATOM     26  H   UNK     1       2.932   1.274  -1.838  1.00  0.00
ATOM     27  H   UNK     1       3.295   1.363  -3.597  1.00  0.00
ATOM     28  H   UNK     1      -0.197   2.665  -4.152  1.00  0.00
ATOM     29  H   UNK     1       0.230   0.910  -4.131  1.00  0.00
ATOM     30  H   UNK     1       1.232   2.073  -5.071  1.00  0.00
ATOM     31  H   UNK     1       2.403   3.634  -1.893  1.00  0.00
ATOM     32  H   UNK     1       1.059   4.192  -2.948  1.00  0.00
CONECT    1   24
CONECT    2    3
CONECT    3    2    4    9   12   17   20
CONECT    4    3    5
CONECT    5    4    6    8
CONECT    6    5    7
CONECT    7    6
CONECT    8    5    9   10
CONECT    9    3    8
CONECT   10    8   11
CONECT   11   10
CONECT   12    3   13
CONECT   13   12   14   16
CONECT   14   13   15
CONECT   15   14
CONECT   16   13   17   18
CONECT   17    3   16
CONECT   18   16   19
CONECT   19   18
CONECT   20    3   21
CONECT   21   20   22   23   24
CONECT   22   21   25   26   27
CONECT   23   21   28   29   30
CONECT   24    1   21   31   32
CONECT   25   22
```

```
CONECT   26   22
CONECT   27   22
CONECT   28   23
CONECT   29   23
CONECT   30   23
CONECT   31   24
CONECT   32   24
```

$[MoO_2(mnt)_2]^{2-}$

```
HEADER    [MoO2(mnt)2]2-
AUTHOR    GENERATED BY BABEL 1.6
ATOM      1  O   UNK     1       1.473   2.087  -1.609  1.00  0.00
ATOM      2  O   UNK     1       0.565   0.001   0.002  1.00  0.00
ATOM      3  MO  UNK     1       0.815   1.748   0.000  1.00  0.00
ATOM      4  S   UNK     1       0.677   2.002   2.523  1.00  0.00
ATOM      5  C   UNK     1       2.275   2.286   3.088  1.00  0.00
ATOM      6  C   UNK     1       2.436   2.478   4.470  1.00  0.00
ATOM      7  N   UNK     1       2.533   2.625   5.617  1.00  0.00
ATOM      8  C   UNK     1       3.341   2.349   2.226  1.00  0.00
ATOM      9  S   UNK     1       3.128   2.238   0.516  1.00  0.00
ATOM     10  C   UNK     1       4.655   2.543   2.671  1.00  0.00
ATOM     11  N   UNK     1       5.758   2.696   3.002  1.00  0.00
ATOM     12  S   UNK     1       0.098   4.209  -0.079  1.00  0.00
ATOM     13  C   UNK     1      -1.426   4.267   0.697  1.00  0.00
ATOM     14  C   UNK     1      -1.931   5.529   1.050  1.00  0.00
ATOM     15  N   UNK     1      -2.334   6.580   1.330  1.00  0.00
ATOM     16  C   UNK     1      -2.163   3.130   0.933  1.00  0.00
ATOM     17  S   UNK     1      -1.585   1.564   0.488  1.00  0.00
ATOM     18  C   UNK     1      -3.437   3.190   1.513  1.00  0.00
ATOM     19  N   UNK     1      -4.474   3.212   1.991  1.00  0.00
CONECT    1    3
CONECT    2    3
CONECT    3    1    2    4    9   12   17
CONECT    4    3    5
CONECT    5    4    6    8
CONECT    6    5    7
CONECT    7    6
CONECT    8    5    9   10
CONECT    9    3    8
CONECT   10    8   11
CONECT   11   10
CONECT   12    3   13
CONECT   13   12   14   16
CONECT   14   13   15
CONECT   15   14
CONECT   16   13   17   18
CONECT   17    3   16
CONECT   18   16   19
CONECT   19   18
MASTER        0    0    0    0    0    0    0    0   19    0   19    0
END
```

$[Mo(OCH_3)(mnt)_2]^-$

