A study of the atmospherically relevant reaction dimethyl sulphide(DMS) + Cl_2 in the absence and presence of a water using electronic structure methods

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Supplementary information

Table S1: Estimated Day-Time and Night-time Concentrations of DMS, H_2O and Cl_2 in the troposphere

	Day-Time	Night-Time
[H_2O]	7.38×10^{17} molecules.cm^{-3} (a)	7.38×10^{17} molecules.cm^{-3} (a)
[Cl_2]	5ppt (c) (1.23×10^{8} molecules.cm^{-3})	50ppt (c) (1.23×10^{9} molecules.cm^{-3})
[DMS]	120ppt (b) (2.95×10^{9} molecules.cm^{-3})	50ppt (b) (1.23×10^{9} molecules.cm^{-3})

See text and references (a) ref.31; 100% humidity = 0.03 atm = 7.38×10^{17} molecules.cm^{-3}
(b) ref.8 and c) refs (14-19);
the number density of air at 1atm and 298 K is 2.46×10^{19} molecules.cm^{-3}.

Table S2: Calculated concentrations (in molecules.cm^{-3}) of complexes at Day-Time and Night-Time using DLPNO-UCCSD(T)/CBS//UM06-2X/aVTZ Keq values (in Table 3) and estimated concentrations in Table S1.

Complex	Day-time	Night-Time
[DMS•H_2O]	3.8×10^{5}	1.6×10^{5}
[Cl_2•H_2O]	9.6×10^{3}	9.6×10^{4}
[DMS•Cl_2]	1.3×10^{-4}	5.3×10^{-4}

Tables S3

Cartesian coordinates for all stationary points for DMS + Cl_2 +H_2O using the M06-2X/aVTZ methods

DMS
Absolute electronic energy = -477.9971871 Hartree

6	0.000000000	1.368528000	-0.514712000
1	-0.890710000	1.338894000	-1.139167000
1	0.000000000	2.291181000	0.059645000
1	0.890710000	1.338894000	-1.139167000
6	0.000000000	-1.368528000	-0.514712000
1	0.000000000	-2.291181000	0.059645000
1	-0.890710000	-1.338894000	-1.139167000
1	0.890710000	-1.338894000	-1.139167000
16	0.000000000	0.000000000	0.663371000

Cl_2
Absolute electronic energy = -920.3757155 Hartree

17	0.000000000	0.000000000	0.997267000
17	0.000000000	0.000000000	-0.997267000

DMS:Cl_2
Absolute electronic energy = -1398.382434 Hartree

6	-1.940232000	0.817267000	1.370029000
1	-1.906247000	0.241705000	2.291346000
1	-1.060465000	1.455827000	1.312918000
1	-2.846309000	1.419152000	1.352593000
6	-1.940232000	0.817267000	-1.370029000
1	-1.060465000	1.455827000	-1.312918000
1	-1.906247000	0.241705000	-2.291346000
1	-2.846309000	1.419152000	-1.352593000
17	2.954881000	-0.191074000	0.000000000
17	0.924681000	-0.416624000	0.000000000
16	-1.940232000	-0.356857000	0.000000000

TS1
Absolute electronic energy = -1398.356275 Hartree

6	-0.120719000	0.775757000	1.386806000
17	1.378679000	-1.349033000	0.067355000
6	1.620436000	1.488443000	-0.567405000
17	-2.430766000	-0.196713000	-0.246477000
1	-0.774951000	0.000692000	1.769397000
1	2.094924000	1.222833000	-1.507422000

1	-0.687896000	1.701010000	1.304762000
1	0.812212000	0.893269000	1.932108000
1	2.326962000	1.462808000	0.256537000
1	1.148324000	2.466968000	-0.651880000
16	0.247975000	0.309056000	-0.310928000

$DMSCl_2$

Absolute electronic energy = -1398.401452 Hartree

16	0.000002	0.000000	-0.291306
6	0.045184	1.402067	0.860455
1	0.851334	1.224095	1.563062
1	0.257912	2.279013	0.255970
1	-0.925501	1.474365	1.335538
6	-0.045202	-1.402065	0.860458
1	-0.851364	-1.224089	1.563051
1	-0.257921	-2.279012	0.255972
1	0.925474	-1.474365	1.335557
17	-2.288257	0.016595	-0.352191
17	2.288265	-0.016597	-0.352146

