Suplementary Information:

Tables of geometric parameters for all species that participate in the oxidation mechanism considering all the solvation models applied in this study. All bond distances are in Å, bond angles and dihedral angles in degrees.

Table 1: Geometric parameters evaluated in gas phase at the uMP2/6-311G(d,p) level. Bond distances in Å and angles in degrees.

DMSO	
$rSO_{(3)}$	1.501
$\theta C_{(1)}SC_{(4)}$	96.53
$\theta C_{(1)}SO_{(3)}$	106.53
Complex 1	
$rSO_{(5)}$	1.513
$rSO_{(3)}$	1.873
$\theta C_{(1)}SC_{(4)}$	102.68
$\theta C_{(1)}SO_{(5)}$	104.45
$\theta O_{(3)}SO_{(5)}$	154.05
$\psi H_{(13)}O_{(3)}SO_{(5)}$	23.32

Complex 2	
$rSO_{(3)}$	1.515
$rO_{(3)}H_{(13)}$	1.793
$\theta C_{(1)}SC_{(4)}$	96.67
$\theta C_{(1)}SO_{(3)}$	106.27
$\theta O_{(5)}H_{(13)}O_{(3)}$	156.53
$\psi O_{(5)}H_{(13)}O_{(3)}S$	0.06
MSIA	
$rSO_{(3)}$	1.473
$rSO_{(4)}$	1.671
$\theta C_{(1)}SO_{(3)}$	104.67
$\theta O_{(3)}SO_{(4)}$	109.30
$\psi O_{(3)}SO_{(4)}H_{(6)}$	37.84

Table 2: Geometric parameters of the species that participate in the water-assisted mechanism in gas phase. Bond distances in Å and angles in degrees.

	Model 1a	Model 1b	Model 1c	Model 1d	Model 1e
			DMSO		
$rSO_{(3)}$	1.517		1.519		
$rO_{(3)}H_{(12)}$	1.811		1.711		
$\theta C_{(1)}SC_{(4)}$	96.61		96.54		
$\theta C_{(1)}SO_{(3)}$	106.36		106.86		
$\theta O_{(5)}H_{(12)}O_{(3)}$	156.53		171.92		
$\psi O_{(5)}H_{(12)}O_{(3)}S$	0.11		-34.97		
			Complex 1		
$rSO_{(5)}$	1.524	1.506	1.526	1.504	1.515
$rSO_{(3)}$	1.857	1.961	1.866	2.000	1.932
$rO_{(3)}H_{(14)}$	-	1.739	-	1.657	1.762
$rO_{(5)}H_{(14)}$	1.908	-	2.013	-	1.964
$\theta C_{(1)}SC_{(4)}$	102.76	103.35	102.73	103.88	102.77
$\theta C_{(1)}SO_{(5)}$	104.02	106.03	104.20	106.90	105.78
$\theta O_{(3)}SO_{(5)}$	156.46	156.28	156.40	155.12	154.39
$\psi H_{(13)}O_{(3)}SO_{(5)}$	33.19	34.59	33.05	1.44	36.16
			Complex 2		
$rSO_{(3)}$	1.527	1.521	1.530	1.524	1.529
$rO_{(3)}H_{(13)}$	1.836	1.702	1.773	1.666	1.740
$rO_{(5)}$-$H_{(14)}$	-	1.951	-	1.865	1.951
$rO_{(3)}H_{(14)}$	1.951	-	2.810	-	2.017
$\theta C_{(1)}SC_{(4)}$	96.86	97.22	97.27	97.22	97.15
$\theta C_{(1)}SO_{(3)}$	105.58	105.96	103.63	105.61	105.58
$\psi O_{(5)}H_{(13)}O_{(3)}S$	60.03	21.70	121.92	33.16	57.66
			MSIA		
$rSO_{(3)}$	1.495	1.495	1.497	1.497	
$rSO_{(4)}$	1.642	1.642	1.627	1.627	
$rO_{(3)}H_{(10)}$	1.891	1.891		1.742	
$\theta C_{(1)}SO_{(3)}$	104.26	104.26	104.25	104.25	
$\theta O_{(3)}SO_{(4)}$	109.19	109.20	110.54	110.54	
$\psi O_{(3)}SO_{(4)}H_{(6)}$	40.42	40.48		52.90	

Table 3: Geometric parameters of transition structures optimized following the microsolvation schemes.