```
HEADER    [Mo(OCH3)(mnt)2]-
AUTHOR    GENERATED BY BABEL 1.6
ATOM      1  O   UNK     1       0.007   0.007  -0.002  1.00  0.00
ATOM      2 MO   UNK     1       1.858  -0.001   0.002  1.00  0.00
ATOM      3  S   UNK     1       2.667  -2.187  -0.110  1.00  0.00
ATOM      4  C   UNK     1       3.101  -2.494  -1.779  1.00  0.00
ATOM      5  C   UNK     1       3.060  -1.490  -2.697  1.00  0.00
ATOM      6  S   UNK     1       2.604   0.129  -2.209  1.00  0.00
ATOM      7  C   UNK     1       3.532  -3.783  -2.107  1.00  0.00
ATOM      8  N   UNK     1       3.881  -4.861  -2.359  1.00  0.00
ATOM      9  C   UNK     1       3.415  -1.695  -4.034  1.00  0.00
ATOM     10  N   UNK     1       3.706  -1.867  -5.144  1.00  0.00
ATOM     11  S   UNK     1       2.464  -0.173   2.226  1.00  0.00
ATOM     12  C   UNK     1       3.013   1.404   2.750  1.00  0.00
ATOM     13  C   UNK     1       3.146   2.412   1.846  1.00  0.00
ATOM     14  S   UNK     1       2.722   2.142   0.165  1.00  0.00
ATOM     15  C   UNK     1       3.339   1.531   4.104  1.00  0.00
ATOM     16  N   UNK     1       3.568   1.603   5.239  1.00  0.00
ATOM     17  C   UNK     1       3.672   3.667   2.178  1.00  0.00
ATOM     18  N   UNK     1       4.097   4.710   2.427  1.00  0.00
ATOM     19  C   UNK     1      -0.938   0.635   0.846  1.00  0.00
ATOM     20  H   UNK     1      -0.818   1.729   0.802  1.00  0.00
ATOM     21  H   UNK     1      -1.947   0.359   0.503  1.00  0.00
ATOM     22  H   UNK     1      -0.791   0.289   1.883  1.00  0.00
CONECT    1    2   19
CONECT    2    1    3    6   11   14
CONECT    3    2    4
CONECT    4    3    5    7
CONECT    5    4    6    9
CONECT    6    2    5
CONECT    7    4    8
CONECT    8    7
CONECT    9    5   10
CONECT   10    9
CONECT   11    2   12
CONECT   12   11   13   15
CONECT   13   12   14   17
CONECT   14    2   13
CONECT   15   12   16
CONECT   16   15
CONECT   17   13   18
CONECT   18   17
CONECT   19    1   20   21   22
CONECT   20   19
CONECT   21   19
CONECT   22   19
MASTER        0    0    0    0    0    0    0    0   22    0   22    0
END
```

{[Mo(OCH$_3$)(OS(CH$_3$)$_2$)(mnt)$_2$]$^-$}‡, TS1

```
HEADER    [MoO(OCH3)(OS(CH3)2)(mnt)2]2-, TS1
AUTHOR    GENERATED BY BABEL 1.6
ATOM      1  O   UNK     1      -0.001  -0.001   0.001  1.00  0.00
ATOM      2 MO   UNK     1       1.866   0.001   0.001  1.00  0.00
ATOM      3  O   UNK     1       0.656   2.739  -0.002  1.00  0.00
ATOM      4  S   UNK     1       2.429  -2.157  -0.589  1.00  0.00
ATOM      5  C   UNK     1       2.847  -2.138  -2.295  1.00  0.00
ATOM      6  C   UNK     1       2.915  -0.959  -2.975  1.00  0.00
ATOM      7  S   UNK     1       2.609   0.549  -2.142  1.00  0.00
ATOM      8  C   UNK     1       3.145  -3.374  -2.880  1.00  0.00
ATOM      9  N   UNK     1       3.380  -4.414  -3.338  1.00  0.00
ATOM     10  C   UNK     1       3.282  -0.901  -4.324  1.00  0.00
ATOM     11  N   UNK     1       3.587  -0.833  -5.444  1.00  0.00
ATOM     12  S   UNK     1       2.168  -0.744   2.194  1.00  0.00
ATOM     13  C   UNK     1       3.183   0.403   3.017  1.00  0.00
ATOM     14  C   UNK     1       3.814   1.380   2.294  1.00  0.00
ATOM     15  S   UNK     1       3.555   1.539   0.580  1.00  0.00
ATOM     16  C   UNK     1       3.426   0.216   4.382  1.00  0.00
ATOM     17  N   UNK     1       3.608   0.055   5.517  1.00  0.00
ATOM     18  C   UNK     1       4.734   2.251   2.890  1.00  0.00
ATOM     19  N   UNK     1       5.494   2.984   3.374  1.00  0.00
ATOM     20  C   UNK     1      -0.964   0.371   0.954  1.00  0.00
ATOM     21  H   UNK     1      -0.961   1.468   1.060  1.00  0.00
ATOM     22  H   UNK     1      -1.953   0.029   0.611  1.00  0.00
ATOM     23  H   UNK     1      -0.723  -0.094   1.928  1.00  0.00
ATOM     24  S   UNK     1       1.178   3.704   1.067  1.00  0.00
ATOM     25  C   UNK     1       0.126   5.135   0.980  1.00  0.00
ATOM     26  H   UNK     1       0.334   5.637   0.025  1.00  0.00
ATOM     27  H   UNK     1      -0.925   4.812   1.043  1.00  0.00
ATOM     28  H   UNK     1       0.390   5.798   1.819  1.00  0.00
ATOM     29  C   UNK     1       0.589   3.075   2.628  1.00  0.00
ATOM     30  H   UNK     1       1.055   2.086   2.781  1.00  0.00
ATOM     31  H   UNK     1       0.917   3.770   3.418  1.00  0.00
ATOM     32  H   UNK     1      -0.509   2.997   2.606  1.00  0.00
CONECT    1    2   20
CONECT    2    1    4    7   12   15
CONECT    3   24
CONECT    4    2    5
CONECT    5    4    6    8
CONECT    6    5    7   10
CONECT    7    2    6
CONECT    8    5    9
CONECT    9    8
CONECT   10    6   11
CONECT   11   10
CONECT   12    2   13
CONECT   13   12   14   16
CONECT   14   13   15   18
CONECT   15    2   14
CONECT   16   13   17
CONECT   17   16
CONECT   18   14   19
CONECT   19   18
CONECT   20    1   21   22   23
CONECT   21   20
CONECT   22   20
CONECT   23   20
CONECT   24    3   25   29
CONECT   25   24   26   27   28
```

