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

The working mechanism of the β-carbonic anhydrase degrading carbonyl sulfide (COSase): a theoretical study

Paolo Piazzetta, Tiziana Marino and Nino Russo

Table of contents

Cartesian coordinates (Å) of B3LYP/6-31+G(d,p) optimized structures of stationary points for conversion of COS in H_2S and CO_2 by COSase taking into account the X-ray position of water molecule.

ES

C -0.26374 0.38799 3.78708
S 0.96173 0.66025 5.12631
C 1.06081 -1.01934 5.84850
C -1.90782 6.45792 -3.28464
C -0.73398 5.79704 -2.61613
N 0.35990 6.52946 -2.19122
C -0.54143 4.46190 -2.32072
C 1.18772 5.64759 -1.65375
N 0.69117 4.38099 -1.70523
C -8.51357 1.62020 2.03876
C -9.19856 0.27082 1.75840
C -7.00561 1.63560 1.75549
C -9.19758 -0.14557 0.28105
C -0.48610 -2.36338 -4.24065
S -1.62008 -1.74486 -2.91343
C 1.87715 0.38780 -2.04416
C 2.86963 1.08378 -1.13627
O 3.94514 0.50177 -0.81113
O 2.54670 2.24481 -0.67492
C 6.53480 1.58832 1.73263
N 5.11470 1.39850 1.46680
C 4.15850 1.46629 2.38629
N 4.46172 1.42775 3.71940
N 2.88747 1.62325 2.01788
C 4.24010 -5.12692 -2.27190
C 3.16423 -4.23889 -1.75302
N 3.39251 -3.15604 -0.91276
C 1.80225 -4.27829 -1.91136
C 2.18792 -2.59568 -0.60976
N 1.21616 -3.25500 -1.20210
C -0.25719 -4.98231 1.23594
S -1.68482 -4.60993 0.11889
S -3.58926 0.08441 -0.00099
C -2.30379 0.92000 -0.35428
Zn -0.84166 -2.64539 -0.88202
O -0.33571 -1.34483 0.54269
H -0.48778 1.36835 3.35922
H -1.18589 -0.02200 4.20690
H 1.77367 -0.97520 6.67563
H 0.08418 -1.32063 6.23658
H 1.40320 -1.74943 5.11059
H -2.36714 7.20478 -2.62573
H -1.59869 6.97711 -4.20001
H -1.15474 3.58740 -2.47495
H 1.16436 3.53871 -1.36212
H 2.14872 5.87088 -1.21012
H -9.00661 2.40247 1.44293
H -6.78219 1.45086 0.70041
H -6.48563 0.86718 2.33975
H -6.56442 2.60414 2.01588
H -10.23709 0.32200 2.11434
H -8.70842 -0.51060 2.35636
H -9.74351 -1.08467 0.13603
H -9.67763 0.61880 -0.34321
H -8.18317 -0.29688 -0.10087
H -0.57753 -3.44663 -4.37729
H 0.56091 -2.12587 -4.02549
H 1.01159 0.06118 -1.45602
H 2.32497 -0.47713 -2.53425
H 6.68740 2.39191 2.46006
H 7.02055 0.67156 2.09641
H 4.77474 1.18196 0.48987
H 2.14775 1.39305 2.66599
H 2.65854 1.88585 1.03848
H 3.67498 1.37044 4.35736
H 5.28562 0.91558 3.99762
H 3.79918 -5.90116 -2.90563
H 4.97592 -4.58261 -2.87910
H 4.28651 -2.75344 -0.67150
H 1.20811 -4.98383 -2.47424
H 2.03892 -1.74124 0.03325
H -0.56867 -5.72314 1.98144
H 0.59145 -5.39365 0.67843
O 4.71190 4.01724 -0.52749
H -0.92875 -1.60051 1.26140
O -1.39556 1.60209 -0.61832
H 4.79857 4.35806 -1.42531
H 3.95483 3.38737 -0.56957
H 0.08197 -4.08234 1.75892
H -0.76447 -1.87517 -5.18018
H 4.78631 -5.63192 -1.46380
H 7.00955 1.88395 0.79564
H 1.49621 1.08603 -2.79563
H -2.67184 5.72051 -3.55097
H -8.68293 1.88766 3.09110
H 0.10945 -0.26616 2.99246

TS1

C -0.54000 0.56500 3.88300
S 0.76800 0.74100 5.15600
C 0.81000 -0.96900 5.80300
C -2.05000 6.33100 -3.50700
C -0.86900 5.70700 -2.81500
N 0.18600 6.47700 -2.36200
C -0.63100 4.37700 -2.52400
C 1.03500 5.62400 -1.81100
N 0.59100 4.34000 -1.88200
C -8.71300 1.48500 1.54600
C -9.41600 0.13500 1.32100
C -7.18400 1.43200 1.42100
C -9.28100 -0.42100 -0.10300
C -0.37200 -2.46000 -4.31500
S -1.36500 -1.67200 -2.96300
C 1.84700 0.37500 -2.07500
C 2.83200 1.10600 -1.18700
O 3.88300 0.51800 -0.79400
O 2.52700 2.30000 -0.80800
C 6.34600 1.73700 1.83700
N 4.94400 1.51600 1.50600
C 3.93700 1.57900 2.37100
N 4.16400 1.55300 3.71900
N 2.68700 1.71800 1.92800
C 4.35700 -5.07800 -2.16200
C 3.28700 -4.17900 -1.64100
N 3.53600 -3.02600 -0.90800
C 1.91800 -4.25900 -1.71100
C 2.33700 -2.46700 -0.58100
N 1.34700 -3.18900 -1.05500
C -0.25500 -5.01300 1.19600
S -1.50400 -4.81700 -0.15600
S -3.14600 0.56400 0.84700
C -1.60000 0.77100 0.51900
Zn -0.79800 -2.71300 -0.94400
O -0.74100 -1.47100 0.62500
H -0.68800 1.55000 3.43400
H -1.47700 0.25800 4.35400
H 1.56900 -1.00500 6.58800
H -0.16000 -1.23100 6.23500
H 1.06600 -1.68100 5.01500
H -2.54900 7.05700 -2.85300
H -1.73800 6.86700 -4.41100
H -1.20600 3.48200 -2.70600
H 1.09100 3.51700 -1.52800
H 1.97700 5.88300 -1.34500
H -9.11300 2.22000 0.83300
H -6.86200 1.14500 0.41500
H -6.75600 0.70500 2.12300
H -6.73600 2.40700 1.63900
H -10.48300 0.24900 1.56000
H -9.02000 -0.59900 2.03700
H -9.84300 -1.35600 -0.21600
H -9.66700 0.29100 -0.84200
H -8.23900 -0.63500 -0.36100
H -0.67500 -3.49800 -4.48600
H 0.70100 -2.44100 -4.09500
H 0.97800 0.05500 -1.49200
H 2.30000 -0.49900 -2.54200
H 6.44500 2.52900 2.58600
H 6.83900 0.82500 2.20400
H 4.66100 1.27400 0.52000
H 1.90800 1.49700 2.53100
H 2.51200 1.97900 0.94000
H 3.34400 1.47700 4.31300
H 4.98100 1.05600 4.04300
H 3.90000 -5.91000 -2.70500
H 5.03300 -4.56100 -2.85700
H 4.42900 -2.57900 -0.75600
H 1.30200 -5.02100 -2.16700
H 2.24100 -1.55200 -0.02000
H -0.56400 -5.83700 1.85100
H 0.73700 -5.24800 0.79500
O 4.73500 4.00600 -0.58300
H -1.38000 -1.89200 1.21500
O -0.55800 1.25400 0.29400
H 4.82200 4.40700 -1.45600
H 3.95800 3.40300 -0.65900
H -0.17300 -4.10200 1.79600
H -0.54600 -1.89300 -5.23500
H 4.96900 -5.50300 -1.35600
H 6.85100 2.06600 0.92700
H 1.46100 1.04600 -2.84800
H -2.78300 5.57000 -3.79500
H -8.97700 1.85600 2.54600
H -0.26400 -0.14900 3.10200

