Effects of Si Substitution on the Ei Reaction of Alkyl Sulfoxides

Supporting Information

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Table S1. Coordinates and Absolute Energies.**(E)-2-methanesulfinylethenylsilane**

HF/6-31G(d,p)

S	16.0	.0114752684	-.1016740872	-.8709818060
C	6.0	-.1430368079	.1154365940	.9071537675
H	1.0	.3324218808	1.0411363315	1.2086246650
H	1.0	.3568417339	-.7200841657	1.3792696053
H	1.0	-1.1910668834	.1147298598	1.1763461198
H	1.0	-2.3420674718	.3028264304	-2.3010232896
C	6.0	-.8715792630	1.3680155668	-1.3598341515
O	8.0	-.8317331451	-1.2667516310	-1.2383872399
H	1.0	-.3917954122	2.2911179673	-1.0760383442
C	6.0	-1.9811749977	1.2948118179	-2.0714852948
SI	14.0	-2.9182210185	2.8070185951	-2.6803608147
H	1.0	-2.2350596712	4.0232955359	-2.1859035187
H	1.0	-4.3083891764	2.7810485360	-2.1747550685
H	1.0	-2.9533413358	2.8257551492	-4.1591891298

Energy -879.4720234183 Hartree
ZPE 0.107516 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	0.0279525483	-0.1248438564	-0.8881577958
C	6.0	-0.1676885408	0.1367730830	0.8929182382
H	1.0	0.3059376734	1.0743710079	1.1799867351
H	1.0	0.3167209966	-0.6922364215	1.4032334882
H	1.0	-1.2293914947	0.1507749629	1.1305444862
H	1.0	-2.3002147557	0.2714990994	-2.2955504873
C	6.0	-0.8390768946	1.3763115033	-1.3565470439
O	8.0	-0.8529414747	-1.2870762281	-1.2860428241
H	1.0	-0.3581135402	2.3054752286	-1.0675459730
C	6.0	-1.9662677306	1.2843558376	-2.0761555663
SI	14.0	-2.9142308783	2.7885759262	-2.6580577756
H	1.0	-2.2121682867	3.9943403096	-2.1666843794
H	1.0	-4.2930694916	2.7703078756	-2.1238642001
H	1.0	-2.9841744303	2.8280541718	-4.1346414025

Energy -880.2990192639 Hartree
ZPE 0.103240 HARTREE/MOLECULE
MP2/6-311+G(3df,2p) -880.6678222418 Hartree
MP2/G3Large -881.3494987954 Hartree

(Z)-2-methanesulfinylethenylsilane

HF/6-31G(d,p)

S	16.0	0.1900832233	-0.0640549234	-0.6198092609
C	6.0	-0.3703663959	-0.1852674043	1.0834945877
H	1.0	0.0587996949	0.6148690564	1.6735792351
H	1.0	-0.0379050484	-1.1438426374	1.4607439338
H	1.0	-1.4519720195	-0.1462863382	1.1119236035
SI	14.0	1.8382596682	3.1051635502	-1.0763261509
C	6.0	-0.6046314685	1.4822147947	-1.0093111175
O	8.0	-0.5555376876	-1.1057657529	-1.3718624641
H	1.0	-1.6698659464	1.3648131113	-1.1408446199
C	6.0	0.0083776093	2.6407323815	-1.1876325241
H	1.0	-0.6408776327	3.4675046837	-1.4438169061
H	1.0	2.6850598462	1.9754315516	-0.6541550725
H	1.0	1.9642243981	4.2069729978	-0.0959865841
H	1.0	2.2758444587	3.5979414290	-2.3997250601

Energy -879.4642809539 Hartree
ZPE 0.107068 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	0.2230529791	-0.0698983342	-0.6368901288
C	6.0	-0.3646553813	-0.1591921343	1.0727132682
H	1.0	0.0654058211	0.6567341553	1.6511302745
H	1.0	-0.0407447372	-1.1163787281	1.4759239210
H	1.0	-1.4520471829	-0.1098887599	1.0846927504
SI	14.0	1.8264228128	3.0916386290	-1.0707083345
C	6.0	-0.6129359325	1.4756746446	-0.9896676879
O	8.0	-0.5062647777	-1.1400154098	-1.4167730293
H	1.0	-1.6854440557	1.3372247117	-1.1119656197
C	6.0	-0.0035269636	2.6589089406	-1.1773404494
H	1.0	-0.6665557026	3.4866554432	-1.4190349265
H	1.0	2.6413414526	1.9356387436	-0.6571756504
H	1.0	1.9872124299	4.1823434817	-0.0843369641
H	1.0	2.2782319377	3.5809811167	-2.3902958235

Energy -880.2904084985 Hartree
ZPE 0.102829 HARTREE/MOLECULE
MP2/6-311+G(3df,2p) -880.6605017582 Hartree

1-methanesulfinylethenylsilane

HF/6-31G(d,p)

S	16.0	.0245167551	-.0097903577	-.9941486058
C	6.0	.0577022419	-.0286559787	.8030085933
H	1.0	.5687455927	.8465541492	1.1835404452
H	1.0	.5940034478	-.9206970698	1.0991126409
H	1.0	-.9573534634	-.0734341398	1.1752353802
H	1.0	-2.5347584205	.3291150802	-1.9669094468
C	6.0	-.9539217324	1.4784734646	-1.2221913881
O	8.0	-.8136288483	-1.1684540452	-1.3969430461
SI	14.0	-.2113746511	3.1856934834	-.9124856563
C	6.0	-2.1614150916	1.3133057427	-1.7404844415
H	1.0	-2.7989265107	2.1533937331	-1.9556913387
H	1.0	.1334036662	3.3667182447	.5154358596
H	1.0	-1.2212751366	4.1875607143	-1.3087300286
H	1.0	1.0228821509	3.3579369791	-1.7078089673

Energy

-879.4707559380 Hartree

ZPE

0.107803 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	.0305909313	-.0343339671	-1.0233448711
C	6.0	.0539351851	-.0000551423	.7851842286
H	1.0	.5561056814	.8972598246	1.1411931705
H	1.0	.5940149999	-.8831623028	1.1184435203
H	1.0	-.9729235025	-.0364127323	1.1434908529
H	1.0	-2.5161817787	.3011067533	-1.9642771903
C	6.0	-.9411663986	1.4801641245	-1.2113152445
O	8.0	-.8432357226	-1.2019659619	-1.4234711716
SI	14.0	-.1983760414	3.1771610183	-.8908888776
C	6.0	-2.1657969662	1.3021443353	-1.7345687863
H	1.0	-2.8220957213	2.1380952274	-1.9366921924
H	1.0	.1434274901	3.3476038865	.5379778631
H	1.0	-1.2064025877	4.1807330911	-1.2867138301
H	1.0	1.0367044313	3.3493818454	-1.6840774713

Energy

-880.3000882174 Hartree

ZPE

.103326 HARTREE/MOLECULE

MP2/6-311+G(3df,2p)

-880.6694030298 Hartree

(E)-2-methanesulfinylethenylsilane TS (H-transfer)

HF/6-31G(d,p)

S	16.0	1.2107399681	-1.1916475922	.5333347057
C	6.0	.9108350487	-.9547301340	2.2849437102
H	1.0	-.0281054087	-.4350749799	2.4158431477
H	1.0	1.7250664322	-.3601068774	2.6835938293
H	1.0	.8870469732	-1.9154900128	2.7807953286
C	6.0	.6862992577	.6533965774	-.1693220487
O	8.0	-.1271739487	-1.8734366830	.0472332179
H	1.0	-.6613445863	-1.0868476547	-.3312243252
H	1.0	1.5333069386	1.2860135471	-.0006347072
C	6.0	-.4925727800	.5987552986	-.6479939991
SI	14.0	-1.5160696032	1.9321358027	-1.4065948391
H	1.0	-.8458049788	3.2585076586	-1.4793742865
H	1.0	-2.7559759351	2.0997600197	-.6125563045
H	1.0	-1.8908073777	1.5403650298	-2.7846834292

Energy -879.4041784888 Hartree
ZPE 0.103789 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	1.1596890557	-1.3773173215	.5258126272
C	6.0	.8681049050	-.9931498432	2.2608657925
H	1.0	.0735012628	-.2545127697	2.3308457838
H	1.0	1.7889158189	-.5857165736	2.6782741261
H	1.0	.5912976794	-1.8953049928	2.7995887537
C	6.0	.9033952272	.7460136108	-.1367654368
O	8.0	-.2980209502	-1.6637047075	-.0315020339
H	1.0	-.6005949715	-.6086470595	-.4162905275
H	1.0	1.8117481534	1.2730768356	.0879961720
C	6.0	-.2720494451	.7698899861	-.6162412985
SI	14.0	-1.5698962223	1.8241832569	-1.3836419322
H	1.0	-1.1166571889	3.2232197449	-1.5496546525
H	1.0	-2.7749608034	1.8148454293	-.5264539304
H	1.0	-1.9290325211	1.2787244041	-2.7094734433

Energy -880.2481329653 Hartree
ZPE .097027 HARTREE/MOLECULE
MP2/6-311+G(3df,2p) -880.6126446114 Hartree
MP2/G3-large -881.2940094489 Hartree

(Z)-2-methanesulfinylethenylsilane TS (Si-transfer)

HF/6-31G(d,p)