```
CONECT   26   25
CONECT   27   25
CONECT   28   25
CONECT   29   24   30   31   32
CONECT   30   29
CONECT   31   29
CONECT   32   29
MASTER        0    0    0    0    0    0    0    0   32    0   32    0
END
```

$[Mo(OCH_3)(OS(CH_3)_2)(mnt)_2]^-$, intermediate

```
HEADER    [Mo(OCH3)(OS(CH3)2)(mnt)2]-, intermediate
AUTHOR    GENERATED BY BABEL 1.6
ATOM      1  O   UNK     1      -0.003    0.003    0.001  1.00  0.00
ATOM      2 MO   UNK     1       1.977    0.002   -0.001  1.00  0.00
ATOM      3  O   UNK     1       1.205    2.029   -0.003  1.00  0.00
ATOM      4  S   UNK     1       1.969   -2.042   -1.142  1.00  0.00
ATOM      5  C   UNK     1       2.836   -1.842   -2.642  1.00  0.00
ATOM      6  C   UNK     1       3.372   -0.630   -2.975  1.00  0.00
ATOM      7  S   UNK     1       3.225    0.708   -1.875  1.00  0.00
ATOM      8  C   UNK     1       2.983   -2.965   -3.462  1.00  0.00
ATOM      9  N   UNK     1       3.098   -3.909   -4.129  1.00  0.00
ATOM     10  C   UNK     1       4.097   -0.432   -4.154  1.00  0.00
ATOM     11  N   UNK     1       4.709   -0.244   -5.123  1.00  0.00
ATOM     12  S   UNK     1       1.884   -1.345    1.906  1.00  0.00
ATOM     13  C   UNK     1       3.104   -0.838    3.041  1.00  0.00
ATOM     14  C   UNK     1       3.997    0.132    2.678  1.00  0.00
ATOM     15  S   UNK     1       3.875    0.893    1.124  1.00  0.00
ATOM     16  C   UNK     1       3.175   -1.487    4.276  1.00  0.00
ATOM     17  N   UNK     1       3.216   -2.023    5.305  1.00  0.00
ATOM     18  C   UNK     1       5.068    0.501    3.500  1.00  0.00
ATOM     19  N   UNK     1       5.967    0.820    4.162  1.00  0.00
ATOM     20  S   UNK     1       2.215    3.221   -0.184  1.00  0.00
ATOM     21  C   UNK     1       1.294    4.375   -1.153  1.00  0.00
ATOM     22  H   UNK     1       1.174    3.944   -2.158  1.00  0.00
ATOM     23  H   UNK     1       0.323    4.563   -0.669  1.00  0.00
ATOM     24  H   UNK     1       1.899    5.294   -1.207  1.00  0.00
ATOM     25  C   UNK     1       2.166    4.053    1.377  1.00  0.00
ATOM     26  H   UNK     1       2.641    3.390    2.116  1.00  0.00
ATOM     27  H   UNK     1       2.756    4.976    1.263  1.00  0.00
ATOM     28  H   UNK     1       1.119    4.272    1.632  1.00  0.00
ATOM     29  C   UNK     1      -0.786   -1.136    0.206  1.00  0.00
ATOM     30  H   UNK     1      -0.592   -1.584    1.202  1.00  0.00
ATOM     31  H   UNK     1      -1.854   -0.860    0.155  1.00  0.00
ATOM     32  H   UNK     1      -0.573   -1.916   -0.553  1.00  0.00
CONECT    1    2   29
CONECT    2    1    3    4    7   12   15
CONECT    3    2   20
CONECT    4    2    5
CONECT    5    4    6    8
CONECT    6    5    7   10
CONECT    7    2    6
CONECT    8    5    9
CONECT    9    8
CONECT   10    6   11
CONECT   11   10
CONECT   12    2   13
CONECT   13   12   14   16
CONECT   14   13   15   18
CONECT   15    2   14
CONECT   16   13   17
CONECT   17   16
CONECT   18   14   19
CONECT   19   18
CONECT   20    3   21   25
CONECT   21   20   22   23   24
CONECT   22   21
CONECT   23   21
CONECT   24   21
CONECT   25   20   26   27   28
```