INT1

C 0.55153 1.78877 5.45359
S 1.91710 0.63655 5.85002
C 1.05421 -0.95473 5.57097
C -2.66419 6.44971 -3.34441
C -1.39707 5.83915 -2.81244
N -0.29880 6.62070 -2.50379
C -1.11033 4.51330 -2.55088
C 0.62313 5.77753 -2.06685
N 0.18533 4.48913 -2.07442
C -8.82237 1.75732 1.92622
C -9.69921 0.49330 1.89967
C -7.31417 1.48073 1.97835
C -9.54084 -0.35863 0.63293
C -1.05925 -2.32737 -4.41098
S -1.97914 -1.59828 -2.98060
C 1.35489 0.48538 -2.35215
C 2.44133 1.24870 -1.61914
O 3.53627 0.67261 -1.35096
O 2.17224 2.44634 -1.23571
C 6.19642 1.80964 1.14145
N 4.77055 1.63668 0.90844
C 3.83325 1.54199 1.85493
N 4.17628 1.29645 3.14882
N 2.55329 1.74338 1.54105
C 3.85144 -4.96125 -2.73830
C 2.86119 -4.03629 -2.12085
N 3.21393 -2.85853 -1.47527
C 1.49559 -4.10078 -2.00941
C 2.07775 -2.27034 -1.01912
N 1.02364 -2.99517 -1.32878
C -0.42889 -4.94644 1.03396
S -1.72214 -4.67562 -0.25613
S -1.05400 -0.60601 0.48670
C 0.09341 -0.81219 1.74583
Zn -1.10787 -2.60656 -1.07201
O 0.64031 -2.06564 1.86276
H 0.95891 2.80192 5.49383
H -0.25003 1.69860 6.19200
H 1.80030 -1.75035 5.64653
H 0.29027 -1.11413 6.33716
H 0.60394 -0.94556 4.57762
H -3.07863 7.17565 -2.63445
H -2.47939 6.98271 -4.28500
H -1.69690 3.61204 -2.65256
H 0.73632 3.67147 -1.78766
H 1.61540 6.04502 -1.72944
H -9.05173 2.37005 1.04233
H -6.96205 0.94744 1.08982
H -7.05471 0.87150 2.85287
H -6.74354 2.41348 2.04355
H -10.75219 0.79169 1.99989
H -9.47014 -0.12026 2.78297
H -10.22323 -1.21627 0.64596
H -9.76277 0.22934 -0.26642
H -8.52462 -0.75157 0.52755
H -1.21839 -3.40790 -4.48808
H 0.01656 -2.13380 -4.34557
H 0.57755 0.17139 -1.64934
H 1.75123 -0.39000 -2.86604
H 6.36791 2.48555 1.98526
H 6.71415 0.85814 1.33302
H 4.42416 1.46834 -0.06327
H 1.79852 1.27356 2.05208
H 2.33679 2.09587 0.59944
H 3.43933 1.16994 3.84280
H 5.03715 0.80246 3.32799
H 3.32908 -5.81194 -3.18383
H 4.43246 -4.47605 -3.53365
H 4.12370 -2.42024 -1.45012
H 0.81700 -4.87129 -2.34684
H 2.08281 -1.32919 -0.49832
H -0.46294 -5.99875 1.33819
H 0.57192 -4.72488 0.65486
O 4.38838 4.15430 -1.24759
H 1.27422 -2.01288 2.59650
O 0.49057 0.05799 2.54880
H 4.44654 4.42796 -2.17030
H 3.61106 3.54803 -1.21579
H -0.60967 -4.31993 1.90980
H -1.43761 -1.85791 -5.32435
H 4.56267 -5.35722 -2.00139
H 6.62467 2.26593 0.24707
H 0.85945 1.13819 -3.07731
H -3.42184 5.68142 -3.52951
H -9.10548 2.36314 2.79825
H 0.16987 1.58159 4.45124

TS2

C -0.02600 1.67900 5.05900
S 1.58100 0.89700 5.45700
C 1.06300 -0.85100 5.62300
C -2.56800 6.46100 -3.40400
C -1.32300 5.85500 -2.81500
N -0.24200 6.64100 -2.46000
C -1.04300 4.53100 -2.53900
C 0.66400 5.80300 -1.98200
N 0.23200 4.51200 -2.00500
C -8.70900 1.86200 1.52600
C -9.70200 0.68600 1.56200
C -7.26300 1.48100 1.86800
C -9.44800 -0.38800 0.49600
C -0.86100 -2.30700 -4.38600
S -1.96300 -1.72200 -3.02300
C 1.49000 0.54200 -2.30300
C 2.55300 1.30300 -1.53800
O 3.66900 0.75700 -1.29900
O 2.23800 2.46900 -1.08900
C 6.25600 1.93400 1.26700
N 4.85100 1.65400 1.00500
C 3.91200 1.51700 1.93600
N 4.23800 1.32600 3.24100
N 2.62100 1.62800 1.60200
C 4.04400 -4.88300 -2.61000
C 2.98600 -3.99900 -2.04400
N 3.25700 -2.82900 -1.34600
C 1.61800 -4.10500 -2.02900
C 2.07600 -2.28500 -0.95200
N 1.06900 -3.03100 -1.35400
C -0.30200 -4.88500 1.08600
S -1.61200 -4.73700 -0.20400
S -1.09100 -0.67000 0.42500
C -0.37300 -1.07900 1.94800
Zn -1.06900 -2.69000 -1.11900
O 1.01200 -1.30500 1.88700
H 0.18000 2.71200 4.76800
H -0.67500 1.67700 5.93800
H 1.96500 -1.46800 5.57300
H 0.58300 -1.01500 6.59200
H 0.37100 -1.11500 4.81900
H -3.01700 7.18400 -2.71200
H -2.34200 6.99600 -4.33400
H -1.62100 3.62700 -2.66400
H 0.77400 3.69800 -1.69700
H 1.63900 6.07600 -1.60100
H -8.73900 2.32500 0.53000
H -6.83900 0.77600 1.14600
H -7.20100 1.01500 2.86000
H -6.61400 2.36300 1.87600
H -10.72000 1.07900 1.43800
H -9.67300 0.22400 2.56000
H -10.21200 -1.17400 0.53800
H -9.47200 0.04500 -0.51200
H -8.47400 -0.87100 0.62300
H -0.90600 -3.39400 -4.50800
H 0.18200 -2.01500 -4.22300
H 0.71200 0.20000 -1.61100
H 1.90900 -0.31600 -2.82800
H 6.35800 2.60500 2.12600
H 6.83900 1.02100 1.45000
H 4.52200 1.49300 0.02200
H 1.92200 1.10500 2.11500
H 2.37600 1.97800 0.66400
H 3.47900 1.23200 3.91600
H 5.12000 0.89500 3.46800
H 3.58000 -5.73700 -3.10900
H 4.66500 -4.36300 -3.35200
H 4.15100 -2.37000 -1.24500
H 0.99000 -4.88600 -2.43200
H 1.99900 -1.38100 -0.37400
H -0.35000 -5.89200 1.51600
H 0.69800 -4.73600 0.66900
O 4.42600 4.21000 -0.95700
H 1.25000 -1.65500 2.76200
O -0.89800 -1.13800 3.05700
H 4.50000 4.55600 -1.85300
H 3.65300 3.59700 -0.98700
H -0.45900 -4.16300 1.89300
H -1.20400 -1.84400 -5.31700
H 4.71300 -5.27500 -1.83200
H 6.66100 2.44100 0.38900
H 0.99500 1.20400 -3.02000
H -3.31200 5.69000 -3.62400
H -9.05300 2.63200 2.23100
H -0.51200 1.14900 4.23700