TS2

Absolute electronic energy = -1398.3585 Hartree

16	-0.580950	-0.079838	-0.475176
6	0.327075	-1.185663	0.436432
1	0.200221	-1.092922	1.510431
1	0.230458	-2.190727	0.043788
1	1.532859	-0.713177	0.173845
6	-0.138322	1.469714	0.310081
1	0.938108	1.561767	0.144037
1	-0.703446	2.258654	-0.175403
1	-0.370385	1.402408	1.369347
17	-2.610208	-0.107222	0.058038
17	2.982848	0.009993	-0.054645

CH_3SClCH_2:HCl

Absolute electronic energy = -1398.368104 Hartree

16	-0.172133	0.926105	-0.795614
6	-0.041448	1.593514	0.878671
1	0.650176	0.995427	1.469745
1	0.339575	2.607000	0.787194
1	-1.024482	1.612946	1.341645
6	-0.792159	-0.707698	-0.394663
1	-0.815397	-1.283044	-1.313808

1	-0.148406	-1.190074	0.335575
1	1.933604	0.023271	-0.477765
17	2.849873	-0.639846	0.166738
17	-2.448655	-0.707100	0.285215

TS3

Absolute electronic energy = -1398.338747 Hartree

6	-0.048228000	0.594378000	-1.334035000
1	-0.763798000	0.785349000	-2.127937000
1	0.895633000	1.101176000	-1.524552000
1	0.054369000	-0.477039000	-1.193678000
6	-0.264953000	0.307883000	1.338381000
1	0.309811000	-0.583150000	1.133129000
1	-0.569229000	0.543323000	2.348277000
16	-0.771964000	1.277826000	0.164739000
17	-2.415840000	-1.080477000	-0.085777000
17	3.027735000	-0.455639000	-0.027999000
1	3.901505000	-1.114466000	0.637047000

trans-CH_3SCH_2Cl:HCl

Absolute electronic energy = -1398.417512 Hartree

6	0.067110000	1.600209000	0.906810000
1	1.038839000	1.578400000	1.393890000
1	-0.281743000	2.627194000	0.838663000
1	-0.655108000	1.009246000	1.466947000
6	0.770395000	-0.677224000	-0.415761000
1	0.110974000	-1.157054000	0.300853000
1	0.784279000	-1.234888000	-1.345713000
16	0.210018000	0.978073000	-0.782102000
17	2.427882000	-0.763782000	0.279997000
17	-2.764755000	-0.576012000	0.083801000
1	-3.655721000	-1.233481000	0.728131000

TS4

Absolute electronic energy = -1398.332813 Hartree

6	-1.299840000	0.844557000	1.372661000
1	-1.339439000	0.254140000	2.283538000
1	-0.307861000	1.276659000	1.230529000
1	-2.091881000	1.590447000	1.360120000
6	-1.300669000	0.838773000	-1.375952000
1	-0.308438000	1.271141000	-1.236441000
1	-1.341261000	0.244654000	-2.284378000
1	-2.092443000	1.584981000	-1.365775000

17	2.587366000	0.434022000	-0.000946000
17	0.269972000	-1.124586000	0.002069000
16	-1.593148000	-0.286401000	0.000817000

DMSCl:Cl

Absolute electronic energy = -1398.3591548 Hartree

6	-0.245584000	-1.062402000	-1.394171000
1	-0.744054000	-0.695713000	-2.287144000
1	0.770886000	-0.656087000	-1.228942000
1	-0.263798000	-2.152028000	-1.358566000
6	-0.245695000	-1.062386000	1.394199000
1	0.770802000	-0.656132000	1.229033000
1	-0.744208000	-0.695627000	2.287119000
1	-0.263963000	-2.152012000	1.358656000
17	2.344477000	0.223198000	0.000020000
17	-0.972718000	1.446951000	-0.000010000
16	-1.243618000	-0.539762000	-0.000031000