```
CONECT   26   25
CONECT   27   25
CONECT   28   25
CONECT   29    1   30   31   32
CONECT   30   29
CONECT   31   29
CONECT   32   29
MASTER        0    0    0    0    0    0    0    0   32    0   32    0
END
```

{[Mo(OCH$_3$)(OS(CH$_3$)$_2$)(mnt)$_2$]$^-$}‡, TS2

```
HEADER    [MoO(OCH3)(OS(CH3)2)(mnt)2]2-, TS2
AUTHOR    GENERATED BY BABEL 1.6
ATOM      1  O   UNK     1      -0.022  -0.020  -0.006  1.00  0.00
ATOM      2  MO  UNK     1       2.002   0.034  -0.038  1.00  0.00
ATOM      3  O   UNK     1       1.596   1.843  -0.051  1.00  0.00
ATOM      4  S   UNK     1       1.849  -2.061  -1.227  1.00  0.00
ATOM      5  C   UNK     1       3.204  -2.058  -2.296  1.00  0.00
ATOM      6  C   UNK     1       3.883  -0.899  -2.592  1.00  0.00
ATOM      7  S   UNK     1       3.401   0.601  -1.889  1.00  0.00
ATOM      8  C   UNK     1       3.544  -3.267  -2.919  1.00  0.00
ATOM      9  N   UNK     1       3.801  -4.283  -3.421  1.00  0.00
ATOM     10  C   UNK     1       4.923  -0.897  -3.530  1.00  0.00
ATOM     11  N   UNK     1       5.784  -0.899  -4.311  1.00  0.00
ATOM     12  S   UNK     1       1.539  -0.892   2.107  1.00  0.00
ATOM     13  C   UNK     1       2.998  -1.054   3.009  1.00  0.00
ATOM     14  C   UNK     1       4.188  -0.631   2.464  1.00  0.00
ATOM     15  S   UNK     1       4.249   0.034   0.877  1.00  0.00
ATOM     16  C   UNK     1       2.926  -1.621   4.285  1.00  0.00
ATOM     17  N   UNK     1       2.863  -2.092   5.346  1.00  0.00
ATOM     18  C   UNK     1       5.398  -0.753   3.157  1.00  0.00
ATOM     19  N   UNK     1       6.405  -0.850   3.730  1.00  0.00
ATOM     20  S   UNK     1       2.780   3.399  -0.435  1.00  0.00
ATOM     21  C   UNK     1       1.602   4.195  -1.485  1.00  0.00
ATOM     22  H   UNK     1       1.671   3.731  -2.480  1.00  0.00
ATOM     23  H   UNK     1       0.598   4.051  -1.052  1.00  0.00
ATOM     24  H   UNK     1       1.849   5.266  -1.550  1.00  0.00
ATOM     25  C   UNK     1       2.367   4.100   1.134  1.00  0.00
ATOM     26  H   UNK     1       2.951   3.568   1.899  1.00  0.00
ATOM     27  H   UNK     1       2.637   5.168   1.128  1.00  0.00
ATOM     28  H   UNK     1       1.286   3.968   1.300  1.00  0.00
ATOM     29  C   UNK     1      -0.764  -1.202  -0.015  1.00  0.00
ATOM     30  H   UNK     1      -0.415  -1.923   0.755  1.00  0.00
ATOM     31  H   UNK     1      -1.824  -0.975   0.195  1.00  0.00
ATOM     32  H   UNK     1      -0.691  -1.717  -0.996  1.00  0.00
CONECT    1    2   29
CONECT    2    1    3    4    7   12   15
CONECT    3    2   20
CONECT    4    2    5
CONECT    5    4    6    8
CONECT    6    5    7   10
CONECT    7    2    6
CONECT    8    5    9
CONECT    9    8
CONECT   10    6   11
CONECT   11   10
CONECT   12    2   13
CONECT   13   12   14   16
CONECT   14   13   15   18
CONECT   15    2   14
CONECT   16   13   17
CONECT   17   16
CONECT   18   14   19
CONECT   19   18
CONECT   20    3   21   25
CONECT   21   20   22   23   24
CONECT   22   21
CONECT   23   21
CONECT   24   21
```

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CONECT   25   20   26   27   28
CONECT   26   25
CONECT   27   25
CONECT   28   25
CONECT   29    1   30   31   32
CONECT   30   29
CONECT   31   29
CONECT   32   29
MASTER        0    0    0    0    0    0    0    0   32    0   32    0
END
```