INT2

C 1.64527 3.62380 3.73675
S 3.20173 2.87277 4.34169
C 2.58288 1.28650 5.01226
C -2.88741 5.44257 -5.03460
C -2.07810 5.33157 -3.78032
N -1.41264 6.41652 -3.24266
C -1.86147 4.21752 -2.99643
C -0.81104 5.95193 -2.15774
N -1.05086 4.62875 -1.96201
C -6.24558 1.27800 2.30393
C -7.40465 0.62051 1.53587
C -6.35454 2.80416 2.42616
C -8.77168 0.73818 2.22521
C -1.39139 -3.25264 -3.32990
S -2.34788 -4.22151 -2.08308
C 1.33300 -0.04114 -2.83730
C 2.40259 0.52844 -1.91086
O 3.60528 0.13563 -1.99788
O 2.02033 1.40480 -1.06007
C 6.73656 2.12692 -0.96648
N 5.42335 1.69059 -0.51454
C 4.92040 2.00806 0.68329
N 5.71504 2.61619 1.61628
N 3.64778 1.76853 0.95473
C 3.78676 -5.42249 -1.80396
C 2.69776 -4.50120 -1.35970
N 2.88113 -3.15093 -1.08164
C 1.37005 -4.73414 -1.10038
C 1.68480 -2.63857 -0.68011
N 0.75746 -3.57159 -0.68405
C 0.31232 -3.91594 2.46335
S -1.37219 -4.44972 1.92205
S -1.67610 -0.96002 -0.18799
C -1.00827 -0.24230 1.24020
Zn -1.35705 -3.45157 -0.14238
O -1.60995 0.99360 1.53496
H 0.93683 3.73520 4.56163
H 1.19658 3.03743 2.93077
H 3.45265 0.72368 5.35868
H 1.91717 1.46840 5.85984
H 2.05965 0.70574 4.24774
H -3.69399 6.17780 -4.92335
H -2.26774 5.76783 -5.87952
H -2.20544 3.19704 -3.07910
H -0.68513 4.02409 -1.20803
H -0.19375 6.53375 -1.48651
H -6.18431 0.83403 3.30820
H -7.24318 3.11106 2.99049
H -6.40928 3.27436 1.43636
H -5.47952 3.22012 2.93845
H -7.16836 -0.44063 1.38843
H -7.46336 1.06027 0.53008
H -9.54693 0.20985 1.65794
H -8.74238 0.30184 3.23199
H -9.09240 1.78148 2.32551
H -0.32224 -3.48154 -3.28333
H -1.52391 -2.17564 -3.18895
H 0.43943 -0.30844 -2.26653
H 1.70713 -0.90529 -3.38860
H 6.87043 3.20528 -0.82328
H 7.55434 1.59393 -0.46012
H 4.79114 1.13406 -1.14234
H 3.31587 1.96303 1.89150
H 2.96027 1.59040 0.14973
H 5.30563 2.76559 2.53124
H 6.70950 2.45147 1.59166
H 3.37176 -6.42062 -1.96629
H 4.24890 -5.09687 -2.74512
H 3.70057 -2.58638 -1.26471
H 0.80988 -5.65423 -1.18674
H 1.53645 -1.61192 -0.38377
H 0.43619 -4.19954 3.51536
H 1.09383 -4.41629 1.88340
O -0.04285 2.87226 -0.01687
H -1.21741 1.24994 2.38641
O -0.10863 -0.61288 1.98825
H 0.60714 2.29014 -0.47400
H -0.71755 2.27275 0.35061
H 0.42824 -2.83460 2.37815
H -1.75698 -3.51486 -4.32865
H 4.58403 -5.50995 -1.05422
H 6.81269 1.90959 -2.03314
H 1.04326 0.73843 -3.55196
H -3.33874 4.47967 -5.29477
H -5.30385 1.02566 1.80256
H 1.89741 4.61348 3.34973

TS3

C 0.40100 2.67500 3.55600
S 2.03000 2.98900 4.33300
C 2.26100 1.40900 5.22200
C -3.42000 5.19700 -4.85400
C -2.58600 5.22800 -3.61200
N -1.98900 6.39000 -3.16100
C -2.27600 4.18600 -2.76300
C -1.33400 6.04000 -2.06400
N -1.47800 4.72000 -1.77700
C -6.39400 0.32200 2.07400
C -7.47800 -0.41400 1.26900
C -6.71700 1.79300 2.37100
C -8.81600 -0.57500 2.00400
C -0.78600 -3.27500 -3.42500
S -1.56100 -4.50500 -2.28400
C 1.45000 0.25700 -2.71200
C 2.40400 0.97200 -1.76000
O 3.64000 0.68300 -1.75100
O 1.89400 1.85600 -0.99100
C 6.44000 3.06500 -0.56500
N 5.17400 2.46000 -0.17900
C 4.55300 2.73400 0.97400
N 5.21400 3.44100 1.94600
N 3.30100 2.36200 1.16200
C 4.59400 -4.77600 -1.79400
C 3.37500 -4.03300 -1.35100
N 3.36700 -2.69500 -0.97000
C 2.08100 -4.45400 -1.17300
C 2.10000 -2.37200 -0.59000
N 1.30400 -3.41500 -0.70400
C 0.81400 -3.94300 2.39800
S -0.80800 -4.60500 1.80800
S -1.65100 -1.27800 -0.32300
C -0.92000 -0.35300 0.93200
Zn -0.81600 -3.63500 -0.27800
O -1.66800 0.84600 1.23200
H -0.38400 2.69300 4.31600
H 0.39900 1.71500 3.03200
H 3.23800 1.44300 5.71000
H 1.48900 1.28500 5.98700
H 2.22700 0.56400 4.53000
H -4.27700 5.87800 -4.77600
H -2.83800 5.50800 -5.73000
H -2.54300 3.14000 -2.77600
H -1.03900 4.18100 -1.01200
H -0.74500 6.70600 -1.44800
H -6.22500 -0.21400 3.02000
H -7.61500 1.90100 2.98900
H -6.88200 2.35400 1.44300
H -5.89200 2.27800 2.90500
H -7.09800 -1.40700 0.99800
H -7.64300 0.11700 0.32100
H -9.53100 -1.14700 1.40100
H -8.68200 -1.11000 2.95300
H -9.27900 0.39200 2.23100
H 0.30700 -3.30700 -3.36600
H -1.11800 -2.25800 -3.19900
H 0.59600 -0.14400 -2.16000
H 1.95600 -0.54400 -3.25500
H 6.42500 4.15100 -0.41800
H 7.29400 2.64200 -0.01600
H 4.65400 1.82700 -0.83600
H 2.87700 2.50400 2.07500
H 2.70300 2.11500 0.31000
H 4.72500 3.57000 2.82100
H 6.21700 3.35700 2.00900
H 4.31700 -5.80000 -2.05500
H 5.06100 -4.32100 -2.67700
H 4.10500 -2.01300 -1.08700
H 1.64700 -5.42700 -1.35800
H 1.80900 -1.40200 -0.21600
H 0.92500 -4.20700 3.45600
H 1.64900 -4.38400 1.84700
O -0.27900 3.08800 0.14400
H -2.21800 0.67100 2.00700
O 0.11900 -0.52000 1.55200
H 0.42000 2.60300 -0.35000
H -0.84800 2.39500 0.52800
H 0.85600 -2.85600 2.30400
H -1.08400 -3.51600 -4.45100
H 5.35400 -4.82600 -1.00300
H 6.59900 2.86300 -1.62600
H 1.05700 0.98700 -3.42900
H -3.80300 4.18900 -5.04100
H -5.45000 0.26700 1.51900
H 0.22300 3.46500 2.82300