	Model 1a	Model 1b	Model 1c	Model 1d	Model 1e
			TS1		
$rSO_{(3)}$	1.744	1.731			1.99518
$rSC_{(1)}$	2.187	2.185			1.83187
$\theta C_{(1)}SC_{(4)}$	94.17	93.32			97.181
$\theta C_{(1)}SO_{(3)}$	152.72	151.40			136.433
$\theta C_{()}SO_{(5)}$	98.68	99.97			104.944
$\psi C_{(1)}SO_{(5)}H_{(13)}$	71.66	-157.75			-159.985
			TS2		
$rO_{(3)}H_{(13)}$	3.228	1.840	3.246	1.818	3.227
$rO_{(5)}H_{(7)}$	1.245	1.275	1.268	1.281	1.273
$\theta C_{(1)}SC_{(4)}$	96.82	96.35	97.94	96.94	96.62
$\theta SO_{(3)}H_{(13)}$	84.98	102.32	87.40	101.74	84.75
$\theta C_{(1)}H_{(7)}O_{(5)}$	173.86	154.34	166.07	155.68	169.99
$\psi SO_{(3)}H_{(13)}O_{(5)}$	4.14	-10.85	-0.79	-17.49	-3.91

Table 4: Geometric parameters of the liquid phase mechanism. Comparison between the two approaches analyzed in this work.

	IEFPCM	IEFPCM + Model 1a	IEFPCM + Model 1b
		DMSO	
$rSO_{(3)}$	1.520	1.531	
$\theta C_{(1)}SC_{(4)}$	96.62	97.21	
$\theta C_{(1)}SO_{(3)}$	106.28	105.90	
		Complex 1	
$rSO_{(5)}$	1.525	1.535	1.506
$rSO_{(3)}$	1.858	1.840	1.961
$\theta C_{(1)}SC_{(4)}$	103.59	103.21	103.35
$\theta C_{(1)}SO_{(5)}$	104.35	103.34	106.03
$\theta O_{(3)}SO_{(5)}$	156.41	156.01	156.28
$\psi H_{(13)}O_{(3)}SO_{(5)}$	46.61	46.80	34.59
		Complex 2	
$rSO_{(3)}$	1.530	1.543	1.521
$rO_{(3)}H_{(13)}$	1.712	1.708	1.702
$\theta C_{(1)}SC_{(4)}$	97.49	97.97	98.22
$\theta C_{(1)}SO_{(3)}$	106.02	105.10	104.96
$\theta O_{(5)}H_{(13)}O_{(3)}$	177.59	179.80	169.34

$\psi O_{(5)}H_{(13)}O_{(3)}S$	-0.22	-71.11	21.71
		MSIA	
$rSO_{(3)}$	1.488		1.501
$rSO_{(4)}$	1.662		1.643
$\theta C_{(1)}SO_{(3)}$	104.87		104.52
$\theta O_{(3)}SO_{(4)}$	109.54		108.44
$\psi O_{(3)}SO_{(4)}H_{(6)}$	51.57		42.16

Table 5: Geometric parameters optimized for the transition structures using the IEFPCM model with Bondi radii to construct the solvent cavity.

TS1		TS2	
$rSO_{(4)}$	1.731	$rO_{(5)}H_{(13)}$	1.880
$rSC_{(1)}$	2.185	$rO_{(5)}H_{(7)}$	1.275
$\theta C_{(1)}SC_{(3)}$	93.32	$\theta C_{(1)}SC_{(3)}$	96.98
$\theta C_{(1)}SO_{(4)}$	151.40	$\theta SO_{(4)}H_{(13)}$	100.53
$\theta C_{(1)}SO_{(5)}$	99.97	$\theta C_{(1)}H_{(7)}O_{(5)}$	156.40
$\psi C_{(1)}SO_{(4)}H_{(13)}$	66.00	$\psi SO_{(4)}H_{(13)}O_{(5)}$	-10.46

Table 5: Geometric parameters of the transition structures using Model 3 and considering Bondi radii to construct the solvent cavity.