$[MoO(OCH_3)(mnt)_2]^-$

```
HEADER    [MoO(OCH3)(mnt)2]-
ATOM      1  O   UNK     1      -0.244   0.163   0.409  1.00  0.00
ATOM      2 MO   UNK     1       1.610   0.236  -0.078  1.00  0.00
ATOM      3  O   UNK     1       1.603   1.762  -0.920  1.00  0.00
ATOM      4  S   UNK     1       1.280  -2.279   0.008  1.00  0.00
ATOM      5  C   UNK     1       2.350  -2.900  -1.164  1.00  0.00
ATOM      6  C   UNK     1       2.929  -2.089  -2.117  1.00  0.00
ATOM      7  S   UNK     1       2.523  -0.423  -2.231  1.00  0.00
ATOM      8  C   UNK     1       2.606  -4.283  -1.149  1.00  0.00
ATOM      9  N   UNK     1       2.811  -5.423  -1.122  1.00  0.00
ATOM     10  C   UNK     1       3.825  -2.593  -3.070  1.00  0.00
ATOM     11  N   UNK     1       4.575  -2.978  -3.867  1.00  0.00
ATOM     12  S   UNK     1       1.672   0.604   2.289  1.00  0.00
ATOM     13  C   UNK     1       3.301   0.483   2.845  1.00  0.00
ATOM     14  C   UNK     1       4.298   0.142   1.977  1.00  0.00
ATOM     15  S   UNK     1       3.971  -0.160   0.309  1.00  0.00
ATOM     16  C   UNK     1       3.552   0.742   4.200  1.00  0.00
ATOM     17  N   UNK     1       3.765   0.971   5.317  1.00  0.00
ATOM     18  C   UNK     1       5.635   0.009   2.381  1.00  0.00
ATOM     19  N   UNK     1       6.751  -0.117   2.668  1.00  0.00
ATOM     20  C   UNK     1      -0.998  -0.683   1.217  1.00  0.00
ATOM     21  H   UNK     1      -0.523  -0.811   2.211  1.00  0.00
ATOM     22  H   UNK     1      -2.006  -0.258   1.344  1.00  0.00
ATOM     23  H   UNK     1      -1.067  -1.685   0.744  1.00  0.00
CONECT    1    2   20
CONECT    2    1    3    4    7   12   15
CONECT    3    2
CONECT    4    2    5
CONECT    5    4    6    8
CONECT    6    5    7   10
CONECT    7    2    6
CONECT    8    5    9
CONECT    9    8
CONECT   10    6   11
CONECT   11   10
CONECT   12    2   13
CONECT   13   12   14   16
CONECT   14   13   15   18
CONECT   15    2   14
CONECT   16   13   17
CONECT   17   16
CONECT   18   14   19
CONECT   19   18
CONECT   20    1   21   22   23
CONECT   21   20
CONECT   22   20
CONECT   23   20
MASTER        0    0    0    0    0    0    0    0   23    0   23    0
END
```