INT3

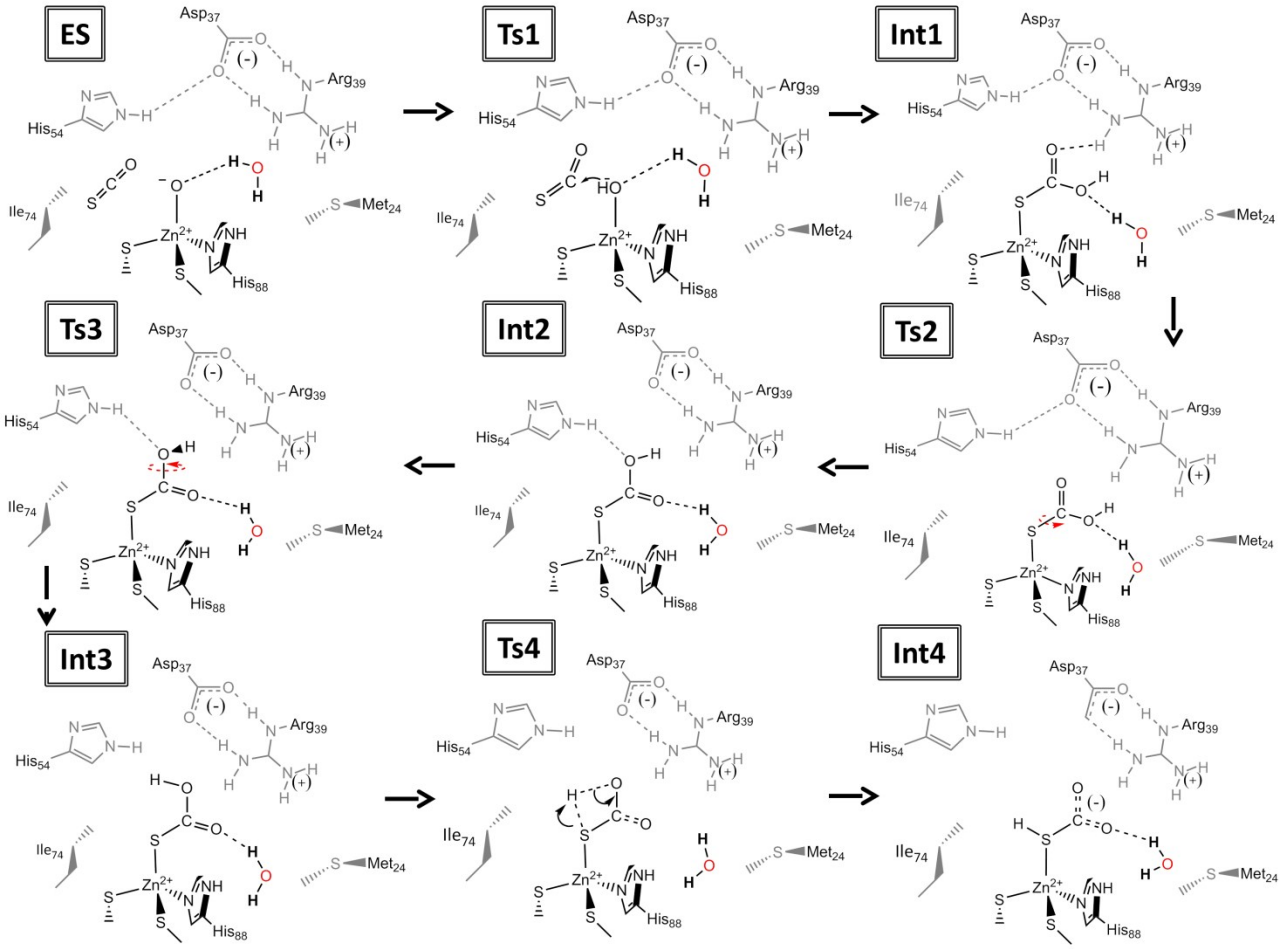
C 1.02670 4.14621 3.89839
S 2.68775 3.49526 4.30427
C 2.24513 1.78965 4.80864
C -4.76009 3.94471 -4.90831
C -4.14817 4.01434 -3.54766
N -4.34103 5.09266 -2.70552
C -3.33605 3.08475 -2.93713
C -3.65127 4.80634 -1.61147
N -3.02823 3.60179 -1.70032
C -6.34823 -0.86968 2.39136
C -7.40026 -1.79445 1.75614
C -6.86650 0.53123 2.74391
C -8.56497 -2.16377 2.68579
C -0.64815 -3.87860 -3.28395
S -1.65441 -3.13166 -1.92437
C 1.01763 0.00660 -2.95373
C 1.82638 1.13992 -2.34612
O 3.09145 1.12449 -2.42515
O 1.17684 2.06821 -1.75098
C 5.62346 3.71837 -1.40197
N 4.39674 3.06037 -0.98851
C 3.86516 3.14356 0.23705
N 4.57246 3.67595 1.27369
N 2.61136 2.75541 0.42039
C 5.01724 -4.38085 -2.05875
C 3.82720 -3.63772 -1.54939
N 3.82316 -2.27373 -1.28648
C 2.56627 -4.06025 -1.21161
C 2.59273 -1.93525 -0.81742
N 1.81134 -2.99311 -0.76739
C 1.49218 -3.89857 2.40137
S 0.05697 -4.72201 1.57473
S -0.68761 -0.80744 0.81507
C 0.54641 0.04418 1.73748
Zn -0.25095 -3.17246 -0.08043
O 0.38613 1.41738 1.80414
H 0.42803 4.24364 4.80836
H 0.52413 3.48276 3.19177
H 3.16294 1.32037 5.17199
H 1.52118 1.82603 5.62737
H 1.85514 1.20961 3.97012
H -5.85517 3.99061 -4.85712
H -4.43152 4.78245 -5.53623
H -2.96273 2.12480 -3.26107
H -2.39346 3.13874 -1.03787
H -3.57598 5.43646 -0.73559
H -5.94617 -1.34961 3.29482
H -7.66250 0.49893 3.49718
H -7.26743 1.03748 1.85675
H -6.06076 1.15689 3.14370
H -6.90245 -2.71455 1.42494
H -7.79575 -1.31831 0.84740
H -9.25588 -2.86029 2.19635
H -8.19863 -2.64764 3.60020
H -9.14465 -1.28345 2.98618
H -0.42320 -4.93267 -3.09056
H 0.29271 -3.34055 -3.43627
H 0.38787 -0.47312 -2.19829
H 1.66496 -0.73725 -3.42080
H 5.63403 4.76840 -1.08827
H 6.52647 3.22499 -1.01181
H 3.89660 2.40600 -1.64643
H 2.24628 2.50314 1.33236
H 2.02820 2.52456 -0.41971
H 4.12878 3.64777 2.19201
H 5.57802 3.59593 1.25906
H 4.76113 -5.43635 -2.18185
H 5.35563 -4.00477 -3.03307
H 4.55517 -1.60900 -1.49176
H 2.15741 -5.06008 -1.23229
H 2.32427 -0.93597 -0.51789
H 1.68091 -4.41231 3.35055
H 2.39638 -3.96998 1.78837
O -1.13354 2.02842 -0.39637
H -0.28413 1.71978 1.14290
O 1.51452 -0.42132 2.32324
H -0.34679 2.03025 -1.00824
H -1.36420 1.07636 -0.30340
H 1.29217 -2.84511 2.60408
H -1.23362 -3.81719 -4.20668
H 5.86608 -4.32310 -1.36506
H 5.67235 3.68405 -2.49205
H 0.33960 0.41795 -3.71022
H -4.48339 3.01322 -5.41263
H -5.50222 -0.77351 1.70054
H 1.15906 5.13396 3.45026