TS5

Absolute electronic energy = -1398.3450259 Hartree

6	0.074548000	-1.262230000	-1.032229000
1	-0.031496000	-1.375341000	-2.102513000
1	1.204003000	-0.555838000	-0.598830000
1	0.325422000	-2.157660000	-0.475372000
6	-1.077318000	-0.945757000	1.374667000
1	-0.033828000	-0.780627000	1.642236000
1	-1.745787000	-0.324870000	1.961649000
1	-1.351545000	-1.996026000	1.440481000
17	2.369068000	0.069706000	0.185254000
17	-0.736715000	1.570134000	-0.086135000
16	-1.256259000	-0.464937000	-0.350456000

cis-CH_3SClCH_2:HCl

Absolute electronic energy =-1398.3765619 Hartree

6	-0.794593000	-1.590586000	-0.940319000
1	-1.006883000	-1.740639000	-1.988257000
1	1.478637000	0.541119000	-0.088802000
1	-0.008832000	-2.157698000	-0.462513000
6	-1.051688000	-0.533055000	1.500905000
1	0.016488000	-0.719835000	1.574248000
1	-1.308948000	0.394895000	1.999269000
1	-1.634870000	-1.369933000	1.875375000
17	2.344904000	-0.445230000	0.064839000

17	-0.162727000	1.790485000	-0.209880000
16	-1.472182000	-0.317212000	-0.237946000

TS6

Absolute electronic energy = -1398.3704238 Hartree

6	-0.537493000	-1.683507000	-0.448666000
1	-0.196732000	-2.133235000	-1.369907000
1	1.308250000	0.539090000	0.026964000
1	-0.305825000	-2.159026000	0.491242000
6	-1.759311000	0.033837000	1.187661000
1	-0.826234000	-0.044513000	1.739568000
1	-2.114534000	1.058495000	1.218304000
1	-2.513240000	-0.664416000	1.540310000
17	1.992629000	-0.776581000	0.239808000
17	0.403209000	1.863278000	-0.204518000
16	-1.393757000	-0.323264000	-0.542525000

cis-CH_3SCH_2Cl:HCl

Absolute electronic energy = -1398.4215178 Hartree

6	1.798561000	0.117611000	-0.402980000
1	2.200640000	0.352410000	-1.382360000
1	-1.467071000	-0.030560000	-0.545419000
1	2.598670000	-0.162695000	0.274586000
6	0.266825000	-1.559928000	1.132679000
1	-0.158108000	-0.671290000	1.594440000
1	-0.469808000	-2.358894000	1.149535000
1	1.163270000	-1.877613000	1.660016000
17	1.066403000	1.617285000	0.252180000
17	-2.626758000	0.332555000	-0.102191000
16	0.641633000	-1.234047000	-0.604925000

TS7

Absolute electronic energy = -1398.4142235 Hartree

6	-0.939165000	-0.354778000	-1.023831000
1	-0.108579000	-0.868521000	-1.497129000
1	1.613419000	0.403086000	-0.262436000
1	-1.775009000	-0.270363000	-1.708076000
6	-0.604269000	1.433494000	1.207353000
1	0.013603000	0.698542000	1.715572000
1	-0.274004000	2.436039000	1.470121000
1	-1.647874000	1.310244000	1.477270000
17	-1.467938000	-1.362471000	0.334250000
17	2.499122000	-0.495703000	0.080780000

16 -0.380692000 1.337977000 -0.584498000

CH_3SCH_2Cl
Absolute electronic energy = -937.6065808 Hartree
16 1.150996 -0.602943 -0.282439
6 1.571835 1.090352 0.182967
1 1.641616 1.184506 1.264636
1 2.539359 1.309664 -0.260627
1 0.828816 1.779832 -0.210122
6 -0.429238 -0.730731 0.538330
1 -0.768390 -1.756235 0.442435
1 -0.347727 -0.458289 1.585827
17 -1.715600 0.319405 -0.154759

HCl
Absolute electronic energy = -460.8074726 Hartree
17 0.000000000 0.000000000 0.071036000
1 0.000000000 0.000000000 -1.207620000

H_2O
Absolute electronic energy = -76.430107 Hartree
8 0.000000000 0.000000000 0.116391000
1 0.000000000 0.762579000 -0.465564000
1 0.000000000 -0.762579000 -0.465564000

DMS•H_2O
Absolute electronic energy =-554.4366248 Hartree
16 0.644375000 0.786118000 0.000000000
6 -0.528486000 0.631366000 1.367783000
1 0.038586000 0.695968000 2.292916000
1 -1.252749000 1.442697000 1.334584000
1 -1.034140000 -0.331270000 1.319595000
6 -0.528486000 0.631366000 -1.367783000
1 -1.252749000 1.442697000 -1.334584000
1 0.038586000 0.695968000 -2.292916000
1 -1.034140000 -0.331270000 -1.319595000
1 0.547916000 -1.623296000 0.000000000
8 -0.063148000 -2.373284000 0.000000000
1 0.485704000 -3.159496000 0.000000000