$\{[MoO(OS(CH_3)_2)(mnt)_2]^{2-}\}^{\ddagger}$, TS

```
HEADER    [MoO(OS(CH3)2)(mnt)2]2-, ts
AUTHOR    GENERATED BY BABEL 1.6
ATOM      1  O   UNK     1       0.007  -0.055   0.094  1.00  0.00
ATOM      2  MO  UNK     1       1.749   0.031   0.027  1.00  0.00
ATOM      3  O   UNK     1       2.168   1.853  -0.049  1.00  0.00
ATOM      4  S   UNK     1       2.097  -2.429   0.306  1.00  0.00
ATOM      5  C   UNK     1       2.493  -2.940  -1.296  1.00  0.00
ATOM      6  C   UNK     1       2.646  -2.084  -2.362  1.00  0.00
ATOM      7  S   UNK     1       2.432  -0.355  -2.207  1.00  0.00
ATOM      8  C   UNK     1       2.698  -4.317  -1.485  1.00  0.00
ATOM      9  N   UNK     1       2.857  -5.460  -1.621  1.00  0.00
ATOM     10  C   UNK     1       3.015  -2.567  -3.619  1.00  0.00
ATOM     11  N   UNK     1       3.325  -2.950  -4.676  1.00  0.00
ATOM     12  S   UNK     1       1.798   0.335   2.549  1.00  0.00
ATOM     13  C   UNK     1       3.311   1.120   2.846  1.00  0.00
ATOM     14  C   UNK     1       4.409   0.952   2.024  1.00  0.00
ATOM     15  S   UNK     1       4.378  -0.065   0.635  1.00  0.00
ATOM     16  C   UNK     1       3.413   1.886   4.012  1.00  0.00
ATOM     17  N   UNK     1       3.482   2.523   4.984  1.00  0.00
ATOM     18  C   UNK     1       5.615   1.596   2.325  1.00  0.00
ATOM     19  N   UNK     1       6.629   2.126   2.539  1.00  0.00
ATOM     20  S   UNK     1       2.722   2.923  -1.616  1.00  0.00
ATOM     21  C   UNK     1       1.956   4.398  -1.017  1.00  0.00
ATOM     22  H   UNK     1       0.912   4.402  -1.359  1.00  0.00
ATOM     23  H   UNK     1       2.010   4.380   0.085  1.00  0.00
ATOM     24  H   UNK     1       2.493   5.271  -1.420  1.00  0.00
ATOM     25  C   UNK     1       4.366   3.133  -0.999  1.00  0.00
ATOM     26  H   UNK     1       4.886   2.171  -1.128  1.00  0.00
ATOM     27  H   UNK     1       4.872   3.933  -1.561  1.00  0.00
ATOM     28  H   UNK     1       4.293   3.381   0.074  1.00  0.00
CONECT    1    2
CONECT    2    1    3    4    7   12   15
CONECT    3    2   20
CONECT    4    2    5
CONECT    5    4    6    8
CONECT    6    5    7   10
CONECT    7    2    6
CONECT    8    5    9
CONECT    9    8
CONECT   10    6   11
CONECT   11   10
CONECT   12    2   13
CONECT   13   12   14   16
CONECT   14   13   15   18
CONECT   15    2   14
CONECT   16   13   17
CONECT   17   16
CONECT   18   14   19
CONECT   19   18
CONECT   20    3   21   25
CONECT   21   20   22   23   24
CONECT   22   21
CONECT   23   21
CONECT   24   21
CONECT   25   20   26   27   28
CONECT   26   25
CONECT   27   25
CONECT   28   25
```