TS4

C -1.05700 -4.11900 3.78100
S -2.71500 -3.53600 4.29200
C -2.29300 -1.82700 4.80500
C 4.68600 -3.92300 -4.94300
C 4.27900 -3.69800 -3.52100
N 5.00000 -4.21900 -2.46300
C 3.20300 -2.98200 -3.04400
C 4.36500 -3.81900 -1.37300
N 3.27000 -3.06700 -1.66900
C 6.28500 0.82500 2.57700
C 7.26500 1.79700 1.89900
C 6.82300 -0.60300 2.74200
C 8.53800 2.08200 2.70900
O 0.62500 3.90800 -3.23200
S 1.59400 3.03400 -1.92200
C -1.06500 0.02900 -2.94000
C -1.69900 -1.29500 -2.55400
O -2.92500 -1.49300 -2.76000
O -0.93400 -2.16600 -1.99300
C -5.69100 -3.67000 -1.42000
N -4.33400 -3.22600 -1.15400
C -3.74400 -3.25400 0.05100
N -4.45200 -3.57500 1.16700
N -2.43800 -3.03500 0.13900
C -5.03600 4.43200 -1.99400
C -3.90000 3.66600 -1.40100
N -4.05800 2.54300 -0.59800
C -2.54500 3.85600 -1.46300
C -2.82300 2.11100 -0.21200
N -1.89100 2.88700 -0.73000
C -1.50800 3.88100 2.45700
S -0.02700 4.57300 1.59400
S 0.60300 0.70100 0.91900
C -0.73200 -0.35300 1.62100
Zn 0.18500 3.03200 -0.09200
O -0.49700 -1.63000 1.56400
H -0.40700 -4.21300 4.65500
H -0.62500 -3.42000 3.06000
H -3.19500 -1.39700 5.24900
H -1.50700 -1.85500 5.56500
H -1.98900 -1.22300 3.94700
H 5.68800 -3.52200 -5.13700
H 4.71400 -4.99300 -5.18300
H 2.41700 -2.43400 -3.54100
H 2.60000 -2.64000 -1.02800
H 4.65700 -4.04400 -0.35700
H 6.00400 1.22600 3.56100
H 7.70700 -0.63800 3.38900
H 7.10400 -1.03100 1.77100
H 6.06500 -1.25900 3.18500
H 6.74400 2.74300 1.70800
H 7.54200 1.39900 0.91200
H 9.17400 2.81700 2.20100
H 8.29100 2.48500 3.70000
H 9.13900 1.17800 2.86000
H 0.38700 4.93800 -2.94500
H -0.30300 3.37900 -3.47100
H -0.67700 0.54100 -2.05400
H -1.78600 0.67600 -3.44100
H -5.86900 -4.66700 -1.00100
H -6.45400 -2.98000 -1.02700
H -3.80900 -2.68500 -1.88400
H -1.99800 -2.64300 0.98000
H -1.90500 -2.85300 -0.73300
H -3.97000 -3.51900 2.06700
H -5.44200 -3.38400 1.18000
H -4.64500 5.27700 -2.56500
H -5.63900 3.81900 -2.67700
H -4.93200 2.11000 -0.33800
H -2.00300 4.63800 -1.97400
H -2.65100 1.28700 0.47100
H -1.61000 4.38800 3.42200
H -2.42400 4.06000 1.88200
O 1.01100 -1.72900 -0.40600
H 0.45200 -1.91700 0.46600
O -1.75800 0.15100 2.10000
H 0.30900 -1.83800 -1.15600
H 1.04000 -0.58900 -0.09200
H -1.40700 2.80800 2.63700
H 1.24000 3.94100 -4.13600
H -5.70700 4.83400 -1.22300
H -5.82100 -3.72500 -2.50300
H -0.20700 -0.14300 -3.59800
H 3.98700 -3.43800 -5.63100
H 5.35900 0.79200 1.98900
H -1.18100 -5.10200 3.32000