S	16.0	0.9079717591	-0.9225359607	0.3170357391
C	6.0	0.4662092956	-0.8374875145	2.0518721934
H	1.0	-0.0940835994	0.0676559669	2.2439849176
H	1.0	1.3888022366	-0.8259679374	2.6216739032
H	1.0	-0.1152916135	-1.7077118414	2.3241635961
C	6.0	1.3573358417	1.2816393236	-0.0528992520
O	8.0	-0.5273212545	-0.9284736527	-0.3666102006
SI	14.0	-1.6259770011	0.2543690155	-0.9763418659
H	1.0	2.3739710843	1.2663954343	0.2534437097
C	6.0	0.2941765252	1.7511088402	-0.5012424008
H	1.0	0.0474267594	2.7512827895	-0.7946277086
H	1.0	-1.3815714486	0.8364867291	-2.3116499171
H	1.0	-2.2688458714	1.1658442312	-0.0052946525
H	1.0	-2.6913755134	-0.7564915237	-1.2450237616

Energy -879.4026929260 Hartree
ZPE 0.103230 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	0.2230529791	-0.0698983342	-0.6368901288
C	6.0	-0.3646553813	-0.1591921343	1.0727132682
H	1.0	0.0654058211	0.6567341553	1.6511302745
H	1.0	-0.0407447372	-1.1163787281	1.4759239210
H	1.0	-1.4520471829	-0.1098887599	1.0846927504
SI	14.0	1.8264228128	3.0916386290	-1.0707083345
C	6.0	-0.6129359325	1.4756746446	-0.9896676879
O	8.0	-0.5062647777	-1.1400154098	-1.4167730293
H	1.0	-1.6854440557	1.3372247117	-1.1119656197
C	6.0	-0.0035269636	2.6589089406	-1.1773404494
H	1.0	-0.6665557026	3.4866554432	-1.4190349265
H	1.0	2.6413414526	1.9356387436	-0.6571756504
H	1.0	1.9872124299	4.1823434817	-0.0843369641
H	1.0	2.2782319377	3.5809811167	-2.3902958235

Energy -880.2386200349 Hartree
ZPE 0.103219 HARTREE/MOLECULE
MP2/6-311+G(3df,2p) -880.6031018145Hartree

1-methanesulfinylethenylsilane TS (H-transfer)

HF/6-31G(d,p)

S	16.0	-.3628804461	-1.4747965549	-.3078393056
C	6.0	-.9821562030	-1.6157997250	1.3695398413
H	1.0	-1.8204812412	-.9450369603	1.4975502715
H	1.0	-.1823160776	-1.3469591652	2.0491126091
H	1.0	-1.2861131688	-2.6375419847	1.5524807902
C	6.0	-.5199319816	.6595818070	-.5752481506
O	8.0	-1.6553993978	-1.7566754453	-1.1642852814
H	1.0	-2.0047703241	-.7940997355	-1.3744884353
SI	14.0	1.0000602589	1.4946944731	.0862968018
C	6.0	-1.6260372103	.7857793725	-1.2054263472
H	1.0	-2.0393129600	1.7340827959	-1.5017029326
H	1.0	2.1898262130	1.1231009430	-.7090578114
H	1.0	1.2439133297	1.0757236949	1.4864695581
H	1.0	.7861786090	2.9550018845	.0306247922

Energy -879.3945157441 Hartree
ZPE .102071 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	-.3407048432	-1.6200478667	-.3507647274
C	6.0	-.9228890173	-1.5860242548	1.3533038297
H	1.0	-1.6483426249	-.7842557847	1.4670401499
H	1.0	-.0682610177	-1.4059911285	2.0040865569
H	1.0	-1.3783074438	-2.5406336767	1.6031150234
C	6.0	-.5221420970	.7484179912	-.5984477609
O	8.0	-1.6830643231	-1.7214329636	-1.1758853345
H	1.0	-1.9370943632	-.5492020861	-1.3661013646
SI	14.0	.9914150594	1.4923358100	.1365420017
C	6.0	-1.6257867487	.7596766411	-1.2221344425
H	1.0	-2.3507615935	1.4312673122	-1.6450149772
H	1.0	2.1680975140	1.0682563043	-.6498796373
H	1.0	1.1488965069	.9961180326	1.5217745094
H	1.0	.9095243922	2.9685710696	.1563925737

Energy -880.2437871827 Hartree
ZPE 0 .096443 HARTREE/MOLECULE
MP2/6-311+G(3df,2p) -880.6081467952 Hartree

Silyl methanesulfenate

HF/6-31G(d,p)

S	16.0	-.0721827537	1.1392803557	.0892813104
C	6.0	-1.5629122837	.6077490780	.9364234745
H	1.0	-1.3087186185	.0570202470	1.8318353443
H	1.0	-2.1893123153	.0047674864	.2926301265
H	1.0	-2.0987559408	1.5097874211	1.2111736166
O	8.0	.6370001322	-.3396585042	-.1678238651
SI	14.0	.5927008603	-1.0589164799	-1.6708890669
H	1.0	1.2795460258	-2.3550334379	-1.5267521660
H	1.0	1.2842041614	-.2200221560	-2.6705581839
H	1.0	-.8076131677	-1.2669495104	-2.0993388904

Energy -802.6550636965 Hartree
ZPE .072652 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	-.0433148266	1.1455804711	.0861129428
C	6.0	-1.5439163356	.5888753486	.8938223281
H	1.0	-1.3033603319	.0744978108	1.8204445438
H	1.0	-2.1290145404	-.0587974569	.2456544262
H	1.0	-2.1263687021	1.4814245557	1.1223764001
O	8.0	.7201603368	-.3693206937	-.0876776203
SI	14.0	.5698754220	-1.0372523834	-1.6409046881
H	1.0	1.2302739017	-2.3524176613	-1.5554271712
H	1.0	1.2344285767	-.1945663456	-2.6551400832
H	1.0	-.8548074008	-1.1999991453	-2.0032793782

Energy -803.2073476404 Hartree
ZPE 0.070377 HARTREE/MOLECULE
MP2/6-311+G(3df,2p) -803.4844863319 Hartree

Ethynylsilane

HF/6-31G(d,p)

H	1.0	.0508282320	.0050566194	-3.0244603491
C	6.0	.0330894913	.0014715873	-1.9665342292
C	6.0	.0130949766	-.0016740538	-.7728092250
SI	14.0	-.0181660243	.0005619279	1.0677613240
H	1.0	1.1768135825	-.6994537195	1.5801549317
H	1.0	-1.2353049843	-.6900863334	1.5390730083
H	1.0	-.0209832736	1.3946917721	1.5544295392

Energy	-366.9204338961 Hartree
ZPE	.046825 HARTREE/MOLECULE

MP2/6-31G(d,p)

H	1.0	.0513164498	.0040557733	-3.0509771069
C	6.0	.0334338188	.0017869180	-1.9867992004
C	6.0	.0127993101	-.0010489978	-.7584470344
SI	14.0	-.0182495663	.0007988578	1.0729761819
H	1.0	1.1751120567	-.6985896055	1.5886690562
H	1.0	-1.2338634801	-.6892028422	1.5477106832
H	1.0	-.0211765889	1.3927676964	1.5644824202

Energy	-367.2713793588 Hartree
ZPE	.043984 HARTREE/MOLECULE
MP2/6-311+G(3df,2p)	-367.4026503109 Hartree
MP2/G3Large	-367.7283468001 Hartree

(E)-methanesulfinylpropene

HF/6-31G(d,p)

S	16.0	-.0536522338	-.1558389921	-.8919769250
C	6.0	-.0884495999	.1345718118	.8813243982
H	1.0	.4673329402	1.0339302347	1.1186578579
H	1.0	.3770401088	-.7174536588	1.3596365348
H	1.0	-1.1169791656	.2220378181	1.2060739642
H	1.0	-2.4788077225	.3489859392	-2.1701175559
C	6.0	-.8577142575	1.3439923312	-1.4001991624
O	8.0	-.9943815920	-1.2762723617	-1.1565513192
H	1.0	-.2994790760	2.2479078815	-1.2193821535
C	6.0	-2.0193043718	1.3123089170	-2.0210470077
C	6.0	-2.7479454614	2.5161230442	-2.5400552894
H	1.0	-2.2087605061	3.4344618164	-2.3395281606
H	1.0	-3.7315372256	2.5876819519	-2.0845015310
H	1.0	-2.8990674365	2.4325856667	-3.6126301507

Energy -628.4333717171 Hartree
ZPE .121127 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	-.0541530790	-.1848707137	-.9074100516
C	6.0	-.0941345928	.1495544560	.8705870309
H	1.0	.4595134858	1.0621208376	1.0855197997
H	1.0	.3715933109	-.6930362052	1.3764573486
H	1.0	-1.1320869668	.2448632005	1.1828123879
H	1.0	-2.4507368893	.3274808897	-2.1831982820
C	6.0	-.8381518322	1.3474496193	-1.3858494749
O	8.0	-1.0368252084	-1.3028007420	-1.1808276792
H	1.0	-.2786536597	2.2552074347	-1.1875738927
C	6.0	-2.0102869159	1.3076570585	-2.0260150860
C	6.0	-2.7468551300	2.5084196242	-2.5279403974
H	1.0	-2.2052258374	3.4288350761	-2.3163870940
H	1.0	-3.7323772286	2.5741817527	-2.0653563118
H	1.0	-2.9033250562	2.4399601116	-3.6051147979

Energy -629.3105656559Hartree
ZPE .116478 HARTREE/MOLECULE
MP2/6-311+G(3df,2p) -629.6641946730 Hartree

(Z)-methanesulfinylpropene

HF/6-31G(d,p)