$[Mo(OCH_3)(OS(CH_3)_2)(mnt)_2]^-$, rotated intermediate

```
HEADER    [Mo(OCH3)(OS(CH3)2)(mnt)2]-, rotated intermediate
AUTHOR    GENERATED BY BABEL 1.6
ATOM      1  O   UNK     1       0.042  -0.048   0.011  1.00  0.00
ATOM      2 MO   UNK     1       2.016  -0.019  -0.007  1.00  0.00
ATOM      3  O   UNK     1       1.360   2.001  -0.004  1.00  0.00
ATOM      4  S   UNK     1       1.992  -1.970  -1.313  1.00  0.00
ATOM      5  C   UNK     1       2.835  -1.651  -2.805  1.00  0.00
ATOM      6  C   UNK     1       3.404  -0.428  -3.023  1.00  0.00
ATOM      7  S   UNK     1       3.295   0.811  -1.809  1.00  0.00
ATOM      8  C   UNK     1       2.921  -2.686  -3.740  1.00  0.00
ATOM      9  N   UNK     1       2.986  -3.560  -4.503  1.00  0.00
ATOM     10  C   UNK     1       4.115  -0.139  -4.192  1.00  0.00
ATOM     11  N   UNK     1       4.708   0.111  -5.159  1.00  0.00
ATOM     12  S   UNK     1       1.961  -1.573   1.738  1.00  0.00
ATOM     13  C   UNK     1       3.136  -1.133   2.943  1.00  0.00
ATOM     14  C   UNK     1       3.948  -0.054   2.728  1.00  0.00
ATOM     15  S   UNK     1       3.790   0.885   1.276  1.00  0.00
ATOM     16  C   UNK     1       3.234  -1.924   4.091  1.00  0.00
ATOM     17  N   UNK     1       3.298  -2.582   5.047  1.00  0.00
ATOM     18  C   UNK     1       4.943   0.312   3.640  1.00  0.00
ATOM     19  N   UNK     1       5.778   0.627   4.384  1.00  0.00
ATOM     20  S   UNK     1      -0.138   2.360   0.373  1.00  0.00
ATOM     21  C   UNK     1       0.056   4.103   0.629  1.00  0.00
ATOM     22  H   UNK     1       0.677   4.237   1.527  1.00  0.00
ATOM     23  H   UNK     1       0.517   4.567  -0.256  1.00  0.00
ATOM     24  H   UNK     1      -0.953   4.506   0.812  1.00  0.00
ATOM     25  C   UNK     1      -1.017   2.432  -1.167  1.00  0.00
ATOM     26  H   UNK     1      -1.161   1.399  -1.513  1.00  0.00
ATOM     27  H   UNK     1      -1.985   2.914  -0.960  1.00  0.00
ATOM     28  H   UNK     1      -0.427   3.027  -1.881  1.00  0.00
ATOM     29  C   UNK     1      -0.768  -1.171   0.196  1.00  0.00
ATOM     30  H   UNK     1      -0.598  -1.631   1.190  1.00  0.00
ATOM     31  H   UNK     1      -1.829  -0.876   0.122  1.00  0.00
ATOM     32  H   UNK     1      -0.554  -1.945  -0.569  1.00  0.00
CONECT    1    2   29
CONECT    2    1    3    4    7   12   15
CONECT    3    2   20
CONECT    4    2    5
CONECT    5    4    6    8
CONECT    6    5    7   10
CONECT    7    2    6
CONECT    8    5    9
CONECT    9    8
CONECT   10    6   11
CONECT   11   10
CONECT   12    2   13
CONECT   13   12   14   16
CONECT   14   13   15   18
CONECT   15    2   14
CONECT   16   13   17
CONECT   17   16
CONECT   18   14   19
CONECT   19   18
CONECT   20    3   21   25
CONECT   21   20   22   23   24
CONECT   22   21
CONECT   23   21
CONECT   24   21
CONECT   25   20   26   27   28
```

```
CONECT   26   25
CONECT   27   25
CONECT   28   25
CONECT   29    1   30   31   32
CONECT   30   29
CONECT   31   29
CONECT   32   29
MASTER        0    0    0    0    0    0    0    0   32    0   32    0
END
```

Me_3NO

```
HEADER    ON(CH3)3
ATOM      1  O   UNK     1      -0.023  -0.003   0.000  1.00  0.00
ATOM      2  N   UNK     1       1.356   0.002   0.001  1.00  0.00
ATOM      3  C   UNK     1       1.845   1.391   0.005  1.00  0.00
ATOM      4  C   UNK     1       1.852  -0.693   1.201  1.00  0.00
ATOM      5  C   UNK     1       1.852  -0.688  -1.201  1.00  0.00
ATOM      6  H   UNK     1       1.442   1.881   0.901  1.00  0.00
ATOM      7  H   UNK     1       1.467   1.879  -0.903  1.00  0.00
ATOM      8  H   UNK     1       2.945   1.400   0.018  1.00  0.00
ATOM      9  H   UNK     1       1.466  -1.721   1.173  1.00  0.00
ATOM     10  H   UNK     1       1.461  -0.160   2.078  1.00  0.00
ATOM     11  H   UNK     1       2.952  -0.692   1.207  1.00  0.00
ATOM     12  H   UNK     1       1.462  -0.151  -2.076  1.00  0.00
ATOM     13  H   UNK     1       1.468  -1.716  -1.177  1.00  0.00
ATOM     14  H   UNK     1       2.953  -0.687  -1.205  1.00  0.00
CONECT    1    2
CONECT    2    1    3    4    5
CONECT    3    2    6    7    8
CONECT    4    2    9   10   11
CONECT    5    2   12   13   14
CONECT    6    3
CONECT    7    3
CONECT    8    3
CONECT    9    4
CONECT   10    4
CONECT   11    4
CONECT   12    5
CONECT   13    5
CONECT   14    5
```