INT4

C 3.79262 2.14318 3.99549
S 4.36382 0.48131 4.51033
C 2.75862 -0.28698 4.95403
C -0.06805 6.42072 -4.80061
C 0.81170 5.88830 -3.71359
N 1.89895 6.59679 -3.24130
C 0.71191 4.68804 -3.04123
C 2.43426 5.82672 -2.30477
N 1.75404 4.66249 -2.14238
C -4.92361 4.24891 2.52971
C -6.27316 4.30873 1.79476
C -4.24586 5.61290 2.71860
C -7.37803 5.05175 2.55811
C -3.12311 -1.90290 -3.33958
S -4.46551 -1.81031 -2.06034
C 0.85718 -0.51770 -2.87359
C 2.19514 -0.96163 -2.29497
O 2.49549 -2.18661 -2.21381
O 2.95952 -0.02714 -1.87542
C 6.65251 -1.43135 -1.14783
N 5.30250 -1.52481 -0.60591
C 4.92921 -0.96608 0.56839
N 5.81771 -0.83913 1.58568
N 3.68950 -0.53977 0.68790
C 0.28555 -6.43667 -2.04496
C -0.31438 -5.14390 -1.60559
N 0.36487 -3.94159 -1.48084
C -1.59732 -4.87644 -1.19711
C -0.50624 -3.01957 -1.01046
N -1.70293 -3.55107 -0.83298
C -1.87283 -3.54449 2.37410
S -3.63253 -3.09362 1.97246
S -0.86392 0.64700 0.80336
C 0.68787 0.27379 1.78671
Zn -3.46717 -2.61824 -0.20961
O 1.64367 1.09454 1.67097
H 3.40097 2.68758 4.85958
H 3.02586 2.05099 3.22210
H 2.98130 -1.29344 5.31815
H 2.29193 0.28413 5.76176
H 2.08921 -0.35383 4.09214
H -0.52782 7.37350 -4.51009
H 0.50253 6.60468 -5.71964
H 0.00793 3.87296 -3.12052
H 1.98187 3.87631 -1.50916
H 3.31206 6.06899 -1.72121
H -5.06883 3.77322 3.51003
H -4.83933 6.28444 3.35001
H -4.09209 6.11228 1.75370
H -3.26384 5.49981 3.19084
H -6.60748 3.28334 1.59167
H -6.12690 4.78090 0.81266
H -8.32643 5.02259 2.00874
H -7.55068 4.59602 3.54147
H -7.12632 6.10578 2.72139
H -2.68809 -2.90309 -3.39622
H -2.33358 -1.17633 -3.13737
H 0.24720 -0.07814 -2.07701
H 0.31307 -1.34320 -3.33624
H 6.99575 -0.39231 -1.22996
H 7.37388 -1.99595 -0.54558
H 4.54027 -1.55946 -1.28928
H 3.28082 -0.13327 1.52824
H 3.20576 -0.35219 -0.20539
H 5.45670 -0.49393 2.47806
H 6.60256 -1.47123 1.62405
H -0.48937 -7.20727 -2.06778
H 0.72433 -6.37005 -3.04847
H 1.30361 -3.65775 -1.79035
H -2.43889 -5.55138 -1.13271
H -0.24100 -1.99629 -0.79512
H -1.87017 -3.89597 3.40992
H -1.51202 -4.34900 1.73062
O 2.35874 2.41770 -0.65757
H 2.05075 2.06079 0.20515
O 0.61910 -0.76591 2.45054
H 2.54508 1.63120 -1.21378
H -0.40738 1.74874 0.17454
H -1.21024 -2.67996 2.29995
H -3.58049 -1.66236 -4.30327
H 1.07566 -6.77279 -1.36183
H 6.64011 -1.87629 -2.14387
H 1.02802 0.26955 -3.61458
H -0.87108 5.71411 -5.03496
H -4.24817 3.58928 1.97196
H 4.65961 2.67857 3.60024



Scheme S1. Proposed reaction mechanism for the conversion of COS in H_2S and CO_2 by considering water molecule in not X-ray position.

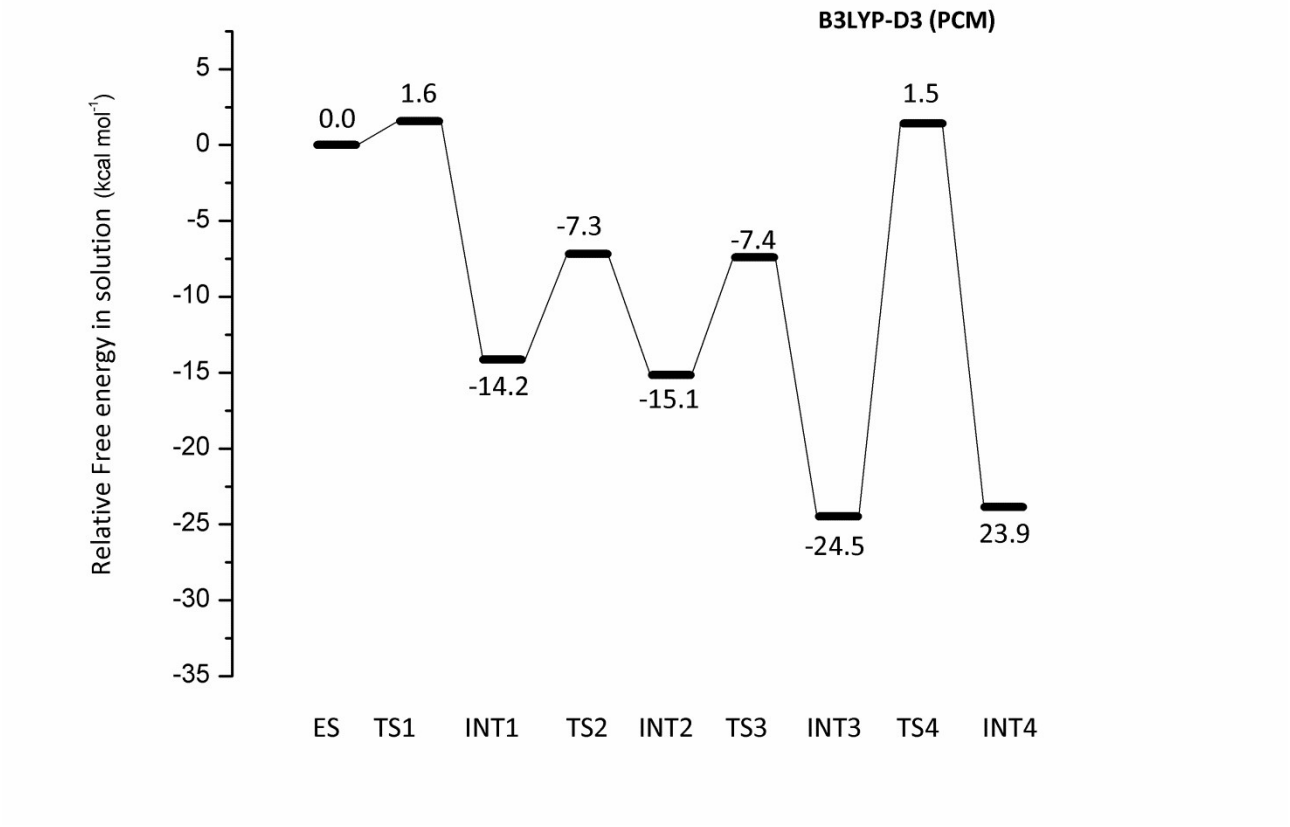


Figure S1. Potential energy surfaces obtained at B3LYP/6-311+G(2d,2p) (PCM, ε=4) level by considering water molecule in not X-ray position.