C	6.0	-0.3299656921	0.5698003330	-0.5484258078
C	6.0	0.3624778957	0.1293751792	-1.8063210487
H	1.0	0.6223109461	1.0052779469	-2.3959120441
H	1.0	-0.2443462114	-0.5321089138	-2.4013496283
H	1.0	1.2957982879	-0.3645513134	-1.5487397821
C	6.0	-1.5417573588	0.2898375288	-0.1015600666
S	16.0	-2.7690665636	-0.7943487907	-0.7934961368
C	6.0	-4.0225467751	0.4559581661	-1.1073333257
H	1.0	-4.8825823961	-0.0516293984	-1.5245372458
H	1.0	-3.6390061115	1.1735075261	-1.8207185934
H	1.0	-4.3007406598	0.9452562868	-0.1819009791
O	8.0	-2.3423892981	-1.2966295069	-2.1257827936
H	1.0	-1.8690396400	0.6863808232	0.8463918344
H	1.0	0.2549654168	1.2170236251	0.0886476525

Energy -628.4278554058 Hartree
ZPE 0.121340 HARTREE/MOLECULE

MP2/6-31G(d,p)

C	6.0	-0.3255803480	0.5858117425	-0.5444050186
C	6.0	0.3549393213	0.1291609159	-1.7982851273
H	1.0	0.6092213698	0.9944720571	-2.4126151348
H	1.0	-0.2703834660	-0.5435824303	-2.3735505504
H	1.0	1.2932645827	-0.3667657043	-1.5461217931
C	6.0	-1.5596434621	0.2958926394	-0.1058663321
S	16.0	-2.7581166522	-0.8219073469	-0.8172325584
C	6.0	-4.0080919868	0.4574067167	-1.0991693700
H	1.0	-4.8875525412	-0.0351418071	-1.5074503082
H	1.0	-3.6171978812	1.1754875964	-1.8168840187
H	1.0	-4.2600529964	0.9469176265	-0.1603979995
O	8.0	-2.3223541332	-1.3190877424	-2.1786808296
H	1.0	-1.9096046399	0.6907886626	0.8430120284
H	1.0	0.2552646731	1.2436965659	0.0966090472

Energy -629.3056277977 Hartree
ZPE 0.116313 HARTREE/MOLECULE
MP2/6-311+G(3df,2p) -629.6586586490 Hartree

2-methanesulfinylpropene

HF/6-31G(d,p)

S	16.0	.0610677465	.0000882178	-.8401603218
C	6.0	-.1684459834	.0986368346	.9405924924
H	1.0	.2969004511	.9921901634	1.3361091166
H	1.0	.3084805668	-.7750680508	1.3650654537
H	1.0	-1.2269149847	.0805962284	1.1653260616
H	1.0	-2.3304893977	.2624715031	-2.2200210989
C	6.0	-.8829858804	1.4509145479	-1.3140970530
O	8.0	-.6979377852	-1.1977816609	-1.2827342487
C	6.0	-.2795279887	2.7869859534	-.9682866292
C	6.0	-1.9898260023	1.2571725675	-2.0005001420
H	1.0	-2.5699989390	2.0893377911	-2.3600688730
H	1.0	.7604015183	2.8391015550	-1.2771761882
H	1.0	-.3154666071	2.9836501087	.0990151412
H	1.0	-.8206756142	3.5792646409	-1.4706765108

Energy -628.4309723270 Hartree
ZPE .121103 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	0.0680685845	-0.0283322135	-0.8771400064
C	6.0	-0.1566155101	0.1264121298	0.9124509904
H	1.0	0.2972368912	1.0464915772	1.2747259760
H	1.0	0.3317442598	-0.7291447393	1.3727680026
H	1.0	-1.2226082878	0.1050232622	1.1306019030
H	1.0	-2.3279161485	0.2431023402	-2.2128000748
C	6.0	-0.8754016656	1.4506500817	-1.3058558222
O	8.0	-0.7316347474	-1.2342066796	-1.3168666257
C	6.0	-0.2731372605	2.7737432568	-0.9387196522
C	6.0	-2.0056350264	1.2516379102	-1.9905964739
H	1.0	-2.6065255112	2.0835142557	-2.3317154615
H	1.0	0.7937796867	2.7955093847	-1.1647155550
H	1.0	-0.3918275133	2.9927296836	0.1228253025
H	1.0	-0.7549466512	3.5704301503	-1.5025753029
H	1.0	0.2552646731	1.2436965659	0.0966090472

Energy -629.3116314154 Hartree
ZPE 0.115965 HARTREE/MOLECULE
MP2/6-311+G(3df,2p) -629.6660595503 Hartree

2-methanesulfinylpropene TS (H-Transfer)

HF/6-31G(d,p)

S	16.0	-.2655812263	-1.3885226591	-.3150314500
C	6.0	-.8645739794	-1.5645822808	1.3674530946
H	1.0	-1.6861771482	-.8801819471	1.5285280400
H	1.0	-.0490464661	-1.3360196920	2.0437209514
H	1.0	-1.1886557178	-2.5838979740	1.5274415900
C	6.0	-.4181560879	.7529798997	-.5423251410
O	8.0	-1.5717520334	-1.6521232200	-1.1620421740
H	1.0	-1.9064393295	-.6865888587	-1.3529942821
C	6.0	.8035795411	1.3358122516	.0731989660
C	6.0	-1.5120184627	.9055737666	-1.1610962192
H	1.0	-1.9393531495	1.8469619788	-1.4533974379
H	1.0	1.7065148566	.9742830694	-.4075984810
H	1.0	.8715647294	1.1203780992	1.1354429051
H	1.0	.7606738735	2.4129829663	-.0472739620

Energy -628.3492140471 Hartree
ZPE .115614 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	-.2513746883	-1.5224384272	-.3580360168
C	6.0	-.8335536323	-1.5423371003	1.3467365752
H	1.0	-1.5601985916	-.7451122938	1.4855161583
H	1.0	.0214380427	-1.3844671162	2.0036417566
H	1.0	-1.2880238410	-2.5037996665	1.5704941680
C	6.0	-.3989147216	.7885403128	-.5364071934
O	8.0	-1.6035314517	-1.6047569904	-1.1885984434
H	1.0	-1.8300481001	-.4663558289	-1.3350520525
C	6.0	.8080960389	1.3349687281	.1129533039
C	6.0	-1.4938204936	.8893433084	-1.1531466494
H	1.0	-2.2021959591	1.5822044140	-1.5635278963
H	1.0	1.7094765244	.9539860275	-.3670380341
H	1.0	.8489615167	1.0539652546	1.1662118870
H	1.0	.8142687564	2.4233147777	.0502788367

Energy -629.2480075355 Hartree
ZPE .109020 HARTREE/MOLECULE MP2/6-
311+G(3df,2p) -629.5973578753 Hartree

(E)-methanesulfinylpropene TS (H-Transfer)

HF/6-31G(d,p)

S	16.0	-.4778581302	-1.4440184371	-.4157408738
C	6.0	-.9454180319	-1.4721289852	1.3155800140
H	1.0	-1.7600156898	-.7795584450	1.4761366965
H	1.0	-.0824623871	-1.1689895072	1.8979908111
H	1.0	-1.2390960249	-2.4733846616	1.6002454204
C	6.0	-.6150510165	.6797987956	-.7829319385
O	8.0	-1.8550105596	-1.7172208680	-1.1414991392
H	1.0	-2.1682970659	-.7626728937	-1.3793739098
H	1.0	.3177435681	1.0394776011	-.4134502803
C	6.0	-1.7288023093	.8667243792	-1.3417986782
C	6.0	-2.4587922889	2.0722766498	-1.8450024531
H	1.0	-1.9202628568	3.0062243773	-1.7061488595
H	1.0	-3.4186778571	2.1539546230	-1.3444803987
H	1.0	-2.6712106500	1.9540082719	-2.9028677108

Energy -628.3451644036 Hartree
ZPE .116122 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	-.5366903539	-1.5791873545	-.4660174563
C	6.0	-.9760788289	-1.4711086492	1.2769689690
H	1.0	-1.6567503962	-.6352549233	1.4176285150
H	1.0	-.0633240044	-1.3004208766	1.8477385602
H	1.0	-1.4432275951	-2.3959222161	1.6047224703
C	6.0	-.4619388620	.7082418709	-.7237456887
O	8.0	-1.9466018649	-1.5324610881	-1.1920688320
H	1.0	-2.0444912488	-.3748216014	-1.3765822197
H	1.0	.4805961608	1.0203835198	-.3205931092
C	6.0	-1.5660064801	.9459183293	-1.2816246851
C	6.0	-2.5124912574	1.9508842992	-1.8331603816
H	1.0	-2.1131275342	2.9610537962	-1.7498958913
H	1.0	-3.4642285683	1.9114243647	-1.3036048581
H	1.0	-2.7188504664	1.7457614292	-2.8831066923

Energy -629.2431852762 Hartree
ZPE .109675 HARTREE/MOLECULE MP2/6-
311+G(3df,2p) -629.5919651656 Hartree

(Z)-methanesulfinylpropene TS (Methyl-Transfer)

HF/6-31G(d,p)

C	6.0	-.4415259919	.7886427793	-.1558910178
C	6.0	-.0093587891	-.1824798335	-2.2972363550
H	1.0	-.0009906595	.8614454231	-2.5182979147
H	1.0	-.2889310353	-.8063057706	-3.1226474138
H	1.0	.8275852313	-.5331283194	-1.7370765832
C	6.0	-1.5753572690	.4720204517	.4136415436
S	16.0	-2.5571786499	-.6823308427	-.5647391713
C	6.0	-3.7833304812	.4274917491	-1.2568418078
H	1.0	-4.4060767903	-.1249706624	-1.9483311463
H	1.0	-3.2719535721	1.2341041247	-1.7646601563
H	1.0	-4.3902316132	.8210943581	-.4497923861
O	8.0	-1.6674334879	-1.0318530645	-1.7594168729
H	1.0	-2.0434496096	.7110461569	1.3560793088
H	1.0	.2023445577	1.4783729422	.3841720080