Cl_2•H_2O
Absolute electronic energy = -996.8075515 Hartree
17 -0.669721000 -1.020235000 -0.000588000

17	-0.851101000	0.967334000	0.001378000
8	2.575947000	0.205686000	-0.009013000
1	3.383312000	-0.307878000	0.058978000
1	1.863098000	-0.438302000	-0.000307000

DMS•H_2O:Cl_2

Absolute electronic energy = -1474.821823 Hartree

16	-1.836095000	-0.842076000	0.000149000
6	-1.982034000	0.320152000	1.370702000
1	-1.787317000	-0.233000000	2.285635000
1	-1.244186000	1.110937000	1.244445000
1	-2.989002000	0.730622000	1.396806000
6	-1.982607000	0.319518000	-1.370834000
1	-1.244643000	1.110302000	-1.245265000
1	-1.788297000	-0.234053000	-2.285601000
1	-2.989546000	0.730081000	-1.396707000
1	0.879232000	3.284621000	0.001081000
8	0.435576000	2.433779000	-0.000471000
1	1.140048000	1.775318000	0.000919000
17	0.708963000	-0.745404000	0.000250000
17	2.803063000	-0.319883000	-0.000199000

DMS•Cl_2:H_2O

Absolute electronic energy = -1474.820668 Hartree

6	-1.364222000	-1.456745000	0.512979000
1	-1.247095000	-2.359855000	-0.080330000
1	-0.564732000	-1.402879000	1.249510000
1	-2.338013000	-1.458912000	0.998251000
6	-1.449509000	1.279717000	0.594267000
1	-0.650200000	1.227288000	1.331045000
1	-1.381747000	2.221920000	0.056598000
1	-2.423235000	1.197379000	1.072584000
1	-3.731008000	-0.122338000	-0.570102000
8	-4.396626000	-0.165039000	0.127552000
1	-5.246451000	-0.175040000	-0.316941000
16	-1.248799000	-0.048818000	-0.614063000
17	1.652923000	0.072900000	-0.299526000
17	3.618763000	0.164512000	0.206614000

TS1•H_2O

Absolute electronic energy = -1474.795889 Hartree

16	-0.301441000	-0.125692000	0.582031000
6	-0.115255000	-1.068353000	-0.936843000

1	-0.691872000	-0.534034000	-1.683535000
1	0.944416000	-1.177414000	-1.153162000
1	-0.615598000	-2.012850000	-0.728718000
6	1.013032000	-0.962481000	1.528816000
1	1.926222000	-1.040216000	0.945296000
1	1.155681000	-0.393126000	2.442712000
1	0.602878000	-1.944596000	1.765174000
1	4.002870000	-0.747220000	-1.333029000
8	3.192343000	-0.499667000	-0.881449000
1	3.091785000	0.446550000	-1.017917000
17	0.742825000	1.554173000	0.049058000
17	-2.890986000	-0.048508000	-0.346091000

DMS•H_2O•Cl_2

Absolute electronic energy = -1474.844166 Hartree

16	0.551712000	0.467661000	0.000440000
6	0.112609000	-0.594537000	1.406594000
1	0.097710000	0.056422000	2.275884000
1	-0.870283000	-1.012644000	1.214139000
1	0.876720000	-1.357355000	1.495094000
6	0.109612000	-0.588434000	-1.409416000
1	-0.864951000	-1.021759000	-1.208019000
1	0.073446000	0.070040000	-2.272354000
1	0.883054000	-1.339596000	-1.514696000
1	-3.610953000	-1.976572000	0.001094000
8	-2.727161000	-1.603995000	-0.001277000
1	-2.832516000	-0.642213000	-0.001476000
17	-1.636750000	1.354208000	0.002097000
17	2.689946000	-0.197096000	-0.000306000

TS2•H_2O-1

Absolute electronic energy = -1474.79628 Hartree

6	-0.459767000	-0.643901000	1.414648000
1	-0.830341000	-1.663931000	1.433198000
1	0.610658000	-0.626852000	1.599968000
1	-1.024520000	-0.001453000	2.084119000
6	-0.254455000	1.590733000	-0.120887000
1	-0.695809000	2.084691000	0.739826000
1	1.226825000	1.583768000	0.084597000
1	-0.420329000	2.101517000	-1.064056000
17	2.328134000	-1.161913000	-0.344688000
1	2.839527000	2.034937000	-0.384521000
8	2.357536000	1.529811000	0.280209000