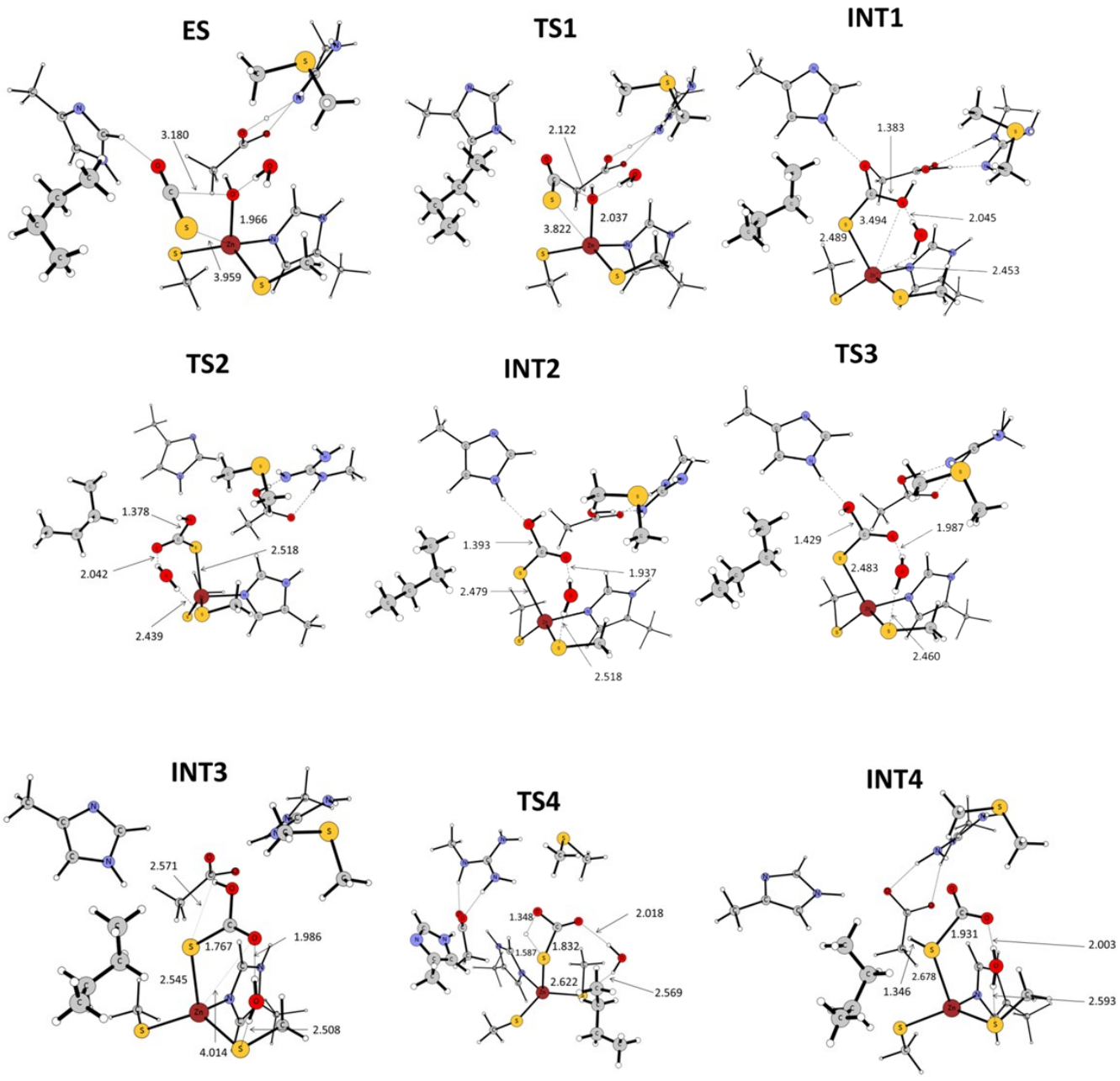


Figure S2. B3LYP/6-31+G(d,p) optimized stationary points present along the PES by considering water molecule in not X-ray position. Distances are in Å.

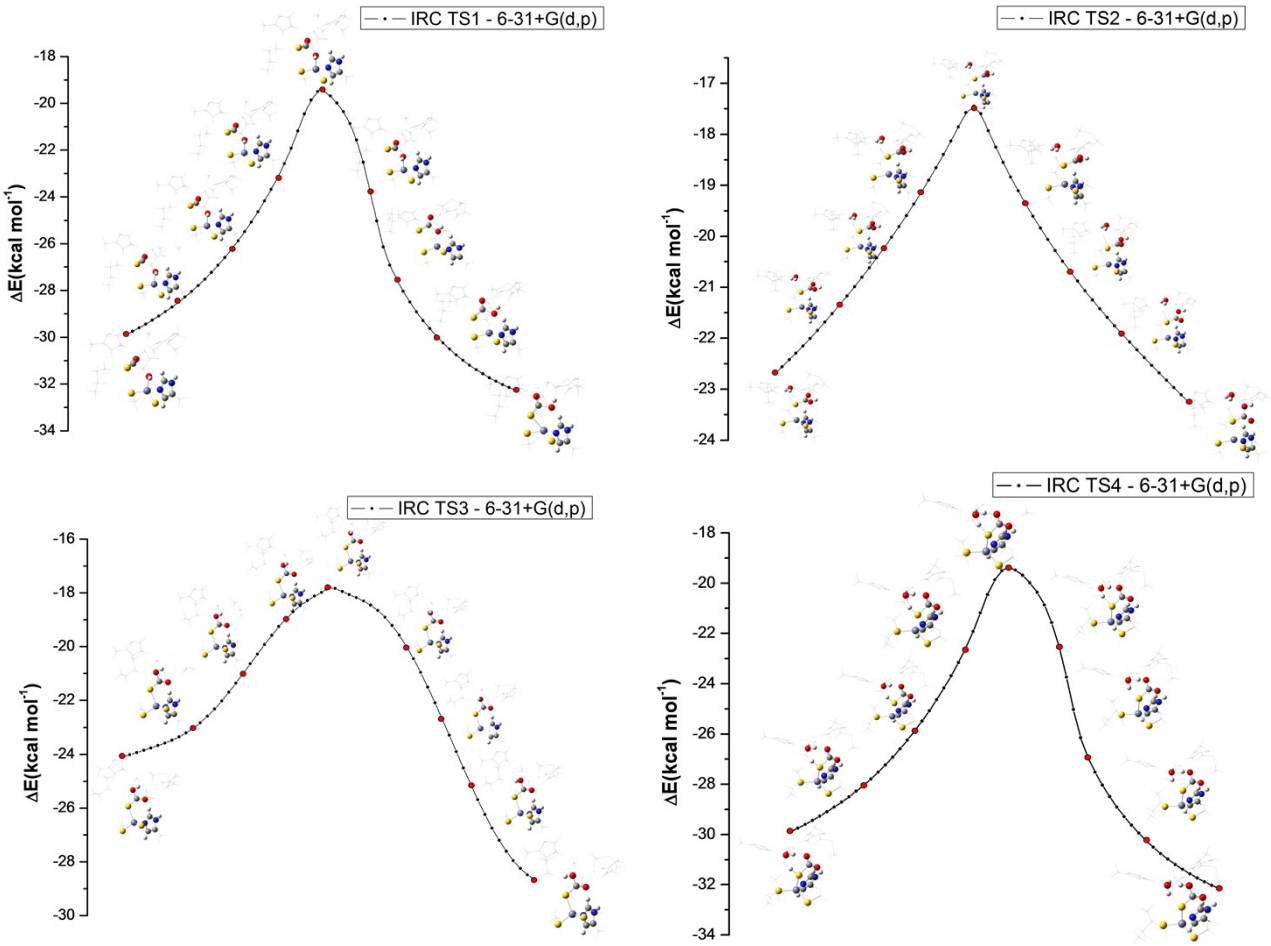


Figure S3. Gas phase intrinsic coordinate results from TS1 to ES and INT1, from TS2 to INT1 and INT2, from TS3 to INT2 and INT3 and from TS4 to INT3 and INT4 minima.