	Model 3a	Model 3b
	TS1	
$rSO_{(4)}$	1.711	1.717
$rSC_{(1)}$	2.183	2.100
$\theta C_{(1)}SC_{(3)}$	93.78	82.20
$\theta C_{(1)}SO_{(4)}$	154.34	153.32
$\theta C_{(1)}SO_{(5)}$	98.07	81.38
$\psi C_{(1)}SO_{(4)}H_{(13)}$	64.74	-120.55
	TS2	
$rO_{(5)}H_{(13)}$	3.190	1.811
$rO_{(5)}H_{(7)}$	1.274	1.456
$\theta C_{(1)}SC_{(3)}$	97.41	97.20
$\theta SO_{(4)}H_{(13)}$	86.35	102.24
$\theta C_{(1)}H_{(7)}O_{(5)}$	173.26	153.34
$\psi SO_{(4)}H_{(13)}O_{(5)}$	9.170	-14.23

Cartesian coordinates for the microsolvated molecules:

DMSO with one water molecule

C	0.577742	1.349626	-0.752527
S	0.926126	-0.003942	0.384784
O	-0.203712	-0.012448	1.397889
C	0.578376	-1.341338	-0.771654
O	-2.320880	0.014098	-0.330774
H	-3.207136	-0.100932	0.011964
H	0.713816	2.276099	-0.192461
H	-0.456865	1.263983	-1.090828
H	0.721005	-2.275834	-0.226714
H	-0.458919	-1.251535	-1.100420
H	1.278338	-1.293018	-1.609068
H	-1.755384	0.003616	0.463175
H	1.282994	1.316653	-1.586287

DMSO with two water molecules

C	-0.199335	0.198444	0.120625
S	-0.111802	-0.020165	1.905527
C	1.644007	0.338115	2.070018
O	-0.278635	-1.505597	2.176221
O	1.203707	-3.430646	1.033955
H	0.551620	-4.019822	0.652086
H	-1.202354	-0.103590	-0.184626
H	0.561636	-0.417276	-0.362874
H	1.912641	0.134556	3.107585
H	2.200568	-0.303566	1.383356
H	1.813949	1.394111	1.845046
H	0.659527	-2.778160	1.522900
H	-0.049209	1.255707	-0.112552
H	2.102700	-2.356592	-0.035804
O	2.495763	-1.605696	-0.520152
H	3.414256	-1.858472	-0.618372

Complex 1: DMSO with one water molecule

C	0.000000	0.000000	0.000000
S	0.000000	0.000000	1.790413
O	1.855491	0.000000	1.866786
C	0.039083	1.740696	2.184701
O	-1.413690	-0.431082	2.162108
O	-2.902035	1.384336	0.665205
H	-0.949637	0.428224	-0.323842
H	0.861684	0.559472	-0.356304
H	0.073915	-1.041154	-0.316606
H	0.927287	2.189836	1.746643
H	-0.890434	2.163213	1.801525
H	0.078516	1.814441	3.271418
H	2.109659	-0.908045	2.065487
H	-2.705494	0.657264	1.273694
H	-3.820346	1.592039	0.839870

Complex 1: OH radical with one water molecule

C	-0.218157	1.492815	-0.413117
S	0.758943	0.219842	0.384299
O	-0.867453	-0.592374	1.119992
O	2.171909	0.740796	0.407435
C	0.744703	-1.115028	-0.802543
O	-2.572577	-0.702265	-0.929481
H	0.419118	1.956428	-1.167687
H	-1.118198	1.050745	-0.836317
H	-0.478823	2.221742	0.354384
H	-0.284644	-1.303306	-1.101311
H	1.376180	-0.801276	-1.634802
H	1.171930	-1.985698	-0.306400
H	-0.940236	-0.297492	2.033955
H	-2.144274	-0.734953	-0.051565
H	-3.158449	-1.459634	-0.928648

Complex 1: DMSO with two water molecules

C	0.969643	-1.391701	-0.694305
S	1.347662	-0.010650	0.380480
O	3.098097	0.101539	-0.257202
C	0.948688	1.400787	-0.637439
O	0.244398	-0.039144	1.428174
O	-1.957196	-0.051586	-0.378580
H	-0.110080	-1.384082	-0.851099
H	1.536435	-1.289714	-1.616663
H	1.275337	-2.295698	-0.165877
H	1.556296	1.375990	-1.538938
H	-0.122186	1.342363	-0.836619
H	1.187433	2.286495	-0.048692
H	3.645413	-0.315597	0.417129
H	-1.536569	-0.046431	0.489622
H	-2.902348	-0.022901	-0.186667
H	-5.235658	-0.706440	-0.332688
O	-4.782484	0.035689	0.071876
H	-5.189164	0.799925	-0.340861