1	2.501017000	0.461029000	0.058277000
16	-0.677368000	-0.039232000	-0.264854000
17	-2.795434000	-0.206644000	-0.262252000

CH_3SClCH_2:HCl•H_2O

Absolute electronic energy = -1474.810466 Hartree

6	-0.336340000	-0.098179000	1.372971000
1	-0.418557000	-1.171641000	1.503670000
1	0.681874000	0.242316000	1.541930000
1	-1.052478000	0.422218000	2.001806000
6	-0.733425000	1.868860000	-0.403754000
1	-0.965168000	2.459729000	0.471747000
1	1.508154000	1.902749000	-0.141765000
1	-0.852819000	2.307187000	-1.383281000
17	2.496830000	-1.413156000	-0.240562000
1	3.013606000	2.278460000	-0.147175000
8	2.375286000	1.660815000	0.217804000
1	2.586894000	-0.123665000	-0.073968000
16	-0.744952000	0.248874000	-0.346742000
17	-2.800710000	-0.716841000	-0.099604000

TS3:HCl•H_2O

Absolute electronic energy = -1474.781316 Hartree

6	-0.245630000	-0.420988000	1.205746000
1	0.038079000	-1.430332000	1.487082000
1	0.556683000	0.279312000	1.418695000
1	-1.200808000	-0.137788000	1.644050000
6	-0.863564000	1.095768000	-0.903006000
1	-0.919973000	1.843130000	-0.124881000
1	2.233453000	2.549860000	-0.401618000
1	-1.099202000	1.351788000	-1.925883000
17	2.938883000	-1.029980000	-0.134003000
1	2.515274000	2.493496000	1.104430000
8	2.089508000	2.017106000	0.385665000
1	2.669320000	0.215298000	0.096899000
16	-0.528864000	-0.436310000	-0.572719000
17	-3.314877000	-0.168216000	0.190648000

CH_3SCH_2Cl•HCl•H_2O-1

Absolute electronic energy = -1474.864331 Hartree

6	0.505816000	0.624833000	1.818098000
1	0.355087000	1.442060000	2.518264000
1	-0.379710000	-0.005863000	1.786223000

1	1.377992000	0.048097000	2.115126000
6	0.981052000	-0.132417000	-0.772483000
1	0.144517000	-0.801377000	-0.592434000
1	-1.341464000	1.639853000	-0.746791000
1	1.020515000	0.154556000	-1.817757000
17	-2.510379000	-1.287389000	0.310007000
1	-2.792689000	2.028107000	-1.143618000
8	-2.143672000	1.321982000	-1.193107000
1	-2.463606000	-0.165941000	-0.376094000
16	0.806585000	1.366930000	0.196712000
17	2.475212000	-1.050301000	-0.405251000

TS2•H_2O-2

Absolute electronic energy = -1474.797815 Hartree

16	0.225671000	-0.908057000	-0.054985000
6	-0.044288000	-0.006379000	1.469503000
1	0.415641000	-0.574598000	2.271546000
1	0.388061000	0.984796000	1.359379000
1	-1.133475000	0.033194000	1.559717000
6	-0.494726000	0.128736000	-1.187488000
1	-0.166657000	1.160428000	-1.108645000
1	-0.477605000	-0.303395000	-2.180955000
1	-1.709175000	0.085726000	-0.718841000
1	1.782060000	3.319352000	-0.067582000
8	1.603025000	2.378378000	-0.001734000
1	2.428416000	1.931681000	-0.209567000
17	2.338176000	-0.800145000	-0.105088000
17	-3.204537000	0.101943000	0.004881000

CH_3SClCH_2•H_2O:HCl-1

Absolute electronic energy = -1474.812493 Hartree

16	0.200955000	-0.741223000	-0.313235000
6	0.004916000	-0.079639000	1.350394000
1	0.532863000	-0.752870000	2.016802000
1	0.442905000	0.915014000	1.372166000
1	-1.062634000	-0.061521000	1.559155000
6	-0.305570000	0.464538000	-1.255695000
1	-0.266478000	1.491390000	-0.918295000
1	-0.396023000	0.243176000	-2.308977000
1	-2.524773000	0.133211000	-0.554947000
1	2.512116000	2.934900000	0.241204000
8	1.867064000	2.235603000	0.119834000
1	2.376065000	1.415442000	0.031433000