Energy -628.2396232386 Hartree
ZPE .115998 HARTREE/MOLECULE

MP2/6-31G(d,p)

C	6.0	-.5258436438	.8842511082	-.1476436368
C	6.0	-.0115534948	-.1569698365	-2.1150075361
H	1.0	.0158302620	.8683742835	-2.4717744256
H	1.0	-.0882967482	-.8398593372	-2.9526190417
H	1.0	.8534537400	-.4115897901	-1.5104459801
C	6.0	-1.5090318394	.5720953215	.5505841204
S	16.0	-2.7448920826	-.9427015333	-.7273145683
C	6.0	-3.8224792773	.4085894322	-1.2356458496
H	1.0	-4.4421663159	.0989818852	-2.0731874460
H	1.0	-3.1976794399	1.2512493935	-1.5215210604
H	1.0	-4.4530265032	.6906550302	-.3924346241
O	8.0	-1.7376423609	-1.0716291046	-1.9119164438
H	1.0	-2.1065218066	.6459635553	1.4339258353
H	1.0	.3639613506	1.4357390841	-.3460373080

Energy -629.1436219431 Hartree
ZPE .109431 HARTREE/MOLECULE MP2/6-
311+G(3df,2p) -629.4950661538 Hartree

Methyl methanesulfenate

HF/6-31G(d,p)

O	8.0	-1.1133328610	-0.3716051619	0.2714427194
C	6.0	-0.8979069966	0.5523114614	1.3125676756
H	1.0	-1.2933495364	0.0981971117	2.2116293253
H	1.0	-1.4155403058	1.4857977749	1.1212909692
H	1.0	0.1594254911	0.7555405361	1.4516631115
S	16.0	-0.6279307420	0.1028110361	-1.2326126333
C	6.0	1.0434773512	-0.5591291869	-1.2605568864
H	1.0	1.4380386849	-0.3523499029	-2.2493785925
H	1.0	1.0279228390	-1.6286993909	-1.1005703315
H	1.0	1.6791961276	-0.0828741706	-0.5254752523

Energy -551.5661258502 Hartree
ZPE 0.086089 HARTREE/MOLECULE

MP2/6-31G(d,p)

O	8.0	-1.1656127152	-0.4091761052	0.2649671396
C	6.0	-0.8804074335	0.5460266784	1.2962526503
H	1.0	-1.2531194431	0.1010962114	2.2158278297
H	1.0	-1.3880761483	1.4922910091	1.1100119978
H	1.0	0.1918258875	0.7270161870	1.3894748590
S	16.0	-0.6487224158	0.1019405148	-1.2610159122
C	6.0	1.0272395494	-0.5444897632	-1.2378223509
H	1.0	1.4572521916	-0.3310232886	-2.2163787848
H	1.0	1.0188413489	-1.6199776635	-1.0820898721
H	1.0	1.6407792304	-0.0637036731	-0.4792274514

Energy -552.1690358081 Hartree
ZPE 0.082989 HARTREE/MOLECULE MP2/6-
311+G(3df,2p) -552.4288311580 Hartree

Propyne

HF/6-31G(d,p)

C	6.0	.0000000001	-.1033741219	.2163365067
C	6.0	.0000000000	-.0243101061	-.9682368835
C	6.0	.0000000002	-.2008234710	1.6804472048
H	1.0	-.0000000001	.0459188556	-2.0223663283
H	1.0	.0000000002	.7865768377	2.1280381582
H	1.0	.8789666549	-.7324939970	2.0268906713
H	1.0	-.8789666551	-.7324939973	2.0268906707

Energy -115.8712460184 Hartree
ZPE .059777 HARTREE/MOLECULE

MP2/6-31G(d,p)

C	6.0	.0000000002	-.1040096863	.2267895793
C	6.0	.0000000000	-.0228595529	-.9904031898
C	6.0	.0000000004	-.2011842875	1.6857842343
H	1.0	-.0000000002	.0477678256	-2.0502155819
H	1.0	-.0000000003	.7886461492	2.1396364129
H	1.0	.8814411695	-.7346802243	2.0382042730
H	1.0	-.8814411694	-.7346802238	2.0382042720

Energy -116.2729956353 Hartree
ZPE .056172 HARTREE/MOLECULE MP2/6-
311+G(3df,2p) -116.3900121684 Hartree

2-methanesulfinylethylsilane

HF/6-31G(d,p)

S	16.0	-.0025329569	.1188298676	-.8128228440
C	6.0	.0249943759	.0151100303	.9794635720
H	1.0	.5146707228	.9108809459	1.3381778168
H	1.0	.5885548313	-.8554371557	1.2938342235
H	1.0	-.9830430060	-.0139082097	1.3698783955
SI	14.0	-3.2236732244	-3.0009892097	-1.4944128596
O	8.0	-.9546165893	1.2083860382	-1.1594096719
C	6.0	-.8355972403	-1.4466096627	-1.1992777113
H	1.0	-.7418217077	-1.5275744270	-2.2772360118
C	6.0	-2.3041878699	-1.5036007782	-.7795245315
H	1.0	-.2415490645	-2.2437502668	-.7624506582
H	1.0	-2.7953592728	-.5926827824	-1.1079492889
H	1.0	-2.3953139781	-1.5381296691	.3028287576
H	1.0	-3.1747500579	-2.9713512953	-2.9745534785
H	1.0	-4.6357830172	-2.9903933174	-1.0502558929
H	1.0	-2.5859380450	-4.2577524081	-1.0314530169

Energy -880.6621832552 Hartree
ZPE .132001 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	-.0205979048	.1426448816	-.8403981267
C	6.0	.0103104783	-.0036802961	.9618735789
H	1.0	.4560228237	.9106436136	1.3457688020
H	1.0	.6166317719	-.8593193212	1.2551216906
H	1.0	-1.0032460507	-.0938336551	1.3452255124
SI	14.0	-3.2186500493	-2.9745468643	-1.4860133250
O	8.0	-1.0394450573	1.2092554474	-1.1841425719
C	6.0	-.8193130871	-1.4705447594	-1.1882976278
H	1.0	-.7249551345	-1.5791442552	-2.2705226924
C	6.0	-2.2799836418	-1.5009127200	-.7648532027
H	1.0	-.2149229725	-2.2505049480	-.7204811397
H	1.0	-2.7470549324	-.5702743454	-1.0982007794
H	1.0	-2.3691509433	-1.5285164783	.3225028645
H	1.0	-3.1555339072	-2.9319338187	-2.9637972384
H	1.0	-4.6328883018	-2.9476082333	-1.0536625020
H	1.0	-2.6031691913	-4.2406965476	-1.0252864423

Energy -881.5152183683 Hartree
ZPE .127650 HARTREE/MOLECULE MP2/6-
311+G(3df,2p) -881.8877948984 Hartree
MP2/G3Large -882.5696425411 Hartree
MP2/G3Large on C also -882.6272469896 Hartree

1-methanesulfinylethylsilane

HF/6-31G(d,p)

S	16.0	.3366239171	-.1880774647	-.6557954123
C	6.0	-.3957474443	.1035360629	.9582082805
H	1.0	.2180420122	.8482343782	1.4482868863
H	1.0	-.3921470161	-.8093092330	1.5420108400
H	1.0	-1.3986646223	.4913796846	.8481539545
H	1.0	-2.7876766421	-1.9225020433	-1.8080618434
O	8.0	.0333107456	1.0189613104	-1.4764044529
C	6.0	-.7214394347	-1.5110687999	-1.2922918894
SI	14.0	-.1757334870	-1.9116497392	-3.0894661276
C	6.0	-2.2213615872	-1.1857209223	-1.2459735640
H	1.0	-.4961906596	-2.3870303856	-.6865246390
H	1.0	-2.4043699493	-.2125628998	-1.6852897029
H	1.0	-2.6110430438	-1.1899900045	-.2342052351
H	1.0	-.7980709457	-.9760560397	-4.0426827215
H	1.0	-.6478876402	-3.2858259830	-3.3811018507
H	1.0	1.2973614976	-1.8683559212	-3.1987590226

Energy -880.6591555905 Hartree
ZPE .131847 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	.3598266764	-.1893184861	-.6733986450
C	6.0	-.4154566723	.0902501324	.9368572666
H	1.0	.1804090323	.8429036808	1.4480033927
H	1.0	-.4186798165	-.8325691320	1.5150464023
H	1.0	-1.4245682215	.4689638642	.7963014629
H	1.0	-2.7862547818	-1.8682277786	-1.8282119709
O	8.0	.0369771091	1.0194192007	-1.5324823555
C	6.0	-.7120261650	-1.5342376743	-1.2749108033
SI	14.0	-.1834921043	-1.9140656873	-3.0734937115
C	6.0	-2.1972644571	-1.1754243655	-1.2264889963
H	1.0	-.4832669676	-2.4096988608	-.6581919798
H	1.0	-2.3338692195	-.1742847670	-1.6356223638
H	1.0	-2.5988223994	-1.2027040020	-.2147328319
H	1.0	-.8429642728	-.9799317552	-4.0030556571
H	1.0	-.6314287509	-3.2941123040	-3.3704896840
H	1.0	1.2858867111	-1.8330000654	-3.2050260255