Me_3N

```
HEADER    N(CH3)3
ATOM      1  N   UNK     1       1.362   0.000   0.001  1.00  0.00
ATOM      2  C   UNK     1       1.828   1.366   0.006  1.00  0.00
ATOM      3  C   UNK     1       1.838  -0.682   1.181  1.00  0.00
ATOM      4  C   UNK     1       1.839  -0.677  -1.181  1.00  0.00
ATOM      5  H   UNK     1       1.454   1.896   0.896  1.00  0.00
ATOM      6  H   UNK     1       1.473   1.894  -0.894  1.00  0.00
ATOM      7  H   UNK     1       2.945   1.413   0.017  1.00  0.00
ATOM      8  H   UNK     1       1.485  -1.725   1.190  1.00  0.00
ATOM      9  H   UNK     1       1.470  -0.178   2.090  1.00  0.00
ATOM     10  H   UNK     1       2.955  -0.693   1.220  1.00  0.00
ATOM     11  H   UNK     1       1.475  -0.166  -2.087  1.00  0.00
ATOM     12  H   UNK     1       1.480  -1.719  -1.196  1.00  0.00
ATOM     13  H   UNK     1       2.954  -0.695  -1.217  1.00  0.00
CONECT    1    2    3    4
CONECT    2    1    5    6    7
CONECT    3    1    8    9   10
CONECT    4    1   11   12   13
CONECT    5    2
CONECT    6    2
CONECT    7    2
CONECT    8    3
CONECT    9    3
CONECT   10    3
CONECT   11    4
CONECT   12    4
CONECT   13    4
```

DMSO

```
HEADER    OS(CH3)2
ATOM      1  C   UNK     1      -0.721   1.373   0.237  1.00  0.00
ATOM      2  S   UNK     1       0.154  -0.025  -0.427  1.00  0.00
ATOM      3  C   UNK     1      -0.904  -1.291   0.236  1.00  0.00
ATOM      4  O   UNK     1       1.461  -0.115   0.364  1.00  0.00
ATOM      5  H   UNK     1      -0.151   2.276  -0.031  1.00  0.00
ATOM      6  H   UNK     1      -0.795   1.255   1.330  1.00  0.00
ATOM      7  H   UNK     1      -1.719   1.403  -0.231  1.00  0.00
ATOM      8  H   UNK     1      -0.460  -2.263  -0.028  1.00  0.00
ATOM      9  H   UNK     1      -1.895  -1.188  -0.236  1.00  0.00
ATOM     10  H   UNK     1      -0.966  -1.162   1.329  1.00  0.00
CONECT    1    2    5    6    7
CONECT    2    1    3    4
CONECT    3    2    8    9   10
CONECT    4    2
CONECT    5    1
CONECT    6    1
CONECT    7    1
CONECT    8    3
CONECT    9    3
CONECT   10    3
MASTER        0    0    0    0    0    0    0    0   10    0   10    0
END
```

DMS

```
HEADER    S(CH3)2
ATOM      1  C   UNK     1      -0.730   1.410   0.220  1.00  0.00
ATOM      2  S   UNK     1       0.162  -0.025  -0.395  1.00  0.00
ATOM      3  C   UNK     1      -0.917  -1.326   0.220  1.00  0.00
ATOM      4  H   UNK     1      -0.144   2.302  -0.045  1.00  0.00
ATOM      5  H   UNK     1      -0.830   1.354   1.315  1.00  0.00
ATOM      6  H   UNK     1      -1.725   1.478  -0.247  1.00  0.00
ATOM      7  H   UNK     1      -0.459  -2.290  -0.048  1.00  0.00
ATOM      8  H   UNK     1      -1.913  -1.256  -0.243  1.00  0.00
ATOM      9  H   UNK     1      -1.004  -1.260   1.316  1.00  0.00
CONECT    1    2    4    5    6
CONECT    2    1    3
CONECT    3    2    7    8    9
CONECT    4    1
CONECT    5    1
CONECT    6    1
CONECT    7    3
CONECT    8    3
CONECT    9    3
MASTER        0    0    0    0    0    0    0    0    9    0    9    0
END
```