17	2.566970000	-0.885866000	0.009729000
17	-3.623553000	0.023902000	0.110646000

TS3•HCl:H_2O

Absolute electronic energy = -1474.811859 Hartree

16	-0.159185000	-1.461041000	-0.356510000
6	-0.377329000	-1.019538000	1.374247000
1	0.454898000	-0.364082000	1.615266000
1	-1.331750000	-0.516494000	1.499337000
1	-0.312617000	-1.949566000	1.936339000
6	-1.590316000	-1.255615000	-1.038091000
1	-2.423988000	-0.798388000	-0.511038000
1	-1.668260000	-1.505353000	-2.088529000
1	1.616595000	0.894618000	-0.111272000
1	-3.429248000	1.597768000	0.839089000
8	-2.801808000	0.911465000	0.604690000
1	-1.983245000	1.372038000	0.324197000
17	-0.000355000	1.745198000	-0.419737000
17	2.697114000	0.078644000	0.145990000

CH_3SClCH_2•H_2O:HCl-2

Absolute electronic energy = -1474.820364 Hartree

16	-0.378613000	-1.019641000	-0.461144000
6	-0.371048000	-0.914480000	1.338469000
1	0.543126000	-0.398780000	1.611580000
1	-1.250656000	-0.355624000	1.646127000
1	-0.376810000	-1.933721000	1.715989000
6	-1.877128000	-1.471337000	-0.800142000
1	-2.677134000	-1.382089000	-0.079206000
1	-2.098467000	-1.700138000	-1.832332000
1	2.033086000	0.744224000	-0.134054000
1	-3.432294000	1.715075000	0.971922000
8	-2.860073000	0.999337000	0.688755000
1	-2.080338000	1.423791000	0.295609000
17	0.045172000	1.520400000	-0.509676000
17	2.999942000	-0.077946000	0.182775000

CH_3SCH_2Cl•HCl•H_2O-2

Absolute electronic energy = -1474.860208 Hartree

16	0.089231000	1.400239000	0.826947000
6	-0.124539000	1.503095000	-0.965689000
1	0.132799000	0.551095000	-1.425632000
1	-1.148752000	1.772188000	-1.207806000

1	0.563309000	2.268204000	-1.316306000
6	-1.134889000	0.151863000	1.193182000
1	-2.087653000	0.399443000	0.736243000
1	-1.223867000	0.074524000	2.270761000
1	2.003166000	0.025280000	0.246391000
1	-3.597371000	-0.548564000	-1.978765000
8	-2.882070000	-0.210905000	-1.435795000
1	-2.331660000	-0.972244000	-1.222186000
17	-0.705709000	-1.494691000	0.587292000
17	2.874854000	-0.518030000	-0.540965000

TS4•H_2O-1

Absolute electronic energy = -1474.79729 Hartree

16	-1.706191000	-0.493536000	0.230509000
6	-1.018612000	0.395425000	1.637016000
1	-0.578957000	-0.355455000	2.288143000
1	-0.268431000	1.091857000	1.258649000
1	-1.856967000	0.893580000	2.121856000
6	-2.062989000	0.860541000	-0.894952000
1	-1.144812000	1.443182000	-1.000374000
1	-2.392158000	0.413192000	-1.828442000
1	-2.870098000	1.431355000	-0.437558000
1	1.247246000	2.761832000	-0.534597000
8	0.754731000	1.950967000	-0.391346000
1	1.464824000	1.252117000	-0.252584000
17	-0.015906000	-1.221969000	-0.546944000
17	2.730622000	-0.200303000	0.157247000

DMSCl:Cl•H2O

Absolute electronic energy = -1474.80375 Hartree

16	-1.440781000	-0.339249000	0.602753000
6	-0.192114000	0.500791000	1.567261000
1	0.807885000	0.078694000	1.278810000
1	-0.198820000	1.553208000	1.299095000
1	-0.441089000	0.308931000	2.606912000
6	-2.168585000	0.985195000	-0.368658000
1	-1.347459000	1.501058000	-0.867522000
1	-2.873133000	0.528107000	-1.057201000
1	-2.683734000	1.623901000	0.347442000
1	1.182188000	2.408533000	-1.564125000
8	0.702849000	1.810487000	-0.987429000
1	1.386791000	1.164238000	-0.670443000
17	-0.457945000	-1.338944000	-0.832712000