Energy	-881.5148264612 Hartree
ZPE	.127400 HARTREE/MOLECULE MP2/6-
311+G(3df,2p)	-881.8877490318 Hartree
MP2/G3Large	-882.5700384610 Hartree

2-methanesulfinylethylsilane TS (H-Transfer)

HF/6-31G(d,p)

S	16.0	-0.9827724727	-0.6127226969	1.2112887883
C	6.0	-0.0906197116	-2.0252802044	1.8678425377
H	1.0	-0.7388588515	-2.8910340975	1.8617847284
H	1.0	0.2030359354	-1.7996183428	2.8869313308
H	1.0	0.7845765586	-2.2242343488	1.2627342435
H	1.0	-0.2496196025	-0.4361839943	-0.7763339265
O	8.0	-1.1886203028	-0.9772701500	-0.2834392211
C	6.0	0.7272570123	0.6699033925	0.7209063178
H	1.0	0.2871667264	1.6154725755	0.9909307830
C	6.0	0.9244677507	0.3564812800	-0.6563766667
H	1.0	1.4244411568	0.3151368725	1.4629180364
SI	14.0	0.7041834993	1.6780877957	-1.9502323136
H	1.0	1.7268020737	-0.3491379536	-0.8351484681
H	1.0	-0.4456490158	2.5370830523	-1.5673902543
H	1.0	0.4345489533	1.0778525612	-3.2785155329
H	1.0	1.8856215904	2.5680537585	-2.1085197828

Energy	-880.5961422286 Hartree
ZPE	0.126106 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	-1.0581031798	-0.6190038338	1.1836983339
C	6.0	-0.1048160586	-1.9983321327	1.8384865721
H	1.0	-0.6854921743	-2.9136047922	1.7629264664
H	1.0	0.1220796547	-1.7919221616	2.8842080155
H	1.0	0.8191028595	-2.1026753502	1.2731761426
H	1.0	-0.1883461731	-0.4176044756	-0.7861465473
O	8.0	-1.1628900250	-0.9684738798	-0.3601184651
C	6.0	0.7657985113	0.6916603870	0.7358271447
H	1.0	0.3138870614	1.6448578869	0.9890855086
C	6.0	0.9678395491	0.3517759044	-0.6204461333
H	1.0	1.4289262989	0.3101432504	1.5060469324
SI	14.0	0.6813849444	1.6476132493	-1.9317815585
H	1.0	1.7521037652	-0.3801704299	-0.7999995394
H	1.0	-0.4155090522	2.5264371903	-1.4637764523
H	1.0	0.2925437771	1.0328351020	-3.2214748136
H	1.0	1.8774515416	2.4890535855	-2.1803310068

Energy	-881.4717449415 Hartree
ZPE	0.121545 HARTREE/MOLECULE MP2/6-
311+G(3df,2p)	-881.8388713332 Hartree
MP2/G3Large	-882.5207198447 Hartree
MP2/G3Large on C as well	-882.5787982013 Hartree

2-methanesulfinylethylsilane TS (Silyl-Transfer)

HF/6-31G(d,p)

S	16.0	-0.9744792812	0.4747020618	0.8823187459
C	6.0	-0.2277682712	-0.5159711908	2.1779746869
H	1.0	-0.8431693931	-1.3864428174	2.3591049590
H	1.0	-0.1891893212	0.0939437428	3.0735315928
H	1.0	0.7701708120	-0.8247134128	1.8973085489
SI	14.0	0.3355981354	-1.0830668075	-1.3933775626
O	8.0	-1.0039423365	-0.5089824955	-0.3419598722
C	6.0	0.7758585371	1.6560296113	0.2085580110
H	1.0	0.2277892584	2.5759914776	0.1065259328
C	6.0	1.2390555506	0.9848590896	-0.9401830609
H	1.0	1.3364958280	1.5989456611	1.1271794126
H	1.0	1.0304935822	1.4853862705	-1.8712703760
H	1.0	2.2405496942	0.5901321862	-0.8730037595
H	1.0	-0.5673971175	-2.2109844929	-1.7880174038
H	1.0	1.3847036778	-1.7501482990	-0.5809238845
H	1.0	0.8358556451	-0.7317656850	-2.7531269705

Energy	-880.6029451172 Hartree
ZPE	0.130350 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	-1.0476385305	.4799686227	.9198744966
C	6.0	-.1615803432	-.5062988650	2.1288774290
H	1.0	-.6857468925	-1.4450456614	2.2874159914
H	1.0	-.1350241428	.0616953837	3.0584845165
H	1.0	.8524903633	-.7031469376	1.7887205098
SI	14.0	.3212407071	-1.0990720214	-1.3776992871
O	8.0	-1.0747606855	-.4808762901	-.3658149158
C	6.0	.7561250270	1.6863324710	.2157968632
H	1.0	.1921681266	2.6014243428	.0854610821
C	6.0	1.2204009190	.9975128265	-.9019864749
H	1.0	1.3047496970	1.6372315931	1.1504594562
H	1.0	1.0010568401	1.4272836822	-1.8686231988
H	1.0	2.1815800956	.5071439853	-.8235538426
H	1.0	-.6562431128	-2.0904024831	-1.9042587413
H	1.0	1.2364941053	-1.8302090610	-.4666758955
H	1.0	1.0653128265	-.7956266878	-2.6358389890

Energy -881.4706864284 Hartree
ZPE .126138 HARTREE/MOLECULE MP2/6-
311+G(3df,2p) -881.8387910632 Hartree

1-methanesulfinylethylsilane TS (H-Transfer)

HF/6-31G(d,p)

S	16.0	-1.0331167039	-1.0642982829	.7778642570
C	6.0	.4057005226	-1.0917868712	1.8547243440
H	1.0	.6956438417	-2.1173295088	2.0409144564
H	1.0	.1400500367	-.6160335328	2.7921961694
H	1.0	1.2299101432	-.5648392456	1.3916289511
H	1.0	-.2580602545	-.4724502150	-1.1531559424
O	8.0	-.4917213441	-1.5602472971	-.5824490067
C	6.0	-.8272964912	1.1488538869	.0245761725
SI	14.0	-2.6140082894	1.7367491785	.1972615781
C	6.0	-.2410473983	.8735753691	-1.2352450036
H	1.0	-.1633891531	1.4483197180	.8215919827
H	1.0	-.8364343967	1.0788038706	-2.1142569730
H	1.0	.8050239140	1.1180142514	-1.3519101516
H	1.0	-2.6908596371	3.1750826244	-.1492431477
H	1.0	-3.0678762604	1.5567395012	1.5941066007
H	1.0	-3.4749544785	.9632237373	-.7201142708

Energy -880.5875338195 Hartree
ZPE .125448 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	-1.0722333582	-1.1125357842	.7776505692
C	6.0	.3851594615	-1.0596096879	1.8367884537
H	1.0	.7261789128	-2.0695567515	2.0492255448
H	1.0	.1106060589	-.5618116752	2.7665548047
H	1.0	1.1763800505	-.5030417037	1.3400067009
H	1.0	-.2651568812	-.4844076214	-1.1570748350
O	8.0	-.4989142299	-1.5701766234	-.6200373332
C	6.0	-.8121223673	1.1543086600	.0453008864
SI	14.0	-2.5798400183	1.7410815998	.2115862141
C	6.0	-.2401730421	.8634371640	-1.2126661456
H	1.0	-.1283760607	1.4367562791	.8433800878
H	1.0	-.8397378234	1.0389892449	-2.1007264158
H	1.0	.8187571512	1.0568818152	-1.3494291331
H	1.0	-2.7057155937	3.1909892385	-.0728242378
H	1.0	-3.0786206243	1.4948163336	1.5849492305
H	1.0	-3.4186275848	.9962566963	-.7541943755

Energy -881.4671181844 Hartree
 ZPE .121062 HARTREE/MOLECULE MP2/6-
 311+G(3df,2p) -881.8354453267 Hartree
 MP2/G3Large -882.5176484006 Hartree

Vinyl silane

HF/6-31G(d,p)

C	6.0	-.9617102281	-.3187948283	.4770779461
C	6.0	-.2249855759	.2128585582	-.4862789449
SI	14.0	1.6391700726	.3958006377	-.3828688504
H	1.0	-2.0326681141	-.4118259760	.3957126523
H	1.0	-.5282112762	-.6863872877	1.3926169619
H	1.0	-.7310390773	.5590923283	-1.3763311007
H	1.0	2.0351318485	1.8200470767	-.4898933585
H	1.0	2.3036559643	-.3411948617	-1.4838317006
H	1.0	2.1076563862	-.1425956472	.9147963948

Energy -368.1208481819 Hartree
 ZPE .071451 HARTREE/MOLECULE

MP2/6-31G(d,p)

C	6.0	-.9573707158	-.3206978985	.4819633244
C	6.0	-.2223107119	.2221336003	-.5036713263
SI	14.0	1.6365394393	.3980530601	-.3875685138
H	1.0	-2.0334740011	-.4209216325	.4105679451
H	1.0	-.5044007477	-.6839201101	1.3960881336
H	1.0	-.7435449431	.5651576719	-1.3920521685
H	1.0	2.0462483785	1.8174099084	-.4838498038
H	1.0	2.3122673946	-.3425563360	-1.4768624293
H	1.0	2.0730459071	-.1476582636	.9163848386

Energy	-368.4912169304 Hartree
ZPE	.068858 HARTREE/MOLECULE MP2/6-
311+G(3df,2p)	-368.6246761487 Hartree
MP2/G3Large	-368.9501140481 Hartree
MP2/G3Large on C also	-368.9899092264 Hartree

Methanesulfenic acid

HF/6-31G(d,p)