Complex 1: OH radical with two water molecules

C	0.000000	0.000000	0.000000
S	0.000000	0.000000	1.789252
C	1.734988	0.000000	2.218118
O	0.089828	-1.997316	1.727958
O	-0.557584	1.328332	2.222141
O	0.912251	-3.451032	-0.310808
O	2.936024	-1.625883	-0.394388
H	0.099282	1.040367	-0.313165
H	0.830291	-0.613065	-0.345756
H	-0.950797	-0.418437	-0.325798
H	2.271139	-0.650273	1.527461
H	2.072297	1.035739	2.153980
H	1.811013	-0.370048	3.239333
H	-0.644606	-2.291131	2.278004
H	0.525134	-2.977887	0.464677
H	1.103412	-4.326335	0.029721
H	2.308896	-2.373318	-0.434398
H	3.144315	-1.468215	-1.316303

Complex 1: DMSO with one water molecule and OH with one water molecule

C	0.019632	-0.016058	-0.020829
S	0.041719	-0.005749	1.768555
O	1.973355	-0.000051	1.818637
O	-1.334588	-0.469865	2.199036
C	0.108612	1.735185	2.152158
O	2.792880	1.819941	0.006856
H	-0.968651	0.338868	-0.316916
H	0.820624	0.623379	-0.387529
H	0.173978	-1.047845	-0.337762
H	0.946665	2.166152	1.609023
H	-0.852049	2.151521	1.846137
H	0.253634	1.820751	3.228607
H	2.253262	-0.908831	1.973406
H	2.720262	1.117529	0.679206
H	3.376649	2.459292	0.416766
H	-2.736327	0.630059	1.373444
O	-2.880917	1.371874	0.772269
H	-3.833859	1.447967	0.716087

Complex 2: DMSO with one water molecule

C	0.000000	0.000000	0.000000
S	0.000000	0.000000	1.799478
O	1.465166	0.000000	2.208835
C	-0.569865	1.689129	2.041166
O	3.532820	-0.545221	0.458455
O	2.373925	2.210515	0.680750
H	0.654048	0.800371	-0.333014
H	0.384288	-0.964059	-0.318623
H	-1.016885	0.128679	-0.361883
H	-0.533268	1.882684	3.108608
H	0.090732	2.366874	1.507858
H	-1.594997	1.769791	1.688008
H	2.885712	-0.518703	1.188425
H	2.287893	1.594093	1.415899
H	3.091193	1.832039	0.173184

Complex 2: OH radical with one water molecule

C	0.012126	0.039547	-0.034356
S	0.046845	-0.028593	1.758232
O	1.515985	0.015750	2.150207
C	-0.533186	1.646936	2.059485
O	2.935587	-2.240795	2.422211
O	0.712928	-2.986636	0.728153
H	0.703960	0.820399	-0.358105
H	0.335594	-0.942245	-0.378717
H	-1.005827	0.242251	-0.375883
H	-0.520825	1.801179	3.139056
H	0.158317	2.342474	1.579662
H	-1.549479	1.765271	1.676824
H	2.492939	-1.357989	2.388393
H	1.528336	-2.900955	1.243524
H	0.170788	-3.548053	1.284246

Complex 2: DMSO with two water molecules

C	-1.44342000	1.45088300	0.45592900
S	-1.12715200	-0.09938700	-0.38663000
O	-0.05323800	-0.80885800	0.43994300
C	-2.64782100	-0.93062300	0.09159100
O	2.17237500	-2.00263000	-0.62474600
O	1.29199100	1.86841700	-0.89551000
H	-1.52955400	1.24434400	1.52507400
H	-0.59483400	2.09863100	0.24005700
H	-2.36356100	1.88936000	0.06241700
H	-2.58847100	-1.95082500	-0.28932500
H	-2.70781300	-0.94635200	1.18156200
H	-3.50648400	-0.41871200	-0.34868800
H	1.30266600	-1.66364400	-0.31877400
H	1.82908000	1.44257400	-0.20467000
H	1.88611400	1.92019700	-1.64462800
H	1.50101500	-0.00308200	1.22627100
O	2.40120700	0.34983000	1.16858600
H	2.85504600	-0.39793100	0.76547500