17	2.561549000	-0.257438000	0.226288000

TS5•H_2O-1

Absolute electronic energy = -1474.795462 Hartree

6	-0.029005000	0.343200000	1.538048000
1	0.076714000	-0.065333000	2.533505000
1	1.170951000	-0.102234000	0.909947000
1	0.109082000	1.405776000	1.385578000
6	-2.131260000	1.050615000	-0.091809000
1	-1.353677000	1.611752000	-0.606845000
1	-2.865820000	0.643737000	-0.779530000
1	-2.603520000	1.637179000	0.693246000
17	2.491947000	-0.397096000	0.219128000
17	-0.663419000	-1.261484000	-1.056366000
16	-1.334643000	-0.333569000	0.734118000
8	0.763388000	2.016437000	-0.985407000
1	1.179581000	2.595879000	-1.626604000
1	1.410479000	1.311814000	-0.816330000

CH_3SClCH_2:HCl•H_2O-3

Absolute electronic energy = -1474.819827 Hartree

6	-0.545488000	-1.118526000	-1.394110000
1	-0.087515000	-0.968483000	-2.360688000
1	1.368166000	0.933099000	0.042404000
1	-0.268764000	-1.968098000	-0.783664000
6	-2.141095000	-0.597441000	0.692910000
1	-1.338438000	-1.082486000	1.242512000
1	-2.541443000	0.244156000	1.247113000
1	-2.920038000	-1.297748000	0.402699000
17	2.386468000	0.174491000	-0.426637000
17	-0.224176000	1.785387000	0.675856000
16	-1.438435000	0.082290000	-0.819705000
8	0.716284000	-2.054167000	1.280570000
1	1.081794000	-2.355492000	2.115068000
1	1.351466000	-1.410371000	0.935747000

TS6•H_2O-1

Absolute electronic energy = -1474.818338 Hartree

6	-0.386678000	-1.131997000	-1.325371000
1	0.015197000	-0.991174000	-2.318246000
1	1.060526000	1.105244000	0.068926000
1	-0.003691000	-1.917469000	-0.685144000
6	-1.981445000	-0.689164000	0.802255000

1	-1.101387000	-1.096782000	1.294379000
1	-2.361044000	0.174410000	1.338070000
1	-2.753403000	-1.440513000	0.655809000
17	2.129915000	0.218144000	-0.512753000
17	-0.186631000	1.942220000	0.654166000
16	-1.490418000	-0.082682000	-0.821869000
8	0.911365000	-2.061425000	1.314182000
1	1.381475000	-2.454115000	2.052357000
1	1.490985000	-1.364512000	0.964968000

$CH_3SCH_2Cl•HCl•H_2O$-3
Absolute electronic energy = -1474.860212 Hartree

6	-1.117164000	0.091509000	-1.201180000
1	-1.172836000	-0.039930000	-2.275792000
1	1.996744000	0.006855000	-0.216931000
1	-2.081919000	0.366711000	-0.787417000
6	-0.142193000	1.525895000	0.921295000
1	0.112499000	0.595465000	1.424924000
1	0.534814000	2.309435000	1.251614000
1	-1.172120000	1.798187000	1.134014000
17	-0.717250000	-1.523668000	-0.498854000
17	2.920518000	-0.481429000	0.547557000
16	0.104054000	1.350151000	-0.861564000
8	-2.958163000	-0.117638000	1.373750000
1	-3.704793000	-0.419807000	1.895041000
1	-2.411368000	-0.896002000	1.220939000

TS4•H_2O-2
Absolute electronic energy = -1474.774147 Hartree

6	-0.864770000	0.624042000	1.309973000
1	-0.822330000	0.053301000	2.233353000
1	0.061275000	1.181736000	1.161297000
1	-1.760507000	1.237425000	1.269165000
6	-0.873792000	0.536115000	-1.444163000
1	0.023651000	1.139371000	-1.310887000
1	-0.791801000	-0.088935000	-2.328760000
1	-1.789979000	1.120041000	-1.460623000
17	3.125374000	0.635119000	0.274650000
17	0.960305000	-1.148076000	0.006517000
16	-0.992375000	-0.571657000	-0.031314000
8	-3.811262000	0.576557000	-0.068371000
1	-4.430029000	1.311901000	-0.065422000
1	-4.356634000	-0.213773000	-0.034963000