S	16.0	.0800853973	.0189420622	-.7668909104
C	6.0	.0323639744	-.0528983013	1.0275143005
H	1.0	-.3691487336	.8965808781	1.3646454971
H	1.0	1.0295886930	-.1786570436	1.4269357743
H	1.0	-.6105138308	-.8505755985	1.3776682904
O	8.0	.8015338285	-1.4328766444	-1.1019985369
H	1.0	.1322298712	-2.0857678525	-1.2396456150

Energy	-512.5418924638 Hartree
ZPE	.056226 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	.0697252069	.0335180435	-.7690048086
C	6.0	.0297830941	-.0526385443	1.0232589234
H	1.0	-.3698312274	.8991530378	1.3734936641
H	1.0	1.0332297674	-.1812418896	1.4202377660
H	1.0	-.6152925101	-.8535805781	1.3771083133
O	8.0	.8297324583	-1.4429941494	-1.1045458235
H	1.0	.1187924108	-2.0874684200	-1.2323192348

Energy	-513.0011201229 Hartree
ZPE	.053758 HARTREE/MOLECULE MP2/6-
311+G(3df,2p)	-513.2241253557 Hartree
MP2/G3Large	-513.5786479620 Hartree
MP2/G3Large on C also	-513.5978861241 Hartree

Methyl Propyl Sulfoxide

HF/6-31G(d,p)

S	16.0	.0044037964	.1002693135	-.8110406959
C	6.0	.0115179366	.0033289489	.9827293705
H	1.0	.5258834362	.8850068302	1.3419121070
H	1.0	.5447786548	-.8827052436	1.3061785752
H	1.0	-1.0001007094	.0068103924	1.3646169420
H	1.0	-2.5709931678	-3.6399466621	-1.0569732950
O	8.0	-.9165359376	1.2129211358	-1.1707171524
C	6.0	-.8520505328	-1.4448930397	-1.2028064318
H	1.0	-.7750225313	-1.5232527189	-2.2825565017
C	6.0	-2.3189322735	-1.4967425613	-.7809077864
H	1.0	-.2679063914	-2.2560193507	-.7767327433
H	1.0	-2.8001567235	-.5807176205	-1.1022135600
H	1.0	-2.3948514312	-1.5340620982	.3015793272
C	6.0	-3.0336894525	-2.7100122865	-1.3758742265
H	1.0	-3.0142882002	-2.6833132188	-2.4613371956
H	1.0	-4.0729494727	-2.7339297207	-1.0647298336

Energy	-629.6232106417 Hartree
ZPE	.146366 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	-.0033837350	.1207957275	-.8393159414
C	6.0	-.0112462256	-.0101597351	.9654029119
H	1.0	.4774338481	.8822924134	1.3482488343
H	1.0	.5423324004	-.8944139682	1.2775535149
H	1.0	-1.0343117836	-.0405646346	1.3319908876
H	1.0	-2.5838126933	-3.6310511572	-1.0707204322
O	8.0	-.9766557010	1.2196483960	-1.2131687415
C	6.0	-.8309493531	-1.4667831867	-1.1903027547
H	1.0	-.7633753909	-1.5698382959	-2.2752419916
C	6.0	-2.2887003401	-1.5016809656	-.7590814407
H	1.0	-.2327719756	-2.2626651627	-.7404646589
H	1.0	-2.7486623406	-.5609758586	-1.0653749060
H	1.0	-2.3579094469	-1.5534588160	.3283765022
C	6.0	-3.0322084515	-2.6838872984	-1.3710477681
H	1.0	-3.0118132251	-2.6334985265	-2.4594224548
H	1.0	-4.0748585860	-2.6910168316	-1.0563046613

Energy -630.5269986050 Hartree
ZPE .141710 HARTREE/MOLECULE
MP2/6-311+G(3df,2p) -630.8833146812 Hartree

Methyl Isopropyl Sulfoxide

HF/6-31G(d,p)

S	16.0	.2609778701	-.0729109300	-.8516989871
C	6.0	-.2757619106	.0242556702	.8591483946
H	1.0	.2832824247	.8301127320	1.3164978671
H	1.0	-.0558181999	-.9039815599	1.3732820384
H	1.0	-1.3305776187	.2557825047	.9105479176
H	1.0	-2.7386136183	-2.0648385333	-1.8596312849
O	8.0	-.2966721452	1.1249603545	-1.5399111818
C	6.0	-.7088553737	-1.5083707142	-1.4189849628
C	6.0	-.2384951520	-1.8339842153	-2.8388236331
C	6.0	-2.2133502474	-1.2504559873	-1.3709790138
H	1.0	-.4343921504	-2.3228476368	-.7530139782
H	1.0	-2.4480506413	-.3278723264	-1.8873704056
H	1.0	-2.5881424205	-1.1834490429	-.3564177333
H	1.0	-.4469373742	-1.0046083957	-3.5053448196
H	1.0	-.7602997749	-2.7103038079	-3.2082768258
H	1.0	.8267120323	-2.0375261118	-2.8689198916

Energy -629.6239780075 Hartree
ZPE .145884 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	.2880957119	-.0731635949	-.8712886271
C	6.0	-.3096018466	.0222390657	.8332396003
H	1.0	.2444650578	.8211835069	1.3199408051
H	1.0	-.1241165537	-.9195034424	1.3477845765
H	1.0	-1.3681772268	.2693705394	.8380121661
H	1.0	-2.7326477234	-2.0118566114	-1.8837261319
O	8.0	-.2792577176	1.1215009551	-1.6136921292
C	6.0	-.6900676432	-1.5322693857	-1.4054246401
C	6.0	-.2472003921	-1.8353859927	-2.8323363264
C	6.0	-2.1827033548	-1.2508242386	-1.3313484595
H	1.0	-.3970606463	-2.3472266351	-.7372125291
H	1.0	-2.3823230767	-.2795272864	-1.7843952155
H	1.0	-2.5554755400	-1.2460631261	-.3091798112
H	1.0	-.4774608558	-.9856737165	-3.4740447977
H	1.0	-.7752238841	-2.7101092502	-3.2091780670
H	1.0	.8237613913	-2.0287287871	-2.8870469133

Energy -630.5309128226 Hartree
ZPE .140909 HARTREE/MOLECULE
MP2/6-311+G(3df,2p) -630.8876957332 Hartree
MP2/G3Large -631.3042371072 Hartree

Methyl Propyl Sulfoxide TS (H-transfer)

HF/6-31G(d,p)

S	16.0	-.9991661606	-.5472691559	1.1148758256
C	6.0	-.1516975325	-1.9417230471	1.8687987506
H	1.0	-.8023576870	-2.8058603446	1.8627141451
H	1.0	.0929093652	-1.6812516359	2.8928230816
H	1.0	.7528926328	-2.1711908462	1.3199012179
H	1.0	-.1215857278	-.3884041348	-.8383460513
O	8.0	-1.1225532007	-.9557212110	-.3746942895
C	6.0	.8592905581	.7272860710	.5831702578
H	1.0	.4694576278	1.6698812915	.9253718062
C	6.0	.9457032513	.4526370920	-.7956723722
H	1.0	1.5309578528	.2544225862	1.2781274046
C	6.0	.6148782679	1.5564064213	-1.7918820356
H	1.0	1.7727588668	-.1860130835	-1.0769524510
H	1.0	-.2951798045	2.0768607100	-1.5058382040
H	1.0	.4512236793	1.1459770194	-2.7827440324
H	1.0	1.4084293113	2.2965517677	-1.8702724534

Energy -629.5457112911 Hartree
 ZPE .139644 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	-1.0553939206	-0.5377369385	1.1005008275
C	6.0	-0.1429269182	-1.9073451268	1.8345165933
H	1.0	-0.7484158694	-2.8094691383	1.8113158375
H	1.0	0.0902345005	-1.6487104912	2.8672281775
H	1.0	0.7784954759	-2.0718324008	1.2800301801
H	1.0	-0.1140691912	-0.3835660359	-0.8515955811
O	8.0	-1.1339285495	-0.9351911503	-0.4278251865
C	6.0	0.8638089417	0.7234950347	0.6103262174
H	1.0	0.4861908252	1.6864475311	0.9353508917
C	6.0	0.9535506713	0.4406693589	-0.7639743986
H	1.0	1.5337921225	0.2441730078	1.3149251817
C	6.0	0.6076584531	1.5223778844	-1.7684437863
H	1.0	1.7551213581	-0.2331049594	-1.0562850185
H	1.0	-0.2830745804	2.0628426389	-1.4472225364
H	1.0	0.3985728383	1.1031695061	-2.7518581556
H	1.0	1.4163451432	2.2463707791	-1.8776086436

Energy -630.4757255639 Hartree
 ZPE 0.134856 HARTREE/MOLECULE
 MP2/6-311+G(3df,2p) -630.8268232990 Hartree

Methyl Propyl Sulfoxide TS (Methyl-transfer)

HF/6-31G(d,p)

S	16.0	-1.0821839316	.2478728476	.9220963824
C	6.0	-.1518416273	-.4773790091	2.2781110264
H	1.0	-.6252785510	-1.3976731012	2.5954435749
H	1.0	-.1330816680	.2239980376	3.1053600590
H	1.0	.8611910326	-.6912020578	1.9569392367
C	6.0	.4627670277	-1.1521848755	-1.6124210476
O	8.0	-.9970067871	-.8029631886	-.1761993413
C	6.0	.7095843257	1.6742279351	.1077623830
H	1.0	.0234723086	2.4664211862	-.1252768671
C	6.0	1.3037731567	.9605222152	-.8938111737
H	1.0	1.1575992588	1.7271027502	1.0835356229
H	1.0	1.1075883052	1.2352961797	-1.9127940320
H	1.0	2.2296688142	.4524246814	-.6977588945
H	1.0	-.4203278775	-1.1186627597	-2.2138078626
H	1.0	.5660368237	-2.0163185661	-.9921265606
H	1.0	1.3586643892	-.8835673749	-2.1344135061