Complex 2: OH radical two water molecules

C	-0.653103	-1.619236	-0.310368
S	-1.152279	-0.029852	0.349823
C	-2.927623	-0.275904	0.212922
O	-0.836678	0.985569	-0.742747
O	1.213339	2.642256	-0.486967
O	2.046344	0.411655	1.019687
H	-1.060107	-1.704951	-1.320640
H	0.437496	-1.651603	-0.334653
H	-1.028776	-2.416161	0.335969
H	-3.407497	0.647026	0.540523
H	-3.167499	-0.465381	-0.835252
H	-3.239340	-1.105768	0.851075
H	0.394133	2.103194	-0.640288
H	1.900311	1.239047	0.531220
H	2.343251	0.694757	1.885362
H	2.617128	-1.106249	0.144886
O	2.731624	-1.897216	-0.402551
H	2.894687	-1.523546	-1.270059

Complex 2: DMSO with one water molecule and OH with one water molecule

C	0.181593	-0.163170	-0.182167
S	-0.067915	-0.107696	1.598195
C	1.666387	-0.046581	2.064849
O	-0.547230	-1.509131	1.980379
O	-2.183060	-3.019108	0.428242
O	1.642618	-2.929306	0.731653
H	0.752843	-1.069052	-0.395592
H	-0.805384	-0.205431	-0.646167
H	0.704319	0.737845	-0.510310
H	1.702002	-0.125665	3.152251
H	2.188431	-0.885248	1.600534
H	2.079827	0.915076	1.751495
H	-1.670442	-2.485125	1.078446
H	0.894678	-2.748248	1.315248
H	1.267878	-3.583533	0.124255
O	-0.071143	-4.523759	-0.858948
H	-0.202300	-4.399116	-1.799544
H	-0.879010	-4.163048	-0.467645

MSIA with one water molecule

C	-1.005434	1.306890	-0.428668
S	-0.868647	-0.409478	0.085411
O	-0.005584	-1.039732	-0.960774
O	0.025227	-0.149428	1.438290
O	2.154120	0.412199	-0.162497
H	0.903867	0.169219	1.128228
H	-1.509944	1.874034	0.354878
H	0.001020	1.693380	-0.601559
H	-1.583717	1.332295	-1.353898
H	1.681242	-0.214961	-0.737735
H	3.048384	0.072026	-0.104639

MSIA with two water molecules

C	1.366574	0.436690	1.309373
S	1.275491	-0.386248	-0.285256
O	0.707370	0.870174	-1.149440
O	0.210930	-1.423873	-0.104396
H	-0.130860	1.204606	-0.731821
H	2.073423	1.264854	1.237386
H	0.371922	0.804111	1.567501
H	1.707955	-0.295865	2.042230
H	-1.498441	-1.255467	0.187057
O	-2.427604	-0.953002	0.228836
H	-2.833252	-1.386380	-0.524004
O	-1.508010	1.541817	0.133263
H	-2.030981	0.710789	0.166373
H	-2.128561	2.232252	-0.102958

TS1: DMSO with one water molecule

C	0.000000	0.000000	0.000000
S	0.000000	0.000000	2.187365
C	1.784017	0.000000	2.317530
O	-0.082173	0.795308	3.737644
O	-0.483656	-1.385133	2.411320
O	0.983829	-1.772920	4.972100
H	2.176982	-0.617015	1.510357
H	2.152073	1.023853	2.243633
H	2.017785	-0.442364	3.286594
H	0.487211	-0.940287	-0.244065
H	-1.060459	0.023843	-0.230248
H	0.543284	0.897245	-0.285100
H	-1.001339	1.077910	3.825819
H	0.436285	-2.037395	4.223751
H	0.627778	-0.897594	5.146907

TS1: DMSO with one water molecule and OH with one water molecule

C	-2.718501	0.538378	0.011082
S	-0.988934	0.062243	-0.212230
O	-0.185575	1.324890	-0.036333
C	-0.811122	-0.902952	1.283321
O	0.028907	-1.371219	-1.383563
O	2.546829	1.495694	-0.065045
O	2.316303	-1.175534	0.347834
H	-1.147488	-0.317303	2.141160
H	-1.389059	-1.822185	1.170852
H	0.248217	-1.149739	1.370755
H	-2.802254	1.097951	0.945987
H	-2.986202	1.172524	-0.834555
H	-3.338704	-0.359440	0.023498
H	0.831296	-1.316806	-0.820086
H	1.582165	1.542580	-0.192566
H	2.695146	2.074010	0.684433
H	2.568407	-0.239007	0.228083
H	3.070507	-1.667905	0.020196