DMSCl•H_2O:Cl
Absolute electronic energy = -1474.800449 Hartree

6	-0.399169000	-0.435607000	-1.399913000
1	-0.475996000	0.193758000	-2.282421000
1	0.609987000	-0.848159000	-1.220933000
1	-1.178796000	-1.194474000	-1.394570000
6	-0.399158000	-0.435579000	1.399940000
1	0.609990000	-0.848151000	1.220958000
1	-0.475944000	0.193826000	2.282423000
1	-1.178824000	-1.194429000	1.394665000
17	2.370283000	-1.345475000	0.000013000
17	0.774398000	1.877665000	-0.000024000
16	-0.790919000	0.614262000	-0.000001000
8	-3.281060000	-0.961912000	-0.000070000
1	-3.620737000	-1.860910000	-0.000328000
1	-4.056107000	-0.394479000	0.000803000

TS5•H_2O-2
Absolute electronic energy = -1474.783702 Hartree

6	-0.272948000	-0.979800000	-0.838801000
1	-0.470385000	-1.120094000	-1.893117000
1	1.096177000	-1.100218000	-0.487110000
1	-0.592253000	-1.770760000	-0.170358000
6	-0.888923000	0.239234000	1.475543000
1	0.034875000	-0.258290000	1.767484000
1	-0.993808000	1.201650000	1.965147000
1	-1.765732000	-0.385722000	1.620681000
17	2.458317000	-1.298876000	0.163869000
17	0.922689000	1.802115000	-0.213064000
16	-0.783439000	0.539725000	-0.294475000
8	-3.451338000	-0.883202000	-0.035071000
1	-4.405116000	-0.771049000	-0.028167000
1	-3.263883000	-1.477180000	-0.766529000

CH_3SCH_2Cl•HCl•H_2O-4
Absolute electronic energy = -1474.820185 Hartree

6	0.614879000	-1.949573000	-0.804231000
1	0.727807000	-2.253560000	-1.834702000
1	1.573855000	1.035886000	-0.032254000
1	1.422278000	-2.114318000	-0.105086000
6	-0.557721000	-0.910527000	1.355743000
1	0.435384000	-0.544652000	1.601429000

1	-1.328571000	-0.206145000	1.647217000
1	-0.743199000	-1.895748000	1.775068000
17	2.715013000	0.497452000	0.368142000
17	-0.349201000	1.500179000	-0.574753000
16	-0.671065000	-1.067241000	-0.437124000
8	-3.166595000	0.533296000	0.479981000
1	-2.540500000	1.165532000	0.098093000
1	-4.039005000	0.823358000	0.207682000

TS6•H_2O-2

Absolute electronic energy = -1474.816297 Hartree

6	0.921285000	-1.764975000	-0.455181000
1	1.410336000	-1.907060000	-1.408159000
1	1.300245000	1.095188000	0.031943000
1	1.433073000	-2.061669000	0.447684000
6	-0.978189000	-1.131977000	1.308686000
1	-1.045896000	-2.153979000	1.670986000
1	-0.198016000	-0.563002000	1.806512000
1	-1.931784000	-0.619021000	1.381159000
17	-0.237833000	1.783568000	0.025926000
17	2.568434000	0.385594000	0.050015000
16	-0.576378000	-1.169637000	-0.451898000
8	-3.101728000	0.439405000	-0.258940000
1	-2.395551000	1.104806000	-0.258737000
1	-3.815325000	0.809652000	-0.781532000

CH_3SCH_2Cl•HCl•H_2O-4

Absolute electronic energy = -1474.860523 Hartree

6	-1.940030000	-0.731921000	0.526511000
1	-2.284233000	-0.709261000	1.554643000
1	0.793103000	0.871317000	0.420895000
1	-2.506476000	-1.461700000	-0.043166000
6	0.076355000	-1.321385000	-1.235473000
1	-0.558953000	-2.106332000	-1.639180000
1	-0.124817000	-0.373804000	-1.730815000
1	1.123228000	-1.586551000	-1.350782000
17	1.549047000	1.869008000	0.035542000
17	-2.296445000	0.873345000	-0.191727000
16	-0.199650000	-1.156663000	0.542400000
8	3.011958000	-1.116386000	0.028386000
1	2.975553000	-0.153248000	0.016127000
1	3.569174000	-1.342881000	0.775705000

$HCl•H_2O$

Absolute electronic energy = -537.2463179 Hartree

17	-1.214515000	-0.000006000	0.007308000
1	0.078915000	0.000393000	-0.070829000
8	1.972394000	0.000031000	-0.084238000
1	2.393936000	-0.767431000	0.310107000
1	2.394755000	0.766898000	0.310388000