Energy -629.4368784316 Hartree
 ZPE .140590 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	-1.1232660766	.3464568431	.8577307248
C	6.0	-.1970942468	-.4972385748	2.1509984189
H	1.0	-.7034184332	-1.4189105647	2.4252945934
H	1.0	-.1222491572	.1593473967	3.0171798985
H	1.0	.7985077109	-.7259925587	1.7758083362
C	6.0	.4379157823	-1.1554006778	-1.4960837304
O	8.0	-1.1222096926	-.6874802194	-.3032896998
C	6.0	.7875241489	1.7137082802	.1869095124
H	1.0	.1585610479	2.5751905519	.0122850681
C	6.0	1.3043061548	1.0134692648	-.8711812562
H	1.0	1.2549732026	1.6598886760	1.1621230494
H	1.0	1.0563092013	1.3075811009	-1.8777076737
H	1.0	2.1739834685	.3899116400	-.7430590985
H	1.0	-.4015257188	-1.6890950020	-1.9242920267
H	1.0	.9934860161	-1.7714523532	-.7952729707
H	1.0	1.0748215917	-.7720689028	-2.2868041460

Energy -630.3803027558 Hartree
 ZPE .135119 HARTREE/MOLECULE
 MP2/6-311+G(3df,2p) -630.7341076509 Hartree

Methyl Isopropyl Sulfoxide TS (H-transfer)

HF/6-31G(d,p)

S	16.0	-1.1002214265	-1.0234046460	.8201183936
C	6.0	.3891721071	-1.0569047139	1.8248007160
H	1.0	.7120644326	-2.0807574109	1.9580624076
H	1.0	.1609553381	-.6221644641	2.7919317185
H	1.0	1.1793538338	-.4934201476	1.3442993739
H	1.0	-.3947702157	-.4354564827	-1.1250480878
O	8.0	-.6169259516	-1.5225939267	-.5677964171
C	6.0	-.9784215621	1.1795368807	.0685554682
C	6.0	-2.4135880469	1.6273231192	.1691607559
C	6.0	-.3787245108	.9219219838	-1.1850221478
H	1.0	-.3464023474	1.5098523561	.8762940660
H	1.0	-.9779629243	1.1516707645	-2.0545548413
H	1.0	.6635328555	1.1860590515	-1.2847814638
H	1.0	-2.4632638705	2.6863462911	-.0736670175
H	1.0	-2.8186797277	1.4894875326	1.1644411939
H	1.0	-3.0385539325	1.0948809965	-.5383041025

Energy -629.5517780930 Hartree
 ZPE .139344 HARTREE/MOLECULE

MP2/6-31G(d,p)

S	16.0	-1.1416565064	-1.0511066112	.8217153184
C	6.0	.3691196771	-1.0226363331	1.8015535818
H	1.0	.7518401982	-2.0326649306	1.9210486041
H	1.0	.1336103638	-.6023104430	2.7791770723
H	1.0	1.1169021193	-.4056779174	1.3073164070
H	1.0	-.4051312269	-.4573622716	-1.1250533550
O	8.0	-.6377784586	-1.5284708307	-.6043600357
C	6.0	-.9622606308	1.1714701044	.0895854157
C	6.0	-2.3932587960	1.6280860765	.1796560936
C	6.0	-.3680434183	.9191765573	-1.1578622969
H	1.0	-.3213502662	1.4969451424	.9047645834
H	1.0	-.9655270923	1.1170180306	-2.0413814448
H	1.0	.6898248936	1.1252363584	-1.2689882713
H	1.0	-2.4607648690	2.6973347035	-.0315712090
H	1.0	-2.8199292314	1.4514031574	1.1664457826
H	1.0	-3.0080327051	1.1059363910	-.5535562302

Energy -630.4796892378 Hartree
 ZPE .134584 HARTREE/MOLECULE
 MP2/6-311+G(3df,2p) -630.8316072064 Hartree
 MP2/G3Large -631.2480691552 Hartree

Propene

HF/6-31G(d,p)

C	6.0	-.7777599990	-.3641775744	.4278484597
C	6.0	-.0145791520	.2806161684	-.4319328997
C	6.0	1.4807842166	.3936636759	-.3492864691
H	1.0	-1.8463119357	-.4070531562	.3102409331
H	1.0	-.3644369507	-.8746728046	1.2819106220
H	1.0	-.4789960100	.7750879872	-1.2719505269
H	1.0	1.7877814556	1.4348625636	-.2888399498
H	1.0	1.9498739470	-.0252763132	-1.2360251634
H	1.0	1.8706444283	-.1260505467	.5190349941

Energy -117.0816139306 Hartree
 ZPE .084965 HARTREE/MOLECULE

MP2/6-31G(d,p)

C	6.0	-.7796021629	-.3674594385	.4323185757
C	6.0	-.0120519314	.2887603128	-.4442776531
C	6.0	1.4790658250	.3949332719	-.3517650496
H	1.0	-1.8532030458	-.4146209381	.3204525970
H	1.0	-.3504404901	-.8751784885	1.2861413033
H	1.0	-.4835926003	.7843895294	-1.2866020160
H	1.0	1.7949693391	1.4368293226	-.2844740760
H	1.0	1.9583724676	-.0286016564	-1.2354092700
H	1.0	1.8534825989	-.1320519152	.5246155887

Energy	-117.5039138387 Hartree
ZPE	.081913 HARTREE/MOLECULE
MP2/6-311+G(3df,2p)	-117.6224988562 Hartree
MP2/G3Large	-117.6827153751 Hartree

Ethene

HF/6-31G(d,p)

H	1.0	-.0000000042	.9153882646	1.2245537659
C	6.0	.0000000007	-.0000003683	.6582259521
C	6.0	-.0000000081	.0000003661	-.6582259527
H	1.0	.0000000056	-.9153880462	1.2245537385
H	1.0	.0000000080	.9153880469	-1.2245537389
H	1.0	-.0000000019	-.9153882631	-1.2245537649

Energy	-78.0388414542 Hartree
ZPE	0.053396 HARTREE/MOLECULE

MP2/6-31G(d,p)

H	1.0	-.0000000059	.9208074722	1.2333218197
C	6.0	.0000000091	-.0000210249	.6676398419
C	6.0	-.0000000199	.0000209377	-.6676398465
H	1.0	.0000000039	-.9207941911	1.2333192656
H	1.0	.0000000114	.9207942319	-1.2333192883
H	1.0	.0000000015	-.9208074259	-1.2333217925

Energy	-78.3172820048 Hartree
ZPE	.052343 HARTREE/MOLECULE
MP2/6-311+G(3df,2p)	-78.4049919373 Hartree

Ethane

MP2/6-31G(d,p)

C	6.0	-0.0000001010	-0.0000008758	-0.4372013274
C	6.0	-0.0000003626	0.0000007552	1.0862013968
H	1.0	0.5076613493	0.8792949809	1.4797193195
H	1.0	0.5076615159	-0.8792958650	1.4797190496
H	1.0	-1.0153226998	-0.0000002911	1.4797189528
H	1.0	1.0153226458	0.0000001559	-0.8307192290
H	1.0	-0.5076617146	0.8792956601	-0.8307189438
H	1.0	-0.5076615271	-0.8792950362	-0.8307189515

Energy -79.5434005239 Hartree
ZPE 0.077460 HARTREE/MOLECULE
MP2/6-311+G(3df,2p) -79.6240909096 Hartree

Methylsilane

MP2/6-31G(d,p)

H	1.0	0.0179145987	0.0310297890	-0.0015281156
C	6.0	0.0047770721	0.0081610536	1.0866534269
H	1.0	1.0350461448	0.0310300902	1.4369466968
SI	14.0	-0.8835255156	-1.5303006628	1.7147436079
H	1.0	-2.2835052532	-1.5544948048	1.2345901132
H	1.0	-0.2044792179	-2.7548202017	1.2345863400
H	1.0	-0.8974867731	-1.5544958526	3.1947125261
H	1.0	-0.4906820677	0.9119439621	1.4369605396

Energy -330.5336325327 Hartree
ZPE 0.063266 HARTREE/MOLECULE
MP2/6-311+G(3df,2p) -330.6314127365 Hartree

Previously Reported compounds: ethyl methyl sulfoxide, methyl vinyl sulfoxide, and their respective transition states and products. See *J. Org. Chem.* **2001**, 66, 8722-8736.

Table S2. Calculated heats of isodesmic reactions (kcal mol⁻¹).