TS2: DMSO with one water molecule

C	0.000000	0.000000	0.000000
S	0.000000	0.000000	1.788319
O	1.447541	0.000000	2.238790
C	-0.613957	1.678647	2.002101
O	1.089122	2.077004	-0.766496
O	3.236132	1.358499	0.754853
H	0.499945	1.032472	-0.432670
H	0.597944	-0.840184	-0.353010
H	-1.017523	-0.022038	-0.396440
H	-0.595582	1.888485	3.072031
H	0.033842	2.361777	1.451689
H	-1.639483	1.730800	1.628205
H	1.952762	1.881694	-0.334652
H	2.688762	0.875572	1.405927
H	3.896040	0.716658	0.489334

TS2: OH radical with one water molecule

C	0.019880	-0.014533	-0.017752
S	-0.020421	-0.015495	1.771358
C	1.766418	-0.009780	2.011010
O	-0.487585	-1.407236	2.150090
O	0.472846	-2.399607	-0.184849
O	-1.873987	-1.795291	-1.891096
H	0.425708	-1.130482	-0.300001
H	-0.985521	0.029764	-0.433239
H	0.700761	0.730679	-0.432558
H	1.940427	-0.152758	3.078231
H	2.195409	-0.840669	1.447370
H	2.182024	0.948307	1.690544
H	0.095367	-2.417960	0.726748
H	-1.539650	-1.918521	-2.780436
H	-1.215539	-2.256978	-1.359041

TS2: DMSO with two water molecules

C	0.000000	0.000000	0.000000
S	0.000000	0.000000	1.786811
C	1.779595	0.000000	2.034985
O	-0.514155	-1.356693	2.236633
O	1.175843	-1.892717	-1.055085
O	0.351737	-3.527031	0.998561
O	3.160330	-2.876666	0.999431
H	0.703720	-0.883131	-0.450377
H	-1.014609	-0.184577	-0.351733
H	0.404827	0.933106	-0.398060
H	1.946075	0.067230	3.111037
H	2.214242	-0.924932	1.647656
H	2.202312	0.879468	1.543172
H	0.747920	-2.575501	-0.494918
H	-0.010891	-2.797275	1.552182
H	-0.270323	-4.249224	1.096005
H	2.344137	-3.357949	1.182586
H	2.970589	-2.531847	0.121862

TS2: OH radical with two water molecules

C	0.295908	0.275822	1.269342
S	1.304902	-0.641159	0.109834
O	0.584981	-0.503073	-1.226345
C	2.668914	0.532450	0.032782
O	-0.498514	1.837820	-0.433867
O	-3.102735	0.646275	-0.029972
H	-0.099788	1.228183	0.619877
H	-0.579450	-0.323392	1.510652
H	0.856663	0.642360	2.130355
H	3.330346	0.191908	-0.764631
H	2.268751	1.519426	-0.206339
H	3.203760	0.537677	0.985274
H	-0.209021	1.122930	-1.052309
H	-3.544567	1.076045	0.703372
H	-2.346031	1.220809	-0.210143
H	-2.353055	-1.120837	0.070254
O	-1.726314	-1.857020	0.109104
H	-1.206798	-1.712090	-0.688166

TS2: DMSO with one water molecule and OH with one water molecule

C	0.247944	-0.161907	-0.198248
S	-0.108504	-0.064224	1.552574
C	1.599535	0.097023	2.103711
O	-0.588338	-1.426159	2.003140
O	1.988367	-1.855906	-0.688169
O	0.352699	-3.555905	0.591757
H	1.173095	-0.920548	-0.400074
H	-0.617226	-0.563412	-0.725517
H	0.564938	0.807727	-0.589150
H	1.580408	0.137287	3.193350
H	2.168673	-0.767805	1.759569
H	2.018916	1.022723	1.702335
H	1.528527	-2.558012	-0.154319
H	-0.060135	-2.929809	1.215555
H	-0.266848	-3.576733	-0.147450
H	0.486599	-2.475530	-1.991861
O	-0.442007	-2.731099	-2.061483
H	-0.491627	-3.209986	-2.889870