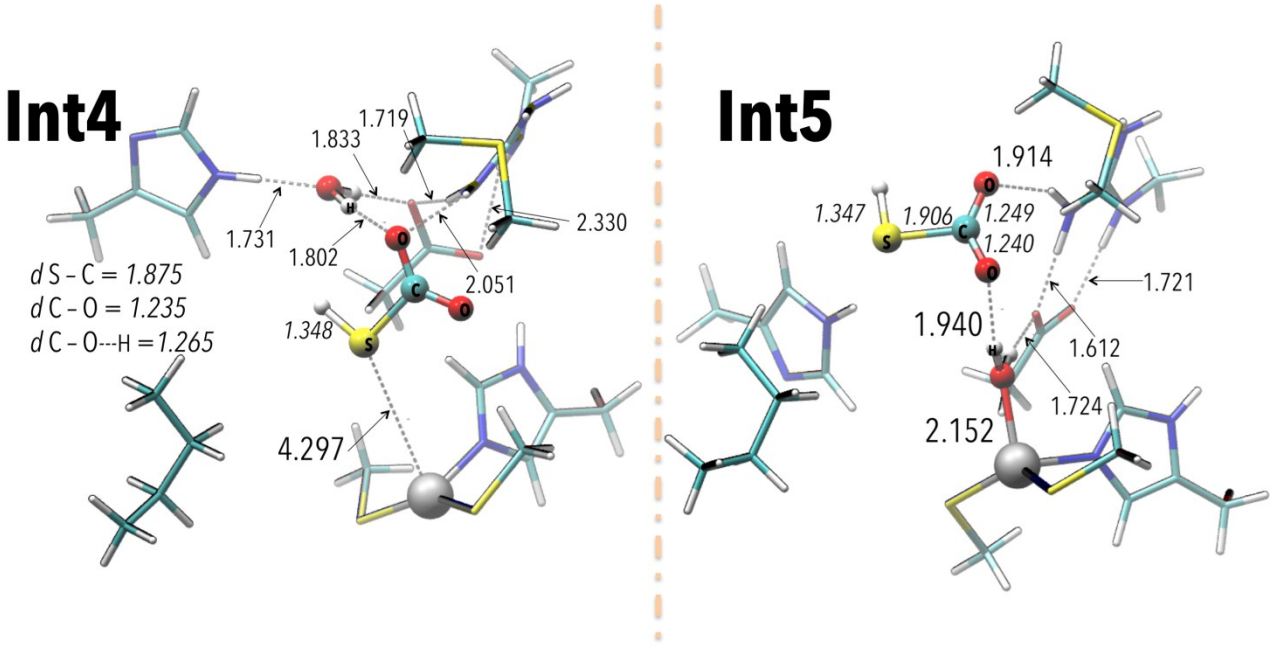


Figure S4. B3LYP/6-31+G(d,p) optimized structures of the intermediates INT4 and INT5 present along the PES for the mechanism with water in X-ray position.

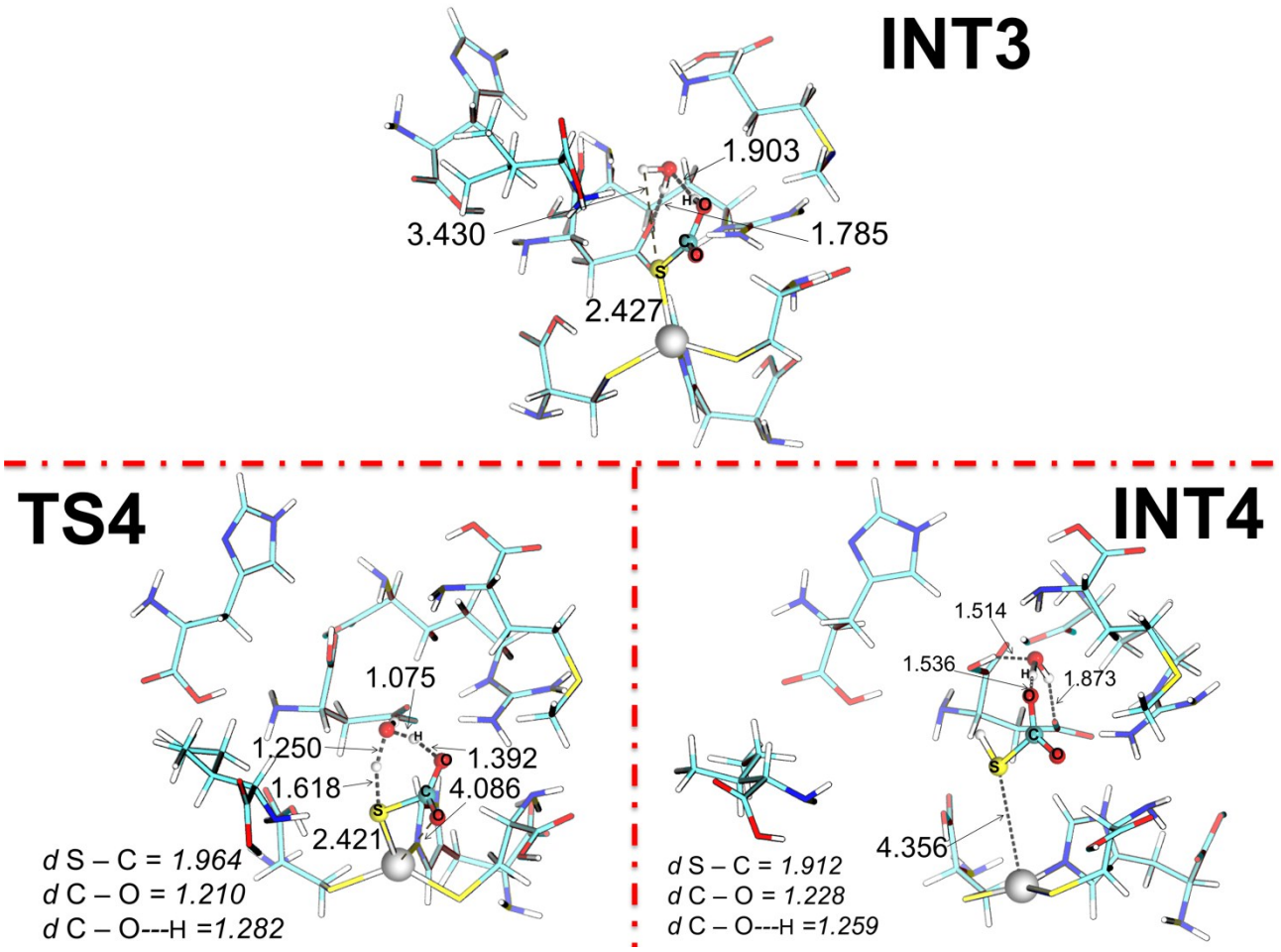


Figure S5. B3LYP/6-31+G(d,p) optimized structures of the species intercepted along the PES related to the rate determining step (INT4-TS4-INT5).