Reaction		ΔH
1		-1.86
2		1.00
3		-4.98
4		0.49
5		-1.50
6		-0.99
7		-3.25
8		-0.16
9		2.37
10		11.33

Table S3. Bond lengths, angles and orders

SM, TS and PR refer to Starting Materials (sulfoxide), Transition State, and PProducts, respectively

θ Dihedral S-C₁-C₂-C₃

Bond lengths and Angles

	S-O	S-C ₁	O-H	C ₂ -H	C ₁ -C ₂	C ₃ -C ₂	θ	ϕ
SM	1.51	1.79	--	1.09	1.33	1.50	-177.543	124.679
TS	1.59	2.30	1.18	1.41	1.26	1.49	178.065	148.202
PR	1.69	--	0.97	--	1.22	1.46	--	180.000

Bond Orders

	S-O	S-C ₁	O-H	C ₂ -H	C ₁ -C ₂	C ₃ -C ₂
SM	1.41	0.80	--	0.90	1.78	0.95
TS	1.06	0.40	0.45	0.39	2.24	0.93
PR	0.82	--	0.83	--	2.76	0.95

Mulliken Charges

	S	O	H	C ₁	C ₂	C ₃
SM	0.83	-0.66	0.16	-0.36	-0.06	-0.37
TS	0.55	-0.62	0.29	-0.28	-0.10	-0.36
PR	0.33	-0.62	0.35	-0.36	0.12	-0.41

θ Dihedral S-C₁-C₂-Si

Bond lengths and Angles

	S-O	S-C ₁	O-H	C ₂ -H	C ₁ -C ₂	Si-C ₂	θ	ϕ
SM	1.51	1.80	--	1.09	1.34	1.87	-178.088	122.542
TS	1.59	2.24	1.16	1.43	1.27	1.84	178.385	145.220
PR	1.69	--	0.97	--	1.22	1.83	--	179.811

Bond Orders

	S-O	S-C ₁	O-H	C ₂ -H	C ₁ -C ₂	Si-C ₂
SM	1.42	0.78	--	0.88	1.76	0.92
TS	1.06	0.43	0.45	0.38	2.11	0.93
PR	0.82	--	0.83	--	2.52	1.00

Mulliken Charges

	S	O	H	C ₁	C ₂	Si
SM	0.83	-0.65	0.17	-0.33	-0.25	0.48
TS	0.58	-0.63	0.30	-0.23	-0.29	0.46
PR	0.33	-0.62	0.35	-0.11	-0.19	0.41

θ Dihedral Si-C₁-C₂-H

Bond lengths and Angles

	S-O	S-C ₁	O-H	C ₂ -H	C ₁ -C ₂	Si-C ₁	θ	ϕ
SM	1.51	1.80	--	1.08	1.34	1.88	175.616	123.101
TS	1.58	2.39	1.21	1.35	1.27	1.84	173.353	155.394
PR	1.69	--	0.97	--	1.22	1.83	--	179.811

Bond Orders

	S-O	S-C ₁	O-H	C ₂ -H	C ₁ -C ₂	Si-C ₁
SM	1.41	0.76	--	0.90	1.75	0.89
TS	1.08	0.37	0.41	0.42	2.13	0.95
PR	0.82	--	0.83	--	2.52	1.00

Mulliken Charges

	S	O	H	C ₁	C ₂	Si
SM	0.84	-0.65	0.17	-0.37	-0.27	0.48
TS	0.55	-0.60	0.29	-0.19	-0.31	0.46
PR	0.33	-0.62	0.35	-0.19	-0.11	0.41

θ Dihedral C₃-C₁-C₂-H

Bond lengths and Angles

	S-O	S-C ₁	O-H	C ₂ -H	C ₁ -C ₂	C ₃ -C ₁	θ	ϕ
SM	1.51	1.81	--	1.08	1.33	1.50	178.686	126.626
TS	1.59	2.32	1.17	1.41	1.26	1.48	-0.712	22.524
PR	1.69	--	0.97	--	1.22	1.46	--	180.000

Bond Orders

	S-O	S-C ₁	O-H	C ₂ -H	C ₁ -C ₂	C ₃ -C ₁
SM	1.41	0.78	--	0.90	1.78	0.92
TS	1.06	0.39	0.46	0.37	2.25	0.94
PR	0.82	--	0.83	--	2.76	0.95

Mulliken Charges

	S	O	H	C ₁	C ₂	C ₃
SM	0.83	-0.66	0.16	-0.18	-0.25	-0.37
TS	0.53	-0.62	0.30	0.00	-0.36	-0.38
PR	0.33	-0.62	0.35	0.13	-0.36	-0.40

Elimination by attack at Si

Bond lengths and Angles

	S-O	S-C ₁	O-Si	C ₁ -C ₂	Si-C ₂
SM	1.51	1.79	--	1.34	1.88
TS	1.61	2.29	1.78	1.25	2.36
PR	1.70	1.79	1.69	1.22	--

Bond Orders

	S-O	S-C ₁	O-Si	C ₁ -C ₂	Si-C ₂
SM	1.42	0.80	--	1.73	0.92
TS	0.88	0.37	0.70	2.38	0.28
PR	0.76	--	0.90	2.84	--

Mulliken Charges

	S	O	Si	C ₁	C ₂
SM	0.83	-0.66	0.48	-0.31	-0.27
TS	0.58	-0.66	0.66	-0.19	-0.31
PR	0.36	-0.67	0.72	-0.19	-0.19

Bond lengths and Angles

	S-O	S-C ₁	O-H	H-C ₂	C ₁ -C ₂
SM	1.52	1.836	--	1.09	1.52
TS	1.59	2.35	1.21	1.38	1.40
PR	1.69	--	0.97	--	1.34

Bond Orders

	S-O	S-C ₁	O-H	H-C ₂	C ₁ -C ₂
SM	1.38	0.77	--	0.91	0.94
TS	1.07	0.42	0.42	0.42	1.29
PR	0.82	--	0.83	--	1.83

Mulliken Charges

	S	O	H	C ₁	C ₂	C ₃
SM	0.83	-0.67	0.16	-0.30	-0.35	-0.35
TS	0.55	-0.62	0.30	-0.16	-0.42	-0.33
PR	0.32	-0.62	0.35	-0.05	-0.25	-0.37

Bond lengths and Angles

	S-O	S-C ₁	O-H	H-C ₂	C ₁ -C ₂	C ₁ -Si
SM	1.52	1.82	--	1.09	1.53	1.91
TS	1.58	2.40	1.23	1.35	1.41	1.87
PR	1.69	--	0.97	--	1.34	1.87

Bond Orders

	S-O	S-C ₁	O-H	H-C ₂	C ₁ -C ₂	C ₁ -Si
SM	1.34	0.79	--	0.91	0.92	0.86
TS	1.09	0.40	0.39	0.45	1.27	0.92
PR	0.82	--	0.83	--	1.80	0.94

Mulliken Charges

	S	O	H	C ₁	C ₂	Si	SiH
SM	0.84	-0.67	0.16	-0.50	-0.36	0.51	-0.10
TS	0.56	-0.61	0.29	-0.35	-0.41	0.50	-0.11
PR	0.32	-0.62	0.35	-0.25	-0.23	0.47	-0.12

θ Dihedral S-C₁-C₂-Si

Bond lengths and Angles

	S-O	S-C ₁	O-H	C ₂ -H	C ₁ -C ₂	Si-C ₂	θ	ϕ
SM	1.51	1.83	--	1.09	1.52	1.89	166.01	112.720
TS	1.59	2.29	1.20	1.40	1.41	1.86	112.72	119.059
PR	1.69	--	0.97	--	1.34	1.87	--	122.404

Bond Orders

	S-O	S-C ₁	O-H	C ₂ -H	C ₁ -C ₂	Si-C ₂
SM	1.39	0.78	--	0.89	0.92	0.90
TS	1.06	0.45	0.41	0.43	1.26	0.91
PR	0.82	--	0.83	--	1.80	0.94

Mulliken Charges

	S	O	H	C ₁	C ₂	Si
SM	0.83	-0.67	0.17	-0.43	-0.42	0.51
TS	0.58	-0.63	0.30	-0.31	-0.45	0.50
PR	0.33	-0.62	0.35	-0.23	-0.25	0.47

θ Dihedral S-C₁-C₂-Si

TS not planar

Attack at Si

Bond lengths and Angles							
	S-O	S-C ₁	O-Si	C ₁ -C ₂	Si-C ₂	θ	ϕ
SM	1.51	1.83	--	1.52	1.89	166.01	
TS	1.60	2.28	1.83	1.39	2.33	-9.48	82.97
PR	1.70	1.79	1.69	1.34	--		

Bond Orders						
	S-O	S-C ₁	O-Si	C ₁ -C ₂	Si-C ₂	
SM	1.39	0.78	--	0.92	0.90	
TS	0.92	0.40	0.40	1.33	0.37	
PR	0.76	--	0.90	1.80	--	

Mulliken Charges					
	S	O	C ₁	C ₂	Si
SM	0.83	-0.67	-0.43	-0.42	0.51
TS	0.61	-0.65	-0.29	-0.41	0.63
PR	0.36	-0.67	-0.23	-0.25	0.72

θ Dihedral S-C₁-C₂-C₃

trans-TS_{propyl methyl sulfoxide elimination}

Bond lengths and Angles								
	S-O	S-C ₁	O-H	C ₂ -H	C ₁ -C ₂	C ₃ -C ₂	θ	ϕ
SM	1.51	1.82	--	1.09	1.52	1.52	165.684	111.805
TS	1.58	2.35	1.23	1.35	1.41	1.52	107.722	119.308
PR	1.69	--	0.97	--	1.34	1.50	--	124.454

Bond Orders						
	S-O	S-C ₁	O-H	C ₂ -H	C ₁ -C ₂	C ₃ -C ₂
SM	1.40	0.79	--	0.91	0.91	0.93
TS	1.08	0.42	0.40	0.44	1.28	0.93
PR	0.82	--	0.83	--	1.83	0.95

Mulliken Charges						
	S	O	H	C ₁	C ₂	C ₃
SM	0.83	-0.67	0.16	-0.43	-0.22	-0.33
TS	0.55	-0.62	0.29	-0.30	-0.28	-0.32
PR	0.33	-0.62	0.35	-0.25	-0.06	-0.33